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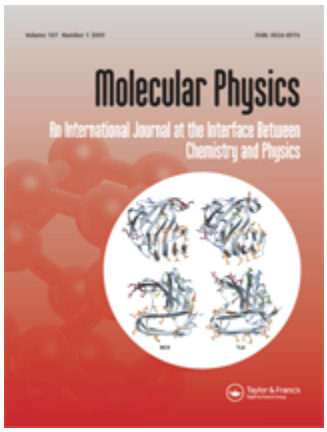

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The accuracy of local MP2 methods for conformational energies

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Abstract

The relative energies of 95 conformers of four peptide models are studied using MP2 and LMP2 methods and correlation consistent basis sets ranging from double-zeta to augmented quintuple-zeta quality. It is found that both methods yield quite similar results, and the differences between MP2 and LMP2 decrease systematically with increasing basis set. Due to reduced intramolecular basis set superposition effects (BSSE) the LMP2 results converge more slowly to basis set limit for most of these rather small systems. However, for larger peptides, the BSSE has a very large effect on the energy difference between extended and helical structures, leading to a very strong basis set dependence of the canonical MP2 results. It is demonstrated for alanine octapeptides that the basis set error exceeds 30 and 20 kJ/mol, respectively, if augmented double-zeta and triple-zeta basis sets are used. On the other hand, the LMP2 results are only slightly affected by the basis set size, and even with augmented double-zeta basis sets reasonably accurate results are obtained. Furthermore, for the larger systems the computation times for the LMP2 calculations are shown to be up to one order or magnitude shorter than for canonical MP2 calculations with the same basis set.

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I. INTRODUCTION

Sampling the low-energy region of the phase-space is an essential element for simulating the behavior of macromolecules at finite temperature conditions. The only realistic energy functions for large-scale simulations are of the force field type, but it is desirable to establish the inherent accuracy of these methods. Two of us have recently shown that most force fields in common use have problems reproducing geometries and relative energies of conformations of small peptide models, typically accounting for only half of the conformations.[1] These conclusions were obtained by generating a reference set of structures and energies by a hierarchy of electronic structure methods, with geometry optimizations at the MP2/aug-cc-pVDZ level and relative energies obtained by extrapolating MP2 energies to the basis set limit and adding corrections for higher order electron correlation effects calculated at the CCSD(T) level. For molecules with localized bonding it is anticipated that relative energies of conformations will be insensitive to electron correlation beyond MP2, and it was found that the MP2/aug-cc-pVTZ level represented a suitable compromise between accuracy and computational cost, producing a typical accuracy of 1 kJ/mol for relative energies. We note that Hartree-Fock and density functional methods will be of limited use for systems with several degrees of conformational freedom, as the inadequacy of describing intramolecular dispersion will lead to artifacts in the resulting energy surface.

Having settled on the MP2 method as a suitable level of theory for generating reliable reference data for parameterizing force fields, there remains a question of the computationally most efficient formulation of MP2 theory. The conventional approach is based on canonical molecular orbitals, which leads to a formal $\mathcal{O}(\mathcal{N}^5)$ scaling of computer time with system size. The local MP2 (LMP2) method[2–9] employs a localization scheme of the molecular orbitals prior to the MP2 step, and by utilizing the locality in the selection of correlating orbitals, the LMP2 method will approach linear scaling for large systems. An additional strategy to reduce the computational requirements is to expand products of functions in an auxiliary basis set,[10–12] a procedure usually called resolution of identity (RI) or density fitting (DF). Both of these procedures involve additional approximations beyond the regular MP2. In the current work we present extensive benchmark data to investigate the accuracy of these approximations relative to conventional MP2. An earlier study on the use of LMP2 for the calculation of conformational energies can be found in Ref. 13.

In section II we summarize the computational details of our calculations. In section III A we report a comparison of MP2, DF-MP2, and DF-LMP2 methods for 95 conformations of small glycine, alanine, serine and cysteine model peptide systems. Finally, in section III B the accuracy and computational savings of the local approximations are investigated for extended and folded structures of larger alanine peptide chains.

II. METHOD

All geometries used in Section III A have been taken as the MP2/aug-cc-pVDZ optimized reported previously,[1] and the performance for energies relative to the lowest energy conformations was evaluated as the mean and maximum absolute deviations (`MAD` and `MAX`) relative to the canonical MP2 results using the cc-pVnZ[14] and aug-cc-pVnZ[15] ($n = 2 - 5$) basis set families. As will be shown below, the additional diffuse functions in the augmented basis sets are essential for achieving rapid basis set convergence at both the Hartree-Fock (HF) and the MP2 levels. These functions are particularly important for the description of the nitrogen and oxygen lone pairs. However, the diffuse functions on the hydrogen atoms have only a rather small effect on the relative energies. Therefore, as a cost effective compromise we recommend mixed basis sets, where the cc-pVnZ sets are used for the hydrogen atoms, and the aug-cc-pVnZ sets for all other atoms. These basis sets will be denoted aug'-cc-pVnZ. For each of the 95 conformers, the MP2 complete basis set limit (CBS) has been estimated using an exponential extrapolation of the HF/aug'-cc-pVnZ energies ($n = 3 - 5$), and a two-point n^{-3} extrapolation of the MP2/aug'-cc-pVnZ ($n = 4 - 5$) correlation energies.[16] These estimates will be denoted MP2/CBS[45].

In Section III B, the initial extended and helical structures of alanine tetra-, hexa- and octapeptide were created in Maestro, the graphic interface program of the MacroModel package.[17] Three, five and seven aminoacid units, respectively, were used for the construction of our peptides. In addition, acetyl and N-methyl functional groups were added to the C-terminus and N-terminus to mimic the environment in a longer peptide chain. Geometries were first pre-optimized at the MM level with the MMFFs[18] force field. The structures were then refined using the B-P86 density functional[19,20] in combination with the TZVP basis set.[21] Since no extensive search of the PES was made, there is no guarantee that the optimized structures are the global minima. However, for the purpose of the present

benchmarks this is of no relevance.

Density fitting approximations[11,12] have been employed in the HF as well as the MP2/LMP2 steps, using, respectively, the cc-pVnZ/JKFIT and cc-pVnZ/MP2FIT or aug-cc-pVnZ/MP2FIT auxiliary basis sets of Weigend et al.[22,23] In each case n corresponds to the orbital basis. Local density fitting approximations[11,12] were disabled, except when otherwise noted. All calculations have been carried out using the MOLPRO[24] program package.

III. RESULTS AND DISCUSSION

A. Small peptide model systems

By comparison of the MP2 and DF-MP2 results it was found that typical errors due to the density fitting approximation are ∼0.01 kJ/mol. The maximum deviations never exceeded 0.1 kJ/mol and are therefore well within the 1 kJ/mol target accuracy. Thus, **in agreement with earlier investigations on conformational energies[25] and other properties**, the errors introduced by density fitting are negligible. Therefore, density fitting was used in all further calculations. For simplicity, the prefix DF will be omitted in the following.

The LMP2 method involves two distinct approximations: first, the excitations are restricted to pair-specific domains of projected atomic orbitals (PAOs). Secondly, distant pairs can be treated by multipole approximations[7,8,26] or neglected. Both approximations together lead to linear scaling of the computational cost with molecular size.[7,8,11] In this benchmark set, however, the systems were rather small and all pairs have always been included, i.e., distant pair approximations were not applied. The impact of pair approximations will be discussed for larger systems in Section III B.

When computing small energy differences using local methods it is essential to make sure that consistent domains are employed for all conformers. In most previous local correlation calculations a method proposed by Boughton and Pulay[27] (BP) has been used to determine the domains automatically. Unfortunately, the domains generated by this procedure are sensitive to the basis set and may also change as a function of the geometry. The former problem may lead to an erratic basis set convergence, the latter to small steps on potential energy surfaces[28–30] and to unbalanced results.[30] This also happens when considering different conformers, and we found that in the present benchmark the BP method leads

to quite unsatisfactory results, with maximum errors of up to about 10 kJ/mol relative to canonical MP2. Since the geometry changes between different conformers are substantial, the problem cannot be avoided by simply freezing the domains. We also tested the LMP2 implementation of the JAGUAR program[31] for the cc-pVDZ and cc-pVTZ basis sets, and in these cases the average and maximum errors were even somewhat larger than with the BP procedure in MOLPRO.

Recently, two of us have developed an alternative method[32] to determine the domains. This procedure is based on the natural population analysis (NPA) and natural localized molecular orbitals (NLMOs) proposed originally by Reed and Weinhold.[33,34] It yields domains that are much more stable with respect to the basis set and geometry than the BP method. In the present work we have applied this NLMO/NPA method in LMP2 calculations for all 95 conformers using 10 different basis sets ranging from cc-pVDZ to aug'-cc-pV5Z. The NPA domain selection criterion[32] was chosen to be 0.03. For each of the four model peptides the domains were consistent (i.e. the same atoms were selected for each orbital domain) for all conformers and 10 different basis sets. This confirms the superior stability of the new NLMO/NPA method.

The results are summarized in Table I, which shows the mean and maximum absolute deviations of the LMP2 and MP2 results for each basis set relative to the MP2/CBS[45] results. In addition, in the last two columns the mean and maximum absolute deviations between the LMP2 and MP2 results for each basis set are presented. The geometries and individual energies can be found in the supplementary material. The canonical MP2 method with an aug-cc-pVTZ basis is capable of reproducing the basis set limiting values within ≈ 1 kJ/mol. For the aug'-cc-pVnZ basis sets, in which the diffuse functions on the hydrogen atoms are omitted, the errors for MP2 are larger, while for LMP2 they perform almost as well as the full sets. On the other hand, the errors of both MP2 and LMP2 increase significantly if the diffuse functions are entirely omitted, at least for the smaller basis sets. These findings can be rationalized by the different contribution of basis set superposition effects (BSSE), as discussed below. It should be noted that the results for the double-zeta basis sets are rather strongly affected by errors of the HF contribution, and these basis sets are clearly too small for obtaining reliable energy differences.

The LMP2 results display convergence towards nearly the same limiting values as the canonical MP2 method. For the aug'-cc-pVnZ basis sets, the absolute deviations of the

LMP2 results from the MP2/CBS[45] reference values are typically twice as large as those of the canonical MP2. Without diffuse functions, the differences between MP2 and LMP2 results are even larger. The different convergence of the two methods with increasing basis set is attributed to the BSSE, which will be discussed below.

A closer inspection of the results for the two glycine conformers (Fig. 1) is presented in Fig. 2. The upper panel shows the convergence of the Hartree-Fock energy differences for the cc-pVnZ and aug'-cc-pVnZ basis sets. It is obvious that the inclusion of diffuse functions is essential to achieve rapid convergence. With the aug'-cc-pVDZ basis sets the error still amounts to 1.4 kJ/mol, but for all larger aug'-cc-pVnZ sets the HF values are very close to the estimated basis set limit. Note that in the present case the HF energy differences are negative, i.e., the energetic order of the two conformers is opposite than for MP2.

The lower panel of Fig. 2 shows the MP2 and LMP2 correlation energy contributions to the energy difference of the two conformers. The energetically lower conformer has a folded structure which is stabilized by hydrogen bonding, while the higher one has a stretched structure. At the more compact folded structure the dynamical correlation energy is larger, and therefore the correlation contribution to the energy difference is positive. This effect should increase with increasing basis set. However, as can be seen in the figure, the MP2 correlation contribution decreases with increasing cardinal number n. This can be attributed to the BSSE, which should decrease with n. Apparently, in the present case the decrease of the BSSE overcompensates the increase of the correlation contribution, leading overall to a decrease of the energy difference.

The behavior is entirely different for the LMP2 method, in which the BSSE is strongly reduced.[6,35,36] When standard NPA domains are used, the correlation contribution converges from below to the basis set limit, as one would anticipate in the absence of BSSE. The convergence is slower than for MP2, because there is no compensation of the incomplete basis set error by the BSSE. If the domains are extended by including the PAOs at the first shell of neighboring atoms (LMP2(ext)), part of the BSSE is re-introduced, and in this case the basis set convergence dependence is remarkably weak. The total (HF + LMP2) triple-zeta value differs only by 0.01 kJ/mol from the quintuple-zeta one. However, the quintuple-zeta result is still 0.2 kJ/mol below the MP2/CBS[45] limit. This may be due to the two missing classes of ionic excitations, which are excluded in the LMP2 ansatz by construction.[36] Interestingly, the extrapolated LMP2(ext) result differs by less than 0.05

kJ/mol from the MP2 one. However, the extrapolation of local correlation energies should be considered with care, since the domains become more complete with increasing cardinal number, and this may lead to a different asymptotic basis set convergence than in the canonical case. Furthermore, it is of course essential that the domains are consistent for all basis sets. In the present applications, this is the case with the NLMO/NPA method, but not with the BP procedure.

The glycine case discussed above demonstrates well the different basis set convergence of MP2 and LMP2, but it is somewhat special in the sense that the MP2 correlation contribution converges from above to the basis set limit. In most other cases of the present benchmark set the MP2 correlation contributions converge from below to the basis set limit (still being positive if the energetically lowest conformer is taken as the reference), indicating that the BSSE is less dominant than in the glycine case. But the BSSE still improves the MP2 results, in particular for the small basis sets, and therefore the convergence of the LMP2 results is slower. This effect is reduced when extended domains are used: For LMP2(ext)/aug'-cc-pVTZ the average and maximum absolute deviations from the MP2/CBS[45] limits are 1.41 and 2.77 kJ/mol, respectively. These values are only 0.4-0.5 kJ/mol larger than the corresponding canonical MP2 values.

B. Alanine peptides

In order to demonstrate the accuracy and computational savings of the LMP2 method for larger peptides, alanine tetra-, hexa- and octapeptides were chosen as model systems. For each of these peptides, an extended and an α-helix conformer were optimized using density functional theory, as described in section III A. The optimized alpha-helix structures are shown in Fig. 3. At these structures, the HF, MP2 and LMP2 conformational energies were computed using aug'-cc-pVnZ basis sets ($n = 2 - 4$). The MP2/CBS[34] basis set limits were estimated by extrapolation of the triple-zeta and quadruple-zeta correlation energies. In these calculations the HF energies were not extrapolated, and the aug'-cc-pVQZ values were taken as the reference. The results are summarized in Table II.

As for the smaller model systems, the MP2 and LMP2 results converge to approximately the same basis set limits. However, the basis set convergence of the two methods is very different. The most striking result in Table II is the slow basis set convergence of the MP2

results for the octapeptide folding energy. The MP2/aug'-cc-pVTZ result has a deviation of 20 kJ/mol relative to the CBS[34] reference. This amounts to 31% of the total folding energy. On the other hand, the LMP2 results show a remarkably low basis set dependence. For the aug'-cc-pVDZ basis set this is partly due to error compensation of the HF and correlation contributions, but nevertheless for all three peptides the LMP2/aug'-cc-pVDZ results are already very close to the aug'-cc-pVQZ ones. Very likely, the strong basis set dependence of the canonical MP2 results is mainly due to BSSE effects, which over-stabilize the folded structure. The BSSE is largely eliminated in the LMP2, and this leads to the much better basis set stability, very similar to the case shown in Fig. 1 for the glycine conformers. **The same effect was observed by Head-Gordon and coworkers, while investigating the stability of 27 alanine tetrapetides.[25]**

The effect is most pronounced for the octapeptide, since the smaller structures, after optimization, tend to distort significantly from the ideal helix conformation, as shown in Fig. 3. In the hexamer, only half of the chain is folded, the other section is extended. In the case of the tetrapeptide, the **polypeptide** chain is too small and the backbone is approximately planar. However, even in this case, the LMP2 results are almost independent of the basis set, while the MP2 ones change by more than 40% from aug'-cc-pVDZ to the CBS[34] limit. Although these examples are simplified models, **the present results confirm earlier findings made for the alanine tetrapeptide.[25] Large basis sets are needed when computing folding energies with canonical correlation methods, since BSSE starts to play a crucial role in larger peptides.** As the chain size increases, the errors accumulate, and at least quadruple-zeta quality basis set are necessary in order to obtain reasonably accurate results with MP2.[37] On the other hand, local correlation methods allow to use much smaller basis sets; moreover, for a given basis set the computational effort is drastically reduced, as will be demonstrated in the following.

The computation times of MP2 and LMP2 calculations for the octapeptides are shown in Table III. The savings made by the local approximations are quite dramatic. As compared to the canonical calculation, the total computational time for the extended structure is reduced by one order of magnitude. As expected, the LMP2 calculations for the α-helix conformer with a more more three-dimensional structure are slower than for the extended peptide, especially for the iterations, but the savings are still significant. The longer computation times for the helix structure are mainly caused by the larger number of pairs included in

the calculation (see below).

Further savings are possible through the use of local density fitting approximations, which asymptotically lead to linear scaling of the computational cost with system size.[11] In the local density fitting method, the 4-index exchange integrals $K_{rs}^{ij} = (ri|sj)$ are decomposed into sums of products of 2- and 3-index integrals

$$K_{rs}^{ij} \approx \sum_{A\in[i]_{\rm fit}} D_{ri}^{A}(sj|A) + \sum_{B\in[j]_{\rm fit}} (ri|B)D_{sj}^{B} - \sum_{A\in[i]_{\rm fit}} \sum_{B\in[j]_{\rm fit}} D_{ri}^{A} J_{AB} D_{sj}^{B}, \quad (1)$$

where the indices $\{A, B\}$ refer to the auxiliary basis set and D_{ri}^{A} are the fitting coefficients obtained by solving systems of linear equations

$$(ri|A) = \sum_{B\in[i]_{\rm fit}} J_{AB} D_{ri}^{B} \quad (2)$$

(for further details see Ref. 11). Note that this *robust* fitting approximation is slightly different than the less symmetric approximation described in Ref. 11.

In a conventional implementation, the summations in eqs. (1) and (2) would run over the full fitting basis, leading to $\mathcal{O}(\mathcal{N}^5)$ scaling. The last two terms in eq. (1) then cancel. In a local calculation, it is possible to use for each orbital pair ij a truncated fitting basis, in which only the auxiliary function in the vicinity of the localized orbitals i and j are included. The default in MOLPRO is to include in the domain $[i]_{\rm fit}$ the fitting functions at all atoms that are separated from the atoms in the orbital domain $[i]$ by at most 3 bonds ($l_f = 3$). Using this value the effect of the local density fitting approximation on the relative energies is negligible. In fact, in the current case even smaller fitting domains with only the atoms that are separated by at most one bond ($l_f = 1$) from the atoms in the domain $[i]$ are sufficient to obtain accurate results (cf. Table III).

The number of pairs included in the LMP2 and therefore onset of linear scaling and the CPU-time depends on the the distance criterium R_{vd} for neglecting very distant pairs.[6,7] Orbital pairs ij are neglected if the closest distance R_{ij} between an atom in the orbital domain $[i]$ and an atom in the orbital domain $[j]$ is larger than R_{vd}. Reducing this distance criterion below its default value of 15 bohr leads to significant savings, but increases the error in the energy difference (cf. Table III). If the distance criterion is set to 12 bohr the errors already exceed 1 kJ/mol. The sensitivity of the energy difference is due to the

different three-dimensional arrangement of the conformers. In the helix structure, more pairs are removed when R_{vd} is decreased: if R_{vd} is reduced from 15 to 12 bohr, about 800 pairs are removed in the helix case, while in the extended conformer only 500 pairs are removed. Therefore, the helix energy is more affected than the energy of the extended conformer, and the energy difference decreases.

Optionally, the integrals for distant pairs ($R_d < R_{ij} \leq R_{vd}$) can be approximated by multipole approximations, which also reduce the overall cost.[8,26] However, as shown in Table III for various choices of R_d, this approximation leads to rather large errors. As already pointed out in Ref. 26, this is due to the neglect of certain exchange contributions, and such approximations are therefore not recommended in the study of intermolecular forces or for cases in which long-range interactions play a crucial role.

Finally, it should be noted that the CPU-time for the Hartree-Fock calculation (about 8.3 hours, using density fitting and the aug'-cc-pVTZ basis) exceeds that of the LMP2 step. The differences are even greater when the aug'-cc-pVQZ basis (3860 contracted functions) is used. The HF and MP2 calculations took about 85 and 110 hours, respectively, while the LMP2 calculation took only 28 hours (helix structure, without local density fitting approximations).

IV. CONCLUSIONS

We have investigated the effect of local approximations on the relative energies of different conformers. In order to obtain reliable LMP2 energy differences it is important that the orbital domains of the different conformers are defined consistently. This can be achieved using a recently proposed method that is based on natural population analysis.[32] With this method consistent domains were obtained for all conformers and all basis sets studied in this work, and a smooth convergence with increasing basis set size to the basis set limit was always achieved.

For all model systems studied, the MP2 and LMP2 methods yield very similar results at the basis set limit. However, due to the reduced BSSE in the LMP2, the convergence of MP2 and LMP2 with increasing basis sets is different. For most of the small systems in the benchmark set the convergence of the LMP2 results is found to be somewhat slower than for MP2, since in these systems the BSSE partly compensates for other basis set deficiencies.

However, the BSSE increases with system size, and our calculations for larger peptide chains demonstrate that canonical MP2 may strongly over-stabilize helical structures. For the alanine-octapeptide the basis set error was found to be more than 30 and 20 kJ/mol, with augmented double-zeta and triple-zeta basis sets, respectively. In contrast, the LMP2 results are only weakly basis set dependent, and already with augmented double-zeta sets results close to the basis set limit are obtained. Moreover, the local approximations reduce the computation times by up to one order of magnitude.

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Tables

TABLE I: Mean (MAD) and maximum (MAX) absolute deviations of relative energies (in kJ/mol) for 91 conformations of four model peptide systems.

Basis set	MP2[a]		LMP2[a]		LMP2[b]	
	MAD	MAX	MAD	MAX	MAD	MAX
cc-pVDZ	3.02	10.55	2.34	7.21	2.39	6.02
cc-pVTZ	0.91	3.48	1.94	4.43	2.20	5.36
cc-pVQZ	0.34	0.86	1.23	2.78	1.16	3.02
cc-pV5Z	0.20	0.47	0.82	2.00	0.67	1.71
aug-cc-pVDZ	1.68	4.30	3.03	5.58	1.99	5.14
aug-cc-pVTZ	0.64	1.64	1.77	3.48	1.38	3.36
aug'-cc-pVDZ[c]	2.13	5.48	3.00	5.51	1.50	4.02
aug'-cc-pVTZ[c]	0.92	2.38	1.85	3.61	1.10	2.79
aug'-cc-pVQZ[c]	0.38	0.89	0.85	1.80	0.54	1.30
aug'-cc-pV5Z[c]	0.19	0.45	0.49	1.06	0.33	0.79
CBS[45][d]	(0.0)	(0.0)	0.12	0.33	0.12	0.33

a) Relative to the MP2/CBS[45] values.

b) Relative to MP2 values for each basis set.

c) aug' indicates that diffuse functions are included only on non-hydrogen atoms.

d) Basis set limits estimated from extrapolations of the aug'-cc-pVnZ energies, see text.

TABLE II: Energy difference $E_{\alpha-\text{helix}} - E_{\text{extended}}$ (in kJ/mol) between the helical and extended conformers of the alanine peptides. The HF contribution is included in the MP2 and LMP2 values.

Peptide	Basis	HF	MP2	LMP2
$(ala)_4$	aug'-cc-pVDZ	27.69	12.58	18.21
	aug'-cc-pVTZ	29.71	15.74	18.61
	aug'-cc-pVQZ	30.71	17.26	19.06
	CBS[**34**][a]	—	18.03	19.06
$(ala)_6$	aug'-cc-pVDZ	42.84	47.29	46.15
	aug'-cc-pVTZ	41.47	45.55	44.27
	aug'-cc-pVQZ	41.61	45.62	45.18
	CBS[**34**][a]	—	45.57	45.75
$(ala)_8$	aug'-cc-pVDZ	-15.32	-94.49	-60.08
	aug'-cc-pVTZ	-2.38	-84.03	-63.19
	aug'-cc-pVQZ	-0.87	-71.78	-60.84
	CBS[**34**][a]	—	-63.95	-60.22

a) Calculated from the aug'-cc-pVTZ and aug'-cc-pVQZ correlation energies and the aug'-cc-pVQZ HF value.

TABLE III: CPU-times (in minutes, using 2.8 **GHz** opteron processors) for conventional and local correlation calculations[a] with the aug'-cc-pVTZ basis set on the extended/helix conformers of the alanine octapeptide. The conformational energies (in kJ/mol) ΔE=E(α-helix)-E(extended) are also shown.

Method	l_f	R_{vd}	R_d	Integrals[b]	Iterations[c]	Total	ΔE
MP2	–	–	–	—	—	1509/1514	-84.03
LMP2	–	–	–	162/176	413/413	590/604	-63.01
LMP2	–	15	–	106/149	95/283	214/448	-63.19
LMP2	1	15	–	45/84	95/283	152/380	-63.13
LMP2	1	12	–	44/78	68/219	124/310	-61.91
LMP2	1	10	–	39/65	43/135	94/212	-58.19
LMP2	1	15	12	44/75	94/256	152/347	-62.30
LMP2	1	15	10	37/70	78/242	128/328	-60.40
LMP2	1	15	8	32/52	70/198	114/264	-52.48

a) R_{vd} and R_d (in bohr) are the distance criteria for neglecting very distant pairs and for using multipole approximations, respectively; l_f determines the size of the local fitting domains, see text.

b) CPU-time for integral evaluation and transformation.

c) CPU-time to solve the first-order LMP2 equations.

Figure Captions

Figure 1: **Ball-and-stick** representation of the two glycine tripeptide conformers discussed in the text and Fig. 2. The upper structure corresponds to the minimum energy conformation.

