A Molecular Mechanics Study of Natural Product Polyphenols Interacting with beta-Amyloid

by

Margaret A.L. Gillis

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Abstract

The most common form of neurodegenerative dementia is Alzheimer's disease. One of the hallmarks of the disease is the presence of plaques, which is an aggregation of a peptide called amyloid-β. This aggregation occurs because of misfolding of the protein. Recent studies have shown that polyphenols within different types of foods may have potential to have an anti-aggregate effect on amyloid-β. This study focused on using molecular modeling to dock various polyphenols to two regions on the amyloid β-peptide that are often the target of anti-aggregate drugs to prevent misfolding: $H_{13}HQK$ and $L_{17}VFF$. The polyphenols studied were (+)-catechin, (-)-epicatechin, cyanidin, and quebecol. Through an analysis of binding energies and interactions obtained using the CHARMM22 force field, these molecules were shown to have some affinity to HHQK but more so toward LVFF. Cyanidin, however, showed very little affinity to HHQK. All of the molecules seemed to interact with an amino acid outside of the two regions: E_{22}. Because of the proximity of E_{22} to LVFF, this may have had a helping hand in the stability of docking the molecules to this region.

List of Abbreviations Used

AD	Alzheimer's disease
Aß	Amyloid β-peptide
His/H	Histidine
Lys/K	Lysine
Leu/L	Leucine
Val/V	Valine
Phe/F	Phenylalanine
Glu/E	Glutamic acid
HH	His13-His14
H13K	His13-Lys16
H14K	His14-Lys16
LV	Leu17-Val18
LF19	Leu17-Phe19
LF20	Leu17-Phe20
VF19	Val18-Phe19
VF20	Val18-Phe20
FF	Phe19-Phe20
AA	Pi-pi interaction
AH	Pi-hydrogen interaction
A+	Pi-cation interaction

SCA	Side chain hydrogen acceptor
SCD	Side chain hydrogen donor
BBA	Backbone hydrogen acceptor
BBD	Backdone hydrogen donor

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1 Introduction

1.1 Computer-aided Drug Design

Computational chemistry is an area of chemistry that is very beneficial to medicinal chemistry today. A technique that is commonly used for studying large protein systems within drug design is called molecular modeling. Molecular modeling, unlike quantum mechanics, ignores electronics of the system under study and solely uses the positions of the atoms to calculate the energy.[1] These methods will be discussed in further detail in Chapter 2. Computational simulations can be used to investigate very specific interactions between proteins/peptides and other molecules, protein folding and conformations, and protein stabilities.[1] This information can provide great insight to the development and potential binding ability of structures for drug candidates. This methodology is employed for discovering drugs and providing insight into the pathology of Alzheimer's disease and will be the basis of this thesis.

1.2 Alzheimer's Disease

One of the major health concerns today that affects the aging population and their families is Alzheimer's disease (AD).[2] It is the most common form of neurodegenerative dementia where neuronal abilities, such as memory and cognitive functions, progressively decline due to damaged brain cells.[3] As a result, this disease includes a vast number of behavioral and psychological changes. The psychological symptoms progress from mild to severe memory loss, where patients cannot recognize family members and close friends.[3,4] Additionally, changes in behavior and mood can occur that severely affect daily life. These include increased irritability, depression, disorientation, deep

confusion, and difficulty speaking.[4] Although AD mainly affects people who are age 65 or older, the disease is not a normal part of aging.[2,4,5]

Two abnormalities that are known to be found within the brains of AD patients are neurofibrillary tangles (NFTs) of tau protein and aggregates of a peptide called β-amyloid (Aβ).[6] Both of these do develop as a normal process of aging, however, they are present in much higher quantities in Alzheimer's. Tau works to stabilize microtubules within the brain cells, providing structural support and intracellular transport. Without this stabilization, the microtubules disassemble which starts a degradation of cellular structure.[6] Although the NFTs contribute greatly to the cell death associated with AD, it seems to occur as a result of AD and is not considered the main cause.[7] The Aβ aggregates are commonly known as plaques and their development is currently the most commonly accepted hypothesis as the cause and progression of AD.[3,5,7] Many of the current curative AD drug design initiatives are aimed toward stabilizing this peptide.

1.3 Amyloid-beta Peptide

Amyloid β-peptide is a 39-43 residue peptide that is generated by proteolytic cleavage of a protein called amyloid precursor protein (APP).[7] The most prevalent fragments of generated Aβ are Aβ(1-40) and Aβ(1-42).[3] The latter form is thought to be more neurotoxic and therefore associated with Alzheimer's disease. The single letter code[8] of amino acids making up Aβ(42) is:

$$\text{DAGFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA}_{42}$$

Aβ is naturally found in the brain in a soluble α-helix or sometimes random coil form.[6] It only becomes neurotoxic when it undergoes a conformational change to a β-

sheet form.[2,3,5] This occurs because of the Aβ peptide interacting with negatively charged regions on lipid membranes which in turn induces misfolding and damage to the Aβ peptide.[6] Once in the β-sheet, the peptide starts to form aggregates of itself into small oligomers. The oligomers form larger protofibrils which can sometimes turn into insoluble fibrils that ultimately become plaques.[6] They are found within the learning, memory, and emotional behavior parts of the brain and as the disease progresses, the number of aggregated Aβ increases as well.[3]

1.4 Drugs for Alzheimer's Disease

1.4.1 Current Drugs

There are many drugs currently on the market that solely treat the symptoms of AD, such as donepezil.[9] This drug is an acetylcholinesterase inhibitor and it works to increase the half-life of the remaining acetylcholine in the brain.[10] Neurons that do not work stop producing acetylcholine and by preventing the breakdown of this remaining neurotransmitter, there is a temporary prevention of progression of the symptoms of AD.[10] However, there are currently no drugs that help cure or prevent the disease. Even with symptomatic drugs, the worldwide cost of dementia was approximately $422 billion in 2009 and in 2010, 35.6 million people were living with Alzheimer's disease.[11] Both of these numbers are expected to increase greatly within the next twenty years.[11] The discovery of a curative drug could contribute greatly to decreasing the psychological and economic burdens of Alzheimer's disease. There are and have been many different approaches to this including designing vaccines to reduce the number of Aβ in the brain and reducing the production of Aβ by preventing the cleavage of APP.[12] A common

current approach is to find an anti-aggregate for Aβ to prevent it from forming deposits without reducing the number of natural Aβ in the brain.[10,12]

1.4.2 Design of Anti-aggregation Drugs

One region that is of particular interest to target on the Aβ peptide is the $\mathbf{H}_{13}\mathbf{H}_{14}\mathbf{Q}_{15}\mathbf{K}_{16}$ region. It has cationic side chains that cause it to be a highly positive region on the peptide. Since it is highly positive, it presents a likely region for interacting with the negative regions on the lipid membranes that induce misfolding.[13,14] Additionally, the imidazole rings on the histidines present a likely opportunity for π- π interactions which would help stabilize binding with a small molecule that also contains aromatic rings. It also follows a commonly found motif within proteins affiliated with AD. This is called the BBXB motif where B represents a basic amino acid and X representing any other amino acid.[13] The advantage here is that since it is a common occurrence, a molecule that binds to one BBXB area could potentially bind to other BBXB areas allowing for the treatment of the disease in multiple ways. Targeting to bind small molecules to this area may help prevent conformational changes to Aβ and ultimately to prevent aggregation.[13] This is the goal in designing anti-aggregate drugs for Alzheimer's disease and many make it to testing in clinical trials with this very design approach.

An additional region that could be targeted is HHQK's neighbor, $\mathbf{L}_{17}\mathbf{V}_{18}\mathbf{F}_{19}\mathbf{F}_{20}$. The LVFF region presents great binding potential for small molecules that contain aromatic rings because of the presence of the benzyl side chains on FF. Furthermore, if the small molecules could bind next to HHQK, it could provide extra stability and help to prevent misfolding.

1.5 Role of Diet in Clinical Trials

Recently, various food extracts have been shown *in vitro* to have an anti-aggregate effect on Aβ.[15] Since one of the current common drug design strategies for AD is to target HHQK in an attempt to prevent aggregation, is it possible that the constituent molecules within these extracts may be acting in the same way to act as anti-aggregants of Aβ. If these molecules are indeed acting in this way, then it may be important to consider the role of diet within clinical trials of an anti-aggregate drug for AD.

1.5.1 Polyphenols potential

Fruits and berries constitute a major portion of the ideal healthy diet for humans. These are sources of an abundant array of polyphenols and antioxidants.[15,16] Polyphenols, which are a family of secondary plant metabolites, are characterized by a general structure[17-19] containing a specific three ring system: two aromatic rings (A/B) bound by three carbon atoms that form an oxygenated heterocycle (C) as shown in Figure 1.1.

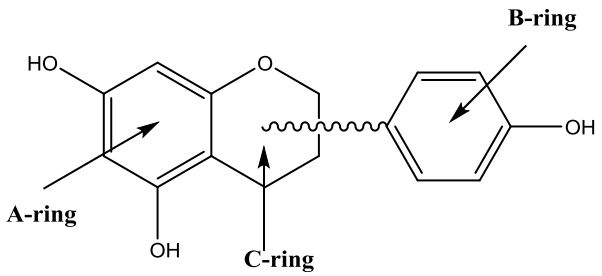


Figure 1.1. General structure of a polyphenol

Polyphenols represent several classes of compounds such as anthocyanins, flavonols, and flavan-3-ols[20] which are based on the variation (e.g. hydroxylation) of the general flavanoid ring. Anthocyanins vary in regards to hydroxylation and methoxylation among the three rings. Examples of this group includes cyanidin, malvidin, and pelargonidin. Flavonols, such as quercetin, are also known as 3-hydroxyflavones due to the hydroxyl

group found in position 3. The compounds vary according to further hydroxylation across the three rings. The flavan-3-ols are characterized by hydroxylation on the B ring and in some cases the presence of gallic acid in position 3. Common flavan-3-ols are catechin, epicatechin, epigallocatechin, and epigallocatechin gallate.[20]

There has been an immense amount of attention toward polyphenols and antioxidants for their potential to improve health, prevent certain diseases, and play a neuroprotective role.[17-22] Polyphenol dietary supplement studies have shown improvements in cognition and memory possibly because of their ability to reduce neuroinflammation in the brain and to interact with neuronal signaling pathways.[17] There are many challenges, however, to studying the beneficial effects of polyphenols. For example, a single piece of fruit contains a large variety of polyphenols with marginally different structures. Considering this along with the possible presence of their metabolites, it is difficult to estimate and analyze their exact concentrations in food.[20] The number of polyphenols will also vary in respect to species, geographical location, and seasonal variations. Moreover, the bioavailability of the molecules can vary between different people.[20] However, both catechin and epicatechin have been shown to cross the blood brain barrier (BBB) in two BBB cell lines.[19,23] Also, in a recent study, the polyphenols found within one of the most basic and accessible fruits, the apple, have been suggested to have anti-aggregation activity on Aβ.[15] In particular, it was the apple peel that was found to possess this quality. Therefore, despite the criticism, these molecules may be playing a role with AD.

1.5.2 Apple Peel

Apples are normally eaten with both the flesh and the peel, or sometimes just the flesh without the peel. It is important to note that in general, although it varies somewhat between apple varieties, the peel contains more and different polyphenols than the flesh.[16,24] The concentration of total and individual polyphenols varies across the diverse variety of apples. There are over 6000 species of apples cultivated worldwide; however, there are a few varieties that are commonly consumed worldwide.[25] These include Golden Delicious, Granny Smith, Fuji, and Gala.[25] On average across a span of common apple varieties, including apples that are common in Canada such as the McIntosh, apple peels are composed of five different groups of polyphenols: 60% flavan-3-ols, 18% flavonols, 9% hydroxycinnamic acids, 8% dichydrochalcones, and 5% anthocyanins.[24] The biggest group, the flavan-3-ols, consist of molecules such as (+)-catechin and (-)-epicatechin.[15,24] Although anthocyanins only constitute about 5% of the apple peel, cyanidin is one molecule that is often seen in high quantities across the different apple varieties.[15,24] These molecules are summarized in Figure 1.2.

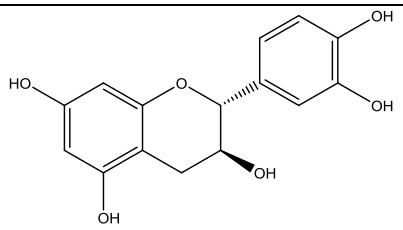
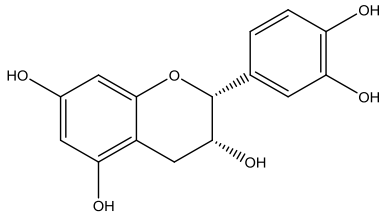
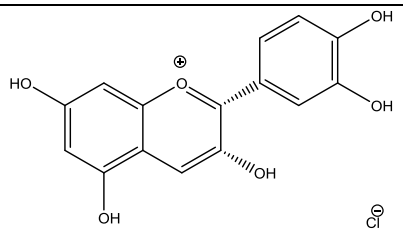
Apple Molecule	Structure
(+)-catechin	
(-)-epicatechin	
Cyanidin [chloride]	

Figure 1.2. Common polyphenols found within apple peels.

Since these polyphenolic molecules compose a high percentage of the apple peel, it is of great interest to investigate their ability to interact with Aβ to see if there are any molecules in particular that are the most bioactive. Apples are one type of food that contains potentially important polyphenols for Aβ, but there is a novel polyphenol found within a Canadian food that could also have similar effects.

1.5.3 Maple Syrup

One particular food condiment that is widely consumed in Canada is maple syrup. Canada accounts for the production of more than 80% of the world's supply of maple syrup.[26] This product is made through an intense heating process of sap, a natural product

collected from deciduous trees. The tree sap contains a large variety of molecular compounds aside from the obvious abundance of sugars. It also contains many polyphenols which are thought to contribute to maple syrup's biological properties (antioxidant, antimutagenic, etc). However, during the process of making sap into syrup, many novel polyphenols are made through the chemical reactions. These novel molecules could be contributing to maple syrups biological activity ability. One molecule that has been recently discovered but not yet tested for potential activity against Alzheimer's is quebecol.[26] This compound, shown in Figure 1.3, will be used to test against amyloid-β because it is a novel polyphenol and has potential to bind with its aromatic rings.

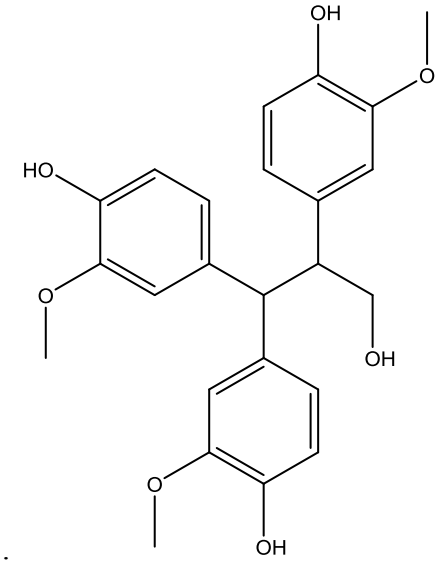


Figure 1.3 The structure of quebecol, a novel polyphenol compound derived from the process of making sap into maple syrup

1.6 Focus of Study

There is an immense amount of research going into developing and discovering a drug to cure Alzheimer's disease. A lot of these efforts involve designing an anti-aggregant for Aβ. The focus of this study is to complement these efforts by investigating molecules commonly found in human diet, through apples, that may act in the same way these drugs are working. The molecules that will be investigated are displayed in Figure 1.2. They were chosen based upon how prevalent they are within apple peel and because of their potential to bind to HHQK and LVFF due to high aromaticity. It is of interest to extend the *in vitro* work that suggested apple polyphenols have anti-aggregate activity to molecular modeling to see if the molecules do bind to the HHQK and LVFF regions of Aβ and if so, in which way and how well. The maple syrup molecule, quebecol, is a novel polyphenol discovered within maple syrup. It is being investigated because it is new and thought to possibly contribute to maple syrup's biological activity.[26] In a similar fashion to the apple molecules, it will be modeled against Aβ in the HHQK and LVFF regions to investigate any possible significant interactions.

2 Computational Methods

2.1 Molecular Modeling and Force Fields

Molecular modeling is a computational technique that uses classical forces to perform calculations on a chemical system. That is, it uses the positions of the atoms to determine energies and structural information instead of electronic wavefunctions like quantum mechanics.[1,27] This can be done because of the Born-Oppenheimer approximation: nuclei are so much heavier than the electrons and as a result it can be assumed that the electrons can quickly redistribute themselves to adjust to nuclear movements.[1] Therefore, as the atoms change position, the energy of the system changes. The energies of these movements are calculated through the use of force field equations.[1,27,28] These equations derive from a simplistic ball-and-stick model of the molecule where the atoms are considered as weights connected by springs. Energies of bond stretching and bending, angles, and rotations are calculated through fairly non-complicated equations such as Hooke's Law. Many versions of force fields are available with each one differing through the use of slightly different equations and parameterizations. They are selected based on the type of system being explored. Since this experiment focuses on proteins and small molecules, an appropriate force field was chosen.

2.2 CHARMM22

This study employed the use of CHARMM22[28] (Chemistry at Harvard Macromolecular Mechanics) through the software package MOE[29] (Molecular Operating Environment Inc.). CHARMM22 is useful for *in vacuo,* or gas phase, calculations

involving proteins as well as solution phase calculations for proteins. CHARMM calculates the energy by a sum of the energies of the bonded and non-bonded interactions within a system. The simple form of the equation[28] is:

$$E_{tot} = E_b + E_\theta + E_\varphi + E_\omega + E_{UB} + E_{NB} + E_{CMAP} \quad \textbf{(1)}$$

The first four terms, E_b, E_θ, E_φ and E_ω, are the bonding terms. Respectively, they represent the energies for 1,2 interactions (bond length), 1,3 interactions (bond angle), 1,4 interactions (torsional angle), and the improper inversion or out-of-plane bending. For the bonding, angle, and improper inversion energies, they are each calculated as a sum of a variation of Hooke's law and are treated as harmonic oscillators.[28] The equations for each are as follows:

$$E_b = \sum k_b (r - r_o)^2 \quad \textbf{(2)}$$

$$E_\theta = \sum k_\theta (\theta - \theta_o)^2 \quad \textbf{(3)}$$

$$E_\omega = \sum k_\omega (\omega - \omega_o)^2 \quad \textbf{(4)}$$

In each equation, k_x, is a force constant that is represented by CHARMM parameters, where x represents the symbol for the equation. In the quadratic portion of the equation, r, θ, and ω all represent the bond length, bond angle, and improper angle being measured while r_0, θ_0, and ω_0 represent the equilibrium values for each of these descriptors.[28] The energy for the third bonding term, the dihedral angles, does not follow the same Hooke's Law pattern. The equation is:

$$E_\varphi = \sum k_\varphi [1 + \cos(\eta\varphi - \delta)] \quad \textbf{(5)}$$

Similarly, k_φ is a force constant, η represents the multiplicity of the function or the periodicity of the dihedral angle, φ is the current dihedral angle for a set of four atoms, and δ is the phase shift.

The next three energy terms, E_{UB}, E_{NB}, and $E_{CMAP,}$ represent the non-bonding energy interactions. E_{UB} is the Urey-Bradley term which accounts for angle bending through 1,3 nonbonded interactons. For three bonded atoms, A-B-C, the Urey-Bradley term is a quadratic function of the distance between atoms A and C.[28] This also follows Hooke's Law and is calculated as:

$$E_{UB} = \sum k_{UB}\left(u - u_o\right)^2 \qquad \textbf{(6)}$$

As above, k_{UB} is a force constant, and u represents the distance between the 1,3 atoms in the harmonic potential. This term is important for calculating in-plane deformations as well as separating symmetric and asymmetric bond stretching modes. The energy calculation for the non-bonded terms accounts for both van der Waals and electronic interactions[11]. The equation is as follows:

$$E_{NB} = \sum \left\{ \varepsilon_{ij}^{\min} \left[\left(\frac{R_{ij}^{\min}}{r_{ij}} \right)^{12} - 2\left(\frac{R_{ij}^{\min}}{r_{ij}} \right)^{6} \right] + \left(\frac{q_i q_j}{4\pi\varepsilon_o \varepsilon r_{ij}} \right) \right\} \qquad \textbf{(7)}$$

The portion within the square brackets represents the 12-6 Lennard Jones (LJ) potential that calculates van der Waals (vdw) energy. The portion within the round brackets is the Coulombic potential which calculates the electrostatic energy. The first term, ε_{ij}^{min}, is the LJ well depth, R_{ij}^{min} is the distance of minimum interaction energy or the distance at the minimum of the LJ, and r_{ij} is the distance between atoms *i* and *j*.[28]

The last term, E_{CMAP}, is an optional term that can be used with CHARMM. This is a spline function that is used as a correctional term to treat the conformational properties of the protein backbone.[30] The backbone, which consists of the $-N-C_{\alpha}-C^{=O}-$ angle, may need a torsional correction term and that is what E_{CMAP} is used for. The angle between N-C_{α} is denoted as Φ, ψ for C_{α}-C=O, and ω for the amide bond.[1] Since the amide bond is planar and has a high energy barrier for rotation, it is unlikely that it will experience any deviation from 0˚ or 180˚ and a correction term is not needed.[1] Therefore, the 2-D dihedral energy correction map (CMAP) is calculated with *ab initio* quantum mechanics calculations and is applied to the Φ/ψ surface only.[30]

2.3 *In vacuo* Calculations

2.3.1 Energy Minimization Algorithms

Studying a particular system for drug design is most useful when it is in the most stable conformation. The optimal conformation corresponds to a minimum point on the potential energy surface (PES) which is a description of the energy variation of a system as the nuclear coordinates change.[1,27] As the atoms change their positions for each iteration, the energy changes. Therefore, in order to find the lowest points on the PES, energy minimization algorithms are employed.

MOE uses three different energy minimization methods sequentially.[29] It starts off with a more versatile method called steepest descent, moves on to conjugate gradient to increase the accuracy of the minimum point, and then to truncated Newton to refine the minimum even more. The steepest descent and conjugate gradient algorithms are both first-order minimization methods where the first derivative of the energy with respect to the coordinates is used to determine the gradient, or the direction of the energy. The

truncated Newton is a second-order method that employs both the first and second derivatives of the energy curves to determine minimum energy points. The second derivative gives details about the curvature of the total-energy function.[1]

The steepest descent algorithm is very helpful to use as an initial minimization technique because it can take a system with high energy and minimize it with ease to a lower energy state. The atomic coordinates are gradually changed to decrease the energy and move along the PES to the minimum point. Each change of coordinates moves parallel to the force and is referred to as an iteration. The change between iterations is known as a step and the starting point of each iteration is the conformation from the previous step. The step sizes are determined by two ways: a line search or arbitrary step.[1]

The line search is as it is called: it tries to locate a minimum along a specific line. It finds three points on the line where two are higher in energy than the middle point. This method is called bracketing. Each iteration after that is done to decrease the distance between the points, pinpointing the minimum more accurately. The gradient at the minimum will be perpendicular to previous steps and the next direction will be orthogonal.[1]

The arbitrary step method involves modifying the step size based on the energy result of the previous iteration. It starts off with a predetermined step size and then is changed based on whether the energy increases or decreases. This method might take more iterations than the steepest descent to locate a minimum point, however, it is advantageous in that it requires fewer energy evaluations. Once the energy gets close to the minimum, a more precise method should be employed and in the case of MOE, it is the conjugate gradient method.[1]

The conjugate gradient method uses the line search method just as the steepest descent does. The difference lies in that the direction of the steps is conjugate; however, the gradient remains orthogonal.[1] This change allows for the minimum to be found in fewer steps.

The truncated Newton method is used to refine the minimum point even more. This algorithm solves the inverse Hessian matrix using an iterative linear equation solver. This is used to help solve the equations and decrease computational expense.[1] After a few iterations, the equation solver is stopped which gives way to the name of truncated Newton.

2.4 Solvent Calculations

Solution calculations in water were performed to mimic the actual environment of the brain and to see if this would change the interactions between the corresponding molecule, like catechin, and Aβ. In MOE and using the CHARMM22 force field, an explicit water model was used. This was chosen because using actual water molecules could show real interactions between the water molecules and the peptide. These potential interactions could change the way that Aβ interacts with the molecules under investigation.

The explicit model used was TIP3P, which treats the water molecules as rigid. It considers three sites of interaction which correspond to the two hydrogens and one oxygen in the molecule.[1] To set up this solvent calculation, a solvent box was placed around the system. For this particular study, water molecules were periodically placed around the system under study with a cutoff distance of 6 Å between a solute atom and an

atom on any of the water molecules. Once this box was set up, an energy minimization was performed. Since water molecules were present to interfere with any intramolecular interactions that Aβ might undergo, the backbone was not constrained.

2.5 Conformers of Aβ Studied

2.5.1 NMR Structures

There are several different NMR structures available of conformers of the Aβ peptide. In this experiment, six particular structures of varying length were obtained from the Protein Data Bank (PDB) which are identified as 1AMB[31], 1AMC[31], 1AML[32], 1BA4[33], 1IYT[34], and 1Z0Q[35]. These six structures were used to see if the polyphenols studied would bind to the HHQK and LVFF regions of each. Two structures, 1AMB and 1AMC, consist of residues 1-28 of Aβ where they both possess an alpha helical conformation.[31] These are represented in Figure 2.1. Another two structures represented residues 1-40, 1AML and 1BA4, as shown in Figure 2.2. Although these two structures are the same in length, they possess different conformations. The AML structure is a random coil whereas BA4 is another alpha helical conformation.[32,33] The last two structures, 1IYT and 1Z0Q, both have residues 1-42. Since it is hypothesized that the 1-42 length of Aβ is the neurotoxic form, these two structures are important to use to model this toxic form. The IYT structure has two alpha helices that are separated by a turn caused by hydrogen bonding[34] whereas Z0Q was obtained from an experiment investigating the change of Aβ from α-helix to β-sheet.[35] These two structures are shown in Figure 2.3.

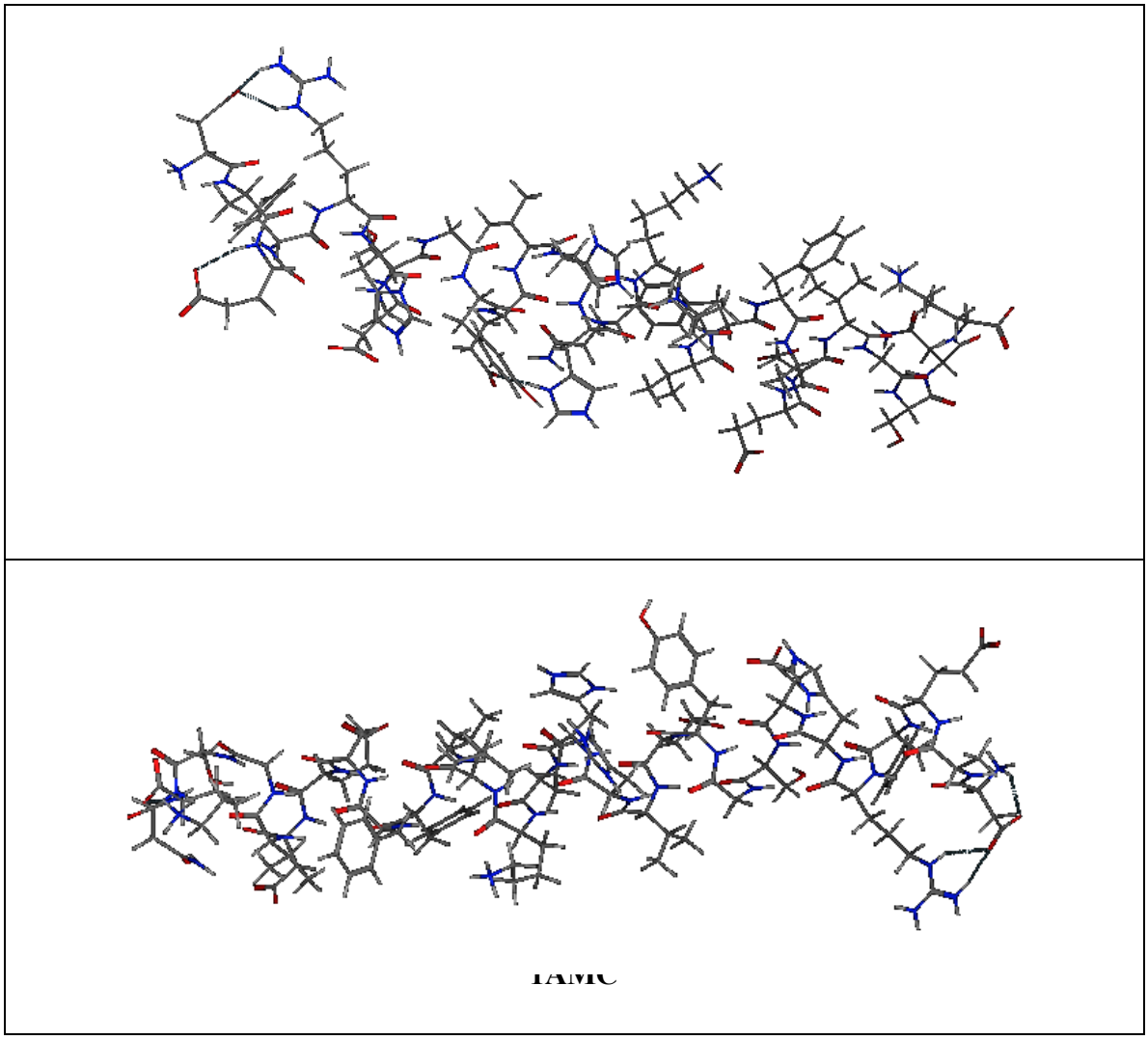


Figure 2.1. Images of the *in vacuo* optimized conformers of β-amyloid(1-28) obtained from the Protein Data Bank.

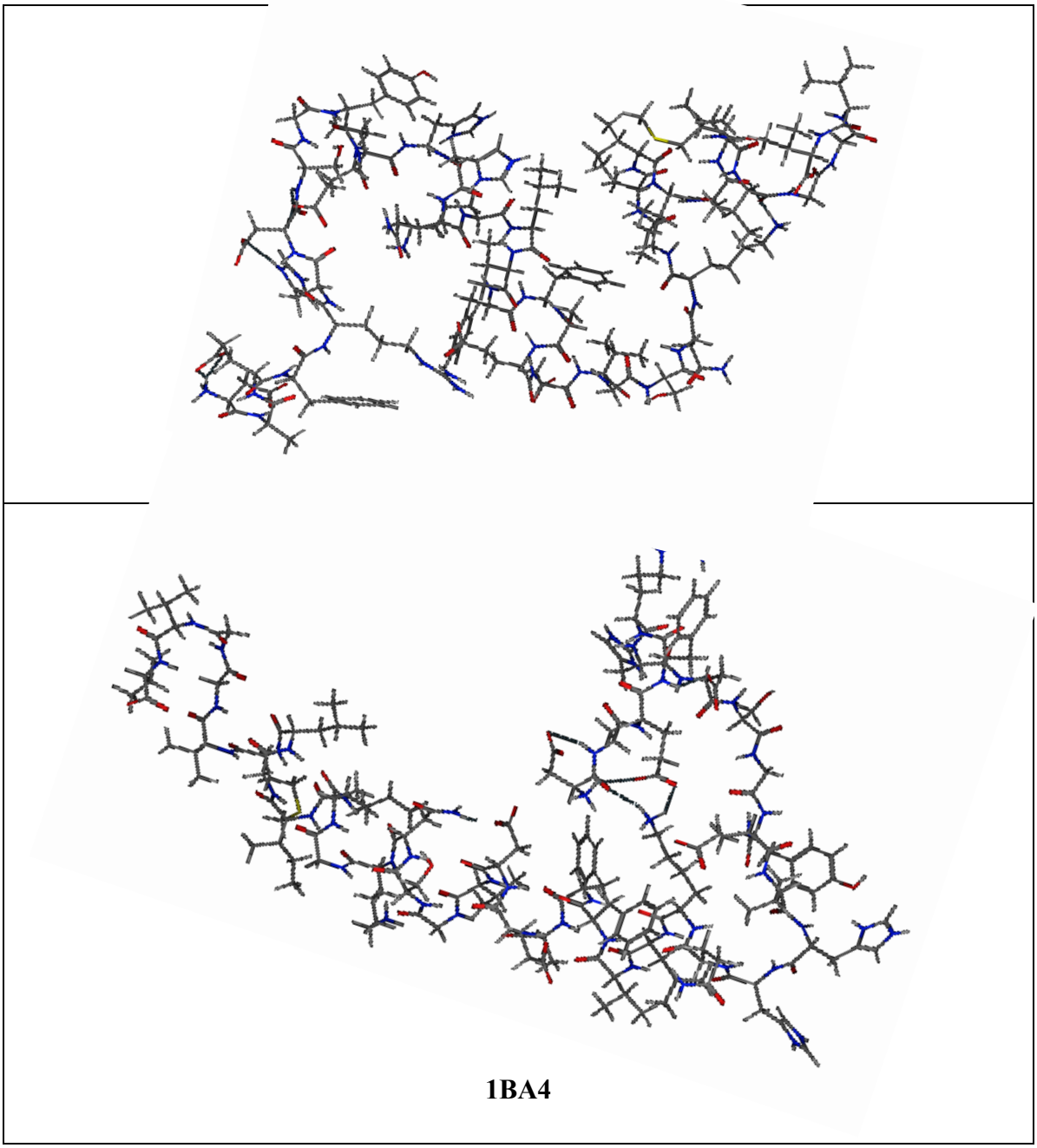


Figure 2.2. Images of the *in vacuo* optimized conformers of β-amyloid(1-40) obtained from the Protein Data Bank.

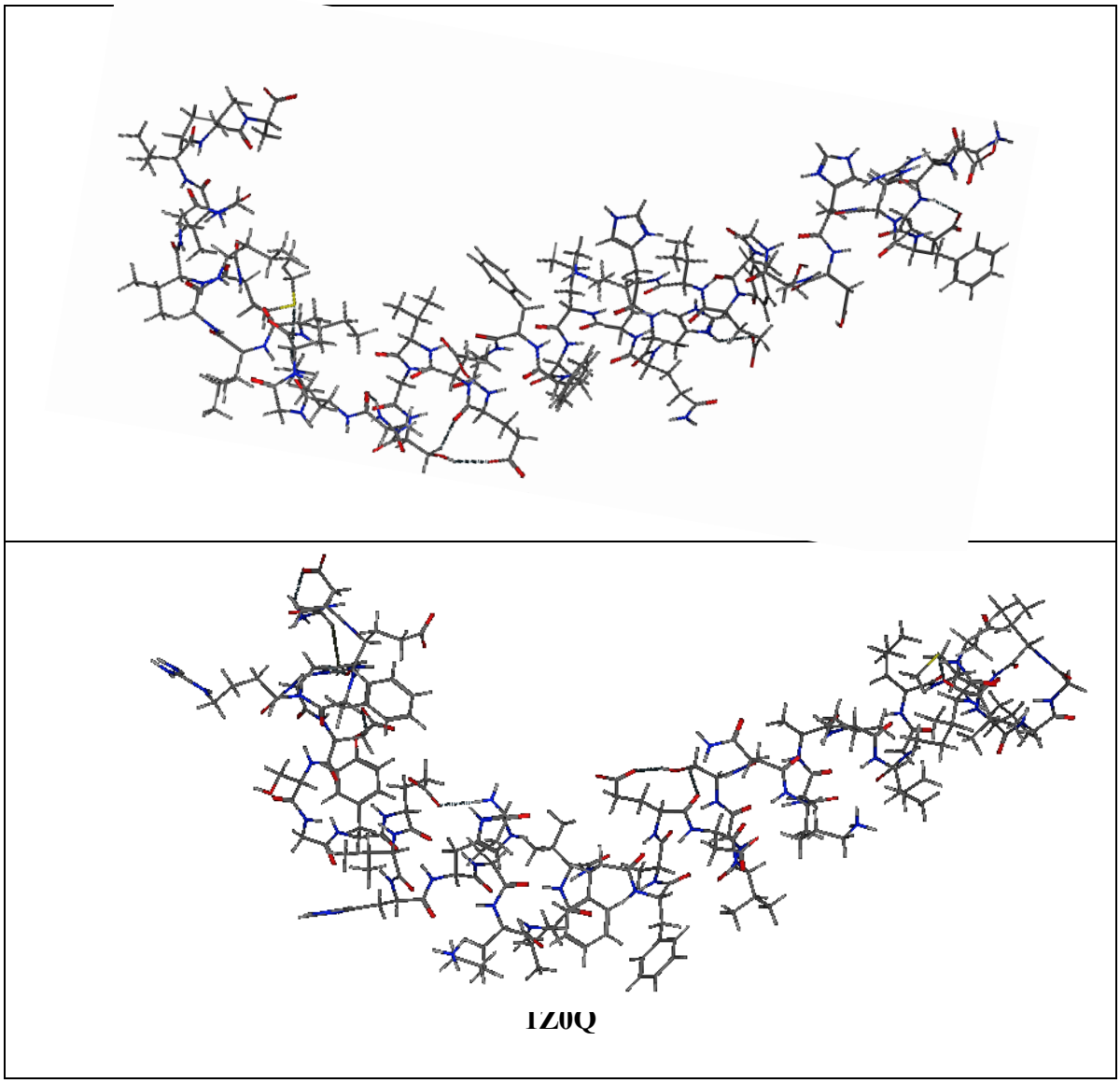


Figure 2.3. Images of the *in vacuo* optimized conformers of β-amyloid(1-42) obtained from the Protein Data Bank.

2.5.2 Preparing the Conformers and Molecules for Calculations

Once obtained from the PDB, each of the six conformations of Aβ were imported into MOE and adjusted for physiological pH to perform gas phase calculations. That is, it was ensured that the terminal ends were charged for zwitterionic form and that the histidine residues were protonated. The protonation occurs because the microcellular area where the Aβ plaques are found is slightly acidic. These structures also needed to be optimized, that is to find the minimum energy conformation on the potential energy surface (PES) in the gas phase. Before optimizing, the backbone atoms of the peptide were fixed so that no intramolecular interactions could occur and change the conformation of the structure. This could possibly happen while performing gas phase calculations since there are many polar side chains within the Aβ structure and there are no interfering atoms to prevent this. Each one was then minimized using a systematic search with the CHARMM22 force field. The systematic search consisted of multiple iterations of changing geometrical parameters such as bond angles and evaluating the energy at each step. After the systematic search, the lowest energy conformation for each structure was chosen to use for the rest of the experiment. These lowest energies for each conformation of Aβ are displayed in Table 2.1. The lowest energy conformations were also found in solution phase (Table 2.1) for when solution calculations were performed. After the conformers of β-amyloid were optimized in gas phase, the target molecules (apple and quebecol molecules) were then built within MOE and minimized as well using the systematic search and CHARMM22 in both gas and solution phase. The energies for each are summarized in Table 2.2.

Table 2.1. Minimum energies of six Aβ conformers obtained from the Protein Data Bank calculated using a systematic search in gas phase and in water.

Conformer of Aβ	Energy *in vacuo* (kcal/mol)	Energy in Water (kcal/mol)
1AMB	36.202	179.624
1AMC	68.118	191.726
1AML	247.209	424.266
1BA4	191.200	400.285
1IYT	213.844	378.721
1Z0Q	176.090	399.488

Table 2.2. Minimum energies of the target molecules calculated using a systematic search in gas and solution phase.

Target Molecule	Energy *in vacuo* (kcal/mol)	Energy in Water (kcal/mol)
(+)-catechin	41.665	47.593
(-)-epicatechin	38.798	44.074
cyanidin	43.747	52.818
quebecol	71.711	79.714

2.6 Manual Docking Method

Once the lowest energy structures were found for both the Aβ conformers and the target molecules, they were paired together to undergo investigation of possible interactions. This was done by taking one molecule, changing its orientation toward the HHQKLVFF region on each Aβ conformation and calculating its energy. This gave information about what orientation the molecule would need to produce a binding interaction to Aβ. This was done in gas phase first and then because there were so many possibilities for orientation, only a select few were chosen to move on to a solvent calculation in water, mimicking the physiological condition of the brain. This was necessary because solvent calculations are much more computer costly in terms of time.

To select the orientation of each target molecule toward HHQKLVFF, each oxygen on the molecule was given a number (example in Figure 2.4). For this particular project, two oxygens were initially oriented toward two amino acids at a time. For example, O1 and O2 to His13His14, then O1-O3, O1-O4, etc. This allows for a wide variety of possible orientations of the target molecule toward two amino acids. By using this method, there are different types of interactions that could occur. First, the hydroxyl groups have potential to form interactions such as hydrogen bonds because they can act as a hydrogen donor. Second, since the oxygens are dispersed among the aromatic rings of the polyphenols, this also allows for the orientation of the rings toward the amino acids. This is important because many amino acids within the HHQKLVFF region have aromatic rings, like histidine and phenylalanine. This was done along the whole HHQK and LVFF regions. For each orientation, the two oxygens were placed 3 Å from the two

amino acids. This distance comes from previous studies that suggest this distance is favorable for interactions between drugs and receptors.

(+)-catechin

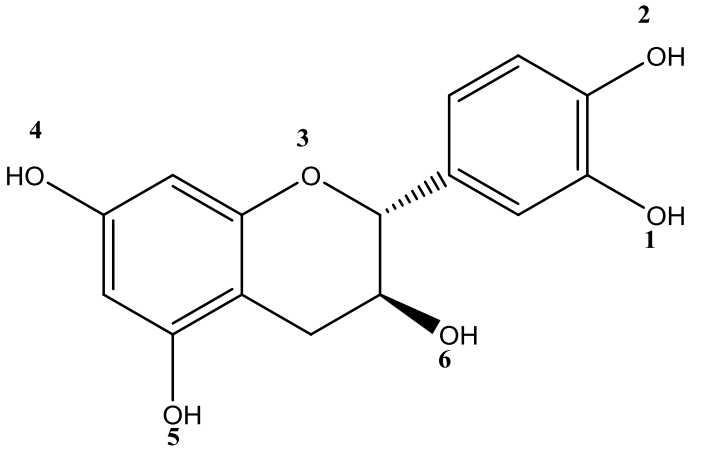


Figure 2.4. Example for numbering the oxygen that were oriented toward HHQK/LVFF on Aβ for (+)-catechin.

After the system was set up, the energy of the system was minimized (while the backbone of Aβ was fixed) and the total potential energy was calculated. This energy led into the calculation of the binding energy which was important to determine how favorable an orientation was. It indicated whether or not the binding increased or decreased the energy of the system. The binding energy was calculated as follows:

$$E_{bind} = E_{system} - E_{A\beta} - E_{molecule} \quad \textbf{(8)}$$

Aside from energies, information about interactions that occur from a particular orientation were obtained. The different types of interactions that were found to occur involved either H-donation/acceptance, pi-pi interactions, pi-cation, or pi-hydrogen

interactions. The pi-pi interactions are denoted as AA, where A indicates aromatic. The pi-cation interactions are written as A+ and the pi-hydrogen as AH. For the hydrogen donations, these are broken down into two different groups. If they occurred from the side chain, it is denoted as SCD/SCA where D is for donation and A is for acceptance. Similarly, if they occurred from the backbone, it is denoted by BBA and BBD.

3 Apple Peel Molecule Results

3.1 Catechin

One of the main molecules found within apple peel is (+)-catechin. It is also important because it is a monomer for further molecules found within apple peels called proanthocyanidins. This molecule was docked toward the HHQK and LVFF regions on each of the six Aβ conformers. It was first oriented toward His13His14 on conformer 1AMB, using 15 different possible initial orientations. These 15 orientations came from the oxygen numbering method described previously in Chapter 2 and as shown in Figure 2.4. Since there are 6 different oxygens, the orientations involved are: 1/2 ; 1/3 ; 1/4; 1/5 ; 1/6 ; 2/3 ; 2/4 ; 2/5 ; 2/6 ; 3/4 ; 3/5; 3/6; 4/5; 4/6 ; 5/6.

Conversely, the orientations could also go in the opposite direction. For example, for 1,2 where 1 is oriented toward His13 and 2 is oriented toward His14, the 2 could be toward H13 and the 1 to H14. This was trialed for 3 sets of calculations for an orientation toward His13-Lys16 using 1AMB, 1AMC, and 1AML. The results are found in Table 3.1. They provided very similar results and because of that, the method of the 15 orientations was continued for the entire project.

Table 3.1. Binding energies in kcal/mol for three trials of the numbering method in reverse for (+)-catechin for systems 1AMB, 1AMC, 1AML for H13K in gas phase.

	1AMB H13K		1AMC H13K		1AML H13K	
	Backwards	Regular	Backwards	Regular	Backwards	Regular
1,2	-20.87	-11.86	-26.26	-26.21	-42.12	-77.83
1,3	-17.10	-15.31	-23.49	-25.20	-76.38	-84.38
1,4	-15.06	-24.10	-27.09	-33.86	-28.21	-38.38
1,5	-21.23	-22.70	-14.53	-27.11	-87.15	-38.93
1,6	-12.03	-13.66	-26.51	-23.62	-39.30	-52.84
2,3	-33.33	-30.68	-24.05	-30.34	-44.78	-26.15
2,4	-15.75	-20.49	-42.87	-18.63	-41.13	-34.93
2,5	-6.99	-12.41	-18.97	-20.84	-56.01	-84.52
2,6	-11.40	-18.22	-28.88	-23.70	-57.94	-38.26
3,4	-21.88	-16.91	-20.49	-29.22	-54.58	-40.81
3,5	-23.26	-15.80	-32.84	-41.89	-66.70	-72.92
3,6	-33.67	-18.61	-21.00	-22.69	-58.74	-57.32
4,5	-16.95	-13.72	-24.26	-10.10	-56.32	-97.76
4,6	-11.66	-22.69	-25.11	-25.86	-69.68	-29.86
5,6	-18.70	-35.12	-11.00	-22.37	-35.41	-64.04
Average	-18.66	-19.48	-24.49	-25.44	-54.30	-55.93

After catechin was docked to 1AMB, then it was docked toward His13His14 on 1AMC. This process continued for the rest of the Aβ conformers and for the entire HHQK LVFF regions. Although there were 15 different possibilities, some orientations were not considered for certain systems if they were not plausible. That is, if they could not be placed 3 Å away or if there was crowding of neighbouring amino acids. To study the affinity of catechin to Aβ, the binding energies and interactions were all analyzed. This was first done in the gas phase, and then in water.

3.1.1 Gas Phase Results

3.1.1.1 His13-His14: An Example

As previously mentioned, there were usually 15 different possible initial orientations for catechin to be positioned toward the two amino acids in question, His13 and His 14. Orientation 3,6 was not plausible for conformers 1AMB and 1Z0Q as well as orientation 1,2 for 1Z0Q. For the each of the Aβ conformers, the binding energies for each were calculated as follows in Table 3.2.

Table 3.2 Binding energies in kcal/mol for the different initial orientations of catechin toward His13His14 as calculated in gas phase using CHARMM22.

Orientation	1AMB	1AMC	1AML	1BA4	1IYT	1Z0Q
1,2	-27.88	-33.06	-18.61	-9.78	-28.18	N/A
1,3	-35.99	-47.26	-41.59	-21.13	-29.59	-8.68
1,4	-48.01	-40.71	-69.91	-14.75	-31.10	-22.01
1,5	-22.82	-20.13	-39.13	-9.04	-25.75	-22.96
1,6	-36.07	-29.90	-41.85	-19.78	-31.39	-25.48
2,3	-29.08	-32.32	-39.42	-18.32	-21.87	-27.78
2,4	-9.57	-29.08	-57.57	-3.60	-31.89	-25.42
2,5	-21.16	-33.90	-60.75	-4.51	-27.58	-11.17
2,6	-47.63	-44.71	-34.85	-12.64	-34.06	-20.79
3,4	-26.53	-44.54	-77.29	-29.01	-44.78	-29.45
3,5	-35.65	-50.47	-59.49	-17.69	-24.75	-22.66
3,6	N/A	-20.07	-51.91	-21.42	-33.63	N/A
4,5	-19.18	-30.02	-46.68	-5.21	-32.10	-18.18
4,6	-23.26	-39.14	-46.79	-20.55	-22.41	-22.61
5,6	-21.06	-34.57	-24.29	-10.51	-19.15	-18.28
Average	-28.85	-35.32	-47.34	-14.53	-29.22	-21.19

For this particular docking, it was found that on average 1AML had the lowest binding energies with -47.34 kcal/mol while 1BA4 had the highest with -14.53 kcal/mol. That is, docking to 1AML lowered the energy of the system the most while docking to 1BA4 lowered it the least. These energies alone do not give much indication as to whether catechin is binding to His13His14. They were considered further when the average binding energies were calculated across the whole HHQK LVFF regions. In addition to the energies, interactions that occurred as a result of the energy minimization of the systems were analyzed. In order to do so, there were a couple of different factors that were considered: the type of interaction that occurred, such as pi-pi (AA) or hydrogen donation through side chain (SCD), what orientation, amino acid and atom/ring on the catechin molecule that produced it. The labeling of the different atoms other than oxygen are found in Figure 3.1

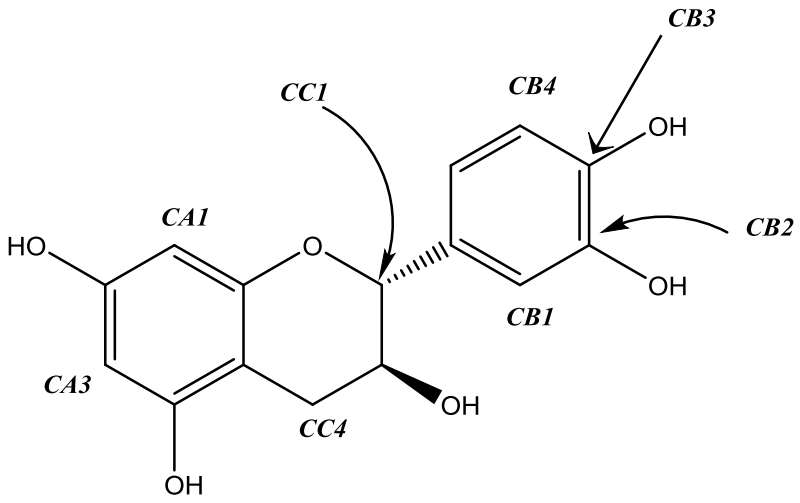


Figure 3.1 Non-oxygen atoms labeled in (+)-catechin.

