Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Hydrogen-bond stabilization in oxyanion holes: grand jeté to three dimensions

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Explanation of the use of theozymes in terms of Warshel thermodynamic analysis.

First of all, we are going to reproduce Warshel deduction that the most relevant term in catalysis is the preorganization energy in water. This is deduced by assuming that the activation free energy for the reaction in water or in the enzyme is the sum of the activation free energy in the gas phase plus a solvation term, either by water or by the protein. The protein is formally considered to "solvate" the charges developed in the reaction transition state:

$$\Delta G^{\ddagger} \cong \Delta G^{\ddagger}_{gas} + \Delta G^{\ddagger}_{sol}$$

The solvation term is decomposed in an electrostatic interaction term (the difference in the interaction energy between the TS and the reactive with the protein or water), and the reorganization term, that accounts for the fact that the dipoles and charges are not pre-organized to stabilize the TS:

$$\Delta G^{w}_{sol} \cong \Delta G^{w}_{Q\mu} + \Delta G^{w}_{\mu\mu} \qquad \Delta G^{p}_{sol} \cong \Delta G^{p}_{Q\mu} + \Delta G^{p}_{\mu\mu}$$

(w and p superscripts refer to water and protein, respectively; $Q\mu$ subscript refers to the electrostatic interaction and $\mu\mu$ subscript to the reorganization term).

The reduction of the energy barrier of the reaction in the enzyme, with respect to the reaction in water is:

$$(\Delta\Delta G^{\ddagger})^{p} = (\Delta G^{\ddagger})^{P} - (\Delta G^{\ddagger})^{W} = (\Delta G^{\ddagger}_{gas} + \Delta G^{\ddagger}_{sol})^{p} - (\Delta G^{\ddagger}_{gas} + \Delta G^{\ddagger}_{sol})^{W}$$

Which is a negative term since the energy barrier in the enzyme is smaller than in water. Assuming that the reaction shares the same mechanism in water and in the enzyme:

$$(\Delta G^{\ddagger}_{gas})^{P} = (\Delta G^{\ddagger}_{gas})^{W}$$

$$(\Delta\Delta G^{\ddagger})^{p} = (\Delta G_{sol}{}^{\ddagger})^{p} - (\Delta G_{sol}{}^{\ddagger})^{w} = \Delta G^{p}_{Q\mu} + \Delta G^{p}_{\mu\mu} - \Delta G^{w}_{Q\mu} - \Delta G^{w}_{\mu\mu}$$

It is reasonable to consider that the preorganization energy in water is much larger than the preorganization energy in the enzyme and that the electrostatic interaction terms are similar in both media:

$$\Delta G^{w}_{\mu\mu} >> \Delta G^{P}_{\mu\mu} \qquad \Delta G^{w}_{Q\mu} \approx \Delta G^{p}_{Q\mu}$$

Therefore: $$(\Delta\Delta G^{\ddagger})^{p} = (\Delta G^{\ddagger})^{p} - (\Delta G^{\ddagger})^{w} \approx -\Delta G^{w}_{\mu\mu}$$

Based on this result, a method which does not calculate the reorganization energy of water cannot quantify the catalytic activity, since this factor is the most relevant in the reduction of the energy barrier.

However, ranking two possible catalysts P and P' is possible without the need of calculating the reorganization energy in water. For each catalyst, we can formulate, in analogy to previous deduction:

$$(\Delta\Delta G^{\ddagger})^{p} = \Delta G^{p}_{Q\mu} + \Delta G^{p}_{\mu\mu} - \Delta G^{w}_{Q\mu} - \Delta G^{w}_{\mu\mu}$$
$$(\Delta\Delta G^{\ddagger})^{p'} = \Delta G^{p'}_{Q\mu} + \Delta G^{p'}_{\mu\mu} - \Delta G^{w}_{Q\mu} - \Delta G^{w}_{\mu\mu}$$

The terms that correspond to water are exactly the same, so:

$$(\Delta\Delta G^{\ddagger})^{p} - (\Delta\Delta G^{\ddagger})^{p'} = \Delta G^{p}_{Q\mu} + \Delta G^{p}_{\mu\mu} - \Delta G^{p'}_{Q\mu} - \Delta G^{p'}_{\mu\mu}$$

The reorganization energies in both catalysts are small and probably similar:

$$\Delta G^{p}_{\mu\mu} \approx \Delta G^{p'}_{\mu\mu}$$
$$(\Delta\Delta G^{\ddagger})^{p} - (\Delta\Delta G^{\ddagger})^{p'} = \Delta G^{p}_{Q\mu} - \Delta G^{p'}_{Q\mu}$$

These terms include entropic and zero-point contributions. If they are similar in both structures, it is possible to write:

$$\Delta S^{p}_{Q\mu} \approx \Delta S^{p'}_{Q\mu}$$
$$(\Delta\Delta G^{\ddagger})^{p} - (\Delta\Delta G^{\ddagger})^{p'} = \Delta E^{p}_{Q\mu} - \Delta E^{p'}_{Q\mu}$$

The energy interaction between the protein and the developing charges in the transition state can be calculated as the difference of the energy interactions with the transition state minus the energy interactions with the reactives:

$$\Delta E^{p}_{Q\mu} = E^{p}_{Q\mu}(TS) - E^{p}_{Q\mu}(RS)$$

If for the two alternative catalysts the interactions with the reactant state is similar, or this interaction is small compared with the interactions with the transition state:

$$\Delta E^{p}_{Q\mu}(RS) \approx \Delta E^{p'}_{Q\mu}(RS)$$
$$or: \Delta E^{p}_{Q\mu}(RS) << \Delta E^{p}_{Q\mu}(TS); and: \Delta E^{p'}_{Q\mu}(RS) << \Delta E^{p'}_{Q\mu}(TS)$$
$$(\Delta\Delta G^{\ddagger})^{p} - (\Delta\Delta G^{\ddagger})^{p'} \approx \Delta E^{p}_{Q\mu} - \Delta E^{p'}_{Q\mu}$$

Since during theozyme calculations the structures are optimized, the arrangement obtained (P) corresponds to a minimum in the potential energy surface. Any other point in this potential energy surface (P') will have a higher energy, which corresponds to a smaller interaction energy between the transition state and the rest of the groups included in the theozyme; since this interaction energy is exothermic, i.e. negative: $\Delta E^{p}_{Q\mu} < \Delta E^{p'}_{Q\mu} \Rightarrow (\Delta\Delta G^{\ddagger})^{p} < (\Delta\Delta G^{\ddagger})^{p'} \Rightarrow (\Delta G^{\ddagger})^{P} < (\Delta G^{\ddagger})^{P'}$

Therefore, the alternative arrangement (P') will be less effective in reducing the energy barrier, and will lead to a higher energy barrier. Accordingly, it is not surprising the similarity in the position of the catalytic groups in the enzyme active center and in theozymes. In Figure 1 (above) we represent these energy terms for water and for an enzyme. Note in this figure that water and the enzyme are nearly as effective stabilizing the charges in the reactants and TS, but the smaller reorganization term in the enzyme reduces the barrier height.

We have found that, for oxyanion holes, in our calculations it is not possible to consider that the interactions with the reactant state are similar for any H-bond dihedral angle. This is also shown in Figure 1 (below), where, for simplicity, the

structure corresponding to a flat oxyanion hole is denote as P-2D (which does not mean it is a 2D structure) and the structure corresponding to the *grand-jeté* as P-3D. The reorganization energies are similar for both arrangements. The p-2D arrangement is more effective at stabilizing the transition state, but much more effective at stabilizing the reactant state. As a consequence, the energetic barrier is increased: $\Delta G^{\ddagger}_{gas} > \Delta G^{\ddagger}_{p-2D} > \Delta G^{\ddagger}_{p-3D}$.

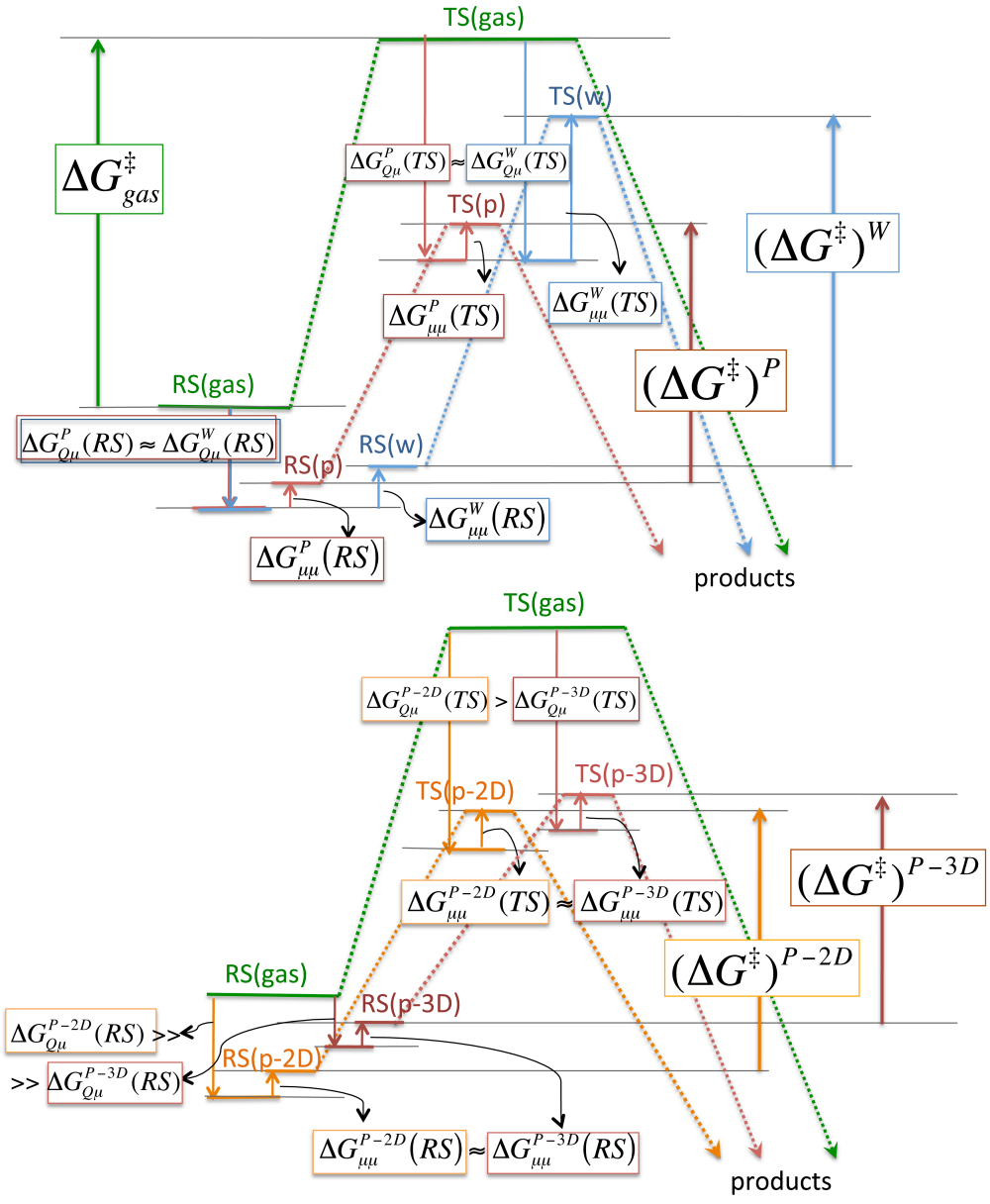

Figure 1

Details of MD calculations

Molecular dynamics simulations on subtilisin used the GROMACS 4.0[1] with OPLSAA force field[2]. Initial coordinates were obtained from the PDB (id: 1tmg). The potential energy of the system was minimized during 500 steps, with 1 nm electrostatic interactions cut-off. The resulting structure was placed in a 8.99 nm × 8.99 nm × 6.35 nm box containing 15 332 SPC[3] water molecules and minimized for 5000 steps using periodic boundary conditions. The solvent was then relaxed in a position-restrained molecular dynamics simulation (2500 steps of 0.001 ps using a leap-frog algorithm) using the Particle-Mesh Ewald summation algorithm[4] with a 1 nm real-space cut-off and a 1.4 nm Van der Waals cut-off. After this was completed, the system was coupled first with a heat bath of 300 K temperature using a Berendsen thermostat[5] and then with a Berendsen barostat[6] of 1 atm (1250 steps of 0.002 ps each). Constraints to all bonds were introduced in these steps using Lincs algorithm[7].

Once the structure was prepared, NPT simulations were run using 2.5 fs time steps for 10 ns. This structure was then simulated for a further 2 ns with the addition of constraints on the oxyanion hole H-bond donors dihedral angle.

References:

(1) Hess, B.; Kutzner, C.; van der Spoel, D.;Lindahl, E. *J. Chem. Theory Comput.*, 4, 435, **2008**.
(2) Kaminski, G. A.; Friesner, R. A.; Tirado-Rives, J.; Jorgensen, W. L. *J. Phys. Chem. B 105*, 6474, **2001**.
(3) Berendsen, H.J.C.; Postma, J.P.M.; van Gunsteren, W.F. ; Hermans, J.; *Intermolecular Forces*, edited by B. Pullman (Reidel, Dordrecht, **1981**), p. 331.
(4) Darden, T.; York, D.; Pedersen, L.;*J. Chem. Phys.*, *98*, 10089, **1993**.
(5) G. Schaftenaar, J. H. Noordik, *Journal of Computer-Aided Molecular Design, 14*, 123, **2000**.
(6) Berendsen, H.J.C.; Postma, J.P.M.; van Gunsteren, W.F.; DiNola, A.; Haak. J.R.; *J. Chem. Phys.*, *81*, 3684, **1984**.
(7) Hess, B; Bekker, H; Berendsen H.J.C.; Fraaije J.G.E.M. *Journal of Computational Chemistry* **18**: 1463, **1997**.