Figure 2: Hartree-Fock (upper panel) and correlation contributions (lower panel) to the relative energy of the glycine conformers as a function of cardinal number n of the basis set.

Figure 3: **Ball-and-stick** representation of the alanine tetra-, hexa- and octapeptide optimized helical conformers.

Figures

FIG. 1: Jakub et al., Molecular Physics

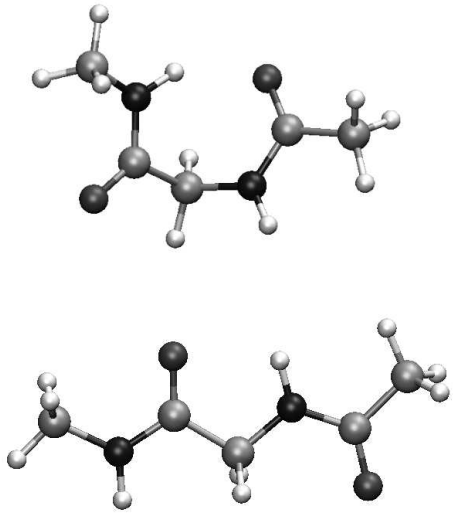


FIG. 2: Jakub et al., Molecular Physics

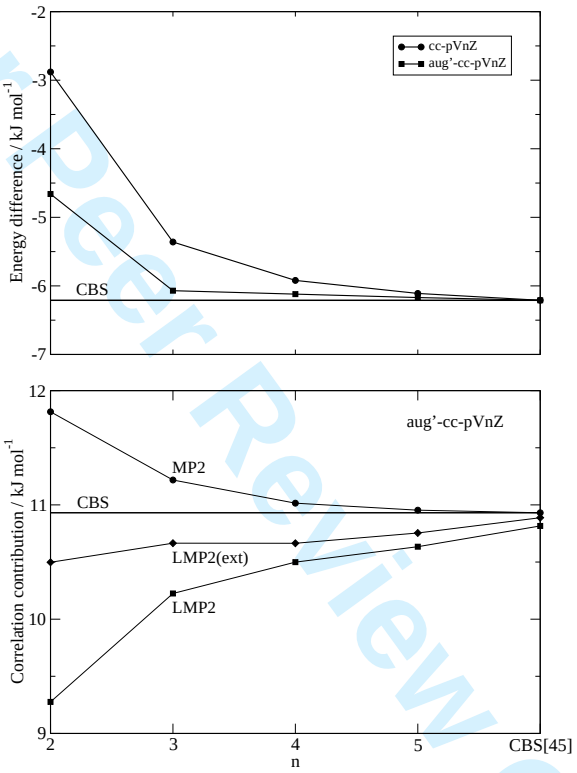
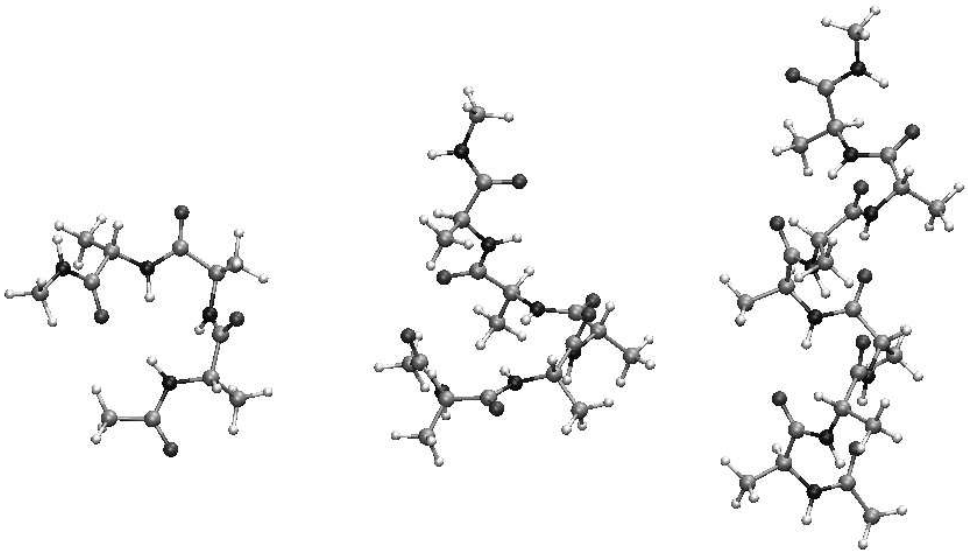
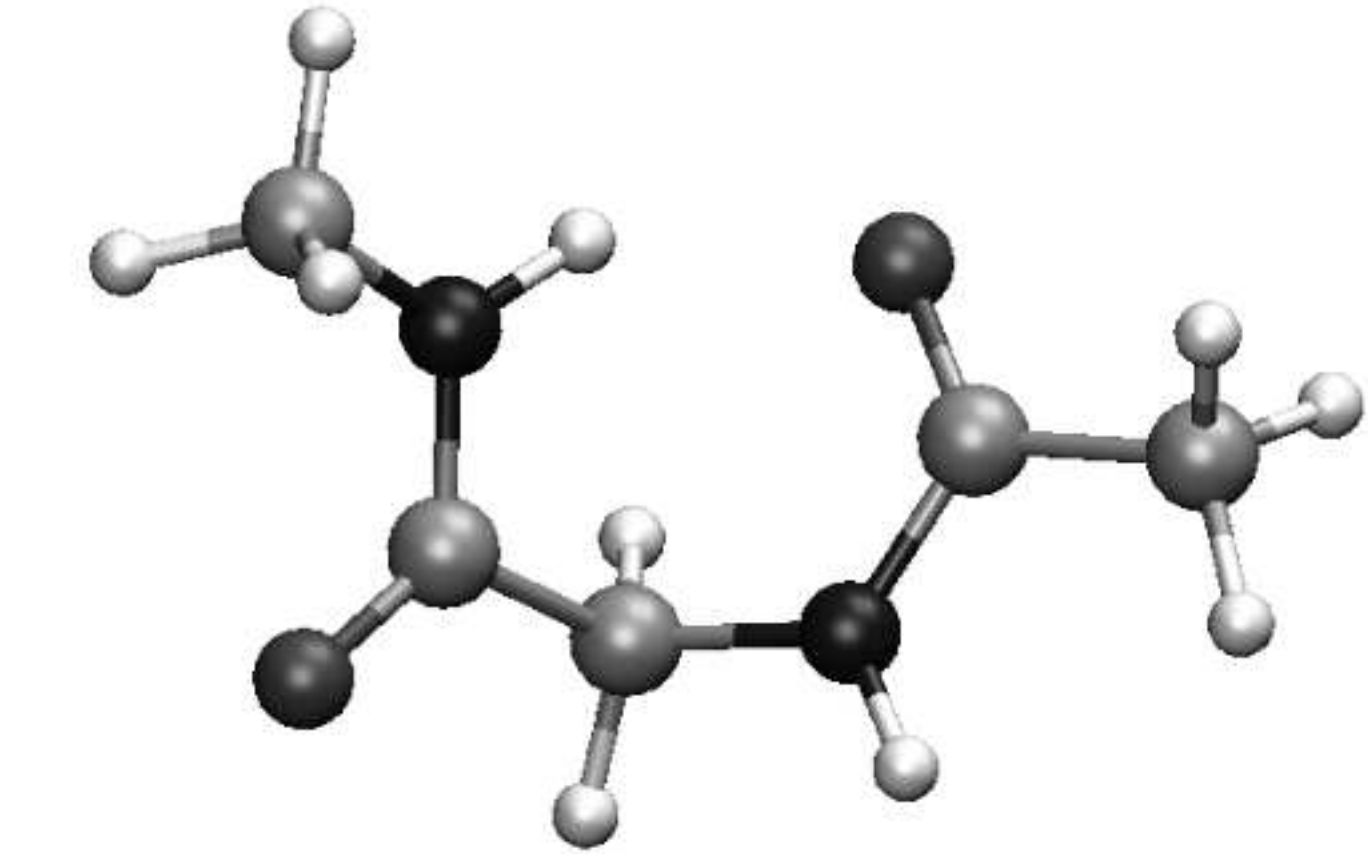
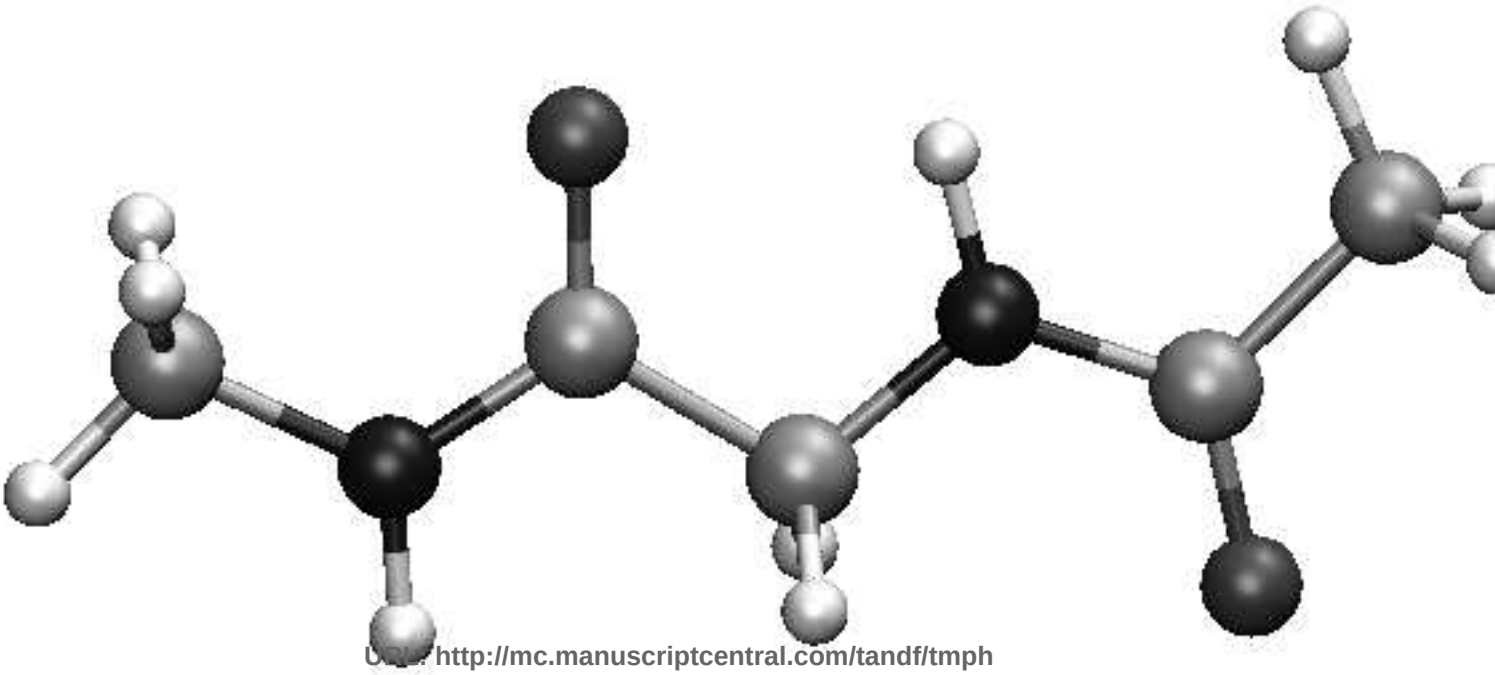
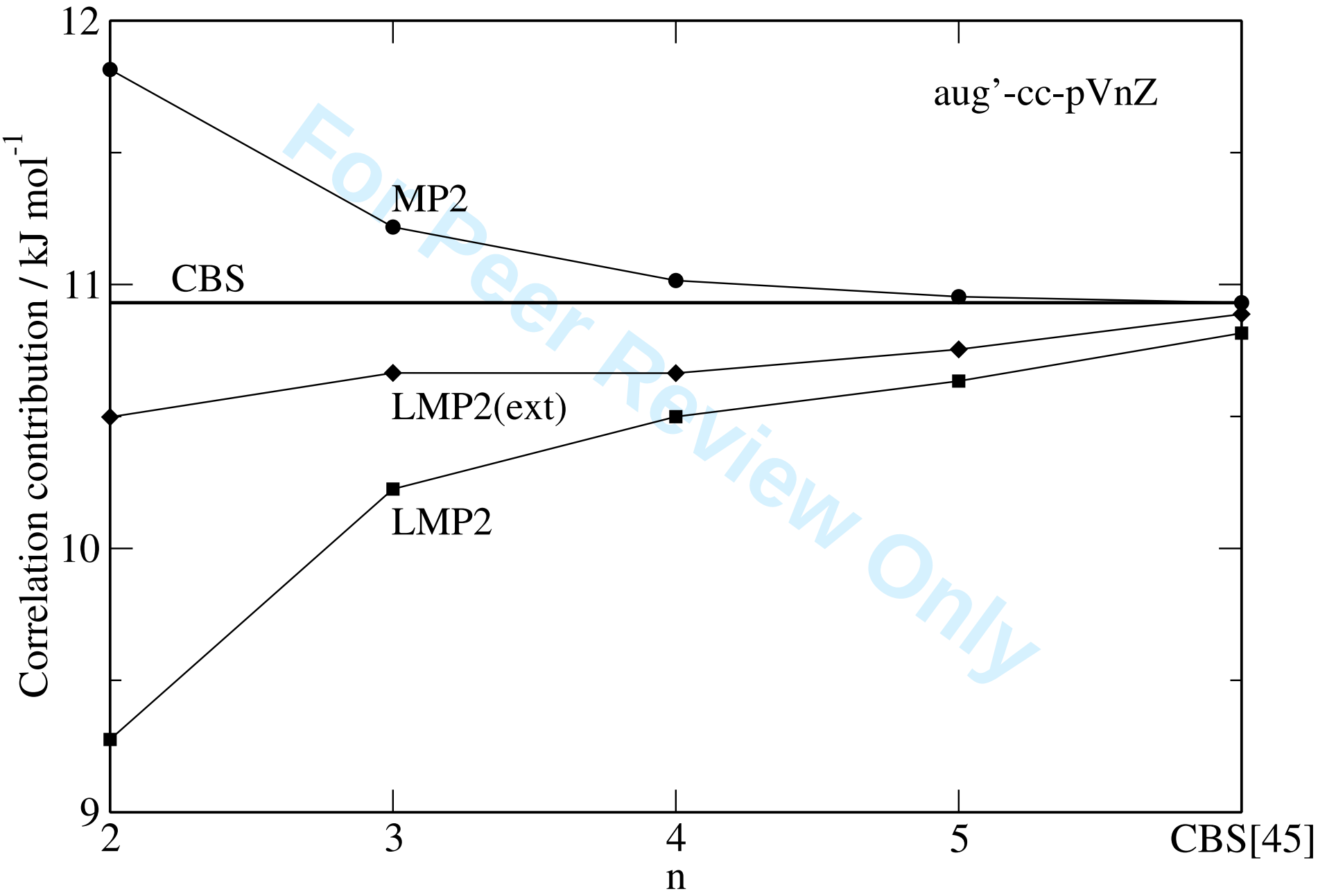


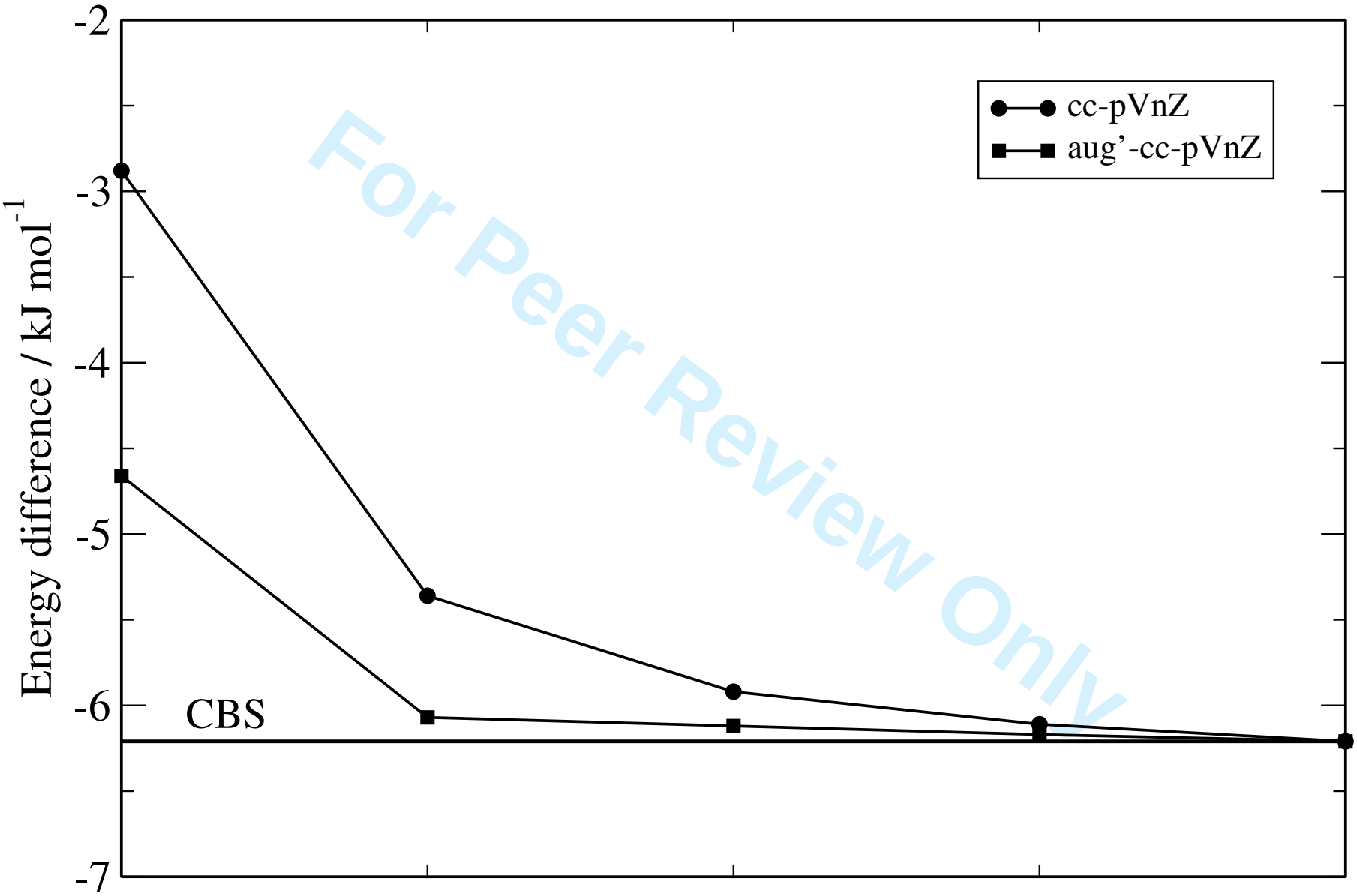
FIG. 3: Jakub et al., Molecular Physics

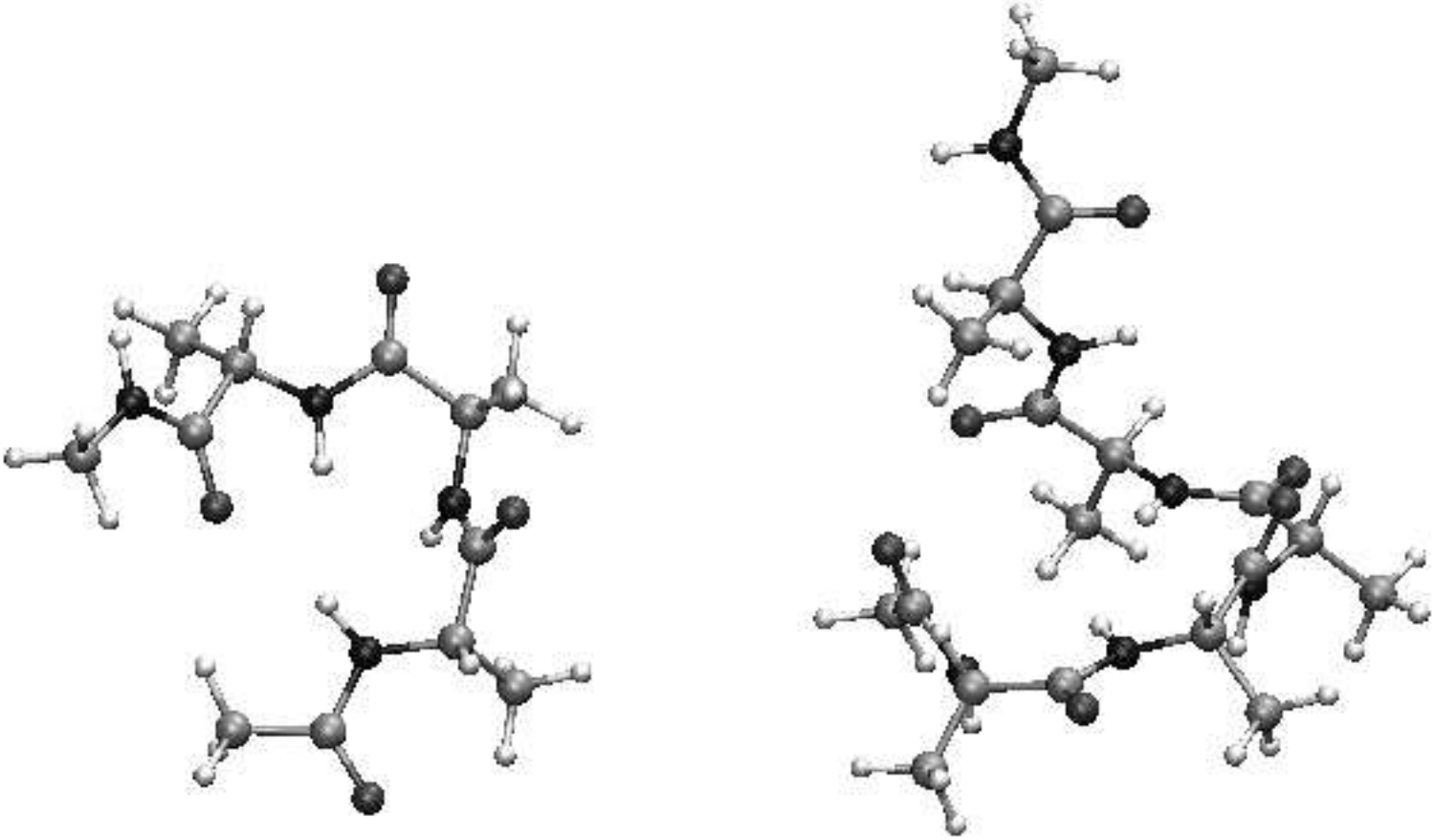












This file contains:

1.) DF-HF results

2.) DF-MP2 results

3.) DF-LMP2 results

4.) Geometries (xyz format)

Basis sets:

DZ: cc-pVDZ

TZ: cc-pVTZ

QZ: cc-pVQZ

5Z: cc-pV5Z

ADZ: aug-cc-pVDZ

ATZ: aug-cc-pVTZ

(A)DZ: (aug)-cc-pVTZ

(A)TZ: (aug)-cc-pVTZ

(A)QZ: (aug)-cc-pVTZ

(A)5Z: (aug)-cc-pVTZ

The (aug)-cc-pVnZ basis sets do not include diffuse function on H-atoms.