For the orientations of catechin toward His13His14, there were 16 different interactions found to be occurring. They are summarized in Table 3.3 .

Table 3.3 Summary of interactions occurring across the different Aβ conformers for docking (+)-catechin to His13His14.

Aβ Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	14	CC4	1,5
1AMB	AH	14	CA4	2,3
1AMB	SCD	14	6	2,6
1AMB	SCA	22	5	2,6
1AMB	AH	17	A-ring	3,4
1AMC	AH	10	2	2,3
1AMC	AH	14	CA1	2,3
1AML	SCA	13	6	4,6
1AML	AH	31	A-ring	5,6
1BA4	SCA	14	6	1,6
1BA4	SCA	14	6	2,3
1BA4	BBD	11	2	3,4
1IYT	AA	13	B-ring	1,4
1IYT	AH	13	CC1	3,4
1IYT	SCA	14	6	4,6
1Z0Q	BBA	14	1	1,4

This method was employed for the rest of the targeted amino acids. The average binding energies and the interactions were recorded for all. These can be found in Appendix A.

3.1.1.2 Overall Energies and Interactions

The average binding energies for (+)-catechin docking to HHQK LVFF are found within Table 3.4 and Figure 3.2.

Table 3.4 Average binding energies in kcal/mol for docking to a specific amino acid pair for (+)-catechin in gas phase.

	HH	**H13K**	**H14K**	**LV**	**LF19**	**LF20**	**VF19**	**VF20**	**FF**
1AMB	-28.85	-19.48	-20.99	-19.13	-27.32	-20.06	-22.33	-29.91	-25.96
1AMC	-35.32	-25.44	-33.98	-39.35	-43.37	-31.10	-29.66	-41.45	-34.19
1AML	-47.34	-55.93	-63.43	-69.66	-80.68	-77.11	-61.52	-66.18	-52.57
1BA4	-14.53	-23.28	-26.45	-16.94	-7.69	-17.91	-8.22	-19.18	-34.02
1IYT	-29.29	-25.78	-25.13	-26.73	-62.22	-60.08	-58.46	-68.25	-52.24
1Z0Q	-21.19	-16.68	-23.00	-22.70	-17.89	-18.04	6.05	-22.15	-13.55
Overall Average	-29.42	-27.70	-32.16	-32.42	-39.86	-37.38	-29.02	-41.19	-35.42

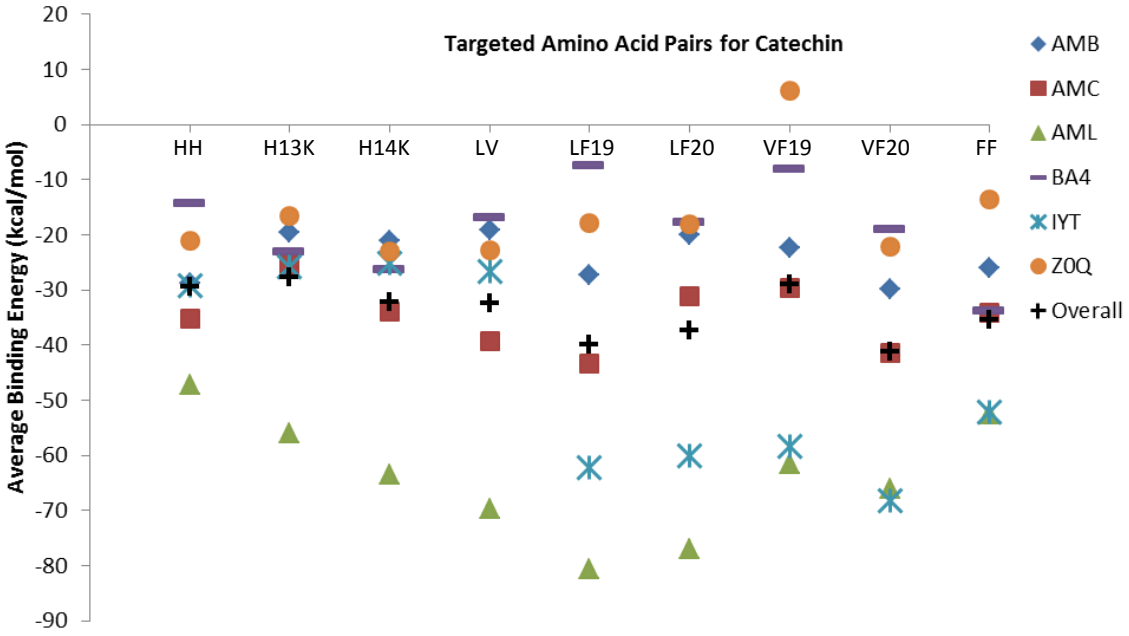


Figure 3.2 Average binding energies in kcal/mol for docking to a specific amino acid pair for (+)-catechin in gas phase.

The comparison of the average binding energies can be used to determine which conformer and which amino acid targets produce the lowest and most stable binding energies. From the overall average, the average across all of the conformers, the two lowest points on the energy scale are when (+)-catechin is being docked toward amino acids Lys16Phe19 (LF20) and Val18Phe20 (VF20). It can be seen that conformer 1AML has the lowest overall binding energies; however 1IYT is close from amino acids LF19 onward. Amino acid target LF19 seems to be a minimum or close to a minimum for most conformers except 1BA4 and 1Z0Q. For those two, H14K and VF20 seem to be minima. It should also be noted that amino acid targets His13His14 (HH) and Val18Phe19 (VF19) were found to have the highest average binding energies indicating they are less stable than the others.

Along with the energies, each calculation provided information about whether or not an interaction was produced. For (+)-catechin, there were a total of 206 interactions. These interactions were summed and correlated across the conformers, the amino acids, specific atoms on catechin, and the initial orientations to see what was contributing the most to produce these interactions. First, the interactions due to certain conformers were summed (Figure 3.3). In this case, conformers 1AML and 1AMC had the highest percentages of interactions with 22% each.

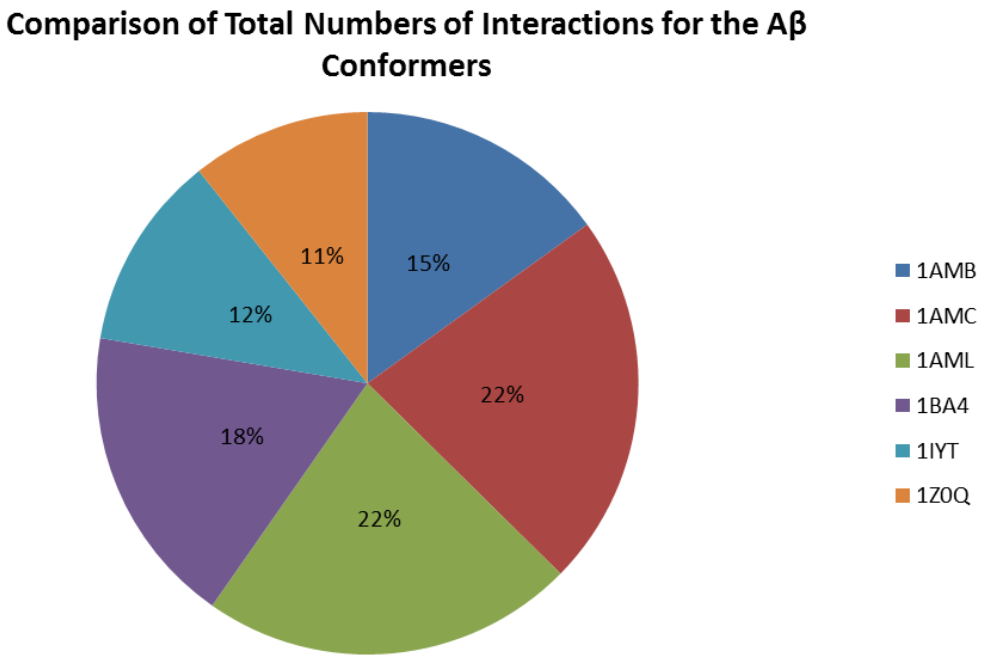


Figure 3.3 Percentages of total interactions due to a particular Aβ conformer.

The total number of interactions that occurred when a particular amino acid was involved is found in Figure 3.4. Most of the interactions occurred with His13 and Lys16 within the HHQK LVFF region. For His13, the majority of the interactions were found to be pi-pi. This is not surprising as both histidine and (+)-catechin contain an aromatic ring.

Although His14 is the same amino acid and is responsible for a fair number of interactions, it is not as prevelant as His13. This could be due to better positioning of the ligand toward His13Lys16 instead of His13His14 and His14Lys16. For Lys16, most interactions were found to be hydrogen donation (to catechin) through the side chain as well as through the backbone. This is reasonable because at physiological pH lysine has a positively charged side chain. In general, multiple interactions were found within the HHQK LVFF region. Although this was the target region for the docking, some of the neighboring amino acids were involved in interactions with catechin as well. Glu22 has a high number of interactions, solely through side chain hydrogen acceptor. Glutamic acid bears a negative charge at physiological pH and it is positioned fairly close to the amino acids in the LVFF regions. Although it is not within the HHQK LVFF regions, this binding should not be ignored.

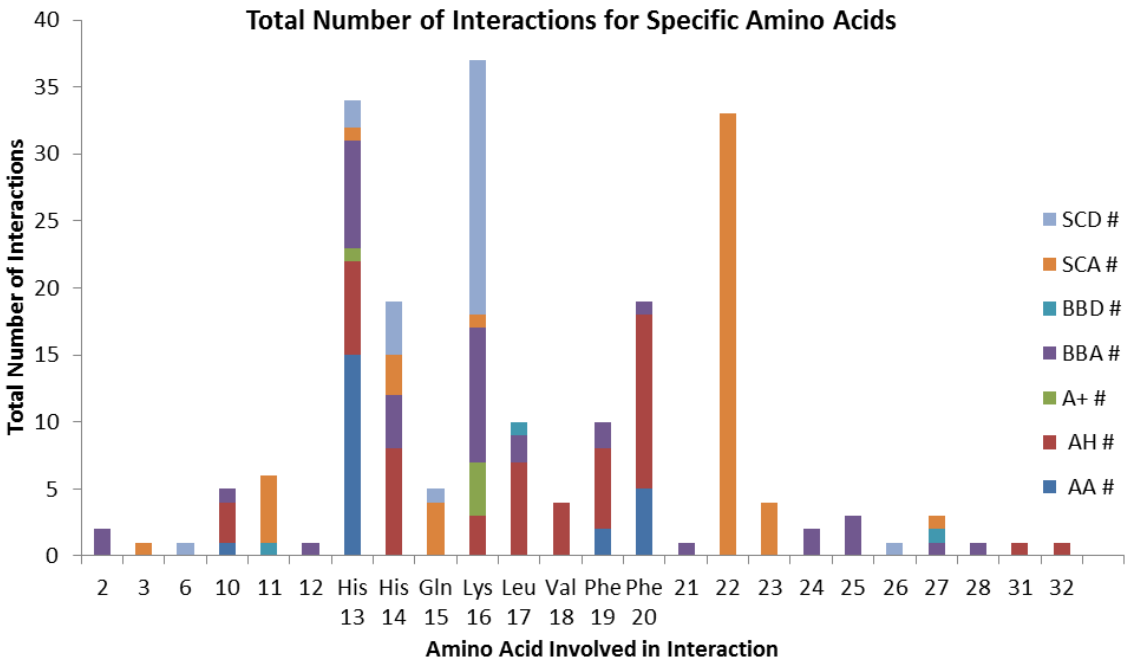


Figure 3.4 Total number of interactions that occur when a particular amino acid is involved in the docking of (+)-catechin to HHQK LVFF across the six Aβ conformers in gas phase calculations.

The total number of interactions occurring with particular atoms or rings on catechin were also investigated and summarized in Figure 3.5. There were many regions of the catechin molecule that were involved in the interactions. Oxygens 2, 4, 5, and the A and B-rings all produced 20 or more interactions. However, oxygen 6 provided the most interactions, almost doubling any other atom. It was involved in mainly all hydrogen donation/acceptance interactions. The A and B-rings participated in the pi type of interactions with the A-ring dominating in pi-hydrogen and the B-ring dominating with pi-pi. The C-ring was not involved in any interactions at all.

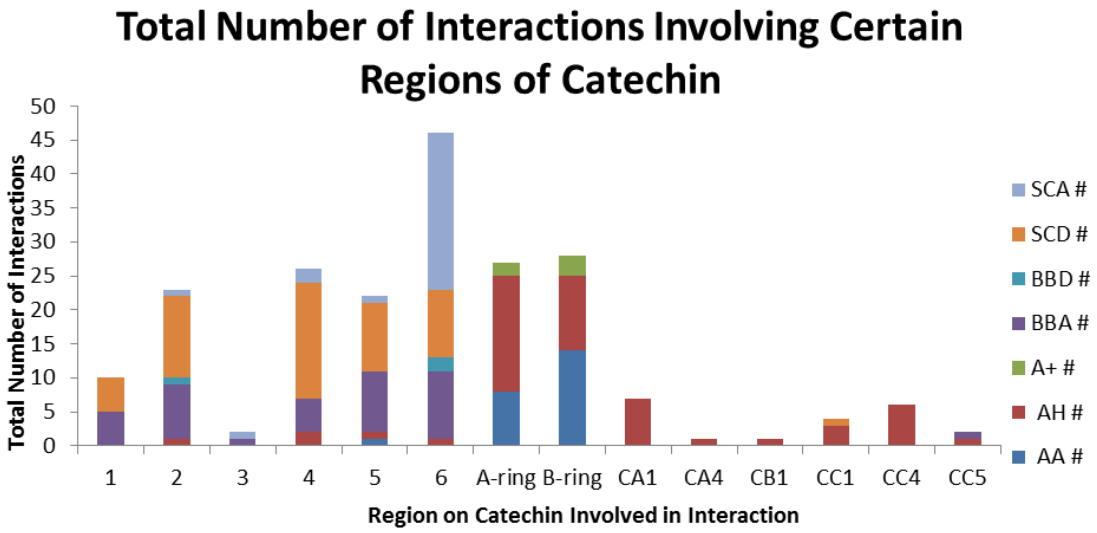


Figure 3.5 Total number of interactions that involve particular atoms or rings on the (+)-catechin molecule in gas phase calculations.

Finally, in addition to the analysis of the atoms and rings on the (+)-catechin molecule, different initial orientations of (+)-catechin gave different numbers of interactions. This is shown in Figure 3.6.

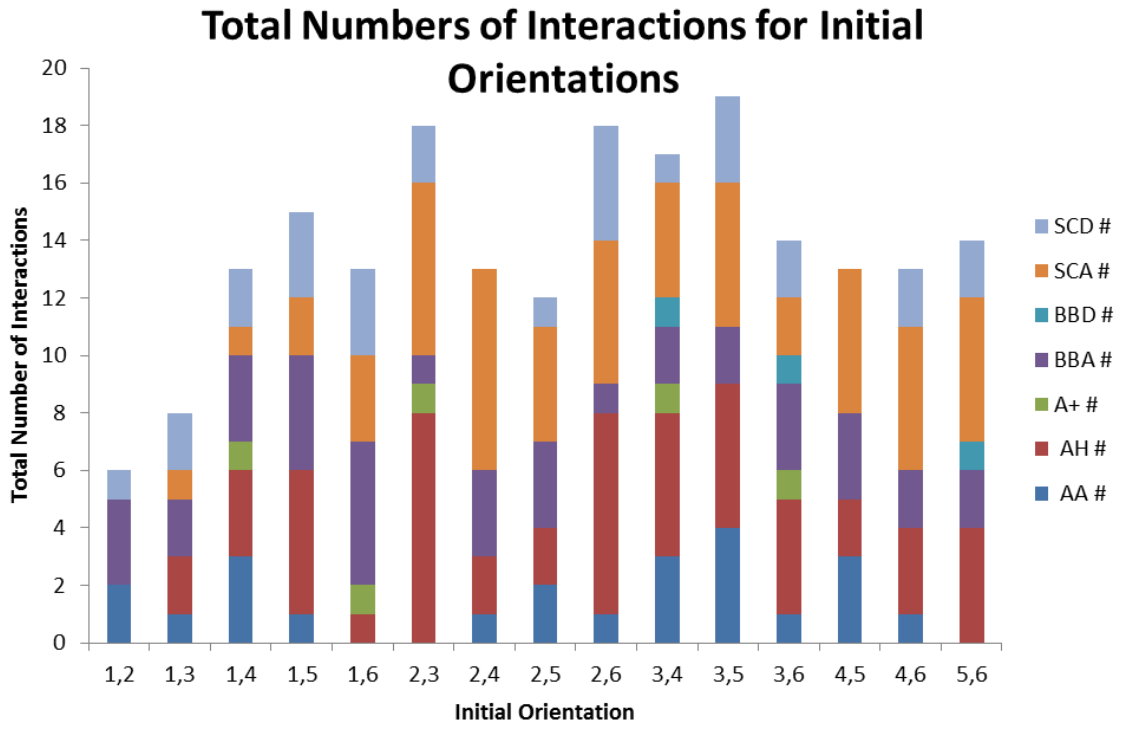


Figure 3.6 Total number of interactions that occur when a particular initial orientation of (+)-catechin is docked toward HHQK LVFF in gas phase.

Many of the orientations provided similar numbers of interactions to occur. From here, it can be seen that orienations 1,2 and 1,3 provide the smallest number of interactions. Orientations 2/3, 2/6, and 3,5 provide the highest number of interactions. The orientations that provide the most pi-pi interactions are 1/4, 3/4, 3/5, and 4/5.

3.1.2 Solvent Phase Results

The systems that were chosen for solvent calculations were based on the ability to produce an interaction and on the relative binding energies. First, they were selected based on whether or not they had an interaction in the gas phase calculation. Then, if there were many interactions, the systems that had the lowest binding energies were selected because solvent calculations take a lot of time. For example, from the

1AMB/His13His14 system with catechin, the following orientations were selected for solvent calculations as described in Table 3.5. They are ordered from lowest to highest binding energy.

Table 3.5 Orientations of the systems chosen from gas phase docking of (+)-catechin to Aβ to continue on with solution phase calculations.

1AMB	1AMC	1AML	1BA4	1IYT	1Z0Q
2,6	2,3	4,6	3,4	3,4	1,4
2,3		5,6	1,6	1,4	
3,4			2,3	4,6	
1,5					

The rest of the solvent calculations chosen across the HHQK LVFF regions for the six conformers are summarized individually within Appendix A. For all of these individual solvent calculations, the binding energies are also summarized in Appendix A.

3.1.2.1 Overall Energies and Interactions

In a similar fashion to the gas phase results, the average binding energies and the total number of interactions were calculated across all of the solvent calculations. The average binding energies are summed in Table 3.6 and Figure 3.7.

Table 3.6 Average binding energies in kcal/mol for docking to a specific amino acid pair for (+)-catechin in water.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-25.78	-15.28	-30.33	-12.24	-31.89	-17.72	-19.99	-27.57	-23.62
1AMC	-24.43	-33.24	-33.33	-35.79	-34.03	-40.44	-33.22	-50.79	-24.85
1AML	-23.43	-41.23	-59.87	-78.01	-66.01	-63.53	-47.94	-79.76	-38.99
1BA4	-26.73	-13.41	-30.01	-31.61	-21.27	-27.25	-17.56	-28.52	-43.36
1IYT	-19.24	-31.38	-10.46	-23.17	-53.87	-66.97	-73.13	-73.93	-55.8
1Z0Q	-37.92	-27.02	-31.35	-17.02	-15.55	-17.39	-20.72	-13.8	-12.9
Overall Average	-26.26	-26.93	-32.56	-32.97	-37.10	-38.88	-28.52	-45.73	-33.25

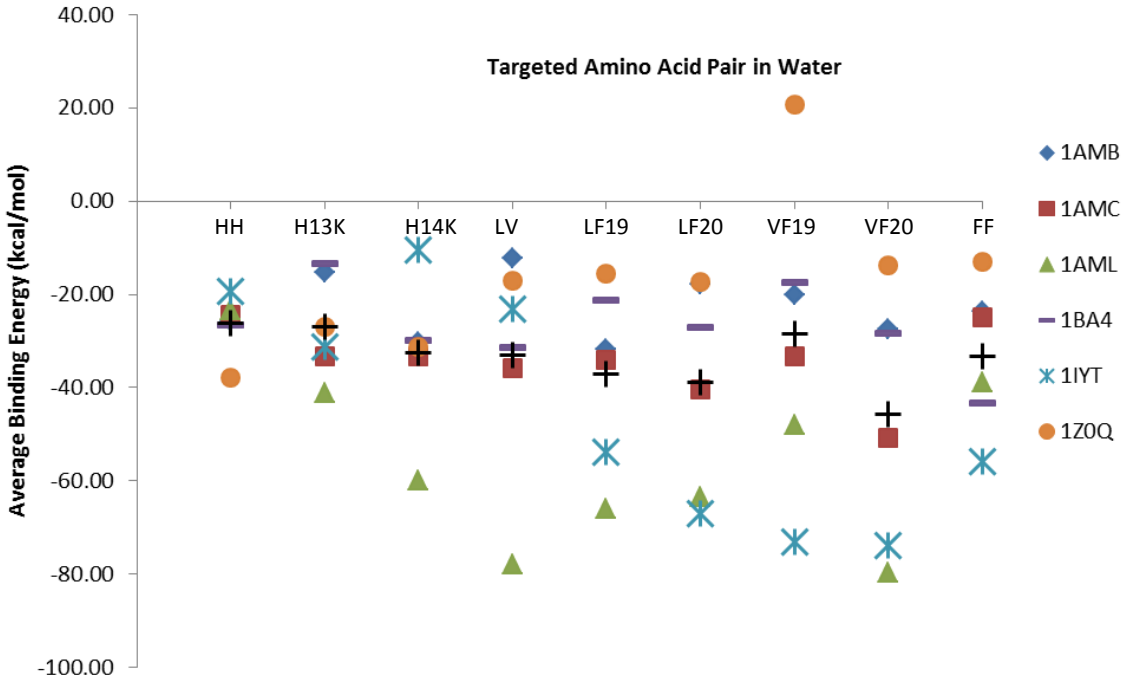


Figure 3.7 Average binding energies in kcal/mol for docking to a specific amino acid pair for (+)-catechin in water.

The amino acid pair that provided the most stable binding energy overall was VF20, similar to the gas phase results. In addition, LF19 and LF20 were both close to

having the lowest energies as well. The highest energies come from HH, H13K and VF19. This was also similar to the gas phase with the exception of the H13K. Conformer 1AML had the lowest binding energies overall. Conformer 1IYT showed higher binding energies toward HHQK but lower binding energies toward LVFF.

After the solvent calculations were finished, the water molecules were deleted to see if the binding interactions had changed or not. The end result was 119 interactions in total that occurred. The total numbers of interactions involving certain amino acids are summarized in Figure 3.8.

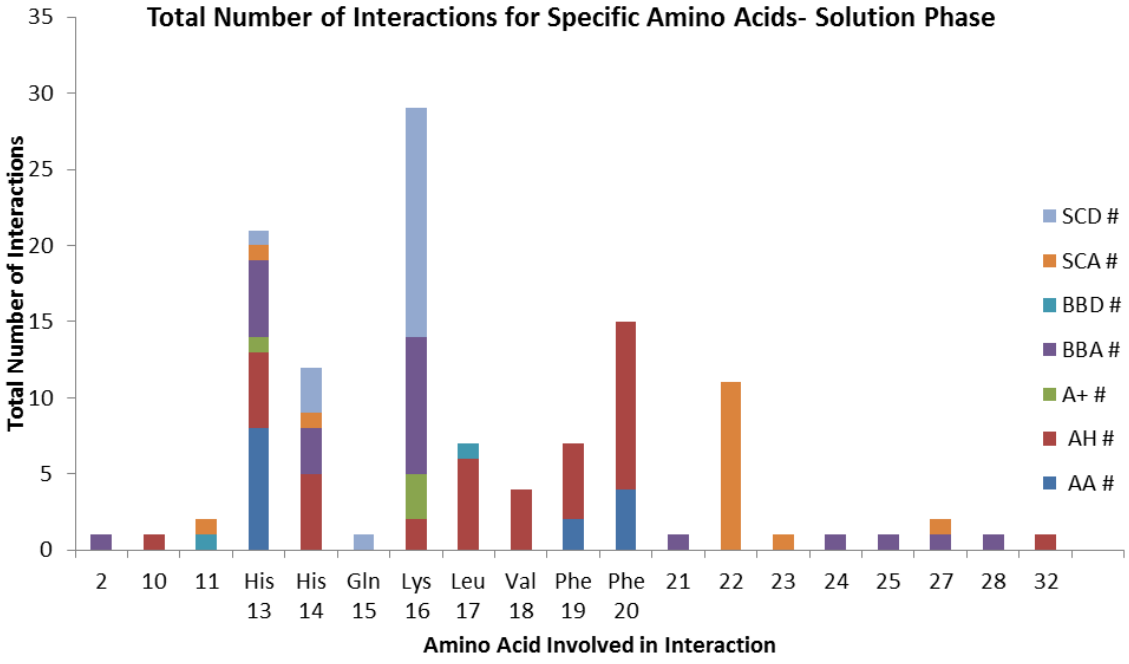


Figure 3.8 Total number of interactions that involve particular amino acids for solution phase of (+)-catechin docking to Aβ.

Similar to the gas phase results, His13 and Lys16 are the predominant amino acids involved in interactions. Again, the His13 is involved in many pi-interactions and Lys16 is involved with side chain hydrogen donation for half of its interactions. In terms

of the catechin molecule itself, oxygen 6 is still involved in a high number of the interactions. However, the relative number of interactions with which the A-ring and the B-ring are involved has increased. These data can be found in Figure 3.9.

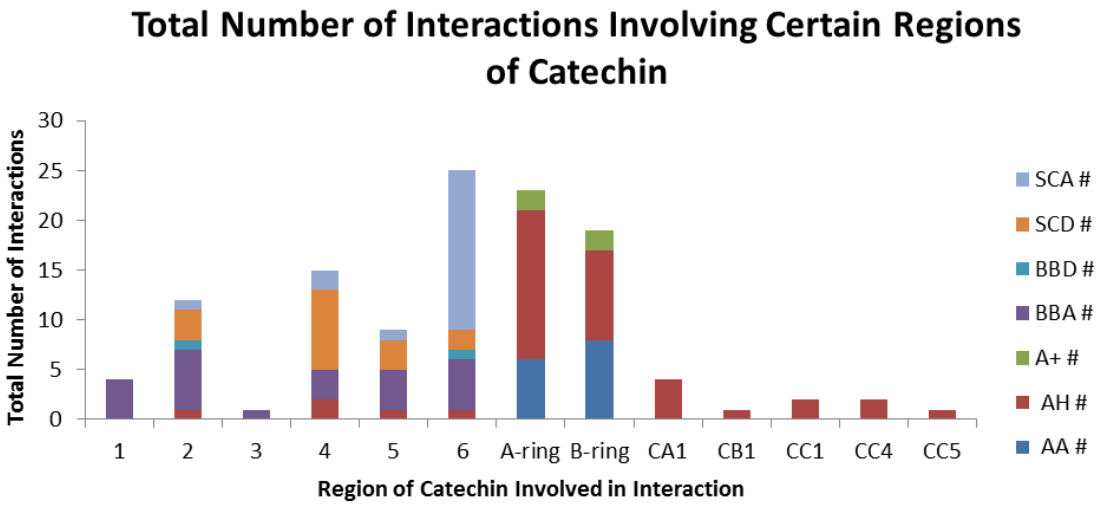


Figure 3.9 Total number of interactions that occur that involved particular atoms or rings on (+)-catechin when it is docked toward HHQK LVFF in water.

3.1.3 Summary

Overall, there were certain trends in the energies and interactions that were shown when (+)-catechin was docked to the HHQK LVFF region of the six Aβ conformers. When catechin was oriented toward amino acids LF19 and VF20, it produced the lowest average binding energies. When the calculations were performed in water, a similar result was shown where targeting VF20 had the lowest average binding energy. However, when catechin was docked toward HH and VF19 in the gas phase, the highest average binding energies were produced. Similarly in water, it was HH and H13K. These observations suggest that (+)-catechin is more prone to bind toward the LVFF region rather than the

HHQK region. Further analysis of the interactions that occurred allowed for more insight into the binding modes.

There were a total of 206 interactions to consider from all of the gas phase calculations. First, the amino acids that were involved in the interactions were analyzed by how often they had an interaction and which type it was. In the gas phase, His13, Lys16, and Glu22 had the highest number of interactions occurring, where His13 consisted of pi-pi interactions, Lys16 in hydrogen donation from the side chain (SCD), and Glu22 in hydrogen acceptance from the side chain (SCA). The same trend was observed in water with the addition of Phe20 producing more interactions. Although the highest binding energies were observed from His13His14 and His13Lys16, it should be noted that they are only relative. The lowest energies were observed for catechin docking to LF19 and VF20, both of which are very close to Glu22. Most of the Glu22 interactions came from these systems. The interaction between (+)-catechin and Glu22 is more stabilizing than the interactions between His13, Lys16, and catechin.

Secondly, the regions on the catechin molecule that were involved in the interactions were analyzed. The C-ring did not produce any binding interactions at all. The A and B-rings played an important role in producing pi-pi and pi-hydrogen interactions. Oxygen 6 also produced many hydrogen interactions. The same result was shown in water.

Lastly, the number of interactions was correlated with the initial orientation of catechin toward Aβ. The best initial orientations were 3/5 and 2/5, where they produced

many pi-type interactions, as well as 2/6 and 3/4. The initial orientations that did not seem to produce many interactions were 1/2 and 1/3.

3.2 Epicatechin

(-)-Epicatechin is another important molecule found within apple peels. Similarly to (+)-catechin, (-)-epicatechin had 15 possible initial orientations. Since (-)-epicatechin has a very similar structure to (+)-catechin, the numbering of the oxygens and atoms were the same and are shown in Figure 3.10. The binding energies and the interactions found for all calculations are found within Appendix B. This subchapter will focus solely on the averages and sums of the interactions found for all.

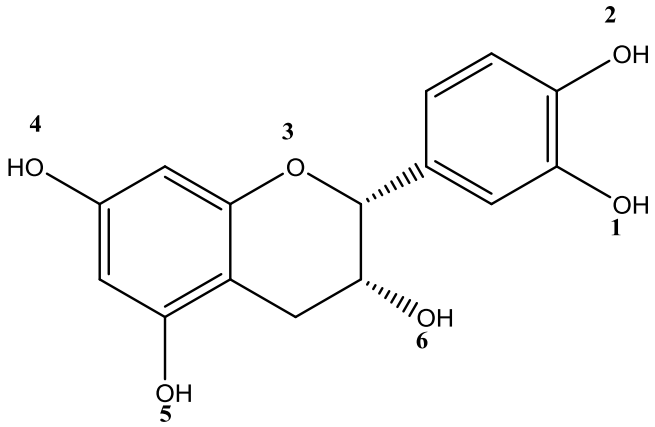


Figure 3.10 The (-)-epicatechin molecule found within apple peel with the numbered oxygens.

3.2.1 Gas Phase Results

3.2.1.1 Overall Energies and Interactions

The average binding energies for (-)-epicatechin docking to HHQK LVFF are found within Table 3.7 and Figure 3.11.

Table 3.7 Average binding energies (kcal/mol) for docking to a specific amino acid pair for (-)-epicatechin in gas phase.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-30.87	-18.38	-6.89	-27.97	-33.79	-18.54	-24.71	-29.90	-27.49
1AMC	-34.80	-24.12	-38.37	-35.45	-42.89	-33.43	-26.02	-40.56	-33.45
1AML	-56.02	-49.58	-66.17	-56.98	-72.69	-62.50	-56.15	N/A	-62.61
1BA4	-15.57	-28.32	-25.01	-16.40	-11.64	-14.32	-2.61	-14.19	-37.20
1IYT	-26.49	-29.40	-29.88	-35.32	-36.57	-24.45	-29.42	-38.87	-26.19
1Z0Q	-24.21	-16.98	-14.15	-14.70	-19.04	-13.29	-18.23	-20.27	-15.36
Average	-31.33	-27.80	-30.08	-31.14	-36.10	-27.75	-26.19	-28.76	-33.72

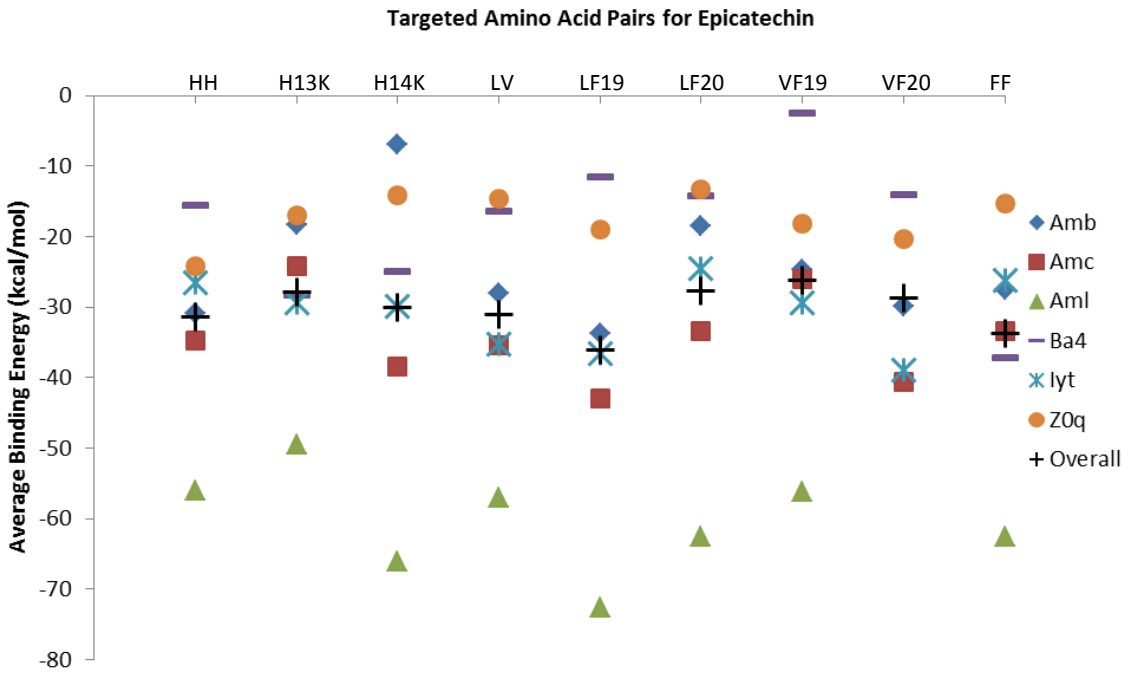


Figure 3.11 Average binding energies (kcal/mol) for docking to a specific amino acid pair for (-)-epicatechin in gas phase.

From these data, the lowest average binding energies are found when amino acid pairs HH, LV, LF19 and FF are targeted; however, LF19 is the lowest out of the four. The highest average binding energies occur for amino acids VF19. Similar to (+)-catechin, conformer 1AML has a much lower average binding energy than the others, with amino acid target LF19 displaying the minimum amongst the points.

All of the interactions that occurred after the energy minimizations were complete were recorded. In this case, there were a total of 208. First, they were summed to see which conformer produced the most interactions as seen in Figure 3.12. It is shown here that they are all fairly similar with the exception of 1AMC having a slightly higher percentage and 1BA4 being responsible for 7-10% more of the interactions.

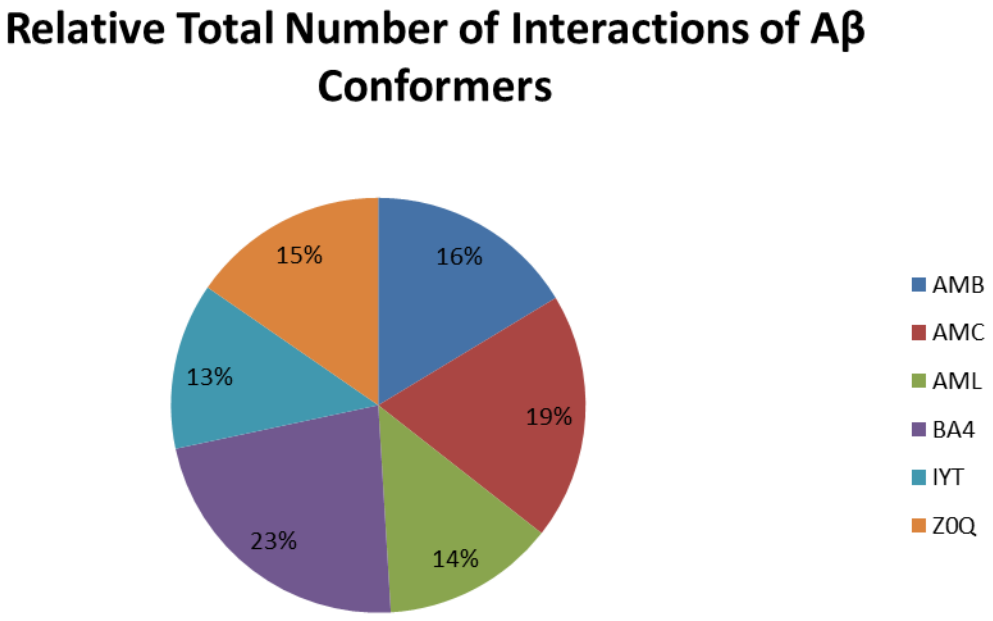


Figure 3.12 The percentages of interactions that occur when a particular conformer of Aβ is used for (-)-epicatechin.

Further analysis of the interactions determined which amino acids were involved in the most interactions. These are summarized in Figure 3.13 along with what types of interactions they were.

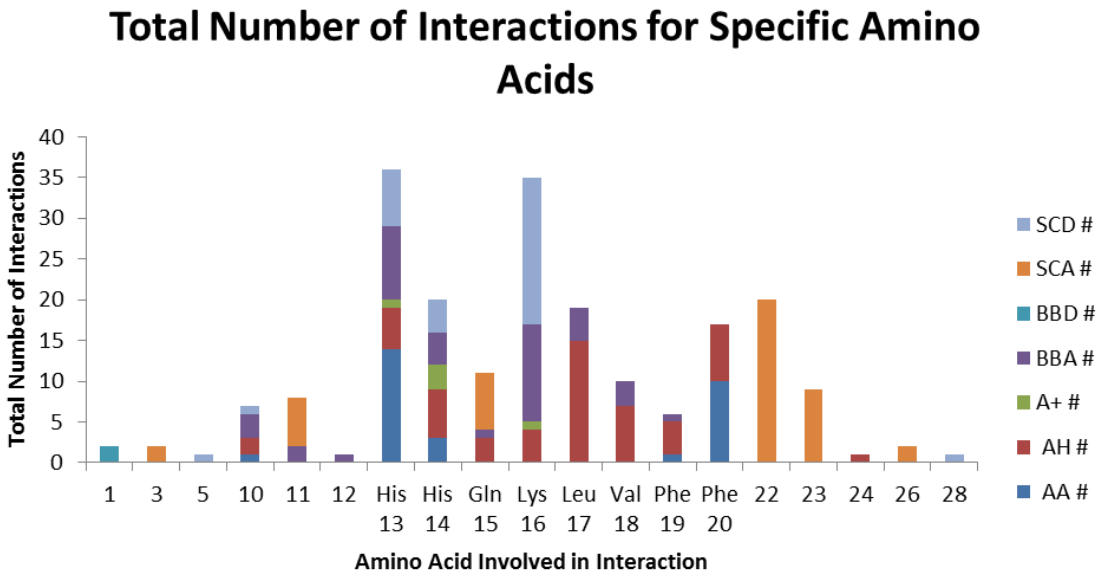


Figure 3.13 Total number of interactions that occur when a particular amino acid is involved in the docking of (-)-epicatechin to HHQK LVFF across the six Aβ conformers in gas phase calculations.

Most of the interactions occurred within the HHQK LVFF regions, with some interactions occurring between neighboring amino acids. Within the HHQK LVFF regions, the amino acids that were involved in the most interactions were His13, His14 and Lys16. For His13, the interactions were primarily pi-pi interactions whereas for Lys16, the interactions were primarily hydrogen donation (from the amino acid to epicatechin) through the side chain. Other amino acids that were involved in many interactions were Leu17, Phe20, and Glu22. Leu17 provided many AH type interactions

and Phe20 provided mainly pi-pi with some AH. As was seen with (+)-catechin, Glu22 participated in all SCA type interactions.

The total number of interactions occurring with particular atoms or rings on (-)-epicatechin were also investigated and summarized in Figure 3.14.

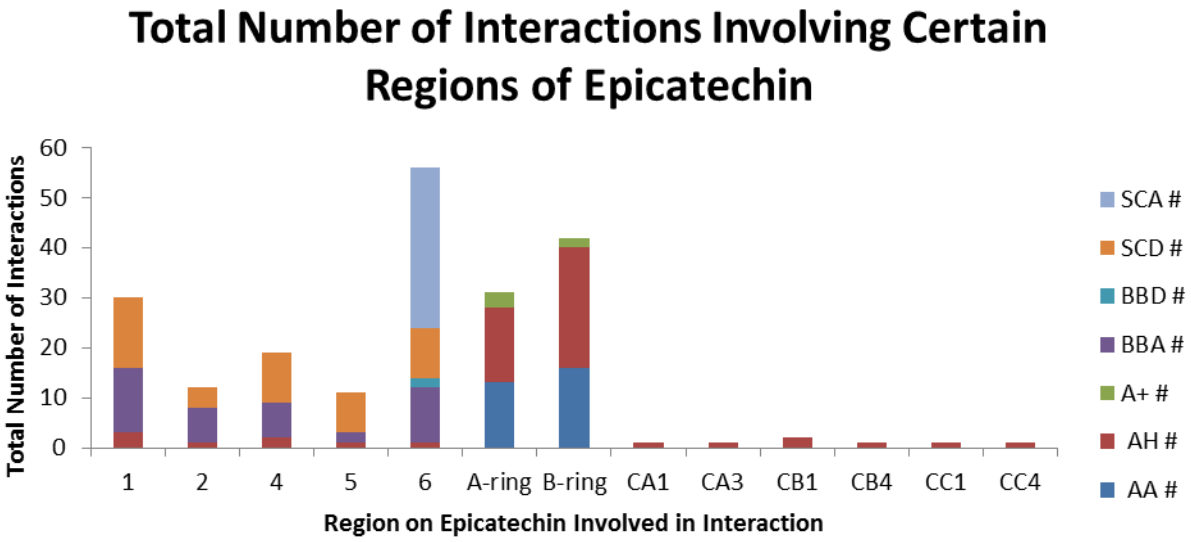


Figure 3.14 Total number of interactions that involve particular atoms or rings on the (-)-epicatechin molecule in gas phase calculations.

The two main aspects of (-)-epicatechin that contributed to interactions were oxygen 6, the B-ring, and the A-ring. The C-ring was not involved in any interactions at all. The sixth oxygen mainly contributed through side chain hydrogen donation while the B and A-rings contributed mainly through AH and pi-pi.

Different initial orientations also gave different total numbers of interactions. As shown in Figure 3.15, orientations 1/3, 2/5, 3/6, and 5/6 provided the most interactions. They all contributed different numbers of the different types of interactions. Orientations

1,3 and 2,5 provided many AA and AH interactions. Orientations 3,6 and 5,6 provided mainly hydrogen donation/acceptance types of interactions. The orientations that provided the least number of interactions were 1/4, 2/3, and 4/6.

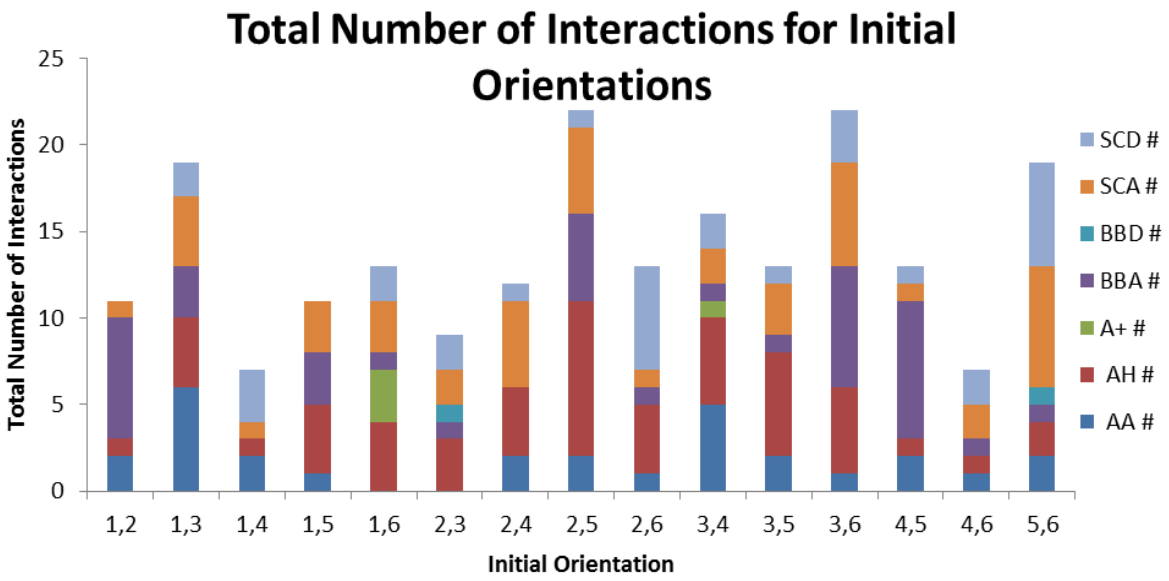


Figure 3.15 Total number of interactions that occur when a particular initial orientation of (-)-epicatechin is docked toward HHQK LVFF in gas phase.

3.2.2 Solvent Phase Results

After the gas phase results were complete, the systems that were chosen to proceed with solution calculations were based on their ability to produce an interaction with HHQK LVFF and lower binding energies. The systems that were chosen along with their individual binding energies in water are found within the Appendix B. The analysis of the average binding energies and total number of interactions will be found within this subchapter. The average binding energies for all of the solvent calculations are found within Table 3.8 and Figure 3.16

Table 3.8 Average binding energies in kcal/mol for docking to a specific amino acid pair for (-)-epicatechin in water.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-21.53	-9.04	-13.78	-30.31	-31.45	-12.86	-17.82	-24.22	-36.13
1AMC	-41.69	-27.68	-29.73	-28.56	-34.54	-42.07	-30.59	-55.23	-26.56
1AML	-47.67	-50.23	-68.51	-50.09	-81.04	-55.61	-46.81	N/A	-63.26
1BA4	-17.91	-24.76	-21.45	-25.74	-16.21	-17.88	0.95	-4.85	-40.76
1IYT	-18.14	-37.75	-38.23	-26.97	-51.24	-26.79	-31.76	-45.76	-25.54
1Z0Q	-29.89	-11.30	-19.83	-17.04	-16.70	-6.40	-14.67	-23.83	-23.71
Overall	-29.47	-26.79	-31.92	-29.79	-38.53	-26.94	-23.45	-30.78	-35.99

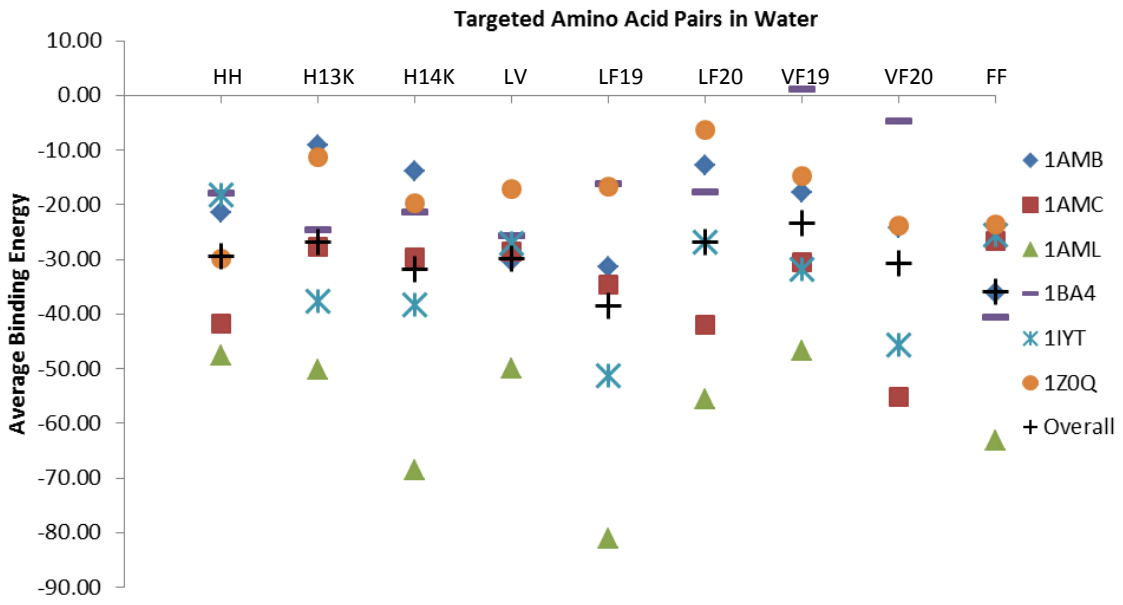


Figure 3.16 Average binding energies in kcal/mol for docking to a specific amino acid pair for (-)-epicatechin in water.