Cartesian coordinates of structures in theozyme calculations

1) Unconstrined water molecules:

d C(4)-O (Asp145): 3.4Å
d C(4)-Cl: 1.76 Å
reaction coordinate: -1.64 Å
Extrapolated ONIOM energy:
-1624.22068944854

C	-1.73600	3.19500	3.51100
C	-0.71700	3.53500	4.41800
C	-1.78500	3.80900	2.24600
C	0.24900	4.49400	4.06400
C	-0.81700	4.76500	1.89100
C	0.19700	5.11100	2.80100
C	-0.79000	7.88500	-2.26200
C	-1.24200	6.46100	-2.00000
C	-2.48700	6.21600	-1.39000
C	-0.41700	5.37800	-2.36100
C	-2.90700	4.89600	-1.14600
C	-0.83800	4.05800	-2.11900
C	-2.08200	3.81600	-1.51000
C	4.15500	5.60400	-1.57000
C	9.10800	1.90800	-0.04000
C	7.61400	1.72600	0.13600
N	6.84600	2.25300	1.16400
C	6.78300	1.01300	-0.68800
C	5.56900	1.86100	0.96500
N	5.51100	1.11200	-0.15100
C	-3.64900	-4.31100	-2.28300
C	-2.48100	-3.55600	-1.72500
C	-2.07200	-2.32200	-2.10500
C	-1.54900	-3.98400	-0.68600
N	-0.93500	-1.97300	-1.39800
C	-0.59300	-2.94500	-0.48800
C	-1.39800	-5.15200	0.09400
C	0.44200	-3.04200	0.44600
C	-0.34600	-5.27100	1.02200
C	0.56000	-4.21200	1.21300
C	-8.45300	-0.83300	0.35200
C	-7.53000	-0.15800	1.38100
C	-7.73300	-1.88700	-0.49800
C	-6.46300	0.74500	0.74900
C	-4.35000	0.48200	-3.06000
C	-5.66900	1.27100	-3.05000
C	-3.30200	1.06600	-4.01600
C	-5.54200	2.66600	-2.42700
C	0.02200	-3.83400	-4.16500
C	1.35500	-3.12300	-4.09300
O	1.87500	-2.73500	-5.13200
N	1.91700	-2.95500	-2.89300
C	3.25600	-2.38600	-2.70300
C	4.00000	-3.04300	-1.52100
O	4.18900	-4.25500	-1.50600
C	3.18400	-0.84100	-2.65700
C	2.38700	-0.22700	-1.47700
O	1.15900	-0.07600	-1.62400
O	3.07200	0.09200	-0.44300
N	4.46200	-2.28000	-0.52900
C	5.34700	-2.74900	0.54000
C	4.59100	-3.35200	1.73100
O	3.81600	-4.43900	1.29800
C	3.70200	-2.33100	2.43800
C	-4.47700	-2.62300	2.52900
S	-3.48900	-1.48900	1.49700
C	-2.09100	-1.20200	2.57900
O	-2.01900	-1.78100	3.66300
C	-1.06000	-0.23800	2.11400
C	-1.14000	0.42200	0.87700
C	-0.15200	1.31300	0.47600
C	0.90700	1.57100	1.33900
C	1.01600	0.92800	2.57000
C	0.04000	0.01300	2.95200
H	-0.67900	3.05700	5.38800
H	-2.56300	3.54000	1.54700
H	1.03000	4.75800	4.76300
H	-0.84900	5.23100	0.91500
H	0.94000	5.84500	2.52500
H	-0.12700	7.91400	-3.12700
H	-1.65500	8.51900	-2.46100
H	-3.12400	7.04200	-1.10900
H	0.54000	5.55700	-2.82800
H	-3.86400	4.71500	-0.67800
H	-0.20200	3.23100	-2.40500
H	-2.40500	2.80200	-1.32100
H	5.03600	5.96000	-1.03700
H	4.28200	4.55300	-1.82900
H	4.02100	6.18700	-2.48100
H	9.43800	1.42100	-0.95900
H	9.34600	2.97100	-0.10000
H	7.05700	0.47200	-1.58700
H	7.18300	2.82700	1.92700
H	4.62600	0.68800	-0.49000
H	4.70000	2.08800	1.57900
H	-3.36800	-5.35100	-2.44600
H	-3.96100	-3.87100	-3.23100
H	-2.54400	-1.71800	-2.86700
H	-0.37100	-1.12400	-1.52100
H	-2.09400	-5.96800	-0.03800
H	-0.22700	-6.18000	1.59900
H	1.13400	-2.22000	0.56100
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H	-9.26600	-1.32300	0.88900
H	-8.45400	-2.36900	-1.16000
H	-7.28600	-2.64400	0.14800
H	-6.95700	-1.42300	-1.10600
H	-7.04300	-0.92200	1.98700
H	-8.14600	0.45400	2.04100
H	-6.94200	1.51300	0.14100
H	-5.78500	0.15900	0.13000
H	-5.88600	1.22700	1.53900
H	-3.93900	0.44900	-2.05000
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H	-8.88500	-0.07400	-0.30200
H	-4.47800	-4.26800	-1.57600
H	9.63600	1.46500	0.80400
H	-0.26000	8.26300	-1.38800
H	3.27500	5.71600	-0.93700
H	-2.48000	2.46300	3.78600
H	6.02300	-3.51000	0.14500
H	-0.17600	-4.35700	-3.23200
H	0.06100	-4.55400	-4.98000
H	-1.98300	-3.77900	3.64000
H	-0.95700	-1.59400	5.32200
O	-0.19300	-1.53400	5.91900
O	-2.10000	-4.69500	3.34600
Cl	2.09200	2.80200	0.90900
H	0.17500	-2.42600	5.89700
H	-1.62700	-4.72000	2.49900

d C(4)-O (Asp145): 2.4Å
d C(4)-Cl: 1.76 Å
reaction coordinate: -0.64 Å
Extrapolated ONIOM energy: 1624.20375360866

C	-2.04100	2.43800	3.58500
C	-0.80400	2.47900	4.25200
C	-2.29100	3.31500	2.51400
C	0.18300	3.39600	3.84900
C	-1.30500	4.23300	2.11200
C	-0.06700	4.27400	2.77800
C	-2.05300	7.48200	-2.04100
C	-2.98700	6.45500	-1.43200
C	-4.23600	6.85700	-0.92100
C	-2.61100	5.09900	-1.36400
C	-5.10600	5.91000	-0.35100
C	-3.48100	4.15300	-0.79200
C	-4.72900	4.55800	-0.28700
C	3.21600	6.13000	-1.30700
C	8.74100	3.37300	0.24200
C	7.26700	3.05600	0.24100
N	6.29200	3.70300	0.98500
C	6.66900	2.05600	-0.47500
C	5.11500	3.09700	0.72300
N	5.32600	2.10300	-0.15800
C	-2.63500	-5.02800	-2.29900
C	-1.66800	-4.01600	-1.75700
C	-1.47300	-2.76000	-2.22700
C	-0.74800	-4.16800	-0.63300
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C	0.01600	-2.97100	-0.51400
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C	1.01100	-2.80500	0.45600
C	0.51400	-5.03700	1.28200
C	1.25500	-3.84600	1.36600
C	-8.02600	-2.53400	0.31400
C	-7.24000	-1.82700	1.43100
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C	-5.63000	1.46900	-2.05300
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C	2.08100	-2.90500	-4.01000
O	2.54000	-2.41300	-5.03500
N	2.57700	-2.65000	-2.79800
C	3.79500	-1.86500	-2.57600
C	4.60100	-2.39500	-1.37000
O	4.91300	-3.58000	-1.31200
C	3.46200	-0.35600	-2.54700
C	2.57600	0.13100	-1.37700
O	1.33700	0.10500	-1.51700
O	3.20000	0.56000	-0.34400
N	4.97700	-1.55300	-0.40600
C	5.88800	-1.90200	0.69000
C	5.16700	-2.52900	1.89200
O	4.54700	-3.72700	1.50200
C	4.12800	-1.59600	2.51200
C	-3.56300	-3.37900	2.89600
S	-3.04100	-2.29400	1.52700
C	-1.67100	-1.42600	2.28600
O	-1.24700	-1.76400	3.39400
C	-1.09900	-0.32600	1.48600
C	-1.72000	0.16800	0.32500
C	-1.11100	1.14500	-0.44700
C	0.15100	1.61100	-0.07300
C	0.73900	1.21200	1.12800
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H	-0.60900	1.80200	5.07200
H	-3.24200	3.28500	2.00400
H	1.13200	3.42000	4.36600
H	-1.49900	4.90800	1.29000
H	0.68700	4.98000	2.46600
H	-1.36500	6.99900	-2.73500

H	-2.63000	8.23300	-2.58200
H	-4.53100	7.89600	-0.96700
H	-1.65100	4.78000	-1.74600
H	-6.06500	6.22300	0.03800
H	-3.18900	3.11600	-0.73400
H	-5.39800	3.83100	0.15200
H	4.03700	6.73900	-0.93000
H	3.58700	5.14500	-1.59200
H	2.77800	6.61500	-2.18000
H	9.19800	3.01900	-0.68300
H	8.89200	4.45000	0.31900
H	7.14700	1.35200	-1.14800
H	6.44200	4.47500	1.62300
H	4.57600	1.45600	-0.46200
H	4.13900	3.32400	1.14800
H	-2.16400	-6.01100	-2.31600
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H	-2.00600	-2.32100	-3.05900
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H	2.01000	-3.73900	2.13300
H	-8.75100	-3.20500	0.77600
H	-7.74900	-3.88400	-1.34400
H	-6.57100	-4.09700	-0.03300
H	-6.43100	-2.71600	-1.14600
H	-6.62200	-2.55500	1.95700
H	-7.95500	-1.41300	2.14300
H	-6.96400	0.05900	0.40800
H	-5.58800	-1.06000	0.25100
H	-5.86300	-0.20400	1.77600
H	-3.77900	-0.60700	-2.01800
H	-2.25700	-0.04900	-3.90100
H	-3.07200	1.40600	-3.31200
H	-3.62200	0.62700	-4.81200
H	-6.24100	-0.55400	-2.39700
H	-5.99800	0.38000	-3.87400
H	-5.10400	2.26800	-2.57500
H	-5.16500	1.30100	-1.08100
H	-6.66500	1.77400	-1.90400
H	0.03100	-3.29200	-4.41000
H	2.96800	-0.14400	-3.49700
H	4.41500	0.19600	-2.53200
H	4.44600	-2.02000	-3.43800
H	2.14300	-3.06900	-1.98700
H	5.91200	-2.76400	2.65300
H	4.61200	-0.68500	2.86000
H	3.36400	-1.33800	1.78100
H	3.65600	-2.09500	3.35800
H	4.60500	-3.79000	0.53400
H	6.40200	-1.00400	1.03000
H	4.50600	-0.65100	-0.40500
H	-2.75900	-4.05700	3.18500
H	-4.41100	-3.94800	2.51100
H	-2.69200	-0.20900	0.02900
H	-1.57600	1.51500	-1.35300
H	1.69900	1.61500	1.41300
H	0.60100	-0.10700	2.80300
H	-3.88000	-2.78200	3.75300
H	-4.28000	-1.39200	-3.51700
H	-8.57200	-1.79400	-0.27300
H	-3.51700	-5.06200	-1.65900
H	9.22200	2.87900	1.08800
H	-1.48300	7.96800	-1.24900
H	2.45400	6.02200	-0.53600
H	-2.80000	1.73400	3.89300
H	6.63800	-2.61100	0.33400
H	0.75000	-4.36300	-3.16600
H	1.13800	-4.59300	-4.88200
H	-0.74400	-3.79200	3.84600
H	0.03400	-0.90700	4.61300
O	0.81000	-0.55100	5.08200
O	-0.81700	-4.66600	4.26200
Cl	0.82700	2.99700	-0.93000
H	1.35400	-1.33600	5.22900
H	-1.20900	-4.46500	5.12200

d C(4)-O (Asp145): 2.2Å
d C(4)-Cl: 1.76 Å
reaction coordinate: -0.44 Å
Extrapolated ONIOM energy:
-1624.19501632936

C	-1.96500	2.47800	3.57700
C	-0.74900	2.55500	4.28000
C	-2.17900	3.29400	2.45300
C	0.25200	3.44800	3.85800
C	-1.17900	4.18800	2.03100
C	0.03700	4.26600	2.73300
C	-1.91100	7.51000	-2.05300
C	-2.84300	6.48300	-1.44200
C	-4.05600	6.89400	-0.85900
C	-2.49800	5.11700	-1.44500
C	-4.92400	5.94600	-0.28700
C	-3.36700	4.17000	-0.87100
C	-4.58000	4.58400	-0.29400
C	3.33500	6.05400	-1.35000
C	8.81400	3.19000	0.17200
C	7.33300	2.91800	0.24000
N	6.42400	3.54200	1.08000
C	6.66200	1.98500	-0.50200
C	5.21400	2.99000	0.85000
N	5.34200	2.05100	-0.10400
C	-2.74500	-4.98600	-2.27600
C	-1.75400	-3.99000	-1.74900
C	-1.54200	-2.73900	-2.22600
C	-0.83000	-4.15100	-0.63000
N	-0.51100	-2.14200	-1.51900
C	-0.04800	-2.96400	-0.51900
C	-0.56600	-5.18100	0.29800
C	0.95100	-2.80600	0.44800
C	0.42500	-5.02800	1.28600
C	1.18200	-3.84600	1.36300
C	-8.06800	-2.37800	0.36500
C	-7.25600	-1.66500	1.45800
C	-7.19700	-3.23700	-0.56100
C	-6.35400	-0.54700	0.92100
C	-4.21200	-0.36000	-2.99000
C	-5.61100	0.26500	-2.87300