All results obtained with density fitting, using the cc-pVnZ/JKFIT sets for DF-HF

the cc-pVnZ/MP2FIT for MP2/cc-pVnZ, and aug-cc-pVnZ/MP2FIT for both MP2/aug-cc-pVnZ and MP2/(aug)-cc-pVnZ

All relative energies in kJ/mol

==========

DF-HF results

	DZ	TZ	QZ	5Z	ADZ	ATZ	(A)DZ	(A)TZ	(A)QZ	(A)5Z	XPOL	REF
Glycine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-2.839	-5.361	-5.925	-6.112	-4.822	-5.984	-4.656	-6.071	-6.119	-6.170	-6.208	-6.208
Alanine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.447	-1.511	-1.840	-1.935	-0.646	-1.767	-0.554	-1.804	-1.916	-1.944	-1.957	-1.957
3	13.250	12.498	12.605	12.609	12.507	12.483	12.606	12.547	12.588	12.610	12.624	12.624
4	13.187	10.404	10.202	10.252	10.718	10.320	10.597	10.290	10.258	10.264	10.272	10.272
5	18.994	20.741	21.444	21.691	20.905	21.692	20.718	21.653	21.712	21.730	21.739	21.739
6	19.124	18.738	19.200	19.311	18.436	19.196	18.248	19.114	19.307	19.330	19.330	19.330
7	23.513	23.057	23.325	23.496	23.671	23.574	23.886	23.563	23.569	23.539	23.513	23.513
Serine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	13.844	10.698	9.746	9.448	10.145	9.502	10.348	9.537	9.444	9.428	9.424	9.424
3	12.472	9.426	8.723	8.424	8.994	8.519	9.020	8.494	8.430	8.395	8.371	8.371
4	17.834	13.502	12.334	11.921	13.667	12.030	14.015	12.091	11.922	11.873	11.848	11.848
5	20.647	22.421	23.008	23.141	21.749	22.941	21.653	22.931	23.131	23.173	23.187	23.187
6	15.426	12.122	11.262	10.867	11.820	10.977	11.857	10.974	10.868	10.826	10.802	10.802
7	23.339	19.539	18.701	18.308	18.518	18.281	18.642	18.364	18.304	18.268	18.244	18.244
8	23.679	20.370	19.553	19.204	19.529	19.194	19.677	19.225	19.194	19.167	19.147	19.147
9	29.021	28.362	28.327	28.249	28.126	28.140	28.188	28.135	28.235	28.258	28.267	28.267
10	22.293	17.524	16.577	16.260	17.495	16.411	17.598	16.382	16.282	16.241	16.215	

16.215

11 27.520 23.690 22.624 22.275 22.546 22.325 22.803 22.354 22.285 22.241 22.210 22.210

12 23.642 18.392 17.537 17.219 18.566 17.366 18.665 17.363 17.230 17.186 17.162 17.162

13 25.152 19.858 18.632 18.239 19.599 18.397 19.359 18.354 18.250 18.211 18.188 18.188

14 27.222 27.371 27.328 27.276 26.983 27.333 26.994 27.316 27.283 27.283 27.286 27.286

15 38.663 32.597 31.414 30.935 31.446 30.807 31.690 30.867 30.890 30.879 30.866 30.866

16 30.655 25.646 25.066 24.864 25.280 24.915 25.198 24.875 24.886 24.861 24.838 24.838

17 36.766 30.626 29.399 28.889 29.370 28.739 29.523 28.811 28.846 28.842 28.835 28.835

18 30.755 23.365 21.634 21.011 23.179 21.175 23.246 21.144 20.991 20.947 20.925 20.925

19 34.717 31.625 31.148 30.920 31.248 30.792 31.669 30.853 30.909 30.901 30.888 30.888

20 39.578 33.338 32.094 31.570 32.100 31.451 32.364 31.490 31.522 31.520 31.516 31.516

21 32.233 26.920 26.226 25.941 26.242 25.980 26.179 25.978 25.957 25.928 25.905 25.905

22 27.087 25.817 25.797 25.743 25.532 25.824 25.560 25.756 25.790 25.766 25.742 25.742

23 33.156 28.584 27.570 27.159 27.746 27.224 27.976 27.144 27.153 27.110 27.071 27.071

24 37.647 35.761 35.374 35.160 34.759 35.076 34.809 35.104 35.162 35.161 35.154 35.154

25 30.682 30.470 30.622 30.493 29.559 30.393 29.511 30.360 30.480 30.481 30.469 30.469

26 33.773 31.498 31.098 30.845 29.987 30.730 29.709 30.704 30.827 30.820 30.800 30.800

27 33.596 33.537 33.620 33.505 32.648 33.427 32.621 33.375 33.488 33.495 33.489 33.489

28 33.054 35.697 36.546 36.734 36.020 36.639 35.749 36.538 36.732 36.770 36.782 36.782

29 32.716 28.178 27.494 27.161 27.544 27.267 27.407 27.193 27.185 27.150 27.119 27.119

30 40.237 38.007 37.389 37.236 38.169 37.370 38.650 37.410 37.289 37.245 37.220 37.220

31 37.942 34.582 33.696 33.370 34.231 33.460 34.239 33.464 33.381 33.358 33.347 33.347

32 39.473 36.612 36.154 35.896 35.278 35.806 35.040 35.734 35.879 35.872 35.852 35.852

33 42.574 38.401 37.711 37.420 37.265 37.393 37.069 37.364 37.386 37.371 37.357 37.357

34 42.537 38.410 37.812 37.540 36.939 37.501 36.874 37.436 37.537 37.528 37.509 37.509

35 48.278 45.415 45.006 44.905 45.541 44.969 46.022 44.999 44.971 44.910 44.861 44.861

36 58.549 53.979 53.472 53.094 54.125 52.971 54.265 53.031 53.049 53.060 53.068 53.068

37 54.922 53.327 53.121 52.909 52.726 52.870 52.556 52.837 52.870 52.901 52.924 52.924

38 61.061 55.832 54.797 54.415 55.292 54.556 55.371 54.544 54.418 54.383 54.366 54.366

39 68.255 60.615 58.704 58.068 60.266 58.412 60.424 58.425 58.107 58.026 57.991 57.991

Cysteine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 6.037 1.573 0.607 0.260 1.298 0.505 1.028 0.388 0.261 0.225 0.209 0.209

3 4.561 2.863 2.382 2.244 3.007 2.440 2.904 2.274 2.234 2.210 2.194 2.194

4 12.161 9.829 9.338 9.181 9.751 9.361 9.180 9.152 9.092 9.075 9.066 9.066

5 6.315 4.609 4.200 4.134 4.500 4.307 4.387 4.217 4.144 4.124 4.114 4.114

6 7.893 6.097 5.630 5.466 6.107 5.687 5.750 5.570 5.443 5.426 5.424 5.424

7 7.516 2.751 2.033 1.774 3.217 2.167 2.821 1.947 1.780 1.726 1.698 1.698

8 9.627 7.264 6.689 6.567 7.328 6.695 7.223 6.679 6.542 6.521 6.516 6.516

9 10.283 7.886 7.342 7.221 8.226 7.494 7.902 7.374 7.198 7.164 7.154 7.154

10 10.677 7.418 6.686 6.437 7.569 6.762 7.094 6.453 6.383 6.352 6.333 6.333

11 11.006 8.186 7.769 7.654 9.238 7.996 8.968 7.856 7.675 7.634 7.618 7.618

12 19.615 15.998 15.397 15.202 15.995 15.303 15.750 15.202 15.137 15.140 15.148 15.148

13 11.807 8.434 8.031 7.912 9.609 8.280 9.436 8.040 7.923 7.877 7.851 7.851

14 17.211 14.253 13.795 13.622 14.379 13.721 14.021 13.599 13.560 13.569 13.580 13.580

15 14.672 11.860 11.371 11.294 11.945 11.553 11.633 11.360 11.272 11.244 11.230 11.230

16 16.248 12.213 11.544 11.381 13.403 11.670 13.391 11.553 11.379 11.341 11.327 11.327

17 17.014 13.658 13.304 13.235 13.596 13.450 13.029 13.300 13.245 13.231 13.224 13.224

18 22.606 19.782 19.367 19.277 19.564 19.247 19.808 19.287 19.232 19.239 19.250 19.250

19 23.240 22.114 21.813 21.694 21.978 21.820 21.751 21.724 21.662 21.671 21.684 21.684

20 18.705 14.050 13.240 13.036 15.010 13.261 14.946 13.128 13.005 12.961 12.936 12.936

21 25.047 22.563 21.875 21.607 22.505 21.830 22.084 21.663 21.559 21.555 21.562 21.562

22 18.202 18.118 18.293 18.339 17.794 18.466 17.102 18.268 18.306 18.313 18.315 18.315

23 21.532 19.960 19.884 19.867 19.783 20.079 19.212 19.887 19.831 19.823 19.822 19.822

24 22.109 17.811 17.297 17.264 17.827 17.387 17.645 17.344 17.251 17.239 17.238 17.238

25 21.793 15.770 14.566 14.212 16.669 14.636 16.249 14.387 14.159 14.094 14.064 14.064

26 29.758 27.651 27.441 27.366 27.791 27.519 27.664 27.398 27.399 27.372 27.350 27.350

27 22.834 22.484 22.672 22.795 22.113 22.815 22.063 22.797 22.796 22.797 22.798 22.798

28 23.435 24.919 25.254 25.382 25.147 25.523 24.853 25.392 25.361 25.364 25.370 25.370

29 31.672 28.385 27.649 27.445 28.200 27.457 28.202 27.411 27.358 27.365 27.375 27.375

30 27.913 27.231 27.222 27.104 26.477 27.163 25.955 27.001 27.089 27.093 27.087 27.087

31 29.731 27.816 27.743 27.758 28.067 27.939 27.863 27.778 27.793 27.769 27.748 27.748

32 37.791 36.611 36.412 36.254 36.170 36.342 36.044 36.181 36.210 36.231 36.247 36.247

33 30.291 28.257 27.869 27.909 28.627 28.102 28.472 28.051 27.899 27.890 27.899 27.899

34 29.825 28.981 29.045 29.033 27.980 28.916 27.876 28.890 29.019 29.034 29.032 29.032

35 43.592 44.209 44.525 44.642 42.943 44.341 43.171 44.468 44.632 44.687 44.715 44.715

36 32.642 36.044 36.830 37.002 36.345 37.058 35.916 36.829 36.986 37.020 37.033 37.033

37 44.943 43.157 43.349 43.310 44.162 43.365 44.080 43.254 43.313 43.313 43.306 43.306

38 34.631 30.509 29.519 29.199 30.511 29.563 30.102 29.401 29.219 29.181 29.167 29.167

39 35.958 35.367 35.257 35.189 35.517 35.506 34.666 35.187 35.083 35.061 35.053 35.053

40 37.001 34.033 33.453 33.363 34.663 33.710 34.631 33.554 33.387 33.337 33.313 33.313

41 46.626 45.445 45.085 44.829 44.072 44.877 43.335 44.588 44.762 44.766 44.752 44.752

42 42.164 38.284 37.451 37.255 38.631 37.644 37.984 37.332 37.178 37.132 37.111 37.111

43 42.729 38.386 37.465 37.232 38.498 37.463 38.369 37.347 37.218 37.176 37.154 37.154

44 43.975 41.187 40.341 40.192 41.761 40.455 42.000 40.415 40.216 40.176 40.163 40.163

45 50.252 50.674 50.588 50.505 49.967 50.570 49.451 50.284 50.401 50.405 50.398 50.398

46 44.696 42.275 41.789 41.650 42.540 41.947 42.534 41.800 41.663 41.619 41.597 41.597

47 51.553 46.740 45.349 44.985 47.109 45.431 46.807 45.196 44.942 44.875 44.845 44.845

MAD

1 3.735 0.837 0.254 0.047 0.865 0.188 0.886 0.128 0.041 0.016 0.000

MaxAD

1 10.264 2.625 0.713 0.149 2.605 0.586 2.433 0.434 0.116 0.049 0.000

==========

DF-MP2 results (using DF-HF reference functions)

	DZ	TZ	QZ	5Z	ADZ	ATZ	(A)DZ	(A)TZ	(A)QZ	(A)5Z	XPOL	REF
Glycine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	7.957	6.321	5.194	4.900	7.348	5.729	7.155	5.418	4.895	4.783	4.680	4.680
Alanine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	8.645	6.555	5.806	5.699	7.115	6.268	7.005	6.025	5.695	5.631	5.582	5.582
3	11.780	9.992	9.945	10.014	9.522	9.526	9.877	9.752	9.928	10.014	10.095	10.095
4	15.921	13.388	12.865	13.005	12.947	12.789	12.652	12.679	12.929	13.022	13.121	13.121
5	17.219	18.962	19.774	20.242	18.582	19.785	18.301	19.705	20.168	20.321	20.471	20.471
6	20.622	20.111	20.314	20.457	18.110	19.754	17.577	19.444	20.222	20.385	20.531	20.531
7	24.756	25.839	26.546	27.002	26.881	26.651	27.017	26.629	27.042	27.117	27.201	27.201
Serine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	18.352	14.933	13.810	13.471	13.939	13.491	14.045	13.469	13.436	13.483	13.546	13.546
3	19.039	16.685	15.493	15.076	16.195	15.244	15.755	15.110	15.039	15.006	14.985	14.985
4	23.293	19.992	18.288	17.776	19.809	18.195	19.960	18.217	17.849	17.769	17.712	17.712
5	15.919	17.941	18.623	19.024	17.218	18.291	17.000	18.295	19.046	19.158	19.246	19.246
6	24.248	20.709	19.182	18.618	20.179	19.064	19.707	18.930	18.604	18.557	18.526	

18.526

7 30.796 26.215 24.645 24.089 23.463 23.958 23.641 23.867 23.951 24.013 24.091 24.091

8 29.240 26.175 24.899 24.427 23.795 24.197 23.842 24.021 24.275 24.351 24.439 24.439

9 28.942 27.567 27.393 27.563 25.725 26.581 26.037 26.648 27.457 27.674 27.887 27.887

10 30.767 27.039 25.699 25.354 26.142 25.553 25.880 25.286 25.327 25.348 25.389 25.389

11 33.022 30.003 28.897 28.540 27.410 28.327 27.549 28.242 28.471 28.528 28.603 28.603

12 32.966 28.572 27.180 26.849 27.485 27.130 27.318 26.833 26.738 26.771 26.828 26.828

13 35.386 29.632 27.642 27.147 27.296 27.277 26.608 26.889 26.970 27.038 27.127 27.127

14 28.518 29.384 29.536 29.653 28.001 29.316 27.768 29.141 29.557 29.733 29.921 29.921

15 41.581 34.244 32.498 31.967 30.185 31.032 30.746 31.107 31.671 31.878 32.095 32.095

16 36.451 32.610 31.906 31.775 30.427 31.236 29.693 30.840 31.570 31.792 32.030 32.030

17 42.603 34.648 32.647 32.063 30.530 31.367 30.689 31.333 31.837 32.027 32.223 32.223

18 43.046 35.972 33.358 32.516 33.430 32.832 32.905 32.419 32.302 32.385 32.497 32.497

19 36.722 32.738 31.928 31.764 31.080 31.195 31.842 31.350 31.704 31.812 31.921 31.921

20 43.729 36.482 34.606 34.043 32.479 33.370 32.726 33.293 33.834 34.018 34.209 34.209

21 39.861 34.791 33.760 33.503 31.982 32.995 31.426 32.683 33.286 33.518 33.769 33.769

22 33.788 34.035 34.164 34.284 33.219 34.156 32.744 33.793 34.214 34.316 34.425 34.425

23 39.815 36.868 35.783 35.430 34.144 35.216 33.835 34.720 35.262 35.388 35.526 35.526

24 38.437 36.847 36.468 36.360 34.504 35.560 34.545 35.664 36.254 36.426 36.601 36.601

25 37.089 36.755 36.802 36.670 33.839 35.864 33.237 35.500 36.304 36.557 36.809 36.809

26 41.671 38.574 37.609 37.305 34.145 36.557 33.661 36.175 36.975 37.223 37.471 37.471

27 37.472 38.249 38.409 38.329 35.462 37.457 34.880 37.052 37.978 38.232 38.484 38.484

28 32.449 36.773 37.914 38.316 34.995 37.287 33.995 36.836 38.000 38.316 38.619 38.619

29 44.335 41.179 40.494 40.270 37.826 39.959 36.633 39.193 40.070 40.288 40.524 40.524

30 40.752 40.301 40.088 40.214 40.242 40.055 40.589 40.028 40.270 40.390 40.537 40.537

31 43.815 41.110 40.189 39.859 38.883 39.708 38.529 39.379 39.728 39.851 39.993 39.993

32 45.850 42.879 41.942 41.677 38.645 40.837 38.116 40.405 41.343 41.605 41.865 41.865

33 48.272 43.064 41.950 41.615 39.155 40.895 38.904 40.621 41.307 41.523 41.751 41.751

34 47.703 43.999 43.154 42.942 39.676 42.018 39.112 41.647 42.616 42.884 43.156 43.156

35 51.056 49.640 49.749 49.975 49.848 49.529 50.290 49.562 50.018 50.119 50.241 50.241

36 59.537 54.486 53.666 53.360 52.099 52.722 51.936 52.582 53.193 53.407 53.627 53.627

37 55.494 54.607 54.558 54.461 50.661 53.240 49.659 52.764 53.975 54.388 54.813 54.813

38 65.537 61.912 61.306 61.117 59.223 60.394 58.639 59.957 60.863 61.208 61.591 61.591

39 77.596 71.888 70.286 69.769 69.614 69.935 69.116 69.451 69.676 69.836 70.053 70.053

Cysteine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 12.862 10.062 8.688 8.239 9.145 8.807 8.748 8.543 8.281 8.247 8.232 8.232

3 9.129 9.710 9.657 9.640 9.013 9.816 8.072 9.237 9.537 9.646 9.770 9.770

4 14.261 12.434 12.032 11.939 11.592 11.734 10.845 11.273 11.637 11.790 11.960 11.960

5	11.784	11.669	11.364	11.346	11.353	11.568	10.729	11.090	11.291	11.339	11.401	11.401
6	12.885	13.472	13.360	13.300	12.953	13.521	12.209	13.021	13.231	13.311	13.411	13.411
7	16.126	14.092	13.268	13.120	13.154	13.781	12.315	13.083	13.056	13.095	13.164	13.164
8	16.735	16.168	15.970	15.965	15.702	16.120	15.089	15.537	15.844	15.950	16.079	16.079
9	16.025	16.316	16.516	16.659	15.996	16.807	15.061	16.366	16.573	16.686	16.830	16.830
10	17.513	17.349	17.235	17.241	16.303	17.407	14.831	16.439	17.032	17.215	17.421	17.421
11	17.417	16.329	16.100	16.100	16.938	16.533	16.028	15.925	16.070	16.129	16.219	16.219
12	21.976	18.728	18.305	18.317	16.583	17.717	16.204	17.423	18.033	18.305	18.596	18.596
13	19.525	17.918	17.546	17.535	17.498	18.064	16.671	17.265	17.450	17.498	17.571	17.571
14	21.413	19.140	19.008	19.093	17.669	18.757	16.848	18.289	18.888	19.128	19.382	19.382
15	21.544	20.718	20.564	20.709	20.594	20.831	19.766	20.134	20.590	20.721	20.874	20.874
16	24.041	22.804	22.214	22.154	22.482	22.664	21.514	22.058	22.063	22.109	22.183	22.183
17	22.111	21.790	22.109	22.331	20.841	22.080	19.416	21.491	22.237	22.482	22.748	22.748
18	25.978	23.423	23.330	23.512	21.889	23.007	21.605	22.574	23.285	23.542	23.815	23.815
19	22.670	23.667	24.076	24.237	22.284	23.747	21.701	23.465	24.080	24.327	24.590	24.590
20	27.296	24.485	23.737	23.649	24.116	23.992	23.180	23.095	23.416	23.544	23.701	23.701
21	26.992	26.232	26.086	25.994	24.554	25.723	23.479	25.180	25.766	26.024	26.306	26.306
22	23.575	25.409	26.053	26.379	23.607	26.127	22.223	25.327	26.143	26.407	26.678	26.678
23	25.902	25.559	25.915	26.194	23.791	25.855	22.768	25.280	25.963	26.213	26.482	26.482

24	29.345	27.632	27.496	27.743	26.493	27.463	25.462	26.877	27.598	27.838	28.101	28.101
25	33.274	30.431	29.575	29.458	29.825	30.003	27.939	28.821	29.154	29.299	29.489	29.489
26	29.391	28.486	28.322	28.346	26.707	27.832	26.824	27.634	28.260	28.398	28.548	28.548
27	28.015	28.777	29.445	29.826	27.193	29.453	26.465	28.810	29.612	29.865	30.131	30.131
28	24.727	28.825	29.902	30.374	28.205	30.145	26.871	29.566	30.174	30.419	30.678	30.678
29	33.764	32.050	31.887	31.919	30.311	31.375	29.739	30.894	31.598	31.914	32.250	32.250
30	31.308	32.721	33.083	33.027	30.047	32.393	29.449	32.029	32.813	33.042	33.272	33.272
31	31.846	31.686	31.850	32.126	30.728	31.681	30.503	31.295	32.083	32.243	32.414	32.414
32	36.645	34.830	34.261	34.200	32.108	33.541	31.827	33.253	33.973	34.197	34.425	34.425
33	31.530	31.977	32.439	32.826	32.003	32.637	31.238	32.265	32.747	32.956	33.192	33.192
34	34.835	35.497	35.837	35.884	32.346	35.079	31.941	34.705	35.625	35.872	36.116	36.116
35	36.253	35.647	35.699	35.822	32.143	34.637	32.945	34.934	35.733	35.953	36.156	36.156
36	29.985	35.045	35.891	36.190	33.010	35.436	31.626	34.595	35.807	36.128	36.441	36.441
37	40.619	39.187	39.392	39.565	38.931	39.209	38.578	38.900	39.566	39.723	39.882	39.882
38	41.100	40.950	40.881	40.840	39.402	40.928	38.203	40.100	40.715	40.964	41.253	41.253
39	38.481	40.856	41.524	41.870	39.328	41.434	37.366	40.442	41.398	41.762	42.159	42.159
40	39.739	40.359	40.694	41.000	39.954	40.799	39.548	40.395	40.890	41.116	41.382	41.382
41	44.276	43.635	43.223	43.004	38.971	41.629	37.794	40.891	42.402	42.834	43.270	43.270
42	45.193	44.781	45.010	45.222	43.867	44.733	42.198	43.731	44.791	45.185	45.623	45.623

43 47.666 47.318 47.409 47.534 46.099 47.274 45.159 46.449 47.287 47.608 47.968 47.968

44 47.003 47.626 47.551 47.641 46.908 47.586 46.602 47.219 47.570 47.731 47.929 47.929

45 47.884 50.067 50.202 50.368 46.862 49.399 45.207 48.344 49.748 50.189 50.639 50.639

46 48.344 49.642 49.966 50.268 48.650 49.946 47.972 49.554 50.037 50.278 50.554 50.554

47 57.296 56.224 55.879 55.901 55.221 55.838 53.951 54.847 55.568 55.853 56.193 56.193

MAD

1 3.024 0.908 0.343 0.203 1.681 0.636 2.128 0.920 0.375 0.194 0.000

MaxAD

1 10.549 3.475 0.861 0.474 4.299 1.640 5.475 2.378 0.891 0.450 0.000

==========

DF-LMP2 results, standard NLMP/NPA domains, npasel=0.03, DF-HF reference functions

Last column: LMP2(ext)/(A)TZ

DZ TZ QZ 5Z ADZ ATZ (A)DZ (A)TZ (A)QZ (A)5Z XPOL REF LMP2(ext)

Glycine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 5.041 3.953 4.048 4.277 4.455 4.286 4.616 4.155 4.379 4.464 4.568 4.680 4.595

Alanine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 6.733 4.608 4.822 5.093 5.149 5.068 5.252 5.015 5.203 5.337 5.495 5.582 5.345

3 11.850 10.262 10.194 10.154 9.991 10.036 10.071 10.116 10.127 10.146 10.158 10.095 10.071

4 14.753 12.026 12.355 12.758 12.054 12.268 11.910 12.225 12.744 12.923 13.113 13.121 12.338

5 17.285 18.875 19.928 20.310 19.100 19.803 18.865 19.762 20.251 20.366 20.477 20.471 19.669

6 21.430 20.111 20.451 20.493 19.312 19.792 19.083 19.732 20.316 20.435 20.535 20.531 19.675

7 23.553 24.278 25.718 26.517 25.148 25.760 25.427 25.829 26.658 26.898 27.155 27.201 26.020

Serine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 15.934 13.560 13.181 13.156 12.803 12.868 13.044 12.930 13.217 13.368 13.540 13.546 13.116

3 15.501 13.659 14.012 14.326 12.638 13.706 12.807 13.723 14.423 14.675 14.953 14.985 14.257

4 19.868 17.657 17.410 17.446 17.555 17.182 18.011 17.297 17.511 17.646 17.816 17.712 17.608

5 16.615 18.897 19.652 19.732 18.715 19.197 18.264 19.208 19.559 19.584 19.580 19.246 18.943

6 20.427 17.595 17.579 17.776 16.090 17.184 16.232 17.175 17.884 18.151 18.451 18.526 17.925

7 27.190 23.252 23.132 23.247 20.786 22.475 21.026 22.531 23.320 23.617 23.942 24.091 23.283

8 25.736 23.234 23.400 23.631 21.432 22.834 21.734 22.892 23.695 23.991 24.311 24.439 23.463

9 28.360 27.707 28.038 28.020 26.845 27.157 26.834 27.232 27.814 27.949 28.076 27.887 27.130

10 27.282 23.806 24.137 24.522 23.121 23.736 23.412 23.760 24.604 24.927 25.284 25.389 24.247

11 29.602 27.098 27.339 27.663 25.173 26.638 25.692 26.735 27.749 28.100 28.483 28.603 27.331

12 28.300 24.607 25.288 25.817 23.907 24.903 24.168 24.928 25.908 26.281 26.695 26.828 25.600

13 31.322 26.038 25.682 25.982 23.770 25.080 23.679 24.994 26.105 26.480 26.892 27.127 25.812

14 26.955 28.215 29.159 29.484 27.671 28.703 27.641 28.698 29.438 29.691 29.960 29.921 28.774

15 38.580 32.211 31.716 31.563 29.541 30.414 29.954 30.541 31.412 31.728 32.059 32.095 30.895

16 32.951 29.107 30.118 30.821 27.616 29.349 27.675 29.338 30.846 31.341 31.864 32.030 29.876

17 39.436 32.386 31.616 31.504 29.055 30.412 29.349 30.500 31.428 31.789 32.165 32.223 31.050

18 38.846 32.124 31.370 31.421 29.735 30.514 30.033 30.491 31.434 31.845 32.301 32.497 31.289

19 34.446 31.501 31.568 31.658 31.136 31.050 31.535 31.171 31.680 31.856 32.035 31.921 31.296

20 40.432 34.025 33.515 33.484 31.173 32.367 31.607 32.463 33.414 33.801 34.203 34.209 32.911

21 36.349 31.334 31.987 32.518 29.081 31.041 29.131 31.024 32.534 33.028 33.554 33.769 31.736

22 30.458 31.199 32.828 33.583 30.854 32.470 30.888 32.452 33.654 34.004 34.373 34.425 32.819

23 36.096 33.310 33.848 34.301 31.558 33.115 32.012 33.103 34.386 34.841 35.325 35.526 33.786

24 36.023 34.906 35.625 35.949 33.377 34.847 33.567 34.991 35.989 36.305 36.630 36.601 35.294

25 35.060 34.864 35.762 36.078 32.408 34.784 32.336 34.742 35.971 36.311 36.655 36.809 35.302

26 38.476 35.859 36.325 36.574 32.490 35.015 32.358 34.970 36.428 36.857 37.296 37.471 35.549

27 35.800 36.540 37.506 37.837 34.459 36.519 34.445 36.501 37.712 38.047 38.386 38.484 36.898

28 32.848 36.546 38.136 38.474 36.271 37.229 35.860 37.121 38.184 38.418 38.637 38.619 37.046