From the overall average binding energies, the amino acid pairs that have the lowest values are LF19 and FF. This was also the case within the gas phase calculations. A difference here between the solution and gas phase is that HH and LV also had low

binding energies. Although they still do here, they are not as low as LF19 and FF. The amino acid pair that has the highest average binding energy is VF19.

After the solvent calculations were complete, there were a total of 130 interactions that occurred. The contribution to these interactions by particular amino acids and the atoms/rings on epicatechin are summarized in Figures 3.17 and 3.18, respectively.

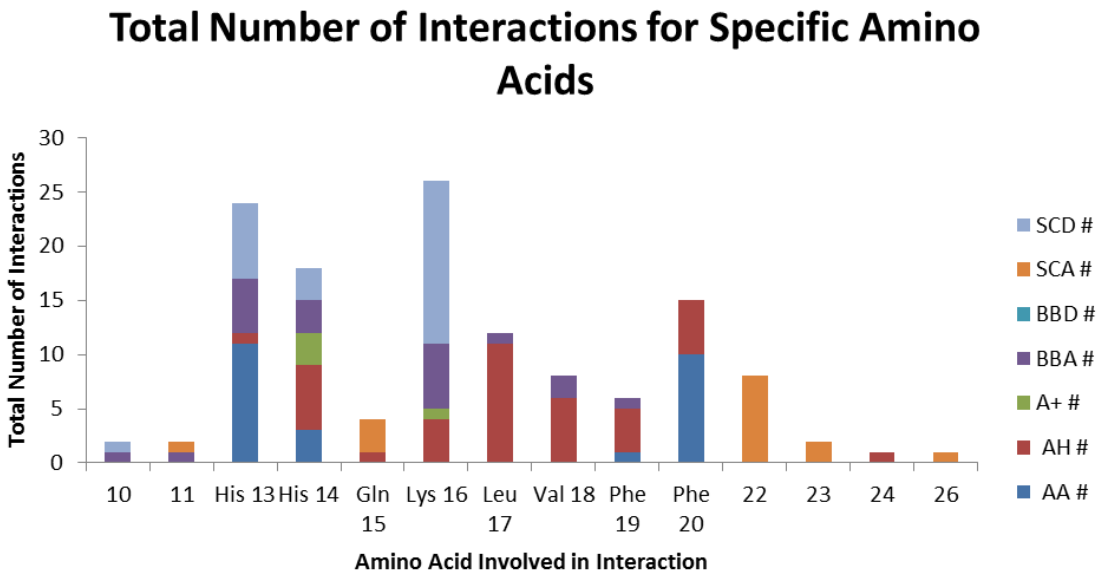


Figure 3.17 Total number of interactions that occur when a particular amino acid is involved in the docking of (-)-epicatechin to HHQK LVFF across the six Aβ conformers in water.

The amino acids that contribute the most to the interactions are His13, His14, Lys16, and Leu17. The same trends follow where His13 participates in mainly pi-pi, Lys16 with SCD, and Phe20 with pi-pi and pi-H. His14 is participating in a variety of interactions, from pi-pi to pi-cation to SCD. Amino acids Val18 and Phe19 are participating the least out of the LVFF region. For the actual (-)-epicatechin molecule, the same trend is shown where oxygen 6, the A-ring, and the B-ring are involved in most of the interactions.

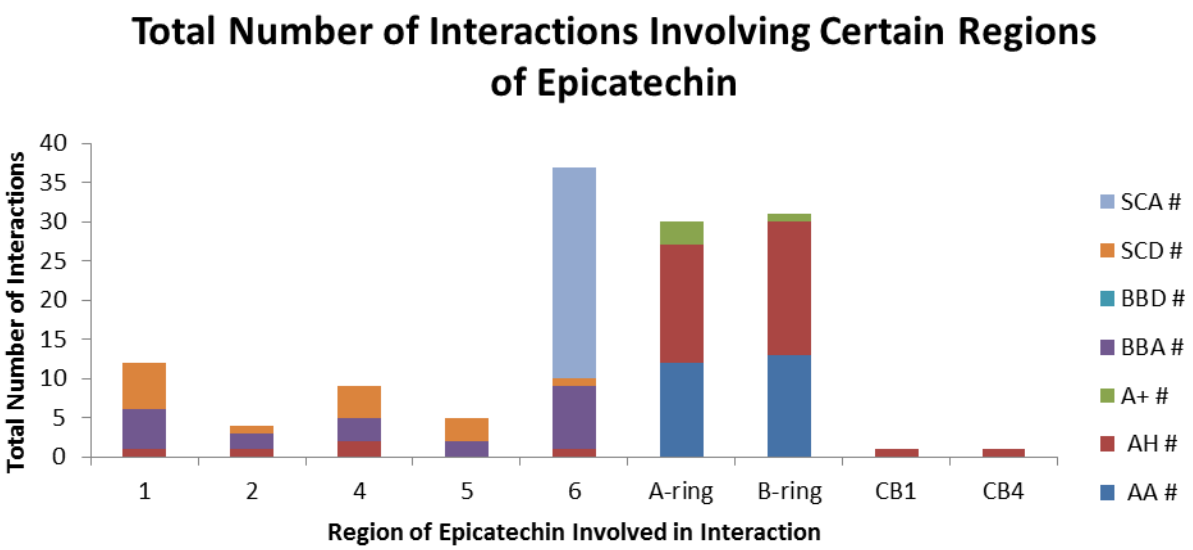


Figure 3.18 Total number of interactions that involve particular atoms or rings on the (-)-epicatechin molecule in water.

3.2.3 Summary

Overall, there were certain trends in the energies and interactions that were shown when (-)-epicatechin was docked to the HHQK LVFF regions of the six Aβ conformers. When epicatechin was oriented toward amino acids LF19, HH, LV, and FF in the gas phase the lowest average binding energies were produced. LF19 had the lowest of the four. When the calculations were performed in water, similar results were shown where targeting LF19 and FF produced the lowest average binding energy. However, when epicatechin was docked toward VF19 in gas phase, the highest average binding energies were produced. This did not change when the solvent calculations were performed. These observations suggest that suggest that (-)-epicatechin is prone to bind toward the LVFF region rather than the HHQK region, however, the HH region is not out of the question.

Further analysis of the interactions that occurred allowed for more insight into the binding modes.

There were a total of 208 interactions to consider from all of the gas phase calculations. First, the amino acids that were involved in the interactions were analyzed by how often they had an interaction and which type it was. In the gas phase, His13, Lys16, Leu17, Phe20 and Glu22 had the highest number of interactions occurring, where His13 and Phe20 consisted of pi-type interactions, Lys16 in hydrogen donation from the side chain (SCD), and Glu22 in hydrogen acceptance from the side chain (SCA). The same trend was observed in water with the addition of His14 producing more interactions. The lowest energies were observed for epicatechin docking to LF19 and FF both of which are very close to Glu22. Most of the Glu22 interactions came from these systems. Similar to (+)-catechin, the interactions with Glu22 is slightly more stabilizing than the interactions with His13 and Lys 16. However, there is still binding occurring in the HHQK region.

Secondly, the regions on the epicatechin molecule that were involved in the interactions were analyzed. The C-ring did not produce any binding interactions at all again, as was found with catechin. The A and B-rings played an important role in producing pi-pi and pi-hydrogen interactions. Oxygen 6 also produced many hydrogen interactions. The same result was shown in water.

Thirdly, the number of interactions was correlated with the initial orientation of epicatechin toward Aβ. The best initial orientations were 1/3 and 2/5, where they produced many pi-type interactions, as well as 3/6 and 5,6. Oxygen 6 was involved in

many interactions so this makes sense that these orientations produced many interactions. The initial orientations that did not seem to produce many interactions were 1/4, 2/3 and 4/6. Although 4/6 contains oxygen 6, the way it has to be oriented toward Aβ could have a role in its inability to produce interactions because the rest of the ring could be interfering with neighbouring atoms.

3.3 Cyanidin

Cyanidin is another molecule found within apple peel. Cyanidin's structure is quite similar to both (+)-catechin and (-)-epicatechin with the exception of the presence of a charged oxygen on the C-ring and the aromaticity of the C-ring (Figure 3.19). The increased aromaticity of the C-ring could provide additional potential for interacting with Aβ. Again, there were 15 different possible initial orientations.

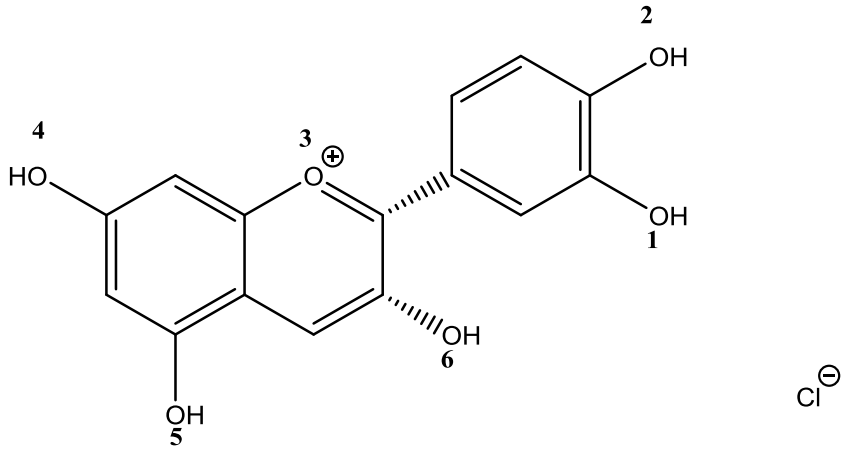


Figure 3.19 Structure of cyanidin (chloride) as found within apple peel.

3.3.1 Gas Phase Results

3.3.1.1 Overall Energies and Interactions

The individual binding energies were calculated for docking cyanidin to the HHQK LVFF regions across the six conformers of Aβ. They are summarized in Appendix C. The average binding energies, however, are shown in Table 3.9 and Figure 3.20

Table 3.9 Average binding energies in kcal/mol for cyanidin docking to HHQK LVFF in gas phase calculations.

	HH	**H13K**	**H14K**	**LV**	**LF19**	**LF20**	**VF19**	**VF20**	**FF**
1AMB	-17.86	-12.06	-9.32	-30.41	-2.87	-12.23	-22.39	-27.66	-21.49
1AMC	-24.47	-26.05	N/A	-44.84	-32.41	-25.95	-37.52	-52.97	-42.68
1AML	-28.01	-55.72	-49.48	-53.76	-65.19	-70.31	-79.71	N/A	-67.45
1BA4	1.51	-17.31	-27.31	-19.34	-16.06	-20.74	-29.37	-23.27	N/A
1IYT	N/A	-26.87	-12.00	-26.99	-30.22	-25.91	-46.82	-27.07	-17.13
1Z0Q	-5.79	-2.96	-12.79	-23.89	-15.73	-14.45	-36.22	-23.15	-12.47

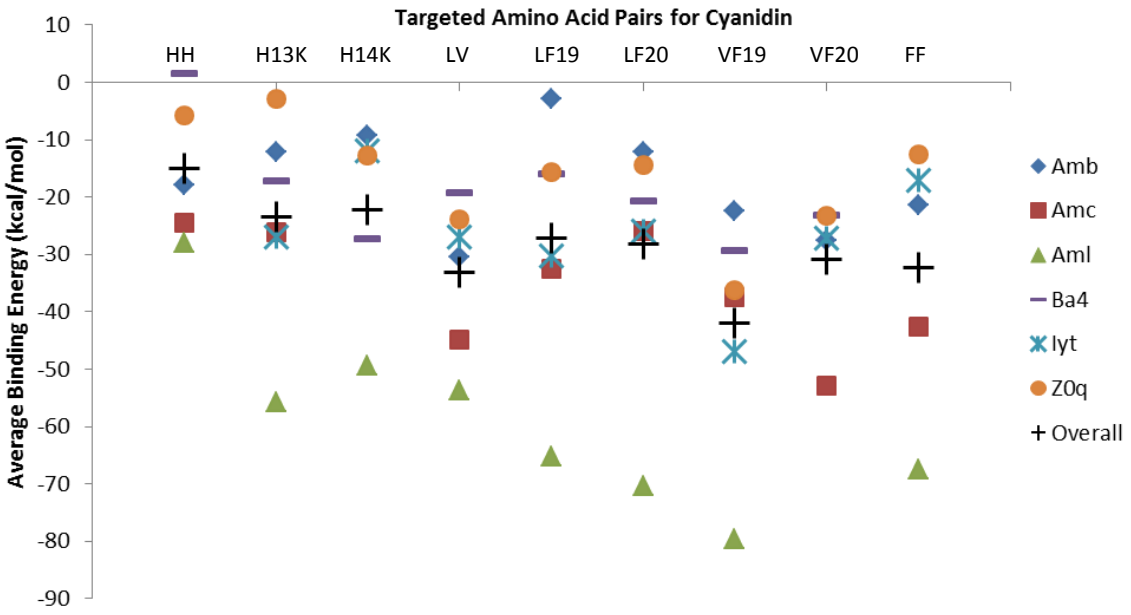


Figure 3.20 Average binding energies in kcal/mol for cyanidin docking to HHQK LVFF in gas phase calculations.

From the overall average of the binding energies, the lowest values are when cyanidin is being docked toward amino acids VF19. It also produces low binding energies when it is docked toward LV and VF20. The amino acids within the HHQK region show the highest average binding energies.

Along with the energies, each calculation provided information about whether or not an interaction was produced. For cyanidin there were a total of 188 interactions. First, the interactions correlated to certain conformers were summed (Figure 3.21). Conformer 1AML has the highest number of interactions with 23%, that is 5% higher than the two with the second most number of interactions, 1BA4 and 1AMC. The number of interactions that occur that involve particular amino acids are summarized in Figure 3.22.

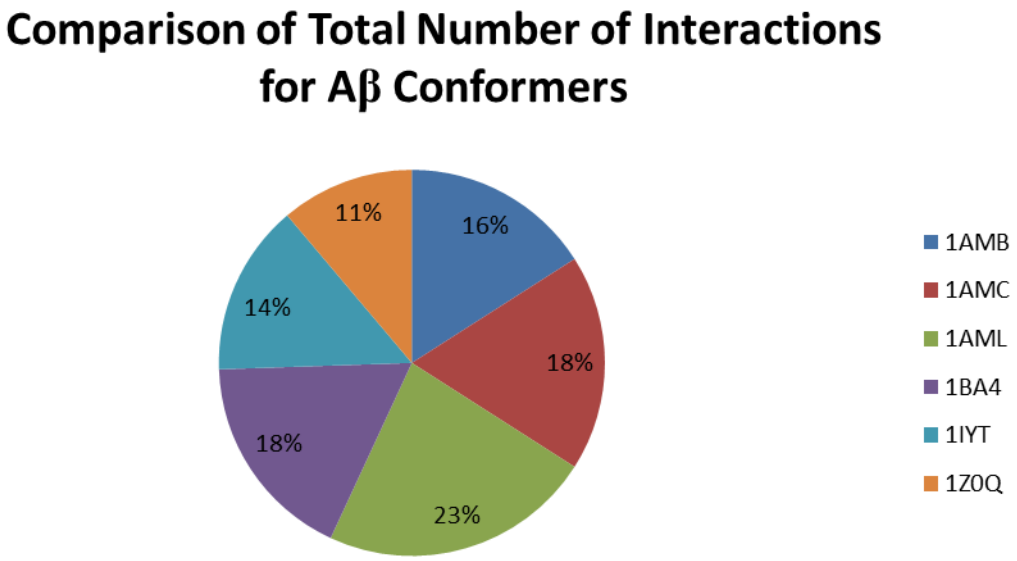


Figure 3.21 Percentages of the total interactions that occur when a particular conformer is used for docking cyanidin to Aβ.

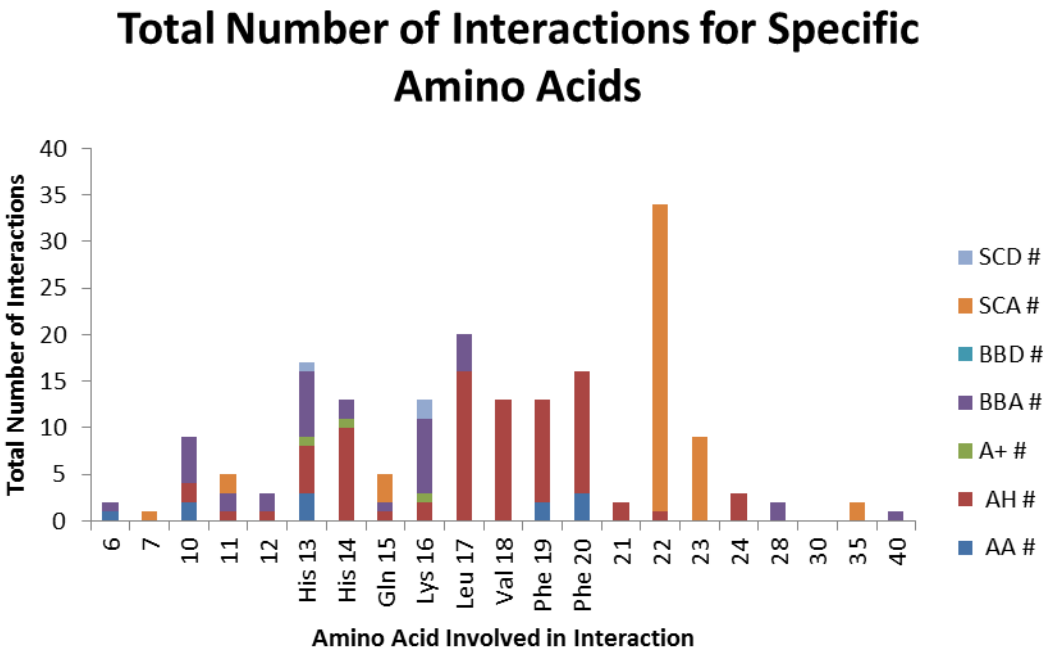


Figure 3.22 Total number of interactions that occur when a particular amino acid is involved in the docking of cyanidin to HHQK LVFF across the six Aβ conformers in gas phase calculations.

Across the HHQK LVFF region, the interactions are occurring fairly evenly with His13, Leu17, and Phe20 being involved in slightly higher numbers of interactions. His13 is involved in a variety of different types of interactions, including pi-pi and BBA. Leu17 is predominately pi-H interactions. A very large portion of these interactions are from Glu22 where they are almost all side chain H-acceptor (where Glu22 is the acceptor). The interaction between Glu22 and cyanidin is sensible because Glu22 bears a negative charge and cyanidin bears a positive charge. The regions on cyanidin that are involved in interactions are summarized in Figure 3.23.

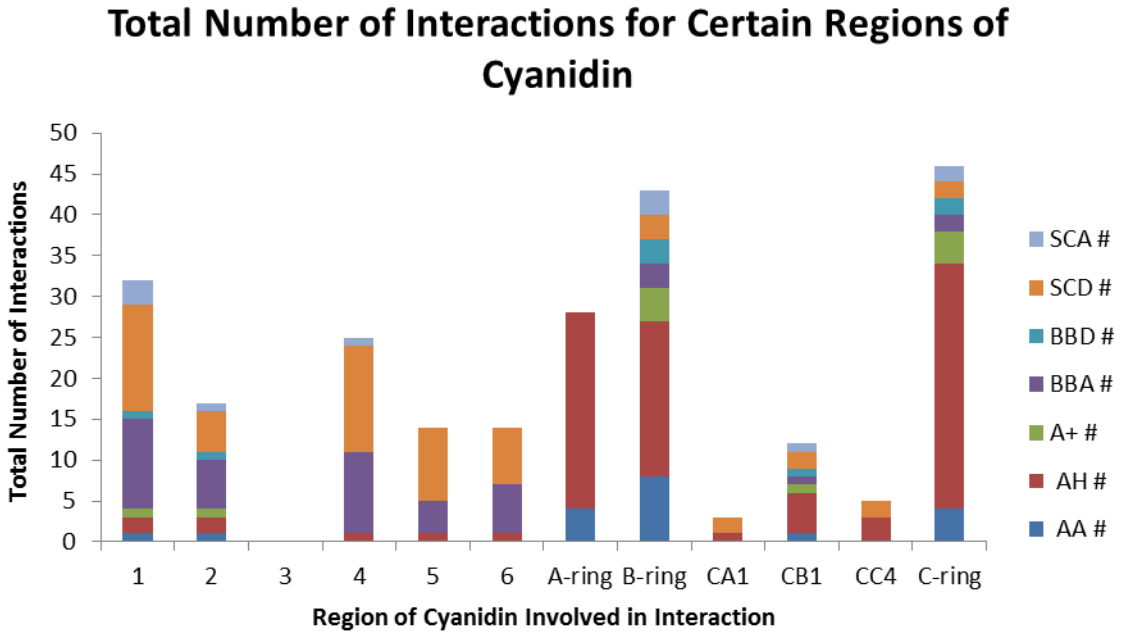


Figure 3.23 Total number of interactions that involve particular atoms or rings on the cyanidin molecule in gas phase calculations.

Most of the interactions involved the C and the B-rings. The cyanidin molecule was involved in a lot of pi type interactions mainly from the C-ring first, then the B-ring,

then the A-ring. These interactions were mainly all pi-H interactions. The hydroxyl groups that were mainly involved were 1 and 4.

The relationship between number of interactions and the initial orientation of cyanidin is displayed in Figure 3.24. The initial orientation that incurred the most interactions was 2,5 by far. It consisted of mainly pi interactions with some pi-pi but mainly pi-H. There were some other orientations that provided many interactions as well, such as 3/6 and 4/6. However, there were many that provided very few interactions.

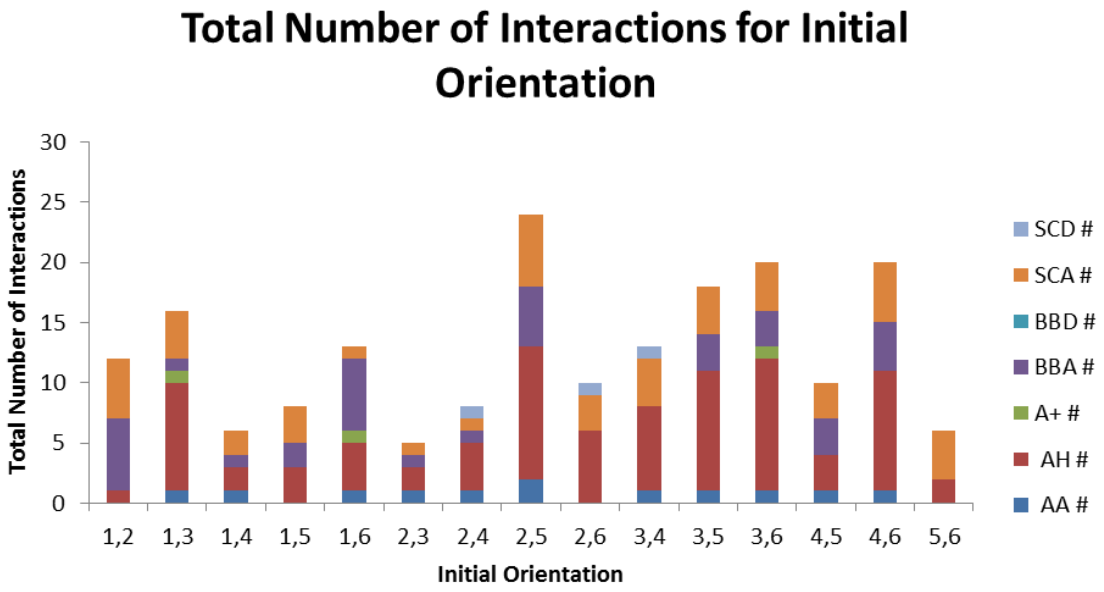


Figure 3.24 Total number of interactions that occur when a particular initial orientation of cyanidin is docked toward HHQK LVFF in gas phase.

3.3.2 Solvent Phase Results

The systems that were chosen along with their individual binding energies and interactions in water are found within Appendix C. The analysis of the average binding energies and total number of interactions will be found within this subchapter. The

average binding energies for all of the solvent calculations of cyanidin docked to Aβ are found within Table 3.10 and Figure 3.25

Table 3.10 Average binding energies in kcal/mol when cyanidin is docked to HHQK LVFF across the six conformers in water.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-15.52	-15.62	-12.88	-21.77	-9.76	-12.88	-25.95	-23.09	-14.60
1AMC	-31.36	-19.16	N/A	-45.49	-40.76	-21.38	-32.95	-46.08	-34.33
1AML	-24.45	-42.14	-51.82	-46.87	-60.62	-55.64	-71.36	N/A	-53.87
1BA4	-13.16	-26.65	-18.96	-15.78	-30.73	-24.30	-38.01	-26.83	N/A
1IYT	N/A	-30.43	-6.32	-31.56	-26.66	-20.23	-38.47	-24.73	-26.47
1Z0Q	-14.14	-8.64	-15.13	-24.54	-29.31	-18.01	-36.87	-26.71	-6.79
Overall	-19.73	-23.77	-21.02	-31.00	-32.97	-25.41	-40.60	-29.49	-27.21

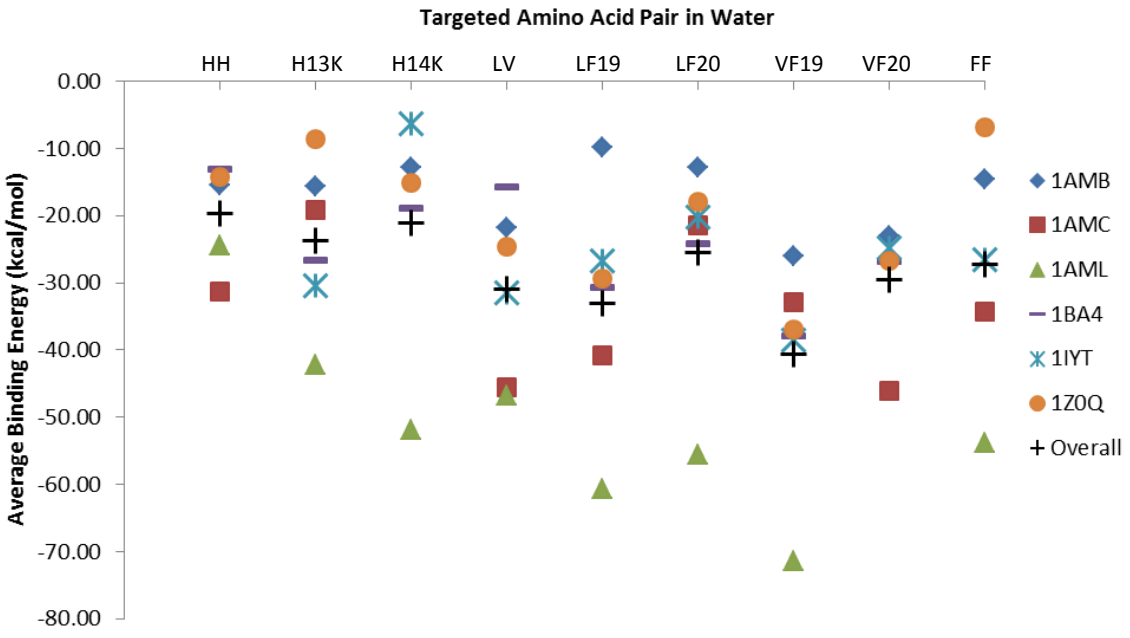


Figure 3.25 Average binding energies in kcal/mol when cyanidin is docked to HHQK LVFF across the six conformers in water.

After the solvent calculations were performed, it was found that docking cyanidin to VF19 produced the lowest average binding energies. This was also the case for the gas phase calculations. Amino acids LF19 were also providing favorable binding energies. The highest binding energies occurred when cyanidin was docking toward HH, H13K, and H14K. Again, this coincides with the gas phase calculation results.

For cyanidin, there were a total of 116 interactions occurring after the solvent calculations were performed. The total numbers of interactions that involved certain amino acids and particular regions on the cyanidin molecule are summarized in Figures 3.26 and 3.27, respectively.

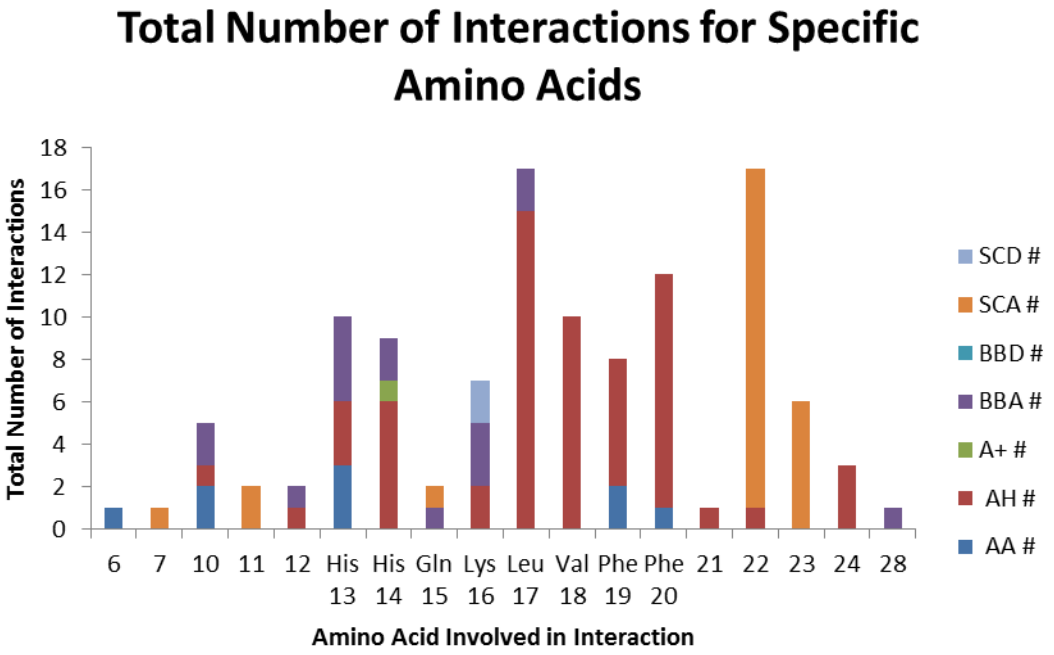


Figure 3.26 Total number of interactions that occur when a particular amino acid is involved in the docking of cyanidin to HHQK LVFF across the six Aβ conformers water.

In water, amino acids Leu17, Phe20, and Glu22 are involved in most of the interactions. The LVFF region in general provides more interactions than the HHQK region. Glu22 is still a predominant amino acid to produce an interaction with cyanidin.

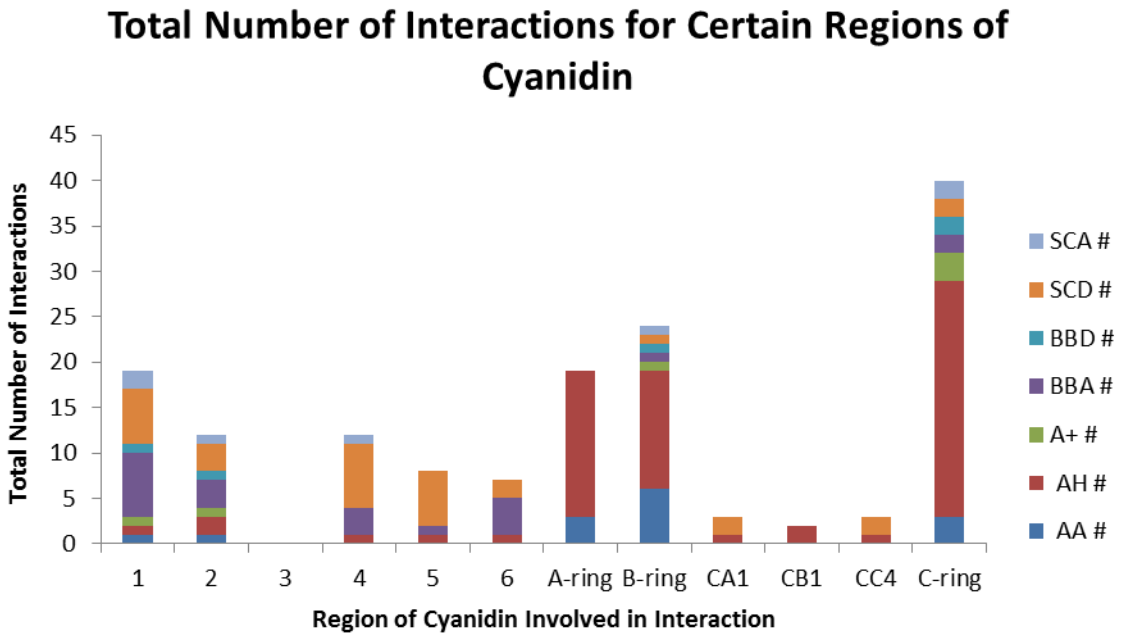


Figure 3.27 Total number of interactions that involve particular atoms or rings on the cyanidin molecule in water.

The region on the cyanidin molecule that partakes in the most interactions in water is clearly the C-ring. The B and A-ring have lots of interactions occurring but relatively less than the C-ring. The predominant interactions that occur with the rings are pi-H interactions with a little bit of pi-pi and a few hydrogen acceptance/donation/ Oxygens 1,2, and 4 are high amongst the oxygens but partake in less interactions than the two rings.

3.3.3 Summary

Overall, there were certain trends in the energies and interactions that were shown when cyanidin was docked to the HHQK LVFF regions of the six Aβ conformers. When cyanidin was oriented toward amino acids VF19, LV, and VF20 in the gas phase the lowest average binding energies were produced. VF19 had the lowest of the four. This is contrary to the results shown with catechin and epicatechin. When the calculations were performed in water, similar results were shown where targeting VF19 produced the lowest average binding energy. However, when cyanidin was docked toward HH and H13K in gas phase, the highest average binding energies were produced. This did not change very much when the solvent calculations were performed except H14K also had higher binding energies. These observations seem to suggest that cyanidin is not prone to bind toward the HHQK region but more toward the LVFF region. Further analysis of the interactions that occurred allowed for more insight into the binding modes.

There were a total of 188 interactions to consider from all of the gas phase calculations. First, the amino acids that were involved in the interactions were analyzed by how often they had an interaction and which type it was. In the gas phase, His13, Leu17 and Phe20 had high numbers of interactions occurring, however, Glu22 had the most by far. Glu22 bears a negative charge in physiological pH and it participated in hydrogen acceptance from the side chain (SCA). It makes sense that Glu22 is highly attracted to cyanidin, for it bears a positive charge. The same trend of amino acids was observed in water where the LVFF region in general produced many interactions. The lowest energies were observed for cyanidin docking to VF19 and VF20 both of which are

very close to Glu22. In general, there were many interactions occurring in the LVFF region. There were not very many binding interactions occurring in the HHQK region.

Secondly, the regions on the cyanidin molecule that were involved in the interactions were analyzed. Here, the C-ring played a much bigger role in producing binding interactions, unlike with catechin and epicatechin. This is most likely due to its increased aromaticity. The A and B-rings also played an important role in producing pi-pi and pi-hydrogen interactions. Oxygen 1 and oxygen 4 also produced many hydrogen interactions. The same results were shown in water.

Thirdly, the number of interactions was correlated with the initial orientation of cyanidin toward Aβ. The best initial orientations were 2/5, 3/6 and 4/6 where they produced many pi-type interactions. There were many initial orientations that did not seem to produce many interactions.

4 Quebecol Results

4.1 Quebecol

Quebecol is a novel polyphenol found within maple syrup. Unlike the polyphenols studied in the apple peel chapter, it has a significantly different structure. Also, there were 21 different orientations since there are seven different oxygens present within the molecule (Figure 4.1). The non-oxygen atoms are described in Figure 4.2.

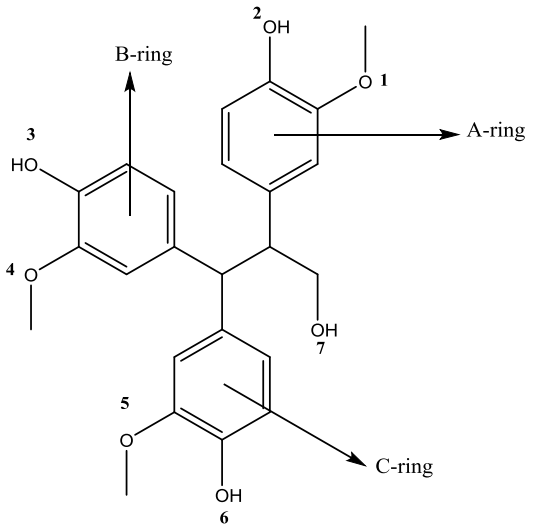


Figure 4.1 Structure of quebecol.

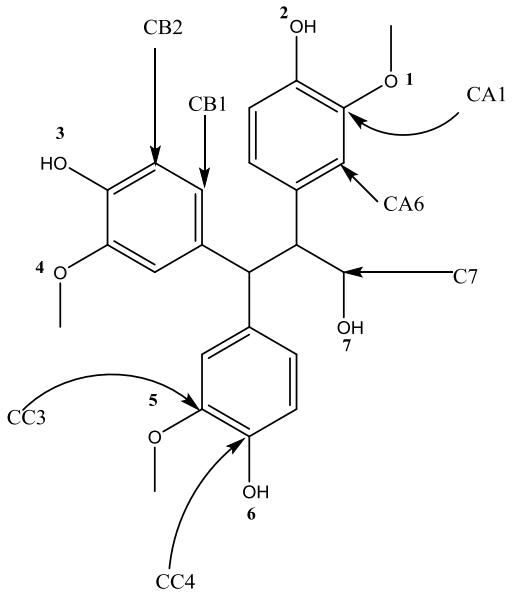


Figure 4.2 Structure of quebecol with the labeling of atoms.

4.2 Gas Phase Results

With the 21 different orientations, quebecol was docked across the HHQK LVFF regions of the six Aβ conformers. The binding energies and interactions for each are summarized in the Appendix D. The overall average binding energies are displayed in Table 4.1 and Figure 4.3.

Table 4.1 Average binding energies in kcal/mol when quebecol is docked to specific amino acid pairs in gas phase.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-24.31	-19.58	-21.80	-27.98	-31.10	-16.61	-25.78	-24.88	-25.37
1AMC	-34.54	-22.92	-30.60	-37.24	-36.55	-30.25	-33.78	-39.89	-35.68
1AML	-55.38	-63.95	-69.47	-55.34	-78.67	-58.75	-45.47	N/A	-61.50
1BA4	-13.49	-25.87	-27.91	-15.57	0.4759	-15.59	3.64	-20.32	-8.17
1IYT	-26.25	-24.07	-11.5	-30.72	-31.76	-24.46	-33.3	-39.26	-27.67
1Z0Q	-14.62	-15.44	-21.09	-21.67	-18.99	-14.28	-7.39	-5.97	-12.35
Average	-28.09	-28.64	-30.42	-31.42	-32.76	-26.64	-23.68	-26.06	-28.46

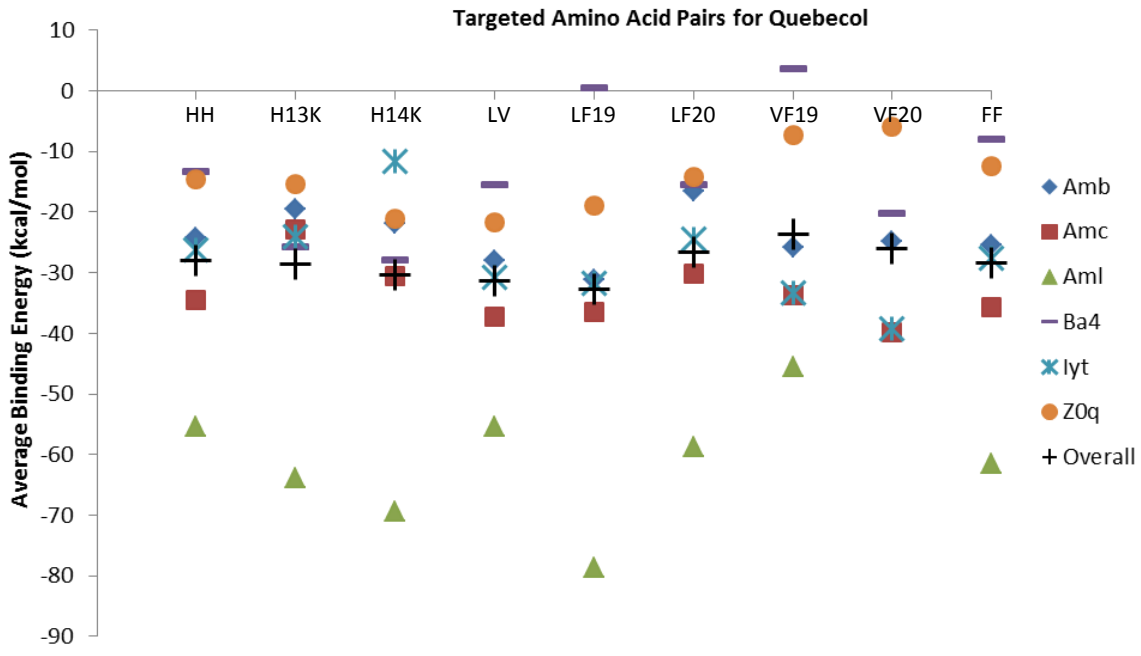


Figure 4.3 Average binding energies in kcal/mol when quebecol is docked to specific amino acid pairs in gas phase.

The lowest average binding energies occur when quebecol is docked to H14K, LV, and LF19. Although the rest of the amino acid pairs are fairly similar in binding energies, the highest binding energy occurs when quebecol is docked to VF19.

In addition to the energies, the interactions that occurred were also analyzed. In total, there were 188 interactions as a result of the gas phase docking calculations. The total number of interactions that occurred when a particular Aβ conformer was used is shown in Figure 4.4. They all contributed fairly evenly towards producing interactions, except 1IYT has a slightly smaller percentage.

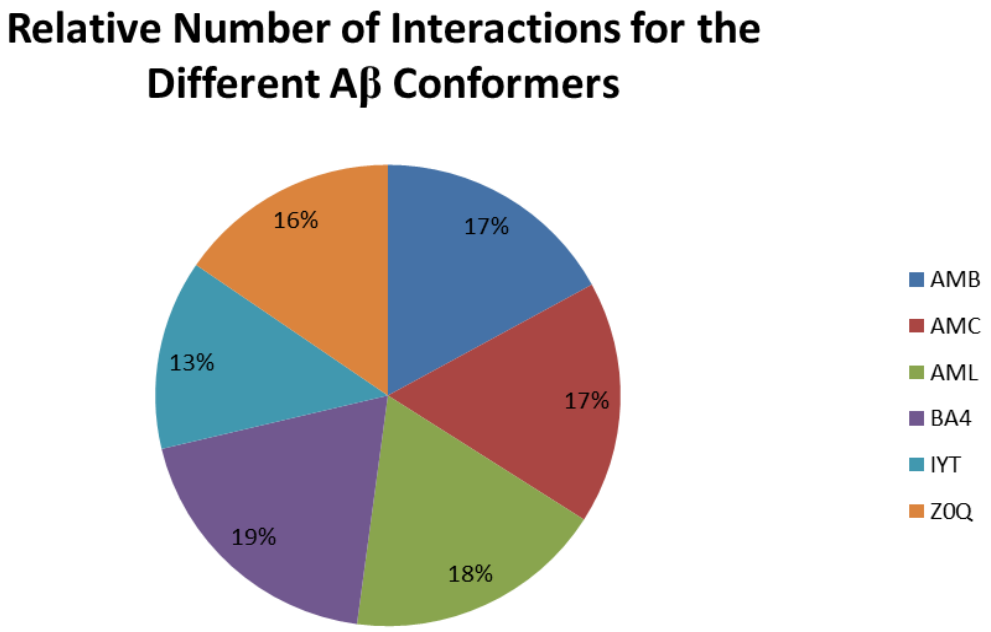


Figure 4.4 Percentage of total interactions that occur when a particular conformer is used in gas phase calculations of docking quebecol to Aβ.

In Figure 4.5, the number of interactions for specific amino acids are displayed. Lys16 is dominating the number of interactions with an equal number of different types

of interactions. It has SCD, BBA, A+ and AH types of interactions. The entire HHQK region is prevelant in terms of interactions. Glu 22 has a high number as well.

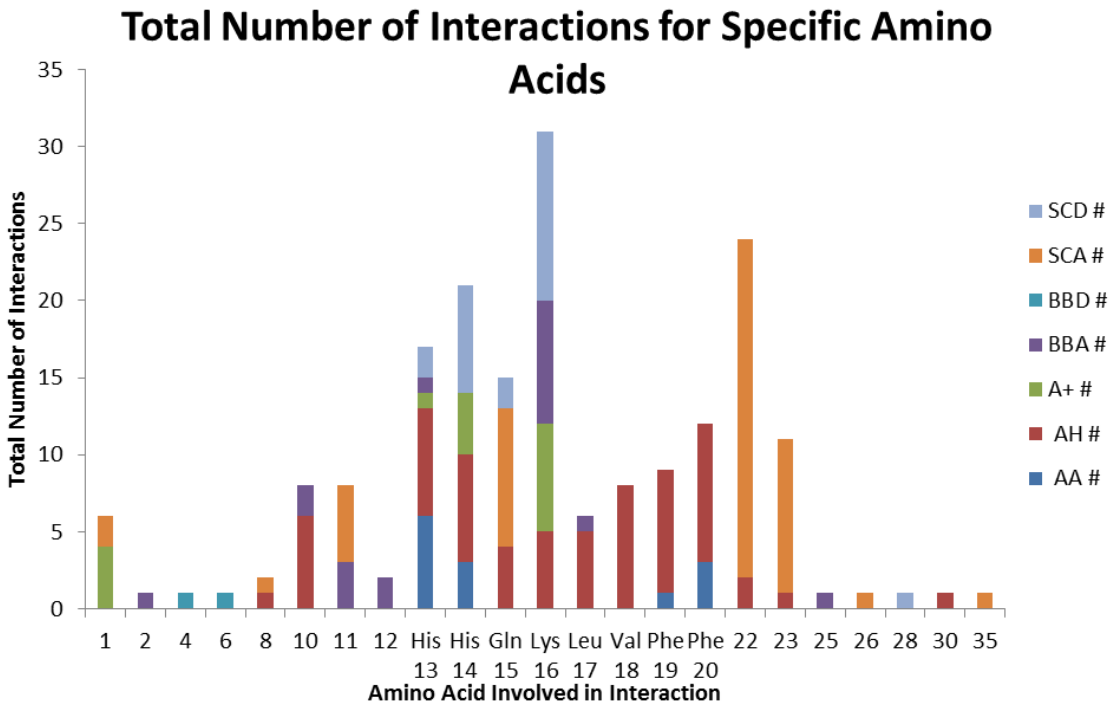


Figure 4.5 Total number of interactions that occur when a particular amino acid is involved in the docking of quebecol to HHQK LVFF across the six Aβ conformers in gas phase calculations.

Certain regions on the quebecol molecule were more prone to producing interactions. In Figure 4.6, it shows that oxygen 7 is contributing a lot with both side chain hydrogen acceptors and donors. Oxygen 3 and the three rings are also involved in a lot of interactions. The oxygen 3 is involved in mainly hydrogen acceptor and donor interactions whereas the rings are mainly involved in pi interactions, with pi-H dominating.

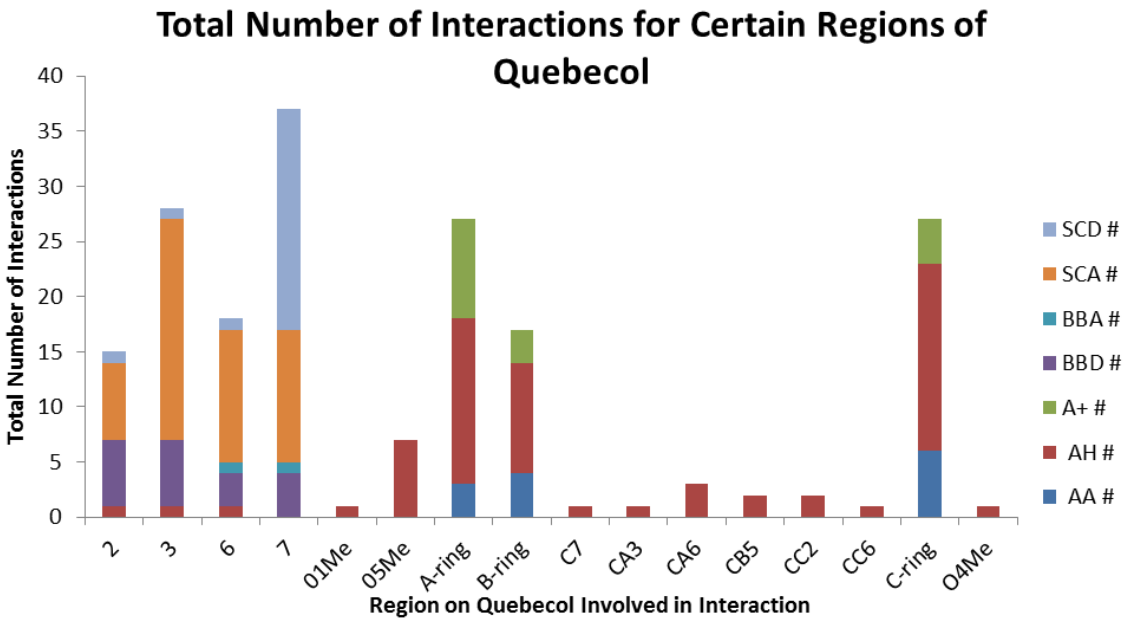


Figure 4.6 Total number of interactions that involve particular atoms or rings on the quebecol molecule in gas phase calculations.

Different initial orientations produced a different number of interactions. The totals are summarized in Figure 4.7. Initial orientations 2/5, 2/6 and 3/7 produced the highest number of interactions. Otherwise, they are all fairly equal except some that did not produce many interactions at all (orientations 3/5 and 4/6). The interactions 2/5 and 2/6 are highest for AH type interactions.