C	-3.23300	0.49700	-3.80300
C	-5.63400	1.56900	-2.06800
C	0.81200	-3.88900	-4.11800
C	1.97200	-2.92900	-4.00900
O	2.41400	-2.41200	-5.02800
N	2.48100	-2.69500	-2.79800
C	3.71100	-1.92900	-2.58000
C	4.51300	-2.47900	-1.38100
O	4.76900	-3.67800	-1.31300
C	3.40100	-0.41500	-2.55100
C	2.56400	0.10500	-1.36400
O	1.31700	0.14700	-1.48300
O	3.21800	0.50100	-0.34200
N	4.94700	-1.64500	-0.43500
C	5.85800	-2.02600	0.65100
C	5.12900	-2.61800	1.86600
O	4.47600	-3.80400	1.49700
C	4.11800	-1.65100	2.48100
C	-3.63700	-3.27300	2.93500
S	-3.07100	-2.23600	1.54500
C	-1.70200	-1.36600	2.30900
O	-1.30300	-1.69000	3.43300
C	-1.10200	-0.30200	1.49300
C	-1.69700	0.17500	0.30900
C	-1.05200	1.10200	-0.49200
C	0.24000	1.51900	-0.14200
C	0.77800	1.17900	1.10600
C	0.13400	0.24500	1.89300
H	-0.58100	1.92300	5.14100
H	-3.11200	3.23200	1.91300
H	1.18400	3.50000	4.40100
H	-1.34600	4.81500	1.16700
H	0.80200	4.95400	2.40600
H	-1.28000	7.04100	-2.80900
H	-2.49100	8.30400	-2.52400
H	-4.32600	7.94100	-0.85000
H	-1.56500	4.79000	-1.88200
H	-5.85600	6.26600	0.15800
H	-3.09900	3.12400	-0.86800
H	-5.24800	3.85700	0.14700
H	4.19000	6.61800	-0.97700
H	3.64000	5.03300	-1.58000
H	2.95400	6.52900	-2.25400
H	9.20800	2.86600	-0.79200
H	9.00300	4.25800	0.28700
H	7.07800	1.31400	-1.24600
H	6.63600	4.26700	1.75600
H	4.56300	1.44400	-0.41100
H	4.27500	3.21800	1.34900
H	-2.29500	-5.97900	-2.28700
H	-3.04400	-4.71600	-3.29000
H	-2.07600	-2.29400	-3.05500
H	-0.13100	-1.20100	-1.65900
H	-1.14300	-6.09300	0.25600
H	0.60400	-5.81900	2.00200
H	1.51500	-1.88700	0.49700
H	1.93800	-3.74500	2.13000
H	-8.79800	-3.02900	0.84800
H	-7.83600	-3.76300	-1.27200
H	-6.64200	-3.97000	0.02500
H	-6.49800	-2.61200	-1.11500
H	-6.64500	-2.39500	1.99100
H	-7.95400	-1.22500	2.17100
H	-6.95700	0.19100	0.39200
H	-5.60200	-0.95500	0.24600
H	-5.84700	-0.06000	1.75500
H	-3.80600	-0.52500	-1.99300
H	-2.27300	-0.01300	-3.88000
H	-3.07500	1.45900	-3.31700
H	-3.62900	0.66300	-4.80600
H	-6.26500	-0.45300	-2.37600
H	-6.01100	0.45200	-3.87000
H	-5.10500	2.35500	-2.60800
H	-5.16500	1.41600	-1.09600
H	-6.66700	1.88500	-1.92000
H	-0.07200	-3.33600	-4.42100
H	2.88800	-0.19900	-3.49000
H	4.36200	0.12100	-2.56100
H	4.35400	-2.09300	-3.44600
H	2.06300	-3.13500	-1.98900
H	5.87300	-2.86100	2.62500
H	4.62500	-0.74400	2.80700
H	3.34900	-1.39100	1.75500
H	3.64600	-2.12500	3.34100
H	4.50500	-3.87000	0.52700
H	6.41200	-1.14700	0.97800
H	4.51700	-0.72300	-0.43500
H	-2.85500	-3.96700	3.24500
H	-4.49900	-3.82600	2.55600
H	-2.68300	-0.17400	0.02300
H	-1.50100	1.46000	-1.41000
H	1.73400	1.58300	1.40000
H	0.57800	-0.05900	2.83400
H	-3.94300	-2.64700	3.77500
H	-4.31100	-1.32900	-3.48100
H	-8.61000	-1.64000	-0.22800
H	-3.62400	-4.99700	-1.63100
H	9.32400	2.64400	0.96600
H	-1.28100	7.93700	-1.27300
H	2.55000	6.03700	-0.59400
H	-2.73500	1.79200	3.90000
H	6.57500	-2.76600	0.28800
H	0.64800	-4.39500	-3.16800
H	1.05100	-4.62800	-4.88000
H	-0.83100	-3.70900	3.88100
H	-0.02600	-0.82700	4.64700
O	0.75200	-0.48300	5.12400
O	-0.89600	-4.58700	4.29100
Cl	0.90600	2.93700	-0.97800
H	1.28100	-1.27700	5.27200
H	-1.28200	-4.39500	5.15500

d C(4)-O (Asp145): 2.0Å
d C(4)-Cl: 1.80 Å
reaction coordinate: -0.20 Å
Extrapolated ONIOM energy:
-1624.18389274655

C	-1.83900	2.53800	3.57100
C	-0.64000	2.58400	4.30400

C	-1.98300	3.32000	2.41200	C	0.88000	1.06500	1.08800
C	0.41500	3.41100	3.87700	C	0.16800	0.20600	1.89500
C	-0.93000	4.14900	1.98600	H	-0.52500	1.97500	5.19000
C	0.26900	4.19500	2.71800	H	-2.90300	3.28100	1.84800
C	-1.62300	7.56900	-2.07500	H	1.33400	3.43700	4.44400
C	-2.56300	6.55200	-1.45900	H	-1.04200	4.74800	1.09300
C	-3.75100	6.98200	-0.83700	H	1.07500	4.83100	2.38600
C	-2.25300	5.17900	-1.49500	H	-1.02000	7.09800	-2.85300
C	-4.62700	6.04500	-0.26000	H	-2.19600	8.38300	-2.51900
C	-3.12900	4.24300	-0.91700	H	-3.99400	8.03400	-0.80200
C	-4.31600	4.67500	-0.30100	H	-1.33900	4.83800	-1.96100
C	3.56400	5.90400	-1.39100	H	-5.53900	6.37900	0.21500
C	8.92900	2.82600	0.11500	H	-2.88700	3.19100	-0.94100
C	7.43300	2.69800	0.24400	H	-4.99000	3.95600	0.14400
N	6.62200	3.40100	1.12200	H	4.42500	6.44500	-1.00100
C	6.64900	1.83600	-0.46900	H	3.84400	4.87400	-1.61200
C	5.35700	2.96400	0.94300	H	3.21500	6.38600	-2.30400
N	5.35900	2.02000	-0.01700	H	9.24500	2.50700	-0.88000
C	-2.96000	-4.88500	-2.26300	H	9.23000	3.86300	0.26200
C	-1.92600	-3.92600	-1.75100	H	6.97000	1.13100	-1.22800
C	-1.67300	-2.68500	-2.23400	H	6.92900	4.09900	1.78900
C	-0.99800	-4.11700	-0.64000	H	4.53200	1.47300	-0.30600
N	-0.61700	-2.12200	-1.53600	H	4.46800	3.27900	1.48400
C	-0.17400	-2.95900	-0.53700	H	-2.55200	-5.89600	-2.26700
C	-0.76800	-5.15300	0.29100	H	-3.25400	-4.61200	-3.27700
C	0.83400	-2.83300	0.42500	H	-2.20100	-2.22300	-3.05700
C	0.23000	-5.02900	1.27700	H	-0.22500	-1.18800	-1.66900
C	1.02800	-3.87500	1.34600	H	-1.37900	-6.04200	0.25800
C	-8.16200	-2.05800	0.39500	H	0.38100	-5.82100	1.99900
C	-7.33700	-1.35800	1.48700	H	1.42800	-1.93300	0.47100
C	-7.31200	-2.95700	-0.51200	H	1.78300	-3.79300	2.11600
C	-6.39200	-0.28000	0.94300	H	-8.91800	-2.67800	0.87900
C	-4.24300	-0.20400	-2.98200	H	-7.96200	-3.47200	-1.22100
C	-5.61700	0.47200	-2.85900	H	-6.78600	-3.70000	0.08900
C	-3.23300	0.61700	-3.79400	H	-6.58800	-2.36300	-1.06700
C	-5.58600	1.77700	-2.05500	H	-6.75700	-2.10100	2.03600
C	0.63000	-3.93600	-4.12200	H	-8.02600	-0.88300	2.18600
C	1.80800	-3.00000	-4.01100	H	-6.96300	0.47000	0.39600
O	2.25300	-2.47700	-5.02600	H	-5.64700	-0.72400	0.28300
N	2.33100	-2.79700	-2.80200	H	-5.87700	0.20200	1.77400
C	3.59100	-2.08500	-2.58700	H	-3.84100	-0.38900	-1.98600
C	4.35400	-2.66200	-1.37500	H	-2.29600	0.06800	-3.88100
O	4.49500	-3.87700	-1.26400	H	-3.03200	1.56800	-3.30000
C	3.34900	-0.55900	-2.58300	H	-3.62800	0.80800	-4.79200
C	2.58900	0.03500	-1.38700	H	-6.29500	-0.22000	-2.36000
O	1.33400	0.16200	-1.48500	H	-6.01300	0.67500	-3.85500
O	3.28000	0.41100	-0.39600	H	-5.03000	2.54200	-2.59700
N	4.88100	-1.83900	-0.46800	H	-5.12000	1.60600	-1.08400
C	5.76800	-2.26600	0.61900	H	-6.60600	2.13200	-1.90200
C	5.01000	-2.76800	1.85800	H	-0.24200	-3.36600	-4.43100
O	4.30500	-3.93700	1.53700	H	2.81900	-0.33800	-3.51200
C	4.04500	-1.73200	2.43200	H	4.33100	-0.06900	-2.63000
C	-3.79800	-3.08300	2.95900	H	4.23000	-2.29100	-3.44600
S	-3.15900	-2.11400	1.55300	H	1.91600	-3.24700	-1.99600
C	-1.75400	-1.29500	2.32200	H	5.74100	-3.01500	2.62800
O	-1.38500	-1.62800	3.45600	H	4.59200	-0.83400	2.71600
C	-1.09700	-0.28200	1.50000	H	3.28400	-1.47100	1.69900
C	-1.65000	0.20900	0.29800	H	3.55600	-2.14600	3.31400
C	-0.94100	1.06300	-0.52400	H	4.28000	-4.01500	0.56800
C	0.39900	1.37900	-0.20200	H	6.39200	-1.42600	0.92100

H	4.54500	-0.87900	-0.49800
H	-3.06400	-3.82100	3.28500
H	-4.69400	-3.58600	2.58800
H	-2.66100	-0.06900	0.02000
H	-1.36700	1.43800	-1.44700
H	1.84800	1.43200	1.39200
H	0.57900	-0.08400	2.85600
H	-4.06400	-2.42400	3.78700
H	-4.38000	-1.16700	-3.47600
H	-8.67400	-1.31000	-0.21300
H	-3.83500	-4.85200	-1.61200
H	9.41700	2.19800	0.86100
H	-0.96600	7.96900	-1.30300
H	2.76100	5.91100	-0.65300
H	-2.65000	1.90200	3.89600
H	6.42100	-3.06800	0.27000
H	0.45100	-4.43700	-3.17300
H	0.85700	-4.68100	-4.88200
H	-1.02800	-3.64100	3.90000
H	-0.10800	-0.79500	4.66500
O	0.67300	-0.49000	5.16400
O	-1.11400	-4.52700	4.29100
Cl	1.07500	2.86300	-0.96800
H	1.16000	-1.30900	5.31900
H	-1.48500	-4.34300	5.16400

d C(4)-O (Asp145): 1.9Å
d C(4)-Cl: 1.83Å
reaction coordinate: -0.1Å
Extrapolated ONIOM energy:
-1624.17849700652

C	-1.68200	2.56400	3.58800
C	-0.47100	2.40600	4.28500
C	-1.74500	3.42100	2.47600
C	0.67700	3.10200	3.86800
C	-0.59800	4.11900	2.05900
C	0.61400	3.95900	2.75500
C	-1.28500	7.66300	-2.04900
C	-2.24900	6.67100	-1.42800
C	-3.46200	7.12300	-0.87600
C	-1.93500	5.29800	-1.39200
C	-4.35900	6.21000	-0.29400
C	-2.83400	4.38500	-0.81000
C	-4.04500	4.84000	-0.26100
C	3.81500	5.73900	-1.39800
C	9.02700	2.39000	0.06700
C	7.53300	2.46100	0.26400
N	6.85800	3.25200	1.18200
C	6.60900	1.71800	-0.41600
C	5.53900	2.98600	1.05900
N	5.37300	2.06200	0.09300
C	-3.24300	-4.70700	-2.28300
C	-2.15100	-3.81700	-1.77400
C	-1.83800	-2.58400	-2.24000
C	-1.22600	-4.07600	-0.67500
N	-0.74300	-2.09200	-1.54900
C	-0.33400	-2.97000	-0.57000
C	-1.05200	-5.13300	0.24300
C	0.68800	-2.91700	0.38300
C	-0.04500	-5.07800	1.22500
C	0.82000	-3.97300	1.29900
C	-8.28500	-1.63700	0.41300
C	-7.45300	-0.97600	1.52500
C	-7.45300	-2.56500	-0.48200
C	-6.45000	0.06100	1.00600
C	-4.29400	0.03400	-2.97600
C	-5.61900	0.79800	-2.82900
C	-3.22800	0.81300	-3.75700
C	-5.49800	2.07800	-1.99400
C	0.38100	-3.93000	-4.15600
C	1.61700	-3.07400	-4.05400
O	2.10700	-2.60200	-5.07300
N	2.13900	-2.88500	-2.84400
C	3.44500	-2.26800	-2.62800
C	4.13400	-2.86700	-1.38500
O	4.11100	-4.08100	-1.19800
C	3.32000	-0.72900	-2.67200
C	2.66900	-0.03500	-1.47100
O	1.40900	0.14500	-1.51200
O	3.43000	0.35900	-0.54800
N	4.77600	-2.06700	-0.53500
C	5.61900	-2.53900	0.56600
C	4.83000	-2.90100	1.83300
O	4.06000	-4.04600	1.58900
C	3.93000	-1.77200	2.33300
C	-3.99700	-2.86100	2.95400
S	-3.28400	-1.94700	1.54600
C	-1.79500	-1.26700	2.30700
O	-1.44500	-1.66100	3.42900
C	-1.06000	-0.30400	1.49800
C	-1.56900	0.26000	0.30700
C	-0.79100	1.05500	-0.50900
C	0.58400	1.24800	-0.20300
C	1.03900	0.85400	1.08300
C	0.25200	0.05800	1.88200
H	-0.42000	1.74000	5.13600
H	-2.67500	3.53900	1.94200
H	1.60500	2.96700	4.40500
H	-0.64800	4.77200	1.19900
H	1.49300	4.49300	2.42600
H	-0.63500	7.15800	-2.76400
H	-1.84100	8.44300	-2.56900
H	-3.70700	8.17500	-0.89700
H	-1.00300	4.93800	-1.80500
H	-5.29000	6.56100	0.12900
H	-2.59000	3.33300	-0.77800
H	-4.73500	4.14000	0.18800
H	4.71200	6.23900	-1.03300
H	4.04500	4.70300	-1.64700
H	3.45100	6.25100	-2.28900
H	9.25300	2.10200	-0.96100
H	9.47800	3.36300	0.26600
H	6.79800	0.98500	-1.19300
H	7.28500	3.89500	1.83800
H	4.48500	1.61000	-0.18000
H	4.72800	3.40900	1.64600
H	-2.89200	-5.73900	-2.30500
H	-3.53300	-4.40500	-3.28900
H	-2.35500	-2.07900	-3.04400