29 40.728 37.575 38.519 39.121 35.176 37.563 35.180 37.455 39.158 39.725 40.328 40.524 38.243

30 38.128 38.310 39.337 39.950 38.566 39.038 39.057 39.162 40.035 40.327 40.655 40.537 39.345

31 40.861 38.087 38.396 38.813 35.750 37.635 35.872 37.637 38.913 39.363 39.848 39.993 38.494

32 42.455 39.882 40.580 40.923 37.095 39.302 37.061 39.264 40.787 41.248 41.717 41.865 39.747

33 44.519 40.230 40.696 40.938 37.535 39.413 37.578 39.415 40.740 41.176 41.633

41.751 39.918

34 45.592 41.848 42.275 42.456 39.310 40.939 39.375 40.939 42.276 42.683 43.101 43.156 41.209

35 48.047 47.186 48.581 49.397 47.785 48.156 48.482 48.327 49.538 49.870 50.234 50.241 48.492

36 56.316 52.093 52.673 52.903 50.476 51.661 50.542 51.683 52.822 53.259 53.713 53.627 52.334

37 54.432 53.090 53.850 54.066 50.532 52.485 50.233 52.407 53.813 54.277 54.755 54.813 52.881

38 61.648 58.243 59.353 60.085 56.173 58.296 56.571 58.316 60.109 60.745 61.433 61.591 59.008

39 71.576 66.527 67.270 68.055 64.475 66.578 65.098 66.666 68.381 69.070 69.842 70.053 67.740

Cysteine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 10.076 7.357 7.447 7.644 6.632 7.278 6.603 7.162 7.725 7.962 8.232 8.232 7.592

3 7.566 7.867 8.538 8.912 7.091 8.333 7.143 8.135 8.911 9.241 9.597 9.770 8.657

4 13.235 11.619 11.577 11.644 10.796 11.150 10.474 10.889 11.388 11.616 11.865 11.960 11.136

5 9.442 9.357 10.086 10.650 9.102 10.029 9.055 9.902 10.710 10.992 11.299 11.401 10.185

6 10.840 11.348 12.203 12.640 10.906 12.164 10.696 11.991 12.680 12.986 13.323 13.411 12.497

7 13.192 10.855 11.611 12.129 10.243 11.493 10.169 11.267 12.189 12.582 13.022 13.164 11.981

8 13.974 13.775 14.540 15.108 13.113 14.584 13.121 14.392 15.156 15.504 15.887 16.079 15.033

9 13.664 13.923 15.093 15.749 13.431 14.970 13.538 14.872 15.810 16.212 16.659 16.830 15.562

10 14.932 14.701 15.681 16.228 13.605 15.295 13.412 14.914 16.143 16.653 17.203 17.421 15.645

11 14.918 14.021 14.897 15.428 14.280 14.865 14.244 14.695 15.412 15.754 16.141 16.219 15.151

12 20.548 17.654 17.861 18.003 15.928 17.118 15.984 17.035 17.805 18.155 18.528

18.596 17.344

13 17.195 15.602 16.338 16.814 15.573 16.172 15.605 15.924 16.755 17.098 17.478 17.571 16.426

14 19.451 17.734 18.338 18.658 16.399 17.802 16.178 17.611 18.495 18.902 19.331 19.382 18.056

15 18.296 17.976 19.063 19.835 17.486 18.847 17.456 18.631 19.805 20.242 20.716 20.874 19.091

16 21.248 19.766 20.565 21.085 19.653 20.469 19.983 20.373 21.168 21.559 21.996 22.183 21.090

17 20.079 19.257 20.818 21.631 18.682 20.404 18.233 20.221 21.613 22.108 22.637 22.748 20.597

18 24.603 22.413 22.775 23.131 20.745 22.301 21.054 22.209 22.966 23.331 23.717 23.815 22.582

19 21.855 22.425 23.392 23.787 21.231 22.881 21.308 22.833 23.769 24.147 24.547 24.590 23.219

20 24.211 21.670 22.169 22.716 21.199 21.844 21.258 21.563 22.567 23.016 23.510 23.701 22.257

21 25.520 24.775 25.269 25.485 23.178 24.621 22.937 24.409 25.378 25.793 26.241 26.306 24.919

22 21.481 23.400 25.069 25.767 22.295 24.583 21.745 24.290 25.627 26.068 26.525 26.678 24.753

23 23.851 23.820 25.091 25.650 22.564 24.495 22.349 24.313 25.491 25.908 26.353 26.482 24.726

24 26.436 24.506 25.908 26.840 23.735 25.557 23.658 25.404 26.818 27.346 27.912 28.101 25.944

25 28.717 26.284 27.187 27.931 25.637 26.919 25.463 26.525 27.890 28.506 29.189 29.489 27.570

26 28.606 27.236 27.852 28.130 26.669 27.167 26.706 27.102 28.051 28.320 28.608 28.548 27.191

27 26.460 27.254 28.593 29.300 25.911 28.195 25.919 28.000 29.163 29.554 29.965 30.131 28.397

28 23.604 27.270 29.067 29.786 26.630 28.785 26.430 28.611 29.710 30.107 30.526 30.678 29.035

29 31.828 30.277 30.843 31.265 28.647 30.145 28.809 29.987 31.095 31.578 32.088 32.250 30.591

30 30.864 31.617 32.517 32.738 30.271 31.722 30.027 31.609 32.668 32.959 33.255 33.272 31.852

31 30.159 29.720 30.970 31.661 29.540 30.538 29.492 30.433 31.644 32.029 32.437 32.414 30.702

32 35.572 34.402 34.427 34.319 32.569 33.460 32.523 33.335 34.052 34.294 34.541 34.425 33.640

33 29.725 29.850 31.247 32.096 29.727 31.149 29.759 31.136 32.171 32.593 33.053 33.192 31.531

34 33.774 34.119 35.096 35.481 32.335 34.298 32.370 34.201 35.383 35.713 36.043 36.116 34.510

35 38.007 36.764 36.684 36.507 35.584 35.863 35.851 36.100 36.366 36.410 36.429 36.156 35.658

36 31.115 35.123 36.236 36.353 34.400 35.362 33.930 35.084 36.028 36.255 36.469 36.441 35.026

37 39.659 38.595 39.452 39.721 38.675 39.036 38.627 38.922 39.601 39.854 40.114 39.882 39.203

38 37.948 37.161 38.666 39.540 35.853 38.154 35.744 37.952 39.622 40.298 41.034 41.253 38.844

39 36.497 38.646 40.355 41.064 37.220 39.622 36.727 39.220 40.737 41.324 41.956 42.159 39.823

40 37.290 37.264 39.000 40.004 37.112 38.674 37.569 38.639 40.072 40.598 41.177 41.382 39.212

41 45.268 43.632 43.383 43.123 41.172 41.839 40.555 41.500 42.627 42.969 43.309 43.270 41.456

42 42.399 41.762 43.243 44.143 40.871 42.570 40.522 42.197 43.933 44.622 45.371 45.623 42.850

43 44.406 43.541 45.185 46.231 42.432 44.544 42.588 44.363 46.204 46.920 47.693 47.968 45.271

44 44.518 44.482 45.727 46.512 43.991 45.411 44.712 45.494 46.706 47.216 47.781 47.929 46.218

45 47.650 49.257 50.010 50.233 47.384 48.754 46.917 48.361 49.719 50.134 50.556 50.639 48.491

46 44.881 46.301 48.255 49.188 45.371 47.722 45.681 47.647 49.193 49.752 50.362 50.554 48.440

47 53.198 52.145 53.442 54.386 51.180 52.865 51.340 52.619 54.397 55.136 55.952 56.193 53.622

MAD

1 2.342 1.936 1.232 0.816 3.032 1.773 2.998 1.853 0.851 0.488 0.123 1.410

MaxAD

1 7.212 4.427 2.783 1.998 5.578 3.475 5.509 3.605 1.796 1.057 0.334 2.774

==========

Geometries (xyz format, in Angstrom)

GLYCINE

glycine_1 -455.33935359386 a.u.

C	3.033948	0.370630	0.782112
C	1.802176	0.176200	-0.078235
O	1.443213	1.023317	-0.915523
H	2.905568	1.288005	1.374728
H	3.227794	-0.476299	1.455992
H	3.899914	0.514703	0.119925
N	1.111247	-0.986642	0.108032
C	-0.095431	-1.292651	-0.659826
C	-1.342397	-0.616305	-0.075338
O	-2.228810	-1.261832	0.504760
H	1.378305	-1.602044	0.866193
H	0.073761	-0.960981	-1.696110
H	-0.262854	-2.376884	-0.636398
N	-1.378961	0.732275	-0.243586
C	-2.451943	1.520840	0.348622
H	-0.553035	1.176987	-0.642171
H	-3.426608	1.141059	0.010760
H	-2.426858	1.467394	1.448811

H -2.335331 2.564465 0.029241

glycine_2 -455.33656092531 a.u.

C 3.408842 0.915890 0.000064

C 2.340217 -0.161251 0.000005

O 2.612265 -1.371075 0.000060

H 4.041608 0.780273 0.889226

H 4.041946 0.780036 -0.888820

H 2.991492 1.933220 -0.000146

N 1.048372 0.279676 -0.000106

C -0.049249 -0.659777 -0.000081

C -1.356984 0.129111 -0.000043

O -1.382383 1.368707 -0.000024

H 0.800691 1.264838 -0.000066

H -0.001905 -1.315939 -0.886760

H -0.001854 -1.315948 0.886590

N -2.490703 -0.622673 -0.000073

C -3.805383 0.011417 0.000114

H -2.412975 -1.631614 0.000163

H -3.927408 0.644016 -0.891310

H -4.571278 -0.774406 -0.000424

H -3.927709 0.643093 0.892160

ALANINE

alanine_1 -494.53336002632 a.u.

C -3.077696 -0.614096 0.770471

C -1.837634 -0.380064 -0.068647

O -1.529867 -1.134105 -1.009779

H	-3.014507	-1.617365	1.215958
H	-3.206763	0.133018	1.566818
H	-3.954515	-0.593649	0.106906
N	-1.085637	0.711655	0.257557
C	0.134480	1.069664	-0.474965
C	1.315236	0.235479	0.061169
O	2.168922	0.706249	0.827271
C	0.403704	2.563351	-0.339710
H	-1.323813	1.247033	1.085193
H	-0.048397	0.794167	-1.526080
H	1.304426	2.833869	-0.908633
H	-0.452033	3.137886	-0.725363
H	0.588562	2.826041	0.712895
N	1.317422	-1.054402	-0.372498
C	2.279406	-2.008300	0.166327
H	0.475135	-1.379089	-0.847767
H	3.295361	-1.603282	0.062520
H	2.097251	-2.207952	1.235029
H	2.199387	-2.944809	-0.400683

alanine_2 -494.53065171909 a.u.

C	-3.366859	-1.142124	-0.000615
C	-2.312419	-0.081812	-0.258627
O	-2.578516	1.000523	-0.803466
H	-3.848821	-1.395499	-0.955887
H	-2.955258	-2.053815	0.456102
H	-4.134449	-0.716837	0.662522
N	-1.045153	-0.392395	0.146127

C	0.048393	0.545547	-0.030045
C	1.345438	-0.255900	0.070600
O	1.409581	-1.318680	0.708184
C	0.026939	1.650336	1.041756
H	-0.818215	-1.277259	0.590800
H	-0.052176	1.003826	-1.028869
H	0.839074	2.375615	0.874530
H	-0.936851	2.176524	0.993300
H	0.150928	1.200185	2.038820
N	2.431426	0.303145	-0.528727
C	3.738664	-0.341795	-0.453976
H	2.301697	1.120310	-1.111200
H	3.996958	-0.535949	0.596426
H	3.737782	-1.301254	-0.993345
H	4.485960	0.328646	-0.897293

alanine_3 -494.52972984894 a.u.

C	-3.146922	-0.743545	-0.625882
C	-1.820406	-0.349990	-0.003653
O	-1.408225	-0.898737	1.035189
H	-3.136531	-1.826777	-0.812937
H	-3.943901	-0.534397	0.102892
H	-3.364878	-0.210896	-1.562710
N	-1.127197	0.629874	-0.651936
C	0.129782	1.254654	-0.203070
C	1.371000	0.356162	-0.357228
O	2.382815	0.779386	-0.940581

C	0.032758	1.824145	1.220232
H	-1.515910	0.967340	-1.523689
H	0.312087	2.080949	-0.905353
H	0.977631	2.335378	1.461016
H	-0.788844	2.554629	1.278311
H	-0.143915	1.028890	1.955771
N	1.294828	-0.871052	0.213667
C	2.436246	-1.775408	0.163178
H	0.435499	-1.118684	0.706234
H	2.729193	-1.966991	-0.880054
H	3.302787	-1.342201	0.686066
H	2.151896	-2.720297	0.644002

alanine_4 -494.52842446812 a.u.

C	3.210523	-0.662723	-0.460988
C	1.902501	-0.329339	0.234014
O	1.592619	-0.795233	1.335459
H	3.389166	-1.743558	-0.378568
H	3.222393	-0.364554	-1.519893
H	4.026069	-0.143867	0.065737
N	1.063614	0.528567	-0.445477
C	-0.109890	1.105277	0.209381
C	-1.337755	0.182224	0.216490
O	-2.351017	0.508207	0.848319
C	-0.482221	2.429954	-0.463158
H	1.409974	0.975421	-1.287344
H	0.136098	1.268574	1.271371
H	-1.380114	2.839518	0.018698

H	0.339979	3.156370	-0.369155
H	-0.702916	2.270943	-1.532093
N	-1.258725	-0.945502	-0.543219
C	-2.326397	-1.937418	-0.487791
H	-0.338347	-1.214934	-0.868032
H	-3.291321	-1.432334	-0.626834
H	-2.174863	-2.666844	-1.294361
H	-2.343712	-2.457830	0.483431

alanine_5 -494.52628258390 a.u.

C	-3.025482	-1.075360	-0.074147
C	-1.673961	-0.442820	0.205604
O	-1.111030	-0.527053	1.302023
H	-3.062202	-2.059331	0.412476
H	-3.806005	-0.443439	0.377657
H	-3.233647	-1.183722	-1.148990
N	-1.092705	0.222116	-0.855711
C	0.054423	1.117537	-0.645550
C	1.294468	0.361408	-0.131136
O	2.172619	0.945485	0.512583
C	-0.280066	2.308181	0.258116
H	-1.670731	0.386489	-1.672458
H	0.331884	1.486839	-1.648165
H	0.603106	2.952842	0.360338
H	-1.105078	2.888571	-0.183820
H	-0.572888	1.953842	1.255792
N	1.406073	-0.939392	-0.533569
C	2.470132	-1.767548	0.024114

H 0.552975 -1.387601 -0.845018

H 3.433815 -1.263280 -0.124568

H 2.326646 -1.934370 1.104246

H 2.478743 -2.731755 -0.501390

alanine_6 -494.52646519902 a.u.

C 2.974570 -1.116271 -0.062307

C 1.699117 -0.341278 -0.322664

O 0.989887 -0.535484 -1.318870

H 3.492270 -1.280126 -1.016614

H 3.644318 -0.603055 0.642957

H 2.699141 -2.097859 0.354607

N 1.364186 0.601008 0.624654

C 0.009715 1.164399 0.603282

C -1.004825 0.000252 0.591930

O -0.935240 -0.881154 1.457888

C -0.140797 2.221470 -0.495396

H 1.801116 0.496087 1.533801

H -0.133757 1.649062 1.582859

H -1.141871 2.678966 -0.455125

H 0.604554 3.014913 -0.338257

H 0.029587 1.782705 -1.489211

N -1.993273 0.042415 -0.348935

C -2.865522 -1.120675 -0.496527

H -1.785949 0.576737 -1.184520

H -3.318936 -1.352210 0.475711

H -3.655464 -0.879325 -1.219954

H -2.302117 -2.004139 -0.838343

alanine_7 -494.52311928750 a.u.

C	-3.057032	-1.512273	-0.105575
C	-2.243919	-0.229609	-0.088498
O	-2.768991	0.886557	-0.142497
H	-3.803773	-1.462314	0.699722
H	-3.596440	-1.570359	-1.062559
H	-2.442470	-2.415128	0.023446
N	-0.875702	-0.395257	0.013556
C	0.014347	0.758107	-0.185154
C	1.450466	0.285311	-0.403506
O	2.211983	0.847603	-1.196767
C	-0.021042	1.713028	1.019355
H	-0.513940	-1.305681	-0.254458
H	-0.282336	1.307966	-1.092609
H	0.671677	2.549888	0.840346
H	-1.037116	2.106567	1.151393
H	0.285158	1.186088	1.937333
N	1.840930	-0.791555	0.357429
C	3.247337	-1.189335	0.368071
H	1.265703	-1.024883	1.159878
H	3.583566	-1.338467	-0.666165
H	3.885179	-0.418690	0.830030
H	3.343311	-2.131957	0.922704

SERINE

serine_1 -569.60448066 a.u.

C	-3.218678	0.093386	-0.805734

C	-1.985847	0.256377	0.058699
O	-1.867557	1.197354	0.867710
H	-3.359884	1.012328	-1.392661
H	-3.155270	-0.770492	-1.482476
H	-4.091405	-0.023707	-0.146631
N	-1.018521	-0.691316	-0.087241
C	0.211863	-0.676130	0.700726
C	1.227497	0.305061	0.085748
O	2.232960	-0.090240	-0.537938
C	0.787063	-2.092439	0.726876
O	0.958958	-2.592093	-0.603138
H	-1.077728	-1.392311	-0.820258
H	1.637259	-2.006543	-0.988627
H	-0.047199	-0.342743	1.719776
H	1.739484	-2.088721	1.283149
H	0.080530	-2.769095	1.230128
N	0.927618	1.611613	0.269056
C	1.728101	2.653416	-0.364879
H	0.010191	1.818727	0.668264
H	2.787348	2.512916	-0.109304
H	1.630566	2.620989	-1.461786
H	1.387550	3.628379	0.006040

serine_2 -569.59916816 a.u.

C	3.403344	-0.419262	0.633643
C	2.106405	-0.182277	-0.112366
O	2.042449	0.571328	-1.099767
H	3.809040	0.552463	0.949173

H	3.283166	-1.070658	1.511169
H	4.123005	-0.876749	-0.061139
N	1.010419	-0.852105	0.353378
C	-0.297874	-0.764813	-0.296104
C	-1.053575	0.502802	0.146948
O	-2.080619	0.446149	0.851479
C	-1.109166	-2.017738	0.050015
O	-2.400124	-1.984675	-0.542770
H	1.087691	-1.381118	1.215297
H	-2.856568	-1.247352	-0.101124
H	-0.124679	-0.715953	-1.383091
H	-0.592296	-2.902798	-0.350518
H	-1.177967	-2.112014	1.150915
N	-0.512085	1.662834	-0.288678
C	-1.083991	2.945885	0.102637
H	0.369481	1.604309	-0.799509
H	-0.998178	3.103035	1.189175
H	-0.546122	3.742082	-0.427296
H	-2.149417	2.979640	-0.166131

serine_3 -569.59831430 a.u.

C	-3.557316	-1.122781	0.178641
C	-2.433710	-0.157088	-0.142845
O	-2.628431	0.925398	-0.716508
H	-0.983564	-1.509072	0.507958
N	-1.180561	-0.540859	0.260039
C	-0.028838	0.232669	-0.157873
C	1.199094	-0.684661	-0.071571

O	1.089033	-1.898208	0.174300
C	0.119537	1.494866	0.714196
O	1.056141	2.427952	0.136415
H	0.591568	2.896329	-0.572500
H	2.389038	0.943388	-0.340747
N	2.390135	-0.072505	-0.282339
C	3.636388	-0.821017	-0.162544
H	-3.210822	-2.012232	0.723865
H	-4.312078	-0.595699	0.779833
H	-4.032047	-1.431511	-0.764340
H	-0.170729	0.562056	-1.204575
H	-0.871779	1.955437	0.835001
H	0.520540	1.228519	1.703497
H	3.801965	-1.159622	0.872260
H	3.601839	-1.706220	-0.812792
H	4.464182	-0.170877	-0.473035

serine_4 -569.59692849 a.u.

C	-3.174638	-1.646694	0.047929
C	-2.233766	-0.480919	-0.176863
O	-2.656332	0.638924	-0.526217
H	-3.949644	-1.337356	0.763484
H	-3.669700	-1.881570	-0.905924
H	-2.661629	-2.543893	0.422001
N	-0.912615	-0.733646	0.010917
C	0.125363	0.262036	-0.202379
C	1.458378	-0.462779	0.015664
O	1.523889	-1.568255	0.576779

C	-0.006407	1.500420	0.726896
O	-0.767689	2.543910	0.138608
H	-0.585382	-1.634627	0.353596
H	-1.597890	2.118643	-0.160038
H	0.074586	0.636017	-1.241575
H	-0.435364	1.157193	1.687321
H	0.990210	1.923416	0.928086
N	2.558641	0.195766	-0.431165
C	3.892652	-0.365129	-0.237063
H	2.444014	1.087307	-0.897040
H	4.100016	-0.501581	0.834369
H	3.972918	-1.343348	-0.733121
H	4.627244	0.326712	-0.667878

serine_5 -569.59791795 a.u.

C	3.088244	-1.111930	-0.434288
C	1.875631	-0.213567	-0.331124
O	1.385296	0.338289	-1.332409
H	3.757186	-0.722215	-1.212194
H	3.629090	-1.197573	0.519061
H	2.743993	-2.113056	-0.738924
N	1.357256	-0.046132	0.925659
C	-0.018867	0.434955	1.117169
C	-0.998438	-0.599732	0.514265
O	-0.834122	-1.804691	0.759098
C	-0.226784	1.913919	0.734464
O	-0.480536	2.163843	-0.649908
H	1.669480	-0.727407	1.610360

H	0.197587	1.637982	-1.130116
H	-0.187546	0.383171	2.206538
H	-1.109325	2.287871	1.276608
H	0.656244	2.477611	1.085594
N	-2.039996	-0.103097	-0.200370
C	-2.981463	-1.025163	-0.828065
H	-1.894941	0.827203	-0.596593
H	-3.360123	-1.727187	-0.073285
H	-3.816429	-0.444928	-1.241756
H	-2.501064	-1.607291	-1.631095

serine_6 -569.59679809 a.u.

C	-3.548102	-1.130719	0.187665
C	-2.441719	-0.149226	-0.149826
O	-2.655824	0.915859	-0.745891
H	-4.333516	-0.597829	0.742387
H	-3.987290	-1.495995	-0.752547
H	-3.193592	-1.984968	0.781955
N	-1.184145	-0.506323	0.265965
C	-0.028681	0.255104	-0.167871
C	1.189917	-0.675612	-0.053277
O	1.061820	-1.878215	0.236689
C	0.104818	1.529231	0.677308
O	1.093120	2.370246	0.042464
H	-0.980022	-1.466725	0.538188
H	1.091608	3.228207	0.487255
H	-0.159477	0.569916	-1.219381
H	-0.876199	2.027139	0.691250

H	0.411111	1.267125	1.705749
N	2.390165	-0.098615	-0.302121
C	3.619476	-0.873990	-0.181428
H	2.413729	0.913811	-0.392797
H	3.799420	-1.180943	0.860923
H	3.548652	-1.780271	-0.798854
H	4.456259	-0.256752	-0.532558

serine_7 -569.59554335 a.u.

C	-2.578215	-1.968971	0.658379
C	-1.386441	-1.325637	-0.020786
O	-0.738116	-1.915707	-0.904570
H	-2.279656	-2.960008	1.027762
H	-2.970861	-1.368976	1.491645
H	-3.369346	-2.110817	-0.093034
N	-1.059087	-0.068630	0.402843
C	-0.107240	0.763369	-0.341706
C	1.348233	0.457994	0.067169
O	2.039414	1.278418	0.693580
C	-0.409066	2.229341	-0.060532
O	-1.801696	2.434332	-0.367993
H	-1.749133	0.429849	0.956072
H	-2.005095	3.365983	-0.209749
H	-0.237469	0.545986	-1.416420
H	-0.194041	2.455989	0.996481
H	0.243305	2.854314	-0.689849
N	1.795515	-0.759357	-0.325855
C	3.119521	-1.219929	0.072559

H	1.107021	-1.396403	-0.730586
H	3.189648	-1.337199	1.165826
H	3.313127	-2.184834	-0.413235
H	3.879943	-0.491322	-0.242465

serine_8 -569.59541496 a.u.

C	-2.519650	-2.018617	0.691781
C	-1.372360	-1.335858	-0.024042
O	-0.738368	-1.899531	-0.935906
H	-1.722558	0.401694	1.004005
N	-1.061938	-0.075542	0.398691
C	-0.117239	0.768628	-0.336044
C	1.337353	0.467597	0.079689
O	2.003650	1.267061	0.756375
C	-0.438062	2.237092	-0.051212
O	-1.825547	2.533882	-0.273713
H	-2.001005	2.457260	-1.222416
H	1.128479	-1.360592	-0.783087
N	1.809156	-0.724419	-0.364618
C	3.127269	-1.191458	0.047524
H	-3.294466	-2.264567	-0.049109
H	-2.152050	-2.961294	1.121863
H	-2.957063	-1.400088	1.488315
H	-0.234349	0.542996	-1.412283
H	-0.244236	2.460133	1.006453
H	0.222751	2.877741	-0.655899
H	3.881333	-0.427179	-0.186762
H	3.163275	-1.388194	1.131164

H 3.357616 -2.113787 -0.500982

serine_9 -569.59467924 a.u.