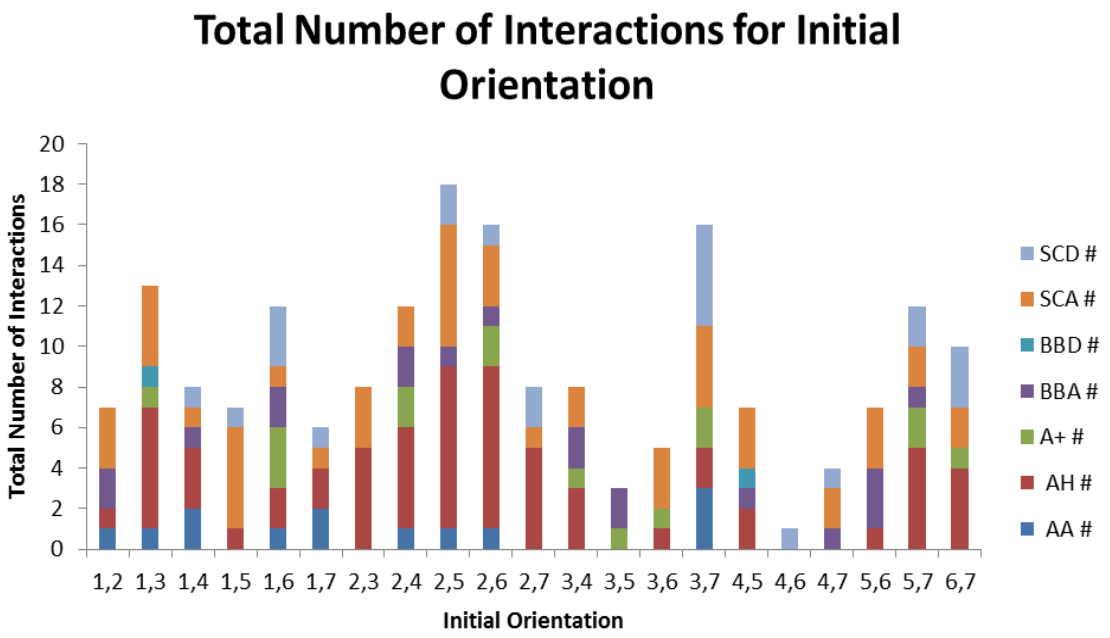


Figure 4.7 Total number of interactions that occur when a particular initial orientation of quebecol is docked toward HHQK LVFF in gas phase.

4.3 Solvent Phase Results

All of the individual binding energies and interactions in water are found within the Appendix D. The analysis of the average binding energies and total number of interactions will be found within this subchapter. The average binding energies for all of the solvent calculations of quebecol docked to Aβ are found within Table 4.2 and Figure 4.8.

Table 4.2 Average binding energies in kcal/mol for docking quebecol to a specific amino acid pair in water.

	HH	H13K	H14K	LV	LF19	LF20	VF19	VF20	FF
1AMB	-21.97	-20.23	-18.24	-30.32	-36.78	-13.05	-17.43	-30.56	-18.48
1AMC	-28.86	-29.81	-38.95	-31.56	-34.21	-23.36	-36.12	-36.33	-36.33
1AML	-58.94	-49.28	-54.80	-45.22	-65.09	N/A	-30.80	N/A	-59.16
1BA4	-9.93	-29.43	-24.35	-22.46	-14.19	N/A	-3.25	-27.21	-4.61
1IYT	-21.68	-20.51	-46.65	-35.29	-23.41	-20.90	-30.96	-38.61	-30.01
1Z0Q	-23.96	-24.78	-17.53	-15.99	-22.55	-22.63	-15.74	-14.32	-20.70
Overall	-27.56	-29.01	-33.42	-30.14	-32.71	-25.55	-22.38	-29.41	-28.22

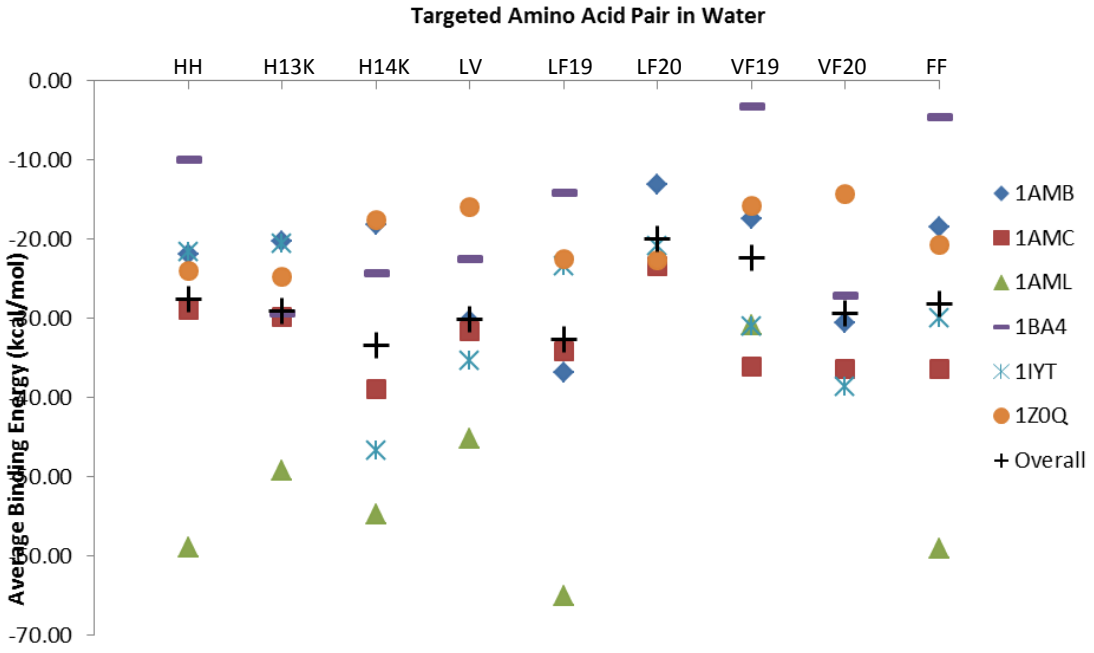


Figure 4.8 Average binding energies in kcal/mol for docking quebecol to a specific amino acid pair in water.

Similar to the gas phase results, the lowest binding energy occurs when quebecol is docked to H14K or LF19. The highest binding energies occur when it is docked to VF19.

After the solvent calculations were complete, there were 114 interactions still occurring. The total number that were occurring that involved a particular amino acid or a specific region on the quebecol molecule are summarized in Figures 4.9 and 4.10 respectively. For the amino acids, Lys16 is involved in many of the interactions, as noted previously for the gas phase results. Glu22 is another amino acid that has many interactions associated with it. His13 and His14 have relatively equal numbers of interactions, however, they differ in the types of interactions they produce. His13 participates in more pi-pi interactions than His14 whereas His14 participates in more SCD interactions. In Figure 4.10, it can be seen that after solvent calculations, the number of interactions occuring with the rings on quebecol decrease and the predominant region participating in interactions is oxygen 7. The rings still participate in many interactions, but not as often as was predicted in the gas phase calculations.

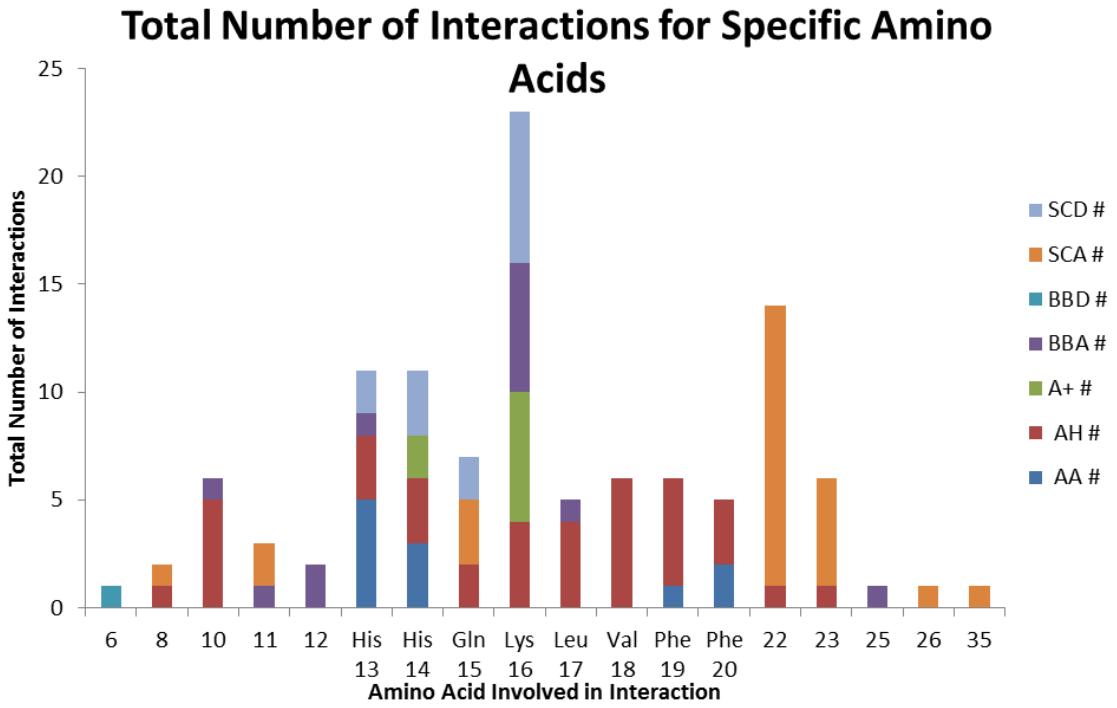


Figure 4.9 Total number of interactions that occur when a particular amino acid is involved in the docking of quebecol to HHQK LVFF across the six Aβ conformers in water.

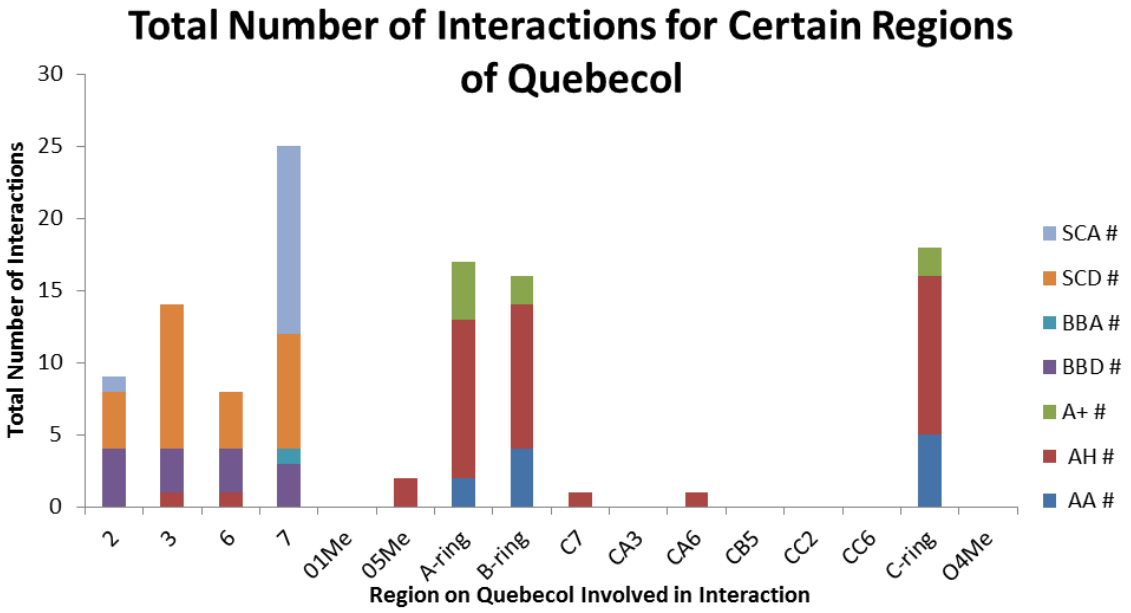


Figure 4.10 Total number of interactions that involve particular atoms or rings on the quebecol molecule in water.

4.4 Summary

Overall, there were certain trends in the energies and interactions that were shown when quebecol was docked to the HHQK LVFF regions of the six Aβ conformers. When quebecol was oriented toward amino acids H14K, LV, and LF19 in the gas phase, the lowest average binding energies were produced. When the calculations were performed in water, similar results were shown where targeting H13K and LF19 produced the lowest average binding energy. However, when quebecol was docked toward VF19 in both gas and solvent phase, the highest average binding energies were produced. From these observations, it seems to suggest that quebecol could have the potential to bind toward both the HHQK region and the LVFF region. Further analysis of the interactions that occurred allowed for more insight into the binding modes.

There were a total of 188 interactions to consider from all of the gas phase calculations. First, the amino acids that were involved in the interactions were analyzed by how often they had an interaction and which type it was. In the gas phase, Lys16 and HHQK in general had the highest number of interactions. Glu22 again had high numbers of interactions. The same trend of amino acids was observed in water. The lowest energies were observed for quebecol docking to parts of both the HHQK region (H14K) and the LVFF region (LF19). Many interactions occurred with the HHQK region, and the stability of the LVFF region might be due to the interactions with the close-by amino acid Glu22.

Secondly, the regions on the quebecol molecule that were involved in the interactions were analyzed. All three rings were responsible for producing most of the pi-type interactions. Oxygen groups 7 and 3 also produced many hydrogen interactions. The same results were shown in water with oxygen 3 producing much less than oxygen 7.

Thirdly, the number of interactions was correlated with the initial orientation of quebecol toward Aβ. The best initial orientations were 2/5, 2/6 and 3/7 where they produced many pi-type interactions. Orientation 3/7 was good because it provided the oxygen 7 that was involved in many interactions but it was a good orientation that did not leave the rest of the molecule to interfere with the neighboring amino acids. The initial orientations that did not produce many interactions were 3/5 and 4/6.

5 Conclusion

5.1 Summary of Molecules and Interactions

For this project, there were a total of four different molecules that were docked to six Aβ conformers to see if there was potential binding within the HHQK LVFF regions. Three molecules are found within apple peel: (+)-catechin, (-)-epicatechin, and cyanidin. The fourth molecule, quebecol, is found within maple syrup. Among the four molecules, there were similarities and differences between the ways they ended up binding to Aβ. These differences were explored through binding energies and interactions.

The average binding energies for the four molecules as they target different amino acid pairs along HHQK LVFF are described in Figure 5.1. Catechin and epicatechin show similar energies up until LF19 is targeted. VF20 is much lower in energy when it is targeted by catechin, rather than the three other molecules. Quebecol shows a trend in energies most similar to epicatechin. Cyanidin seems to show an opposite trend to the other three, where VF19 is lowest in energy instead of highest in energy. The highest binding energy for cyanidin is HH which is not the case for the other three molecules. In general for the four molecules, the lowest binding energies are produced between LV and LF20.

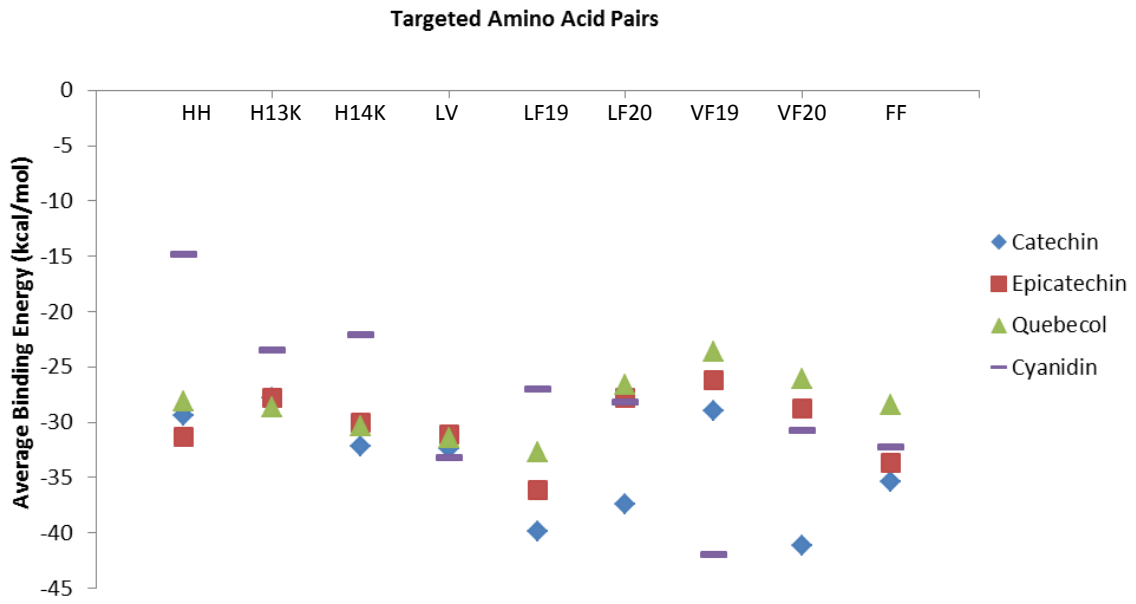


Figure 5.1 Overall average binding energies in kcal/mol of the four molecules examined in gas phase.

In terms of interactions, one amino acid that seemed to play a role in all molecules was Glu22. These interactions mainly occurred when the LVFF region was targeted so this could have been playing a role in the stability of the LVFF region. Catechin, epicatechin, and quebecol also produced many interactions within the HHQK region, particular on K16 (Lys16). Cyanidin, however, was the opposite and did not bind as readily to this region. The rings on each of the molecules provided many opportunities for pi type binding because they are aromatic. This, along with the many hydroxyl groups present on the molecules, helped immensely with forming interactions in general with Aβ.

5.2 Relevance of Work to Aβ/Diet/Drug trials

This project was primarily designed to see if some molecules within common foods are likely to bind to Aβ in the same way that some drug molecule candidates are designed to bind to Aβ. If so, it would be important to consider the diet of patients within clinical trials of a particular drug. If some patients in a clinical trial were consuming apples on a daily basis and other patients were not, then this single uncontrolled variable could possibly influence the validity of the trial results. Moreover, these concerns are not restricted to apples. As shown with the quebecol study, other polyphenols from other plant-based foods could likewise conceivably interfere with statistical analyses of clinical trial data. The clinical relevance of these molecular mechanics calculations is thus highly significant.

From the results shown here, multiple polyphenol molecules showed potential binding to the LVFF regions mainly, focusing on Glu22. HHQK was also a potential binding spot, except with cyanidin. These results, however, are not sufficiently conclusive to say with certainty that patient diets should be highly controlled during clinical trials. More polyphenols will have to be researched and docked to the same region because apple peels contain many more polyphenols. Furthermore, these *in silico* results must be experimentally validated by, for example, NMR binding studies. This project, however, provides very detailed manual docking data of some polyphenols to the important Aβ regions. This could be used for comparison in a much faster docking experiment where the receptor site has to be defined on the Aβ conformers. By confirming that method, then multiple polyphenols from a diversity of plant and fruit products could be tested *in silico* much more easily and efficiently against Aβ to

determine whether the diets do actually need to be considered in clinical trials for drugs for Alzheimer's.

5.3 Future Considerations

This work could be expanded to provide more conclusive results. First of all, the number of polyphenols found within fruits, vegetables, and drinks such as tea and wine, is rather vast. Therefore, a future consideration is of course to do calculations on more polyphenols.

Another consideration is to employ a better docking method. Here, the HHQK LVFF regions were the amino acids that the molecules were actually oriented toward. It would be better to have docked it to another region of the Aβ conformer to be able to compare directly how much better or worse it is to dock these molecules to the HHQK LVFF regions.

Furthermore, there are two fairly new NMR structures for full length Aβ that were found on the Protein Data Bank after this project was well underway. These new structures could be either added to the six conformers that were already used or replace some of the shorter chain conformers. It would be interesting to see if they produce any different types of interactions or different binding energies.

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APPENDIX A: DATA FOR (+)-CATECHIN

Tables of energies for gas phase calculations of (+)-catechin. All energies are in kcal/mol. The order of the tables for each pair of amino acids is always 1AMB, 1AMC, 1AML, 1BA4, 1IYT, 1Z0Q.

ABBREVIATION LEGEND:

E=Potential Energy

VDW= van der waals energy

ELE= Electrostatic energy

BE= Binding energy

HH

Orientation	E	VDW	ELE	Binding Energy (BE)
1,2	49.987	109.107	-324.689	-27.88
1,3	41.871	101.959	-325.112	-35.996
1,4	29.86	96.090	-340.385	-48.007
1,5	55.044	100.742	-313.440	-22.823
1,6	41.798	107.315	-330.060	-36.069
2,3	48.791	100.052	-321.437	-29.076
2,4	68.296	102.948	-306.723	-9.571
2,5	56.703	102.565	-316.684	-21.164
2,6	30.233	96.076	-338.236	-47.634
3,4	51.335	101.115	-319.481	-26.532
3,5	42.22	105.635	-333.144	-35.647
3,6	n/a			
4,5	58.685	104.807	-313.682	-19.182
4,6	54.605	96.614	-308.909	-23.262
5,6	56.806	103.758	-315.534	-21.061

Orientation	E	VDW	ELE	BE
1,2	76.727	110.014	-310.914	-33.056
1,3	62.527	100.954	-314.991	-47.256
1,4	69.074	105.36	-315.553	-40.709
1,5	89.654	102.135	-294.221	-20.129
1,6	79.884	101.054	-296.471	-29.899
2,3	77.459	98.744	-300.33	-32.324

2,4	80.707	101.718	-297.271	-29.076
2,5	75.882	104.469	-303.842	-33.901
2,6	65.075	100.483	-311.276	-44.708
3,4	65.245	103.199	-319.049	-44.538
3,5	59.313	103.656	-312.866	-50.47
3,6	89.709	108.739	-294.803	-20.074
4,5	79.758	108.083	-307.908	-30.025
4,6	70.645	105.211	-314.192	-39.138
5,6	75.21	104.396	-306.755	-34.573

Orientation	E	VDW	ELE	BE
1,2	270.264	148.496	-241.9	-18.61
1,3	247.277	147.071	-260.816	-41.597
1,4	218.964	146.351	-292.955	-69.91
1,5	249.739	152.163	-258.41	-39.135
1,6	247.021	145.957	-271.903	-41.853
2,3	249.452	141.528	-258.95	-39.422
2,4	231.305	148.254	-269.891	-57.569
2,5	228.126	145.268	-287.303	-60.748
2,6	254.027	146.624	-259.883	-34.847
3,4	211.579	144.353	-288.178	-77.295
3,5	229.381	135.046	-266.986	-59.493
3,6	236.96	140.24	-266.693	-51.914
4,5	242.194	146.429	-264.594	-46.68
4,6	242.088	147.806	-270.485	-46.786
5,6	264.581	147.696	-246.292	-24.293

Orientation	E	VDW	ELE	BE
1,2	223.081	160.669	-314.985	-9.784
1,3	211.734	158.475	-325.294	-21.131
1,4	218.111	159.369	-320.764	-14.754
1,5	223.827	162.426	-317.351	-9.038
1,6	213.082	161.07	-326.325	-19.783
2,3	214.546	158.563	-323.583	-18.319
2,4	229.266	163.574	-311.473	-3.599
2,5	228.35	160.483	-311.296	-4.515
2,6	220.228	161.079	-319.707	-12.637
3,4	203.85	152.125	-327.073	-29.015
3,5	215.173	158.397	-321.79	-17.692
3,6	211.444	159.116	-324.754	-21.421
4,5	227.659	162.21	-312.407	-5.206

4,6	212.312	158.118	-324.728	-20.553
5,6	222.359	160.252	-316.436	-10.506

Orientation	E	VDW	ELE	BE
1,2	227.331	141.448	-303.698	-28.178
1,3	225.923	144.148	-305.646	-29.586
1,4	224.409	135.968	-311.424	-31.1
1,5	229.754	136.938	-300.166	-25.755
1,6	224.115	143.734	-311.593	-31.394
2,3	233.623	136.549	-299.087	-21.886
2,4	223.61	139.276	-310.888	-31.899
2,5	227.927	140.073	-302.467	-27.582
2,6	221.447	138.783	-311.081	-34.062
3,4	210.726	137.216	-320.984	-44.783
3,5	230.759	134.697	-300.71	-24.75
3,6	221.874	140.256	-310.143	-33.635
4,5	223.41	141.615	-308.762	-32.099
4,6	233.094	139.097	-300.716	-22.415
5,6	236.362	138.801	-296.437	-19.147

Orientation	E	VDW	ELE	BE
1,2	N/A			
1,3	209.07	147.618	-338.79	-8.685
1,4	195.74	145.995	-340.771	-22.015
1,5	194.798	144.622	-340.573	-22.957
1,6	192.276	146.171	-345.051	-25.479
2,3	189.97	141.154	-347.084	-27.785
2,4	192.336	144.524	-343.393	-25.419
2,5	206.589	148.074	-331.658	-11.166
2,6	196.959	146.301	-342.381	-20.796
3,4	188.309	141.488	-345.387	-29.446
3,5	195.099	141.549	-339.212	-22.656
3,6	n/a			
4,5	199.577	146.504	-336.364	-18.178
4,6	195.142	147.771	-344.588	-22.613
5,6	199.474	148.733	-339.229	-18.281

H13K

Orientation	E	VDW	ELE	BE
1,2	66.009	107.32	-308.368	-11.858
1,3	62.56	94.068	-309.391	-15.307
1,4	53.765	99.142	-315.148	-24.102
1,5	55.172	106.49	-316.435	-22.695
1,6	64.211	108.801	-313.135	-13.656
2,3	47.186	103.445	-325.264	-30.681
2,4	57.378	105.543	-314.821	-20.489
2,5	65.456	107.118	-308.558	-12.411
2,6	59.648	105.992	-316.098	-18.219
3,4	60.955	104.209	-311.928	-16.912
3,5	62.068	97.969	-313.061	-15.799
3,6	59.254	102.532	-316.832	-18.613
4,5	64.15	104.972	-310.937	-13.717
4,6	55.175	110.66	-320.519	-22.692
5,6	42.748	101.111	-329.457	-35.119

Orientation	E	VDW	ELE	BE
1,2	83.577	112.09	-299.008	-26.206
1,3	84.587	103.03	-293.673	-25.196
1,4	75.923	105.122	-307.237	-33.86
1,5	82.672	105.545	-298.832	-27.111
1,6	86.162	103.855	-293.271	-23.621
2,3	79.443	107.169	-299.068	-30.34
2,4	91.151	109.138	-293.624	-18.632
2,5	88.94	108.91	-295.002	-20.843
2,6	86.08	106.523	-299.469	-23.703
3,4	80.565	102.154	-296.302	-29.218
3,5	67.89	96.59	-312.419	-41.893
3,6	87.09	106.383	-291.717	-22.693
4,5	99.686	110.101	-285.209	-10.097
4,6	83.925	102.8	-292.331	-25.858
5,6	87.418	103.009	-294.199	-22.365

Orientation	E	VDW	ELE	BE
1,2	211.047	143.05	-282.345	-77.827
1,3	204.495	151.124	-295.112	-84.379
1,4	250.494	152.912	-267.334	-38.38
1,5	249.94	154.207	-263.049	-38.934
1,6	236.032	149.02	-279.209	-52.842

2,3	262.723	152.207	-254.384	-26.151
2,4	253.944	153.128	-266.421	-34.93
2,5	204.354	150.131	-304.521	-84.52
2,6	250.618	153.457	-270.632	-38.256
3,4	248.063	149.225	-262.956	-40.811
3,5	215.951	148.684	-291.367	-72.923
3,6	231.557	138.927	-273.78	-57.317
4,5	191.118	150.893	-307.253	-97.756
4,6	259.018	152.907	-254.717	-29.856
5,6	224.832	147.867	-283.072	-64.042

Orientation	E	VDW	ELE	BE
1,2	207.578	152.22	-322.132	-25.287
1,3	206.488	152.353	-323.796	-26.377
1,4	206.23	150.776	-323.543	-26.635
1,5	250.475	142.337	-330.713	17.61
1,6	202.926	148.645	-323.603	-29.939
2,3	204.563	157.275	-325.322	-28.302
2,4	209.084	151.375	-317.428	-23.781
2,5	220.919	154.452	-314.42	-11.946
2,6	201.146	149.372	-327.088	-31.719
3,4	194.722	147.259	-328.294	-38.143
3,5	204.729	154.176	-312.12	-28.136
3,6	199.258	148.05	-324.47	-33.607
4,5	218.528	154.796	-316.862	-14.337
4,6	201.679	147.167	-325.089	-31.186
5,6	215.465	152.328	-315.094	-17.4

Orientation	E	VDW	ELE	BE
1,2	232.601	136.156	-294.252	-22.908
1,3	224.881	136.723	-304.718	-30.628
1,4	237.36	136.972	-295.393	-18.149
1,5	238.801	137.6	-291.349	-16.708
1,6	221.386	138.846	-304.608	-34.123
2,3	221.596	136.427	-303.78	-33.913
2,4	224.03	137.447	-302.919	-31.479
2,5	245.233	138.5	-288.741	-10.276
2,6	233.103	140.87	-299.862	-22.406
3,4	212.208	144.348	-320.085	-43.301
3,5	233.296	139.469	-295.571	-22.213
3,6	231.459	137.438	-296.54	-24.05
4,5	224.571	137.804	-302.381	-30.938
4,6	236.993	138.422	-295.328	-18.516
5,6	228.401	139.829	-303.761	-27.108

Orientation	E	VDW	ELE	BE
1,2	199.548	146.55	-338.414	-18.207
1,3	198.97	146.75	-341.737	-18.785
1,4	203.31	150.627	-337.032	-14.445
1,5	202.347	146.177	-338.684	-15.408
1,6	198.651	149.766	-341.688	-19.104
2,3	207.748	148.612	-334.316	-10.007
2,4	208.137	151.845	-332.367	-9.618
2,5	213.048	151.72	-329.926	-4.707
2,6	198.469	150.513	-344.759	-19.286
3,4	197.958	150.654	-342.149	-19.797
3,5	191.919	144.412	-343.689	-25.836
3,6	189.316	146.772	-349.208	-28.439
4,5	206.063	149.928	-333.754	-11.692
4,6	202.139	147.967	-337.805	-15.616
5,6	198.494	147.979	-340.251	-19.261

H14K

Orientation	E	VDW	ELE	BE
1,2	72.248	106.367	-310.409	-5.619
1,3	53.418	98.585	-317.277	-24.449
1,4	52.921	99.161	-318.829	-24.946
1,5	57.66	99.315	-311.185	-20.207
1,6	49.797	106.653	-331.943	-28.07
2,3	49.884	99.217	-322.189	-27.983
2,4	51.206	97.581	-320.955	-26.661
2,5	59.559	100.535	-320.022	-18.308
2,6	64.701	99.315	-312.8	-13.166
3,4	57.874	97.776	-315.293	-19.993
3,5	50.911	95.083	-319.007	-26.956
3,6	32.622	96.099	-331.826	-45.245
4,5	66.07	100.695	-310.178	-11.797
4,6	65.273	103.672	-314.775	-12.594
5,6	68.883	107.13	-314.702	-8.984

Orientation	E	VDW	ELE	BE
1,2	83.565	102.577	-308.058	-26.218
1,3	73.092	109.455	-321.188	-36.691
1,4	87.474	101.267	-288.728	-22.309
1,5	71.207	106.182	-314.018	-38.576
1,6	74.543	98.383	-303.382	-35.24
2,3	73.726	108.398	-311.109	-36.057
2,4	88.069	100.634	-290.491	-21.714
2,5	85.615	100.859	-292.747	-24.168
2,6	37.7	106.592	-333.238	-72.083

3,4	66.175	94.366	-307.336	-43.608
3,5	65.486	93.369	-300.804	-44.297
3,6	65.977	107.53	-317.834	-43.806
4,5	89.38	106.352	-302.965	-20.403
4,6	94.977	114.488	-299.774	-14.806
5,6	80.09	109.61	-307.127	-29.693

Orientation	E	VDW	ELE	BE
1,2	228.122	138.105	-277.44	-60.752
1,3	223.746	141.592	-275.376	-65.128
1,4	178.712	145.359	-324.081	-110.162
1,5	235.661	151.219	-274.775	-53.213
1,6	195.491	144.189	-304.423	-93.383
2,3	237.364	143.897	-263.692	-51.51
2,4	231.957	143.555	-267.897	-56.917
2,5	232.121	137.053	-268.299	-56.753
2,6	238.884	153.064	-272.439	-49.99
3,4	208.312	154.687	-324.183	-80.562
3,5	247.899	138.571	-255.432	-40.975
3,6	211.679	138.655	-293.468	-77.195
4,5	249.207	142.172	-254.711	-39.667
4,6	203.522	140.249	-291.624	-85.352
5,6	258.937	143.353	-247.67	-29.937

Orientation	E	VDW	ELE	BE
1,2	204.773	149.92	-323.66	-28.092
1,3	198.852	142.485	-325.085	-34.013
1,4	209.551	155.054	-322.681	-23.314
1,5	212.273	151.954	-319.232	-20.592
1,6	208.815	154.135	-324.753	-24.05
2,3	206.039	151.232	-322.579	-26.826
2,4	199.01	147.968	-330.665	-33.855
2,5	211.382	155.036	-321.947	-21.483
2,6	196.348	152.123	-333.743	-36.517
3,4	208.312	154.687	-324.183	-24.553
3,5	210.782	148.301	-322.304	-22.083
3,6	205.662	154.952	-328.241	-27.203
4,5	214.41	152.003	-313.531	-18.455
4,6	206.577	151.739	-327.274	-26.288

5,6	203.357	149.724	-324.117	-29.508

Orientation	E	VDW	ELE	BE
1,2	212.961	138.541	-309.728	-42.548
1,3	263.918	136.383	-312.554	8.409
1,4	252.144	128.947	-319.887	-3.365
1,5	217.608	136.227	-305.311	-37.901
1,6	209.746	137.105	-317.126	-45.763
2,3	262.262	132.987	-316.058	6.753
2,4	233.511	136.748	-295.287	-21.998
2,5	227.223	137.37	-304.512	-28.286
2,6	229.383	136.032	-304.12	-26.126
3,4	236.807	130.497	-292.844	-18.702
3,5	207.815	138.985	-316.299	-47.694
3,6	240.357	140.691	-305.666	-15.152
4,5	230.173	136.07	-301.204	-25.336
4,6	215.082	134.614	-314.019	-40.427
5,6	216.633	134.776	-309.012	-38.876

Orientation	E	VDW	ELE	BE
1,2	198.597	147.986	-339.945	-19.158
1,3	192.815	146.797	-344.018	-24.94
1,4	193.732	142.996	-340.658	-24.023
1,5	196.278	143.488	-341.168	-21.477
1,6	195.634	146.031	-344.339	-22.121
2,3	192.186	143.97	-344.948	-25.569
2,4	186.737	145.102	-348.516	-31.018
2,5	203.442	145.136	-334.394	-14.313
2,6	189.151	142.589	-347.399	-28.604
3,4	192.068	145.372	-344.582	-25.687
3,5	201.806	148.16	-344.002	-15.949
3,6	191.107	144.995	-345.804	-26.648
4,5	198.834	145.015	-336.501	-18.921
4,6	198.266	150.744	-343.946	-19.489
5,6	190.61	142.055	-340.561	-27.145

LV

Orientation	E	VDW	ELE	BE
1,2	59.999	104.898	-318.262	-19.866

1,3	177.442	101.363	-307.187	97.577
1,4	48.527	95.781	-308.918	-31.338
1,5	50.592	98.094	-321.872	-29.273
1,6	45.606	101.531	-325.555	-34.259
2,3	60.695	99.319	-310.575	-19.17
2,4	56.938	102.688	-312.79	-22.927
2,5	56.92	101.042	-322.273	-22.945
2,6	46.141	97.364	-323.047	-33.724
3,4	30.11	101.068	-340.062	-49.755
3,5	44.376	102.552	-325.104	-35.489
3,6	52.642	100.407	-316.044	-27.223
4,5	54.638	105.785	-319.875	-25.227
4,6	63.215	102.631	-308.728	-16.65
5,6	63.213	103.636	-309.829	-16.652

Orientation	E	VDW	ELE	BE
1,2	87.506	104.049	-292.395	-22.277
1,3	64.827	103.818	-317.523	-44.956
1,4	69.762	105.573	-307.591	-40.021
1,5	76.993	108.914	-304.095	-32.79
1,6	70.999	102.384	-307.961	-38.784
2,3	65.838	102.204	-307.954	-43.945
2,4	66.037	105.99	-308	-43.746
2,5	77.267	103.114	-305.157	-32.516
2,6	53.655	101.004	-317.599	-56.128
3,4	73.938	99.815	-302.555	-35.845
3,5	69.882	103.822	-305.179	-39.901
3,6	58.455	97.896	-313.73	-51.328
4,5	78.687	114.418	-311.213	-31.096
4,6	70.264	101.321	-301.136	-39.519
5,6	72.374	105.131	-311.002	-37.409

Orientation	E	VDW	ELE	BE
1,2	252.926	144.928	-256.476	-35.948
1,3	182.189	143.439	-324.903	-106.685
1,4	216.054	137.009	-281.75	-72.82
1,5	208.775	136.088	-299.229	-80.099
1,6	245.773	148.151	-264.986	-43.101
2,3	244.226	144.699	-271.766	-44.648
2,4	212.379	142.361	-292.242	-76.495
2,5	187.879	143.941	-315.144	-100.995
2,6	195.861	145.881	-315.875	-93.013
3,4	236.356	146.455	-261.427	-52.518

3,5	231.393	136.959	-268.156	-57.481
3,6	247.804	138.91	-257.753	-41.07
4,5	194.188	148.871	-311.622	-94.686
4,6	207.373	143.233	-298.544	-81.501
5,6	225.062	143.523	-295.117	-63.812

Orientation	E	VDW	ELE	BE
1,2	217.479	160.149	-320.871	-15.386
1,3	213.18	151.307	-314.621	-19.685
1,4	218.129	157.62	-320.427	-14.736
1,5	216.746	158.825	-321.69	-16.119
1,6	214.03	157.481	-319.918	-18.835
2,3	216.767	156.09	-318.523	-16.098
2,4	223.917	155.465	-309.734	-8.948
2,5	211.976	156.446	-326.371	-20.889
2,6	213.916	156.446	-321.429	-18.949
3,4	216.86	155.772	-319.461	-16.005
3,5	210.079	155.318	-321.992	-22.786
3,6	211.024	155.172	-320.702	-21.841
4,5	219.479	156.421	-314.524	-13.386
4,6	216.911	155.778	-316.061	-15.954
5,6	218.407	154.742	-315.857	-14.458

Orientation	E	VDW	ELE	BE
1,2	221.838	140.933	-311.225	-33.671
1,3	234.523	134.818	-298.829	-20.986
1,4	234.91	135.276	-299.177	-20.599
1,5	227.155	134.801	-306.766	-28.354
1,6	223.833	139.819	-316.679	-31.676
2,3	221.119	138.075	-313.619	-34.39
2,4	226.158	142.254	-318.195	-29.351
2,5	225.474	137.143	-310.685	-30.035
2,6	234.036	136.512	-299.849	-21.473
3,4	228.076	135.023	-302.95	-27.433
3,5	229.422	133.581	-301.486	-26.087
3,6	218.982	136.249	-305.588	-36.527
4,5	243.272	140.512	-291.793	-12.237
4,6	222.625	139.245	-303.776	-32.884
5,6	240.261	138.822	-291.587	-15.248

Orientation	E	VDW	ELE	BE
1,2	201.49	149.385	-340.656	-16.265
1,3	200.083	147.886	-336.487	-17.672
1,4	199.98	147.005	-335.642	-17.775
1,5	191.161	142.559	-342.319	-26.594
1,6	186.958	144.324	-350.581	-30.797
2,3	192.818	143.326	-344.272	-24.937
2,4	199.305	148.716	-338.576	-18.45
2,5	193.934	137.678	-333.519	-23.821
2,6	184.546	142.594	-351.058	-33.209
3,4	203.211	143.584	-331.906	-14.544
3,5	189.297	142.688	-342.628	-28.458
3,6	193.883	140.812	-337.55	-23.872
4,5	197.265	147.428	-341.987	-20.49
4,6	192.438	143.277	-342.867	-25.317
5,6	199.376	146.147	-336.209	-18.379

LF19

Orientation	E	VDW	ELE	BE
1,2	54.747	105.738	-313.775	-23.12
1,3	58.017	97.943	-316.971	-19.85
1,4	50.568	96.61	-323.734	-27.299
1,5	50.849	97.08	-321.951	-27.018
1,6	46.632	100.321	-325.58	-31.235
2,3	47.237	103.63	-321.824	-30.63
2,4	46.335	99.75	-320.495	-31.532
2,5	48.504	94.774	-316.156	-29.363
2,6	52.671	96.121	-328.976	-25.196
3,4	37.839	98.465	-331.434	-40.028
3,5	50.69	96.916	-322.715	-27.177
3,6	59.088	101.145	-311.76	-18.779
4,5	51.745	104.165	-321.114	-26.122
4,6	49.03	102.733	-321.414	-28.837
5,6	54.182	97.979	-310.455	-23.685

Orientation	E	VDW	ELE	BE
1,2	69.838	100.012	-300.666	-39.945
1,3	60.835	99.808	-310.131	-48.948
1,4	62.352	97.851	-322.495	-47.431

1,5	45.903	92.83	-319.677	-63.88
1,6	67.883	103.442	-311.047	-41.9
2,3	66.572	103.317	-309.169	-43.211
2,4	75.733	85.714	-317.336	-34.05
2,5	63.804	108.701	-325.81	-45.979
2,6	77.277	100.514	-296.678	-32.506
3,4	69.971	99.278	-314.408	-39.812
3,5	67.233	95.755	-299.045	-42.55
3,6	61.034	97.901	-303.613	-48.749
4,5	64.993	104.236	-322.233	-44.79
4,6	73.085	105.723	-308.904	-36.698
5,6	69.607	98.257	-302.989	-40.176

Orientation	E	VDW	ELE	BE
1,2	205.783	146.141	-298.114	-83.091
1,3	196.822	143.442	-298.655	-92.052
1,4	202.515	151.676	-304.783	-86.359
1,5	195.262	142.263	-307.779	-93.612
1,6	202.458	147.63	-301.691	-86.416
2,3	217.947	143.919	-286.7	-70.927
2,4	227.619	141.802	-282.729	-61.255
2,5	194.906	140.424	-309.321	-93.968
2,6	233.05	146.086	-286.841	-55.824
3,4	196.735	145.066	-320.549	-92.139
3,5	293.481	147.206	-276.238	4.607
3,6	229.193	151.152	-291.854	-59.681
4,5	175.191	140.741	-327.378	-113.683
4,6	171.768	146.17	-331.936	-117.106
5,6	180.17	141.071	-319.01	-108.704

Orientation	E	VDW	ELE	BE
1,2	209.106	150.616	-325.28	-23.759
1,3	266.437	152.766	-320.627	33.572
1,4	213.268	150.563	-316.092	-19.597
1,5	214.828	152.666	-314.381	-18.037
1,6	207.488	154.973	-326.961	-25.377
2,3	281.05	148.835	-312.51	48.185
2,4	217.053	157.13	-316.174	-15.812
2,5	206.497	152.886	-329.499	-26.368
2,6	207.806	156.273	-325.817	-25.059
3,4	218.824	149.627	-317.554	-14.041
3,5	216.733	149.015	-313.481	-16.132
3,6	218.602	156.415	-316.11	-14.263

4,5	210.298	157.108	-328.833	-22.567
4,6	268.328	156.028	-320.952	35.463
5,6	221.251	157.115	-314.228	-11.614

Orientation	E	VDW	ELE	BE
1,2	217.482	140.976	-313.113	-70.367
1,3	226.12	133.124	-302.053	-61.729
1,4	238.811	136.958	-291.529	-49.038
1,5	223.527	138.928	-310.986	-64.322
1,6	217.483	140.229	-308.86	-70.366
2,3	224.819	131.022	-299.843	-63.03
2,4	234.58	133.807	-295.814	-53.269
2,5	241.001	133.975	-287.165	-46.848
2,6	222.259	137.376	-308.903	-65.59
3,4	212.907	137.831	-306.977	-74.942
3,5	244.827	139.212	-290.158	-43.022
3,6	220.697	138.589	-301.911	-67.152
4,5	217.44	137.561	-301.999	-70.409
4,6	220.534	136.448	-309.093	-67.315
5,6	222.008	134.506	-306.291	-65.841

Orientation	E	VDW	ELE	BE
1,2	204.612	149.205	-331.915	-13.143
1,3	190.186	142.263	-345.114	-27.569
1,4	198.948	144.455	-336.716	-18.807
1,5	205.524	147.797	-333.03	-12.231
1,6	200.942	146.346	-337.621	-16.813
2,3	189.992	141.965	-344.924	-27.763
2,4	207.284	150.453	-332.256	-10.471
2,5	200.802	148.501	-336.973	-16.953
2,6	202.967	143.554	-331.451	-14.788
3,4	196.649	147.831	-339.524	-21.106
3,5	197.357	143.065	-341.388	-20.398
3,6	190.209	142.969	-345.332	-27.546
4,5	205.547	148.764	-334.064	-12.208
4,6	200.015	145.78	-336.861	-17.74
5,6	206.878	147.326	-330.293	-10.877

LF20

Orientation	E	VDW	ELE	BE
1,2	60.715	104.619	-311.961	-17.152
1,3	50.678	101.375	-313.815	-27.189
1,4	57.376	108.025	-317.853	-20.491
1,5	63.114	100.944	-302.752	-14.753
1,6	56.083	104.704	-313.103	-21.784
2,3	57.922	104.887	-315.497	-19.945
2,4	58.997	104.112	-314.29	-18.87
2,5	50.055	107.051	-322.922	-27.812
2,6	70.213	107.092	-305.42	-7.654
3,4	59.586	103.329	-314.337	-18.281
3,5	60.334	104.581	-314.124	-17.533
3,6	41.97	104.293	-330.615	-35.897
4,5	57.274	104.082	-315.306	-20.593
4,6	62.698	103.054	-310.573	-15.169
5,6	60.097	105.371	-314.425	-17.77

Orientation	E	VDW	ELE	BE
1,2	78.57	106.046	-303.854	-31.213
1,3	91.045	106.171	-291.018	-18.738
1,4	86.531	102.39	-293.585	-23.252
1,5	74.543	103.838	-303.468	-35.24
1,6	86.416	105.06	-293.529	-23.367
2,3	66.649	98.233	-315.373	-43.134
2,4	76.036	106.19	-303.472	-33.747
2,5	73.78	106.489	-314.579	-36.003
2,6	93.817	105.858	-293.286	-15.966
3,4	71.307	105.358	-304.421	-38.476
3,5	73.158	101.999	-304.228	-36.625
3,6	76.94	105.485	-297.189	-32.843
4,5	85.68	108.163	-298.454	-24.103
4,6	72.826	105.896	-307.716	-36.957
5,6	72.987	106.129	-310.50	-36.796

Orientation	E	VDW	ELE	BE
1,2	219.133	151.096	-289.706	-69.716
1,3	227.773	148.518	-280.315	-61.076
1,4	192.72	141.457	-308.998	-96.129
1,5	238.208	149.734	-266.869	-50.641
1,6	196.083	143.006	-314.785	-92.766
2,3	219.631	152.552	-289.625	-69.218
2,4	176.511	143.878	-321.868	-112.338
2,5	245.786	152.603	-264.811	-43.063
2,6	218.104	145.718	-296.592	-70.745
3,4	214.293	146.567	-290.821	-74.556

3,5	192.78	149.948	-308.948	-96.069
3,6	216.923	151.52	-285.639	-71.926
4,5	199.701	153.852	-306.275	-89.148
4,6	191.262	149.307	-320.424	-97.587
5,6	227.21	149.327	-282.932	-61.639

Orientation	E	VDW	ELE	BE
1,2	220.893	158.237	-315.695	-11.972
1,3	217.272	158.757	-320.715	-15.593
1,4	208.162	156.86	-325.216	-24.703
1,5	215.668	158.347	-323.536	-17.197
1,6	220.446	159.197	-317.921	-12.419
2,3	216.392	155.999	-316.836	-16.473
2,4	216.815	157.74	-317.972	-16.05
2,5	220.689	160.256	-319.173	-12.176
2,6	218.117	158.186	-319.994	-14.748
3,4	208.736	154.276	-324.61	-24.129
3,5	206.203	150.341	-326.994	-26.662
3,6	215.115	158.134	-319.986	-17.75
4,5	220.508	156.611	-316.232	-12.357
4,6	209.277	155.958	-324.447	-23.588
5,6	210	154.521	-323.554	-22.865

Orientation	E	VDW	ELE	BE
1,2	233.603	139.593	-300.163	-54.246
1,3	215.045	136.516	-309.179	-72.804
1,4	223.744	139.179	-304.503	-64.105
1,5	219.741	137.897	-299.485	-68.108
1,6	227.387	139.951	-307.719	-60.462
2,3	221.372	137.649	-308.656	-66.477
2,4	229.98	140.642	-303.493	-57.869
2,5	229.452	140.267	-299.517	-58.397
2,6	231.709	140.853	-293.794	-56.14
3,4	230.833	139.174	-306.017	-57.016
3,5	235.722	135.576	-296.876	-52.127
3,6	207.967	142.239	-327.348	-79.882
4,5	236.66	139.434	-299.306	-51.189
4,6	224.659	138.464	-301.671	-63.19
5,6	248.638	139.497	-286.289	-39.211

Orientation	E	VDW	ELE	BE
1,2	199.273	147.958	-337.426	-18.482
1,3	201.274	147.521	-337.959	-16.481
1,4	196.324	147.218	-342.688	-21.431
1,5	198.579	143.129	-336.616	-19.176
1,6	204.567	148.9	-338.188	-13.188
2,3	197.846	144.014	-336.454	-19.909
2,4	202.765	145.392	-334.016	-14.99
2,5	198.999	145.543	-337.621	-18.756