H	-0.32400	-1.16800	-1.66000
H	-1.71700	-5.98300	0.20800
H	0.05800	-5.88200	1.94200
H	1.33700	-2.05700	0.43200
H	1.57600	-3.93900	2.07200
H	-9.07400	-2.22800	0.87900
H	-8.10900	-3.05100	-1.20500
H	-6.96800	-3.33000	0.12500
H	-6.69600	-1.99700	-1.02100
H	-6.91900	-1.74500	2.08500
H	-8.13700	-0.47300	2.21000
H	-6.97600	0.83800	0.45100
H	-5.71200	-0.41300	0.35900
H	-5.93200	0.51600	1.85000
H	-3.90800	-0.21100	-1.98600
H	-2.33400	0.20000	-3.87400
H	-2.95500	1.72300	-3.22300
H	-3.61000	1.07600	-4.74400
H	-6.34100	0.14100	-2.34300
H	-6.00400	1.05200	-3.81700
H	-4.89200	2.81600	-2.52000
H	-5.04000	1.85300	-1.03000
H	-6.49000	2.49700	-1.82800
H	-0.45700	-3.30200	-4.44200
H	2.77200	-0.49700	-3.58600
H	4.33300	-0.31800	-2.77400
H	4.08000	-2.54900	-3.47000
H	1.68700	-3.28700	-2.03300
H	5.54400	-3.13900	2.62200
H	4.53100	-0.89400	2.56000
H	3.18800	-1.51300	1.58000
H	3.41400	-2.09700	3.23700
H	3.96400	-4.14400	0.62500
H	6.33300	-1.75800	0.82500
H	4.58400	-1.07200	-0.62900
H	-3.33400	-3.66900	3.26500
H	-4.94100	-3.27200	2.59100
H	-2.60400	0.08600	0.03100
H	-1.19300	1.49200	-1.41600
H	2.04000	1.12200	1.38800
H	0.64300	-0.28400	2.83400
H	-4.18800	-2.18600	3.79000
H	-4.49500	-0.90000	-3.50200
H	-8.75300	-0.86600	-0.20000
H	-4.10600	-4.63400	-1.62100
H	9.45300	1.65000	0.74600
H	-0.67600	8.11500	-1.26600
H	3.04200	5.76300	-0.62900
H	-2.56400	2.02800	3.90300
H	6.18100	-3.42000	0.24900
H	0.18800	-4.43500	-3.21200
H	0.54600	-4.67700	-4.93100
H	-1.27000	-3.70300	3.81700
H	-0.07800	-0.97400	4.63300
O	0.73700	-0.74800	5.12000
O	-1.43500	-4.58100	4.20100
Cl	1.30900	2.79500	-0.85300
H	1.15800	-1.61000	5.23700
H	-1.76100	-4.37200	5.08500

d C(4)-O (Asp145): 1.85Å
d C(4)-Cl: 1.85Å
reaction coordinate: 0.0Å
Extrapolated ONIOM energy:
-1624.17700408572

C	-1.33100	2.67200	3.76200
C	-0.59000	1.69400	4.44800
C	-0.67100	3.74900	3.14400
C	0.81200	1.79100	4.51200
C	0.73100	3.84300	3.20200
C	1.47200	2.86400	3.88800
C	-0.25000	7.88500	-2.30600
C	-1.07100	6.91500	-1.47700
C	-2.40900	7.21600	-1.15900
C	-0.49800	5.71600	-1.01300
C	-3.17100	6.32100	-0.38500
C	-1.25900	4.82400	-0.23600
C	-2.59500	5.12500	0.07800
C	4.51000	5.25900	-1.54600
C	9.16600	1.22100	0.05100
C	7.71200	1.59600	0.22100
N	7.20400	2.59400	1.04000
C	6.65800	0.97600	-0.39000
C	5.85700	2.57400	0.92600
N	5.51200	1.60000	0.06200
C	-3.96600	-4.07700	-2.38300
C	-2.73400	-3.45900	-1.79800
C	-2.18400	-2.27200	-2.15000
C	-1.90100	-3.98000	-0.72000
N	-1.03700	-2.05300	-1.40700
C	-0.82700	-3.06900	-0.50000
C	-1.95400	-5.12900	0.09600
C	0.15200	-3.29000	0.47700
C	-0.98400	-5.35200	1.09100
C	0.06200	-4.43500	1.28500
C	-8.54900	-0.26800	0.18700
C	-7.75300	0.33800	1.35500
C	-7.73200	-1.27300	-0.63600
C	-6.60100	1.24800	0.90900
C	-4.31400	0.75300	-3.16400
C	-5.19900	1.92900	-2.72200
C	-3.10100	1.19000	-3.99500
C	-4.51200	2.87000	-1.72500
C	-0.24300	-3.86200	-4.21100
C	1.11100	-3.21300	-4.11000
O	1.68600	-2.85400	-5.13100
N	1.63400	-3.07600	-2.89500
C	3.01800	-2.67400	-2.66600
C	3.55600	-3.31200	-1.37000
O	3.26000	-4.47100	-1.08500
C	3.15300	-1.13900	-2.78200
C	2.67800	-0.29700	-1.59800
O	1.44900	0.06000	-1.59600
O	3.53100	0.02500	-0.73600
N	4.36100	-2.60800	-0.57800
C	5.07700	-3.15800	0.57100
C	4.23300	-3.24200	1.85000
O	3.25000	-4.22700	1.69200
C	3.57000	-1.92100	2.22400
C	-4.54100	-2.05400	2.79700

S	-3.66000	-1.27400	1.40200
C	-2.02100	-1.03300	2.13100
O	-1.74300	-1.59400	3.20000
C	-1.10700	-0.19600	1.36700
C	-1.49100	0.53900	0.22000
C	-0.57300	1.22300	-0.54900
C	0.81600	1.14300	-0.23600
C	1.17600	0.58100	1.02000
C	0.24900	-0.11500	1.76000
H	-1.09400	0.86000	4.91700
H	-1.24200	4.50500	2.62500
H	1.37700	1.02800	5.03100
H	1.23300	4.66900	2.71800
H	2.54900	2.93100	3.93600
H	0.53600	7.34900	-2.83900
H	-0.89000	8.38600	-3.03300
H	-2.85600	8.13500	-1.50900
H	0.52800	5.47300	-1.24900
H	-4.19900	6.55400	-0.14400
H	-0.81300	3.90600	0.12200
H	-3.17900	4.43600	0.67300
H	5.50200	5.58400	-1.23400
H	4.54200	4.20900	-1.84000
H	4.18300	5.85900	-2.39500
H	9.32500	0.79300	-0.94000
H	9.79600	2.10500	0.15600
H	6.69400	0.14300	-1.08300
H	7.75000	3.21100	1.63000
H	4.55900	1.28900	-0.19500
H	5.14600	3.20800	1.44900
H	-3.80900	-5.14700	-2.51900
H	-4.19200	-3.62100	-3.34700
H	-2.58100	-1.60700	-2.90500
H	-0.47400	-1.20300	-1.43800
H	-2.76200	-5.83300	-0.02900
H	-1.05200	-6.22600	1.72600
H	0.94900	-2.57800	0.62300
H	0.78800	-4.61700	2.06500
H	-9.41800	-0.78400	0.59500
H	-8.37200	-1.72100	-1.39600
H	-7.34900	-2.06100	0.01400
H	-6.89900	-0.77400	-1.12900
H	-7.35500	-0.46400	1.97800
H	-8.43700	0.93000	1.96400
H	-6.98400	2.04800	0.27500
H	-5.85400	0.67400	0.36100
H	-6.12700	1.68600	1.78800
H	-3.97300	0.21100	-2.28100
H	-2.56700	0.31300	-4.35900
H	-2.42100	1.78700	-3.38800
H	-3.43100	1.78100	-4.85100
H	-6.09400	1.52500	-2.24900
H	-5.50900	2.50000	-3.59800
H	-3.66700	3.37100	-2.19700
H	-4.16400	2.30700	-0.85900
H	-5.22400	3.62700	-1.39300
H	-0.98200	-3.09800	-4.43700
H	2.62300	-0.85400	-3.69300
H	4.21700	-0.91300	-2.92900
H	3.61800	-3.10000	-3.47200
H	1.11700	-3.39800	-2.08800
H	4.88400	-3.54300	2.67100
H	4.32600	-1.14600	2.34300
H	2.86800	-1.62500	1.44900
H	3.02900	-2.04200	3.16200
H	3.13300	-4.38100	0.73700
H	5.94000	-2.52800	0.78000
H	4.39700	-1.60700	-0.75500
H	-4.10700	-3.02400	3.04400
H	-5.57100	-2.18300	2.45800
H	-2.53800	0.58400	-0.06300
H	-0.88500	1.79400	-1.41500
H	2.20500	0.65000	1.34400
H	0.56700	-0.59800	2.67800
H	-4.52400	-1.40000	3.67100
H	-4.92000	0.07600	-3.76800
H	-8.90200	0.53100	-0.46600
H	-4.80500	-3.92100	-1.70400
H	9.44700	0.48600	0.80600
H	0.20200	8.62900	-1.65000
H	3.80600	5.38500	-0.72400
H	-2.40700	2.59600	3.71000
H	5.44100	-4.15900	0.33400
H	-0.48800	-4.37700	-3.28500
H	-0.21800	-4.58500	-5.02400
H	-2.11900	-3.81700	3.33300
H	-0.16300	-1.55900	4.33500
O	0.71900	-1.63800	4.74400
O	-2.58500	-4.53900	3.78500
C	1.79700	2.63400	-0.72100
H	0.98400	-2.53500	4.50100
H	-2.69300	-4.19000	4.68000

d C(4)-O (Asp145): 1.8Å
d C(4)-Cl: 1.87Å
reaction coordinate: 0.07Å
Extrapolated ONIOM energy:
-1624.17524745117

C	-1.32500	2.66700	3.75800
C	-0.57800	1.69300	4.44500
C	-0.66800	3.73100	3.11500
C	0.82500	1.78200	4.48500
C	0.73600	3.81600	3.14700
C	1.48200	2.84200	3.83400
C	-0.23500	7.89500	-2.28100
C	-1.06200	6.92700	-1.45700
C	-2.38600	7.25200	-1.10400
C	-0.50900	5.70500	-1.03000
C	-3.15300	6.35900	-0.33300
C	-1.27500	4.81400	-0.25700
C	-2.59700	5.14000	0.09200
C	4.51900	5.25500	-1.53000
C	9.16600	1.20200	0.05300
C	7.71600	1.59200	0.23100
N	7.22300	2.59500	1.05300
C	6.65300	0.98600	-0.37600
C	5.87500	2.59000	0.94500
N	5.51500	1.62200	0.08100
C	-3.98200	-4.05700	-2.38500

C	-2.74400	-3.45500	-1.79500	H	6.67600	0.15400	-1.07100
C	-2.19400	-2.26400	-2.13000	H	7.77800	3.20600	1.64200
C	-1.90900	-3.99700	-0.73000	H	4.55800	1.32200	-0.17500
N	-1.04600	-2.05900	-1.38500	H	5.17300	3.23300	1.47100
C	-0.83400	-3.09000	-0.49500	H	-3.83400	-5.12700	-2.53100
C	-1.96000	-5.16000	0.06600	H	-4.20400	-3.59000	-3.34400
C	0.14500	-3.32700	0.47700	H	-2.59300	-1.58500	-2.87000
C	-0.99000	-5.40100	1.05500	H	-0.49300	-1.20200	-1.39500
C	0.05600	-4.48700	1.26500	H	-2.76900	-5.86200	-0.07000
C	-8.55300	-0.24300	0.19700	H	-1.05600	-6.28500	1.67600
C	-7.74300	0.35200	1.36100	H	0.94100	-2.61700	0.63700
C	-7.74900	-1.24700	-0.63900	H	0.78300	-4.68100	2.04100
C	-6.58900	1.25700	0.91100	H	-9.42100	-0.75700	0.61100
C	-4.31800	0.77600	-3.15400	H	-8.39900	-1.68700	-1.39600
C	-5.19200	1.96000	-2.71100	H	-7.36400	-2.04000	0.00200
C	-3.10600	1.20200	-3.99200	H	-6.91900	-0.74800	-1.13800
C	-4.49600	2.89400	-1.71500	H	-7.34500	-0.45600	1.97600
C	-0.25900	-3.84700	-4.21500	H	-8.41800	0.94500	1.98000
C	1.09300	-3.19200	-4.11100	H	-6.97200	2.06300	0.28400
O	1.66700	-2.82700	-5.13000	H	-5.85100	0.68200	0.35300
N	1.61600	-3.05700	-2.89600	H	-6.10400	1.68700	1.78700
C	3.00400	-2.66400	-2.66900	H	-3.97700	0.23400	-2.27100
C	3.54000	-3.30800	-1.37500	H	-2.57700	0.32000	-4.35200
O	3.24300	-4.46800	-1.09600	H	-2.42100	1.80000	-3.39100
C	3.15300	-1.13100	-2.79000	H	-3.43600	1.78900	-4.85000
C	2.69800	-0.28000	-1.60600	H	-6.09000	1.56300	-2.23700
O	1.46800	0.09000	-1.60600	H	-5.49800	2.53300	-3.58700
O	3.55300	0.03600	-0.74800	H	-3.64500	3.38600	-2.18700
N	4.34600	-2.61000	-0.57700	H	-4.15400	2.32900	-0.84800
C	5.06600	-3.16800	0.56600	H	-5.20000	3.65800	-1.38400
C	4.22400	-3.27400	1.84500	H	-1.00300	-3.08500	-4.43100
O	3.24800	-4.26400	1.67900	H	2.62000	-0.84300	-3.69700
C	3.55300	-1.96100	2.23400	H	4.21800	-0.91600	-2.94500
C	-4.54500	-2.04200	2.80500	H	3.59900	-3.09600	-3.47500
S	-3.66600	-1.26400	1.40700	H	1.10000	-3.38200	-2.08900
C	-2.02200	-1.03000	2.13300	H	4.88000	-3.57800	2.66200
O	-1.74800	-1.59500	3.20200	H	4.30300	-1.18300	2.36400
C	-1.10400	-0.20200	1.36700	H	2.85000	-1.66200	1.46000
C	-1.48000	0.53200	0.21700	H	3.01000	-2.09700	3.17000
C	-0.55600	1.19300	-0.56400	H	3.12600	-4.40600	0.72300
C	0.83800	1.10200	-0.25800	H	5.92500	-2.53500	0.78100
C	1.19200	0.53400	1.00100	H	4.39200	-1.61000	-0.75300
C	0.25700	-0.13900	1.75100	H	-4.11500	-3.01600	3.04400
H	-1.08000	0.86900	4.93300	H	-5.57800	-2.16300	2.47100
H	-1.24200	4.48300	2.59400	H	-2.52700	0.59100	-0.06400
H	1.39300	1.02300	5.00500	H	-0.86500	1.76000	-1.43500
H	1.23500	4.63000	2.64200	H	2.22200	0.59100	1.32300
H	2.55900	2.90100	3.86200	H	0.57400	-0.62200	2.66900
H	0.53200	7.35500	-2.83500	H	-4.51700	-1.39200	3.68000
H	-0.87600	8.42100	-2.98900	H	-4.93100	0.10200	-3.75300
H	-2.81700	8.19000	-1.42500	H	-8.90800	0.56200	-0.44700
H	0.50600	5.44200	-1.29200	H	-4.81800	-3.90000	-1.70400
H	-4.17000	6.61200	-0.06600	H	9.44100	0.46000	0.80400
H	-0.84500	3.87900	0.07300	H	0.24000	8.62000	-1.61900
H	-3.18400	4.45300	0.68500	H	3.80700	5.39300	-0.71700
H	5.51300	5.56000	-1.20500	H	-2.40200	2.59700	3.72400
H	4.53300	4.20700	-1.82800	H	5.43600	-4.16400	0.31700
H	4.21400	5.86500	-2.38100	H	-0.49900	-4.37200	-3.29200
H	9.31600	0.77700	-0.94000	H	-0.23300	-4.56200	-5.03500
H	9.80600	2.07800	0.16100	H	-2.11900	-3.82000	3.30800