C -3.155250 -1.068773 -0.408166
C -1.885407 -0.355699 0.006988
O -1.547512 -0.297165 1.208270
H -1.468706 0.013290 -1.939512
N -1.146907 0.189103 -0.995155
C 0.151226 0.874566 -0.867016
C 1.356257 -0.044947 -0.604006
O 2.448657 0.221768 -1.122489
C 0.156340 2.047443 0.141475
O 0.367623 1.672551 1.494683
H -0.333942 1.028476 1.706690
H 0.319510 -1.082550 0.802330
N 1.142857 -1.119316 0.205589
C 2.289947 -1.909321 0.645627
H -3.386474 -0.958174 -1.476979
H -3.045221 -2.136856 -0.168207
H -3.986836 -0.672357 0.191239
H 0.342732 1.314543 -1.857924
H 1.001482 2.697899 -0.128309
H -0.784035 2.616598 0.010741
H 2.863748 -2.233962 -0.232353
H 2.956294 -1.322523 1.298373
H 1.920975 -2.789747 1.187754

serine_10 -569.59451888 a.u.

C	-3.413970	-1.128540	0.444231
C	-2.370408	-0.276987	-0.253336
O	-2.644249	0.467487	-1.204042
H	-4.248313	-0.481482	0.750243
H	-3.803155	-1.862299	-0.277234
H	-3.015751	-1.656031	1.322765
N	-1.094650	-0.367448	0.250708
C	0.010525	0.254244	-0.459983
C	1.281189	-0.503850	-0.052210
O	1.251642	-1.429183	0.773531
C	0.102851	1.743596	-0.090808
O	0.451137	1.918807	1.283630
H	-0.829078	-1.144709	0.854308
H	-0.232832	1.467976	1.802495
H	-0.156869	0.169165	-1.549947
H	0.893245	2.244772	-0.670942
H	-0.860455	2.219732	-0.337249
N	2.427563	-0.107840	-0.664507
C	3.711799	-0.676974	-0.265732
H	2.409409	0.720129	-1.245555
H	3.970144	-0.389346	0.765067
H	3.658896	-1.772699	-0.319586
H	4.484211	-0.314022	-0.955703

serine_11 -569.59403494 a.u.

C	-2.162173	-2.277649	0.819050
C	-1.291874	-1.392197	-0.049447
O	-0.810226	-1.788123	-1.121775

H	-1.272204	0.070973	1.392330
N	-1.089312	-0.111164	0.408908
C	-0.174687	0.804174	-0.285862
C	1.274292	0.521710	0.135680
O	1.865091	1.211972	0.980818
C	-0.581341	2.242469	0.021452
O	-1.871375	2.546855	-0.519878
H	-2.475929	1.846179	-0.233339
H	1.206309	-1.143375	-1.035107
N	1.828920	-0.555408	-0.483636
C	3.148367	-1.035076	-0.088191
H	-2.531450	-1.767649	1.720295
H	-3.017722	-2.619253	0.218562
H	-1.579629	-3.163746	1.110354
H	-0.301453	0.607596	-1.361541
H	-0.544673	2.418441	1.111307
H	0.128591	2.933270	-0.452541
H	3.865962	-0.203954	-0.121820
H	3.140069	-1.441063	0.936305
H	3.461444	-1.817639	-0.791117

serine_12 -569.59401144 a.u.

C	3.563474	-1.113873	-0.181315
C	2.441949	-0.188591	0.251538
O	2.631201	0.787285	0.991175
H	1.023452	-1.330645	-0.785074
N	1.197525	-0.498360	-0.228684
C	0.035962	0.278175	0.153516

C	-1.195580	-0.596268	-0.068735
O	-1.177063	-1.570516	-0.837682
C	-0.044298	1.561211	-0.705116
O	-1.108705	2.430831	-0.302740
H	-1.935637	2.052821	-0.633435
H	-2.235732	0.528577	1.284536
N	-2.326655	-0.187359	0.572996
C	-3.559762	-0.964472	0.471837
H	3.224313	-1.911363	-0.858042
H	4.337827	-0.514232	-0.681064
H	4.011551	-1.562463	0.717352
H	0.131155	0.580052	1.210266
H	0.889102	2.119907	-0.554291
H	-0.129208	1.274874	-1.768592
H	-3.786488	-1.151576	-0.586365
H	-3.464373	-1.935533	0.982126
H	-4.375989	-0.388267	0.926027

serine_13 -569.59381212 a.u.

C	3.382938	0.237140	-0.014381
C	1.890335	0.095646	0.219638
O	1.352324	0.370460	1.296531
H	3.720863	1.183113	0.430315
H	3.895813	-0.584744	0.508488
H	3.656027	0.208801	-1.079461
N	1.151005	-0.338232	-0.865183
C	-0.241930	-0.760868	-0.699821
C	-1.129027	0.369559	-0.152318
O	-2.125359	0.116973	0.544396

C	-0.380351	-2.022674	0.173565
O	-1.684566	-2.583478	0.057672
H	1.658848	-0.697897	-1.665794
H	-2.276722	-1.885360	0.391749
H	-0.627739	-1.008197	-1.703433
H	0.326889	-2.782289	-0.195331
H	-0.128780	-1.774741	1.217734
N	-0.813634	1.628493	-0.556283
C	-1.514091	2.770626	0.023106
H	0.117573	1.760685	-0.932985
H	-2.596307	2.621182	-0.083444
H	-1.278527	2.881797	1.093728
H	-1.215958	3.677605	-0.518823

serine_14 -569.59297755 a.u.

C	2.710020	-1.743500	0.582667
C	1.568943	-0.910238	0.032302
O	1.183610	-1.035156	-1.147255
H	2.410354	-2.801531	0.555465
H	3.579392	-1.623814	-0.079653
H	2.991667	-1.471666	1.609913
N	0.992236	-0.035089	0.901421
C	-0.081507	0.916785	0.584865
C	-1.476793	0.280399	0.462397
O	-2.445022	0.749098	1.081205
C	0.215602	1.769781	-0.665891
O	1.492505	2.406519	-0.583293
H	1.366779	0.000341	1.841272

H	2.154317	1.752617	-0.848773
H	-0.143538	1.594679	1.447742
H	0.129995	1.165622	-1.580086
H	-0.536298	2.572543	-0.696810
N	-1.567702	-0.773814	-0.388162
C	-2.852578	-1.423694	-0.616166
H	-0.732849	-1.048347	-0.906220
H	-3.276018	-1.775578	0.336218
H	-3.570990	-0.724919	-1.071756
H	-2.695412	-2.278502	-1.286432

serine_15 -569.59288500 a.u.

C	2.877630	-1.628808	-0.386827
C	1.591186	-1.102213	0.221581
O	1.013025	-1.660412	1.159156
H	2.798082	-2.718977	-0.495857
H	3.104758	-1.172077	-1.361041
H	3.703814	-1.417922	0.309742
N	1.079412	0.046043	-0.356683
C	0.044774	0.792243	0.351608
C	-1.344670	0.147036	0.310979
O	-2.226707	0.537149	1.086958
C	-0.074601	2.183137	-0.285477
O	1.193560	2.855321	-0.343599
H	1.721996	0.612673	-0.905612
H	1.428448	3.121504	0.557102
H	0.300255	0.879985	1.422751
H	-0.400772	2.082229	-1.332059

H	-0.827717	2.765123	0.267578
N	-1.552201	-0.766146	-0.676625
C	-2.803536	-1.514011	-0.726835
H	-0.725431	-1.139283	-1.128419
H	-3.642950	-0.811279	-0.644701
H	-2.861810	-2.043230	-1.687026
H	-2.872872	-2.238795	0.100401

serine_16 -569.59284583 a.u.

C	2.833451	-1.624179	0.532462
C	1.551548	-0.976733	0.047861
O	1.051629	-1.272835	-1.054246
H	2.794951	-2.697575	0.303622
H	3.672626	-1.183303	-0.027402
H	3.007413	-1.479075	1.608471
N	0.991913	-0.062690	0.891991
C	-0.056597	0.901191	0.528820
C	-1.480036	0.323892	0.431302
O	-2.428384	0.907313	0.981551
C	0.281692	1.682609	-0.743519
O	1.536132	2.339328	-0.498572
H	1.527331	0.166995	1.720278
H	1.807916	2.777071	-1.316506
H	-0.103931	1.620703	1.358638
H	0.351123	1.002793	-1.606300
H	-0.528409	2.414224	-0.910700
N	-1.618527	-0.797653	-0.315490
C	-2.933617	-1.398891	-0.495908

H	-0.786057	-1.170611	-0.776691
H	-3.613262	-0.706446	-1.016118
H	-2.817890	-2.315522	-1.088422
H	-3.379176	-1.644629	0.479647

serine_17 -569.59174969 a.u.

C	-3.448900	-1.071357	0.480615
C	-2.384893	-0.274624	-0.249959
O	-2.655105	0.488600	-1.191900
H	-4.186382	-0.370540	0.898143
H	-3.966702	-1.712141	-0.247913
H	-3.037078	-1.692833	1.288667
N	-1.106306	-0.439816	0.196678
C	-0.001341	0.221804	-0.460635
C	1.280803	-0.517996	-0.051132
O	1.271131	-1.429782	0.786136
C	0.075273	1.705852	-0.083030
O	0.504457	1.776174	1.282510
H	-0.861258	-1.116258	0.914522
H	0.265269	2.644350	1.632642
H	-0.142496	0.158568	-1.554861
H	0.790222	2.228724	-0.747485
H	-0.923387	2.145971	-0.229199
N	2.417214	-0.113884	-0.682781
C	3.714029	-0.640974	-0.268352
H	2.380826	0.713175	-1.264710
H	3.687226	-1.738576	-0.294702
H	4.478910	-0.278157	-0.966976

H 3.964800 -0.322546 0.755580

serine_18 -569.59263641 a.u.

C 3.487401 0.279265 -0.331846

C 2.037430 0.144939 0.090241

O 1.636955 0.565601 1.190398

H 3.785510 1.331918 -0.226821

H 4.102311 -0.316027 0.359421

H 3.674825 -0.055856 -1.361964

N 1.205718 -0.453257 -0.812332

C -0.193631 -0.829873 -0.587730

C -1.215286 0.307070 -0.460072

O -2.403616 0.068657 -0.753363

C -0.383697 -1.774612 0.624678

O -1.638795 -2.447107 0.542666

H 1.611641 -0.738338 -1.694840

H -2.300738 -1.787772 0.266947

H -0.504275 -1.398101 -1.477379

H 0.397245 -2.550019 0.594218

H -0.284086 -1.208090 1.565712

N -0.789080 1.496870 0.027489

C -1.767529 2.540618 0.321183

H 0.102545 1.486329 0.525217

H -2.391759 2.713694 -0.565488

H -2.426498 2.253755 1.156466

H -1.227683 3.461563 0.576080

serine_19 -569.59210256 a.u.

C	2.855595	-1.620455	0.520731
C	1.565296	-0.985291	0.042645
O	1.050542	-1.301498	-1.046182
H	1.546789	0.168114	1.710395
N	1.016816	-0.054245	0.877047
C	-0.049383	0.891636	0.520447
C	-1.469703	0.305710	0.432327
O	-2.419302	0.908797	0.960657
C	0.274328	1.677979	-0.762406
O	1.498104	2.413755	-0.636724
H	1.320984	3.193485	-0.092073
H	-0.775791	-1.207070	-0.749464
N	-1.606705	-0.833972	-0.284939
C	-2.924531	-1.428224	-0.470125
H	3.041801	-1.460968	1.592735
H	2.819557	-2.696744	0.305831
H	3.685587	-1.182294	-0.054757
H	-0.108733	1.606257	1.355552
H	0.418369	0.988698	-1.603787
H	-0.579729	2.341294	-0.984099
H	-3.391911	-1.627813	0.505450
H	-3.585893	-0.751788	-1.033471
H	-2.806172	-2.370209	-1.020783

serine_20 -569.59229424 a.u.

C	2.872406	-1.637078	-0.364256
C	1.568505	-1.121698	0.215685
O	0.960386	-1.697748	1.122853

H	2.831668	-2.733293	-0.413498
H	3.082645	-1.223658	-1.361518
H	3.690899	-1.355929	0.316999
N	1.079689	0.042190	-0.353055
C	0.052021	0.791658	0.366616
C	-1.346294	0.165091	0.305826
O	-2.234303	0.565729	1.069395
C	-0.051378	2.189077	-0.240773
O	1.273634	2.753746	-0.225730
H	1.749461	0.615821	-0.860539
H	1.220259	3.654972	-0.571624
H	0.310784	0.864992	1.436259
H	-0.428986	2.115172	-1.277003
H	-0.754901	2.780301	0.364946
N	-1.552206	-0.748038	-0.682338
C	-2.807742	-1.488244	-0.737934
H	-0.723609	-1.133184	-1.120413
H	-3.643765	-0.779842	-0.671132
H	-2.859670	-2.026560	-1.693457
H	-2.890016	-2.204513	0.095601

serine_21 -569.59182483 a.u.

C	2.819149	-1.682427	-0.630213
C	1.902472	-0.842759	0.235314
O	2.228513	-0.437775	1.355491
H	0.608990	-0.673724	-1.327362
N	0.656805	-0.571332	-0.315819
C	-0.123461	0.529307	0.244211

C	-1.632051	0.305941	0.125255
O	-2.428933	1.249312	0.219811
C	0.269285	1.879012	-0.382951
O	1.689991	2.049967	-0.408276
H	2.024094	1.896661	0.489325
H	-1.315843	-1.702457	-0.022314
N	-2.025758	-0.982088	-0.087774
C	-3.442926	-1.327577	-0.078888
H	3.442733	-2.312719	0.016523
H	2.264528	-2.307639	-1.345426
H	3.477783	-1.000374	-1.191420
H	0.121132	0.550406	1.319853
H	-0.055642	1.914664	-1.435093
H	-0.239796	2.689360	0.160964
H	-3.556041	-2.362457	-0.427078
H	-3.876010	-1.227017	0.929011
H	-3.984633	-0.651774	-0.754406

serine_22 -569.59147111 a.u.

C	3.360974	-0.323472	0.619450
C	2.061561	-0.225220	-0.153356
O	1.971459	0.410743	-1.215804
H	1.052193	-1.219244	1.340311
N	0.991240	-0.900189	0.378506
C	-0.336415	-0.768235	-0.222914
C	-0.981868	0.534850	0.277301
O	-1.647952	0.576185	1.320128
C	-1.199365	-1.979317	0.125655

O	-2.440238	-1.950687	-0.583558
H	-2.252234	-2.116208	-1.518185
H	0.056124	1.516819	-1.161651
N	-0.708906	1.621999	-0.498122
C	-1.091118	2.954449	-0.042484
H	3.287858	-0.975165	1.501817
H	4.139139	-0.708111	-0.055237
H	3.656861	0.687948	0.934709
H	-0.178689	-0.720025	-1.312451
H	-0.629879	-2.902796	-0.082513
H	-1.465681	-1.945947	1.192111
H	-2.154975	2.949642	0.229192
H	-0.510241	3.264737	0.841687
H	-0.925576	3.667423	-0.860526

serine_23 -569.59133060 a.u.

C	3.415234	-0.572591	0.244905
C	1.989986	-0.223614	-0.137416
O	1.523968	-0.537806	-1.247116
H	3.690331	-0.237032	1.254926
H	3.535622	-1.663313	0.175610
H	4.091889	-0.110872	-0.488724
N	1.271611	0.457991	0.805346
C	-0.123939	0.896566	0.655632
C	-1.109567	-0.288903	0.649246
O	-1.793877	-0.557454	1.645424
C	-0.305181	1.837787	-0.548814
O	-1.663877	2.273868	-0.635402

H	1.707406	0.602875	1.707799
H	-2.186537	1.516338	-0.939424
H	-0.375042	1.455697	1.568385
H	0.300058	2.741847	-0.383507
H	0.031171	1.358624	-1.480021
N	-1.200831	-0.962312	-0.537884
C	-2.000812	-2.183907	-0.597426
H	-0.379297	-0.880270	-1.141845
H	-3.017674	-1.969298	-0.242921
H	-2.040026	-2.525664	-1.639894
H	-1.577403	-2.979573	0.037362

serine_24 -569.59159155 a.u.

C	-3.368232	-0.697605	-0.005877
C	-2.044779	-0.023753	0.287920
O	-1.582025	0.086522	1.426521
H	-4.014268	-0.622803	0.877715
H	-3.871624	-0.258975	-0.880328
H	-3.165531	-1.761470	-0.209930
N	-1.378254	0.480070	-0.820537
C	0.063347	0.678185	-0.710789
C	0.752395	-0.664955	-0.371925
O	0.187176	-1.747456	-0.580849
C	0.409001	1.829697	0.242811
O	1.749321	2.261712	-0.109384
H	-1.673375	0.064693	-1.699466
H	1.998720	2.967613	0.503024
H	0.422195	0.985451	-1.708688

H	-0.313497	2.645681	0.079739
H	0.364080	1.498595	1.288988
N	2.012849	-0.565238	0.121370
C	2.786644	-1.766373	0.409616
H	2.429266	0.359853	0.179781
H	2.243591	-2.401946	1.123922
H	2.963479	-2.351768	-0.506152
H	3.748763	-1.466145	0.844722

serine_25 -569.59147579 a.u.

C	-2.298150	-2.206374	-0.045689
C	-1.173185	-1.221967	0.209726
O	-0.549658	-1.170848	1.274720
H	-2.136371	-3.100163	0.570135
H	-3.247728	-1.737991	0.259419
H	-2.372354	-2.487088	-1.106940
N	-0.867875	-0.382972	-0.850072
C	-0.114319	0.849221	-0.593627
C	1.316832	0.582489	-0.106396
O	1.913930	1.411359	0.591411
C	-0.842794	1.782666	0.372318
O	-2.149696	1.990623	-0.204110
H	-1.588321	-0.303609	-1.561586
H	-2.630368	2.602861	0.368536
H	-0.029891	1.363649	-1.566170
H	-0.913872	1.314258	1.365915
H	-0.279868	2.724265	0.450280
N	1.894328	-0.557402	-0.580756

C	3.189303	-0.977159	-0.056314
H	1.262252	-1.256855	-0.952739
H	3.897224	-0.142026	-0.136463
H	3.116779	-1.274059	1.002736
H	3.554611	-1.822937	-0.653616

serine_26 -569.59097222 a.u.

C	-3.365625	-0.664387	0.016355
C	-2.024299	-0.024972	0.304893
O	-1.522386	0.013097	1.430844
H	-1.708016	0.160547	-1.684808
N	-1.385237	0.532836	-0.796138
C	0.062488	0.710077	-0.711620
C	0.739112	-0.650642	-0.414875
O	0.173044	-1.716945	-0.695004
C	0.437816	1.841261	0.264401
O	1.810007	2.259018	0.086308
H	1.875721	2.725536	-0.759103
H	2.395588	0.328823	0.275979
N	1.982807	-0.586843	0.122096
C	2.717777	-1.810415	0.418795
H	-3.184390	-1.716010	-0.259233
H	-3.980037	-0.636950	0.924852
H	-3.892393	-0.166897	-0.811558
H	0.397421	1.019723	-1.718753
H	-0.254313	2.685592	0.112165
H	0.358847	1.498261	1.301435
H	2.143094	-2.439612	1.114249

H 2.899485 -2.389888 -0.499271

H 3.677072 -1.537960 0.877454

serine_27 -569.59115753 a.u.

C 2.635444 -1.766647 -0.064499

C 1.331236 -0.996526 -0.133435

O 0.588345 -1.026346 -1.118118

H 2.544084 -2.676786 -0.670966

H 3.427139 -1.136085 -0.499751

H 2.918239 -2.028300 0.966223

N 1.013513 -0.277358 1.009439

C 0.043823 0.821603 0.962536

C -1.229279 0.403514 0.202584

O -1.729109 1.134575 -0.660751

C 0.635807 2.105708 0.368111

O 1.195401 1.899935 -0.923659

H 1.760038 -0.179200 1.691012

H 0.467185 1.589085 -1.486775

H -0.261965 1.032327 2.003800

H -0.149793 2.881098 0.359822

H 1.465068 2.449624 1.007215

N -1.803338 -0.759658 0.630890

C -2.843819 -1.367795 -0.196209

H -1.181032 -1.384706 1.133187

H -3.650641 -0.640161 -0.349831

H -2.443285 -1.666259 -1.178965

H -3.242638 -2.245974 0.328417

serine_28 -569.59007297 a.u.

C	-3.216704	-0.696178	0.676629
C	-2.021913	-0.566542	-0.244372
O	-1.701209	-1.438451	-1.059664
H	-3.985394	-1.306365	0.185589
H	-2.886447	-1.214759	1.591114
H	-3.631230	0.283333	0.956535
N	-1.302894	0.609579	-0.120273
C	0.043145	0.609502	-0.658353
C	0.948338	-0.319405	0.175617
O	0.682315	-0.627100	1.339808
C	0.585106	2.036046	-0.684979
O	0.555834	2.518630	0.666643
H	-1.392782	1.096748	0.768550
H	0.829259	3.445714	0.665419
H	-0.006516	0.230311	-1.692487
H	1.614931	2.033067	-1.082784
H	-0.059816	2.649008	-1.338440
N	2.095486	-0.719118	-0.458693
C	2.983345	-1.674846	0.199203
H	2.103541	-0.676379	-1.471064
H	3.244392	-1.291690	1.194232
H	2.502106	-2.658503	0.320844
H	3.896388	-1.779811	-0.401515

serine_29 -569.58914106 a.u.

C	2.702645	-2.086065	0.129949
C	2.057523	-0.714097	0.059420

O	2.731314	0.296810	-0.188213
H	3.347017	-2.213859	-0.750655
H	3.342525	-2.120745	1.024613
H	1.973022	-2.907310	0.176274
N	0.701436	-0.692555	0.270381
C	-0.112451	0.516692	0.480220
C	-1.595314	0.135149	0.453333
O	-2.424065	0.703371	1.171490
C	0.101714	1.617701	-0.591567
O	1.162618	2.507653	-0.303826
H	0.304650	-1.554458	0.632035
H	1.959772	1.943804	-0.260035
H	0.084667	0.966611	1.467127
H	0.224035	1.127565	-1.578102
H	-0.812406	2.230593	-0.615872
N	-1.938572	-0.839096	-0.446965
C	-3.347612	-1.140230	-0.687990
H	-1.242358	-1.121641	-1.127647
H	-3.839905	-1.351070	0.270601
H	-3.865516	-0.291638	-1.162137
H	-3.413515	-2.023863	-1.335926

serine_30 -569.58967453 a.u.

C	3.120214	-1.062621	-1.125943
C	2.276523	-0.430251	-0.034762
O	2.772866	0.070824	0.983023
H	3.827923	-0.310085	-1.502676
H	3.702620	-1.883094	-0.682018

H	2.521428	-1.454016	-1.961169
N	0.919918	-0.467512	-0.234064
C	0.013194	0.169596	0.716171
C	-1.382747	-0.447859	0.553388
O	-1.859133	-1.218111	1.396025
C	0.049307	1.697548	0.598937
O	-0.275028	2.061592	-0.762286
H	0.554513	-0.755243	-1.133920
H	-0.143464	3.013965	-0.859671
H	0.350483	-0.090272	1.730658
H	-0.679304	2.133670	1.305476
H	1.063990	2.037798	0.856805
N	-2.018465	-0.135593	-0.618054
C	-3.373065	-0.626740	-0.852744
H	-1.688641	0.695860	-1.103714
H	-3.392564	-1.716021	-0.713925
H	-4.096194	-0.179632	-0.151470
H	-3.661164	-0.383662	-1.883933

serine_31 -569.58976019 a.u.

C	-2.263067	-2.254733	-0.056877
C	-1.149658	-1.258005	0.200014
O	-0.504585	-1.222996	1.252641
H	-2.061388	-3.169131	0.515490
H	-3.209422	-1.819550	0.302588
H	-2.370911	-2.494153	-1.125325
N	-0.880662	-0.385583	-0.843230
C	-0.138070	0.850099	-0.570972

C	1.302184	0.594006	-0.102971
O	1.898086	1.429404	0.588530
C	-0.885321	1.755107	0.417003
O	-2.204613	2.046592	-0.087426
H	-1.611775	-0.306208	-1.543371
H	-2.146049	2.848210	-0.623982
H	-0.058352	1.379281	-1.537285
H	-1.017581	1.228751	1.371161
H	-0.301198	2.668626	0.596165
N	1.889604	-0.535642	-0.590219
C	3.193185	-0.943158	-0.076611
H	1.261713	-1.244139	-0.951920
H	3.889396	-0.098032	-0.153681
H	3.130330	-1.250093	0.980188
H	3.566027	-1.778882	-0.683364

serine_32 -569.58956384 a.u.

C	-2.262481	-2.253727	-0.112639
C	-1.243826	-1.174527	0.209494
O	-0.724776	-1.063125	1.326255
H	-1.471793	-0.370793	-1.667727
N	-0.896382	-0.343169	-0.834101
C	-0.087707	0.859048	-0.614245
C	1.341247	0.551844	-0.141392
O	1.999023	1.409182	0.461219
C	-0.757341	1.857994	0.345597
O	-2.077971	2.188122	-0.114630
H	-2.683390	1.518210	0.229287

H	1.182911	-1.360234	-0.808491
N	1.848611	-0.659515	-0.506853
C	3.142979	-1.084638	0.015500
H	-2.602266	-2.232751	-1.158278
H	-1.813661	-3.234002	0.104524
H	-3.127596	-2.128697	0.555107
H	0.000033	1.347900	-1.599042
H	-0.771579	1.450944	1.366716
H	-0.174430	2.786743	0.343097
H	3.884205	-0.298166	-0.177292
H	3.098716	-1.264119	1.101931
H	3.445822	-2.005642	-0.499790

serine_33 -569.58936549 a.u.