2,6	195.919	148.743	-338.311	-21.836
3,4	199.849	145.072	-337.499	-17.906
3,5	195.612	142.312	-339.004	-22.143
3,6	200.025	145.914	-338.038	-17.73
4,5	203.027	149.004	-336.39	-14.728
4,6	201.027	145.765	-336.15	-16.728
5,6	200.68	145.407	-334.231	-17.075

VF19

Orientation	E	VDW	ELE	BE
1,2	63.563	107.783	-315.358	-14.304
1,3	62.625	104.151	-309.385	-15.242
1,4	65.619	106.548	-314.401	-12.248
1,5	53.261	101.854	-318.942	-24.606
1,6	61.221	106.548	-313.9	-16.646
2,3	63.593	106.291	-312.461	-14.274
2,4	55.08	107.843	-323.929	-22.787
2,5	41.769	103.823	-326.123	-36.098
2,6	41.443	104.553	-325.132	-36.424
3,4	48.038	104.676	-324.703	-29.829
3,5	55.576	104.392	-320.43	-22.291
3,6	55.866	103.951	-319.414	-22.001
4,5	51.676	111.805	-329.895	-26.191
4,6	54.131	105.619	-320.172	-23.736
5,6	59.625	104.968	-314.806	-18.242

Orientation	E	VDW	ELE	BE
1,2	99.681	106.824	-283.453	-10.102
1,3	60.679	110.348	-326.065	-49.104
1,4	85.583	107.615	-295.742	-24.2
1,5	80.583	102.03	-293.511	-29.2
1,6	83.636	112.314	-304.225	-26.147
2,3	83.862	106.778	-292.363	-25.921
2,4	81.217	104.17	-296.145	-28.566
2,5	83.505	105.822	-300.019	-26.278
2,6	65.327	107.436	-321.619	-44.456
3,4	71.013	107.599	-320.837	-38.77
3,5	70.014	100.834	-302.817	-39.769
3,6	84.724	106.323	-299.717	-25.059
4,5	83.344	102.739	-294.609	-26.439
4,6	82.997	103.948	-303.033	-26.786

5,6	85.683	107.896	-300.872	-24.1

Orientation	E	VDW	ELE	BE
1,2	219.831	150.913	-294.579	-69.043
1,3	236.712	147.22	-272.74	-52.162
1,4	254.875	144.517	-254.529	-33.999
1,5	219.209	142.573	-289.073	-69.665
1,6	220.567	147.125	-282.358	-68.307
2,3	216.512	143.686	-302.23	-72.362
2,4	165.572	139.823	-319.537	-123.302
2,5	234.518	148.998	-275.635	-54.356
2,6	237.848	140.954	-275.774	-51.026
3,4	295.453	137.919	-258.833	6.579
3,5	210.476	135.882	-289.467	-78.398
3,6	215.137	143.075	-298.084	-73.737
4,5	243.249	149.865	-279.655	-45.625
4,6	215.336	139.428	-297.555	-73.538
5,6	225.053	143.452	-290.787	-63.821

Orientation	E	VDW	ELE	BE
1,2	225.199	160.857	-312.417	-7.666
1,3	215.104	155.798	-319.678	-17.761
1,4	221.857	155.498	-311.606	-11.008
1,5	264.893	152.776	-317.146	32.028
1,6	263.279	156.758	-321.811	30.414
2,3	215.912	157.531	-321.78	-16.953
2,4	216.002	159.701	-321.458	-16.863
2,5	213.545	156.259	-323.263	-19.32
2,6	208.563	152.547	-326.22	-24.302
3,4	220.012	158.262	-316.645	-12.853
3,5	214.437	159.928	-323.14	-18.428
3,6	235.321	160.9	-302.811	2.456
4,5	217.686	159.14	-320.135	-15.179
4,6	219.814	157.353	-321.491	-13.051
5,6	218	159.292	-320.33	-14.865

Orientation	E	VDW	ELE	BE
1,2	239.051	136.305	-294.874	-48.798
1,3	215.617	135.547	-315.216	-72.232
1,4	236.67	130.501	-290.088	-51.179
1,5	218.266	135.178	-306.988	-69.583
1,6	222.36	136.919	-309.832	-65.489
2,3	229.497	134.356	-297.63	-58.352
2,4	234.625	135.724	-296.952	-53.224

2,5	233.642	135.655	-301.62	-54.207
2,6	225.4	132.366	-301.991	-62.449
3,4	231.066	133.012	-296.001	-56.783
3,5	226.109	136.106	-300.618	-61.74
3,6	249.442	141.804	-286.652	-38.407
4,5	227.772	140.29	-304.528	-60.077
4,6	222.329	135.892	-310.726	-65.52
5,6	229.032	136.334	-308.744	-58.817

Orientation	E	VDW	ELE	BE
1,2	196.406	149.033	-343.315	-21.349
1,3	181.398	143.055	-354.211	-36.357
1,4	249.921	147.632	-342.955	32.166
1,5	254.774	147.729	-345.035	37.019
1,6	221.219	140.68	-363.144	3.464
2,3	191.893	145.465	-347.102	-25.862
2,4	241.118	148.803	-347.596	23.363
2,5	196.455	144.123	-340.985	-21.3
2,6	254.801	154.907	-345.098	37.046
3,4	191.354	141.243	-345.82	-26.401
3,5	243.759	146.383	-345.389	26.004
3,6	184.939	142.599	-348.691	-32.816
4,5	195.274	149.115	-346.379	-22.481
4,6	247.67	150.631	-344.589	29.915
5,6	306.107	157.044	-340.97	88.352

VF20

Orientation	E	VDW	ELE	BE
1,2	64.26	103.686	-308.734	-13.607
1,3	37.711	104.564	-332.298	-40.156
1,4	31.422	104.147	-340.292	-46.445
1,5	50.59	105.431	-342.289	-27.277
1,6	48.458	102.572	-326.35	-29.409
2,3	41.536	97.911	-319.732	-36.331
2,4	41.654	96.017	-320.672	-36.213
2,5	38.252	96.894	-329.818	-39.615
2,6	50.774	99.725	-315.397	-27.093
3,4	48.058	100.622	-320.712	-29.809
3,5	61.61	101.868	-315.734	-16.257
3,6	41.794	101.123	-340.261	-36.073
4,5	56.259	105.837	-317.399	-21.608
4,6	50.977	101.985	-320.422	-26.89
5,6	55.919	102.674	-317.067	-21.948

Orientation	E	VDW	ELE	BE
1,2	74.994	109.706	-315.248	-34.789
1,3	58.551	98.371	-324.365	-51.232
1,4	53.958	99.136	-319.84	-55.825
1,5	77.898	98.117	-292.684	-31.885
1,6	78.717	99.585	-301.015	-31.066
2,3	56.69	104.176	-321.242	-53.093
2,4	49.818	102.009	-326.407	-59.965
2,5	66.012	104.159	-314.6	-43.771
2,6	80.849	102.733	-298.531	-28.934
3,4	65.501	95.056	-312.992	-44.282
3,5	73.423	104.292	-312.46	-36.36
3,6	68.529	103.611	-314.032	-41.254
4,5	79.468	106.157	-306.859	-30.315
4,6	74.196	101.176	-305.73	-35.587
5,6	66.337	101.842	-309.093	-43.446

Orientation	E	VDW	ELE	BE
1,2	242.181	143.419	-265.655	-46.693
1,3	165.431	130.229	-333.032	-123.443
1,4	181.515	141.675	-328.51	-107.359
1,5	236.313	139.408	-271.17	-52.561
1,6	180.684	143.446	-333.117	-108.19
2,3	248.398	138.29	-313.089	-40.476
2,4	224.672	150.519	-285.541	-64.202
2,5	233.981	156.245	-301.895	-54.893
2,6	206.406	131.454	-291.098	-82.468
3,4	239.606	139.169	-279.915	-49.268
3,5	237.682	141.395	-271.345	-51.192
3,6	254.08	137.502	-260.865	-34.794
4,5	230.865	145.497	-281.412	-58.009
4,6	215.21	131.794	-283.144	-73.664
5,6	243.353	154.661	-290.748	-45.521

Orientation	E	VDW	ELE	BE
1,2	219.111	157.487	-316.273	-13.754
1,3	211.509	153.602	-326.994	-21.356
1,4	212.296	154.458	-325.65	-20.569
1,5	214.609	155.801	-322.177	-18.256
1,6	215.606	155.84	-317.766	-17.259

2,3	212.829	157.753	-324.984	-20.036
2,4	215.349	155.703	-318.018	-17.516
2,5	207.907	151.038	-323.949	-24.958
2,6	215.142	156.081	-324.928	-17.723
3,4	211.8	153.673	-320.689	-21.065
3,5	213.241	153.57	-319.65	-19.624
3,6	211.278	153.839	-326.577	-21.587
4,5	214.676	157.517	-320.414	-18.189
4,6	217.086	154.487	-314.956	-15.779
5,6	212.823	154.591	-322.806	-20.042

Orientation	E	VDW	ELE	BE
1,2	232.428	140.641	-300.542	-55.421
1,3	217.48	134.607	-302.321	-70.369
1,4	205.184	136.018	-326.704	-82.665
1,5	222.339	132.257	-308.102	-65.51
1,6	226.59	139.172	-305.451	-61.259
2,3	207.21	138.752	-315.808	-80.639
2,4	224.623	140.231	-308.15	-63.226
2,5	232.693	134.69	-297.787	-55.156
2,6	218.201	136.542	-311.8	-69.648
3,4	207.692	135.047	-315.706	-80.157
3,5	222.056	135.852	-309.137	-65.793
3,6	213.609	131.975	-311.881	-74.24
4,5	220.914	138.588	-309.996	-66.935
4,6	218.271	137.449	-311.637	-69.578
5,6	224.72	134.609	-302.237	-63.129

Orientation	E	VDW	ELE	BE
1,2	203.371	148.262	-334.401	-14.384
1,3	195.761	141.952	-337.659	-21.994
1,4	185.876	142.095	-346.622	-31.879
1,5	187.38	141.986	-345.261	-30.375
1,6	195.872	146.693	-339.308	-21.883
2,3	197.02	144.742	-335.884	-20.735
2,4	200.607	146.239	-336.24	-17.148
2,5	199.967	146.783	-336.344	-17.788
2,6	196.357	142.727	-336.636	-21.398
3,4	192.577	143.531	-340.818	-25.178
3,5	189.435	142.27	-345.177	-28.32
3,6	192.546	145.751	-340.641	-25.209
4,5	197.637	146.735	-341.587	-20.118

4,6	198.455	145.142	-337.839	-19.3
5,6	201.178	144.558	-334.991	-16.577

FF

Orientation	E	VDW	ELE	BE
1,2	57.767	106.035	-316.714	-20.1
1,3	48.38	100.754	-324.166	-29.487
1,4	63.3	103.334	-311.132	-14.567
1,5	55.689	102.99	-315.133	-22.178
1,6	50.64	103.972	-325.24	-27.227
2,3	54.961	98.544	-311.445	-22.906
2,4	60.703	104.11	-314.251	-17.164
2,5	43.023	106.541	-332.277	-34.844
2,6	51.168	101.876	-315.541	-26.699
3,4	38.242	99.911	-330.545	-39.625
3,5	52.552	103.975	-319.771	-25.315
3,6	46.138	107.133	-327.07	-31.729
4,5	46.39	104.719	-326.694	-31.477
4,6	62.846	106.058	-314.091	-15.021
5,6	46.766	106.128	-329.24	-31.101

Orientation	E	VDW	ELE	BE
1,2	97.156	107.284	-287.544	-12.627
1,3	77.379	96.376	-295.618	-32.404
1,4	88.48	102.947	-290.168	-21.303
1,5	69.95	99.877	-307.515	-39.833
1,6	65.738	106.461	-317.579	-44.045
2,3	70.18	104.492	-320.11	-39.603
2,4	80.872	105.184	-301.69	-28.911
2,5	85.334	106.277	-295.763	-24.449
2,6	58.099	99.35	-317.75	-51.684
3,4	64.82	105.991	-320.934	-44.963
3,5	72.984	104.445	-304.626	-36.799
3,6	84.564	103.427	-296.573	-25.219
4,5	79.438	105.95	-310.469	-30.345
4,6	66.444	105.342	-321.855	-43.339
5,6	72.506	103.068	-306.273	-37.277

Orientation	E	VDW	ELE	BE
1,2	275.304	154.887	-246.656	-13.57
1,3	261.53	152.815	-252.111	-27.344
1,4	281.321	149.519	-236.94	-7.553
1,5	228.847	145.793	-282.36	-60.027
1,6	231.986	153.678	-282.299	-56.888
2,3	191.248	139.287	-312.228	-97.626
2,4	229.56	155.97	-278.972	-59.314
2,5	248.555	154.449	-264.856	-40.319
2,6	221.859	146.799	-279.475	-67.015
3,4	231.623	147.491	-273.164	-57.251
3,5	211.131	145.344	-297.885	-77.743
3,6	221.164	144.395	-280.248	-67.71
4,5	225.513	153.266	-283.064	-63.361
4,6	235.815	148.926	-273.236	-53.059
5,6	249.028	147.919	-268.445	-39.846

Orientation	E	VDW	ELE	BE
1,2	200.129	152.709	-331.599	-32.736
1,3	195.683	148.065	-342.306	-37.182
1,4	188.877	137.616	-342.523	-43.988
1,5	200.289	145.916	-333.442	-32.576
1,6	251.734	141.661	-320.464	18.869
2,3	196.304	146.088	-340.443	-36.561
2,4	196.445	146.223	-339.297	-36.42
2,5	192.862	148.593	-344.139	-40.003
2,6	176.7	143.883	-356.098	-56.165
3,4	192.46	147.731	-338.643	-40.405
3,5	217.938	149.989	-318.44	-14.927
3,6	193.702	148.628	-348.113	-39.163
4,5	185.735	149.668	-348.868	-47.13
4,6	190.513	148.743	-338.76	-42.352
5,6	203.223	144.581	-324.808	-29.642

Orientation	E	VDW	ELE	BE
1,2	232.655	142.141	-298.66	-55.194
1,3	238.251	136.856	-289.937	-49.598
1,4	239.008	140.368	-297.236	-48.841
1,5	227.435	141.111	-307.916	-60.414
1,6	226.66	142.08	-307.655	-61.189
2,3	239.758	137.948	-291.553	-48.091
2,4	238.861	144.245	-301.889	-48.988

2,5	245.987	140.535	-290.86	-41.862
2,6	238.334	136.519	-293.066	-49.515
3,4	235.785	139.641	-295.63	-52.064
3,5	226.493	140.366	-301.152	-61.356
3,6	236.595	137.49	-296.578	-51.254
4,5	231.89	142.008	-301.561	-55.959
4,6	240.998	137.868	-293.101	-46.851
5,6	235.418	142.669	-301.326	-52.431

Orientation	E	VDW	ELE	BE
1,2	210.603	150.697	-330.956	-7.152
1,3	209.73	148.765	-328.661	-8.025
1,4	201.091	146.597	-337.924	-16.664
1,5	198.593	144.197	-338.23	-19.162
1,6	208.637	149.402	-330.83	-9.118
2,3	206.197	147.467	-331.93	-11.558
2,4	195.734	145.519	-339.746	-22.021
2,5	201.097	147.832	-335.655	-16.658
2,6	195.535	145.467	-339.746	-22.22
3,4	201.702	146.68	-336.555	-16.053
3,5	203.262	145.361	-334.66	-14.493
3,6	203.359	149.13	-337.412	-14.396
4,5	211.903	150.357	-329.414	-5.852
4,6	205.803	148.586	-333.328	-11.952
5,6	209.872	148.303	-330.026	-7.883

INTERACTIONS IN GAS PHASE

Legend of Amino Acids for $A\beta_{42:}$

$$D_1A_2G_3F_4R_5H_6D_7S_8G_9Y_{10}E_{11}V_{12}H_{13}H_{14}Q_{15}K_{16}L_{17}V_{18}F_{19}F_{20}-$$

$$-A_{21}E_{22}D_{23}V_{24}G_{25}S_{26}N_{27}K_{28}G_{29}A_{30}I_{31}I_{32}G_{33}L_{34}M_{35}V_{36}G_{37}G_{38}V_{39}V_{40}I_{41}A_{42}$$

HH

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	14	CC4	1/5
1AMB	AH	14	CA4	2/3
1AMB	14=SCD	14	6	2/6
1AMB	22=SCA	22	5	2/6
1AMB	AH	17	A-ring	3/4
1AMC	AH	10	2	2/3
1AMC	AH	14	Ca1	2/3
1AML	6=SCA	His 13	6	4/6
1AML	AH	Ile 31	A-ring	5/6
1BA4	6=SCA	His 14	6	1/6
1BA4	6=SCA	His 14	6	2/3
1BA4	2=BBD	Glu 11	2	3/4
1IYT	AA	His 13	B-ring	1/4
1IYT	AH	His 13	CC1	3/4

1IYT	6=SCA	His 14	6	4/6
1Z0Q	BBA(14)	His 14	1	1/4

H13K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AA	His 13	B-ring	3/5
1AMC	16=SCD	Lys 16	6	1/6
1AMC	16=SCD	Lys 16	5	2/5
1AMC	16=SCD	Lys 16	6	2/6
1AMC	AA	His 13	B-ring	3/4
1AMC	AA	His 13	B-ring	3/5
1AMC	16=SCD	Lys 16	6	4/6
1AMC	16=SCD	Lys 16	6	5/6
1AML	16=SCD	Lys 16	4	1/3
1AML	AH	Lys 16	A-ring	3/5
1AML	AA	His 13	B-ring	3/6
1AML	AH	Lys 16	A-ring	4/6
1AML	AH	Lys 16	A-ring	5/6
1BA4	10=BBA	Tyr 10	Cc5	1/6
1BA4	13=BBA	His 13	2	2/4
1BA4	AA	Tyr 10	B-ring	3/5

1BA4	AH	Tyr 10	A-ring	4/5
1IYT	--	--	--	--
1Z0Q	16=SCD	Lys 16	6	1/3
1Z0Q	16=SCD	Lys 16	6	1/6
1Z0Q	16=SCD	Lys 16	6	2/6

H14K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	13=BBA	His 13	1	1/2
1AMB	13=SCD	His 13	6	1/4
1AMB	AH	His 13	Cc1	2/3
1AMB	AA	His 13	B-ring	2/4
1AMB	AA	His 13	B-ring	2/5
1AMB	AH	His 13	Cc5	2/6
1AMB	AH	His 14	B-ring	2/6
1AMB	AA	His 13	A-ring	3/4
1AMB	13=SCD	His 6	6	3/6
1AMB	AA	His 13	A-ring	4/5
1AMC	AA	His 13	B-ring	1/2
1AMC	AA	His 13	A-ring	1/4
1AMC	AH	Leu 17	A-ring	1/4
1AMC	AH	His 13	Cc4	1/5

1AMC	A+	His 13	B-ring	1/6
1AMC	13=SCD	His 13	6	2/3
1AMC	AH	His 14	B-ring	3/4
1AMC	AH	Tyr 10	Cc1	3/5
1AMC	AH	His 13	Cc4	3/5
1AMC	13=BBA	His 13	6	3/6
1AMC	17=BBD	Leu 17	6	3/6
1AMC	AH	His 14	A-ring	3/6
1AMC	13=BBA	His 13	5	4/5
1AMC	AA	His 13	5	4/5
1AML	AA	His 13	B-ring	1/2
1AML	13=BBA	His 13	3	1/3
1AML	AA	His 13	A-ring	1/5
1AML	AH	His 13	B-ring	2/4
1AML	13=BBA	His 13	5	3/5
1AML	AA	His 13	A-ring	4/5
1BA4	13=BBA	His 13	1	1/2
1BA4	AH	Leu 17	B-ring	1/3
1BA4	12=BBA	Val 12	6	1/3
1IYT	AA	Phe 19	A-ring	1/4
1IYT	11=SCA	Glu 11	2	2/3
1IYT	11=SCA	Glu 11	1	2/3
1IYT	11=SCA	Glu 11	2	2/6

1IYT	15=SCA	Gln 15	4	4/6
1Z0Q	14=BBA	His 14	1	1/2
1Z0Q	AH	His 14	B-ring	1/4
1Z0Q	13=BBA	His 13	6	1/6
1Z0Q	AH	His 14	A-ring	5/6

LV

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	22=SCA	Glu 22	6	1/3
1AMB	22=SCA	Glu 22	5	1/6
1AMB	22=SCA	Glu 22	5	2/6
1AMB	22=SCA	Glu 22	4	3/4
1AMB	22=SCA	Glu 22	5	4/5
1AMC	14=SCD	His 14	6	1/5
1AMC	AH	Leu 17	B-ring	2/6
1AML	14=SCD	His 14	6	1/5
1AML	AH	Val 18	B-ring	2/5
1AML	AH	Val 18	B-ring	2/6
1AML	AH	Leu 17	A-ring	4/6
1BA4	AH	Val 18	A-ring	3/5
1IYT	--	--	--	--
1Z0Q	22=SCA	Glu 22	4	2/4

LF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	16=SCD	Lys 16	6	1/4
1AMB	16=BBD/BBA	Lys 16	6	1/6
1AMB	AA	Phe 20	B-ring	2/5
1AMB	AA	Phe 20	B-ring	2/6
1AMB	16=BBA	Lys 16	4	4/5
1AMB	16=BBA	Lys 16	5	5/6
1AMB	16=SCD	Lys 16	6	5/6
1AMC	AH	Phe 19	CA1	1/3
1AMC	16=BBA	Lys 16	2	1/5
1AMC	16=SCD	Lys 16	2	2/3
1AMC	16=BBA	Lys 16	2	2/5
1AMC	16=BBA	Lys 16	6	3/4
1AMC	19=BBA	Phe 19	5	4/6
1AMC	16=BBA	Lys 16	5	5/6
1AMC	23=SCA	Asp 23	2	5/6
1AML	AA	Phe 20	B-ring	3/4
1AML	AH	Phe 19	6	3/6
1AML	AH	Phe 20	A-ring	4/5
1BA4	14=SCD	His 14	6	1/2
1BA4	14=BBA	His 14	2	1/4

1BA4	14=BBA	His 14	2	1/5
1BA4	22=SCA	Glu 22	6	1/6
1BA4	22=SCA	Glu 22	6	2/3
1BA4	22=SCA	Glu 22	4	2/5
1BA4	15=SCA	Gln 15	2	4/5
1IYT	AA	Phe 20	B-ring	1/3
1IYT	A+	Lys 16	B-ring	1/4
1IYT	A+	Lys 16	B-ring	2/3
1IYT	AH	Phe 20	A-ring	2/4
1IYT	AH	Phe 20	CB1	2/6
1IYT	26=SCD	Ser 26	6	3/4
1IYT	16=SCD	Lys 16	6	3/5
1IYT	AH	Phe 20	CA1	3/5
1IYT	AH	Phe 20	AH	3/6
1Z0Q	AH	Phe 20	CC4	1/5

LF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	A+	Lys 16	A-ring	3/4
1AMC	16=SCD	Lys 16	6	3/5
1AML	AH	His 13	4	5/6
1BA4	AA	Phe 20	A-ring	4/6
1IYT	--	--	--	--
1Z0Q	AH	Phe 20	CA1	1/4
1Z0Q	AH	Phe 20	CC4	1/5
1Z0Q	AH	Phe 20	CA1	2/3
1Z0Q	16=BBA	Lys 16	1	2/3
1Z0Q	AH	Phe 20	CC4	2/5
1Z0Q	16=BBA	Lys 16	2	2/6

VF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	22=SCA	Glu 22	1	1/5
1AMC	22=SCA	Glu 22	2	2/5
1AMC	22=SCA	Glu 22	1	2/6
1AMC	22=SCA	Glu 22	6	3/4
1AMC	AA	Phe 19	A-ring	3/5
1AMC	22=SCA	Glu 22	4	4/5
1AMC	22=SCA	Glu 22	4	5/6
1AML	22=SCA	Glu 22	2	2/3
1AML	1=SCA	Asp 1	5	2/3
1AML	15=SCA	Gln 15	2	2/4
1AML	16=SCA	Lys 16	4	2/4
1AML	1=SCA	Asp 1	5	2/4
1AML	22=SCA	Glu 22	1	2/4
1AML	15=SCA	Gln 15	1	2/5
1AML	22=SCA	Glu 22	6	3/5
1AML	22=SCA	Glu 22	CC1	3/6
1AML	22=SCA	Glu 22	4	4/5
1AML	22=SCA	Glu 22	4	4/6
1AML	2=BBA	Ala 2	2	4/6
1AML	22=SCA	Glu 22	5	5/6

1BA4	22=SCA	Glu 22	6	3/5
1BA4	15=SCD	Gln 15	6	4/6
1BA4	22=SCA	Glu 22	4	5/6
1IYT	AH	Phe 19	5	1/5
1IYT	AH	Phe 19	CA1	2/3
1IYT	22=SCA	Glu 22	5	3/5
1Z0Q	22=SCA	Glu 22	4	4/6
1Z0Q	22=SCA	Glu 22	4	5/6

VF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	22=SCA	22	2	2/5
1AMB	22=SCA	22	5	3/6
1AMC	22=SCA	22	2	2/4
1AMC	AH	17	A-ring	3/4
1AMC	22=SCA	22	2	3/4
1AML	25=BBA	25	5	1/5
1AML	20=BBA	20	6	1/6
1AML	25=BBA	25	5	2/4
1AML	27=BBA	27	6	2/4
1AML	21=BBA	21	6	2/5
1AML	AH	18	B-ring	2/6

1AML	27=SCA	27	4	2/6
1AML	28=BBA	28	4	¾
1AML	17=BBA	17	6	3/6
1AML	25=BBA	25	5	3/6
1AML	AH	32	A-ring	3/6
1AML	27=BBD	27	6	5/6
1BA4	17=BBA	17	4	4/5
1IYT**	17			
1Z0Q	24=BBA	24	2	1/4
1Z0Q	AH	20	CA1	2/3
1Z0Q	AH	17	A-ring	3/4
1Z0Q	24=BBA	24	4	3/5

FF

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	16=BBA	16	6	1/5
1AMC	AH	19	B-ring	2/6
1AML	--	--	--	--
1BA4	SCA	11	2	1/4
1BA4	SCA	22	2	1/5
1BA4	SCD	16	6	1/6

1BA4	BBA	2	5	1/6
1BA4	SCA	23	4	2/4
1BA4	BBA	19	4	2/5
1BA4	SCD	16	6	2/6
1BA4	SCA	23	4	3/4
1BA4	SCA	23	5	3/5
1BA4	SCA	3	4	3/5
1BA4	SCD	16	4	3/5
1BA4	SCD	16	3	3/6
1BA4	SCA	11	4	4/5
1BA4	AH	19	4	4/6
1IYT	SCD	16	6	1/5
1IYT	AH	20	B-ring	2/3
1IYT	A+	16	A-ring	3/6
1IYT	AH	20	A-ring	4/6
1Z0Q	--	--	--	--

APPENDIX B: (-)-EPICATECHIN DATA

Tables of energies for gas phase calculations of (+)-epicatechin. All energies are in kcal/mol. The order of the tables for each pair of amino acids is always 1AMB, 1AMC, 1AML, 1BA4, 1IYT, 1Z0Q.

HH

Orientation	E	VDW	ELE	Binding Energy (BE)
1,2	57.969	102.93	-306.204	-17.031
1,3	40.713	106.369	-332.087	-34.287
1,4	35.275	100.966	-328.942	-39.725
1,5	36.882	93.933	-324.211	-38.118
1,6	48.058	99.286	-318.362	-26.942
2,3	47.299	103.289	-321.743	-27.701
2,4	55.739	105	-313.056	-19.261
2,5	46.216	97.326	-316.731	-28.784
2,6	31.995	102.63	-334.356	-43.005
3,4	48.737	102.402	-318.53	-26.263
3,5	47.941	103.11	-320.249	-27.059
3,6	43.338	99.451	-322.876	-31.662
4,5	60.456	106.823	-310.551	-14.544
4,6	25.229	93.416	-336.53	-49.771
5,6	36.161	98.623	-323.303	-38.839

Orientation	E	VDW	ELE	BE
1,2	88.176	108.164	-291.122	-18.74
1,3	68.031	96.695	-306.959	-38.885
1,4	75.693	107.706	-305.537	-31.223
1,5	79.296	104.875	-296.378	-27.62
1,6	68.37	103.988	-310.834	-38.546
2,3	66.468	94.419	-305.137	-40.448
2,4	65.509	103.706	-312.411	-41.407
2,5	76.06	98.747	-300.076	-30.856
2,6	71.305	98.59	-301.177	-35.611
3,4	54.132	99.287	-317.238	-52.784
3,5	54.622	98.712	-315.236	-52.294
3,6	66.456	95.86	-298.127	-40.46
4,5	90.574	103.519	-282.632	-16.342
4,6	80.54	105.041	-296.97	-26.376
5,6	76.562	106.049	-304.876	-30.354

Orientation	E	VDW	ELE	BE
1,2	220.354	150.261	-282.913	-65.653
1,3	246.241	144.654	-258.092	-39.766
1,4	267.267	151.653	-247.303	-18.74
1,5	226.917	138.472	-275.466	-59.09
1,6	228.783	148.921	-273.065	-57.224
2,3	213.888	140.903	-292.953	-72.119
2,4	224.814	146.596	-281.227	-61.193
2,5	255.52	149.026	-249.59	-30.487
2,6	208.196	147.574	-292.456	-77.811
3,4	220.702	146.461	-275.594	-65.305
3,5	203.514	143.495	-284.825	-82.493
3,6	218.902	141.87	-286.175	-67.105
4,5	244.174	153.13	-260.518	-41.833
4,6	254.509	145.626	-250.174	-31.498
5,6	215.971	150.614	-280.843	-70.036

Orientation	E	VDW	ELE	BE
1,2	209.145	157.513	-319.586	-20.853
1,3	211.218	159.779	-322.399	-18.78
1,4	217.425	161.54	-317.117	-12.573
1,5	208.93	157.645	-321.934	-21.068
1,6	218.684	161.469	-317.299	-11.314
2,3	206.218	159.721	-327.47	-23.78
2,4	209.201	158.195	-322.841	-20.797
2,5	213.914	158.306	-319.55	-16.084
2,6	216.261	160.26	-315.932	-13.737
3,4	214.221	161.219	-318.485	-15.777
3,5	214.898	157.576	-316.114	-15.1
3,6	211.321	158.882	-323.485	-18.677
4,5	227.789	160.24	-304.845	-2.209
4,6	217.563	161.213	-317.311	-12.435
5,6	219.645	160.946	-313.828	-10.353

Orientation	E	VDW	ELE	BE
1,2	217.648	141.99	-311.766	-34.994
1,3	224.195	141.669	-303.708	-28.447
1,4	237.773	141.649	-294.388	-14.869
1,5	230.501	139.374	-305.919	-22.141
1,6	236.236	140.151	-296.048	-16.406
2,3	230.786	138.835	-301.692	-21.856
2,4	229.673	138.673	-298.429	-22.969

2,5	222.508	139.756	-308.234	-30.134
2,6	217.627	141.502	-310.398	-35.015
3,4	230.946	136.666	-296.062	-21.696
3,5	219.037	137.469	-310.266	-33.605
3,6	209.56	136.391	-316.286	-43.082
4,5	225.638	142.843	-306.522	-27.004
4,6	229.592	136.474	-301.584	-23.05
5,6	230.603	139.242	-300.551	-22.039

Orientation	E	VDW	ELE	BE
1,2				
1,3	185.291	140.729	-342.21	-29.597
1,4	189.912	147.332	-344.569	-24.976
1,5	194.952	146.105	-337.096	-19.936
1,6	196.346	147.297	-336.338	-18.542
2,3	184.77	144.181	-347.117	-30.118
2,4	192.094	148.563	-343.006	-22.794
2,5	184.937	141.152	-344.385	-29.951
2,6	193.986	147.854	-343.181	-20.902
3,4	194.104	144.104	-338.088	-20.784
3,5	187.311	143.335	-342.535	-27.577
3,6				
4,5	205.767	150.679	-330.135	-9.121
4,6	186.32	149.041	-347.953	-28.568
5,6	183.02	141.638	-347.009	-31.868

H13K

Orientation	E	VDW	ELE	BE
1,2	52.262	105.496	-315.081	-22.738
1,3	45.324	101.823	-319.34	-29.676
1,4	60.838	110.674	-311.905	-14.162
1,5	58.309	105.45	-312.862	-16.691
1,6	61.693	107.175	-309.181	-13.307
2,3	53.086	107.308	-315.971	-21.914
2,4	60.55	107.685	-310.316	-14.45
2,5	60.601	106.119	-309.003	-14.399
2,6	60.972	105.997	-307.755	-14.028
3,4	59.4	105.268	-310.526	-15.6
3,5	46.185	105.749	-320.474	-28.815
3,6	53.412	101.883	-313.204	-21.588
4,5	67.473	108.525	-304.758	-7.527
4,6	62.791	110.553	-310.195	-12.209

5,6	46.429	99.194	-312.528	-28.571

Orientation	E	VDW	ELE	BE
1,2	82.558	110.929	-298.429	-24.358
1,3	81.357	106.61	-294.608	-25.559
1,4	81.047	108.687	-299.288	-25.869
1,5	92.293	107.894	-285.826	-14.623
1,6	88.821	104.379	-311.608	-18.095
2,3	83.378	106.979	-291.788	-23.538
2,4	85.161	106.302	-291.491	-21.755
2,5	69.708	107.5	-304.737	-37.208
2,6	86.941	109.298	-292.304	-19.975
3,4	76.831	103.701	-297.36	-30.085
3,5	78.968	104.518	-295.687	-27.948
3,6	75.239	103.598	-298.591	-31.677
4,5	83.066	109.579	-292.581	-23.85
4,6	90.415	109.692	-288.522	-16.501
5,6	86.103	105.931	-292.113	-20.813

Orientation	E	VDW	ELE	BE
1,2	243.62	158.706	-270.196	-42.387
1,3	209.702	150.58	-291.05	-76.305
1,4	248.235	154.94	-265.211	-37.772
1,5	267.541	154.324	-247.098	-18.466
1,6	266.862	153.361	-248.803	-19.145
2,3	233.369	154.319	-275.307	-52.638
2,4	190.205	153.184	-315.01	-95.802
2,5	198.481	146.981	-308.397	-87.526
2,6	235.64	152.541	-263.373	-50.367
3,4	225.131	154.479	-277.757	-60.876
3,5	216.52	157.636	-290.09	-69.487
3,6	245.48	147.099	-258.494	-40.527
4,5	248.456	159.468	-262.406	-37.551
4,6	259.089	151.699	-253.322	-26.918
5,6	258.009	143.328	-330.429	-27.998

Orientation	E	VDW	ELE	BE
1,2	207.802	156.316	-320.29	-22.196
1,3	204.626	150.453	-324.347	-25.372
1,4	204.516	148.639	-321.488	-25.482
1,5	198.349	145.689	-331.412	-31.649
1,6	193.858	150.957	-330.546	-36.14
2,3	189.686	150.602	-340.841	-40.312
2,4	192.698	149.776	-332.02	-37.3
2,5	200.906	149.339	-323.263	-29.092

2,6	186.504	148.466	-338.531	-43.494
3,4	206.569	154.957	-326.525	-23.429
3,5	205.529	147.631	-325.865	-24.469
3,6	211.486	153.517	-336.805	-18.512
4,5	210.828	154.488	-316.601	-19.17
4,6	208.896	153.404	-322.098	-21.102
5,6	202.962	152.24	-327.506	-27.036

Orientation	E	VDW	ELE	BE
1,2	226.135	138.348	-303.089	-26.507
1,3	224.51	142.916	-307.856	-28.132
1,4	221.163	139.432	-304.554	-31.479
1,5	221.539	138.815	-305.928	-31.103
1,6	223.87	137.016	-305.254	-28.772
2,3	232.827	139.089	-296.18	-19.815
2,4	221.411	143.292	-305.734	-31.231
2,5	227.749	142.415	-305.162	-24.893
2,6	226.385	141.803	-298.736	-26.257
3,4	215.958	139.223	-308.506	-36.684
3,5	229.11	137.749	-294.136	-23.532
3,6	209.846	141.446	-324.156	-42.796
4,5	231.491	142.95	-300.598	-21.151
4,6	220.452	139.475	-310.609	-32.19
5,6	216.18	135.715	-309.791	-36.462

Orientation	E	VDW	ELE	BE
1,2	195.495	152.057	-342.995	-19.393
1,3	198.413	149.082	-335.712	-16.475
1,4	198.4	150.098	-337.566	-16.488
1,5	191.477	148.623	-341.947	-23.411
1,6	204.586	149.666	-333.372	-10.302
2,3	197.581	149.337	-338.284	-17.307
2,4	200.288	151.411	-336.506	-14.6
2,5	197.689	150.306	-339.4	-17.199
2,6	193.851	148.588	-342.2	-21.037
3,4	198.692	149.549	-335.065	-16.196
3,5	199.438	143.661	-332.509	-15.45
3,6	189.389	148.73	-343.909	-25.499
4,5	204.24	148.776	-331.892	-10.648
4,6	200.624	149.742	-336.53	-14.264
5,6	198.522	149.775	-336.408	-16.366

H14K

Orientation	E	VDW	ELE	BE
1,2	65.447	107.174	-311.276	-9.553
1,3	48.774	107.535	-319.502	-26.226
1,4	49.01	103.521	-321.267	-25.99
1,5	58.971	101.038	-319.052	-16.029
1,6	61.205	98.833	-314.119	-13.795
2,3	61.768	106.904	-316.293	-13.232
2,4	55.34	104.141	-315.14	-19.66
2,5	64.918	102.582	-314.177	-10.082
2,6	58.093	109.643	-320.558	-16.907
3,4	54.085	101.181	-315.609	-20.915
3,5	66.993	106.921	-311.672	-8.007
3,6	55.972	103.67	-317.329	-19.028
4,5	62.568	103.266	-305.601	-12.432
4,6	53.449	99.114	-315.067	-21.551
5,6	204.989	110.444	-314.204	129.989

Orientation	E	VDW	ELE	BE
1,2	72.026	98.945	-300.224	-34.89
1,3	70.98	102.557	-302.315	-35.936
1,4	63.979	105.517	-315.513	-42.937
1,5	47.852	104.809	-326.563	-59.064
1,6	72.917	101.866	-304.992	-33.999
2,3	95.047	103.973	-288.14	-11.869
2,4	66.055	98.472	-296.572	-40.861
2,5	70.79	105.554	-310.058	-36.126
2,6	60.559	101.012	-312.907	-46.357
3,4	57.842	104.29	-326.083	-49.074
3,5	62.777	98.468	-304.812	-44.139
3,6	52.058	113.091	-328.032	-54.858
4,5	78.481	101.63	-295.187	-28.435
4,6	83.26	103.355	-302.13	-23.656
5,6	73.631	104.248	-312.148	-33.285

Orientation	E	VDW	ELE	BE
1,2	237.286	152.213	-264.212	-48.721
1,3	190.779	137.822	-303.58	-95.228
1,4	230.188	150.738	-277.249	-55.819
1,5	245.011	145.402	-261.03	-40.996
1,6	242.41	152.675	-264.994	-43.597

2,3	196.946	147.178	-304.368	-89.061
2,4	222.282	146.185	-277.403	-63.725
2,5	230.829	145.2	-272.084	-55.178
2,6	242.243	146.865	-256.919	-43.764
3,4	220.715	145.622	-279.925	-65.292
3,5	191.326	136.979	-313.697	-94.681
3,6	214.22	135.798	-289.714	-71.787
4,5	198.4	137.92	-291.218	-87.607
4,6	192.222	147.427	-315.47	-93.785
5,6	242.668	145.812	-258.326	-43.339

Orientation	E	VDW	ELE	BE
1,2	206.429	152.14	-317.02	-23.569
1,3	202.922	147.029	-321.034	-27.076
1,4	202.493	157.24	-327.719	-27.505
1,5	201.659	149.492	-321.701	-28.339
1,6	186.666	148.959	-334.528	-43.332
2,3	271.196	156.557	-328.714	41.198
2,4	209.014	156.128	-321.339	-20.984
2,5	206.264	154.229	-321.685	-23.734
2,6	197.358	152.796	-332.295	-32.64
3,4	189.919	151.966	-333.661	-40.079
3,5	195.116	149.493	-320.766	-34.882
3,6	193.994	150.413	-332.417	-36.004
4,5	210.214	155.179	-319.589	-19.784
4,6	205.786	162.302	-325.466	-24.212
5,6	195.841	155.864	-335.709	-34.157

Orientation	E	VDW	ELE	BE
1,2	236.613	137.569	-294.619	-16.029
1,3	213.492	133.391	-309.008	-39.15
1,4	207.749	137.766	-322.761	-44.893
1,5	217.381	130.404	-303.246	-35.261
1,6	218.587	138.707	-311.936	-34.055
2,3	239.946	142.4	-302.414	-12.696
2,4	213.028	136.343	-312.639	-39.614
2,5	209.359	140.32	-317.822	-43.283
2,6	214.721	139.087	-306.87	-37.921
3,4	223.579	134.082	-303.945	-29.063
3,5	n/a			
3,6	n/a			
4,5	242.387	136.979	-285.719	-10.255
4,6	246.261	129.863	-317.645	-6.381

5,6	212.824	133.464	-311.963	-39.818

Orientation	E	VDW	ELE	BE
1,2	194.942	145.703	-338.403	-19.946
1,3	190.774	142.932	-338.736	-24.114
1,4	187.049	142.258	-344.295	-27.839
1,5	336.758	154.965	-330.051	121.87
1,6	192.246	146.099	-339.665	-22.642
2,3	188.849	147.614	-343.436	-26.039
2,4	188.789	145.561	-342.301	-26.099
2,5	193.668	144.301	-335.476	-21.22
2,6	189.851	147.538	-345.854	-25.037
3,4	183.729	141.812	-343.984	-31.159
3,5	195.292	145.134	-339.075	-19.596
3,6	190.488	144.604	-341.797	-24.4
4,5	196.263	146.283	-338.006	-18.625
4,6	186.759	142.047	-344.958	-28.129
5,6	195.66	145.111	-337.253	-19.228

LV

Orientation	E	VDW	ELE	BE
1,2	59.996	109.406	-312.139	-15.004
1,3	46.569	104.077	-326.298	-28.431
1,4	40.58	102.921	-328.21	-34.42
1,5	46.075	103.73	-321.686	-28.925
1,6	47.769	105.691	-323.067	-27.231
2,3	33.796	103.711	-334.997	-41.204
2,4	46.902	100.293	-317.668	-28.098
2,5	38.357	94.841	-321.623	-36.643
2,6	43.444	104.459	-325.033	-31.556
3,4	54.112	105.066	-316.242	-20.888
3,5	42.675	99.061	-319.593	-32.325
3,6	52.443	100.869	-320.527	-22.557
4,5	55.422	96.143	-302.671	-19.578
4,6	54.619	101.904	-312.967	-20.381
5,6	42.637	101.919	-326.607	-32.363

Orientation	E	VDW	ELE	BE
1,2	71.979	109.109	-303.446	-34.937

1,3	64.284	105.943	-312.421	-42.632
1,4	68.294	107.811	-316.836	-38.622
1,5	72.178	102.341	-301.266	-34.738
1,6	79.685	103.459	-293.68	-27.231
2,3	85.38	105.728	-294.098	-21.536
2,4	66.775	106.146	-320.088	-40.141
2,5	56.687	104.353	-322.936	-50.229
2,6	64.203	108.499	-318.63	-42.713
3,4	64.683	108.328	-324.612	-42.233
3,5	71.415	98.351	-301.659	-35.501
3,6	59.652	94.23	-309.044	-47.264
4,5	92.81	106.832	-284.509	-14.106
4,6	67.241	106.16	-308.266	-39.675
5,6	86.711	105.629	-289.672	-20.205

Orientation	E	VDW	ELE	BE
1,2	253.457	148.567	-254.585	-32.55
1,3	234.4	145.536	-271.182	-51.607
1,4	171.617	150.014	-331.138	-114.39
1,5	249.295	144.738	-257.191	-36.712
1,6	238.448	146.869	-266.864	-47.559
2,3	209.521	138.311	-293.01	-76.486
2,4	210.265	144.631	-284.721	-75.742
2,5	188.458	143.104	-321.711	-97.549
2,6	260.282	148.759	-252.315	-25.725
3,4	237.184	140.459	-259.386	-48.823
3,5	211.475	141.01	-298.269	-74.532
3,6	221.676	138.401	-267.443	-64.331
4,5	255.401	149.697	-256.308	-30.606
4,6	249.426	148.854	-261.649	-36.581
5,6	244.482	150.31	-263.578	-41.525

Orientation	E	VDW	ELE	BE
1,2	224.925	162.275	-310.535	-5.073
1,3	214.027	158.477	-316.007	-15.971
1,4	209.872	156.952	-323.43	-20.126
1,5	214.325	158.244	-317.255	-15.673
1,6	211.775	160.089	-320.788	-18.223
2,3	214.953	161.534	-321.256	-15.045
2,4	212.928	160.569	-322.107	-17.07
2,5	206.418	157.602	-324.446	-23.58
2,6	214.775	157.83	-317.588	-15.223
3,4	216.739	158.612	-313.874	-13.259
3,5	206.614	154.406	-321.146	-23.384

3,6	212.69	157.719	-320.458	-17.308
4,5	218.627	160.3	-311.72	-11.371
4,6	210.026	159.915	-322.634	-19.972
5,6	215.221	160.968	-320.027	-14.777

Orientation	E	VDW	ELE	BE
1,2	224.602	145.838	-309.378	-30.907
1,3	213.675	139.747	-320.103	-41.834
1,4	210.951	139.192	-319.547	-44.558
1,5	218.601	138.837	-307.637	-36.908
1,6	235.142	140.89	-297.527	-20.367
2,3	206.884	137.762	-323.294	-48.625
2,4	225.833	138.259	-306.999	-29.676
2,5	229.573	138.24	-299.515	-25.936
2,6	224.405	141.681	-301.718	-31.104
3,4	233.185	137.984	-296.13	-22.324
3,5	213.06	133.697	-301.332	-42.449
3,6	214.293	133.382	-312.61	-41.216
4,5	240.264	140.043	-288.955	-15.245
4,6	192.211	136.794	-336.271	-63.298
5,6	220.158	141.589	-316.887	-35.351

Orientation	E	VDW	ELE	BE
1,2	204.979	150.831	-331.897	-9.909
1,3	315.985	159.642	-346.769	101.097
1,4	185.619	145.145	-342.945	-29.269
1,5	186.367	144.462	-340.554	-28.521
1,6	180.534	141.996	-347.627	-34.354
2,3	188.859	143.284	-337.681	-26.029
2,4	186.413	144.085	-343.544	-28.475
2,5	188.678	146.024	-337.792	-26.21
2,6	190.871	145.515	-340.869	-24.017
3,4	198.83	147.208	-333.188	-16.058
3,5	188.689	145.568	-347.403	-26.199
3,6	195.599	147.615	-338.337	-19.289
4,5	197.956	148.366	-334.815	-16.932
4,6	195.748	145.551	-336.268	-19.14
5,6	197.405	145.664	-332.961	-17.483

LF19

Orientation	E	VDW	ELE	BE
1,2	60.759	109.175	-313.405	-14.241
1,3	39.383	98.87	-323.23	-35.617
1,4	42.301	94.481	-309.835	-32.699
1,5	37.19	103.469	-334.225	-37.81
1,6	30.164	97.012	-326.109	-44.836
2,3	33.994	94.943	-320.372	-41.006
2,4	37.685	98.041	-317.93	-37.315
2,5	38.489	100.665	-326.925	-36.511
2,6	30.7	97.856	-326.553	-44.3
3,4	37.489	99.681	-322.833	-37.511
3,5	40.062	92.317	-314.115	-34.938
3,6	52.193	102.048	-314.844	-22.807
4,5	46.178	106	-322.578	-28.822
4,6	42.196	100.356	-325.295	-32.804
5,6	49.391	103.656	-315.105	-25.609

Orientation	E	VDW	ELE	BE
1,2	77.808	99.773	-299.807	-29.108
1,3	60.835	99.808	-310.131	-46.081
1,4	73.444	100.615	-298.323	-33.472
1,5	45.903	92.83	-319.677	-61.013
1,6	81.323	105.047	-301.859	-25.593
2,3	61.904	99.598	-301.675	-45.012
2,4	72.785	102.718	-299.566	-34.131
2,5	61.614	97.416	-302.639	-45.302
2,6	53.196	95.322	-309.81	-53.72
3,4	48.349	97.371	-318.36	-58.567
3,5	48.299	95.139	-323.181	-58.617
3,6	45.319	97.709	-337.265	-61.597
4,5	80.324	106.593	-293.993	-26.592
4,6	76.103	100.433	-290.686	-30.813
5,6	73.138	102.026	-300.865	-33.778

Orientation	E	VDW	ELE	BE
1,2	251.341	155.132	-261.05	-34.666
1,3	202.104	138.163	-290.064	-83.903
1,4	212.834	144.761	-278.867	-73.173
1,5	239.36	147.757	-263.657	-46.647
1,6	232.278	146.27	-271.269	-53.729
2,3	191.16	145.633	-309.442	-94.847

2,4	209.626	145.519	-282.671	-76.381
2,5	184.559	138.404	-312.193	-101.448
2,6	179.122	142.55	-314.897	-106.885
3,4	230.099	135.903	-263.747	-55.908
3,5	230.184	135.721	-272.298	-55.823
3,6	213.154	134.386	-287.166	-72.853
4,5	257.201	149.324	-255.486	-28.806
4,6	164.837	151.052	-336.373	-121.17
5,6	201.946	147.658	-310.113	-84.061