H	-0.18000	-1.54700	4.33400
O	0.69800	-1.62700	4.75500
O	-2.58300	-4.54200	3.76000
Cl	1.81300	2.63800	-0.69600
H	0.94700	-2.53800	4.54900
H	-2.70100	-4.18700	4.65100

d C(4)-O (Asp145): 1.75Å
d C(4)-Cl: 1.91Å
reaction coordinate: 0.16Å
Extrapolated ONIOM energy:
-1624.17400545207

C	-1.33500	2.59200	3.76700
C	-0.61700	1.63500	4.50600
C	-0.64600	3.58400	3.04800
C	0.78900	1.67100	4.52500
C	0.76000	3.61400	3.05500
C	1.47700	2.65700	3.79600
C	-0.23400	7.92600	-2.19300
C	-1.07800	6.95300	-1.39300
C	-2.37500	7.31600	-0.98300
C	-0.56600	5.68700	-1.04600
C	-3.15700	6.41800	-0.23300
C	-1.34800	4.79200	-0.29400
C	-2.64300	5.15700	0.11300
C	4.52000	5.28300	-1.45500
C	9.16500	1.21800	0.10200
C	7.71900	1.63000	0.26500
N	7.23600	2.66300	1.05500
C	6.64900	1.01900	-0.32600
C	5.88800	2.67200	0.94300
N	5.51800	1.68300	0.10800
C	-3.96900	-4.02900	-2.43200
C	-2.73200	-3.44000	-1.83000
C	-2.18500	-2.24100	-2.13900
C	-1.89800	-4.00200	-0.77500
N	-1.04100	-2.04800	-1.38600
C	-0.82700	-3.09700	-0.51800
C	-1.94700	-5.18300	-0.00400
C	0.15000	-3.35100	0.45300
C	-0.97800	-5.44100	0.98300
C	0.06400	-4.52800	1.21500
C	-8.55200	-0.24500	0.17500
C	-7.78800	0.37200	1.35900
C	-7.71300	-1.25700	-0.61600
C	-6.62300	1.27600	0.93600
C	-4.30700	0.81200	-3.15200
C	-5.20800	1.97400	-2.70300
C	-3.09800	1.26800	-3.97800
C	-4.53400	2.91100	-1.69400
C	-0.24100	-3.79600	-4.24800
C	1.10500	-3.12800	-4.13100
O	1.67800	-2.74400	-5.14300
N	1.62600	-3.00300	-2.91300
C	3.01500	-2.61700	-2.68000
C	3.54800	-3.27700	-1.39200
O	3.25700	-4.44300	-1.13500
C	3.17600	-1.08300	-2.79300
C	2.73500	-0.23600	-1.60500
O	1.50300	0.14500	-1.61100
O	3.58300	0.06700	-0.74100
N	4.34400	-2.58800	-0.57700
C	5.06800	-3.16100	0.55600
C	4.22600	-3.31600	1.83000
O	3.26200	-4.31400	1.63400
C	3.53700	-2.02400	2.25400
C	-4.56400	-2.03500	2.78600
S	-3.66800	-1.27500	1.39000
C	-2.03000	-1.03800	2.13000
O	-1.76500	-1.60500	3.20000
C	-1.10500	-0.21400	1.37000
C	-1.46900	0.52300	0.21700
C	-0.53600	1.15900	-0.57200
C	0.86000	1.05900	-0.26500
C	1.20600	0.47200	0.99000
C	0.25800	-0.17400	1.74800
H	-1.14300	0.86400	5.05200
H	-1.19800	4.32300	2.48600
H	1.33600	0.92400	5.08500
H	1.28300	4.36800	2.48600
H	2.55600	2.67200	3.80300
H	0.49900	7.38300	-2.79000
H	-0.87100	8.50600	-2.86100
H	-2.77300	8.28600	-1.24200
H	0.42800	5.39500	-1.35200
H	-4.15300	6.70000	0.08000
H	-0.94800	3.82400	-0.02600
H	-3.24300	4.46600	0.68900
H	5.51900	5.54600	-1.10900
H	4.50700	4.24600	-1.79000
H	4.24200	5.93200	-2.28600
H	9.31200	0.75700	-0.87600
H	9.81500	2.09000	0.17900
H	6.66300	0.16800	-0.99700
H	7.79700	3.28500	1.62600
H	4.55800	1.39000	-0.14600
H	5.19400	3.34100	1.44600
H	-3.82900	-5.09900	-2.58100
H	-4.17900	-3.55600	-3.39200
H	-2.58500	-1.54500	-2.86300
H	-0.50100	-1.18400	-1.36900
H	-2.75400	-5.88400	-0.15600
H	-1.04400	-6.33700	1.58500
H	0.94200	-2.64100	0.63100
H	0.79000	-4.73500	1.98900
H	-9.43300	-0.75800	0.56400
H	-8.33200	-1.71100	-1.39100
H	-7.34900	-2.04000	0.05000
H	-6.86600	-0.76200	-1.09000
H	-7.40900	-0.42500	2.00000
H	-8.48900	0.97000	1.94200
H	-6.98600	2.06900	0.28300
H	-5.86100	0.69600	0.41700
H	-6.17400	1.72300	1.82400
H	-3.96200	0.26700	-2.27300
H	-2.54900	0.39800	-4.33800
H	-2.42900	1.87600	-3.36800
H	-3.43300	1.85300	-4.83500
H	-6.10000	1.55400	-2.23700

H	-5.52000	2.55000	-3.57500
H	-3.69200	3.42500	-2.15800
H	-4.18300	2.34300	-0.83200
H	-5.25400	3.65700	-1.35700
H	-0.99300	-3.03900	-4.45200
H	2.64100	-0.78600	-3.69700
H	4.24100	-0.87600	-2.95100
H	3.60800	-3.04700	-3.48900
H	1.11000	-3.34100	-2.11100
H	4.88300	-3.63500	2.63900
H	4.27700	-1.24100	2.40900
H	2.83400	-1.71300	1.48700
H	2.99400	-2.19300	3.18400
H	3.14300	-4.43100	0.67400
H	5.91600	-2.51900	0.79200
H	4.39500	-1.58600	-0.74000
H	-4.15800	-3.01900	3.02100
H	-5.60100	-2.12800	2.45400
H	-2.51500	0.59500	-0.06500
H	-0.83500	1.71800	-1.45100
H	2.23700	0.51200	1.31100
H	0.57000	-0.66100	2.66600
H	-4.51900	-1.38800	3.66300
H	-4.90300	0.13200	-3.76200
H	-8.88700	0.54800	-0.49500
H	-4.81000	-3.86600	-1.75800
H	9.43200	0.49900	0.87800
H	0.28400	8.60100	-1.51200
H	3.80300	5.41100	-0.64400
H	-2.41500	2.56400	3.75000
H	5.45700	-4.14400	0.28400
H	-0.47600	-4.33800	-3.33400
H	-0.20500	-4.49700	-5.07900
H	-2.16500	-3.81400	3.28200
H	-0.19100	-1.58600	4.33000
O	0.68500	-1.70600	4.74300
O	-2.63000	-4.56200	3.69100
Cl	1.83300	2.66400	-0.62900
H	0.90500	-2.61600	4.50400
H	-2.75300	-4.25900	4.60000

d C(4)-O (Asp145): 1.57Å
d C(4)-Cl: 1.9Å
reaction coordinate: 0.33
Extrapolated ONIOM energy:
-1624.17467009707

C	-1.79000	2.76200	3.71000
C	-0.77800	2.00600	4.32800
C	-1.45700	3.72900	2.74500
C	0.56700	2.21400	3.97700
C	-0.11200	3.93200	2.38900
C	0.89900	3.17200	3.00300
C	-1.45300	8.00200	-2.16900
C	-2.09100	6.75700	-1.58300
C	-3.47900	6.72100	-1.34500
C	-1.30200	5.63500	-1.26300
C	-4.07400	5.57100	-0.79300
C	-1.89700	4.48700	-0.71000
C	-3.28200	4.45400	-0.47400
C	3.62700	6.06600	-1.40600
C	8.80200	2.73600	0.22400
C	7.30800	2.93300	0.37400
N	6.67400	3.86300	1.18500
C	6.34200	2.19800	-0.25300
C	5.33900	3.68700	1.04900
N	5.12100	2.68200	0.17900
C	-3.50300	-4.35300	-1.96600
C	-2.20400	-4.02700	-1.30500
C	-1.86400	-2.80500	-0.84400
C	-1.06600	-4.89600	-1.01700
N	-0.60500	-2.85300	-0.28000
C	-0.06100	-4.11400	-0.37100
C	-0.76100	-6.25200	-1.26700
C	1.17500	-4.64700	0.01000
C	0.48600	-6.79500	-0.89800
C	1.45200	-5.99600	-0.26100
C	-8.54200	-1.15000	0.57400
C	-7.70600	-0.22500	1.47400
C	-7.69900	-2.21400	-0.14000
C	-6.73000	0.67000	0.70000
C	-4.51200	0.36700	-2.84100
C	-5.73700	1.23900	-3.15800
C	-3.21200	0.88700	-3.46600
C	-5.67700	2.63400	-2.52500
C	0.14200	-3.67200	-3.83600
C	1.47000	-2.94800	-3.82800
O	1.94200	-2.54600	-4.88500
N	2.08300	-2.78200	-2.65400
C	3.43100	-2.21500	-2.53400
C	4.15700	-2.71000	-1.25600
O	4.36000	-3.91100	-1.10400
C	3.39700	-0.68300	-2.77000
C	2.85100	0.18100	-1.65200
O	1.54600	0.30800	-1.62700
O	3.63100	0.72000	-0.85500
N	4.55300	-1.84400	-0.31600
C	5.35300	-2.14700	0.87500
C	4.57200	-2.87100	1.98700
O	4.27800	-4.18300	1.58400
C	3.27700	-2.16900	2.38300
C	-4.29200	-2.15700	3.27100
S	-3.55400	-1.45400	1.75900
C	-1.87200	-1.05400	2.34700
O	-1.51800	-1.48400	3.46100
C	-1.02400	-0.30400	1.44900
C	-1.45300	0.32000	0.24100
C	-0.58400	0.90700	-0.64000
C	0.84800	0.97100	-0.38600
C	1.26200	0.37400	0.87200
C	0.36800	-0.21800	1.72500
H	-1.03200	1.25500	5.06300
H	-2.23500	4.30900	2.27000
H	1.34000	1.61600	4.44100
H	0.13900	4.65900	1.63000
H	1.92900	3.31000	2.71200
H	-0.53500	7.74000	-2.69700
H	-2.13900	8.47600	-2.87200
H	-4.09200	7.57800	-1.58500
H	-0.23600	5.64800	-1.43900

H	-5.13900	5.54700	-0.61300
H	-1.28900	3.63100	-0.45800
H	-3.73300	3.57000	-0.04500
H	4.62200	6.37300	-1.08400
H	3.66100	5.04400	-1.78300
H	3.28200	6.73000	-2.19900
H	9.01800	2.23700	-0.72200
H	9.31000	3.70100	0.23600
H	6.48300	1.37600	-0.94700
H	7.13500	4.53800	1.78400
H	4.21800	2.26600	-0.10800
H	4.55400	4.23800	1.56100
H	-3.43500	-5.32600	-2.45400
H	-3.73900	-3.59300	-2.71000
H	-2.50700	-1.93600	-0.88300
H	-0.19800	-2.06400	0.21700
H	-1.50000	-6.88100	-1.74200
H	0.70100	-7.83800	-1.08900
H	1.90300	-4.03800	0.51900
H	2.40400	-6.42000	0.03400
H	-9.28200	-1.65700	1.19500
H	-8.35800	-2.88600	-0.69100
H	-7.13400	-2.79300	0.59100
H	-7.01100	-1.74500	-0.84300
H	-7.14700	-0.82600	2.19200
H	-8.38900	0.41800	2.03100
H	-7.27400	1.25600	-0.04200
H	-5.97200	0.06400	0.20400
H	-6.23300	1.34800	1.39400
H	-4.38700	0.29800	-1.76000
H	-2.40500	0.18300	-3.26200
H	-2.94900	1.85600	-3.04000
H	-3.33300	0.98800	-4.54500
H	-6.62400	0.73100	-2.77900
H	-5.84000	1.34000	-4.23900
H	-4.85600	3.21000	-2.95200
H	-5.53800	2.54800	-1.44700
H	-6.61100	3.16100	-2.72100
H	-0.59100	-3.07200	-3.30600
H	2.82200	-0.52900	-3.68500
H	4.42500	-0.35100	-2.94900
H	4.01600	-2.62600	-3.35900
H	1.65300	-3.15700	-1.82000
H	5.21100	-2.92800	2.86900
H	3.49600	-1.16500	2.74400
H	2.60100	-2.11000	1.53200
H	2.79200	-2.73300	3.17900
H	4.27900	-4.20300	0.60900
H	5.73500	-1.21400	1.28800
H	4.32400	-0.87000	-0.47400
H	-3.80000	-3.09200	3.53800
H	-5.34100	-2.33900	3.02900
H	-2.51300	0.33800	-0.00100
H	-0.94500	1.36400	-1.55400
H	2.30800	0.43300	1.14000
H	0.74400	-0.63800	2.65200
H	-4.22300	-1.44200	4.09200
H	-4.69800	-0.63700	-3.22400
H	-9.07300	-0.55200	-0.16900
H	-4.29300	-4.38200	-1.21500
H	9.17600	2.12000	1.04400
H	-1.21900	8.70200	-1.36600
H	2.93400	6.11900	-0.56600
H	-2.82200	2.59900	3.97400
H	6.20300	-2.77100	0.59500
H	0.26700	-4.64700	-3.37100
H	-0.18000	-3.80700	-4.86700
H	-1.73100	-3.44800	3.86200
H	0.05600	-1.07200	4.52500
O	0.93600	-1.03800	4.94600
O	-2.00100	-4.34600	4.12400
Cl	1.47700	2.75400	-0.57800
H	1.13700	-1.97100	5.09000
H	-2.18500	-4.25500	5.06800

d C(4)-O (Asp145): 1.53Å
d C(4)-Cl: 1.95Å
reaction coordinate: 0.42Å
Extrapolated ONIOM energy:
-1624.17680145385