C	2.475785	-2.053480	-0.104962
C	1.430630	-0.983725	-0.338442
O	0.705849	-0.954067	-1.338906
H	2.873627	-2.382786	-1.073295
H	3.295058	-1.704336	0.540484
H	1.982479	-2.911012	0.380261
N	1.324283	-0.020564	0.651226
C	0.113913	0.808349	0.675184
C	-1.128049	-0.100300	0.578995
O	-1.236876	-1.073151	1.334345
C	0.228514	1.944725	-0.349905
O	1.383708	2.745174	-0.085455
H	1.713268	-0.273322	1.553902
H	2.137020	2.134424	-0.081052

H	0.074073	1.271790	1.674427
H	0.260523	1.533240	-1.373092
H	-0.633346	2.621327	-0.249539
N	-2.104559	0.273189	-0.299644
C	-3.233496	-0.630273	-0.516979
H	-1.815212	0.850072	-1.080938
H	-3.705833	-0.850288	0.448871
H	-3.959323	-0.133415	-1.173905
H	-2.905630	-1.579494	-0.970407

serine_34 -569.58548889 a.u.

C	3.287362	-1.508146	-0.028550
C	2.364738	-0.306753	0.074195
O	2.783505	0.840620	0.234580
H	0.758195	-1.548332	0.196578
N	1.009359	-0.591784	-0.039184
C	0.029727	0.437762	0.318817
C	-1.373281	-0.141806	0.437597
O	-2.242623	0.433014	1.110285
C	-0.044785	1.541016	-0.766167
O	-0.861680	2.629650	-0.348963
H	-1.641757	2.265065	0.102871
H	-0.987019	-1.503722	-1.034579
N	-1.636790	-1.272309	-0.290236
C	-3.016269	-1.746895	-0.398412
H	2.768355	-2.423022	-0.349363
H	4.089391	-1.272055	-0.741462
H	3.749593	-1.677782	0.955805

H	0.286338	0.919481	1.276653
H	0.962444	1.941013	-0.935297
H	-0.418053	1.087624	-1.706102
H	-3.434930	-1.856102	0.610141
H	-3.645462	-1.038336	-0.960056
H	-3.013635	-2.722515	-0.901347

serine_35 -569.58463816 a.u.

C	-3.288880	-0.819234	-0.424296
C	-1.834561	-0.580782	-0.051986
O	-1.335686	-1.137270	0.936529
H	-3.509933	-1.888000	-0.302829
H	-3.918624	-0.257450	0.282748
H	-3.536420	-0.503888	-1.448592
N	-1.164516	0.271937	-0.893674
C	0.142348	0.937899	-0.751922
C	1.405317	0.081023	-0.532562
O	2.486328	0.545880	-0.935722
C	0.117762	2.083065	0.264366
O	-0.098032	1.521891	1.562812
H	-1.718366	0.618575	-1.667605
H	-0.005626	2.230308	2.214423
H	0.330248	1.405866	-1.731468
H	1.087749	2.606181	0.199183
H	-0.694833	2.783892	-0.004221
N	1.275501	-1.106357	0.093797
C	2.468403	-1.880646	0.412939
H	0.387657	-1.279798	0.578270

H 3.069236 -2.027101 -0.495502

H 3.094490 -1.364113 1.158551

H 2.154320 -2.855487 0.807996

serine_36 -569.58518761 a.u.

C 3.128904 -1.010278 -0.318829

C 1.710453 -0.470511 -0.328149

O 0.897950 -0.749991 -1.212976

H 3.511581 -1.008899 -1.347981

H 3.803833 -0.430807 0.328313

H 3.098277 -2.052231 0.036123

N 1.388661 0.347566 0.735073

C 0.009553 0.752931 1.005775

C -0.964353 -0.406390 0.692525

O -0.902710 -1.443946 1.361609

C -0.329581 2.119451 0.408988

O -0.261770 2.054098 -1.025550

H 2.035157 0.358927 1.514630

H -0.395503 2.947728 -1.370621

H -0.071339 0.875571 2.099667

H -1.342684 2.408299 0.744201

H 0.399447 2.853530 0.794747

N -1.906393 -0.165856 -0.265592

C -2.708460 -1.297052 -0.725632

H -1.610513 0.511778 -0.966400

H -3.204952 -1.761969 0.135790

H -3.467296 -0.928192 -1.428505

H -2.078738 -2.055896 -1.219069

serine_37 -569.58191740 a.u.

C	-3.448036	-0.344564	-0.374990
C	-2.067579	-0.117312	0.213981
O	-1.856220	0.649850	1.155911
H	-3.948946	0.627191	-0.482656
H	-3.420352	-0.856961	-1.347981
H	-4.033544	-0.950370	0.333526
N	-1.034945	-0.815241	-0.386210
C	0.278519	-0.858125	0.257787
C	0.939590	0.527594	0.331762
O	1.677284	0.837070	1.267507
C	1.149593	-1.821887	-0.556702
O	2.390796	-1.966897	0.127289
H	-1.286792	-1.578661	-1.006624
H	2.988924	-2.474568	-0.437233
H	0.201738	-1.210573	1.299345
H	0.624539	-2.795018	-0.634847
H	1.290441	-1.408890	-1.572572
N	0.726851	1.327695	-0.763051
C	1.183755	2.713781	-0.717124
H	-0.096990	1.110952	-1.313221
H	2.254866	2.728948	-0.477342
H	1.025182	3.171529	-1.702782
H	0.647653	3.292137	0.053281

serine_38 -569.57795927 a.u.

C	2.873379	-1.643738	-0.852648
C	2.065133	-0.756007	0.077880

O	2.488694	-0.392232	1.176244
H	3.237631	-2.508755	-0.281146
H	2.301669	-1.993627	-1.725141
H	3.747013	-1.072906	-1.201064
N	0.829548	-0.379125	-0.408442
C	-0.060751	0.494068	0.342427
C	-1.436883	-0.162293	0.505221
O	-1.842558	-0.603319	1.584499
C	-0.157711	1.888221	-0.283546
O	1.148016	2.463572	-0.228556
H	0.520605	-0.759589	-1.294602
H	1.095024	3.368113	-0.566158
H	0.375001	0.586315	1.347696
H	-0.503670	1.819779	-1.334835
H	-0.891331	2.485805	0.289024
N	-2.172442	-0.282018	-0.649916
C	-3.512169	-0.862667	-0.599564
H	-1.909784	0.268300	-1.457784
H	-3.460397	-1.851761	-0.125035
H	-4.201879	-0.235396	-0.013122
H	-3.888815	-0.967942	-1.625446

CYSTEINE

cysteine_1 -892.21081947086 a.u.

C	-2.250475	-2.429025	-0.803597
C	-1.705008	-1.313294	0.063364
O	-2.443769	-0.622773	0.792264
H	-2.718237	-3.179529	-0.149367

H	-3.032565	-2.016087	-1.456741
H	-1.475334	-2.912408	-1.415119
N	-0.358239	-1.117616	0.006890
C	0.327371	-0.108090	0.807715
C	0.238126	1.293364	0.164326
O	1.241303	1.917042	-0.224971
C	1.782348	-0.525004	1.040149
S	2.681147	-0.977895	-0.500053
H	0.208275	-1.609646	-0.680558
H	2.610078	0.269090	-1.021316
H	-0.196100	-0.063949	1.779520
H	2.322010	0.287929	1.544295
H	1.809625	-1.424789	1.673800
N	-1.023164	1.778410	0.075788
C	-1.278214	3.070030	-0.550455
H	-1.784325	1.183804	0.407467
H	-0.717473	3.862809	-0.033882
H	-0.966190	3.061603	-1.606209
H	-2.353453	3.279909	-0.487142

cysteine_2 -892.20733413107 a.u.

C	-3.779963	-1.000497	0.125086
C	-2.552638	-0.167719	-0.188375
O	-2.620707	0.938535	-0.747450
H	-4.452654	-0.407498	0.761596
H	-4.306892	-1.213791	-0.816389
H	-3.535755	-1.945305	0.631419
N	-1.352565	-0.699240	0.196431

C	-0.119117	-0.022078	-0.146425
C	1.009726	-1.055123	-0.017833
O	0.800504	-2.187716	0.449573
C	0.091440	1.194582	0.785608
S	1.272374	2.441199	0.126578
H	-1.259249	-1.652596	0.540139
H	0.468274	2.854183	-0.879441
H	-0.187717	0.343966	-1.185900
H	-0.878258	1.684709	0.941265
H	0.493774	0.871713	1.758979
N	2.231351	-0.644850	-0.440111
C	3.397387	-1.506892	-0.273791
H	2.344417	0.336802	-0.680404
H	3.617403	-1.680981	0.791061
H	3.210186	-2.478909	-0.750785
H	4.257597	-1.023032	-0.753620

cysteine_3 -892.20737742594 a.u.

C	3.453412	-1.281508	0.523441
C	2.215467	-0.757578	-0.175347
O	2.279015	-0.126889	-1.244419
H	3.980631	-1.956834	-0.166067
H	4.118577	-0.433174	0.740149
H	3.227096	-1.818487	1.455760
N	1.018490	-1.034948	0.428544
C	-0.249306	-0.560703	-0.136710
C	-0.480714	0.899623	0.294913
O	-1.222700	1.198054	1.246003

C	-1.390105	-1.459657	0.328725
S	-2.980843	-1.028295	-0.473449
H	1.018575	-1.417538	1.368160
H	-3.136455	0.129468	0.206984
H	-0.147099	-0.611156	-1.231629
H	-1.175579	-2.501094	0.042784
H	-1.509875	-1.397143	1.420737
N	0.218742	1.806260	-0.432477
C	0.221985	3.214254	-0.052476
H	0.930343	1.436487	-1.062197
H	-0.813087	3.564270	0.060312
H	0.745933	3.373398	0.903930
H	0.718843	3.789427	-0.844161

cysteine_4 -892.20640260508 a.u.

C	-2.291869	-2.368868	-0.833364
C	-1.726852	-1.292512	0.070467
O	-2.453325	-0.612504	0.819979
H	-2.796282	-3.119221	-0.206945
H	-3.047684	-1.914303	-1.489990
H	-1.521974	-2.862129	-1.443667
N	-0.374682	-1.123872	0.024483
C	0.318058	-0.118470	0.823905
C	0.250125	1.277488	0.170647
O	1.269319	1.864880	-0.225919
C	1.774584	-0.530576	1.043904
S	2.656412	-0.847426	-0.549478
H	0.171391	-1.566894	-0.710937

H 2.933473 -2.147656 -0.303493

H -0.200222 -0.072622 1.797671

H 2.302100 0.281539 1.561164

H 1.815272 -1.443416 1.654074

N -1.001657 1.790519 0.077471

C -1.226843 3.078253 -0.567851

H -1.775986 1.218787 0.415187

H -0.644374 3.864488 -0.065454

H -0.918925 3.046218 -1.624405

H -2.296179 3.316595 -0.503977

cysteine_5 -892.20648452460 a.u.

C 3.365309 -0.457956 -0.966367

C 2.306650 -0.508623 0.119937

O 2.545941 -0.919973 1.259138

H 3.871696 -1.432341 -1.011211

H 2.953812 -0.208472 -1.955245

H 4.114303 0.297748 -0.685406

N 1.047243 -0.085495 -0.267561

C 0.007599 0.170911 0.718670

C -1.302774 -0.564928 0.402333

O -2.383883 -0.185360 0.878618

C -0.263415 1.670818 0.881924

S -0.786072 2.457067 -0.698267

H 0.965721 0.437521 -1.137125

H -2.000968 1.862636 -0.724410

H 0.385494 -0.233973 1.674398

H -1.038589 1.835246 1.641390

H	0.662921	2.182914	1.184114
N	-1.189550	-1.653609	-0.399459
C	-2.351036	-2.485135	-0.690703
H	-0.267371	-1.897836	-0.739031
H	-3.147766	-1.876232	-1.142113
H	-2.050574	-3.274650	-1.391310
H	-2.745851	-2.939755	0.230545

cysteine_6 -892.20587470359 a.u.

C	0.630535	3.168306	0.719844
C	0.092708	1.952937	-0.006196
O	-0.690372	2.052903	-0.968863
H	1.281345	0.720300	1.118803
N	0.503515	0.738546	0.466546
C	0.223084	-0.492953	-0.272537
C	-1.174454	-1.029581	0.112049
O	-1.320801	-2.006065	0.862881
C	1.269952	-1.564344	0.030782
S	3.002304	-0.996643	-0.188787
H	2.871023	-0.603975	-1.476046
H	-1.962230	0.549163	-0.891267
N	-2.200983	-0.337961	-0.445065
C	-3.576880	-0.638358	-0.066306
H	-0.218887	3.759068	1.091712
H	1.290561	2.908107	1.559525
H	1.182970	3.787182	-0.002332
H	0.226305	-0.242218	-1.348600
H	1.186089	-1.883077	1.080819

H	1.077457	-2.445813	-0.595377
H	-4.250979	-0.062699	-0.713504
H	-3.768401	-1.711910	-0.199617
H	-3.770144	-0.382685	0.988143

cysteine_7 -892.20580222661 a.u.

C	3.830761	-0.896459	-0.226683
C	2.605398	-0.140534	0.249977
O	2.679696	0.851213	0.990307
H	4.483269	-0.197466	-0.769786
H	4.381673	-1.257482	0.653973
H	3.583109	-1.747618	-0.877107
N	1.400071	-0.625846	-0.180282
C	0.159129	0.027205	0.192588
C	-0.967196	-0.966732	-0.086905
O	-0.880461	-1.789497	-1.013853
C	-0.024274	1.314855	-0.639102
S	-1.471709	2.333269	-0.146445
H	1.326807	-1.410762	-0.821606
H	-2.404214	1.601387	-0.795068
H	0.204484	0.299348	1.259575
H	0.855528	1.952088	-0.466487
H	-0.087513	1.065601	-1.708790
N	-2.049831	-0.876325	0.728544
C	-3.250615	-1.661097	0.458087
H	-2.100372	-0.076461	1.350141
H	-2.967821	-2.711910	0.311988
H	-3.925281	-1.579063	1.319750

H -3.767103 -1.311929 -0.450711

cysteine_8 -892.20482964037 a.u.

C 0.604532 3.161764 0.744382

C 0.103053 1.946643 -0.007465

O -0.630617 2.044038 -1.008023

H -0.256886 3.788183 1.015600

H 1.171159 2.901798 1.649942

H 1.248428 3.743788 0.068395

N 0.503318 0.733003 0.473793

C 0.227606 -0.510795 -0.249291

C -1.177173 -1.039704 0.111889

O -1.343899 -2.030771 0.839090

C 1.273842 -1.566086 0.094121

S 2.942421 -0.894069 -0.312602

H 1.153666 0.700979 1.251855

H 3.629099 -1.994624 0.062770

H 0.256589 -0.270305 -1.326244

H 1.209732 -1.825116 1.160255

H 1.074607 -2.467631 -0.499881

N -2.188496 -0.320146 -0.436614

C -3.573585 -0.615598 -0.089866

H -1.934999 0.557461 -0.892877

H -3.779388 -1.680511 -0.265999

H -3.778335 -0.396587 0.970509

H -4.229677 -0.005824 -0.724105

cysteine_9 -892.20471439220 a.u.

C	0.039098	3.214162	0.797306
C	-0.114054	1.954424	-0.030270
O	-0.681828	1.955005	-1.135035
H	0.706373	0.818919	1.478874
N	0.433370	0.815702	0.500816
C	0.316083	-0.477656	-0.176940
C	-1.046256	-1.115185	0.156028
O	-1.166572	-2.032246	0.982722
C	1.459990	-1.394285	0.244165
S	3.089934	-0.823637	-0.378985
H	2.986488	0.437990	0.094291
H	-1.894842	0.278056	-1.062832
N	-2.086424	-0.567853	-0.527118
C	-3.456966	-0.965747	-0.226088
H	-0.958969	3.636390	0.982417
H	0.549065	3.040679	1.755867
H	0.611758	3.946538	0.209557
H	0.373439	-0.266883	-1.256405
H	1.477481	-1.518234	1.337117
H	1.304908	-2.390646	-0.194713
H	-4.124357	-0.510023	-0.968679
H	-3.542067	-2.059804	-0.279259
H	-3.757017	-0.646087	0.784944

cysteine_10 -892.20459812865 a.u.

C	3.446707	-1.271764	0.498584
C	2.190761	-0.785520	-0.195492
O	2.226731	-0.197735	-1.289169

H	4.091716	-0.404494	0.701937
H	3.240413	-1.803785	1.438335
H	3.986190	-1.940323	-0.187770
N	1.007076	-1.051215	0.443558
C	-0.261958	-0.553357	-0.096667
C	-0.446868	0.912663	0.336576
O	-1.063848	1.216797	1.367845
C	-1.421082	-1.409217	0.400509
S	-3.000101	-0.933650	-0.404074
H	1.033279	-1.358626	1.410414
H	-2.750328	-1.560485	-1.575379
H	-0.177132	-0.615151	-1.192477
H	-1.217303	-2.476011	0.228453
H	-1.578355	-1.231642	1.475383
N	0.162751	1.811242	-0.481082
C	0.221255	3.220235	-0.108449
H	0.821974	1.432875	-1.158986
H	-0.789666	3.569869	0.140340
H	0.868657	3.381836	0.768963
H	0.607430	3.793413	-0.961138

cysteine_11 -892.20436303871 a.u.

C	3.511505	-0.953218	-0.779221
C	2.450561	-0.466059	0.188846
O	2.722383	-0.065165	1.329707
H	4.261090	-0.158955	-0.906999
H	4.015372	-1.823878	-0.334427
H	3.099500	-1.229827	-1.760276

N	1.163233	-0.475382	-0.284006
C	0.058506	-0.182157	0.607041
C	-1.197781	-0.796708	-0.025741
O	-1.153211	-1.405550	-1.104662
C	-0.080405	1.333440	0.840934
S	-0.613220	2.245827	-0.659492
H	0.912858	-0.986768	-1.128682
H	0.433348	1.848674	-1.417430
H	0.253521	-0.656591	1.588073
H	-0.846358	1.545780	1.604720
H	0.878745	1.721599	1.210237
N	-2.348526	-0.648439	0.681964
C	-3.621446	-1.084787	0.114718
H	-2.345732	-0.064283	1.507751
H	-3.874530	-0.497339	-0.781352
H	-3.554482	-2.143809	-0.169235
H	-4.403773	-0.958443	0.873950

cysteine_12 -892.20449191511 a.u.

C	-1.786700	2.689061	0.544688
C	-0.917816	1.550353	0.048906
O	-0.522400	1.500197	-1.132224
H	-1.308085	3.639346	0.269802
H	-2.755349	2.636461	0.024877
H	-1.958524	2.662434	1.630169
N	-0.602772	0.593979	0.966319
C	0.065116	-0.679141	0.674272
C	1.587886	-0.564253	0.469417

O	2.360974	-1.325519	1.072234
C	-0.550881	-1.442704	-0.513915
S	-2.354369	-1.725257	-0.341197
H	-0.997875	0.693728	1.893105
H	-2.724594	-0.494921	-0.759897
H	-0.053266	-1.294635	1.577474
H	-0.356297	-0.932878	-1.465090
H	-0.086595	-2.440986	-0.545286
N	1.994908	0.367761	-0.427496
C	3.411454	0.518251	-0.737135
H	1.279365	0.896628	-0.927556
H	3.814277	-0.399704	-1.192423
H	3.526845	1.356668	-1.435968
H	3.982103	0.722969	0.180705

cysteine_13 -892.20415032168 a.u.

C	3.362888	-0.982904	-0.923683
C	2.294666	-0.787978	0.133770
O	2.556463	-0.695091	1.342571
H	0.814157	-0.634445	-1.324296
N	1.008100	-0.716456	-0.329961
C	-0.064917	-0.330456	0.558068
C	-1.382043	-0.549981	-0.182421
O	-1.451912	-0.504045	-1.420663
C	0.037675	1.139454	1.032608
S	0.162540	2.361761	-0.327196
H	-0.945523	1.963799	-0.993715
H	-2.345722	-0.866480	1.599779

N	-2.477539	-0.718451	0.607189
C	-3.800860	-0.893041	0.015044
H	4.108721	-1.695099	-0.545966
H	2.951527	-1.341523	-1.878323
H	3.863665	-0.016727	-1.091344
H	-0.016946	-0.965019	1.461053
H	-0.815891	1.380846	1.685487
H	0.967651	1.248165	1.610252
H	-4.547358	-0.890802	0.819377
H	-4.006671	-0.065640	-0.677975
H	-3.863044	-1.838385	-0.545368

cysteine_14 -892.20407501523 a.u.

C	-1.849657	2.673025	0.528754
C	-0.885127	1.605062	0.055740
O	-0.392217	1.628868	-1.087781
H	-1.521403	3.644854	0.137582
H	-2.842236	2.447224	0.108481
H	-1.930537	2.719037	1.624555
N	-0.601913	0.619371	0.957577
C	0.040001	-0.659793	0.634162
C	1.569314	-0.592596	0.456808
O	2.297448	-1.418688	1.031221
C	-0.583742	-1.363065	-0.585623
S	-2.388341	-1.646400	-0.416314
H	-1.115659	0.648943	1.829863
H	-2.298261	-2.596782	0.541342
H	-0.099607	-1.300415	1.517481

H	-0.468296	-0.745389	-1.486877
H	-0.067586	-2.321528	-0.744503
N	2.030750	0.363521	-0.383843
C	3.458420	0.473445	-0.656054
H	1.345226	0.955089	-0.856772
H	3.837395	-0.441699	-1.136544
H	3.619756	1.331888	-1.320600
H	4.015717	0.623033	0.280635

cysteine_15 -892.20296328273 a.u.

C	3.192541	-1.034334	-0.980308
C	2.199831	-0.799667	0.143599
O	2.491306	-0.972619	1.330322
H	3.597561	-2.051811	-0.884016
H	2.749346	-0.909425	-1.979055
H	4.027928	-0.328565	-0.860615
N	0.932756	-0.411746	-0.259641
C	-0.024861	0.089923	0.716751
C	-1.460446	-0.352915	0.399169
O	-2.435691	0.262942	0.850339
C	0.030804	1.614361	0.867502
S	-0.281874	2.477235	-0.732086
H	0.839686	-0.032831	-1.199339
H	1.014723	2.627822	-1.081005
H	0.256244	-0.366104	1.682273
H	-0.763179	1.937444	1.554031
H	1.007613	1.924508	1.264247
N	-1.579203	-1.464811	-0.374674

C	-2.892057	-2.038903	-0.644701
H	-0.731072	-1.947310	-0.645267
H	-3.556277	-1.263259	-1.050920
H	-2.778469	-2.846848	-1.378967
H	-3.348779	-2.436860	0.274856

cysteine_16 -892.20224663189 a.u.

C	2.647402	-2.234413	-0.413084
C	1.784274	-1.211729	0.297180
O	2.070415	-0.767330	1.420294
H	0.415775	-1.221016	-1.274249
N	0.684644	-0.785833	-0.397013
C	-0.242731	0.172088	0.165083
C	-1.658990	-0.270842	-0.210302
O	-1.894141	-0.803026	-1.305330
C	-0.038045	1.603119	-0.370722
S	1.687163	2.211342	-0.185581
H	1.949135	1.531995	0.955329
H	-2.356736	0.339865	1.616196
N	-2.631119	0.022961	0.694850
C	-4.025435	-0.319221	0.427509
H	2.920865	-3.022440	0.301860
H	2.150744	-2.679039	-1.287704
H	3.571303	-1.734406	-0.741468
H	-0.092637	0.166414	1.257788
H	-0.258128	1.623968	-1.450268
H	-0.736648	2.282156	0.143127
H	-4.654934	0.147204	1.195974

H	-4.310219	0.062321	-0.562430
H	-4.176828	-1.409550	0.436574

cysteine_17 -892.20286745792 a.u.

C	-0.512386	3.294322	-0.377796
C	0.021526	2.004517	0.215788
O	0.863764	1.973598	1.117621
H	0.313671	4.012097	-0.470090
H	-0.988650	3.142145	-1.357313
H	-1.254308	3.716862	0.317785
N	-0.485023	0.838241	-0.335903
C	-0.290036	-0.412864	0.388467
C	1.148036	-0.947427	0.325091
O	1.521025	-1.807845	1.131803
C	-1.193933	-1.508285	-0.193742
S	-2.976794	-1.060434	-0.230077
H	-1.374075	0.918885	-0.827127
H	-3.105728	-0.889853	1.105247
H	-0.504349	-0.275514	1.463201
H	-0.925575	-1.698798	-1.245924
H	-1.046234	-2.433486	0.378882
N	1.903435	-0.503547	-0.716930
C	3.313999	-0.866989	-0.798765
H	1.571364	0.327150	-1.193236
H	3.410987	-1.952732	-0.668661
H	3.696682	-0.581179	-1.787383
H	3.904484	-0.367173	-0.013957

cysteine_18 -892.20247180682 a.u.

C	-1.915259	2.588281	0.523677
C	-0.928778	1.542406	0.047740
O	-0.447263	1.567506	-1.098996
H	-1.616718	3.565682	0.122766
H	-2.904952	2.332243	0.113894
H	-1.987546	2.639593	1.619943
N	-0.619431	0.563102	0.950585
C	0.073417	-0.693437	0.633114
C	1.598734	-0.573253	0.450689
O	2.356831	-1.374793	1.020331
C	-0.538606	-1.415001	-0.578138
S	-2.353633	-1.576706	-0.293676
H	-1.060445	0.617825	1.860749
H	-2.556299	-2.547124	-1.210376
H	-0.050717	-1.336525	1.516484
H	-0.357136	-0.854166	-1.503521
H	-0.083716	-2.414229	-0.639822
N	2.024393	0.407388	-0.381048
C	3.446356	0.566422	-0.658716
H	1.316786	0.965331	-0.862182
H	3.850484	-0.322876	-1.166906
H	3.578372	1.447881	-1.299195
H	4.003568	0.706015	0.279357

cysteine_19 -892.20231698181 a.u.