Orientation	E	VDW	ELE	BE
1,2	216.177	156.984	-316.825	-13.821
1,3	254.095	151.666	-322.661	24.097
1,4	204.456	155.61	-322.79	-25.542
1,5	204.157	155.814	-325.069	-25.841
1,6	206.572	155.512	-321.736	-23.426
2,3	212.012	154.877	-316.563	-17.986
2,4	203.278	155.989	-324.884	-26.72
2,5	209.233	153.357	-322.222	-20.765
2,6	252.578	155.109	-327.655	22.58
3,4	208.879	152.103	-318.368	-21.119
3,5	261.129	156.232	-325.07	31.131
3,6	209.655	152.585	-320.646	-20.343
4,5	208.786	155.397	-319.681	-21.212
4,6	211.63	156.264	-328.144	-18.368
5,6	212.783	153.912	-312.746	-17.215

Orientation	E	VDW	ELE	BE
1,2	213.837	140.881	-310.668	-38.805
1,3	205.177	136.981	-313.202	-47.465
1,4	215.667	138.709	-301.344	-36.975
1,5	207.601	133.758	-306.274	-45.041
1,6	215.257	137.401	-308.332	-37.385
2,3	234.368	138.957	-296.423	-18.274
2,4	219.315	138.814	-301.178	-33.327
2,5	214.687	136.908	-307.078	-37.955
2,6	243.694	142.036	-288.556	-8.948
3,4	206.01	134.69	-306.926	-46.632
3,5	195.055	134.355	-317.611	-57.587
3,6	n/a			
4,5	221.785	140.352	-296.704	-30.857
4,6	204.215	135.856	-309.193	-48.427
5,6	228.32	145.354	-302.693	-24.322

Orientation	E	VDW	ELE	BE
1,2	198.208	149.412	-332.918	-16.68
1,3	197.383	148.316	-335.811	-17.505
1,4	205.255	152.665	-333.215	-9.633
1,5	196.277	145.854	-334.874	-18.611
1,6	193.128	147.504	-337.958	-21.76
2,3	195.078	148.33	-339.206	-19.81
2,4	196.607	145.643	-334.809	-18.281
2,5	195.657	145.493	-335.359	-19.231
2,6	193.102	145.435	-340.911	-21.786
3,4	195.071	146.546	-336.014	-19.817
3,5	193.14	147.817	-341.88	-21.748
3,6	192.912	140.437	-334.253	-21.976
4,5	197.112	149.455	-333.758	-17.776
4,6	191.99	146.643	-340.276	-22.898
5,6	196.854	145.55	-335.405	-18.034

LF20

Orientation	E	VDW	ELE	BE
1,2	55.631	108.659	-315.883	-19.369
1,3	54.76	101.151	-307.787	-20.24
1,4	63.143	108.646	-306.674	-11.857
1,5	52.841	107.766	-318.201	-22.159
1,6	54.603	106.939	-314.799	-20.397
2,3	52.33	107.399	-315.884	-22.67
2,4	57.209	106.565	-312.423	-17.791
2,5	55.065	103.398	-311.04	-19.935
2,6	56.86	103.411	-311.983	-18.14
3,4	51.642	106.296	-329.475	-23.358
3,5	52.41	95.577	-303.909	-22.59
3,6	55.366	105.212	-317.75	-19.634
4,5	65.179	106.022	-304.237	-9.821
4,6	65.073	108.286	-308.874	-9.927
5,6	54.78	104.666	-314.902	-20.22

Orientation	E	VDW	ELE	BE
1,2	85.602	106.93	-293.31	-21.314
1,3	55.019	99.048	-318.431	-51.897
1,4	92.509	107.242	-284.309	-14.407
1,5	71.454	105.511	-304.525	-35.462
1,6	70.489	103.538	-306.29	-36.427
2,3	66.862	107.336	-311.186	-40.054
2,4	70.763	105.405	-303.659	-36.153
2,5	81.27	103.928	-296.195	-25.646
2,6	67.726	102.569	-302.31	-39.19
3,4	61.637	107.871	-319.003	-45.279
3,5	72.446	105.865	-306.592	-34.47
3,6	68.867	105.605	-317.813	-38.049
4,5	86.607	108.426	-297.159	-20.309

4,6	76.897	104.435	-303.114	-30.019
5,6	74.093	103.439	-306.837	-32.823

Orientation	E	VDW	ELE	BE
1,2	218.263	156.295	-289.072	-67.744
1,3	262.866	152.077	-251.093	-23.141
1,4	246.928	151.515	-256.761	-39.079
1,5	183.891	148.174	-327.159	-102.116
1,6	244.473	150.304	-265.12	-41.534
2,3	220.716	156.389	-286.69	-65.291
2,4	212.694	147.317	-283.321	-73.313
2,5	212.886	141.856	-287.502	-73.121
2,6	187.256	146.265	-313.671	-98.751
3,4	209.507	146.372	-290.487	-76.5
3,5	205.925	143.595	-290.385	-80.082
3,6	221.062	148.713	-282.303	-64.945
4,5	253.231	153.081	-260.57	-32.776
4,6	207.905	151.716	-291.693	-78.102
5,6	264.961	151.112	-241.236	-21.046

Orientation	E	VDW	ELE	BE
1,2	217.081	162.181	-318.268	-12.917
1,3	217.264	156.787	-314.086	-12.734
1,4	221.041	160.847	-311.53	-8.957
1,5	212.484	158.951	-321.101	-17.514
1,6	222.937	162.758	-312.54	-7.061
2,3	217.855	160.93	-315.759	-12.143
2,4	216.859	161.494	-318.17	-13.139
2,5	211.828	156.575	-318.669	-18.17
2,6	218.205	162.583	-317.396	-11.793
3,4	207.742	156.764	-324.704	-22.256
3,5	211.025	156.2	-319.211	-18.973
3,6	208.449	157.284	-321.716	-21.549
4,5	223.001	163.036	-310.573	-6.997
4,6	216.059	157.353	-314.771	-13.939
5,6	213.377	160.761	-321.331	-16.621

Orientation	E	VDW	ELE	BE
1,2	219.104	142.021	-306.04	-33.538
1,3	226.248	140.787	-300.962	-26.394
1,4	240.013	140.729	-291.085	-12.629
1,5	218.909	143.596	-312.856	-33.733
1,6	232.818	140.827	-298.992	-19.824
2,3	224.354	143.198	-307.627	-28.288
2,4	225.088	140.679	-301.474	-27.554
2,5	219.036	141.179	-305.553	-33.606
2,6	233.12	141.663	-299.867	-19.522
3,4	217.041	136.434	-308.096	-35.601

3,5	220.478	138.249	-304.936	-32.164
3,6	222.661	140.203	-305.491	-29.981
4,5	245.351	142.011	-284.817	-7.291
4,6	235.114	140.188	-297.501	-17.528
5,6	243.566	140.129	-287.606	-9.076

Orientation	E	VDW	ELE	BE
1,2	200.218	150.735	-331.541	-14.67
1,3	198.935	147.733	-333.216	-15.953
1,4	206.698	152.188	-331.445	-8.19
1,5	202.993	150.312	-334.295	-11.895
1,6	202.331	150.685	-333.585	-12.557
2,3	205.118	149.994	-331.537	-9.77
2,4	198.342	148.863	-336.731	-16.546
2,5	199.556	150.526	-337.973	-15.332
2,6	206.989	150.596	-328.784	-7.899
3,4	202.929	148.024	-329.798	-11.959
3,5	202.571	147.314	-330.594	-12.317
3,6	191.363	149.09	-340.442	-23.525
4,5	202.54	152.365	-335.009	-12.348
4,6	200.623	150.169	-335.49	-14.265
5,6	202.727	149.966	-330.829	-12.161

VF19

Orientation	E	VDW	ELE	BE
1,2	56.481	115.502	-322.334	-18.519
1,3	53.091	108.207	-321.26	-21.909
1,4	55.949	106.181	-316.072	-19.051
1,5	49.536	103.952	-318.65	-25.464
1,6	64.982	107.635	-307.068	-10.018
2,3	46.245	110.006	-325.674	-28.755
2,4	54.029	102.921	-312.167	-20.971
2,5	38.708	95.176	-326.442	-36.292
2,6	60.996	109.134	-309.583	-14.004
3,4	47.442	103.324	-320.463	-27.558
3,5	37.192	103.285	-331.54	-37.808
3,6	32.86	101.917	-331.432	-42.14
4,5	61.566	107.304	-311.003	-13.434
4,6	49.835	106.652	-320.128	-25.165
5,6	45.364	110.641	-329.398	-29.636

Orientation	E	VDW	ELE	BE
1,2	92.054	107.388	-284.221	-14.862
1,3	142.228	149.427	-276.053	35.312
1,4	67.857	106.457	-308.861	-39.059
1,5	69.832	108.791	-304.19	-37.084
1,6	78.701	107.538	-297.711	-28.215
2,3	69.877	109.042	-312.247	-37.039
2,4	79.371	106.859	-298.089	-27.545
2,5	73.977	100.61	-295.311	-32.939
2,6	63.496	103.945	-305.57	-43.42
3,4	88.479	104.039	-287.037	-18.437
3,5	68.655	106.489	-309.432	-38.261
3,6	62.433	104.367	-308.753	-44.483
4,5	94.955	109.282	-285.965	-11.961
4,6	75.552	107.591	-306.195	-31.364
5,6	85.902	106.97	-296.946	-21.014

Orientation	E	VDW	ELE	BE
1,2	217.414	149.267	-297.46	-68.593
1,3	197.302	138.532	-304.986	-88.705
1,4	227.142	144.107	-283.944	-58.865
1,5	224.898	147.82	-287.013	-61.109
1,6	223.315	147.854	-282.739	-62.692
2,3	205.923	144.739	-298.032	-80.084
2,4	165.688	143.48	-335.603	-120.319
2,5	367.481	152.354	-263.485	81.474
2,6	226.461	146.686	-279.052	-59.546
3,4	227.418	146.883	-280.218	-58.589
3,5	227.387	144.591	-287.842	-58.62
3,6	180.825	140.774	-332.67	-105.182
4,5	256.694	146.188	-257.687	-29.313
4,6	260.585	146.975	-256.503	-25.422
5,6	239.282	145.165	-264.081	-46.725

Orientation	E	VDW	ELE	BE
1,2	222.88	162.9898	-312.915	-7.118
1,3	211.235	156.329	-315.849	-18.763
1,4	219.143	160.749	-315.439	-10.855
1,5	211.222	158.558	-320.917	-18.776
1,6	211.75	159.251	-321.204	-18.248
2,3	219.515	157.845	-310.547	-10.483
2,4	210.603	158.649	-319.987	-19.395
2,5	273.394	157.926	-311.872	43.396
2,6	217.55	156.922	-316.941	-12.448
3,4	210.981	156.997	-320.744	-19.017

3,5	207.827	157.367	-325.443	-22.171
3,6	352.087	160.724	-319.785	122.089
4,5	213.006	158.881	-322.621	-16.992
4,6	217.569	158.141	-314.714	-12.429
5,6	212.086	157.137	-321.449	-17.912

Orientation	E	VDW	ELE	BE
1,2	225.486	141.842	-302.892	-27.156
1,3	223.596	130.85	-296.727	-29.046
1,4	220.521	139.832	-309.138	-32.121
1,5	227.813	138.841	-300.215	-24.829
1,6	233.916	138.238	-298.15	-18.726
2,3	227.687	144.21	-308.217	-24.955
2,4	218.759	138.867	-311.508	-33.883
2,5	212.847	137.764	-316.202	-39.795
2,6	233.251	134.424	-295.85	-19.391
3,4	230.603	139.878	-302.873	-22.039
3,5	212.302	132.7	-313.339	-40.34
3,6	207.074	132.274	-307.476	-45.568
4,5	221.914	142.284	-305.692	-30.728
4,6	219.529	133.899	-309.396	-33.113
5,6	233.072	137.394	-296.254	-19.57

Orientation	E	VDW	ELE	BE
1,2	198.077	146.827	-331.031	-16.811
1,3	180.722	142.325	-349.395	-34.166
1,4	195.025	146.732	-339.517	-19.863
1,5	190.03	145.289	-343.161	-24.858
1,6	200.788	148.316	-334.383	-14.1
2,3	185.48	147.568	-349.082	-29.408
2,4	213.606	146.91	-325.555	-1.282
2,5	196.255	148.331	-344.495	-18.633
2,6	192.093	146.185	-341.55	-22.795
3,4	181.909	145.529	-356.209	-32.979
3,5	199.049	145.46	-340.049	-15.839
3,6	191.298	147.036	-346.31	-23.59
4,5	195.307	148.483	-340.472	-19.581
4,6	237.19	147.921	-346.337	22.302
5,6	193.001	148.238	-343.015	-21.887

VF20

Orientation	E	VDW	ELE	BE
1,2	59.294	103.677	-308.87	-15.706
1,3	33.766	99.224	-329.347	-41.234
1,4	44.747	98.362	-317.131	-30.253
1,5	48.17	104.829	-322.649	-26.83
1,6	32.637	97.112	-333.847	-42.363
2,3	45.036	104.833	-320.702	-29.964
2,4	47.512	100.449	-319.348	-27.488
2,5	52.982	103.167	-315.581	-22.018
2,6	56.603	106.736	-315.636	-18.397
3,4	44.354	101.131	-323.415	-30.646
3,5	37.28	101.05	-334.595	-37.72
3,6	42.49	99.108	-329.213	-32.51
4,5	51.022	105.348	-320.007	-23.978
4,6	32.138	102.104	-336.015	-42.862
5,6	48.508	105.043	-320.014	-26.492

Orientation	E	VDW	ELE	BE
1,2	78.78	107.655	-300.526	-28.136
1,3	67.451	99.618	-306.733	-39.465
1,4	67.161	106.894	-308.311	-39.755
1,5	44.488	105.192	-334.314	-62.428
1,6	55.339	99.286	-315.85	-51.577
2,3	62.802	100.019	-317.247	-44.114
2,4	60.927	99.803	-307.268	-45.989
2,5	59.851	99.085	-315.644	-47.065
2,6	74.334	102.423	-300.111	-32.582
3,4	76.605	105.105	-299.837	-30.311
3,5	78.125	105.642	-302.177	-28.791
3,6	62.628	102.589	-316.159	-44.288
4,5	81.831	106.034	-295.563	-25.085
4,6	63.006	102.031	-312.517	-43.91
5,6	62.076	98.291	-309.639	-44.84

NO AML DATA

Orientation	E	VDW	ELE	BE
1,2	213.383	161.564	-320.569	-16.615
1,3	238.359	151.635	-316.474	8.361
1,4	209.001	157.953	-323.465	-20.997
1,5	206.886	152.977	-321.8	-23.112
1,6	206.972	155.944	-323.275	-23.026
2,3	209.049	156.79	-335.819	-20.949
2,4	208.931	158.165	-323.943	-21.067
2,5	203.035	154.529	-330.428	-26.963
2,6	216.357	156.764	-316.922	-13.641
3,4	282.883	158.791	-324.154	-52.885
3,5	209.45	155.304	-315.524	-20.548
3,6	193.562	148.522	-324.283	-36.436
4,5	213.586	156.21	-316.09	-16.412
4,6	213.223	157.534	-319.744	-16.775
5,6	212.374	156.083	-319.018	-17.624

Orientation	E	VDW	ELE	BE
1,2	219.366	138.802	-305.915	-33.276
1,3	232.124	138.268	-297.291	-20.518
1,4	219.18	141.174	-307.325	-33.462
1,5	209.657	138.559	-316.143	-42.985
1,6	192.641	134.697	-326.628	-60.001
2,3	205.879	136.09	-313.895	-46.763
2,4	219.312	138.043	-310.585	-33.33
2,5	222.359	131.239	-299.832	-30.283
2,6	213.238	137.945	-318.694	-39.404
3,4	207.174	139.922	-317.807	-45.468
3,5	223.096	142.459	-310.432	-29.546
3,6	199.266	134.598	-326.285	-53.376
4,5	226.924	141.647	-303.682	-25.718
4,6	204.525	138.025	-311.172	-48.117
5,6	211.858	138.623	-307.9	-40.784

Orientation	E	VDW	ELE	BE
1,2	197.612	147.727	-335.394	-17.276
1,3	198.343	147.392	-331.84	-16.545
1,4	189.986	141.882	-335.551	-24.902
1,5	189.793	139.805	-330.245	-25.095
1,6	190.223	142.029	-338.727	-24.665
2,3	196.347	145.284	-334.593	-18.541
2,4	193.443	147.243	-338.747	-21.445
2,5	216.849	143.984	-339.299	1.961
2,6	192.317	147.553	-342.255	-22.571
3,4	182.693	146.724	-346.083	-32.195

3,5	206.513	146.202	-336.316	-8.375
3,6	177.181	140.912	-349.518	-37.707
4,5	198.368	149.415	-337.098	-16.52
4,6	190.092	147.352	-343.012	-24.796
5,6	199.525	145.759	-335.168	-15.363

FF

Orientation	E	VDW	ELE	BE
1,2	53.615	103.398	-313.401	-21.385
1,3	51.954	109.566	-321.085	-23.046
1,4	33.852	103.621	-332.227	-41.148
1,5	47.04	103.297	-321.274	-27.96
1,6	55.578	102.226	-310.424	-19.422
2,3	35.876	103.678	-335.354	-39.124
2,4	49.641	106.214	-321.27	-25.359
2,5	48.871	102.884	-317.361	-26.129
2,6	47.557	105.19	-325.005	-27.443
3,4	51.699	104.661	-317.596	-23.301
3,5	46.52	109.213	-328.132	-28.48
3,6	57.229	104.806	-312.471	-17.771
4,5	50.835	107.739	-319.469	-24.165
4,6	52.246	106.543	-320.458	-22.754
5,6	30.145	102.964	-334.065	-44.855

Orientation	E	VDW	ELE	BE
1,2	91.769	108.852	-289.288	-15.147
1,3	66.934	107.048	-311.351	-39.982
1,4	87.441	108.726	-293.968	-19.475
1,5	81.607	105.251	-297.83	-25.309
1,6	67.404	104.721	-311.517	-39.512
2,3	69.155	103.6	-305.513	-37.761
2,4	57.362	102.21	-312.642	-49.554
2,5	82.035	104.694	-293.448	-24.881
2,6	69.507	102.729	-303.583	-37.409
3,4	81.605	99.934	-289.617	-25.311
3,5	75.786	97.448	-293.621	-31.13
3,6	62.043	100.093	-321.228	-44.873
4,5	73.447	108.865	-315.309	-33.469
4,6	66.403	104.299	-309.499	-40.513
5,6	69.424	105.761	-303.113	-37.492

Orientation	E	VDW	ELE	BE
1,2	276.478	153.721	-240.324	-9.529
1,3	194.3	151.903	-316.405	-91.707
1,4	206.357	147.271	-300.26	-79.65
1,5	207.257	155.053	-296.763	-78.75
1,6	219.467	157.099	-288.293	-66.54
2,3	234.533	150.432	-272.32	-51.474
2,4	264.192	155.702	-246.46	-21.815
2,5	211.15	148.451	-294.541	-74.857
2,6	243.812	151.729	-263.998	-42.195
3,4	184.974	145.857	-319.927	-101.033
3,5	228.127	146.876	-271.931	-57.88
3,6	195.866	144.011	-307.03	-90.141
4,5	271.055	155.65	-246.846	-14.952
4,6	204.493	148.582	-296.062	-81.514
5,6	208.849	144.99	-293.984	-77.158

Orientation	E	VDW	ELE	BE
1,2	201.161	155.358	-342.62	-28.837
1,3	199.222	148.487	-324.755	-30.776
1,4	186.082	151.829	-347.184	-43.916
1,5	210.42	149.508	-325.903	-19.578
1,6	193.346	142.31	-341.849	-36.652
2,3	205.207	149.565	-324.38	-24.791
2,4	195.285	147.773	-340.723	-34.713
2,5	176.876	141.625	-351.522	-53.122
2,6	196.121	144.072	-332.051	-33.877
3,4	197.728	149.372	-332.583	-32.27
3,5	176.683	138.138	-344.929	-53.315
3,6	193.78	141.172	-334.598	-36.218
4,5	196.274	148.428	-334.319	-33.724
4,6	195.103	148.58	-341.519	-34.895
5,6	168.672	136.007	-354.312	-61.326

Orientation	E	VDW	ELE	BE
1,2	227.48	143.143	-309.418	-25.162
1,3	219.513	141.441	-309.126	-33.129
1,4	231.676	142.806	-299.81	-20.966
1,5	229.067	142.149	-303.712	-23.575
1,6	228.13	141.272	-302.655	-24.512
2,3	218.769	140.289	-307.908	-33.873
2,4	238.309	142.096	-292.934	-14.333
2,5	211.225	135.847	-304.07	-41.417

2,6	217.368	138.802	-314.86	-35.274
3,4	224.683	141.521	-303.504	-27.959
3,5	231.402	142.106	-302.296	-21.24
3,6	226.585	137.183	-307.629	-26.057
4,5	232.576	144.665	-297.26	-20.066
4,6	236.875	138.459	-290.748	-15.767
5,6	223.06	141.082	-303.163	-29.582

Orientation	E	VDW	ELE	BE
1,2	211.57	152.495	-325.588	-3.318
1,3	201.297	150.64	-333.671	-13.591
1,4	199.339	149.679	-334.666	-15.549
1,5	195.641	146.91	-336.853	-19.247
1,6	207.793	151.706	-328.665	-7.095
2,3	201.249	150.503	-333.996	-13.639
2,4	193.771	146.579	-337.801	-21.117
2,5	197.752	149.227	-335.503	-17.136
2,6	197.804	149.799	-336.238	-17.084
3,4	188.98	144.637	-342.401	-25.908
3,5	186.757	144.278	-342.248	-28.131
3,6	193.51	146.079	-337.146	-21.378
4,5	206.171	150.561	-329.834	-8.717
4,6	203.915	148.15	-328.492	-10.973
5,6	207.423	149.605	-328.006	-7.465

GAS PHASE INTERACTIONS

Legend of Amino Acids for $A\beta_{42:}$

$$D_1A_2G_3F_4R_5H_6D_7S_8G_9Y_{10}E_{11}V_{12}H_{13}H_{14}Q_{15}K_{16}L_{17}V_{18}F_{19}F_{20-}$$

$$-A_{21}E_{22}D_{23}V_{24}G_{25}S_{26}N_{27}K_{28}G_{29}A_{30}I_{31}I_{32}G_{33}L_{34}M_{35}V_{36}G_{37}G_{38}V_{39}V_{40}I_{41}A_{42}$$

HH

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	AA	14	A-ring	1/3
1AMC	AH	17	B-ring	1/6
1AMC	AA	14	A-ring	3/5
1AMC	AH	10	Ca3	3/6
1AML	AA	13	B-ring	3/4
1AML	SCD	14	6	5/6
1BA4	AA	13	B-ring	1/5
1BA4	SCD	14	6	2/3
1BA4	AA	13	B-ring	2/4
1IYT	SCD	14	6	5/6
1Z0Q	AA	13	B-ring	3/4
1Z0Q	BBA	10	4	4/5
1Z0Q	AH	14	CB1	5/6

H13K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	A+	16	A-ring	1/6
1AMC	SCD	16	6	2/6
1AMC	AH	13	1	3/5
1AMC	SCD	16	6	3/6
1AML	AH	16	A-ring	3/5
1BA4	AA	10	B-ring	1/4
1BA4	BBA	10	4	3/5
1BA4	AA	13	B-ring	3/6
1IYT	SCD	16	6	2/6
1IYT	AH	20	4	3/4
1IYT	SCD	16	6	4/6
1IYT	SCD	16	6	5/6
1Z0Q	SCD	16	6	2/6
1Z0Q	AA	13	B-ring	3/5
1Z0Q	SCD	16	6	3/6
1Z0Q	SCD	16	6	5/6

H14K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	13	2	1/2
1AMB	SCD	13	6	1/4
1AMB	SCD	13	6	2/3
1AMB	AA	13	A-ring	3/4
1AMB	AH	13	CA1	3/5
1AMB	BBA	13	4	4/5
1AMB	AH	13	B-ring	4/6
1AMB	BBA	13	6	5/6
1AMB	AA	13	A-ring	5/6
1AMC	BBA	13	2	1/2
1AMC	AH	17	B-ring	1/2
1AMC	SCD	13	6	1/4
1AMC	AH	14	B-ring	1/5
1AMC	AH	16	A-ring	1/6
1AMC	SCD	13	6	2/4
1AMC	AH	13	1	2/5
1AMC	AH	14	B-ring	2/5
1AMC	AA	13	B-ring	2/6
1AMC	SCD	13	6	3/4
1AMC	AA	13	A-ring	3/4

1AMC	AH	17	A-ring	3/4
1AMC	BBA	13	5	4/5
1AMC	AA	13	A-ring	4/5
1AMC	BBA	13	6	4/6
1AMC	AA	13	A-ring	4/6
1AMC	AA	13	A-ring	5/6
1AML	BBA	13	2	1/2
1AML	AA	13	B-ring	1/2
1AML	AH	17	B-ring	1/3
1AML	SCD	13	6	1/4
1AML	AH	13	CC4	1/5
1AML	BBA	14	6	2/5
1AML	SCD	10	6	3/5
1AML	AH	10	5	3/6
1AML	SCD	13	6	4/5
1BA4	AH	17	A-ring	1/5
1BA4	BBA	10	1	3/6
1IYT	BBA	11	2	1/2
1IYT	SCA	15	1	1/3
1IYT	SCA	11	1	1/5
1IYT	SCA	11	2	2/5
1IYT	BBA	11	4	4/5
1IYT	SCA	11	5	5/6

1Z0Q	BBA	14	1	1/3
1Z0Q	BBA	13	6	1/5
1Z0Q	BBA	13	6	2/5
1Z0Q	AA	14	B-ring	3/4
1Z0Q	AH	14	A-ring	3/5
1Z0Q	BBA	12	1	3/6

LV

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	14	6	2/5
1AMB	BBA	17	1	3/6
1AMB	SCA	22	1	5/6
1AMC	A+	14	A-ring	1/6
1AMC	AH	17	B-ring	2/5
1AMC	BBA	18	1	3/6
1AML	SCD	14	6	1/6
1BA4	--	--	--	--
1IYT	AH	17	A-ring	3/5
1Z0Q	SCA	26	4	1/3
1Z0Q	SCA	22	4	2/4
1Z0Q	AH	17	B-ring	2/5

1Z0Q	SCA	26	2	5/6

LF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	16	1	1/3
1AMB	SCD	16	6	1/3
1AMB	AA	20	B-ring	1/3
1AMB	AA	20	B-ring	1/4
1AMB	BBA	16	6	1/5
1AMB	SCD	16	6	2/6
1AMB	BBA	16	1	2/6
1AMB	BBA	16	4	4/5
1AMB	SCD	16	6	5/6
1AMC	A+	14	A-ring	1/6
1AMC	AH	17	B-ring	2/5
1AMC	BBA	18	1	3/6
1AML	AH	20	A-ring	2/4
1AML	AH	16	A-ring	4/5
1BA4	BBA	15	2	1/2
1BA4	AH	14	CB4	1/4
1BA4	AH	18	B-ring	1/6
1BA4	AH	18	B-ring	2/3

1BA4	AH	18	A-ring	2/4
1BA4	BBA	14	1	2/5
1BA4	SCA	15	1	2/6
1BA4	AH	18	B-ring	2/6
1BA4	AH	17	B-ring	3/4
1BA4	SCA	15	4	3/5
1BA4	SCA	15	5	4/6
1IYT	AA	20	B-ring	1/2
1IYT	BBA	16	1	1/3
1IYT	SCD	16	6	1/3
1IYT	AA	20	B-ring	1/3
1IYT	AH	20	1	1/6
1IYT	AA	20	B-ring	2/5
1IYT	AH	20	2	2/6
1IYT	SCD	16	6	2/6
1IYT	AH	20	CC1	3/4
1IYT	AA	20	A-ring	4/5
1Z0Q	BBA	16	6	1/5
1Z0Q	BBA	16	6	1/6
1Z0Q	BBA	16	1	2/3
1Z0Q	BBA	16	6	2/5
1Z0Q	AH	16	A-ring	3/4
1Z0Q	BBA	16	6	3/6

1Z0Q	AH	17	A-ring	3/6
1Z0Q	BBA	16	4	4/5

LF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	20	6	1/3
1AMB	AH	17	B-ring	2/3
1AMB	A+	13	B-ring	B-ring
1AMC	--	--	--	--
1AML	AH	17	B-ring	2/6
1AML	BBA	16	4	4/5
1BA4	AA	20	A-ring	2/5
1IYT	--	--	--	--
1Z0Q	AA	20	A-ring	1/3

VF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	18	B-ring	2/5
1AMB	A+	14	B-ring	3/4
1AMB	SCA	22	1	3/4

1AMB	SCA	11	5	3/6
1AMB	SCA	23	2	3/6
1AMC	SCA	22	1	1/2
1AMC	SCA	22	1	2/4
1AMC	AH	18	B-ring	2/6
1AMC	AH	14	4	3/6
1AMC	SCA	15	5	4/6
1AMC	SCA	22	5	5/6
1AML	SCA	22	1	1/3
1AML	SCA	22	6	1/5
1AML	SCA	22	6	1/6
1AML	AH	15	B-ring	2/4
1AML	SCA	22	1	2/4
1AML	SCA	15	1	2/5
1AML	SCA	22	6	2/5
1AML	SCD	5	6	3/4
1AML	SCA	22	6	3/6
1AML	SCA	22	6	5/6
1BA4	AH	15	B-ring	1/3
1BA4	AH	18	B-ring	2/5
1BA4	AH	19	A-ring	2/5
1BA4	SCA	22	4	3/5
1BA4	AH	19	A-ring	5/6

1IYT	AH	19	B-ring	1/3
1IYT	SCA	22	1	2/3
1Z0Q	SCA	15	1	1/6
1Z0Q	SCA	22	2	1/6
1Z0Q	AH	15	B-ring	2/4
1Z0Q	SCA	22	1	3/4

VF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	17	2	1/2
1AMB	SCD	28	6	5/6
1AMC	AH	20	A-ring	1/5
1AMC	SCA	22	4	3/6
1AML	n/a	n/a	n/a	n/a
1BA4	AH	17	B-ring	2/5
1BA4	BBA	18	1	3/4
1IYT	AH	24	A-ring	2/3
1IYT	BBA	17	5	4/5
1Z0Q	BBA	17	2	1/2
1Z0Q	AH	17	B-ring	3/6

FF

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	SCD	16	6	1/6
1AMB	SCD	16	6	2/5
1AMC	AA	20	A-ring	1/3
1AMC	BBA	19	1	3/6
1AML	SCA	23	4	5/6
1BA4	AA	20	A-ring	1/3
1BA4	SCA	23	6	1/3
1BA4	SCA	23	4	1/4
1BA4	SCA	11	4	1/5
1BA4	BBD	1	6	2/3
1BA4	SCA	23	6	2/3
1BA4	SCA	23	4	2/4
1BA4	AA	19	B-ring	2/4
1BA4	SCA	22	1	2/4
1BA4	SCA	23	5	2/5
1BA4	SCA	11	6	2/5
1BA4	SCD	16	6	2/6
1BA4	SCA	3	4	3/5
1BA4	AH	19	CB1	3/5
1BA4	SCA	23	6	3/6

1BA4	SCA	3	5	3/6
1BA4	SCA	23	6	4/5
1BA4	SCD	16	6	4/6
1BA4	SCA	22	5	5/6
1BA4	BBD	1	6	5/6
1IYT	SCD	16	6	3/6
1Z0Q	--	--	--	--

APPENDIX C: DATA FOR CYANIDIN

Tables of energies for gas phase calculations of cyanidin. All energies are in kcal/mol. The order of the tables for each pair of amino acids is always 1AMB, 1AMC, 1AML, 1BA4, 1IYT, 1Z0Q.

HH

Orientation	E			Binding Energy (BE)
1,2	65.834	111.188	-310.147	-14.115
1,3	63.201	109.049	-310.821	-16.748
1,4	54.14	111.173	-326.351	-25.809
1,5	59.874	112.498	-318.899	-20.075
1,6	48.588	108.51	-328.788	-31.361
2,3	83.636	112.429	-295.825	3.687
2,4	61.978	115.995	-318.907	-17.971
2,5	56.958	108.132	-316.519	-22.991
2,6	44.802	109.713	-330.989	-35.147
3,4	78.144	109.304	-299.496	-1.805
3,5	61.211	101.016	-307.231	-18.738
3,6	51.258	99.959	-319.868	-28.691
4,5	76.646	111.242	-302.49	-3.303
4,6	65.27	102.956	-312.816	-14.679
5,6	59.777	112.158	-313.856	-20.172

Orientation	E	VDW	ELE	BE
1,2	87.671	109.862	-296.251	-24.194
1,3	81.792	101.547	-297.811	-30.073
1,4	62.731	103.693	-324.496	-49.134
1,5	100.086	112.352	-287.686	-11.779
1,6	98.893	107.728	-277.589	-12.972
2,3	57.233	114.171	-327.036	-54.632
2,4	101.387	108.217	-280.365	-10.478
2,5	105.221	104.273	-278.011	-6.644
2,6	85.989	107.413	-301.6	-25.876
3,4	92.259	109.735	-297.311	-19.606
3,5	81.146	100.978	-294.067	-30.719
3,6	75.512	108.204	-309.432	-36.353
4,5	96.403	111.036	-288.18	-15.462
4,6	91.031	99.009	-288.982	-20.834
5,6	93.487	110.81	-289.706	-18.378

Orientation	E	VDW	ELE	BE
1,2	270.666	153.124	-239.695	-20.29
1,3	281.662	152.02	-232.138	-9.294
1,4	283.746	155.129	-233.161	-7.21
1,5	280.753	154.599	-236.123	-10.203
1,6	272.334	153.174	-245.9	-18.622
2,3	231.918	150.987	-275.735	-59.038
2,4	268.655	157.108	-250.665	-22.301
2,5	269.78	152.847	-245.923	-21.176
2,6	260.18	160.257	-260.479	-30.776
3,4	262.295	144.857	-238.275	-28.661
3,5	273.997	147.8	-239.252	-16.959
3,6	256.05	151.607	-263.784	-34.906
4,5	250.771	156.962	-249.882	-40.185
4,6	268.005	152.899	-242.774	-22.951
5,6	213.301	152.332	-310.121	-77.655

Orientation	E	VDW	ELE	BE
1,2	226.291	166.642	-314.68	-8.656
1,3	245.142	165.724	-297.943	10.195
1,4	234.766	164.29	-307.301	-0.181
1,5	240.381	165.743	-301.509	5.434
1,6	234.356	166.362	-306.6	-0.591
2,3	235.088	163.37	-305.546	0.141
2,4	235.636	162.657	-301.177	0.689
2,5	231.068	164.894	-308.011	-3.879
2,6	238.433	164.503	-301.792	3.486
3,4	233.626	164.695	-306.439	-1.321
3,5	247.431	165.107	-294.92	12.484
3,6	241.399	162.547	-299.47	6.452
4,5	233.546	166.735	-310.108	-1.401
4,6	238.575	168.543	-302.244	3.628
5,6	231.081	166.662	-312.652	-3.866

No IYT data

Orientation	E	VDW	ELE	BE
1,2				
1,3	213.76	150.62	-328.854	-6.077
1,4	216.877	155.035	-328.78	-2.96
1,5	216.6	151.828	-326.819	-3.237

1,6	207.968	151.292	-332.567	-11.869
2,3	210.791	148.378	-326.552	-9.046
2,4	213.596	153.46	-330.98	-6.241
2,5	215.456	150.457	-323.019	-4.381
2,6	208.301	154.607	-333.957	-11.536
3,4	211.188	147.504	-326.802	-8.649
3,5	220.061	144.152	-327.756	0.224
3,6				
4,5	213.76	154.308	-327.972	-6.077
4,6	219.985	150.949	-319.915	0.148
5,6	214.226	149.71	-324.578	-5.611

H13K

Orientation	E	VDW	ELE	BE
1,2	73.342	112.894	-303.535	-6.607
1,3	73.321	112.166	-304.153	-6.628
1,4	80.8	112.117	-296.215	0.851
1,5	66.126	114.507	-315.175	-13.823
1,6	65.409	110.384	-311.411	-14.54
2,3	61.095	112.577	-313.65	-18.854
2,4	78.224	112.944	-296.945	-1.725
2,5	57.723	113.183	-319.315	-22.226
2,6	60.375	117.227	-319.889	-19.574
3,4	60.83	106.735	-313.82	-19.119
3,5	75.342	111.784	-302.241	-4.607
3,6	69.445	106.772	-298.494	-10.504
4,5	69.505	116.942	-307.984	-10.444
4,6	61.626	110.502	-318.094	-18.323
5,6	65.079	109.627	-308.5	-14.87

Orientation	E	VDW	ELE	BE
1,2	80.401	114.069	-302.781	-31.464
1,3	74.844	114.038	-314.608	-37.021
1,4	92.034	112.803	-297.472	-19.831
1,5	91.092	115.054	-296.465	-20.773
1,6	82.278	113.426	-299.19	-29.587
2,3	82.312	113.817	-300.566	-29.553
2,4	88.303	116.518	-303.142	-23.562
2,5	81.103	117.826	-315.386	-30.762
2,6	77.376	112.231	-303.198	-34.489
3,4	90.737	108.687	-288.383	-21.128
3,5	94.503	111.562	-288.2	-17.362

3,6	93.321	109.874	-291.83	-18.544
4,5	87.415	114.211	-295.673	-24.45
4,6	81.954	113.613	-306.992	-29.911
5,6	89.576	113.438	-293.673	-22.289

Orientation	E	VDW	ELE	BE
1,2	258.312	160.49	-258.792	-32.644
1,3	225.141	151.887	-289.767	-65.815
1,4	283.708	160.695	-239.388	-7.248
1,5	241.56	158.596	-267.891	-49.396
1,6	198.205	153.772	-309.618	-92.751
2,3	221.628	148.345	-287.22	-69.328
2,4	217.378	160.139	-295.367	-73.578
2,5	259.325	154.637	-249.675	-31.631
2,6	209.323	161.966	-299.758	-81.633
3,4	260.388	156.883	-253.697	-30.568
3,5	259.245	152.383	-255.471	-31.711
3,6	200.137	147.557	-304.944	-90.819
4,5	250.907	158.314	-255.145	-40.049
4,6	201.18	149.883	-311.84	-89.776
5,6	242.087	157.543	-267.255	-48.869

Orientation	E	VDW	ELE	BE
1,2	213.265	157.177	-318.253	-21.682
1,3	211.893	150.685	-322.308	-23.054
1,4	224.653	153.568	-313.03	-10.294
1,5	209.397	155.187	-322.365	-25.55
1,6	207.998	157.103	-329.523	-26.949
2,3	204.665	151.104	-327.219	-30.282
2,4	222.668	158.919	-315.251	-12.279
2,5	220.346	162.566	-323.113	-14.601
2,6	210.798	158.296	-320.875	-24.149
3,4	232.614	157.878	-301.768	-2.333
3,5	229.94	151.76	-302.759	-5.007
3,6	225.485	152.174	-316.553	-9.462
4,5	219.783	160.685	-314.849	-15.164
4,6	214.214	159.316	-321.389	-20.733
5,6	216.856	162.3	-320.129	-18.091

Orientation	E	VDW	ELE	BE
1,2	225.903	146.724	-303.385	-31.688
1,3	210.46	149.978	-322.316	-47.131
1,4	204.475	150.104	-320.228	-53.116
1,5	240.829	149.482	-295.263	-16.762
1,6	261.927	143.588	-274.7	4.336

2,3	207.012	151.372	-321.316	-50.579
2,4	227.03	146.092	-308.372	-30.561
2,5	246.521	143.565	-283.696	-11.07
2,6	234.985	141.633	-302.319	-22.606
3,4	215.146	148.733	-312.134	-42.445
3,5	245.838	141.696	-283.806	-11.753
3,6	259.182	140.061	-272.881	1.591
4,5	215.168	149.956	-313.686	-42.423
4,6	233.801	148.42	-309.931	-23.79
5,6	232.554	147.723	-306.517	-25.037

Orientation	E	VDW	ELE	BE
1,2	213.132	156.352	-330.307	-6.705
1,3	222.836	153.481	-318.704	2.999
1,4	221.349	157.664	-328.416	1.512
1,5	207.427	155.542	-340.025	-12.41
1,6	223.271	155.797	-320.754	3.434
2,3	219.94	154.671	-323.652	0.103
2,4	222.115	156.518	-323.855	2.278
2,5	222.386	154.02	-322.598	2.549
2,6	210.438	152.933	-334.055	-9.399
3,4	220.967	151.198	-325.142	1.13
3,5	193.347	151.34	-343.414	-26.49
3,6	218.015	149.347	-319.896	-1.822
4,5	214.12	153.216	-329.855	-5.717
4,6	225.205	155.28	-321.59	5.368
5,6	218.67	155.859	-328.192	-1.167

H14K

Orientation	E	VDW	ELE	BE
1,2	59.416	109.511	-315.86	-20.533
1,3	73.432	108.48	-305.697	-6.517
1,4				
1,5	76.301	112.378	-309.419	-3.648
1,6	55.984	110.337	-319.383	-23.965
2,3	65.854	111.19	-315.919	-14.095
2,4	69.732	109.163	-304.294	-10.217
2,5	58.869	103.499	-317.018	-21.08
2,6	62.521	117.125	-322.585	-17.428
3,4	77.664	104.855	-303.193	-2.285
3,5	75.107	110.423	-310.021	-4.842
3,6				
4,5	70.597	112.766	-309.527	-9.352
4,6	81.903	108.249	-307.842	1.954

5,6	90.77	110.733	-293.95	10.821

No AMC data

Orientation	E	VDW	ELE	BE
1,2	254.932	152.431	-261.171	-36.024
1,3	243.084	145.82	-269.643	-47.872
1,4	232.213	150.365	-281.809	-58.743
1,5	253.526	156.131	-251.31	-37.43
1,6	255.844	151.437	-253.13	-35.112
2,3	246.495	143.217	-257.759	-44.461
2,4	259.528	145.353	-251.085	-31.428
2,5	221.386	144.525	-276.999	-69.57
2,6	206.074	149.637	-301.739	-84.882
3,4	256.962	141.795	-249.588	-33.994
3,5	224.163	147.167	-293.352	-66.793
3,6	216.068	143.76	-296.503	-74.888
4,5	239.132	148.904	-255.349	-51.824
4,6	262.539	148.551	-251.63	-28.417
5,6	250.155	146.552	-260.85	-40.801

Orientation	E	VDW	ELE	BE
1,2	207.219	156.68	-324.093	-27.728
1,3	190.992	150.111	-338.884	-43.955
1,4	211.768	155.081	-319.237	-23.179
1,5	206.312	156.194	-322.446	-28.635
1,6	209.576	155.715	-320.027	-25.371
2,3	186.168	141.87	-337.377	-48.779
2,4	203.152	153.895	-330.428	-31.795
2,5	209.399	157.014	-327.441	-25.548
2,6	200.897	154.605	-334.183	-34.05
3,4	212.364	156.194	-315.927	-22.583
3,5	216.923	152.525	-313.741	-18.024
3,6	214.564	159.041	-318.932	-20.383
4,5	212.688	159.065	-319.391	-22.259
4,6	223.83	162.719	-316.075	-11.117
5,6	208.743	156.94	-324.8	-26.204

Orientation	E	VDW	ELE	BE
1,2	194.192	138.462	-329.75	-63.399
1,3	217.956	137.488	-317.762	-39.635
1,4	217.027	136.945	-313.064	-40.564

1,5	266.071	143.858	-319.646	8.48
1,6	348.309	152.31	-312.471	90.718
2,3	241.85	140.861	-292.141	-15.741
2,4	367.111	158.452	-299.315	109.52
2,5	287.055	134.519	-308.448	29.464
2,6	225.092	144.337	-314.865	-32.499
3,4	210.724	135.636	-324.287	-46.867
3,5	214.976	138.128	-317.42	-42.615
3,6	2008			
4,5	226.379	143.138	-305.132	-31.212
4,6	198.749	145.26	-331.834	-58.842
5,6	222.782	140.76	-315.203	-34.809

Orientation	E	VDW	ELE	BE
1,2	205.518	151.537	-334.369	-14.319
1,3	201.102	145.537	-335.584	-18.735
1,4	200.974	146.108	-335.9	-18.863
1,5	206.154	151.864	-335.558	-13.683
1,6	212.497	152.396	-330.712	-7.34
2,3	200.78	151.312	-343.969	-19.057
2,4	197.772	149.508	-339.699	-22.065
2,5	210.754	145.815	-324.227	-9.083
2,6	201.003	153.089	-338.646	-18.834
3,4	218.143	150.685	-319.956	-1.694
3,5	217.771	148.694	-321.517	-2.066
3,6	212.069	151.419	-336.31	-7.768
4,5	207.737	152.802	-331.086	-12.1
4,6	204.124	147.683	-334.921	-15.713
5,6	209.199	152.292	-330.543	-10.638

LV

Orientation	E	VDW	ELE	BE
1,2	44.948	113.925	-336.376	-35.001
1,3	54.925	107.325	-324.203	-25.024
1,4	64.235	108.759	-314.787	-15.714
1,5	54.689	107.524	-321.09	-25.26
1,6	48.536	110.166	-333.56	-31.413
2,3	33.837	101.225	-340.746	-46.112
2,4	58.419	110.347	-322.027	-21.53
2,5	56.231	108.917	-326.705	-23.718
2,6	36.045	106.242	-341.292	-43.904
3,4	49.276	107.034	-326.815	-30.673
3,5	45.772	108.891	-333.031	-34.177

3,6	45.1	102.244	-322.838	-34.849
4,5	59.958	112.105	-317.703	-19.991
4,6	45.131	110.225	-327.035	-34.818
5,6	45.95	107.576	-330.281	-33.999

Orientation	E	VDW	ELE	BE
1,2	93.288	112.055	-292.763	-18.577
1,3	54.124	106.496	-320.995	-57.741
1,4	75.05	110.838	-316.677	-36.815
1,5	49.217	107.312	-334.577	-62.648
1,6	56.748	113.317	-334.563	-55.117
2,3	54.325	103.625	-322.224	-57.54
2,4	50.383	100.604	-329.736	-61.482
2,5	69.049	102.31	-305.425	-42.816
2,6	82.021	109.307	-295.036	-29.844
3,4	76.46	112.303	-308.509	-35.405
3,5	64.233	100.02	-310.726	-47.632
3,6	48.093	109.746	-335.44	-63.772
4,5	98.189	111.91	-286.679	-13.676
4,6	61.421	107.868	-319.557	-50.444
5,6	72.714	116.651	-314.697	-39.151

Orientation	E	VDW	ELE	BE
1,2	216.78	152.163	-299.009	-74.176
1,3	237.782	150.552	-273.466	-53.174
1,4	258.928	150.104	-256.685	-32.028
1,5	170.333	147.128	-337.916	-120.623
1,6	206.143	154.046	-294.764	-84.813
2,3	260.207	153.314	-258.688	-30.749
2,4	248.464	151.581	-263.741	-42.492
2,5	244.772	152.227	-277.308	-46.184
2,6	269.232	153.557	-246.684	-21.724
3,4	244.024	153.986	-268.881	-46.932
3,5	240.468	141.715	-268.359	-50.488
3,6	213.48	149.199	-290.227	-77.476
4,5	229.737	147.672	-282.934	-61.219
4,6	259.887	142.514	-249.843	-31.069
5,6	257.692	150.678	-255.652	-33.264

Orientation	E	VDW	ELE	BE
1,2	225.787	165.105	-314.268	-9.16
1,3	205.284	164.166	-337.631	-29.663
1,4	212.429	160.536	-322.81	-22.518

1,5	211.828	159.845	-326.647	-23.119
1,6	214.893	165.699	-323.654	-20.054
2,3	212.868	163.51	-327.549	-22.079
2,4	215.295	167.019	-326.254	-19.652
2,5	211.663	163.92	-327.098	-23.284
2,6	216.075	163.004	-323.882	-18.872
3,4	219.934	160.696	-315.444	-15.013
3,5	222.979	164.097	-315.335	-11.968
3,6	216.323	157.209	-314.418	-18.624
4,5	223.229	165.804	-316.739	-11.718
4,6	210.93	159.678	-325.825	-24.017
5,6	214.579	163.276	-321.831	-20.368

Orientation	E	VDW	ELE	BE
1,2	239.736	151.717	-297.786	-17.855
1,3	233.499	142.616	-309.173	-24.092
1,4	225.45	146.098	-314.147	-32.141
1,5	224.085	146.775	-313.941	-33.506
1,6	229.409	149.441	-306.89	-28.182
2,3	228.671	139.361	-307.77	-28.92
2,4	221.703	145.54	-314.923	-35.888
2,5	242.516	139.007	-292.728	-15.075
2,6	241.437	143.513	-295.549	-16.154
3,4	235.421	142.857	-302.334	-22.17
3,5	222.262	142.727	-313.658	-35.329
3,6	216.492	139.147	-315.814	-41.099
4,5	238.758	145.761	-301.497	-18.833
4,6	--			
5,6	228.975	141.108	-303.812	-28.616

Orientation	E	VDW	ELE	BE
1,2	205.819	155.618	-336.2	-14.018
1,3	197.408	149.631	-339.354	-22.429
1,4	198.33	149.679	-339.576	-21.507
1,5	184.995	150.701	-353.914	-34.842
1,6	188.593	148.981	-350.433	-31.244
2,3	192.648	147.736	-348.194	-27.189
2,4	192.479	151.602	-349.503	-27.358
2,5	193.76	144.909	-338.659	-26.077
2,6	195.456	152.049	-345.522	-24.381
3,4	208.988	152.772	-333.397	-10.849
3,5	204.464	155.085	-340.14	-15.373
3,6	205.656	154.941	-335.691	-14.181

4,5	195.737	152.629	-348.667	-24.1
4,6	185.065	148.728	-351.138	-34.772
5,6	189.834	147.735	-344.62	-30.003