C	-1.80000	2.75900	3.71200
C	-0.79900	1.99400	4.33700
C	-1.45400	3.71000	2.73600
C	0.54900	2.17800	3.98200
C	-0.10800	3.88900	2.37600
C	0.89300	3.12000	2.99600
C	-1.43700	8.02200	-2.15500
C	-2.06400	6.76600	-1.58000
C	-3.45000	6.72000	-1.32900
C	-1.26700	5.64300	-1.28200
C	-4.03400	5.56000	-0.78700
C	-1.85200	4.48500	-0.74000
C	-3.23400	4.44200	-0.49100
C	3.63600	6.07300	-1.38200
C	8.79900	2.72900	0.25600
C	7.30500	2.93900	0.39100
N	6.67000	3.88300	1.18600
C	6.33600	2.20600	-0.23600
C	5.33500	3.71800	1.04000
N	5.11500	2.70600	0.17900
C	-3.51700	-4.32900	-1.97100
C	-2.21500	-4.01900	-1.30700
C	-1.86500	-2.80500	-0.83400
C	-1.08200	-4.89900	-1.02900
N	-0.60500	-2.86600	-0.27300
C	-0.07000	-4.13000	-0.37900
C	-0.78800	-6.25500	-1.29300
C	1.16500	-4.67500	-0.01000
C	0.45700	-6.81000	-0.93500
C	1.43200	-6.02400	-0.29500
C	-8.55500	-1.11700	0.56100
C	-7.72600	-0.18400	1.45900
C	-7.70700	-2.19100	-0.13200
C	-6.74100	0.70100	0.68500
C	-4.51300	0.39500	-2.84300
C	-5.73300	1.27300	-3.16300
C	-3.21000	0.90700	-3.46500
C	-5.66600	2.66800	-2.53100
C	0.13400	-3.65500	-3.83200

C	1.46700	-2.93900	-3.82200
O	1.94200	-2.54000	-4.87900
N	2.08200	-2.77600	-2.64800
C	3.43400	-2.21500	-2.53000
C	4.16000	-2.71100	-1.25100
O	4.38300	-3.91000	-1.11100
C	3.40900	-0.68400	-2.77300
C	2.87200	0.18300	-1.65600
O	1.56300	0.30600	-1.62600
O	3.65100	0.72000	-0.86000
N	4.53400	-1.85100	-0.29800
C	5.33700	-2.14700	0.89400
C	4.57100	-2.90300	1.99400
O	4.29400	-4.21200	1.57100
C	3.26500	-2.22900	2.40400
C	-4.32100	-2.11400	3.27400
S	-3.57000	-1.43400	1.75700
C	-1.88800	-1.03700	2.34900
O	-1.54100	-1.46200	3.46700
C	-1.02800	-0.30000	1.44800
C	-1.44500	0.32200	0.23600
C	-0.56200	0.87500	-0.65400
C	0.86900	0.91400	-0.40000
C	1.27300	0.30200	0.85200
C	0.36700	-0.25200	1.71800
H	-1.06300	1.25600	5.08100
H	-2.22400	4.29600	2.25500
H	1.31500	1.57500	4.45100
H	0.15400	4.60200	1.60800
H	1.92400	3.23800	2.70100
H	-0.52200	7.77100	-2.69200
H	-2.13200	8.50000	-2.84700
H	-4.06800	7.57700	-1.55100
H	-0.20300	5.66200	-1.46800
H	-5.09800	5.52900	-0.59600
H	-1.23700	3.62700	-0.50600
H	-3.67700	3.55000	-0.07000
H	4.64600	6.34900	-1.08000
H	3.63100	5.05000	-1.76000
H	3.29500	6.74700	-2.16800
H	9.01800	2.19600	-0.67100
H	9.31200	3.69100	0.23800
H	6.47600	1.37500	-0.92000
H	7.13200	4.56200	1.78000
H	4.20900	2.29800	-0.11100
H	4.55000	4.28200	1.53700
H	-3.45700	-5.29700	-2.47000
H	-3.74800	-3.55900	-2.70700
H	-2.50200	-1.93100	-0.86400
H	-0.19000	-2.08500	0.22900
H	-1.53200	-6.87400	-1.77200
H	0.66400	-7.85200	-1.13800
H	1.90100	-4.07700	0.50200
H	2.38200	-6.45700	-0.00800
H	-9.30200	-1.61500	1.18000
H	-8.36100	-2.86700	-0.68300
H	-7.15100	-2.76300	0.61100
H	-7.01000	-1.73200	-0.83300
H	-7.17600	-0.77800	2.18900
H	-8.41300	0.46600	2.00200
H	-7.27600	1.28000	-0.06800
H	-5.97900	0.08900	0.20300
H	-6.24900	1.38500	1.37700
H	-4.39000	0.32500	-1.76100
H	-2.40800	0.19700	-3.26400
H	-2.94000	1.87300	-3.03600
H	-3.32900	1.01300	-4.54400
H	-6.62400	0.77000	-2.78500
H	-5.83300	1.37400	-4.24400
H	-4.84100	3.23900	-2.95700
H	-5.53200	2.58200	-1.45300
H	-6.59800	3.19900	-2.73100
H	-0.59300	-3.05300	-3.29500
H	2.83300	-0.52900	-3.68800
H	4.43900	-0.36000	-2.95500
H	4.01500	-2.63300	-3.35400
H	1.64900	-3.14600	-1.81400
H	5.21100	-2.96400	2.87400
H	3.46700	-1.22600	2.77900
H	2.58500	-2.17000	1.55700
H	2.79200	-2.81300	3.19300
H	4.30200	-4.21900	0.59600
H	5.69500	-1.21000	1.31800
H	4.29600	-0.87800	-0.44800
H	-3.84200	-3.05400	3.54900
H	-5.37200	-2.28300	3.03100
H	-2.50400	0.36000	-0.00700
H	-0.91100	1.32400	-1.57700
H	2.32400	0.32600	1.11200
H	0.73600	-0.68000	2.64400
H	-4.24300	-1.39200	4.08800
H	-4.70400	-0.60900	-3.22600
H	-9.07700	-0.52600	-0.19400
H	-4.30700	-4.36100	-1.22000
H	9.16500	2.14000	1.09800
H	-1.20300	8.71300	-1.34600
H	2.96200	6.14700	-0.52800
H	-2.83400	2.61500	3.97900
H	6.20300	-2.74700	0.61000
H	0.25400	-4.63400	-3.37500
H	-0.19200	-3.77900	-4.86300
H	-1.77800	-3.42900	3.87600
H	0.05000	-1.07600	4.52700
O	0.93400	-1.06400	4.94100
O	-2.06000	-4.32500	4.13300
Cl	1.51500	2.74800	-0.54000
H	1.11200	-2.00200	5.08800
H	-2.23900	-4.23800	5.07800

d C(4)-O (Asp145): 1.51Å
d C(4)-Cl: 2.0Å
reaction coordinate: 0.49Å
Extrapolated ONIOM energy:
-1624.17892797965

C	-1.80000	2.75700	3.72000
C	-0.81500	1.98000	4.35400
C	-1.43500	3.69500	2.73800
C	0.53700	2.13800	4.00300
C	-0.08400	3.84700	2.38300

C	0.90100	3.06600	3.01200	H	-2.19200	4.29100	2.24900
C	-1.40600	8.04200	-2.14200	H	1.29100	1.52600	4.48000
C	-2.02400	6.77800	-1.57500	H	0.19400	4.54900	1.60900
C	-3.40800	6.72000	-1.32200	H	1.93500	3.16300	2.71800
C	-1.21900	5.65800	-1.28900	H	-0.48900	7.80300	-2.67900
C	-3.98400	5.55200	-0.78800	H	-2.10400	8.51900	-2.83200
C	-1.79600	4.49100	-0.75500	H	-4.03300	7.57600	-1.53500
C	-3.17700	4.43700	-0.50400	H	-0.15500	5.68500	-1.47500
C	3.65700	6.07000	-1.36300	H	-5.04700	5.51300	-0.59600
C	8.80200	2.70000	0.28000	H	-1.17400	3.63600	-0.53000
C	7.30700	2.92600	0.40100	H	-3.61300	3.53900	-0.09000
N	6.67700	3.88900	1.17700	H	4.66200	6.33700	-1.03900
C	6.33500	2.19400	-0.22200	H	3.65500	5.05400	-1.76000
C	5.34100	3.73500	1.02400	H	3.33100	6.76000	-2.14100
N	5.11500	2.71300	0.17700	H	9.02000	2.12300	-0.62000
C	-3.54100	-4.30000	-1.97700	H	9.32100	3.65700	0.21700
C	-2.23700	-4.00400	-1.31100	H	6.47000	1.35200	-0.89300
C	-1.87600	-2.79600	-0.83000	H	7.14000	4.57200	1.76500
C	-1.11000	-4.89500	-1.04100	H	4.20500	2.31400	-0.11400
N	-0.61500	-2.87000	-0.27400	H	4.55700	4.31500	1.50500
C	-0.09000	-4.13800	-0.38900	H	-3.48200	-5.25400	-2.50100
C	-0.82800	-6.25100	-1.31400	H	-3.77800	-3.51100	-2.69200
C	1.14300	-4.69400	-0.02900	H	-2.50600	-1.91600	-0.85500
C	0.41400	-6.81700	-0.96400	H	-0.19100	-2.09500	0.23000
C	1.39800	-6.04300	-0.32300	H	-1.57900	-6.86100	-1.79400
C	-8.57000	-1.06800	0.55000	H	0.61300	-7.86000	-1.17300
C	-7.74100	-0.12700	1.44100	H	1.88700	-4.10600	0.48300
C	-7.72400	-2.15800	-0.11900	H	2.34600	-6.48600	-0.04300
C	-6.74400	0.74000	0.66100	H	-9.32600	-1.55100	1.17000
C	-4.51500	0.43000	-2.84500	H	-8.37900	-2.83800	-0.66500
C	-5.72000	1.32400	-3.17700	H	-7.17800	-2.72400	0.63800
C	-3.19900	0.92400	-3.45700	H	-7.01700	-1.71500	-0.82100
C	-5.64100	2.71900	-2.54500	H	-7.20100	-0.71400	2.18400
C	0.11600	-3.63900	-3.83100	H	-8.42800	0.53600	1.96800
C	1.45400	-2.93300	-3.82000	H	-7.27000	1.31200	-0.10400
O	1.93200	-2.53900	-4.87700	H	-5.98400	0.11500	0.19400
N	2.07200	-2.77500	-2.64600	H	-6.25300	1.43000	1.34700
C	3.42800	-2.22300	-2.52900	H	-4.40200	0.36000	-1.76200
C	4.15500	-2.72300	-1.25100	H	-2.41000	0.20200	-3.24900
O	4.39400	-3.92000	-1.12300	H	-2.91900	1.88500	-3.02500
C	3.41500	-0.69200	-2.77700	H	-3.30800	1.03000	-4.53600
C	2.88700	0.17700	-1.65800	H	-6.62100	0.83400	-2.80700
O	1.57500	0.30400	-1.62500	H	-5.80900	1.42600	-4.25900
O	3.66700	0.70700	-0.86200	H	-4.80300	3.27800	-2.96200
N	4.51100	-1.86800	-0.28500	H	-5.52000	2.63200	-1.46600
C	5.31700	-2.16100	0.90500	H	-6.56100	3.26300	-2.75600
C	4.56300	-2.94200	1.99700	H	-0.60600	-3.03500	-3.29000
O	4.29500	-4.24700	1.55600	H	2.83800	-0.53400	-3.69000
C	3.25200	-2.28700	2.42200	H	4.44600	-0.37600	-2.96100
C	-4.35200	-2.07300	3.27200	H	4.00500	-2.64700	-3.35300
S	-3.58800	-1.40900	1.75400	H	1.63500	-3.14000	-1.81200
C	-1.90600	-1.02100	2.35100	H	5.20800	-3.01000	2.87300
O	-1.56500	-1.44400	3.46900	H	3.44500	-1.28800	2.81000
C	-1.03300	-0.29500	1.44800	H	2.56700	-2.22500	1.57900
C	-1.43900	0.33400	0.23700	H	2.79000	-2.88700	3.20600
C	-0.54300	0.86000	-0.65900	H	4.31100	-4.24300	0.58000
C	0.88400	0.86700	-0.40400	H	5.65800	-1.22200	1.34000
C	1.28100	0.24200	0.83900	H	4.26500	-0.89700	-0.42800
C	0.36300	-0.28300	1.71400	H	-3.88600	-3.01800	3.55200
H	-1.09500	1.25200	5.10300	H	-5.40400	-2.22800	3.02800

H	-2.49700	0.39200	-0.00600
H	-0.88200	1.30800	-1.58600
H	2.33300	0.23200	1.09100
H	0.72400	-0.72300	2.63700
H	-4.26500	-1.34900	4.08400
H	-4.71600	-0.57200	-3.22800
H	-9.08100	-0.48500	-0.21800
H	-4.32800	-4.35200	-1.22400
H	9.16200	2.15000	1.15000
H	-1.17800	8.73000	-1.32800
H	2.96800	6.12800	-0.52000
H	-2.83800	2.63400	3.98300
H	6.19400	-2.74300	0.61700
H	0.22900	-4.62200	-3.38000
H	-0.21300	-3.75600	-4.86200
H	-1.82700	-3.41700	3.88200
H	0.04500	-1.09300	4.52800
O	0.93300	-1.10600	4.93300
O	-2.12300	-4.31000	4.13200
Cl	1.56300	2.74600	-0.49900
H	1.08700	-2.04800	5.07700
H	-2.30000	-4.23100	5.07800

d C(4)-O (Asp145): 1.49Å
d C(4)-Cl: 2.05Å
reaction coordinate: 0.55Å
Extrapolated ONIOM energy:
-1624.18107301731