C	-3.679907	-0.450545	0.165650
C	-2.205160	-0.330866	-0.165787

O	-1.822551	-0.010798	-1.305738
H	-1.739638	-0.791304	1.768909
N	-1.340975	-0.607079	0.856154
C	0.129463	-0.579356	0.761866
C	0.668484	0.862168	0.660991
O	1.256814	1.391340	1.614500
C	0.645849	-1.506201	-0.349434
S	2.477012	-1.615591	-0.340097
H	2.686659	-0.335371	-0.721133
H	-0.230188	1.058213	-1.151173
N	0.479547	1.471449	-0.543095
C	0.847094	2.875086	-0.702147
H	-4.165617	0.509580	-0.060281
H	-4.120019	-1.214613	-0.491659
H	-3.870213	-0.720181	1.214268
H	0.506520	-0.945657	1.727735
H	0.287784	-2.530418	-0.157771
H	0.289973	-1.194797	-1.338520
H	0.706968	3.155239	-1.754210
H	0.235746	3.530087	-0.060057
H	1.900786	3.012023	-0.422899

cysteine_20 -892.20163042237 a.u.

C	3.479346	-0.888263	-0.870725
C	2.412063	-0.595657	0.165546
O	2.682368	-0.354207	1.352719
H	4.155660	-1.656612	-0.470709
H	3.060956	-1.224672	-1.830207

H	4.065095	0.028812	-1.034233
N	1.123925	-0.605420	-0.288984
C	0.024941	-0.276074	0.589453
C	-1.266650	-0.700044	-0.117565
O	-1.296904	-0.929661	-1.335607
C	-0.013279	1.223978	0.947729
S	-0.386986	2.212774	-0.563396
H	0.890591	-0.773483	-1.263767
H	-0.029836	3.400649	-0.029123
H	0.148106	-0.833841	1.535061
H	-0.786653	1.404467	1.711058
H	0.971106	1.501810	1.347598
N	-2.371880	-0.767536	0.669966
C	-3.684277	-1.022402	0.082661
H	-2.290142	-0.552605	1.655309
H	-3.946051	-0.230024	-0.634438
H	-3.680127	-1.985184	-0.447742
H	-4.427817	-1.051283	0.889174

cysteine_21 -892.20145215785 a.u.

C	-3.693405	-0.396087	0.184280
C	-2.218737	-0.300921	-0.155609
O	-1.836793	-0.008109	-1.302870
H	-4.146305	-1.165264	-0.458242
H	-3.882438	-0.645664	1.238129
H	-4.167753	0.566369	-0.055471
N	-1.353617	-0.564722	0.868933
C	0.115631	-0.567374	0.766358

C	0.708038	0.851315	0.652950
O	1.396978	1.321994	1.570578
C	0.599671	-1.525517	-0.333687
S	2.426816	-1.553283	-0.464477
H	-1.752094	-0.728227	1.785546
H	2.663247	-1.951139	0.805956
H	0.481852	-0.933104	1.737947
H	0.213643	-2.537248	-0.136177
H	0.240178	-1.203056	-1.320130
N	0.434276	1.508875	-0.501591
C	0.921511	2.868386	-0.698389
H	-0.273836	1.108046	-1.116607
H	2.012372	2.893185	-0.565200
H	0.668765	3.184122	-1.718824
H	0.470965	3.565546	0.026215

cysteine_22 -892.20181857175 a.u.

C	1.102074	2.986967	-0.082923
C	0.395113	1.677871	0.208287
O	-0.164081	1.433290	1.282163
H	0.666512	3.774438	0.544863
H	2.166680	2.876093	0.179745
H	1.033139	3.267708	-1.144632
N	0.399579	0.758925	-0.829690
C	0.111965	-0.648988	-0.542765
C	-1.343870	-0.875941	-0.093951
O	-1.649089	-1.865230	0.582963
C	1.078943	-1.266243	0.478613

S	2.832761	-1.131610	-0.052328
H	1.091604	0.923634	-1.554785
H	2.781317	-2.097734	-0.996712
H	0.219825	-1.185380	-1.501871
H	1.007476	-0.723694	1.431939
H	0.815217	-2.315622	0.657635
N	-2.256044	0.009730	-0.583171
C	-3.635841	-0.045061	-0.112187
H	-1.889206	0.882283	-0.944236
H	-4.013033	-1.070033	-0.223074
H	-3.709471	0.241756	0.949397
H	-4.243928	0.635610	-0.722440

cysteine_23 -892.20174893625 a.u.

C	1.165494	2.962890	-0.106197
C	0.485616	1.643621	0.210875
O	0.005282	1.387380	1.320361
H	0.583272	3.777753	0.345083
H	2.163034	2.962912	0.360529
H	1.277298	3.138321	-1.186217
N	0.415747	0.739381	-0.831326
C	0.074991	-0.661819	-0.575068
C	-1.384582	-0.849926	-0.120908
O	-1.723655	-1.869404	0.492397
C	1.016793	-1.349234	0.425911
S	2.772860	-1.279169	-0.103036
H	1.004767	0.922295	-1.636892
H	2.996190	-0.001762	0.276982

H	0.166044	-1.177935	-1.545889
H	0.908750	-0.913088	1.426702
H	0.753936	-2.414391	0.481359
N	-2.263221	0.109146	-0.524333
C	-3.640460	0.074542	-0.044303
H	-1.867723	0.985872	-0.840926
H	-4.059014	-0.924029	-0.225637
H	-3.694850	0.285201	1.036007
H	-4.225277	0.821632	-0.596829

cysteine_24 -892.20071350906 a.u.

C	-0.700967	3.252451	-0.399680
C	-0.110184	2.000100	0.219215
O	0.667381	2.019533	1.177572
H	0.051507	4.051570	-0.373923
H	-1.042541	3.089962	-1.432567
H	-1.560350	3.570609	0.211432
N	-0.489935	0.806304	-0.372007
C	-0.253376	-0.441141	0.350650
C	1.203752	-0.926259	0.294445
O	1.581467	-1.829728	1.050390
C	-1.119725	-1.560623	-0.236225
S	-2.900288	-1.102148	-0.067983
H	-1.317757	0.829108	-0.963887
H	-3.375026	-2.030378	-0.925814
H	-0.477197	-0.304377	1.423341
H	-0.878337	-1.698436	-1.301680
H	-0.910710	-2.484895	0.317554

N	1.981211	-0.372206	-0.674707
C	3.406209	-0.678810	-0.729775
H	1.629521	0.471811	-1.111277
H	3.539649	-1.767393	-0.679602
H	3.813078	-0.302940	-1.677726
H	3.948788	-0.221716	0.113408

cysteine_25 -892.19944915731 a.u.

C	2.644242	-2.266022	-0.408406
C	1.777603	-1.241269	0.296839
O	2.046150	-0.802208	1.422550
H	2.913081	-3.053715	0.308562
H	2.152185	-2.711070	-1.285636
H	3.570299	-1.767072	-0.732348
N	0.689138	-0.803963	-0.415471
C	-0.228931	0.174084	0.129812
C	-1.651409	-0.265089	-0.221494
O	-1.907919	-0.790861	-1.314840
C	-0.009772	1.575851	-0.468698
S	1.674041	2.172532	-0.018913
H	0.421180	-1.244093	-1.290236
H	1.618499	3.279596	-0.792797
H	-0.066081	0.202003	1.220290
H	-0.104645	1.511404	-1.563264
H	-0.770152	2.266642	-0.071884
N	-2.605009	0.020334	0.706094
C	-4.002746	-0.328655	0.467849
H	-2.310195	0.326133	1.624988

H	-4.313353	0.060347	-0.511382
H	-4.146829	-1.420068	0.469568
H	-4.617323	0.125941	1.255289

cysteine_26 -892.20064029699 a.u.

C	2.997166	-1.471871	-1.030993
C	2.196993	-0.702582	0.004229
O	2.735085	0.003574	0.868071
H	3.649177	-0.765687	-1.565193
H	3.640774	-2.193271	-0.506496
H	2.366236	-2.007008	-1.755452
N	0.834747	-0.821345	-0.086871
C	-0.060805	-0.227290	0.900822
C	-1.510056	-0.605592	0.585785
O	-2.292031	-0.970305	1.470991
C	0.076456	1.312631	1.005437
S	0.084613	2.194992	-0.605102
H	0.439818	-1.471153	-0.756823
H	1.360818	1.879629	-0.919300
H	0.154288	-0.634948	1.903169
H	-0.788182	1.702673	1.566151
H	0.996777	1.567002	1.543636
N	-1.860062	-0.505105	-0.737223
C	-3.265306	-0.665128	-1.109404
H	-1.283486	0.127704	-1.291508
H	-3.628964	-1.627920	-0.727667
H	-3.893384	0.134090	-0.683562
H	-3.341604	-0.652989	-2.204410

cysteine_27 -892.20045719276 a.u.

C	1.395409	2.832856	-0.071384
C	0.576057	1.592403	0.222169
O	0.054880	1.365135	1.317757
H	1.053463	3.648326	0.578418
H	2.449427	2.613423	0.163544
H	1.327900	3.137496	-1.126717
N	0.433694	0.708960	-0.836803
C	0.029455	-0.677895	-0.580035
C	-1.434745	-0.802448	-0.122554
O	-1.815489	-1.804292	0.495025
C	0.939683	-1.397236	0.425644
S	2.681440	-1.166521	-0.135869
H	1.033629	0.865015	-1.640868
H	3.208517	-2.177729	0.585743
H	0.099300	-1.199420	-1.550026
H	0.805299	-0.976403	1.429700
H	0.685287	-2.464026	0.428771
N	-2.268085	0.194581	-0.528880
C	-3.643358	0.228504	-0.043498
H	-1.828212	1.052683	-0.839148
H	-4.105307	-0.753763	-0.207407
H	-3.684187	0.458815	1.033463
H	-4.197547	0.991279	-0.606084

cysteine_28 -892.20006965072 a.u.

C	3.018038	-1.952719	-0.036010
C	1.794409	-1.092053	0.216812

O	1.571803	-0.544687	1.300881
H	3.901587	-1.431520	0.357881
H	2.903378	-2.893029	0.524570
H	3.169196	-2.184678	-1.100415
N	0.939501	-0.926912	-0.856925
C	-0.384177	-0.323594	-0.659753
C	-0.257860	1.107647	-0.098122
O	-1.085136	1.571848	0.695213
C	-1.300808	-1.183841	0.225661
S	-3.082925	-0.844698	-0.046198
H	1.063643	-1.537121	-1.657694
H	-3.028530	0.407878	0.458861
H	-0.841901	-0.237231	-1.659801
H	-1.163042	-2.242463	-0.046425
H	-1.047083	-1.048462	1.284945
N	0.769014	1.843480	-0.612363
C	1.063642	3.153483	-0.039594
H	1.515327	1.325028	-1.060535
H	0.158933	3.774461	-0.072972
H	1.389650	3.066924	1.009547
H	1.853243	3.628572	-0.636480

cysteine_29 -892.19926080892 a.u.

C	-3.687937	-0.466515	0.228138
C	-2.223020	-0.334585	-0.140763
O	-1.871304	-0.023942	-1.292916
H	-4.188287	0.487734	0.009261
H	-4.136878	-1.238240	-0.414087

H	-3.849961	-0.732066	1.282556
N	-1.332676	-0.584404	0.865062
C	0.133033	-0.559711	0.742845
C	0.709168	0.866353	0.627777
O	1.477430	1.305373	1.497638
C	0.622574	-1.490337	-0.377789
S	2.465221	-1.529892	-0.303614
H	-1.710280	-0.769675	1.786259
H	2.613610	-2.337789	-1.375952
H	0.521468	-0.931271	1.703455
H	0.220442	-2.499258	-0.201310
H	0.296299	-1.124262	-1.358319
N	0.343063	1.561180	-0.476933
C	0.836513	2.916813	-0.684105
H	-0.369671	1.155138	-1.082988
H	0.475738	3.596180	0.104248
H	1.935918	2.921961	-0.664324
H	0.484360	3.268830	-1.662271

cysteine_30 -892.19936668052 a.u.

C	3.659957	-0.258078	-0.009699
C	2.188227	-0.442957	0.291014
O	1.710921	-0.334725	1.423458
H	4.243191	-0.492837	0.889445
H	3.992831	-0.884238	-0.850830
H	3.818656	0.800947	-0.270460
N	1.393876	-0.755620	-0.805614
C	-0.037762	-0.475640	-0.694136

C	-0.233149	1.032294	-0.384812
O	0.664071	1.846854	-0.641227
C	-0.698692	-1.463363	0.289351
S	-2.515023	-1.666499	0.064104
H	1.803122	-0.486195	-1.696078
H	-2.474693	-2.022626	-1.239782
H	-0.463215	-0.651294	-1.698386
H	-0.214396	-2.443401	0.178140
H	-0.565497	-1.126520	1.325842
N	-1.433295	1.397580	0.133242
C	-1.722747	2.805662	0.381026
H	-2.168386	0.699437	0.200886
H	-1.709703	3.383826	-0.556153
H	-2.714083	2.879773	0.846695
H	-0.966461	3.228840	1.057303

cysteine_31 -892.19910741984 a.u.

C	3.216666	-1.248422	-1.017932
C	2.359884	-0.524992	0.004034
O	2.845101	0.145817	0.923009
H	3.816796	-0.502161	-1.558968
H	3.908019	-1.915961	-0.483864
H	2.626823	-1.830259	-1.741011
N	0.999114	-0.637116	-0.171850
C	0.084487	-0.108422	0.836319
C	-1.328161	-0.658767	0.649883
O	-2.068003	-0.868038	1.617205
C	0.061248	1.434819	0.837093

S	-0.471741	2.194602	-0.752174
H	0.655646	-1.361136	-0.793002
H	-1.798192	2.185412	-0.492070
H	0.415970	-0.421152	1.841539
H	-0.590132	1.790434	1.648842
H	1.083216	1.794758	1.018045
N	-1.705349	-0.893239	-0.651962
C	-3.102497	-1.235562	-0.919576
H	-1.225721	-0.316084	-1.341628
H	-3.377923	-2.105661	-0.310203
H	-3.783891	-0.407309	-0.663483
H	-3.205648	-1.486206	-1.983348

cysteine_32 -892.19858623738 a.u.

C	3.489315	-0.677007	-0.065923
C	2.047336	-0.217198	-0.154329
O	1.533332	0.088361	-1.246687
H	1.852271	-0.508948	1.843052
N	1.362175	-0.175007	1.022329
C	-0.031390	0.247487	1.234112
C	-1.119418	-0.703936	0.709375
O	-2.183851	-0.797406	1.336439
C	-0.321822	1.710213	0.800895
S	-1.086806	1.991050	-0.843192
H	-0.037374	1.532066	-1.560153
H	-0.086605	-1.010630	-1.005236
N	-0.841667	-1.387123	-0.432686
C	-1.918893	-2.123618	-1.088027

H	4.124737	0.090772	-0.530138
H	3.828471	-0.858313	0.963888
H	3.594290	-1.601281	-0.652841
H	-0.159935	0.218430	2.327311
H	-1.066053	2.118941	1.501310
H	0.600260	2.303687	0.894445
H	-1.493860	-2.696120	-1.922811
H	-2.378181	-2.812936	-0.367337
H	-2.699282	-1.440835	-1.462551

cysteine_33 -892.19861635228 a.u.

C	-3.470899	-1.367935	-0.309820
C	-2.216876	-0.733676	0.262301
O	-2.204691	-0.095698	1.318115
H	-4.306094	-0.663535	-0.196814
H	-3.362637	-1.650029	-1.367554
H	-3.704777	-2.268638	0.278576
N	-1.063224	-0.898307	-0.484277
C	0.230841	-0.566759	0.117524
C	0.454163	0.948220	0.227674
O	1.310871	1.406831	0.998970
C	1.344560	-1.185076	-0.746214
S	2.980324	-1.237262	0.083438
H	-1.078484	-1.582403	-1.234112
H	2.880421	0.008938	0.607567
H	0.280688	-0.962180	1.145085
H	1.096439	-2.240209	-0.950414
H	1.416997	-0.648775	-1.706319

N	-0.258387	1.721854	-0.633909
C	-0.175725	3.175846	-0.544286
H	-1.055832	1.288692	-1.084112
H	0.878847	3.480123	-0.572540
H	-0.705599	3.612106	-1.401037
H	-0.619701	3.544499	0.394208

cysteine_34 -892.19849231317 a.u.

C	3.659020	-0.286207	-0.014330
C	2.185758	-0.446939	0.292448
O	1.712045	-0.316390	1.424710
H	4.241792	-0.526845	0.883599
H	3.978952	-0.920360	-0.854396
H	3.834157	0.769180	-0.279229
N	1.383605	-0.763547	-0.795252
C	-0.044207	-0.476832	-0.674032
C	-0.236091	1.035769	-0.391618
O	0.640122	1.851085	-0.710172
C	-0.708634	-1.424009	0.345757
S	-2.481380	-1.673223	-0.125866
H	1.786582	-0.511453	-1.693506
H	-2.876606	-2.217282	1.045461
H	-0.479569	-0.671832	-1.671206
H	-0.191173	-2.391773	0.310998
H	-0.646844	-1.008563	1.357737
N	-1.413723	1.402383	0.175009
C	-1.703509	2.812716	0.408705
H	-2.131721	0.698361	0.321071

H	-0.934628	3.251711	1.060693
H	-1.714645	3.374146	-0.538285
H	-2.684749	2.889882	0.894743

cysteine_35 -892.19856656126 a.u.

C	3.313770	-0.639440	-0.482950
C	1.872911	-0.190529	-0.374524
O	1.116007	-0.144500	-1.355380
H	2.076928	-0.096543	1.641855
N	1.448739	0.155408	0.886964
C	0.020943	0.193241	1.227822
C	-0.703024	-1.001582	0.561878
O	-0.245605	-2.141051	0.715611
C	-0.597348	1.595442	1.116612
S	-0.847063	2.293054	-0.578894
H	0.038743	1.458636	-1.185841
H	-1.989794	0.217202	-0.422882
N	-1.874625	-0.734224	-0.074339
C	-2.543287	-1.817259	-0.791525
H	3.711517	-0.331657	-1.458255
H	3.942914	-0.235181	0.323721
H	3.329355	-1.739778	-0.429291
H	-0.024962	-0.053191	2.304050
H	-1.590673	1.580229	1.593890
H	0.044410	2.286676	1.683290
H	-3.500208	-1.441707	-1.176760
H	-1.923442	-2.185961	-1.624739
H	-2.727585	-2.650701	-0.100836

cysteine_36 -892.19825551109 a.u.

C	-1.638194	2.710046	-0.050439
C	-0.674815	1.541096	-0.100495
O	-0.033348	1.243683	-1.111340
H	-1.312283	3.471962	-0.769756
H	-2.631725	2.342376	-0.353854
H	-1.715867	3.150452	0.955158
N	-0.544040	0.843211	1.092119
C	-0.010776	-0.519126	1.136910
C	1.242107	-0.668985	0.250108
O	1.383663	-1.632901	-0.508593
C	-1.051442	-1.608315	0.834442
S	-2.028502	-1.351892	-0.692907
H	-1.219394	1.075735	1.814195
H	-0.957566	-1.322127	-1.517481
H	0.341146	-0.685805	2.172565
H	-0.541381	-2.581569	0.795022
H	-1.796143	-1.633211	1.647204
N	2.217996	0.262047	0.481182
C	3.314880	0.363514	-0.479826
H	1.889344	1.127996	0.896719
H	3.798070	-0.616930	-0.575279
H	2.945741	0.676186	-1.470589
H	4.045320	1.092776	-0.105240

cysteine_37 -892.19598788871 a.u.

C	3.138837	-1.351654	0.332765
C	1.690349	-0.987975	0.061231

O	1.152220	-1.303815	-1.012003
H	1.670468	-0.152412	1.887361
N	1.072605	-0.314177	1.084513
C	-0.173014	0.469915	1.133394
C	-1.495245	-0.122648	0.604438
O	-2.546810	0.350299	1.071594
C	-0.001101	1.901446	0.583490
S	0.598784	1.998709	-1.145304
H	-0.368292	1.217913	-1.677610
H	-0.549292	-1.313798	-0.757845
N	-1.460491	-1.080561	-0.343883
C	-2.709796	-1.612557	-0.875239
H	3.338119	-2.343535	-0.093252
H	3.773882	-0.618037	-0.188324
H	3.395552	-1.347117	1.402383
H	-0.389848	0.582849	2.209024
H	-0.958668	2.431277	0.698031
H	0.765395	2.431467	1.172499
H	-2.469591	-2.422584	-1.575802
H	-3.332524	-2.003099	-0.057214
H	-3.284001	-0.830132	-1.396004

cysteine_38 -892.19580040690 a.u.

C	3.699460	-1.054154	-0.412018
C	2.584355	-0.121854	0.021817
O	2.797750	0.982882	0.535043
H	1.155034	-1.518215	-0.541246
N	1.304815	-0.579738	-0.188601

C	0.158904	0.186678	0.303670
C	-1.015003	-0.772722	0.524535
O	-1.383677	-1.110222	1.652587
C	-0.153936	1.353322	-0.644845
S	-1.668702	2.267055	-0.154048
H	-1.214966	2.637571	1.064195
H	-1.412496	-0.788062	-1.481767
N	-1.557312	-1.303768	-0.621329
C	-2.764773	-2.122979	-0.519349
H	4.398897	-0.492797	-1.047229
H	4.244706	-1.382760	0.485291
H	3.334507	-1.937026	-0.956797
H	0.418109	0.594441	1.293208
H	0.711709	2.029189	-0.678644
H	-0.339795	0.992276	-1.670317
H	-2.993954	-2.536755	-1.510070
H	-2.581087	-2.943308	0.186331
H	-3.620573	-1.533908	-0.152562

cysteine_39 -892.19583377205 a.u.

C	3.083231	-1.872603	-0.026662
C	1.833021	-1.047972	0.217587
O	1.597757	-0.490333	1.293623
H	3.951528	-1.311952	0.346486
H	3.006093	-2.802525	0.557079
H	3.233731	-2.124470	-1.086667
N	0.968833	-0.930592	-0.854262
C	-0.366768	-0.352017	-0.673240

C	-0.282486	1.077211	-0.100630
O	-1.103021	1.484298	0.726245
C	-1.277461	-1.212300	0.215015
S	-3.046633	-0.731801	0.032153
H	1.116952	-1.540362	-1.650973
H	-3.421414	-1.836686	-0.650785
H	-0.815647	-0.274471	-1.677662
H	-1.170852	-2.270185	-0.064892
H	-0.996211	-1.082940	1.268032
N	0.695154	1.864719	-0.641232
C	0.961909	3.169236	-0.041642
H	1.455746	1.378932	-1.102503
H	0.032468	3.753010	-0.023064
H	1.331513	3.067832	0.991809
H	1.707743	3.692680	-0.654359

cysteine_40 -892.19558730201 a.u.

C	3.651888	-1.157321	-0.141174
C	2.536053	-0.149817	0.066103
O	2.750704	1.039777	0.315944
H	1.140579	-1.655584	-0.001178
N	1.252293	-0.648013	-0.058928
C	0.111924	0.183734	0.345219
C	-1.131198	-0.690557	0.510732
O	-1.911446	-0.563097	1.461064
C	-0.150904	1.269836	-0.717046
S	-1.420065	2.487573	-0.200937
H	-2.336712	1.585029	0.217626

H	-0.790062	-1.515223	-1.337313
N	-1.328264	-1.616169	-0.483533
C	-2.570878	-2.385086	-0.520610
H	4.356376	-0.751384	-0.880629
H	4.192159	-1.277996	0.809724
H	3.288822	-2.138349	-0.480411
H	0.310744	0.670320	1.312959
H	0.772891	1.849406	-0.854501
H	-0.427883	0.804429	-1.676647
H	-2.483820	-3.158095	-1.295119
H	-2.726469	-2.861141	0.456278
H	-3.439154	-1.741493	-0.733990

cysteine_41 -892.19597944300 a.u.

C	3.095863	-1.155546	-0.553282
C	1.729342	-0.532301	-0.364109
O	0.932130	-0.359383	-1.292781
H	3.502099	-0.831279	-1.520106
H	3.795358	-0.891409	0.253382
H	2.972926	-2.249933	-0.576956
N	1.407828	-0.166552	0.925568
C	0.017090	0.144988	1.257321
C	-0.929709	-0.873275	0.578854
O	-0.765144	-2.079348	0.795781
C	-0.315369	1.637775	1.120156
S	-0.124236	2.305389	-0.596576
H	1.982752	-0.552206	1.665910
H	-0.594666	3.530918	-0.266097

H	-0.094799	-0.078925	2.332631
H	-1.353778	1.796074	1.450834
H	0.362659	2.196962	1.781733
N	-1.969696	-0.367026	-0.144268
C	-2.791701	-1.303213	-0.908968
H	-1.805923	0.548811	-0.559485
H	-3.194190	-2.066824	-0.230862
H	-3.620238	-0.747517	-1.367450
H	-2.200323	-1.806559	-1.691250

cysteine_42 -892.19409950680 a.u.