LF19

Orientation	E	VDW	ELE	BE
1,2	48.067	103.293	-319.863	-31.882
1,3	191.67	106.103	-329.394	111.721
1,4	44.649	105.604	-323.793	-35.3
1,5	64.772	107.184	-310.307	-15.177
1,6	61.987	108.548	-313.303	-17.962
2,3	220.636	111.588	-297.015	140.687
2,4	57.445	108.214	-322.517	-22.504
2,5	59.197	105.304	-315.59	-20.752
2,6	65.79	99.313	-297.339	-14.159
3,4	40.926	98.178	-324.107	-39.023
3,5				
3,6	61.42	108.569	-313.051	-18.529
4,5	66.858	112.44	-309.679	-13.091
4,6	32.789	105.023	-336.139	-47.16
5,6	62.862	113.481	-318.18	-17.087

Orientation	E	VDW	ELE	BE
1,2	220.787	118.963	-308.495	108.922
1,3	43.682	96.018	-326.497	-68.183
1,4	51.8	103.925	-329.242	-60.065
1,5	61.772	108.113	-312.817	-50.093
1,6	64.669	110.121	-312.937	-47.196
2,3	62.957	101.744	-317.016	-48.908
2,4	54.717	103.805	-328.437	-57.148
2,5	64.896	98.052	-307.696	-46.969
2,6	71.539	110.769	-310.443	-40.326
3,4	81.142	105.747	-297.256	-30.723
3,5	124.237	102.902	-302.317	12.372
3,6	66.786	100.21	-306.038	-45.079
4,5	66.763	110.026	-317.734	-45.102
4,6	82.258	106.188	-325.057	-29.607
5,6	73.831	106.769	-301.298	-38.034

Orientation	E	VDW	ELE	BE
1,2	234.125	158.795	-277.203	-56.831

1,3	174.818	144.049	-332.022	-116.138
1,4	175.332	144.724	-328.842	-115.624
1,5	175.273	141.697	-335.322	-115.683
1,6	203.267	150.974	-301.367	-87.689
2,3	261.714	151.998	-256.787	-29.242
2,4	197.163	152.466	-313.881	-93.793
2,5	188.361	139.103	-318.784	-102.595
2,6	225.616	155.656	-289.635	-65.34
3,4	351.223	145.078	-292.291	60.267
3,5	221.524	148.003	-280.388	-69.432
3,6				
4,5	278.088	157.567	-242.005	-12.868
4,6	221.931	147.302	-297.697	-69.025
5,6	252.268	148.868	-262.63	-38.688

Orientation	E	VDW	ELE	BE
1,2	218.582	159.945	-322.458	-16.365
1,3	-			
1,4	260.302	158.758	-325.046	25.355
1,5	204.274	159.378	-333.246	-30.673
1,6	202.873	157.91	-330.121	-32.074
2,3	185.698	154.978	-351.889	-49.249
2,4	210.371	156.005	-320.47	-24.576
2,5	206.953	156.191	-332.863	-27.994
2,6	216.575	162.503	-321.063	-18.372
3,4	230.306	154.791	-301.13	-4.641
3,5	212.212	160.022	-330.529	-22.735
3,6	-			
4,5	218.623	161.64	-323.384	-16.324
4,6	207.596	160.967	-330.786	-27.351
5,6	271.103	154.834	-313.541	36.156

Orientation	E	VDW	ELE	BE
1,2	-			
1,3	217.431	143.013	-308.705	-40.16
1,4	224.748	143.147	-304.13	-32.843
1,5	233.991	146.348	-311.568	-23.6
1,6	235.601	142.205	-291.793	-21.99
2,3	199.242	135.104	-318.229	-58.349
2,4	227.701	143.445	-298.487	-29.89
2,5	235.741	143.537	-291.619	-21.85
2,6	224.334	146.003	-306.241	-33.257
3,4	232.955	138.603	-294.295	-24.636
3,5	-			
3,6	-			

4,5	233.032	143.045	-293.423	-24.559
4,6	234.338	145.086	-292.546	-23.253
5,6	229.296	146.598	-302.225	-28.295

Orientation	E	VDW	ELE	BE
1,2	202.926	154.307	-334.016	-16.911
1,3	206.716	150.749	-334.305	-13.121
1,4	200.88	154.623	-343.307	-18.957
1,5	202.543	155.508	-343.04	-17.294
1,6	206.4	151.334	-332.644	-13.437
2,3	205.016	149.399	-338.428	-14.821
2,4	208.047	154.67	-333.896	-11.79
2,5	206.416	150.415	-335.751	-13.421
2,6	207.55	153.69	-333.394	-12.287
3,4	198.7	150.439	-339.894	-21.137
3,5	201.289	149.755	-338.419	-18.548
3,6	199.649	147.891	-338.273	-20.188
4,5	204.414	153.159	-336.127	-15.423
4,6	203.842	150.962	-340.194	-15.995
5,6	207.206	153.538	-333.629	-12.631

LF20

Orientation	E	VDW	ELE	BE
1,2	70.686	113.235	-306.342	-9.263
1,3	67.88	110.94	-304.443	-12.069
1,4	75.589	111.092	-302.201	-4.36
1,5	78.472	113.286	-299.949	-1.477
1,6	68.371	114.349	-312.83	-11.578
2,3	81.278	111.218	-299.051	1.329
2,4	61.954	115.747	-320.038	-17.995
2,5	59.241	114.328	-318.574	-20.708
2,6	65.969	113.778	-308.793	-13.98
3,4	67.472	115.113	-314.718	-12.477
3,5	58.063	111.658	-317.071	-21.886
3,6	61.789	114.761	-318.021	-18.16
4,5	66.987	114.641	-312.561	-12.962
4,6	60.286	111.142	-313.096	-19.663
5,6	71.781	110.568	-304.027	-8.168

Orientation	E	VDW	ELE	BE
1,2	90.346	116.695	-296.53	-21.519
1,3	156.881	110.036	-282.25	45.016
1,4	79.837	111.766	-301.407	-32.028
1,5	70.764	113.396	-315.721	-41.101
1,6	79.042	109.792	-306.984	-32.823
2,3	78.886	110.45	-306.235	-32.979
2,4	75.224	116.318	-312.251	-36.641
2,5	95.41	115.106	-290.619	-16.455
2,6	84.261	110.005	-300.916	-27.604
3,4	85.31	112.075	-296.789	-26.555
3,5	90.227	115.486	-299.411	-21.638
3,6	81.735	114.96	-306.16	-30.13
4,5	74.564	114.668	-304.72	-37.301
4,6	67.361	116.681	-325.171	-44.504
5,6	78.853	113.085	-303.287	-33.012

Orientation	E	VDW	ELE	BE
1,2	219.788	153.38	-299.072	-71.168
1,3	198.731	147.621	-310.235	-92.225
1,4	226.788	155.391	-285.609	-64.168
1,5	195.997	152.841	-311.393	-94.959
1,6	213.639	150.722	-281.909	-77.317
2,3	202.638	152.184	-306.048	-88.318
2,4	226.389	153.334	-287.004	-64.567
2,5	252.314	147.883	-260.484	-38.642
2,6	220.544	159.623	-289.915	-70.412
3,4	223.535	151.154	-288.265	-67.421
3,5	256.802	155.791	-260.405	-34.154
3,6	199.411	149.316	-314.142	-91.545
4,5	228.106	160.343	-290.236	-62.85
4,6	252.578	155.211	-256.082	-38.378
5,6	192.442	152.804	-307.877	-98.514

Orientation	E	VDW	ELE	BE
1,2	224.186	164.676	-316.475	-10.761
1,3	208.052	161.244	-331.345	-26.895
1,4	212.808	162.928	-325.019	-22.139
1,5	213.189	160.856	-320.298	-21.758
1,6	224.586	166.029	-315.549	-10.361
2,3	183.974	151.518	-357.463	-50.973
2,4	223.207	162.634	-316.362	-11.74
2,5	218.637	161.022	-320.018	-16.31
2,6	219.003	164.221	-322.933	-15.944
3,4	209.102	160.571	-324.558	-25.845
3,5	209.77	156.033	-324.194	-25.177
3,6	210.305	157.444	-321.201	-24.642
4,5	221.661	165.028	-318.441	-13.286
4,6	217.046	161.415	-324.574	-17.901
5,6	217.514	166.203	-324.271	-17.433

Orientation	E	VDW	ELE	BE
1,2	241.463	149.352	-295.806	-16.128
1,3	243.062	142.067	-293.585	-14.529
1,4	228.675	146.111	-298.449	-28.916
1,5	225.953	150.478	-306.219	-31.638
1,6	249.087	146.776	-293.281	-8.504
2,3	227.862	142.362	-305.388	-29.729
2,4	223.022	147.017	-311.862	-34.569
2,5	235.764	144.05	-295.625	-21.827
2,6	233.861	147.599	-306.404	-23.73
3,4	215.806	146.167	-316.447	-41.785
3,5	241.518	140.956	-295.674	-16.073
3,6	209.431	144.507	-319.43	-48.16
4,5	240.899	148.114	-296.868	-16.692
4,6	220.59	146.566	-316.663	-37.001
5,6	238.261	144.394	-299.397	-19.33

Orientation	E	VDW	ELE	BE
1,2	204.062	153.089	-335.001	-15.775
1,3	211.848	151.635	-329.068	-7.989
1,4	200.408	153.881	-343.575	-19.429
1,5	204.402	154.487	-337.613	-15.435
1,6	204.475	154.957	-338.503	-15.362
2,3	207.692	154.881	-334.316	-12.145
2,4	204.867	156.193	-336.895	-14.97
2,5	208.136	151.421	-334.522	-11.701
2,6	203.734	150.289	-333.339	-16.103
3,4	202.177	150.294	-338.513	-17.66
3,5	204.456	149.712	-333.887	-15.381
3,6	200.438	147.596	-336.321	-19.399
4,5	210.908	155.813	-332.836	-8.929
4,6	204.918	153.945	-337.816	-14.919
5,6	208.331	156.807	-335.368	-11.506

VF19

Orientation	E	VDW	ELE	BE
1,2	58.971	112.521	-319.283	-20.978
1,3	55.744	107.802	-318.164	-24.205
1,4	60.84	110.82	-319.207	-19.109
1,5	54.957	110.744	-327.391	-24.992
1,6	60.898	111.616	-318.522	-19.051
2,3	58.628	113.016	-327.787	-21.321
2,4	55.654	104.249	-312.915	-24.295
2,5	69.801	111.486	-305.809	-10.148
2,6	57.993	109.037	-320.809	-21.956
3,4	53.012	111.4	-326.735	-26.937
3,5	51.65	106.804	-322.344	-28.299
3,6	46.336	107.828	-328.008	-33.613
4,5	65.425	112.35	-311.396	-14.524
4,6	54.866	109.396	-322.597	-25.083

5,6	58.534	112.158	-318.592	-21.415

Orientation	E	VDW	ELE	BE
1,2	78.389	116.728	-320.602	-33.476
1,3	80.603	111.942	-303.959	-31.262
1,4	65.987	110.791	-317.528	-45.878
1,5	55.248	111.915	-327.418	-56.617
1,6	79.171	111.285	-304.363	-32.694
2,3	66.569	108.993	-311.989	-45.296
2,4	88.442	112.093	-295.188	-23.423
2,5	76.185	108.837	-304.824	-35.68
2,6	66.606	113.482	-327.514	-45.259
3,4	69.452	107.361	-314.19	-42.413
3,5	61.843	112.121	-315.885	-50.022
3,6	65.568	104.157	-312.254	-46.297
4,5	79.612	111.55	-303.883	-32.253
4,6	83.821	110.983	-298.398	-28.044
5,6	97.682	116.156	-289.183	-14.183

Orientation	E	VDW	ELE	BE
1,2	228.77	144.045	-300.662	-62.186
1,3	174.084	147.599	-322.425	-116.872
1,4	181.193	149.16	-326.111	-109.763
1,5	221.038	150.435	-294.603	-69.918
1,6	185.569	156.285	-321.765	-105.387
2,3	224.025	150.681	-289.474	-66.931
2,4	172.362	150.876	-331.862	-118.594
2,5	221.275	146.025	-290.271	-69.681
2,6	186.835	149.112	-322.078	-104.121
3,4	207.778	145.844	-299.446	-83.178
3,5	171.599	143.632	-346.24	-119.357
3,6	250.491	146.931	-319.314	-40.465
4,5	207.42	146.664	-304.279	-83.536
4,6	199.488	147.022	-311.255	-91.468
5,6	336.791	158.917	-307.694	45.835

Orientation	E	VDW	ELE	BE
1,2	224.14	165.665	-316.46	-10.807
1,3	210.129	160.084	-330.78	-24.818
1,4	208.553	161.414	-328.641	-26.394
1,5	193.864	157.07	-342.753	-41.083
1,6	195.942	159.162	-344.496	-39.005
2,3	207.041	163.913	-332.491	-27.906
2,4	218.472	162.936	-321.473	-16.475
2,5	193.051	159.772	-347.5	-41.896

2,6	207.844	159.027	-332.512	-27.103
3,4	202.862	160.707	-335.07	-32.085
3,5	201.183	161.756	-336.732	-33.764
3,6	197.397	159.355	-338.03	-37.55
4,5	206.791	164.449	-335.436	-28.156
4,6	206.622	158.403	-330.783	-28.325
5,6	209.702	164.13	-330.319	-25.245

Orientation	E	VDW	ELE	BE
1,2	224.177	146.465	-305.964	-33.414
1,3	212.079	138.079	-317.437	-45.512
1,4	208.758	142.261	-325.76	-48.833
1,5	202.571	140.802	-334.396	-55.02
1,6	207.101	141.228	-321.46	-50.49
2,3	209.186	138.425	-321.49	-48.405
2,4	209.527	141.438	-324.667	-48.064
2,5	203.713	139.209	-326.618	-53.878
2,6	210.66	143.821	-326.915	-46.931
3,4	210.289	138.703	-321.741	-47.302
3,5	220.139	142.164	-324.455	-37.452
3,6	200.442	136.57	-332.433	-57.149
4,5	203.852	144.486	-319.782	-53.739
4,6	210.433	142.821	-320.06	-47.158
5,6	228.647	142.25	-308.294	-28.944

Orientation	E	VDW	ELE	BE
1,2	171.012	150.542	-365.742	-48.825
1,3	180.093	148.907	-357.831	-39.744
1,4	231.91	145.638	-355.718	12.073
1,5	189.421	149.642	-343.665	-30.416
1,6	154.139	149.04	-379.308	-65.698
2,3	229.006	148.804	-360.866	9.169
2,4	178.208	151.014	-361.983	-41.629
2,5	175.044	155.536	-370.519	-44.793
2,6	196.762	153.304	-345.189	-23.075
3,4	163.943	152.395	-376.612	-55.894
3,5	148.354	140.926	-386.413	-71.483
3,6	-			
4,5	178.344	152.102	-360.962	-41.493
4,6	209.089	146.444	-375.858	-10.748
5,6	165.313	151.135	-372.371	-54.524

VF20

Orientation	E	VDW	ELE	BE
1,2	50.704	107.084	-327.341	-29.245
1,3	56.763	108.379	-318.912	-23.186
1,4	47.954	101.069	-322.251	-31.995
1,5	52.267	111.794	-328.694	-27.682
1,6	60.494	110.654	-316.498	-19.455
2,3	59.241	109.144	-318.326	-20.708
2,4	40.47	110.951	-341.989	-39.479
2,5	56.958	108.422	-311.996	-22.991
2,6	64.854	106.015	-346.449	-15.095
3,4	48.632	109.104	-335.339	-31.317
3,5	1801			
3,6	43.953	105.202	-332.655	-35.996
4,5	60.02	113.432	-322.55	-19.929
4,6	35.148	106.05	-333.241	-44.801
5,6	54.553	107.908	-321.969	-25.396

Orientation	E	VDW	ELE	BE
1,2	89.3	110.633	-291.805	-22.565
1,3	55.238	107.813	-321.28	-56.627
1,4	41.929	101.599	-331.559	-69.936
1,5	45.34	101.822	-336.551	-66.525
1,6	62.892	110.412	-320.421	-48.973
2,3	46.14	109.841	-339.808	-65.725
2,4	45.738	105.802	-335.417	-66.127
2,5	65.937	111.996	-320.553	-45.928
2,6	68.478	114.167	-314.78	-43.387
3,4	68.172	105.118	-311.985	-43.693
3,5	42.149	104.796	-332.996	-69.716
3,6	80.57	107.458	-303.591	-31.295
4,5	69.758	106.181	-308.953	-42.107
4,6	56.506	105.245	-322.235	-55.359
5,6	45.217	106.4	-333.743	-66.648

No AML data

Orientation	E	VDW	ELE	BE
1,2	220.174	164.859	-324.102	-14.773
1,3	195.398	152.375	-340.176	-39.549
1,4	206.779	158.719	-327.658	-28.168

1,5	207.721	155.392	-322.189	-27.226
1,6	206.718	154.826	-328.155	-28.229
2,3	207.751	160.197	-329.1	-27.196
2,4	207.125	155.197	-329.544	-27.822
2,5	204.671	156.966	-326.217	-30.276
2,6	219.345	160.264	-319.372	-15.602
3,4	213.846	161.536	-323.628	-21.101
3,5	213.39	162.638	-329.306	-21.557
3,6	216.722	155.769	-327.979	-18.225
4,5	219.435	163.303	-319.48	-15.512
4,6	216.708	162.629	-323.215	-18.239
5,6	219.349	161.693	-317.649	-15.598

Orientation	E	VDW	ELE	BE
1,2	210.659	147.512	-318.146	-46.932
1,3	218.868	139.662	-311.217	-38.723
1,4	221.03	140.99	-313.618	-36.561
1,5	220.722	144.375	-311.81	-36.869
1,6	224.539	144.38	-308.835	-33.052
2,3	210.321	140.186	-322.823	-47.27
2,4	221.093	141.724	-313.154	-36.498
2,5	224.609	144.221	-314.686	-32.982
2,6	228.635	142.106	-308.762	-28.956
3,4	207.949	140.45	-315.891	-49.642
3,5	228.5	138.719	-297.783	-29.091
3,6	245.635	150.71	-306.181	-11.956
4,5	222.387	145.757	-302.989	-35.204
4,6	357.04	155.836	-307.568	99.449
5,6	215.762	139.092	-310.228	-41.829

Orientation	E	VDW	ELE	BE
1,2	208.624	153.365	-332.212	-11.213
1,3	185.631	148.635	-343.683	-34.206
1,4	181.809	144.233	-351.848	-38.028
1,5	182.742	145.681	-350.733	-37.095
1,6	193.851	149.75	-348.399	-25.986
2,3	195.312	152.192	-343.105	-24.525
2,4	189.249	149.123	-347.339	-30.588
2,5	184.819	141.376	-351.248	-35.018
2,6	199.092	150.062	-340.18	-20.745
3,4	181.432	148.109	-354.897	-38.405
3,5	194.382	151.554	-341.006	-25.455
3,6	-			

4,5	203.018	153.922	-337.077	-16.819
4,6	255.55	149.26	-346.602	35.713
5,6	198.041	150.451	-340.534	-21.796

FF

Orientation	E	VDW	ELE	BE
1,2	66.283	112.877	-310.358	-13.666
1,3	62.728	112.985	-315.018	-17.221
1,4	65.439	110.28	-308.606	-14.51
1,5	46.534	111.575	-330.734	-33.415
1,6	58.215	109.927	-315.76	-21.734
2,3	62.054	114.352	-322.14	-17.895
2,4	77.037	111.962	-300.078	-2.912
2,5	45.091	106.253	-327.141	-34.858
2,6	58.247	111.913	-317.538	-21.702
3,4	47.411	110.826	-328.817	-32.538
3,5	60.447	110.196	-316.54	-19.502
3,6	48.952	106.724	-328.214	-30.997
4,5	59.281	115.594	-326.689	-20.668
4,6	66.144	106.548	-306.23	-13.805
5,6	53.057	113.529	-329.954	-26.892

Orientation	E	VDW	ELE	BE
1,2	95.198	109.461	-288.184	-16.667
1,3	73.07	107.848	-308.463	-38.795
1,4	76.653	106.322	-304.972	-35.212
1,5	67.282	103.766	-311.199	-44.583
1,6	70.432	104.459	-306.949	-41.433
2,3	71.683	103.836	-305.785	-40.182
2,4	77.855	109.923	-303.127	-34.01
2,5	50.469	99.39	-323.797	-61.396
2,6	75.326	106.037	-307.767	-36.539
3,4	62.568	110.575	-317.405	-49.297
3,5	53.656	110.419	-330.364	-58.209
3,6	53.972	105.943	-326.799	-57.893
4,5	79.496	113.448	-301.887	-32.369
4,6	65.205	109.937	-319.013	-46.66
5,6	64.835	104.371	-309.201	-47.03

Orientation	E	VDW	ELE	BE
1,2	265.139	156.597	-254.665	-25.817
1,3	209.929	151.889	-302.178	-81.027
1,4	246.443	161.085	-266.843	-44.513
1,5	239.58	156.89	-276.996	-51.376
1,6	226.652	154.582	-285.983	-64.304
2,3	192.737	160.394	-323.262	-98.219
2,4	239.04	161.591	-271.885	-51.916
2,5	218.435	154.671	-291.763	-72.521
2,6	226.448	157.596	-283.065	-64.508
3,4	200.772	151.616	-313.081	-90.184
3,5	240.981	154.936	-271.329	-49.975
3,6	258.641	153.133	-259.992	-32.315
4,5	201.829	154.18	-310.626	-89.127
4,6	180.502	152.882	-329.052	-110.454
5,6	205.49	155.145	-305.279	-85.466

NO BA4

Orientation	E	VDW	ELE	BE
1,2	235.164	150.161	-301.143	-22.427
1,3	255.077	142.004	-283.879	-2.514
1,4	242.343	148.64	-293.3	-15.248
1,5	241.348	144.815	-293.267	-16.243
1,6	253.211	145.191	-288.007	-4.38
2,3	229.483	141.065	-301.132	-28.108
2,4	246.792	145.288	-289.2	-10.799
2,5	229.869	140.569	-299.035	-27.722
2,6	235.132	145.681	-291.822	-22.459
3,4	230.088	141.28	-296.715	-27.503
3,5	240.182	146.835	-294.385	-17.409
3,6	249.756	143.477	-290.774	-7.835
4,5	235.171	147.981	-298.16	-22.42
4,6	231.702	142.009	-299.076	-25.889
5,6	251.534	145.264	-283.12	-6.057

Orientation	E	VDW	ELE	BE
1,2	219.533	157.186	-323.943	-0.304
1,3	205.609	151.046	-333.517	-14.228
1,4	201.079	152.499	-342.496	-18.758
1,5	204.598	152.964	-340.246	-15.239
1,6	204.434	155.485	-338.407	-15.403
2,3	209.428	155.207	-333.336	-10.409

2,4	201.176	152.602	-342.524	-18.661
2,5	206.55	151.789	-337.36	-13.287
2,6	207.068	156.283	-335.97	-12.769
3,4	205.577	155.975	-337.986	-14.26
3,5	205.681	149.303	-333.959	-14.156
3,6	200.053	152.235	-341.847	-19.784
4,5	214.035	154.807	-327.373	-5.802
4,6	200.071	147.695	-342.264	-19.766
5,6	225.645	154.24	-314.672	5.808

INTERACTIONS IN GAS PHASE

HH

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	14	CC4	1,5
1AMB	AH	14	CC4	2,5
1AMB	AH	17	C-ring	3,6
1AMB	AH	17	CB1	4,6
1AMC	AH	17	A-ring	3,5
1AMC	AH	14	CB1	4,6
1AML	SCD	13	1	3,4
1BA4	AA	13	B-ring	3,6
1Z0Q	AH	14	C-ring	1,3

H13K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMC	AH	17	B-ring	1,6
1AMC	SCD	16	4	2,4
1AMC	A+	13	C-ring	3,6
1AMC	AH	17	B-ring	3,6
1AML	AH	16	C-ring	2,5
1AML	AH	16	A-ring	2,5
1BA4	AH	10	B-ring	1,2
1BA4	AA	10	B-ring	1,4
1BA4	BBA	10	6	1,6
1BA4	BBA	10	5	3,5
1BA4	AA	10	A-ring	3,5
1BA4	BBA	11	4	3,5
1BA4	AH	13	C-ring	3,5
1BA4	AH	13	A-ring	3,5
1BA4	BBA	12	5	4,6
1BA4	AH	10	C-ring	4,6
1BA4	BBA	10	6	4,6
1IYT	AH	20	2	4,6
1Z0Q	AH	12	C-ring	3,5

H14K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	13	1	1,6
1AMB	BBA	13	2	1,6
1AMB	AA	13	B-ring	2,5
1AMB	BBA	13	5	4,6
1AML	BBA	13	2	1,2
1AML	BBA	13	6	1,3
1AML	AH	13	CA1	1,4
1AML	BBA	16	6	1,5
1AML	AA	13	A-ring	2,5
1AML	AH	13	C-ring	2,5
1AML	AH	17	A-ring	3,4
1AML	BBA	13	6	3,6
1AML	AH	14	C-ring	3,6
1AML	AH	13	CC4	4,6
1BA4	BBA	10	6	1,6
1BA4	BBA	10	4	2,5
1BA4	AH	20	5	2,6
1BA4	AH	17	C-ring	3,4
1BA4	AH	17	C-ring	3,6
I1YT	SCA	11	2	1,3
1IYT	SCA	7	1	1,5
1IYT	BBA	12	1	2,5
1IYT	AH	14	B-ring	3,5
1IYT	BBA	11	4	4,5
1IYT	AH	11	A-ring	4,6
1Z0Q	AH	14	B-ring	2,5
1Z0Q	AH	17	C-ring	2,6
1Z0Q	AH	14	A-ring	3,5
1Z0Q	AH	17	C-ring	4,5

LV

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	17	B-ring	2,5
1AMB	SCA	22	4	2,5
1AMB	SCA	22	4	3,4
1AMB	SCA	22	6	4,6
1AMB	SCA	22	6	5,6
1AMC	AH	18	A-ring	1,3
1AMC	SCA	22	4	1,3
1AMC	AH	18	A-ring	1,4
1AMC	SCA	22	5	1,5
1AMC	SCA	22	CC4	1,5
1AMC	SCA	22	4	2,3
1AMC	AH	17	B-ring	2,4
1AMC	AH	18	A-ring	3,4
1AMC	SCA	22	5	3,5
1AMC	AH	18	C-ring	4,6
1AML	SCA	35	6	1,2
1AML	BBA	40	4	1,2
1AML	AH	14	B-ring	2,4
1AML	AH	14	CB1	3,5
1AML	AH	18	A-ring	3,6
1AML	AH	18	C-ring	3,6
1AML	AH	18	A-ring	4,5
1AML	SCA	35	4	5,6
1IYT	AH	17	C-ring	3,6
1Z0Q	A+	14	C-ring	1,3
1Z0Q	SCA	22	4	1,4
1Z0Q	SCA	22	4	2,4
1Z0Q	AH	18	A-ring	2,5

LF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	16	1	1,5
1AMB	BBA	16	1	1,6
1AMB	SCA	23	4	2,5
1AMB	BBA	16	4	3,6
1AMB	AH	20	B-ring	3,6
1AMB	BBA	16	4	4,5
1AMC	BBA	16	1	2,5
1AMC	SCD	16	1	2,6
1AMC	BBA	16	4	4,6
1AMC	SCA	23	CC4	4,6
1AML	SCA	23	5	1,3
1AML	SCA	23	4	1,4
1AML	AH	20	C-ring	1,5
1AML	AA	20	C-ring	4,6
1AML	SCA	23	1	4,6
1BA4	BBA	15	2	1,2
1BA4	AH	18	C-ring	1,5
1BA4	AH	19	6	1,6
1BA4	BBA	14	1	2,5
1BA4	SCA	15	6	2,5
1BA4	AH	18	C-ring	2,5
1BA4	SCA	22	4	2,5
1BA4	BBA	14	1	3,5
1IYT	AH	20	B-ring	1,3
1IYT	BBA	16	1	1,6
1IYT	AA	20	A-ring	1,6

1IYT	AA	20	C-ring	2,4
1IYT	AH	20	CB1	2,5
1IYT	AH	20	1	2,5
1Z0Q	AH	20	A-ring	1,3
1Z0Q	AH	19	A-ring	2,5

LF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	SCD	13	1	3,4
1AMB	AH	17	B-ring	3,4
1AMC	AH	16	B-ring	1,3
1AML	AH	30	B-ring	3,6
1AML	AH	20	C-ring	4,6
1BA4	AA	20	C-ring	2,3
1Z0Q	BBA	16	2	1,2
1Z0Q	AH	20	CB1	4,6

VF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	15	A-ring	2,4
1AMB	SCA	22	2	3,4
1AMB	AH	18	A-ring	3,5
1AMB	SCA	11	2	3,6
1AMC	SCA	22	1	1,2
1AMC	SCA	22	6	1,6
1AMC	SCA	22	1	2,6
1AMC	SCA	22	5	3,6
1AML	SCA	22	1	1,2
1AML	SCA	22	2	1,2
1AML	SCA	15	1	1,3
1AML	AH	19	A-ring	1,3

VF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	17	B-ring	2,5
1AMB	BBA	17	1	2,5
1AMB	AH	17	C-ring	3,4
1AMB	SCA	22	1	3,4
1AMB	AH	17	C-ring	5,6
1AMC	BBA	28	4	1,4
1AMC	AH	21	B-ring	1,6
1AMC	BBA	28	5	2,3
1AMC	SCA	22	1	3,5
1BA4	AH	24	A-ring	1,6
1BA4	AH	18	A-ring	3,6
1BA4	BBA	17	4	4,5
1IYT	BBA	17	2	1,2
1IYT	AH	24	C-ring	2,3
1IYT	AH	24	C-ring	2,6
1IYT	BBA	13	4	3,6
1Z0Q	BBA	17	2	1,2
1Z0Q	AH	20	4	2,3
1Z0Q	AH	21	C-ring	2,4

FF

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	19	B-ring	1,3
1AMB	AA	19	B-ring	3,4
1AMC	AH	19	B-ring	2,6
1AMC	SCA	23	4	3,5
1AMC	AH	19	A-ring	4,6
1AMC	AH	19	A-ring	5,6
1AMC	SCA	23	6	5,6
1AML	AH	20	C-ring	1,3
1AML	SCA	23	CA1	3,4
1AML	AH	19	C-ring	3,4
1AML	AH	19	C-ring	3,6
1AML	SCA	23	5	3,6
1IYT	AH	20	C-ring	1,3
1IYT	A+	16	B-ring	1,6
1IYT	AH	20	B-ring	2,6
1IYT	AH	20	A-ring	3,5

APPENDIX D: DATA FOR QUEBECOL

Tables of energies for gas phase calculations of quebecol. All energies are in kcal/mol. The order of the tables for each pair of amino acids is always 1AMB, 1AMC, 1AML, 1BA4, 1IYT, 1Z0Q.

HH

	E	VDW	ELE	BE
1,2	86.36	113.513	-300.246	-21.553
1,3	86.657	112.581	-304.049	-21.256
1,4	76.171	112.145	-305.51	-31.742
1,5	89.401	113.96	-300.645	-18.512
1,6	93.055	113.043	-301.126	-14.858
1,7	81.969	111.284	-303.444	-25.944
2,3	87.031	114.189	-302.164	-20.882
2,4	83.78	111.715	-301.747	-24.133
2,5	81.652	110.644	-304.967	-26.261
2,6	89.129	109.762	-293.135	-18.784
2,7	90.191	113.809	-294.305	-17.722
3,4	77.18	108.685	-302.398	-30.733
3,5	79.607	113.511	-303.664	-28.306
3,6	87.254	112.54	-295.586	-20.659
3,7	58.5	106.679	-324.244	-49.413
4,5	82.714	109.974	-297.269	-25.199
4,6	88.578	114.79	-298.772	-19.335
4,7	79.532	105.593	-298.603	-28.381
5,6	83.883	113.17	-301.416	-24.03
5,7	87.335	117.066	-299.304	-20.578
6,7	85.594	113.314	-298.327	-22.319

	E	VDW	ELE	BE
1,2	110.074	116.137	-292.597	-29.755
1,3	104.127	113.761	-288.979	-35.702
1,4	105.343	108.957	-292.557	-34.486
1,5	114.295	112.541	-278.253	-25.534
1,6	102.867	107.397	-291.072	-36.962
1,7	112.208	115.083	-280.908	-27.621
2,3	116.072	113.448	-277.125	-23.757
2,4	103.24	110.463	-289.298	-36.589

2,5	90.419	106.506	-296.81	-49.41
2,6	105.301	107.137	-280.781	-34.528
2,7	95.034	119.833	-300.437	-44.795
3,4	110.214	113.818	-290.706	-29.615
3,5	109.748	112.487	-280.358	-30.081
3,6	111.546	110.442	-280.159	-28.283
3,7	91.528	108.224	-295.216	-48.301
4,5	109.086	109.962	-281.916	-30.743
4,6	80.491	117.511	-320.633	-59.338
4,7	105.738	114.139	-296.384	-34.091
5,6	122.098	112.353	-272.438	-17.731
5,7	109.333	115.529	-294.168	-30.496
6,7	102.316	114.283	-293.362	-37.513

	E	VDW	ELE	BE
1,2	257.241	160.338	-255.316	-61.679
1,3	297.762	159.768	-231.238	-21.158
1,4	282.642	156.965	-240.368	-36.278
1,5	295.874	158.752	-230.411	-23.046
1,6	283.763	154.713	-238.717	-35.157
1,7	292.264	164.125	-240.547	-26.656
2,3	274.334	156.055	-246.073	-44.586
2,4	246.684	159.86	-266.671	-72.236
2,5	274.501	156.019	-248.394	-44.419
2,6	258.134	154.681	-263.503	-60.786
2,7	251.605	154.414	-255.089	-67.315
3,4	260.821	153.366	-245.686	-58.099
3,5	244.4	145.274	-264.809	-74.52
3,6	266.564	158.926	-257.365	-52.356
3,7	247.657	151.222	-273.836	-71.263
4,5	249.601	151.323	-270.457	-69.319
4,6	250.473	152.929	-255.519	-68.447
4,7	286.107	150.989	-232.683	-32.813
5,6	226.42	152.939	-293.2	-92.5
5,7	266.273	155.871	-256.552	-52.647
6,7	221.226	147.566	-295.615	-97.694

	E	VDW	ELE	BE
1,2	251.113	171.206	-301.437	-11.798
1,3	244.874	169.131	-304.26	-18.037
1,4	260.538	172.896	-293.119	-2.373
1,5	245.388	168.111	-300.494	-17.523
1,6	247.64	169.621	-303.846	-15.271
1,7	247.767	169.199	-303.326	-15.144
2,3	249.401	170.607	-303.817	-13.51
2,4	247.044	169.789	-303.128	-15.867
2,5	244.474	169.348	-303.044	-18.437
2,6	250.731	165.723	-295.879	-12.18
2,7	252.951	170.197	-300.235	-9.96
3,4	255.168	170.906	-297.212	-7.743
3,5	254.132	169.945	-297.654	-8.779
3,6	250.572	169.869	-302.775	-12.339
3,7	246.219	169.28	-303.533	-16.692
4,5	239.009	163.888	-306.893	-23.902
4,6	248.983	170.74	-303.718	-13.928
4,7	249.396	167.957	-301.381	-13.515
5,6	252.698	170.539	-300.206	-10.213
5,7	248.663	169.175	-300.454	-14.248
6,7	250.998	170.528	-301.632	-11.913

	E	VDW	ELE	BE
1,2	249.907	150.419	-297.456	-35.648
1,3	258.396	151.841	-293.16	-27.159
1,4	264.401	144.137	-282.873	-21.154
1,5	255.131	152.316	-297.341	-30.424
1,6	259.43	154.597	-291.113	-26.125
1,7	273.857	151.293	-275.994	-11.698
2,3	254.127	151.434	-293.646	-31.428
2,4	255.269	150.386	-290.673	-30.286
2,5	247.859	146.112	-295.024	-37.696
2,6	248.7	145.247	-297.522	-36.855
2,7	263.553	150.304	-283.221	-22.002
3,4	257.154	152.868	-289.456	-28.401
3,5	269.418	149.2	-278.546	-16.137

3,6	270.458	149.905	-279.504	-15.097
3,7	252.909	146.336	-288.318	-32.646
4,5	266.38	149.256	-283.207	-19.175
4,6	267.273	150.731	-282.522	-18.282
4,7	256.618	152.523	-293.751	-28.937
5,6	257.256	151.056	-288.557	-28.299
5,7	255.087	146.063	-283.787	-30.468
6,7	262.234	153.325	-288.677	-23.321

	E	VDW	ELE	BE
1,2	236.014	160.201	-316.456	-11.787
1,3	221.273	152.759	-324.923	-26.528
1,4	223.01	152.418	-323.398	-24.791
1,5	225.603	153.918	-319.01	-22.198
1,6	297.002	160.253	-322.358	49.201
1,7	233.803	153.051	-320.318	-13.998
2,3	220.805	156.528	-330.298	-26.996
2,4	222.306	156.642	-329.447	-25.495
2,5	294.095	154.171	-321.093	46.294
2,6	223.845	149.682	-320.49	-23.956
2,7	228.741	154.184	-319.36	-19.06
3,4	229.795	158.899	-322.932	-18.006
3,5	232.988	158.286	-321.185	-14.813
3,6	221.776	157.411	-330.523	-26.025
3,7	219.919	151.235	-324.833	-27.882
4,5	231.146	155.958	-320.182	-16.655
4,6	226.074	155.165	-323.961	-21.727
4,7	224.4	154.409	-331.825	-23.401
5,6	231.83	161.752	-325.274	-15.971
5,7	224.356	149.842	-322.12	-23.445
6,7	227.943	155.351	-328.028	-19.858

H13K

	E	VDW	ELE	BE
1,2	86.01	110.778	-293.956	-21.903
1,3	95.987	118.851	-293.932	-11.926
1,4	94.753	118.842	-296.303	-13.16

1,5	94.512	118.598	-293.212	-13.401
1,6	82.179	121.682	-307.782	-25.734
1,7	84.302	120.003	-303.42	-23.611
2,3	85.616	119.436	-304.425	-22.297
2,4	87.553	115.159	-298.033	-20.36
2,5	89.478	115.066	-297.838	-18.435
2,6	83.573	117.576	-304.474	-24.34
2,7	92.153	117.482	-296.005	-15.76
3,4	82.558	119.4	-306.671	-25.355
3,5	85.868	113.763	-299.45	-22.045
3,6	95.077	115.693	-290.997	-12.836
3,7	80.91	116.946	-307.168	-27.003
4,5	85.338	114.535	-299.158	-22.575
4,6	83.16	121.758	-307.334	-24.753
4,7	95.315	116.743	-293.137	-12.598
5,6	93.031	116.278	-295.169	-14.882
5,7	89.179	114.188	-296.956	-18.734
6,7	88.417	116.02	-298.32	-19.496

	E	VDW	ELE	BE
1,2	107.383	115.209	-284.609	-32.446
1,3	105.948	118.784	-288.83	-33.881
1,4	121.75	116.014	-272.585	-18.079
1,5	121.37	121.802	-278.419	-18.459
1,6	104.036	114.34	-289.421	-35.793
1,7	125.175	120.426	-271.353	-14.654
2,3	118.844	115.454	-272.723	-20.985
2,4	117.741	114.502	-273.293	-22.088
2,5	111.029	118.836	-286.437	-28.8
2,6	93.667	109.322	-301.116	-46.162
2,7	132.291	120.125	-264.445	-7.538
3,4	106.28	116.745	-288.967	-33.549
3,5	121.634	117.832	-277.196	-18.195
3,6	113.567	117.93	-278.84	-26.262
3,7	130.222	115.279	-263.676	-9.607
4,5	126.341	117.062	-271.497	-13.488
4,6	126.258	119.776	-271.08	-13.571
4,7	119.219	118.874	-276.314	-20.61

5,6	114.659	119.447	-288.768	-25.17
5,7	115.576	117.141	-277.804	-24.253
6,7	122.014	117.958	-274.576	-17.815

	E	VDW	ELE	BE
1,2	223.237	166.265	-298.716	-95.683
1,3	224.256	164.072	-294.273	-94.664
1,4	256.828	162.328	-264.828	-62.092
1,5	276.522	161.312	-247.085	-42.398
1,6	260.014	158.132	-250.048	-58.906
1,7	276.667	162.569	-249.439	-42.253
2,3	280.907	161.843	-247.726	-38.013
2,4	280.474	160.811	-247.314	-38.446
2,5	206.761	156.004	-311.642	-112.159
2,6	217.001	153.599	-291.622	-101.919
2,7	234.213	163.574	-290.935	-84.707
3,4	297.493	164.354	-231.031	-21.427
3,5	219.088	157.549	-294.61	-99.832
3,6	257.515	159.955	-253.205	-61.405
3,7	293.483	157.492	-237.157	-25.437
4,5	274.886	160.739	-252.568	-44.034
4,6	245.525	161.587	-277.835	-73.395
4,7	217.543	161.669	-297.415	-101.377
5,6	278.185	163.716	-244.516	-40.735
5,7	258.118	158.79	-268.811	-60.802
6,7	275.637	161.417	-248.383	-43.283

	E	VDW	ELE	BE
1,2	246.463	164.738	-301.287	-16.448
1,3	236.985	161.829	-307.858	-25.926
1,4	235.533	164.325	-313.924	-27.378
1,5	223.477	160.482	-323.743	-39.434
1,6	223.937	157.085	-322.975	-38.974
1,7	241.286	149.316	-301.843	-21.625
2,3	222.857	154.237	-316.369	-40.054
2,4	227.015	159.082	-319.437	-35.896
2,5	220.815	150.638	-315.983	-42.096
2,6	224.289	157.993	-321.792	-38.622
2,7	236.384	159.143	-308.697	-26.527
3,4	294.171	152.619	-301.623	31.26

3,5	230.627	160.991	-308.726	-32.284
3,6	237.457	162.453	-306.327	-25.454
3,7	244.789	160.326	-305.597	-18.122
4,5	239.134	163.335	-305.336	-23.777
4,6	231.756	164.15	-312.246	-31.155
4,7	n/a			
5,6	247.602	164.801	-300.131	-15.309
5,7	234.317	162.156	-309.035	-28.594
6,7	241.833	156.373	-301.793	-21.078

	E	VDW	ELE	BE
1,2	317.219	148.628	-286.784	32.264
1,3	246.003	144.962	-292.632	-38.952
1,4	259.013	146.815	-284.407	-25.942
1,5	263.869	153.343	-285.006	-21.086
1,6	256.536	147.863	-282.656	-28.419
1,7	243.146	154.301	-304.266	-41.809
2,3	263.884	150.334	-279.981	-21.071
2,4	259.369	152.954	-285.808	-25.586
2,5	250.739	143.354	-287.569	-34.216
2,6	265.165	144.432	-280.164	-19.79
2,7	274.541	149.548	-273.681	-10.414
3,4	271.849	148.906	-276.074	-13.106
3,5	262.522	151.822	-285.375	-22.433
3,6	262.629	151.643	-285.698	-22.326
3,7	248.173	145.585	-293.464	-36.782
4,5	251.683	147.833	-288.389	-33.272
4,6	251.203	149.353	-295.338	-33.752
4,7	255.006	146.328	-285.574	-29.949
5,6	250.592	150.658	-294.084	-34.363
5,7	263.921	151.824	-283.787	-21.034
6,7	261.449	151.046	-284.763	-23.506

	E	VDW	ELE	BE
1,2	232.746	161.663	-321.589	-15.055
1,3	236.464	162.835	-319.168	-11.337
1,4	230.902	159.179	-321.314	-16.899
1,5	231.709	160.343	-322.967	-16.092
1,6	231.341	159.039	-324.055	-16.46
1,7	236.564	162.059	-318.055	-11.237

2,3	236.574	161.677	-320.324	-11.227
2,4	234.451	161.261	-321.757	-13.35
2,5	228.157	159.981	-324.952	-19.644
2,6	230.043	154.272	-317.429	-17.758
2,7	235.654	159.046	-318.045	-12.147
3,4	231.284	156.734	-319.718	-16.517
3,5	232.007	158.514	-319.847	-15.794
3,6	232.882	160.155	-321.222	-14.919
3,7	230.084	158.015	-322.641	-17.717
4,5	235.6	161.003	-319.63	-12.201
4,6	227.81	157.014	-323.221	-19.991
4,7	222.849	156.867	-327.295	-24.952
5,6	231.305	159.661	-320.598	-16.496
5,7	237.505	159.897	-315.543	-10.296
6,7	233.547	158.747	-321.495	-14.254

H14K

	E	VDW	ELE	BE
1,2	82.755	112.561	-303.764	-25.158
1,3	132.816	109.478	-304.07	24.903
1,4	66.124	105.251	-308.669	-41.789
1,5	83.005	109.69	-302.82	-24.908
1,6	81.449	110.211	-303.389	-26.464
1,7	87.69	113.516	-302.742	-20.223
2,3	73.021	106.029	-305.133	-34.892
2,4	86.513	110.81	-301.358	-21.4
2,5	57.493	105.172	-319.613	-50.42
2,6	139.812	111.073	-302.693	31.899
2,7	78.233	109.763	-306.246	-29.68
3,4	132.808	109.696	-304.422	24.895
3,5	91.823	113.641	-304.453	-16.09
3,6	75.364	113.143	-310.273	-32.549
3,7	72.45	108.775	-313.123	-35.463
4,5	76.657	109.203	-306.836	-31.256
4,6	89.047	111.133	-297.834	-18.866
4,7	74.209	108.018	-309.696	-33.704
5,6	76.937	111.984	-309.267	-30.976
5,7	69.218	104.539	-307.929	-38.695
6,7	80.84	113.028	-303.95	-27.073

	E	VDW	ELE	BE
1,2	98.574	112.771	-299.345	-41.255
1,3	107.132	114.187	-289.228	-32.697
1,4	230.849	109.961	-303.367	91.02
1,5	122.15	108.485	-282.864	-17.679
1,6	87.263	111.639	-298.77	-52.566
1,7	104.946	113.906	-293.025	-34.883
2,3	100.786	114.385	-295.098	-39.043
2,4	96.699	113.894	-302.522	-43.13
2,5	113.358	109.515	-285.164	-26.471
2,6	92.595	106.756	-301.486	-47.234
2,7	111.938	109.267	-275.186	-27.891
3,4	113.873	117.226	-314.76	-25.956
3,5	109.191	116.567	-285.943	-30.638
3,6	110.415	119.867	-296.278	-29.414
3,7	101.983	109.39	-293.893	-37.846
4,5	98.376	120.723	-297.791	-41.453
4,6	102.191	113.586	-298.539	-37.638
4,7	95.625	114.462	-295.4	-44.204
5,6	106.439	115.353	-288.418	-33.39
5,7	89.732	109.147	-295.062	-50.097
6,7	99.644	112.793	-292.265	-40.185

	E	VDW	ELE	BE
1,2	285.949	151.589	-235.116	-32.971
1,3	240.267	153.726	-281.862	-78.653
1,4	234.616	144.084	-279.791	-84.304
1,5	226.899	158.977	-297.671	-92.021
1,6	272.045	156.356	-247.478	-46.875
1,7	250.772	157.964	-259.565	-68.148
2,3	213.769	158.211	-307.549	-105.151
2,4	267.825	147.419	-253.824	-51.095
2,5	246.871	139.944	-262.692	-72.049
2,6	269.602	146.686	-248.069	-49.318
2,7	253.014	156.114	-269.778	-65.906
3,4	256.548	158.055	-260.156	-62.372
3,5	253.075	147.113	-254.78	-65.845
3,6	254.548	158.922	-264.601	-64.372

3,7	244.201	150.602	-267.375	-74.719
4,5	210.414	141.252	-306.611	-108.506
4,6	240.345	155.825	-276.935	-78.575
4,7	231.737	147.626	-285.807	-87.183
5,6	258.441	150.807	-261.513	-60.479
5,7	251.452	143.669	-264.187	-67.468
6,7	276.019	158.3	-260.298	-42.901

	E	VDW	ELE	BE
1,2	241.4	162.3	-301.354	-21.511
1,3	227.939	161.567	-316.903	-34.972
1,4	223.582	157.825	-316.751	-39.329
1,5	236.737	164.859	-312.073	-26.174
1,6	249.884	151.231	-306.346	-13.027
1,7	242.284	165.816	-307.198	-20.627
2,3	226.437	160.228	-319.57	-36.474
2,4	225.549	159.559	-316.063	-37.362
2,5	228.288	159.588	-321.249	-34.623
2,6	239.433	157.67	-299.377	-23.478
2,7	237.56	167.02	-310.961	-25.351
3,4	242.489	162.256	-304.429	-20.422
3,5	233.99	162.792	-310.878	-28.921
3,6	234.737	164.879	-314.189	-28.174
3,7	245.837	159.205	-294.802	-17.074
4,5	236.166	159.658	-310.215	-26.745
4,6	228.955	163.656	-313.662	-33.956
4,7	233.368	163.669	-310.622	-29.543
5,6	234.409	161.895	-310.408	-28.502
5,7	234.847	162.882	-308.834	-28.064
6,7	231.146	169.105	-314.86	-31.765

	E	VDW	ELE	BE
1,2	311.876	144.468	-285.996	26.321
1,3	241.876	144.348	-300.617	-43.679
1,4	228.073	143.776	-313.653	-57.482
1,5	248.308	144.556	-299.618	-37.247
1,6	284.879	139.568	-310.821	-0.676
1,7	315.075	148.024	-287.304	29.52
2,3	283.367	147.672	-322.268	-2.188
2,4	303.998	148.509	-297.059	18.443
2,5	244.747	133.144	-294.339	-40.808
2,6	235.987	144.215	-301.585	-49.568

2,7	242.288	146.196	-298.336	-43.267
3,4	247.692	145.132	-301.035	-37.863
3,5	239.23	145.636	-301.901	-46.325
3,6	245.89	151.779	-303.385	-39.665
3,7	246.22	143.389	-292.323	-39.335
4,5	306.283	146.273	-290.591	20.728
4,6	407.225	158.668	-309.663	121.67
4,7	285.574	147.024	-309.132	0.019
5,6	300.105	150.824	-302.235	14.55
5,7	286.142	138.887	-297.099	0.587
6,7	247.067	149.396	-295.334	-38.488