C	-1.80200	2.75600	3.72400
C	-0.83000	1.96900	4.36700
C	-1.42100	3.68300	2.73900
C	0.52600	2.10600	4.01900
C	-0.06700	3.81500	2.38700
C	0.90500	3.02300	3.02400
C	-1.38100	8.05800	-2.13300
C	-1.99000	6.78600	-1.57300
C	-3.37300	6.71800	-1.31900
C	-1.17700	5.67000	-1.29300
C	-3.94100	5.54300	-0.79200
C	-1.74500	4.49700	-0.76500
C	-3.12600	4.43100	-0.51400
C	3.67400	6.06700	-1.34800
C	8.80400	2.67700	0.30000
C	7.30900	2.91500	0.41000
N	6.68100	3.89000	1.17300
C	6.33300	2.18600	-0.21200
C	5.34400	3.74600	1.01300
N	5.11500	2.71800	0.17400
C	-3.56100	-4.27600	-1.98400
C	-2.25400	-3.99100	-1.31600
C	-1.88600	-2.78600	-0.83100
C	-1.13300	-4.88900	-1.04900
N	-0.62400	-2.87100	-0.27600
C	-0.10600	-4.14100	-0.39700
C	-0.86000	-6.24700	-1.32600
C	1.12400	-4.70600	-0.04100
C	0.37900	-6.82200	-0.98100
C	1.36900	-6.05600	-0.34000
C	-8.58200	-1.02800	0.53900
C	-7.75700	-0.08700	1.43200
C	-7.73400	-2.12400	-0.12200
C	-6.75200	0.77400	0.65700
C	-4.51600	0.45800	-2.84800
C	-5.71600	1.35900	-3.17900
C	-3.19700	0.94900	-3.45400
C	-5.63100	2.75200	-2.54400
C	0.10100	-3.62700	-3.83100
C	1.44500	-2.93000	-3.81900
O	1.92600	-2.53900	-4.87600
N	2.06400	-2.77500	-2.64500
C	3.42400	-2.23100	-2.52900
C	4.15200	-2.73300	-1.25100
O	4.40800	-3.92800	-1.13500
C	3.42000	-0.69900	-2.78000
C	2.90000	0.17100	-1.66000
O	1.58600	0.30100	-1.62600
O	3.68100	0.69300	-0.86200
N	4.49000	-1.88400	-0.27300
C	5.30000	-2.17200	0.91500
C	4.55700	-2.97300	2.00000
O	4.29400	-4.27400	1.54300
C	3.24400	-2.33300	2.44000
C	-4.37400	-2.04400	3.26900
S	-3.60300	-1.38900	1.75100
C	-1.92100	-1.00900	2.35000
O	-1.58400	-1.43100	3.46900
C	-1.03700	-0.29000	1.44700
C	-1.43400	0.34600	0.23700
C	-0.52700	0.85000	-0.66300
C	0.89600	0.82800	-0.40900
C	1.28500	0.19400	0.82800
C	0.35900	-0.30700	1.70900
H	-1.12200	1.25000	5.11900
H	-2.16800	4.28700	2.24400
H	1.27100	1.48800	4.50100
H	0.22400	4.50800	1.61000
H	1.94100	3.10400	2.73100
H	-0.46100	7.82800	-2.67100
H	-2.08200	8.53300	-2.82200
H	-4.00400	7.57000	-1.52800
H	-0.11300	5.70600	-1.47900
H	-5.00300	5.49500	-0.59900
H	-1.11600	3.64600	-0.54500
H	-3.55600	3.52800	-0.10500
H	4.68900	6.32600	-1.05000
H	3.65200	5.05000	-1.74100
H	3.33500	6.75700	-2.12100
H	9.02100	2.07300	-0.58200
H	9.32800	3.62900	0.21100
H	6.46500	1.33700	-0.87600
H	7.14600	4.57500	1.75700
H	4.20100	2.32800	-0.11700
H	4.56200	4.33600	1.48300
H	-3.50400	-5.22400	-2.51800
H	-3.79700	-3.47900	-2.68900
H	-2.51000	-1.90200	-0.85300
H	-0.19300	-2.10000	0.22700
H	-1.61600	-6.85000	-1.80700
H	0.57000	-7.86600	-1.19300

H	1.87300	-4.12500	0.47000
H	2.31500	-6.50500	-0.06400
H	-9.34300	-1.50800	1.15500
H	-8.38800	-2.80300	-0.67000
H	-7.19600	-2.68900	0.64000
H	-7.02200	-1.68400	-0.81900
H	-7.22300	-0.67400	2.18100
H	-8.44500	0.57900	1.95400
H	-7.27100	1.34600	-0.11300
H	-5.99100	0.14600	0.19500
H	-6.26300	1.46500	1.34400
H	-4.40700	0.38300	-1.76600
H	-2.41100	0.22100	-3.25000
H	-2.91300	1.90600	-3.01700
H	-3.30300	1.06300	-4.53400
H	-6.62000	0.87200	-2.81100
H	-5.80400	1.46300	-4.26100
H	-4.79100	3.30800	-2.96100
H	-5.50800	2.66200	-1.46500
H	-6.55000	3.30000	-2.75200
H	-0.61600	-3.01900	-3.28800
H	2.84300	-0.54000	-3.69300
H	4.45300	-0.39000	-2.96500
H	3.99800	-2.65900	-3.35300
H	1.62600	-3.13600	-1.81100
H	5.20600	-3.04800	2.87200
H	3.43100	-1.33600	2.83700
H	2.55400	-2.26800	1.60100
H	2.79100	-2.94500	3.22000
H	4.32000	-4.26100	0.56800
H	5.62600	-1.23100	1.35600
H	4.23600	-0.91500	-0.41000
H	-3.91700	-2.99400	3.54900
H	-5.42800	-2.18900	3.02400
H	-2.49100	0.42100	-0.00400
H	-0.85800	1.29700	-1.59300
H	2.33800	0.15600	1.07300
H	0.71400	-0.75600	2.63100
H	-4.28000	-1.32000	4.08000
H	-4.72100	-0.54100	-3.23600
H	-9.08600	-0.44700	-0.23500
H	-4.34700	-4.33500	-1.23000
H	9.15900	2.15000	1.18700
H	-1.15900	8.74400	-1.31500
H	3.00600	6.13500	-0.48800
H	-2.84200	2.64900	3.98400
H	6.18600	-2.73800	0.62300
H	0.20900	-4.61200	-3.38400
H	-0.22900	-3.73800	-4.86200
H	-1.86300	-3.41200	3.88100
H	0.03800	-1.10800	4.52900
O	0.92800	-1.13900	4.92800
O	-2.16900	-4.30300	4.12500
Cl	1.60900	2.74900	-0.46700
H	1.06700	-2.08400	5.06600
H	-2.34200	-4.22700	5.07200

d C(4)-O (Asp145): 1.48Å
d C(4)-Cl: 2.10Å
reaction coordinate: 0.61Å
Extrapolated ONIOM energy:
-1624.1832500946

C	-1.80100	2.75800	3.72900
C	-0.84500	1.95700	4.37900
C	-1.40100	3.67600	2.74400
C	0.51400	2.07200	4.03800
C	-0.04300	3.78600	2.40000
C	0.91300	2.98000	3.04300
C	-1.35200	8.07400	-2.12900
C	-1.95000	6.79500	-1.57200
C	-3.33300	6.71500	-1.31800
C	-1.12800	5.68500	-1.29500
C	-3.89000	5.53400	-0.79400
C	-1.68600	4.50500	-0.77200
C	-3.06600	4.42800	-0.52100
C	3.69300	6.06000	-1.33800
C	8.80700	2.64700	0.31500
C	7.31200	2.89800	0.41800
N	6.68900	3.88400	1.17000
C	6.33100	2.17200	-0.20200
C	5.35200	3.75100	1.00600
N	5.11500	2.71800	0.17500
C	-3.58500	-4.25100	-1.99000
C	-2.27700	-3.97500	-1.32100
C	-1.89900	-2.77500	-0.83300
C	-1.16100	-4.88200	-1.05600
N	-0.63700	-2.86900	-0.28100
C	-0.12800	-4.14200	-0.40500
C	-0.89700	-6.24100	-1.33700
C	1.10000	-4.71600	-0.05400
C	0.33800	-6.82500	-0.99500
C	1.33500	-6.06700	-0.35600
C	-8.59500	-0.98300	0.52700
C	-7.77700	-0.03200	1.41600
C	-7.74500	-2.09100	-0.10800
C	-6.76100	0.81500	0.63900
C	-4.51900	0.48700	-2.85300
C	-5.70400	1.40500	-3.19200
C	-3.18700	0.96200	-3.44600
C	-5.60400	2.79600	-2.55400
C	0.08200	-3.61700	-3.83200
C	1.43200	-2.93000	-3.81800
O	1.91500	-2.54200	-4.87500
N	2.05300	-2.77800	-2.64400
C	3.41700	-2.24100	-2.53000
C	4.14600	-2.74700	-1.25300
O	4.42100	-3.93800	-1.14900
C	3.42200	-0.71000	-2.78400
C	2.91200	0.16300	-1.66200
O	1.59500	0.29800	-1.62600
O	3.69400	0.67600	-0.86200
N	4.46500	-1.90500	-0.26300
C	5.28100	-2.18700	0.92300
C	4.55000	-3.00800	2.00100
O	4.29000	-4.30400	1.52700
C	3.23700	-2.38200	2.45900
C	-4.40000	-2.01000	3.26400

S	-3.62000	-1.36600	1.74600
C	-1.93800	-0.99500	2.34800
O	-1.60500	-1.41800	3.46800
C	-1.04100	-0.28500	1.44500
C	-1.42900	0.36100	0.23900
C	-0.51100	0.84600	-0.66300
C	0.90600	0.79100	-0.41100
C	1.28800	0.14700	0.81800
C	0.35400	-0.33300	1.70600
H	-1.15300	1.24400	5.13100
H	-2.13500	4.29100	2.24400
H	1.24800	1.44500	4.52600
H	0.26300	4.47200	1.62300
H	1.95100	3.04500	2.75500
H	-0.43000	7.85300	-2.66700
H	-2.05600	8.54400	-2.81700
H	-3.97000	7.56300	-1.52400
H	-0.06400	5.73000	-1.48100
H	-4.95200	5.47700	-0.60100
H	-1.04900	3.65900	-0.55500
H	-3.48900	3.52000	-0.11500
H	4.70600	6.32500	-1.03800
H	3.68100	5.04700	-1.74100
H	3.34800	6.75400	-2.10400
H	9.01800	2.00200	-0.53900
H	9.33400	3.59200	0.18100
H	6.45600	1.31700	-0.85800
H	7.15700	4.57100	1.74900
H	4.19600	2.33900	-0.11600
H	4.57100	4.35200	1.46600
H	-3.52600	-5.18500	-2.54900
H	-3.82900	-3.43800	-2.67400
H	-2.51700	-1.88600	-0.85300
H	-0.19800	-2.10200	0.22200
H	-1.65800	-6.83800	-1.81800
H	0.52200	-7.87000	-1.21000
H	1.85600	-4.14100	0.45600
H	2.27900	-6.52300	-0.08300
H	-9.36500	-1.45100	1.14200
H	-8.39400	-2.77500	-0.65400
H	-7.21800	-2.64700	0.66900
H	-7.02300	-1.66400	-0.80300
H	-7.25300	-0.60900	2.17900
H	-8.46900	0.64400	1.92000
H	-7.27000	1.37600	-0.14500
H	-5.99600	0.17800	0.19600
H	-6.27800	1.51500	1.32100
H	-4.42000	0.40800	-1.77000
H	-2.41300	0.22400	-3.23600
H	-2.89500	1.91500	-3.00300
H	-3.28200	1.08000	-4.52600
H	-6.61700	0.93000	-2.83300
H	-5.78100	1.51300	-4.27500
H	-4.75500	3.34200	-2.96400
H	-5.49000	2.70200	-1.47400
H	-6.51500	3.35600	-2.76700
H	-0.63100	-3.00600	-3.28700
H	2.84200	-0.54700	-3.69500
H	4.45600	-0.40800	-2.97200
H	3.98600	-2.67300	-3.35500
H	1.61100	-3.13400	-1.80900
H	5.20600	-3.09200	2.86700
H	3.42100	-1.38800	2.86400
H	2.53900	-2.31400	1.62700
H	2.79500	-3.00500	3.23600
H	4.32700	-4.28200	0.55300
H	5.59200	-1.24400	1.37100
H	4.20100	-0.93800	-0.39100
H	-3.95500	-2.96500	3.54500
H	-5.45600	-2.14200	3.01800
H	-2.48500	0.45600	-0.00100
H	-0.83400	1.29600	-1.59500
H	2.34100	0.08200	1.05900
H	0.70100	-0.79200	2.62500
H	-4.29900	-1.28600	4.07400
H	-4.73300	-0.50800	-3.24600
H	-9.08900	-0.41100	-0.26000
H	-4.36700	-4.33400	-1.23400
H	9.16100	2.16000	1.22400
H	-1.13600	8.75900	-1.31000
H	3.02500	6.11300	-0.47800
H	-2.84500	2.66700	3.98300
H	6.17500	-2.73800	0.62600
H	0.18300	-4.60300	-3.38700
H	-0.24900	-3.72300	-4.86300
H	-1.90600	-3.40300	3.88600
H	0.03200	-1.12600	4.52900
O	0.92400	-1.17900	4.91900
O	-2.22500	-4.29200	4.11800
Cl	1.66200	2.75000	-0.42700
H	1.04200	-2.12900	5.05200
H	-2.39500	-4.22900	5.06700

d C(4)-O (Asp145): 1.47Å
d C(4)-Cl: 2.15Å
reaction coordinate: 0.68Å
Extrapolated ONIOM energy:
-1624.18547089439

C	-1.79900	2.75700	3.73600
C	-0.86400	1.94000	4.39500
C	-1.37300	3.66800	2.75400
C	0.50000	2.02900	4.06600
C	-0.01100	3.75200	2.42200
C	0.92400	2.92900	3.07400
C	-1.32200	8.09000	-2.12800
C	-1.90800	6.80600	-1.57100
C	-3.29100	6.71100	-1.32100
C	-1.07500	5.70500	-1.29100
C	-3.83800	5.52400	-0.79800
C	-1.62300	4.51900	-0.76800
C	-3.00300	4.42700	-0.52200
C	3.71300	6.05300	-1.33200
C	8.80900	2.61500	0.32400
C	7.31400	2.87700	0.42400
N	6.69700	3.86800	1.17400
C	6.32700	2.15800	-0.19600
C	5.35900	3.74600	1.00800
N	5.11500	2.71500	0.17700
C	-3.61300	-4.22400	-1.99700