C	-3.568131	-1.153410	-0.356039
C	-2.286367	-0.601206	0.239651
O	-2.261412	0.096488	1.256473
H	-4.328377	-0.360416	-0.352918
H	-3.435352	-1.535908	-1.378813
H	-3.927980	-1.969983	0.288602
N	-1.122106	-0.912458	-0.439725
C	0.169900	-0.637610	0.191039
C	0.478497	0.863378	0.282986
O	1.250326	1.287142	1.149442
C	1.252812	-1.348987	-0.632395
S	2.919951	-1.067585	0.101392
H	-1.165162	-1.636266	-1.150182
H	3.504864	-2.059445	-0.608000
H	0.174522	-1.003910	1.230938
H	1.046491	-2.430927	-0.626680
H	1.231373	-0.971892	-1.667659

N	-0.056343	1.640040	-0.703260
C	0.103494	3.089340	-0.642122
H	-0.841128	1.247569	-1.210396
H	1.166783	3.324425	-0.503405
H	-0.246715	3.524167	-1.587603
H	-0.461941	3.522798	0.198689

cysteine_43 -892.19324683884 a.u.

C	3.702306	-1.063987	-0.308642
C	2.583930	-0.099248	0.038732
O	2.793892	1.050417	0.440262
H	4.394433	-0.563646	-1.000394
H	4.255450	-1.299595	0.612777
H	3.339848	-1.997791	-0.762615
N	1.305071	-0.582581	-0.128481
C	0.158290	0.198513	0.340504
C	-1.040741	-0.735521	0.535075
O	-1.599364	-0.874049	1.626728
C	-0.148266	1.335749	-0.648492
S	-1.676638	2.200993	-0.088816
H	1.171850	-1.570904	-0.312999
H	-1.582105	3.218381	-0.972014
H	0.387924	0.632636	1.325983
H	0.701886	2.030639	-0.650518
H	-0.292785	0.928310	-1.662036
N	-1.413865	-1.438354	-0.585449
C	-2.649850	-2.220061	-0.554608
H	-1.105183	-1.075244	-1.480866

H	-2.609221	-2.919020	0.290685
H	-3.531909	-1.572152	-0.428298
H	-2.732667	-2.784575	-1.492483

cysteine_44 -892.19294326763 a.u.

C	2.259781	-2.393616	-0.826023
C	1.686580	-1.310332	0.066121
O	2.261939	-0.923770	1.090861
H	0.041402	-1.157854	-1.173813
N	0.496031	-0.767271	-0.356988
C	-0.194029	0.256556	0.417544
C	-1.682595	-0.108350	0.514079
O	-2.199093	-0.507298	1.561623
C	0.020639	1.681638	-0.118447
S	1.796855	2.139905	-0.263720
H	2.217851	1.367342	0.764884
H	-1.998935	0.528507	-1.417022
N	-2.382586	-0.032340	-0.666159
C	-3.816708	-0.316405	-0.673592
H	2.556542	-3.244026	-0.196640
H	1.555739	-2.733890	-1.599510
H	3.163587	-1.996223	-1.311875
H	0.202336	0.194337	1.441901
H	-0.386238	1.794739	-1.137512
H	-0.502493	2.390377	0.543589
H	-4.169455	-0.317450	-1.713168
H	-3.989119	-1.304535	-0.227078
H	-4.379786	0.429076	-0.090162

cysteine_45 -892.19297152350 a.u.

C	-1.680035	2.688722	0.011972
C	-0.742441	1.502958	-0.088041
O	-0.198027	1.160399	-1.140763
H	-1.394487	3.433233	-0.742035
H	-2.698601	2.334525	-0.214667
H	-1.678175	3.146136	1.012896
N	-0.513801	0.828724	1.102639
C	0.035725	-0.528134	1.109742
C	1.312042	-0.653338	0.251509
O	1.555067	-1.682077	-0.383851
C	-0.988464	-1.629044	0.791760
S	-1.957836	-1.295422	-0.742595
H	-1.122888	1.070416	1.878199
H	-2.944452	-2.164320	-0.427954
H	0.377554	-0.715098	2.144497
H	-0.441610	-2.576652	0.685773
H	-1.697921	-1.697179	1.630727
N	2.200277	0.379019	0.389475
C	3.330399	0.447891	-0.534221
H	1.796266	1.257580	0.695446
H	3.881020	-0.500517	-0.496242
H	2.990768	0.618125	-1.569245
H	3.992896	1.265391	-0.220084

cysteine_46 -892.19227693245 a.u.

C	2.332237	-2.747840	-0.021593
C	1.839087	-1.317023	0.082037

O	2.611505	-0.353099	0.147900
H	-0.096989	-1.969637	0.265300
N	0.472239	-1.150794	0.074678
C	-0.111405	0.162157	0.375459
C	-1.630720	0.031223	0.479385
O	-2.285978	0.633460	1.334282
C	0.229326	1.205620	-0.734138
S	1.216676	2.634609	-0.158540
H	2.297986	1.885159	0.155563
H	-1.647939	-1.050635	-1.263420
N	-2.212818	-0.779199	-0.465619
C	-3.669093	-0.812591	-0.586794
H	3.044757	-2.812046	-0.856066
H	2.872781	-2.997017	0.903669
H	1.520686	-3.473519	-0.176007
H	0.249890	0.534136	1.346490
H	0.752624	0.701748	-1.559672
H	-0.696483	1.649656	-1.134243
H	-3.945218	-1.597551	-1.302844
H	-4.104993	-1.042885	0.394090
H	-4.070685	0.156656	-0.923240

cysteine_47 -892.18977633428 a.u.

C	2.256111	-2.433423	-0.804541
C	1.690433	-1.328668	0.067554
O	2.274201	-0.904520	1.068383
H	2.586519	-3.256410	-0.155902
H	1.535442	-2.811925	-1.544469

H	3.137703	-2.038165	-1.331355
N	0.487439	-0.803470	-0.355372
C	-0.187234	0.248941	0.395944
C	-1.676047	-0.102542	0.515551
O	-2.184492	-0.484571	1.572976
C	0.029574	1.641684	-0.217416
S	1.818892	2.073842	-0.128694
H	0.007650	-1.233647	-1.137221
H	1.691490	3.233962	-0.811874
H	0.223717	0.226020	1.416363
H	-0.278995	1.651029	-1.275737
H	-0.562738	2.380873	0.345166
N	-2.388886	-0.037140	-0.658292
C	-3.825468	-0.307376	-0.645347
H	-2.007071	0.507787	-1.421823
H	-4.002274	-1.287846	-0.183851
H	-4.374954	0.450821	-0.065237
H	-4.190527	-0.318674	-1.680648

ALANINE PEPTIDES

Tetrapeptide (extended)

C	-1.7307169	-1.9998193	2.4398450
C	-1.7097793	-0.8547348	1.4381148
O	-2.7331081	-0.2460801	1.1122687
H	0.3399725	-1.1321307	1.1057528
N	-0.4815890	-0.5546139	0.9193524
C	-0.3049099	0.4209427	-0.1429185
C	0.9752746	0.0212053	-0.9041798

O	1.7890205	-0.7821991	-0.4277562
C	-0.2141688	1.8598615	0.4020435
H	-2.3492830	-1.7082871	3.2978703
H	-2.2065653	-2.8728977	1.9702484
H	-0.7316886	-2.2903146	2.7925998
H	-1.1764994	0.3562927	-0.8156046
H	-0.1251338	2.5918091	-0.4138146
H	-1.1259607	2.0849493	0.9697891
H	0.6558929	1.9666558	1.0649776
H	0.5042038	1.3318417	-2.4600477
N	1.1499928	0.6211133	-2.1075591
C	2.3618694	0.4597004	-2.8985189
C	2.4705975	1.7126959	-3.7914620
O	1.4961277	2.4520774	-3.9871938
C	2.3387540	-0.8315821	-3.7387636
H	3.2183819	0.4169620	-2.2060526
H	3.2732523	-0.9541708	-4.3048091
H	2.2232795	-1.6947458	-3.0713953
H	1.4994302	-0.8145745	-4.4482407
H	4.4664927	1.2745949	-4.2320421
N	3.6863544	1.9265814	-4.3491845
C	3.9380344	2.9938027	-5.3061713
C	5.1903624	2.5711036	-6.1053237
O	5.9213548	1.6565450	-5.7116738
C	4.1392074	4.3548152	-4.6123572
H	4.7616485	4.0125554	-7.4966754
N	5.4266357	3.2904298	-7.2357533
C	6.5940226	3.0779876	-8.0828869

H	3.0676617	3.0633957	-5.9800374
H	4.2826566	5.1607312	-5.3464066
H	3.2498130	4.5912478	-4.0150548
H	5.0178897	4.3245858	-3.9534336
H	7.1639666	2.2445437	-7.6570785
H	6.2929684	2.8199577	-9.1082906
H	7.2323661	3.9735146	-8.1091971

Tetrapeptide (alpha-helix)

C	-5.2517434	-2.0228398	0.7780798
C	-4.8625137	-0.5517560	0.7325422
O	-5.5925336	0.3304254	1.1814779
H	-3.2468464	-1.0469982	-0.4047796
N	-3.6131928	-0.3039855	0.1936698
C	-3.1178851	1.0615508	-0.0685251
C	-1.7262370	0.9878734	-0.7290987
O	-1.4639211	1.5783618	-1.7734027
C	-3.0555640	1.9271467	1.2022938
H	-6.2949817	-2.1176460	0.4506971
H	-4.6105689	-2.6679419	0.1636226
H	-5.2045696	-2.3636619	1.8226802
H	-3.7643212	1.5600933	-0.8077555
H	-2.6139898	2.9036408	0.9575397
H	-4.0642812	2.0735442	1.6015975
H	-2.4399311	1.4514300	1.9803264
H	-1.0743581	-0.1370730	0.8696851
N	-0.8053020	0.2230847	-0.0443091
C	0.5751754	0.0423786	-0.4887049

C	0.8320892	-1.3386175	-1.1474921
O	1.9299767	-1.6255600	-1.6274862
C	1.5748296	0.2853630	0.6460407
H	0.7306093	0.7793531	-1.2916747
H	2.5927162	0.1043997	0.2795442
H	1.5024151	1.3187428	1.0101867
H	1.3903442	-0.3988468	1.4890283
H	-1.1402482	-1.8183899	-0.8301867
N	-0.2371053	-2.1786707	-1.1385930
C	-0.3020475	-3.4272486	-1.8714773
C	-1.7869380	-3.6163954	-2.2563637
O	-2.6893041	-2.9937801	-1.6767274
C	0.2240130	-4.6168323	-1.0456462
H	-1.2182257	-4.9588337	-3.6846560
N	-2.0199070	-4.5168943	-3.2440336
C	-3.3540002	-4.8607962	-3.7221645
H	0.3135974	-3.3248260	-2.7813050
H	0.2042205	-5.5504236	-1.6266284
H	1.2623667	-4.4172411	-0.7507604
H	-0.3826724	-4.7565815	-0.1400023
H	-4.0694367	-4.2025039	-3.2174844
H	-3.4263386	-4.7057978	-4.8077443
H	-3.6022480	-5.9065505	-3.4893921

Hexapeptide (extended)

C	-0.3608532	-1.6602936	0.6496324
C	-0.1276226	-0.5560681	-0.3627130
O	-0.6332025	-0.5884094	-1.4949245

H	1.1136119	0.4378538	0.9547199
N	0.6655882	0.4785102	0.0434593
C	0.9183939	1.6653896	-0.7855861
C	2.0432127	1.3826641	-1.8183614
O	3.1668942	1.9025595	-1.7305239
C	1.2518372	2.8647625	0.0934572
H	-1.4405553	-1.7411778	0.8344402
H	-0.0308438	-2.6144382	0.2175455
H	0.1539205	-1.5005216	1.6061688
H	-0.0114654	1.8462696	-1.3484788
H	1.3957978	3.7592300	-0.5247347
H	0.4352338	3.0558902	0.8028889
H	2.1887511	2.7007938	0.6438141
H	0.7477894	0.1077843	-2.7435510
N	1.6836146	0.5323857	-2.8110937
C	2.6441820	-0.0159074	-3.7813257
C	2.9052129	0.9682584	-4.9560747
O	2.6590893	0.6709650	-6.1352698
C	2.1639305	-1.3705320	-4.2885396
H	3.6043398	-0.1265423	-3.2480599
H	2.8886842	-1.7857816	-4.9990594
H	2.0459071	-2.0703850	-3.4503032
H	1.2059472	-1.2761816	-4.8172679
H	3.6489079	2.2922453	-3.5813462
N	3.4488557	2.1518179	-4.5813551
C	3.7113546	3.2378847	-5.5347050
C	5.0764346	3.0156435	-6.2388999
O	6.0670616	3.7212666	-6.0045546

C	3.6596470	4.5903524	-4.8345397
H	2.9260912	3.1728707	-6.3057079
H	3.8304095	5.3960568	-5.5592767
H	2.6775127	4.7377128	-4.3651184
H	4.4454649	4.6677181	-4.0713944
H	4.2282191	1.4191696	-7.1967284
N	5.0832175	1.9840880	-7.1221608
C	6.3178694	1.5017346	-7.7554772
C	6.6420725	2.3252622	-9.0346569
O	6.5579031	1.8469197	-10.1691426
C	6.2064926	0.0150805	-8.0722042
H	7.1311247	1.6834701	-7.0336599
H	7.1394001	-0.3453565	-8.5223731
H	6.0109312	-0.5569795	-7.1547789
H	5.4025361	-0.1718295	-8.7963133
H	7.0371163	3.9398624	-7.8015823
N	7.0364581	3.6029448	-8.7736644
C	7.3528233	4.5441033	-9.8391315
C	8.5474872	5.4037628	-9.3875122
O	8.6185333	5.8621288	-8.2470668
C	6.1558599	5.4501898	-10.1861235
H	9.3690370	5.1932384	-11.2592796
N	9.4824237	5.6454142	-10.3574375
C	10.6466073	6.4905728	-10.1345023
H	7.6123680	3.9350113	-10.7187164
H	6.4075892	6.1408801	-11.0044347
H	5.3047415	4.8317078	-10.5016124
H	5.8641729	6.0424284	-9.3081541

H 11.5798958 5.9257748 -10.2774155

H 10.6456082 7.3588508 -10.8106350

H 10.5980034 6.8434755 -9.0977057

Hexapeptide (alpha-helix)

C -1.8566174 0.1013342 -1.9406248

C -0.6159223 0.8384601 -1.4770731

O -0.0408217 1.6717919 -2.1748291

H -0.7847461 -0.0470457 0.3731835

N -0.1532925 0.4972252 -0.2114070

C 0.8350031 1.3237120 0.4864251

C 2.1262977 0.5703329 0.8770376

O 2.9514878 1.0810749 1.6339012

C 0.2317379 2.0336121 1.7032682

H -1.6721523 -0.3443433 -2.9291980

H -2.1894172 -0.6807089 -1.2432468

H -2.6683791 0.8330278 -2.0611781

H 1.1506859 2.0733709 -0.2589486

H 1.0093333 2.6136293 2.2138784

H -0.5759802 2.7080001 1.3894721

H -0.1741294 1.3075339 2.4253439

H 1.6311483 -0.9320797 -0.4098080

N 2.3012168 -0.6625102 0.3077921

C 3.5930601 -1.3591072 0.4159509

C 3.7708568 -2.3936471 -0.7078489

O 4.7768092 -2.4192256 -1.4070539

C 3.7831743 -2.0094174 1.7979309

H 4.3929224 -0.6202898 0.2663661

H	4.7582001	-2.5140905	1.8461581
H	3.7524435	-1.2309259	2.5699467
H	2.9942150	-2.7459844	2.0106728
H	2.0708731	-3.3635589	-0.0808724
N	2.7285183	-3.2972024	-0.8580411
C	2.8919019	-4.5149742	-1.6671273
C	1.8199460	-4.6737204	-2.7714605
O	1.6536886	-5.7503863	-3.3444868
C	2.9637108	-5.7710448	-0.7946527
H	3.8503666	-4.3767379	-2.1940940
H	3.0454878	-6.6573026	-1.4346774
H	3.8351909	-5.7240078	-0.1282801
H	2.0545032	-5.8837677	-0.1832286
H	1.3207904	-2.7068747	-2.5343001
N	1.1260131	-3.5406179	-3.0837727
C	0.0703038	-3.5090196	-4.0983918
C	0.0687065	-2.1310410	-4.8073730
O	-0.9571256	-1.4494301	-4.9121580
C	-1.3040347	-3.8524465	-3.5232059
H	0.3478475	-4.2785249	-4.8380595
H	-2.0667795	-3.8256912	-4.3116260
H	-1.2747678	-4.8592363	-3.0865012
H	-1.5992763	-3.1298349	-2.7501844
H	2.0843882	-2.3666941	-5.2885405
N	1.2744435	-1.7407302	-5.2958974
C	1.4595059	-0.5220795	-6.0717129
C	2.6441301	-0.7914453	-7.0248753
O	3.4413066	-1.7099068	-6.8136647

C	1.7365610	0.7024881	-5.1780155
H	2.0391566	0.7889611	-8.1806001
N	2.7494898	0.0710105	-8.0738173
C	3.8488613	0.0275524	-9.0286965
H	0.5356948	-0.3472868	-6.6474843
H	1.8358314	1.6173242	-5.7804419
H	0.9126422	0.8546859	-4.4686694
H	2.6693302	0.5604624	-4.6144159
H	3.4771353	-0.1394299	-10.0501367
H	4.4310723	0.9606611	-9.0052481
H	4.4986555	-0.8072828	-8.7438783

Octapeptide (extended)

C	-1.6015296	-1.8805714	2.3774044
C	-1.5896908	-0.7306424	1.3785058
O	-2.6094311	-0.1101131	1.0646801
H	0.4556586	-1.0288983	1.0302893
N	-0.3629157	-0.4451823	0.8465530
C	-0.1794910	0.5369091	-0.2084299
C	1.1185258	0.1575073	-0.9505692
O	1.9276758	-0.6496631	-0.4719438
C	-0.1122078	1.9732887	0.3469699
H	-2.4978417	-1.7947855	3.0002755
H	-1.6439709	-2.8405352	1.8406806
H	-0.7068681	-1.8864723	3.0156836
H	-1.0368833	0.4670951	-0.8989338
H	-0.0087441	2.7105548	-0.4620455
H	-1.0380597	2.1876806	0.8958275

H	0.7423157	2.0803974	1.0299777
H	0.6506303	1.4733871	-2.5038881
N	1.3119669	0.7847594	-2.1358599
C	2.5276427	0.6390056	-2.9237133
C	2.5803622	1.8540920	-3.8747794
O	1.5727058	2.5395584	-4.0979809
C	2.5523364	-0.6834855	-3.7136442
H	3.3904430	0.6609613	-2.2378115
H	3.4887864	-0.7862934	-4.2799114
H	2.4747221	-1.5255520	-3.0143948
H	1.7099749	-0.7244231	-4.4187203
H	4.5947864	1.4836750	-4.2814716
N	3.7822829	2.0825615	-4.4532108
C	4.0017993	3.0977434	-5.4750496
C	5.3102714	2.7037495	-6.1961988
O	6.0905495	1.8786016	-5.6991653
C	4.0973451	4.5142943	-4.8773453
H	3.1590616	3.0665025	-6.1853032
H	4.2357462	5.2659153	-5.6670283
H	3.1694611	4.7438782	-4.3386000
H	4.9439464	4.5806466	-4.1796563
H	4.9024601	4.0383758	-7.7515172
N	5.5418904	3.3356261	-7.3688287
C	6.7739321	3.1809251	-8.1318552
C	6.8272164	4.3793928	-9.1060793
O	5.8233301	5.0736310	-9.3219788
C	6.8269205	1.8408566	-8.8890685
H	7.6258549	3.2303409	-7.4337131

H	7.7727365	1.7372440	-9.4389300
H	6.7508317	1.0140720	-8.1719565
H	5.9968311	1.7716675	-9.6060509
H	8.8297231	3.9797614	-9.5463669
N	8.0208922	4.5872271	-9.7062894
C	8.2344116	5.5960364	-10.7358215
C	9.5282188	5.1865242	-11.4736300
O	10.3026473	4.3482072	-10.9915355
C	8.3504851	7.0139539	-10.1455658
H	7.3820528	5.5678200	-11.4344996
H	8.4850147	7.7613994	-10.9399236
H	7.4320060	7.2549652	-9.5958989
H	9.2069816	7.0755026	-9.4597313
H	9.1279535	6.5496705	-13.0041748
N	9.7525629	5.8208360	-12.6466286
C	10.9785868	5.6640012	-13.4178378
C	11.0588900	6.8969748	-14.3444767
O	10.0769264	7.6332401	-14.5210763
C	11.0003841	4.3498742	-14.2203810
H	11.8321066	5.6692899	-12.7200418
H	11.9440695	4.2406624	-14.7729617
H	10.9046496	3.5016692	-13.5311966
H	10.1694126	4.3231249	-14.9393564
H	13.0357480	6.4413992	-14.8414239
N	12.2537178	7.0944159	-14.9452741
C	12.4856634	8.1405319	-15.9308424
C	13.7511292	7.7163324	-16.7111764
O	14.4710101	6.7967250	-16.3084263

C	12.6550890	9.5246106	-15.2767141
H	13.3539844	9.1700411	-18.0953314
N	14.0068515	8.4372266	-17.8345002
C	15.1824831	8.2211709	-18.6692389
H	11.6200916	8.1724511	-16.6143716
H	12.7903922	10.3102774	-16.0338891
H	11.7563733	9.7630731	-14.6944967
H	13.5287121	9.5317528	-14.6105597
H	15.7486604	7.3902307	-18.2337197
H	14.8913797	7.9584096	-19.6962512
H	15.8196219	9.1173292	-18.6931048

Octapeptide (alpha-helix)

C	-2.8430480	-2.3803383	3.9023715
C	-3.0538594	-1.8363243	2.5035294
O	-2.7836173	-2.4919837	1.4915857
H	-3.8569117	-0.1003200	3.2723942
N	-3.5583057	-0.5598854	2.4154666
C	-4.0665677	-0.0190382	1.1489268
C	-2.9781513	0.1647379	0.0729983
O	-3.2931440	0.2072438	-1.1207359
C	-4.7978553	1.3039449	1.3958417
H	-3.5787775	-3.1779732	4.0794207
H	-1.8470415	-2.8361068	3.9648552
H	-2.9494038	-1.6242085	4.6915507
H	-4.7616677	-0.7488252	0.7041859
H	-5.1666415	1.7006690	0.4423677
H	-5.6604154	1.1541580	2.0611183

H	-4.1279579	2.0525977	1.8442321
H	-1.5187619	0.1861333	1.5068839
N	-1.6976340	0.2892916	0.5104867
C	-0.5705616	0.4094077	-0.4107890
C	-0.4052511	-0.8021026	-1.3554030
O	0.2573997	-0.6656526	-2.3925774
C	0.7260205	0.6646916	0.3631593
H	-0.7663353	1.2529362	-1.0892194
H	1.5610473	0.7455489	-0.3427813
H	0.6610323	1.6026213	0.9326422
H	0.9432099	-0.1607753	1.0581392
H	-1.5759524	-2.0382463	-0.1599737
N	-0.9962036	-1.9723041	-1.0035100
C	-0.9045453	-3.1394802	-1.8810718
C	-1.5550713	-2.9226893	-3.2641194
O	-1.2128669	-3.6405593	-4.2140314
C	-1.4960212	-4.3777593	-1.2012488
H	0.1567165	-3.3149260	-2.1130279
H	-1.4248723	-5.2318548	-1.8855582
H	-0.9435179	-4.6159463	-0.2820716
H	-2.5517991	-4.2218969	-0.9387775
H	-2.7105766	-1.3358022	-2.5898847
N	-2.4949418	-1.9487594	-3.3811631
C	-3.1223837	-1.6775833	-4.6749696
C	-2.1300869	-1.1789715	-5.7530320
O	-2.4309332	-1.2794123	-6.9479043
C	-4.2808358	-0.6891345	-4.5172831
H	-3.4986878	-2.6289977	-5.0790550

H	-4.7222552	-0.4925332	-5.5021290
H	-5.0576208	-1.1043722	-3.8600946
H	-3.9355262	0.2621456	-4.0886080
H	-0.7259529	-0.6400848	-4.3227596
N	-0.9638933	-0.6267951	-5.3186576
C	0.0485349	-0.1458367	-6.2551487
C	0.9465330	-1.2563850	-6.8576035
O	1.8287855	-0.9534608	-7.6635438
C	0.9010784	0.9546998	-5.6196850
H	-0.4910589	0.2567826	-7.1265873
H	1.6847703	1.2537409	-6.3257611
H	0.2805202	1.8291576	-5.3803149
H	1.3771904	0.6000622	-4.6942200
H	-0.0166890	-2.7273855	-5.7475537
N	0.6675057	-2.5417732	-6.4865284
C	1.3989015	-3.6755369	-7.0373421
C	0.5984915	-4.4755708	-8.0878659
O	1.1001815	-5.4945528	-8.5978532
C	1.9147072	-4.6080238	-5.9346112
H	2.2485835	-3.2437092	-7.5896835
H	2.4145844	-5.4718395	-6.3891978
H	2.6285832	-4.0715466	-5.2952709
H	1.0850109	-4.9676360	-5.3093718
H	-0.9622809	-3.1393469	-8.0083769
N	-0.6273129	-4.0102510	-8.4252799
C	-1.5129296	-4.7137892	-9.3649903
C	-1.1573292	-4.3740252	-10.8448140
O	-1.9268554	-3.7587794	-11.5859216

C	-2.9707169	-4.3989073	-9.0537608
H	0.6317408	-5.2948489	-10.4899651
N	0.0644358	-4.8470018	-11.2203689
C	0.6387883	-4.5803014	-12.5280619
H	-1.3120784	-5.7884185	-9.2228596
H	-3.6241623	-4.9180967	-9.7657089
H	-3.2191039	-4.7242166	-8.0341439
H	-3.1703845	-3.3231642	-9.1448066
H	-0.1334391	-4.1065456	-13.1456395
H	1.5036959	-3.9014689	-12.4570813
H	0.9638790	-5.5150307	-13.0090573