	E	VDW	ELE	BE
1,2	241.711	157.548	-315.468	-6.09
1,3	222.742	152.876	-327.967	-25.059
1,4	224.783	153.188	-324.101	-23.018
1,5	220.811	153.849	-330.621	-26.99
1,6	232.256	152.318	-318.554	-15.545
1,7	218.662	151.585	-326.472	-29.139
2,3	224.662	155.273	-325.74	-23.139
2,4	224.854	155.217	-324.13	-22.947
2,5	220.023	149.996	-323.825	-27.778
2,6	221.182	149.058	-325.796	-26.619
2,7	230.458	157.473	-324.711	-17.343
3,4	231.096	158.092	-321.921	-16.705
3,5	226.903	155.753	-326.487	-20.898
3,6	232.613	159.531	-325.075	-15.188
3,7	222.3	149.398	-323.95	-25.501
4,5	227.06	156.45	-324.567	-20.741
4,6	233.06	159.923	-323.912	-14.741
4,7	221.735	155.417	-331.285	-26.066
5,6	222.591	157.632	-329.315	-25.21
5,7	229.714	159.344	-328.72	-18.087
6,7	231.708	155.945	-324.165	-16.093

LV

	E	VDW	ELE	BE
1,2	92.609	118.015	-298.092	-15.304
1,3	68.629	117.619	-326.3	-39.284
1,4	107.184	115.526	-279.527	-0.729
1,5	77.482	111.474	-302.889	-30.431
1,6	79.875	108.968	-297.913	-28.038
1,7	88.642	113.684	-298.957	-19.271
2,3	80.993	113.643	-305.497	-26.92
2,4	81.088	110.196	-303.123	-26.825
2,5	69.12	105.838	-305.318	-38.793
2,6	76.775	108.798	-308.808	-31.138
2,7	74.432	112.149	-310.902	-33.481
3,4	85.942	116.337	-303.436	-21.971
3,5	82.907	110.728	-299.136	-25.006
3,6	95.716	115.751	-300.294	-12.197
3,7	69.057	109.672	-315.569	-38.856
4,5	74.083	118.413	-319.147	-33.83
4,6	83.543	115.002	-302.849	-24.37
4,7	72.487	105.097	-306.96	-35.426
5,6	80.149	113.661	-305.818	-27.764
5,7	76.859	113.038	-311.716	-31.054
6,7	61.004	109.298	-319.687	-46.909

	E	VDW	ELE	BE
1,2	108.125	115.521	-282.434	-31.704
1,3	106.789	114.837	-287.382	-33.04
1,4	93.97	114.078	-301.939	-45.859
1,5	97.277	117.353	-297.475	-42.552
1,6	102.042	110.667	-287.49	-37.787
1,7	108.081	115.071	-286.04	-31.748
2,3	110.382	112.018	-286.317	-29.447
2,4	101.035	115.088	-289.076	-38.794
2,5	93.153	106.432	-297.187	-46.676
2,6	88.494	116.557	-312.866	-51.335
2,7	101.542	113.255	-292.928	-38.287
3,4	110.125	119.318	-287.002	-29.704
3,5	115.843	116.376	-281.202	-23.986

3,6	110.49	115.239	-279.433	-29.339
3,7	91.154	107.184	-299.494	-48.675
4,5	114.583	111.634	-279.257	-25.246
4,6	108.729	113.953	-286.359	-31.1
4,7	90.071	102.707	-290.488	-49.758
5,6	110.218	115.953	-288.086	-29.611
5,7	96.539	114.07	-290.725	-43.29
6,7	95.794	114.932	-297.648	-44.035

	E	VDW	ELE	BE
1,2	262.806	158.364	-256.853	-56.114
1,3	243.195	154.127	-274.152	-75.725
1,4	280.684	158.326	-246.363	-38.236
1,5	255.946	152.471	-264.518	-62.974
1,6	299.233	159.866	-236.351	-19.687
1,7	277.501	159.7	-251.929	-41.419
2,3	232.254	144.982	-277.625	-86.666
2,4	273.523	156.65	-248.23	-45.397
2,5	263.989	149.694	-251.997	-54.931
2,6	231.116	151.228	-287.702	-87.804
2,7	287.487	158.995	-241.283	-31.433
3,4	277.349	157.469	-249.7	-41.571
3,5	260.01	149.024	-253.315	-58.91
3,6	284.739	160.046	-245.575	-34.181
3,7	233.245	145.287	-279.481	-85.675
4,5	244.408	154.837	-278.598	-74.512
4,6	271.967	157.839	-253.981	-46.953
4,7	241.324	152.196	-276.594	-77.596
5,6	270.894	154.934	-247.299	-48.026
5,7	268.682	154.301	-250.6	-50.238
6,7	274.72	155.664	-248.455	-44.2

	E	VDW	ELE	BE
1,2	254.628	170.455	-299.339	-8.283
1,3	249.947	170.539	-301.416	-12.964

1,4	248.903	169.038	-302.935	-14.008
1,5	242.101	165.866	-306.298	-20.81
1,6	242.839	164.643	-301.685	-20.072
1,7	256.556	171.387	-296.597	-6.355
2,3	243.535	168.522	-305.711	-19.376
2,4	251.008	168.757	-300.76	-11.903
2,5	237.53	162.697	-306.139	-25.381
2,6	245.554	165.072	-305.428	-17.357
2,7	244.558	169.154	-306.407	-18.353
3,4	248.048	171.08	-302.772	-14.863
3,5	251.139	171.818	-305.773	-11.772
3,6	248.92	169.751	-300.611	-13.991
3,7	247.309	165.322	-299.845	-15.602
4,5	243.761	167.884	-307.728	-19.15
4,6	253.324	169.776	-300.306	-9.587
4,7	244.173	166.608	-303.916	-18.738
5,6	253.776	170.86	-302.344	-9.135
5,7	245.304	170.909	-304.557	-17.607
6,7	241.18	165.89	-308.391	-21.731

	E	VDW	ELE	BE
1,2	268.948	148.732	-280.079	-16.607
1,3	266.114	148.966	-283.021	-19.441
1,4	264.054	145.604	-281.199	-21.501
1,5	249.484	151.572	-307.607	-36.071
1,6	250.088	151.008	-292.508	-35.467
1,7	251.059	145.214	-295.638	-34.496
2,3	240.482	149.569	-307.162	-45.073
2,4	254.225	147.537	-285.688	-31.33
2,5	256.174	146.228	-289.608	-29.381
2,6	257.494	140.604	-281.181	-28.061
2,7	267.935	144.954	-276.005	-17.62
3,4	251.963	153.268	-301.31	-33.592
3,5	263.745	148.247	-286.869	-21.81
3,6	244.541	148.608	-300.193	-41.014
3,7	247.871	144.351	-298.902	-37.684
4,5	263.434	149.154	-287.283	-22.121
4,6	265.519	146.453	-279.725	-20.036
4,7	234.852	146.758	-301.015	-50.703
5,6	265.73	149.959	-288.065	-19.825
5,7	248.23	146.876	-291.378	-37.325

6,7	239.669	147.501	-303.239	-45.886

	E	VDW	ELE	BE
1,2	237.357	160.771	-316.195	-10.444
1,3	229.972	157.14	-321.691	-17.829
1,4	237.44	156.781	-316.188	-10.361
1,5	227.923	157.84	-324.747	-19.878
1,6	220.36	153.817	-332.264	-27.441
1,7	229.54	156.915	-322.534	-18.261
2,3	222.011	151.339	-323.26	-25.79
2,4	224.688	159.425	-328.928	-23.113
2,5	224.65	161.658	-332.469	-23.151
2,6	219.94	150.978	-329.729	-27.861
2,7	232.327	158.695	-319.764	-15.474
3,4	224.303	161.009	-332.826	-23.498
3,5	229.843	153.879	-317.632	-17.958
3,6	221.096	155.214	-328.759	-26.705
3,7	224.029	155.072	-329.508	-23.772
4,5	219.609	154.781	-330.823	-28.192
4,6	219.821	154.901	-330.088	-27.98
4,7	219.539	151.1	-326.942	-28.262
5,6	230.632	158.748	-321.809	-17.169
5,7	231.858	158.847	-321.638	-15.943
6,7	221.8	152.144	-326.882	-26.001

LF19

	E	VDW	ELE	BE
1,2	89.069	110.761	-292.322	-18.844
1,3	64.988	105.789	-304.181	-42.925
1,4	59.285	108.176	-314.646	-48.628
1,5	80.803	110.464	-301.321	-27.11
1,6	76.85	102.147	-308.758	-31.063
1,7	79.48	113.931	-304.473	-28.433
2,3	68.47	109.446	-307.628	-39.443
2,4	68.247	110.154	-310.292	-39.666
2,5	76.134	107.472	-303.96	-31.779
2,6	74.557	104.042	-297.902	-33.356
2,7	80.553	104.818	-304.7	-27.36
3,4	82.99	114.05	-301.18	-24.923

3,5	85.265	111.838	-298.094	-22.648
3,6	75.612	113.991	-306.663	-32.301
3,7	64.35	101.087	-313.074	-43.563
4,5	85.491	117.849	-303.445	-22.422
4,6	90.063	113.383	-300.335	-17.85
4,7	72.784	111.153	-315.482	-35.129
5,6	91.634	108.169	-291.681	-16.279
5,7	74.361	107.145	-300.6	-33.552
6,7	71.999	106.035	-307.05	-35.914

	E	VDW	ELE	BE
1,2	112.113	115.297	-277.802	-27.716
1,3	93.312	107.02	-293.933	-46.517
1,4	96.39	102.997	-285.988	-43.439
1,5	91.967	104.593	-292.062	-47.862
1,6	128.526	112.779	-285.978	-11.303
1,7	111.735	114.161	-283.894	-28.094
2,3	159.223	113.393	-292.722	19.394
2,4	99.423	110.597	-300.371	-40.406
2,5	100.835	105.288	-283.764	-38.994
2,6	89.393	111.571	-298.665	-50.436
2,7	99.095	111.286	-287.942	-40.734
3,4	112.498	109.657	-277.614	-27.331
3,5	96.38	111.879	-295.602	-43.449
3,6	96.338	109.889	-289.27	-43.491
3,7	95.14	101.674	-279.798	-44.689
4,5	99.598	108.744	-289.73	-40.231
4,6	105.998	111.635	-281.73	-33.831
4,7	91.706	110.008	-303.9	-48.123
5,6	97.011	109.384	-288.486	-42.818
5,7	94.323	109.446	-293.029	-45.506
6,7	97.764	112.326	-287.635	-42.065

	E	VDW	ELE	BE
1,2	228.618	159.721	-299.232	-90.302
1,3	254.621	158.407	-264.7	-64.299
1,4	237.444	150.701	-279.587	-81.476
1,5	258.339	156.394	-267.139	-60.581
1,6	234.939	152.201	-284.504	-83.981
1,7	283.049	160.119	-241.024	-35.871
2,3	237.181	154.943	-285.398	-81.739
2,4	234.722	153.598	-279.92	-84.198
2,5	327.659	152.003	-253.333	8.739
2,6	218.442	150.202	-294.677	-100.478
2,7	211.697	153.796	-305.132	-107.223
3,4	250.256	154.166	-270.301	-68.664

3,5	249.397	164.326	-271.822	-69.523
3,6	231.399	157.219	-294.811	-87.521
3,7	218.224	149.625	-302.318	-100.696
4,5	247.399	157.936	-271.516	-71.521
4,6	203.999	151.356	-311.71	-114.921
4,7	254.965	155.861	-281.736	-63.955
5,6	182.343	151.989	-328.394	-136.577
5,7	248.645	160.335	-275.318	-70.275
6,7	231.985	162.058	-291.458	-86.935

	E	VDW	ELE	BE
1,2	247.067	168.004	-302.965	-15.844
1,3	236.466	160.891	-302.725	-26.445
1,4	237.344	161.482	-304.077	-25.567
1,5	243.343	164.475	-306.679	-19.568
1,6	308.931	167.324	-298.776	46.02
1,7	302.044	162.317	-302.641	39.133
2,3	244.125	162.927	-301.683	-18.786
2,4	243.42	161.218	-299.201	-19.491
2,5	294.984	162.448	-308.045	32.073
2,6	295.844	161.936	-303.77	32.933
2,7	300.548	162.952	-303.386	37.637
3,4	248.796	162.659	-300.995	-14.115
3,5	244.002	165.49	-301.959	-18.909
3,6	260.641	168.65	-297.019	-2.27
3,7	244.712	161.632	-308.536	-18.199
4,5	243.163	163.318	-309.297	-19.748
4,6	297.058	166.359	-305.222	34.147
4,7	260.124	167.998	-305.386	-2.787
5,6	253.686	168.846	-304.456	-9.225
5,7	234.55	160.51	-305.555	-28.361
6,7	290.278	164.896	-311.672	27.367

	E	VDW	ELE	BE
1,2	n/a			
1,3	242.955	147.812	-298.051	-42.6
1,4	252.361	142.759	-287.62	-33.194
1,5	243.803	138.724	-286.483	-41.752
1,6	269.115	147.612	-274.676	-16.44
1,7	250.683	146.341	-280.965	-34.872

2,3	265.056	143.461	-277.68	-20.499
2,4	266.046	145.538	-274.331	-19.509
2,5	226.074	148.33	-312.541	-59.481
2,6	259.811	147.41	-291.545	-25.744
2,7	255.227	150.262	-288.109	-30.328
3,4	255.126	145.597	-295.51	-30.429
3,5	250.219	143.434	-288.053	-35.336
3,6	248.433	143.417	-288.502	-37.122
3,7	246.558	149.218	-290.762	-38.997
4,5	260.037	147.708	-283.774	-25.518
4,6	265.63	150.546	-287.16	-19.925
4,7	261.504	148.215	-297.326	-24.051
5,6	240.401	154.807	-304.301	-45.154
5,7	247.977	142.648	-291.915	-37.578
6,7	268.79	146.694	-272.595	-16.765

	E	VDW	ELE	BE
1,2	231.11	157.479	-320.028	-16.691
1,3	226.689	159.165	-327.669	-21.112
1,4	233.772	159.212	-320.118	-14.029
1,5	230.32	157.777	-322.587	-17.481
1,6	225.09	155.744	-323.104	-22.711
1,7	225.814	157.278	-326.181	-21.987
2,3	227.51	159.083	-327.384	-20.291
2,4	226.697	159.281	-327.678	-21.104
2,5	225.202	155.902	-326.88	-22.599
2,6	235.635	159.609	-319.415	-12.166
2,7	235.237	158.658	-317.548	-12.564
3,4	231.266	156.349	-317.356	-16.535
3,5	228.362	156.764	-322.674	-19.439
3,6	230.128	157.455	-321.445	-17.673
3,7	224.546	152.677	-323.519	-23.255
4,5	230.078	156.743	-320.738	-17.723
4,6	228.679	155.756	-323.987	-19.122
4,7	220.54	151.2	-323.532	-27.261
5,6	229.537	156.72	-321.37	-18.264
5,7	230.121	156.453	-321.103	-17.68
6,7	228.759	156.007	-323.166	-19.042

LF20

	E	VDW	ELE	BE
1,2	95.491	119.219	-294.84	-12.422
1,3	88.073	115.246	-299.227	-19.84
1,4	78.978	109.11	-301.363	-28.935
1,5	100.562	118.455	-289.298	-7.351
1,6	88.832	115.818	-299.377	-19.081
1,7	96.682	117.533	-294.271	-11.231
2,3	99	117.46	-291.523	-8.913
2,4	93.349	116.889	-296.127	-14.564
2,5	91.574	114.836	-297.926	-16.339
2,6	71.112	117.12	-322.415	-36.801
2,7	90.433	117.258	-297.247	-17.48
3,4	85.468	118.496	-305.698	-22.445
3,5	92.073	117.279	-296.333	-15.84
3,6	86.076	122.623	-305.518	-21.837
3,7	86.632	113.84	-299.706	-21.281
4,5	97.076	116.077	-293.229	-10.837
4,6	100.967	117.998	-289.286	-6.946
4,7	92.04	116.236	-296.048	-15.873
5,6	99.125	118.522	-292.104	-8.788
5,7	85.357	113.239	-296.831	-22.556
6,7	98.52	118.8	-292.183	-9.393

	E	VDW	ELE	BE
1,2	113.643	118.996	-280.94	-26.186
1,3	106.098	115.59	-290.325	-33.731
1,4	96.099	115.559	-296.48	-43.73
1,5	108.317	117.826	-286.058	-31.512
1,6	109.447	110.84	-287.355	-30.382
1,7	112.871	117.503	-281.101	-26.958
2,3	105.581	113.987	-285.084	-34.248
2,4	116.345	115.2	-276.043	-23.484
2,5	110.368	115.788	-285.977	-29.461
2,6	105.938	111.58	-286.13	-33.891
2,7	104.769	111.614	-289.553	-35.06
3,4	114.141	115.947	-282.032	-25.688
3,5	126.244	119.349	-272.211	-13.585

3,6	113.85	113.901	-282.313	-25.979
3,7	96.609	114.16	-292.805	-43.22
4,5	97.667	116.106	-295.493	-42.162
4,6	109.719	114.33	-285.359	-30.11
4,7	108.657	111.183	-280.329	-31.172
5,6	123.768	114.592	-269.115	-16.061
5,7	113.528	113.02	-283.769	-26.301
6,7	107.569	117.576	-290.563	-32.26

	E	VDW	ELE	BE
1,2	193.61	153.646	-329.183	-125.31
1,3	257.888	160.917	-255.691	-61.032
1,4	288.109	155.405	-228.097	-30.811
1,5	239.018	161.083	-264.836	-79.902
1,6	253.215	155.989	-260.197	-65.705
1,7	270.15	167.445	-264.946	-48.77
2,3	244.941	156.855	-271.333	-73.979
2,4	253.23	159.44	-259.737	-65.69
2,5	252.589	154.849	-267.985	-66.331
2,6	282.39	157.167	-243.294	-36.53
2,7	262.028	156.281	-251.298	-56.892
3,4	253.707	160.665	-266.074	-65.213
3,5	238.098	162.25	-278.855	-80.822
3,6	264.327	168.239	-263.724	-54.593
3,7	209.972	150.996	-297.051	-108.948
4,5	284.941	165.402	-247.965	-33.979
4,6	268.616	160.04	-253.019	-50.304
4,7	293.907	158.312	-238.011	-25.013
5,6	253.987	153.177	-264.276	-64.933
5,7	296.196	163.041	-235.336	-22.724
6,7	302.668	160.614	-230.573	-16.252

	E	VDW	ELE	BE
1,2	250.743	169.429	-301.371	-12.168
1,3	249.776	169.667	-301.522	-13.135
1,4	250.305	168.736	-300.564	-12.606
1,5	249.175	169.259	-300.483	-13.736
1,6	231.1	161.414	-309.066	-31.811
1,7	238.674	162.888	-307.965	-24.237
2,3	268.126	180.629	-293.327	5.215
2,4	249.955	169.837	-300.081	-12.956

2,5	241.661	166.009	-306.614	-21.25
2,6	246.577	166.738	-308.185	-16.334
2,7	253.435	170.164	-299.211	-9.476
3,4	254.662	169.061	-295.795	-8.249
3,5	247.097	169.753	-303.75	-15.814
3,6	253.58	169.402	-296.971	-9.331
3,7	238.599	163.21	-311.027	-24.312
4,5	243.903	169.806	-308.699	-19.008
4,6	244.025	167.815	-304.15	-18.886
4,7	244.881	168.666	-305.002	-18.03
5,6	236.84	163.533	-314.371	-26.071
5,7	254.352	171.959	-297.933	-8.559
6,7	246.509	167.992	-305.412	-16.402

	E	VDW	ELE	BE
1,2	258.387	153.192	-291.191	-27.168
1,3	263.877	151.95	-284.892	-21.678
1,4	259.338	149.609	-285.394	-26.217
1,5	269.29	148.903	-276.866	-16.265
1,6	259.898	150.89	-283.866	-25.657
1,7	256.807	148.895	-291.439	-28.748
2,3	263.316	148.498	-285.423	-22.239
2,4	259.527	148.953	-285.198	-26.028
2,5	245.552	148.861	-292.434	-40.003
2,6	248.168	147.682	-287.093	-37.387
2,7	255.537	153.125	-288.165	-30.018
3,4	280.989	151.529	-268.779	-4.566
3,5	269.61	149.794	-281.155	-15.945
3,6	255.447	150.047	-292.162	-30.108
3,7	255.748	148.73	-281.861	-29.807
4,5	257.047	148.96	-286.618	-28.508
4,6	272.528	151.055	-276.466	-13.027
4,7	260.697	147.69	-280.74	-24.858
5,6	274.99	151.413	-274.451	-10.565
5,7	265.891	149.726	-284.389	-19.664
6,7	250.291	155.283	-294.372	-35.264

	E	VDW	ELE	BE
1,2	231.427	157.244	-320.043	-16.374
1,3	231.497	158.546	-321.142	-16.304
1,4	226.155	158.093	-318.034	-21.646
1,5	240.277	161.433	-316.039	-7.524

1,6	233.615	157.605	-319.221	-14.186
1,7	236.994	159.723	-318.332	-10.807
2,3	239.04	160.471	-315.469	-8.761
2,4	232.593	158.115	-319.932	-15.208
2,5	226.347	155.14	-321.871	-21.454
2,6	231.87	156.053	-319.094	-15.931
2,7	238.076	160.409	-317.725	-9.725
3,4	233.936	161.243	-320.997	-13.865
3,5	237.739	160.65	-317.974	-10.062
3,6	235.336	160.27	-318.528	-12.465
3,7	227.859	158.231	-324.079	-19.942
4,5	236.528	159.985	-317.556	-11.273
4,6	238.643	159.427	-314.826	-9.158
4,7	220.984	156.402	-332.228	-26.817
5,6	228.541	158.361	-321.054	-19.26
5,7	239.312	160.459	-315.787	-8.489
6,7	237.12	159.941	-318.675	-10.681

VF19

	E	VDW	ELE	BE
1,2	91.217	117.152	-297.202	-16.696
1,3	80.9	110.604	-305.143	-27.013
1,4	91.658	111.378	-303.854	-16.255
1,5	81.599	111.148	-299.966	-26.314
1,6	98.962	113.612	-286.314	-8.951
1,7	77.249	113.08	-308.132	-30.664
2,3	73.897	116.626	-311.385	-34.016
2,4	81.572	117.101	-308.397	-26.341
2,5	80.752	116.101	-306.969	-27.161
2,6	55.283	108.737	-320.253	-52.63
2,7	81.175	116.765	-305.785	-26.738
3,4	96.606	118.138	-293.356	-11.307
3,5	87.043	115.191	-300.495	-20.87
3,6	90.263	116.04	-298.048	-17.65
3,7	84.522	111.562	-306.225	-23.391
4,5	70.094	113.036	-315.887	-37.819
4,6	79.323	110.028	-308.097	-28.59
4,7	81.1	109.314	-306.351	-26.813
5,6	79.259	114.381	-307.73	-28.654
5,7	77.855	111.904	-312.384	-30.058
6,7	84.432	112.633	-303.469	-23.481

	E	VDW	ELE	BE
1,2	110.966	117.659	-280.637	-28.863
1,3	99.560	117.068	-297.885	-40.269
1,4	89.084	111.467	-297.274	-50.745
1,5	100.656	114.720	-290.613	-39.173
1,6	105.337	112.323	-284.648	-34.492
1,7	100.379	113.913	-287.255	-39.450
2,3	126.178	117.525	-269.793	-13.651
2,4	108.543	115.661	-285.971	-31.286
2,5	89.774	113.988	-297.333	-50.055
2,6	114.242	109.736	-272.073	-25.587
2,7	104.324	119.311	-291.532	-35.505
3,4	122.851	117.481	-272.299	-16.978
3,5	107.560	116.154	-285.745	-32.269
3,6	92.394	117.093	-302.585	-47.435
3,7	105.397	112.221	-286.150	-34.432
4,5	115.794	114.296	-284.247	-24.035
4,6	109.042	116.218	-286.061	-30.787
4,7	107.371	112.36	-284.579	-32.458
5,6	117.825	115.601	-275.586	-22.004
5,7	101.041	115.29	-289.701	-38.788
6,7	98.71	117.368	-293.659	-41.119

	E	VDW	ELE	BE
1,2	256.044	159.252	-275.88	-62.876
1,3	267.425	148.008	-255.381	-51.495
1,4	230.018	151.607	-283.011	-88.902
1,5	252.309	155.748	-271.911	-66.611
1,6	370.174	157.455	-305.208	51.254
1,7	266.159	155.634	-263.615	-52.761
2,3	269.624	150.823	-247.735	-49.296
2,4	222.579	158.469	-299.306	-96.341
2,5	243.062	145.378	-272.918	-75.858
2,6	257.926	154.197	-261.592	-60.994
2,7	401.708	162.203	-258.502	82.788
3,4	266.353	150.539	-256.822	-52.567
3,5	327.224	163.675	-273.532	8.304
3,6	257.556	142.899	-264.933	-61.364
3,7	250.553	155.266	-273.286	-68.367
4,5	219.302	146.237	-304.039	-99.618
4,6	264.425	153.746	-272.164	-54.495
4,7	227.085	153.076	-300.121	-91.835
5,6	366.483	157.485	-281.858	47.563
5,7	257.766	149.464	-263.985	-61.154
6,7	268.613	150.896	-254.785	-50.307

	E	VDW	ELE	BE
1,2	250.827	168.272	-297.802	-12.084
1,3	243.917	167.084	-303.101	-18.994
1,4	296.954	164.677	-298.922	34.043
1,5	291.765	163.703	-307.635	28.854
1,6	245.151	166.848	-302.041	-17.76
1,7	249.904	169.118	-301.639	-13.007
2,3	249.134	167.825	-301.329	-13.777
2,4	248.665	166.329	-296.648	-14.246
2,5	303.154	164.131	-308.135	40.243
2,6	297.925	162.24	-297.999	35.014
2,7	249.8181	167.328	-298.486	-13.0929
3,4	247.851	168.78	-304.28	-15.06
3,5	243.677	170.574	-308.587	-19.234
3,6	303.256	168.722	-296.234	40.345
3,7	300.044	170.606	-306.106	37.133
4,5	295.159	168.206	-309.795	32.248
4,6	248.675	165.524	-298.339	-14.236
4,7	298.238	161.963	-299.478	35.327
5,6	248.888	169.57	-303.108	-14.023
5,7	246.325	166.134	-304.821	-16.586
6,7	238.316	165.708	-307.367	-24.595

	E	VDW	ELE	BE
1,2	257.924	148.764	-288.84	-27.631
1,3	251.232	146.681	-293.055	-34.323
1,4	254.397	144.409	-288.327	-31.158
1,5	261.369	145.023	-284.242	-24.186
1,6	233.058	147.133	-307.757	-52.497
1,7	258.887	148.362	-287.629	-26.668
2,3	256.718	149.08	-290.148	-28.837
2,4	261.439	147.187	-282.37	-24.116
2,5	256.797	138.537	-282.395	-28.758
2,6	235.292	144.642	-297.261	-50.263
2,7	251.66	151.074	-292.623	-33.895
3,4	254.134	148.082	-286.594	-31.421
3,5	249.249	150.125	-289.399	-36.306
3,6	248.316	149.618	-298.53	-37.239
3,7	247.243	145.454	-297.944	-38.312
4,5	260.935	149.729	-288.104	-24.62
4,6	246.009	147.398	-295.746	-39.546
4,7	245.547	144.634	-291.681	-40.008
5,6	252.037	152.348	-290.442	-33.518

5,7	262.692	147.556	-285.402	-22.863
6,7	252.419	148.577	-293.323	-33.136

	E	VDW	ELE	BE
1,2	226.32	155.977	-325.424	-21.481
1,3	215.552	153.912	-334.083	-32.249
1,4	216.673	154.223	-332.717	-31.128
1,5	204.927	154.287	-343.716	-42.874
1,6	270.106	153.907	-331.417	22.305
1,7	228.462	156.643	-323.179	-19.339
2,3	216.462	150.915	-330.109	-31.339
2,4	218.871	152.379	-328.411	-28.93
2,5	276.064	150.916	-333.542	28.263
2,6	210.242	149.033	-333.204	-37.559
2,7	284.97	157.974	-319.521	37.169
3,4	232.726	159.122	-319.883	-15.075
3,5	223.096	156.663	-328.851	-24.705
3,6	226.051	159.512	-322.121	-21.75
3,7	387.776	163.196	-326.804	139.975
4,5	226.453	154.316	-321.44	-21.348
4,6	258.352	149.996	-337.148	10.551
4,7	211.334	148.549	-328.384	-36.467
5,6	218.308	154.082	-331.636	-29.493
5,7	227.316	153.37	-320.424	-20.485
6,7	268.536	158.652	-334.23	20.735

VF20

	E	VDW	ELE	BE
1,2	91.327	115.695	-298.342	-16.586
1,3	72.614	111.466	-310.249	-35.299
1,4	73.622	110.853	-321.422	-34.291
1,5	80.657	114.747	-304.086	-27.256
1,6	79.54	113.516	-304.134	-28.373
1,7	80.139	110.238	-299.924	-27.774
2,3	88.617	111.585	-296.694	-19.296
2,4	75.997	107.186	-306.113	-31.916
2,5	85.148	111.554	-305.285	-22.765
2,6	80.003	109.168	-309.038	-27.91
2,7	78.667	110.824	-304.65	-29.246
3,4	81.166	112.538	-309.426	-26.747

3,5	83.365	116.442	-305.836	-24.548
3,6	129.731	113.137	-317.928	21.818
3,7	68.067	114.374	-320.93	-39.846
4,5	95.276	109.57	-292.678	-12.637
4,6	80.449	111.246	-303.23	-27.464
4,7	70.087	104.055	-309.513	-37.826
5,6	90.272	117.273	-304.617	-17.641
5,7	76.214	111.728	-313.182	-31.699
6,7	82.799	114.285	-303.795	-25.114

	E	VDW	ELE	BE
1,2	99.664	120.582	-294.224	-40.165
1,3	91.618	109.495	-297.391	-48.211
1,4	95.506	103.382	-292.835	-44.323
1,5	93.204	107.078	-297.357	-46.625
1,6	113.757	109.028	-294.383	-26.072
1,7	95.727	110.662	-295.871	-44.102
2,3	101.304	108.782	-289.504	-38.525
2,4	109.156	107.791	-280.513	-30.673
2,5	98.416	107.366	-285.387	-41.413
2,6	105.395	108.154	-288.802	-34.434
2,7	84.043	114.656	-304.954	-55.786
3,4	104.674	107.307	-283.064	-35.155
3,5	99.9	113.138	-294.944	-39.929
3,6	92.738	116.938	-299.367	-47.091
3,7	125.097	111.471	-279.476	-14.732
4,5	92.917	112.408	-301.967	-46.912
4,6	97.926	109.976	-293.866	-41.903
4,7	94.36	115.46	-298.4	-45.469
5,6	110.526	113.004	-283.202	-29.303
5,7	100.111	108.396	-297.337	-39.718
6,7	92.693	116.684	-308.631	-47.136

No AML data

	E	VDW	ELE	BE
1,2	246.264	169.051	-303.317	-16.647
1,3	244.586	166.639	-303.167	-18.325
1,4	241.203	165.179	-304.728	-21.708
1,5	232.565	161.652	-313.235	-30.346
1,6	259.801	160.782	-295.555	-3.11
1,7	243.997	168.296	-307.109	-18.914

2,3	244.083	163.737	-303.258	-18.828
2,4	240.001	164.684	-306.494	-22.91
2,5	233.641	161.705	-310.599	-29.27
2,6	243.173	161.447	-308.953	-19.738
2,7	251.617	168.147	-298.334	-11.294
3,4	243.363	171.098	-309.925	-19.548
3,5	239.586	167.187	-311.707	-23.325
3,6	239.536	166.976	-309.298	-23.375
3,7	225.187	166.915	-320.019	-37.724
4,5	244.327	163.239	-304.278	-18.584
4,6	241.678	165.39	-307.292	-21.233
4,7	235.504	160.142	-310.533	-27.407
5,6	251.627	169.999	-299.103	-11.284
5,7	246.384	163.516	-302.304	-16.527
6,7	246.306	165.853	-303.416	-16.605

	E	VDW	ELE	BE
1,2	248.368	149.572	-295.299	-37.187
1,3	244.216	141.412	-291.924	-41.339
1,4	238.125	139.717	-296.854	-47.43
1,5	245.767	144.974	-295.898	-39.788
1,6	247.72	144.37	-287.342	-37.835
1,7	240.515	144.452	-300.888	-45.04
2,3	249.6	144.646	-295.761	-35.955
2,4	249.473	141.94	-291.758	-36.082
2,5	241.933	143.099	-300.16	-43.622
2,6	235.28	147.473	-307.32	-50.275
2,7	250.817	145.346	-297.071	-34.738
3,4	252.708	148.386	-289.721	-32.847
3,5	242.332	145.603	-295.001	-43.223
3,6	249.273	145.405	-296.475	-36.282
3,7	255.159	149.01	-289.446	-30.396
4,5	251.811	147.671	-290.818	-33.744
4,6	251.215	148.697	-297.908	-34.34
4,7	244.51	146.201	-297.511	-41.045
5,6	241.704	148.611	-295.922	-43.851
5,7	241.172	145.294	-297.625	-44.383
6,7	250.512	149.43	-294.157	-35.043

	E	VDW	ELE	BE
1,2	294.691	153.957	-320.837	46.89
1,3	218.303	146.827	-325.526	-29.498
1,4	221.147	152.26	-326.438	-26.654
1,5	215.886	147.295	-328.614	-31.915
1,6	220.715	153.373	-324.321	-27.086
1,7	229.52	155.921	-326.522	-18.281
2,3	220.447	146.883	-322.497	-27.354
2,4	220.508	150.268	-323.358	-27.293
2,5	375.319	154.258	-316.156	127.518
2,6	214.062	150.474	-327.573	-33.739
2,7	220.68	158.036	-330.692	-27.121
3,4	232.338	157.793	-320.422	-15.463
3,5	232.13	159.402	-318.45	-15.671
3,6	387.185	171.582	-317.881	139.384
3,7	218.807	151.517	-336.389	-28.994
4,5	244.922	159.084	-317.11	-2.879
4,6	233.945	153.627	-322.663	-13.856
4,7	213.071	152.68	-335.023	-34.73
5,6	232.432	155.908	-322.608	-15.369
5,7	218.626	159.459	-328.706	-29.175
6,7	213.666	153.505	-333.343	-34.135

FF

	E	VDW	ELE	BE
1,2	80.959	113.261	-307.516	-26.954
1,3	94.716	116.522	-293.699	-13.197
1,4	73.093	115.353	-311.377	-34.82
1,5	84.018	114.601	-302.259	-23.895
1,6	66.08	116.015	-319.626	-41.833
1,7	70.026	116.428	-319.445	-37.887
2,3	92.48	113.387	-293.702	-15.433
2,4	89.359	113.332	-296.159	-18.554
2,5	83.876	114.073	-302.5	-24.037
2,6	84.454	111.129	-295.717	-23.459
2,7	90.349	114.37	-295.748	-17.564
3,4	87.227	113.761	-298.515	-20.686
3,5	80.006	114.459	-307.869	-27.907
3,6	93.965	116.739	-294.227	-13.948
3,7	79.263	111.687	-304.307	-28.65
4,5	83.03	112.832	-299.58	-24.883

4,6	76.743	113.247	-307.041	-31.17
4,7	72.639	110.534	-310.747	-35.274
5,6	81.78	113.265	-306.748	-26.133
5,7	87.547	117.166	-303.911	-20.366
6,7	81.776	115.582	-306.094	-26.137

	E	VDW	ELE	BE
1,2	115.702	110.736	-273.793	-24.127
1,3	107.516	112.016	-287.168	-32.313
1,4	103.601	112.04	-288.249	-36.228
1,5	110.789	115.511	-285.021	-29.04
1,6	90.323	114.721	-304.722	-49.506
1,7	114.291	109.685	-274.691	-25.538
2,3	108.991	117.755	-288.066	-30.838
2,4	99.584	112.7	-294.544	-40.245
2,5	99.681	118.714	-300.169	-40.148
2,6	111.615	114.941	-277.591	-28.214
2,7	120.956	114.764	-272.064	-18.873
3,4	102.517	111.904	-290.844	-37.312
3,5	102.231	115.206	-293.744	-37.598
3,6	94.712	114.805	-300.311	-45.117
3,7	91.619	112.555	-298.9	-48.21
4,5	98.281	116.269	-295.934	-41.548
4,6	108.207	115.834	-286.945	-31.622
4,7	85.619	110.84	-303.571	-54.21
5,6	112.363	111.343	-276.673	-27.466
5,7	98.805	113.416	-292.385	-41.024
6,7	109.614	112.858	-278.914	-30.215

	E	VDW	ELE	BE
1,2	274.086	163.684	-247.307	-44.834
1,3	255.276	168.078	-273.777	-63.644
1,4	198.005	152.454	-319.113	-120.915
1,5	210.423	161.151	-316.185	-108.497
1,6	281.473	163.834	-252.614	-37.447
1,7	224.095	157.579	-298.98	-94.825
2,3	229.655	166.2	-296.943	-89.265
2,4	278.761	168.87	-243.483	-40.159
2,5	261.278	159.985	-262.071	-57.642
2,6	261.437	163.696	-258.63	-57.483
2,7	304.98	163.87	-228.781	-13.94
3,4	283.156	161.156	-246.774	-35.764

3,5	215.668	163.05	-304.083	-103.252
3,6	253.207	169.157	-275.324	-65.713
3,7	255.394	161.068	-275.305	-63.526
4,5	298.099	167.186	-238.297	-20.821
4,6	281.723	166.73	-245.219	-37.197
4,7	217.805	151.043	-294.734	-101.115
5,6	221.028	157.381	-287.492	-97.892
5,7	300.542	164.333	-228.357	-18.378
6,7	299.777	164.713	-232.433	-19.143

	E	VDW	ELE	BE
1,2	220.908	164.451	-337.804	-42.003
1,3	279.146	147.547	-327.183	16.235
1,4	243.34	150.591	-298.508	-19.571
1,5	225.034	158.503	-334.745	-37.877
1,6	229.882	156.715	-324.395	-33.029
1,7	297.055	163.3	-322.374	34.144
2,3	233.526	154.949	-312.024	-29.385
2,4	241.216	159.242	-318.435	-21.695
2,5	227.381	153.635	-328.991	-35.53
2,6	231.676	164.782	-324.349	-31.235
2,7	286.305	157.732	-321.84	23.394
3,4	291.131	144.974	-310.216	28.22
3,5	347.825	167.098	-324.913	84.914
3,6	222.87	153.176	-333.356	-40.041
3,7	268.534	164.738	-301.004	5.623
4,5	228.95	158.859	-322.726	-33.961
4,6	237.687	165.977	-315.587	-25.224
4,7	232.372	152.412	-320.999	-30.539
5,6	336.529	157.428	-338.512	73.618
5,7	230.106	151.757	-317.629	-32.805
6,7	237.975	154.358	-317.272	-24.936

	E	VDW	ELE	BE
1,2	259.715	151.668	-283.876	-25.84
1,3	261.32	152.568	-286.121	-24.235
1,4	271.574	149.643	-278.068	-13.981
1,5	262.593	147.652	-285.326	-22.962
1,6	247.372	147.768	-285.637	-38.183
1,7	254.16	149.177	-293.77	-31.395
2,3	243.075	150.666	-302.477	-42.48
2,4	271.547	149.749	-278.663	-14.008
2,5	248.16	146.482	-289.063	-37.395

2,6	247.384	149.292	-298.558	-38.171
2,7	256.761	149.092	-288.75	-28.794
3,4	259.177	154.569	-287.804	-26.378
3,5	258.687	150.482	-284.415	-26.868
3,6	254.171	151.928	-290.56	-31.384
3,7	245.187	150.005	-290.248	-40.368
4,5	263.641	150.699	-287.792	-21.914
4,6	268.91	148.255	-279.253	-16.645
4,7	249.775	147.123	-294.456	-35.78
5,6	273.784	150.393	-276.955	-11.771
5,7	260.455	151.622	-294.488	-25.1
6,7	258.022	151.174	-289.544	-27.533

	E	VDW	ELE	BE
1,2	239.952	161.064	-315.348	-7.849
1,3	231.865	155.116	-320.088	-15.936
1,4	234.066	156.176	-317.701	-13.735
1,5	231.139	158.395	-320.501	-16.662
1,6	227.744	160.226	-324.46	-20.057
1,7	233.973	160.051	-319.785	-13.828
2,3	230.407	153.938	-318.898	-17.394
2,4	234.89	154.634	-314.165	-12.911
2,5	226.916	158.186	-325.156	-20.885
2,6	n/a			
2,7	229.338	157.812	-321.401	-18.463
3,4	229.534	158.89	-320.254	-18.267
3,5	240.24	159.195	-313.891	-7.561
3,6	242.914	158.679	-310.49	-4.887
3,7	229.294	157.716	-325.223	-18.507
4,5	238.843	157.487	-313.859	-8.958
4,6	237.03	160.027	-316.958	-10.771
4,7	251.582	161.376	-317.393	3.781
5,6	239.45	160.171	-314.362	-8.351
5,7	238.149	159.142	-314.702	-9.652
6,7	241.665	157.545	-311.143	-6.136

GAS PHASE INTERACTIONS

HH

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	AA	14	B-ring	1-4
1AMC	AA	14	A-ring	1-6
1AMC	AH	14	CA6	2-5
1AMC	AH	10	B-ring	2-6
1AMC	AH	14	CB5	2-6
1AML	AH	10	C7	2-7
1AML	SCD	14	7	6-7
1BA4	SCD	14	7	3-7
1BA4	SCD	14	7	4-7
1IYT	AH	13	05Me	2-7
1IYT	AH	13	3	3-7
1IYT	SCD	14	6	4-6
1IYT	AH	13	A-ring	5-7
1Z0Q	BBA	10	7	1-6
1Z0Q	AH	14	CA3	3-6
1Z0Q	AH	14	A-ring	5-7

H13K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	13	05Me	1-7
1AMB	SCD	16	7	3-7
1AMC	AH	16	A-ring	2-6
1AMC	SCD	16	7	6-7
1AML	AH	16	C-ring	1-3
1AML	BBA	12	3	2-5
1AML	SCD	16	7	3-7
1AML	SCD	16	7	5-7
1BA4	BBA	12	6	1-2
1BA4	AH	10	B-ring	1-3
1BA4	AH	10	C-ring	2-5
1IYT	AH	16	A-ring	2-6
1IYT	A+	16	A-ring	2-6
1IYT	A+	16	A-ring	3-7
1Z0Q	AA	13	C-ring	2-6
1Z0Q	SCD	16	7	3-7
1Z0Q	SCD	16	7	5-7

H14K

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	AH	15	C-ring	1-4
1AMB	AH	19	B-ring	1-4
1AMB	SCA	15	6	1-7
1AMB	BBA	11	6	2-4
1AMB	AH	19	C-ring	2-4
1AMB	AH	15	C-ring	2-5
1AMB	BBA	11	3	3-4
1AMB	BBA	11	3	3-5
1AMC	AA	13	B-ring	1-3
1AMC	AA	13	B-ring	1-4
1AMC	BBA	13	3	1-4
1AMC	AH	17	B-ring	2-4
1AMC	AA	13	A-ring	3-7
1AMC	AH	17	A-ring	4-5
1AMC	A+	13	A-ring	5-7
1AML	SCD	13	7	1-7
1AML	AH	13	CB5	2-4
1AML	AA	13	B-ring	2-5
1AML	AH	17	C-ring	2-7
1AML	AA	13	A-ring	3-7

1AML	BBA	16	2	4-5
1AML	BBA	16	7	5-7
1BA4	AH	10	B-ring	1-3
1BA4	BBA	10	7	2-6
1BA4	AH	10	CC6	3-4
1BA4	AH	17	A-ring	6-7
1IYT	SCA	8	3	1-2
1IYT	SCA	11	6	2-3
1IYT	SCA	11	6	2-4
1IYT	SCA	11	3	3-6
1IYT	AH	8	C-ring	3-7
1IYT	SCA	11	3	5-7
1Z0Q	AH	13	01Me	1-7

LV

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	SCA	22	3	1-3
1AMB	SCA	22	3	1-5
1AMB	SCD	14	7	2-6
1AMB	SCD	13	2	2-7
1AMB	SCA	22	7	6-7
1AMC	--	--	--	--
1AML	SCA	35	7	1-2
1AML	A+	14	C-ring	1-6
1AML	A+	14	C-ring	2-4
1AML	SCD	14	7	2-5
1AML	AH	14	A-ring	3-4
1AML	AA	14	C-ring	3-7
1AML	SCD	14	7	6-7
1BA4	AH	18	A-ring	6-7
1IYT	--	--	--	--
1Z0Q	A+	14	A-ring	1-6
1Z0Q	AH	18	A-ring	1-6
1Z0Q	A+	14	A-ring	6-7
1Z0Q	AH	18	A-ring	6-7

LF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	BBA	16	6	1-2
1AMB	AA	20	C-ring	1-2
1AMB	BBA	16	7	1-6
1AMB	AA	20	C-ring	1-7
1AMB	AH	20	CC2	2-3
1AMB	SCD	16	7	2-7
1AMB	BBA	16	3	3-5
1AMB	A+	16	A-ring	3-5
1AMB	BBA	16	2	5-6
1AMB	A+	16	B-ring	5-7
1AMC	AH	20	05Me	1-3
1AMC	SCA	23	7	1-5
1AMC	AA	20	C-ring	1-7
1AMC	AH	16	B-ring	2-5
1AMC	BBA	16	2	5-6
1AML	AH	16	B-ring	2-5
1AML	AH	20	05Me	2-5
1BA4	SCA	15	7	1-5
1BA4	AH	14	05Me	2-3
1BA4	AH	18	B-ring	2-3

1BA4	SCA	22	3	2-5
1BA4	SCD	15	7	3-7
1BA4	SCA	15	3	4-5
1IYT	AH	20	CC2	1-5
1IYT	A+	16	B-ring	2-4
1IYT	A+	16	C-ring	3-4
1IYT	AH	20	CA6	5-7
1Z0Q	AH	20	C-ring	1-2

LF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	--	--	--	--
1AML	AH	30	C-ring	2-7
1BA4	--	--	--	--
1IYT	AH	13	O5Me	1-3
1Z0Q	AH	20	CA6	2-5

VF19

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	SCA	22	6	1-3
1AMB	SCA	22	6	2-5
1AMB	AH	18	C-ring	2-6
1AMB	SCA	11	3	4-5
1AMB	AH	19	2	4-5
1AMB	AH	18	A-ring	5-7
1AMC	AH	18	C-ring	1-4
1AMC	AH	14	O5Me	1-6
1AMC	AH	19	O4Me	3-4
1AMC	SCA	22	3	3-4
1AMC	SCA	22	2	3-7
1AMC	SCA	22	3	5-6
1AML	SCA	22	6	1-2
1AML	BBD	6	7	1-3
1AML	SCA	22	7	1-6
1AML	SCA	1	2	2-3
1AML	SCA	22	6	2-7
1AML	SCA	22	3	3-4
1AML	BBD	4	6	4-5
1AML	SCA	15	3	4-5

1AML	SCA	22	2	5-6
1AML	SCA	22	7	5-7
1AML	SCA	22	7	6-7
1BA4	AH	15	C-ring	2-4
1BA4	SCA	22	3	2-5
1BA4	AH	18	C-ring	2-6
1BA4	SCA	22	7	2-6
1BA4	AH	15	C-ring	2-7
1BA4	AH	19	A-ring	6-7
1IYT	SCD	15	7	1-6
1IYT	AH	22	C-ring	2-5
1IYT	SCA	22	7	2-6
1Z0Q	AH	22	C-ring	2-6
1Z0Q	SCA	22	2	3-7
1Z0Q	SCA	22	3	4-7
1Z0Q	SCA	15	2	5-6

VF20

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	SCD	28	3	1-4
1AMC	BBA	25	3	2-4
1AMC	BBA	17	2	5-6
1AML	--N/A	--	--	--
1BA4	--	--	--	--
1IYT	AH	17	B-ring	1-3
1Z0Q	SCA	23	3	1-3
1Z0Q	SCA	15	6	1-4
1Z0Q	SCA	15	6	2-3
1Z0Q	SCA	15	6	2-4
1Z0Q	AH	19	C-ring	2-4
1Z0Q	SCA	23	3	2-5
1Z0Q	SCA	15	3	3-6
1Z0Q	SCA	23	6	4-7

FF

AB Conformer	Type of Interaction	Amino Acid Involved	Part on Molecule Involved	Initial Orientation
1AMB	--	--	--	--
1AMC	SCD	16	7	1-6
1AMC	AH	19	6	2-3
1AMC	SCA	23	3	2-5
1AMC	SCA	23	7	2-6
1AMC	AH	19	A-ring	5-6
1AML	--	--	--	--
1BA4	A+	1	A-ring	1-3
1BA4	SCA	22	6	1-3
1BA4	SCA	23	2	1-5
1BA4	SCA	23	3	1-5
1BA4	A+	1	A-ring	1-6
1BA4	SCD	16	7	1-6
1BA4	SCA	23	3	2-5
1BA4	AH	23	A-ring	2-6
1BA4	BBA	2	2	3-4
1BA4	A+	1	A-ring	3-6
1BA4	SCA	1	7	3-6
1BA4	A+	1	C-ring	3-7
1BA4	SCA	23	7	3-7

1BA4	SCA	26	2	3-7
1IYT	SCD	16	7	1-5
1IYT	SCD	16	7	2-5
1IYT	A+	16	B-ring	2-6
1Z0Q	AH	20	B-ring	2-3
1Z0Q	AA	19	C-ring	2-4
1Z0Q	BBA	16	2	4-7
1Z0Q	AH	20	A-ring	5-7