C	-2.30200	-3.95600	-1.32800	H	6.44700	1.30100	-0.85100
C	-1.91700	-2.75700	-0.84000	H	7.16900	4.55300	1.75300
C	-1.19200	-4.86900	-1.06400	H	4.19000	2.34800	-0.11300
N	-0.65400	-2.85900	-0.29000	H	4.58200	4.35400	1.46500
C	-0.15200	-4.13500	-0.41600	H	-3.55200	-5.14900	-2.57100
C	-0.93600	-6.22900	-1.34500	H	-3.86100	-3.40100	-2.66700
C	1.07300	-4.71500	-0.06700	H	-2.52800	-1.86400	-0.86000
C	0.29700	-6.82100	-1.00500	H	-0.20800	-2.09500	0.21100
C	1.30000	-6.06800	-0.36900	H	-1.70100	-6.82300	-1.82400
C	-8.61000	-0.93500	0.51700	H	0.47400	-7.86600	-1.22000
C	-7.79300	0.02200	1.40200	H	1.83400	-4.14400	0.44000
C	-7.76100	-2.05600	-0.09600	H	2.24100	-6.53000	-0.09800
C	-6.76500	0.85300	0.62400	H	-9.38900	-1.38900	1.13000
C	-4.52300	0.51900	-2.85900	H	-8.41100	-2.74200	-0.64100
C	-5.69100	1.45600	-3.20400	H	-7.24600	-2.60700	0.69100
C	-3.17900	0.97700	-3.43400	H	-7.02900	-1.64300	-0.79000
C	-5.57600	2.84200	-2.55800	H	-7.28000	-0.55000	2.17600
C	0.06000	-3.60600	-3.83500	H	-8.48500	0.70800	1.89100
C	1.41500	-2.92900	-3.82000	H	-7.26400	1.40800	-0.17200
O	1.90100	-2.54400	-4.87700	H	-6.00100	0.20600	0.19500
N	2.03900	-2.78100	-2.64600	H	-6.28400	1.55800	1.30100
C	3.40600	-2.25100	-2.53400	H	-4.43700	0.43100	-1.77500
C	4.14100	-2.75900	-1.26000	H	-2.41800	0.22700	-3.21900
O	4.44600	-3.94500	-1.17300	H	-2.87700	1.92300	-2.98300
C	3.42000	-0.71900	-2.79100	H	-3.26000	1.10200	-4.51400
C	2.92100	0.15400	-1.66600	H	-6.61500	0.99300	-2.85600
O	1.60300	0.29800	-1.62600	H	-5.75600	1.57000	-4.28700
O	3.70700	0.65800	-0.86600	H	-4.71600	3.37800	-2.96000
N	4.43300	-1.92700	-0.25400	H	-5.47000	2.74100	-1.47700
C	5.26000	-2.20300	0.92600	H	-6.47700	3.41600	-2.77300
C	4.54700	-3.04700	1.99800	H	-0.64900	-2.99000	-3.29000
O	4.28300	-4.33500	1.50400	H	2.83700	-0.55500	-3.70000
C	3.23800	-2.43400	2.48400	H	4.45500	-0.42500	-2.98400
C	-4.42500	-1.97900	3.25700	H	3.97000	-2.68600	-3.36000
S	-3.63800	-1.34100	1.74000	H	1.59500	-3.13300	-1.81100
C	-1.95400	-0.98500	2.34500	H	5.21500	-3.14400	2.85400
O	-1.62600	-1.41100	3.46400	H	3.42300	-1.44400	2.90100
C	-1.04500	-0.28100	1.44400	H	2.52800	-2.35700	1.66300
C	-1.42300	0.37900	0.24300	H	2.81100	-3.07000	3.25900
C	-0.49600	0.84900	-0.66000	H	4.34000	-4.30200	0.53100
C	0.91500	0.75700	-0.41100	H	5.55700	-1.25800	1.38100
C	1.29000	0.10200	0.81000	H	4.14900	-0.96400	-0.36700
C	0.34800	-0.35900	1.70100	H	-3.99200	-2.94000	3.53600
H	-1.19200	1.23500	5.14600	H	-5.48200	-2.09700	3.01100
H	-2.09200	4.29600	2.24600	H	-2.47800	0.49500	0.00600
H	1.21900	1.39100	4.56200	H	-0.81100	1.30500	-1.59100
H	0.31500	4.43100	1.64700	H	2.34300	0.01000	1.04400
H	1.96600	2.97500	2.79400	H	0.68800	-0.83100	2.61700
H	-0.39600	7.87800	-2.66200	H	-4.31500	-1.25800	4.06800
H	-2.02900	8.55100	-2.81800	H	-4.74800	-0.47000	-3.26000
H	-3.93700	7.55200	-1.52900	H	-9.09200	-0.36900	-0.28200
H	-0.01100	5.76000	-1.47300	H	-4.39100	-4.32100	-1.24000
H	-4.89900	5.45700	-0.60800	H	9.16100	2.14100	1.24100
H	-0.97700	3.68100	-0.54800	H	-1.11700	8.77900	-1.30800
H	-3.41700	3.51500	-0.11700	H	3.03600	6.09000	-0.47800
H	4.72000	6.32600	-1.01900	H	-2.84700	2.68800	3.98000
H	3.71500	5.04300	-1.74400	H	6.16300	-2.73500	0.62000
H	3.36700	6.75000	-2.09500	H	0.15300	-4.59400	-3.39100
H	9.01600	1.95500	-0.51900	H	-0.27200	-3.70900	-4.86600
H	9.34100	3.55500	0.17400	H	-1.94900	-3.40500	3.87700

H	0.02500	-1.16000	4.52600
O	0.92000	-1.23500	4.90500
O	-2.28300	-4.29100	4.09800
Cl	1.71900	2.75100	-0.38400
H	1.02300	-2.18700	5.02500
H	-2.44600	-4.24000	5.04900

d C(4)-O (Asp145): 1.46Å
d C(4)-Cl: 2.2Å
reaction coordinate: 0.74Å
Extrapolated ONIOM energy:
-1624.18773320491

C	-1.79600	2.76000	3.74100
C	-0.87600	1.93000	4.40700
C	-1.35200	3.66200	2.75900
C	0.49100	1.99900	4.08500
C	0.01300	3.72600	2.43500
C	0.93300	2.89100	3.09300
C	-1.29000	8.10500	-2.12400
C	-1.86500	6.81400	-1.57000
C	-3.24700	6.70800	-1.32100
C	-1.02300	5.72000	-1.29200
C	-3.78400	5.51600	-0.80000
C	-1.56100	4.52900	-0.77200
C	-2.94000	4.42500	-0.52700
C	3.73400	6.04300	-1.32600
C	8.81200	2.58000	0.33300
C	7.31900	2.85300	0.42900
N	6.70900	3.85800	1.16900
C	6.32500	2.13700	-0.18500
C	5.37000	3.74500	1.00200
N	5.11700	2.70800	0.18200
C	-3.64000	-4.19900	-2.00200
C	-2.32700	-3.93800	-1.33300
C	-1.93400	-2.74200	-0.84500
C	-1.22300	-4.85900	-1.06900
N	-0.67100	-2.85200	-0.29700
C	-0.17800	-4.13100	-0.42200
C	-0.97600	-6.22100	-1.35000
C	1.04500	-4.71900	-0.07600
C	0.25400	-6.82000	-1.01200
C	1.26300	-6.07300	-0.37700
C	-8.62300	-0.88600	0.50900
C	-7.80400	0.07100	1.39000
C	-7.77900	-2.01700	-0.09400
C	-6.76900	0.89100	0.61000
C	-4.52700	0.54900	-2.86200
C	-5.68200	1.50000	-3.21300
C	-3.17300	0.99400	-3.42700
C	-5.55500	2.88300	-2.56400
C	0.03700	-3.59700	-3.83700
C	1.39800	-2.93100	-3.82100
O	1.88700	-2.55100	-4.87800
N	2.02400	-2.78600	-2.64700
C	3.39500	-2.26300	-2.53700
C	4.13500	-2.77400	-1.26700
O	4.46600	-3.95400	-1.19500
C	3.41700	-0.73100	-2.79700
C	2.92900	0.14300	-1.66900
O	1.61000	0.29500	-1.62600
O	3.72000	0.63700	-0.86800
N	4.40400	-1.95200	-0.24500
C	5.24000	-2.22100	0.92900
C	4.54300	-3.08600	1.99500
O	4.27300	-4.36500	1.48300
C	3.23800	-2.48200	2.50600
C	-4.44900	-1.94700	3.25200
S	-3.65400	-1.31800	1.73700
C	-1.96900	-0.97200	2.34400
O	-1.64500	-1.39900	3.46200
C	-1.04900	-0.27600	1.44200
C	-1.41800	0.39500	0.24700
C	-0.48200	0.85000	-0.65800
C	0.92300	0.72500	-0.41200
C	1.29100	0.06200	0.80300
C	0.34300	-0.38200	1.69800
H	-1.21800	1.23200	5.15700
H	-2.05800	4.30000	2.24700
H	1.19800	1.35200	4.58500
H	0.35400	4.39900	1.66100
H	1.97600	2.92100	2.81800
H	-0.36100	7.90200	-2.65700
H	-2.00000	8.56100	-2.81500
H	-3.90000	7.54400	-1.52700
H	0.04000	5.78500	-1.47300
H	-4.84500	5.43900	-0.61000
H	-0.90700	3.69600	-0.55400
H	-3.34700	3.50800	-0.12400
H	4.74000	6.32100	-1.01100
H	3.74300	5.03500	-1.74400
H	3.38400	6.74200	-2.08400
H	9.01500	1.91100	-0.50500
H	9.35200	3.51400	0.17500
H	6.43700	1.27400	-0.83200
H	7.18600	4.54400	1.74100
H	4.18600	2.35300	-0.10600
H	4.59600	4.36400	1.45000
H	-3.58200	-5.11800	-2.58500
H	-3.88800	-3.36900	-2.66500
H	-2.54000	-1.84500	-0.86500
H	-0.21900	-2.09100	0.20400
H	-1.74500	-6.80900	-1.82800
H	0.42400	-7.86600	-1.22700
H	1.81100	-4.15300	0.43000
H	2.20100	-6.54100	-0.10700
H	-9.40700	-1.33200	1.12300
H	-8.43100	-2.70200	-0.63600
H	-7.27100	-2.56600	0.70000
H	-7.04200	-1.61300	-0.78700
H	-7.29600	-0.49800	2.17000
H	-8.49400	0.76400	1.87400
H	-7.26200	1.44500	-0.19000
H	-6.00800	0.23700	0.18700
H	-6.28500	1.59800	1.28500
H	-4.44900	0.45800	-1.77800
H	-2.42200	0.23600	-3.20800
H	-2.86500	1.93700	-2.97300
H	-3.24600	1.12200	-4.50800
H	-6.61300	1.04700	-2.87000

H	-5.74000	1.61600	-4.29600
H	-4.68900	3.41100	-2.96300
H	-5.45400	2.78000	-1.48400
H	-6.44900	3.46800	-2.78200
H	-0.66700	-2.97600	-3.29200
H	2.83100	-0.56400	-3.70300
H	4.45400	-0.44400	-2.99400
H	3.95500	-2.70200	-3.36600
H	1.57800	-3.13300	-1.81100
H	5.22100	-3.19500	2.84200
H	3.42500	-1.49700	2.93300
H	2.51800	-2.39800	1.69600
H	2.82300	-3.13000	3.27800
H	4.34800	-4.32400	0.51200
H	5.52400	-1.27600	1.39000
H	4.10200	-0.99300	-0.34700
H	-4.02500	-2.91200	3.53200
H	-5.50700	-2.05500	3.00500
H	-2.47100	0.53100	0.01300
H	-0.79000	1.31300	-1.58800
H	2.34300	-0.05200	1.03300
H	0.67600	-0.86300	2.61100
H	-4.33200	-1.22700	4.06400
H	-4.76000	-0.43700	-3.26700
H	-9.09900	-0.32300	-0.29500
H	-4.41700	-4.30100	-1.24500
H	9.16100	2.11100	1.25400
H	-1.09200	8.79400	-1.30400
H	3.05700	6.07000	-0.47200
H	-2.84500	2.70600	3.97900
H	6.14900	-2.73800	0.61500
H	0.12300	-4.58600	-3.39400
H	-0.29500	-3.69600	-4.86900
H	-1.98800	-3.40000	3.87800
H	0.01800	-1.17900	4.52500
O	0.91500	-1.27300	4.89400
O	-2.33400	-4.28200	4.09500
Cl	1.77600	2.75200	-0.34400
H	0.99900	-2.22800	5.01300
H	-2.49600	-4.23400	5.04600

d C(4)-O (Asp145): 1.45Å
d C(4)-Cl: 2.25Å
reaction coordinate: 0.8Å
Extrapolated ONIOM energy:
-1624.19001489262

C	-1.79500	2.76100	3.74400
C	-0.89200	1.91700	4.41600
C	-1.33200	3.65800	2.76700
C	0.47800	1.96800	4.10300
C	0.03600	3.70200	2.45100
C	0.93900	2.85300	3.11400
C	-1.26400	8.11700	-2.12500
C	-1.82800	6.82200	-1.57100
C	-3.20900	6.70400	-1.31800
C	-0.97700	5.73400	-1.29400
C	-3.73500	5.50800	-0.79700
C	-1.50400	4.53900	-0.77300
C	-2.88300	4.42300	-0.52600
C	3.75200	6.03400	-1.32200
C	8.81400	2.55100	0.34000
C	7.32100	2.83300	0.43600
N	6.71700	3.84500	1.17000
C	6.32200	2.12200	-0.17600
C	5.37800	3.74200	1.00400
N	5.11700	2.70300	0.18800
C	-3.66300	-4.17700	-2.01000
C	-2.34900	-3.92200	-1.33900
C	-1.95100	-2.72700	-0.85300
C	-1.24900	-4.84700	-1.07500
N	-0.68800	-2.84200	-0.30500
C	-0.20000	-4.12300	-0.42900
C	-1.00700	-6.21000	-1.35300
C	1.02000	-4.71600	-0.08200
C	0.22000	-6.81400	-1.01400
C	1.23200	-6.07100	-0.38100
C	-8.63500	-0.84600	0.49800
C	-7.81800	0.11500	1.37700
C	-7.79300	-1.98600	-0.08900
C	-6.77400	0.92400	0.59700
C	-4.53000	0.57400	-2.86900
C	-5.66900	1.54200	-3.22500
C	-3.16500	1.00400	-3.41700
C	-5.52900	2.92100	-2.56800
C	0.01900	-3.59000	-3.84000
C	1.38500	-2.93200	-3.82200
O	1.87500	-2.55400	-4.88000
N	2.01200	-2.79100	-2.64900
C	3.38600	-2.27200	-2.54100
C	4.13200	-2.78500	-1.27400
O	4.49400	-3.95700	-1.21900
C	3.41400	-0.74100	-2.80300
C	2.93700	0.13400	-1.67000
O	1.61600	0.29300	-1.62600
O	3.73000	0.61700	-0.86800
N	4.37500	-1.97300	-0.23700
C	5.22200	-2.23700	0.93100
C	4.54200	-3.12100	1.99200
O	4.26500	-4.39200	1.46100
C	3.24400	-2.52800	2.53000
C	-4.47300	-1.91900	3.24500
S	-3.66900	-1.29800	1.73000
C	-1.98400	-0.96200	2.34200
O	-1.66500	-1.39000	3.46000
C	-1.05300	-0.27300	1.44100
C	-1.41500	0.41000	0.25100
C	-0.47100	0.85200	-0.65500
C	0.92800	0.69400	-0.41300
C	1.29000	0.02600	0.79600
C	0.33600	-0.40300	1.69400
H	-1.24900	1.22400	5.16400
H	-2.02500	4.30600	2.25000
H	1.17400	1.31200	4.60800
H	0.39200	4.37100	1.68000
H	1.98500	2.86900	2.84600
H	-0.33400	7.92100	-2.66000
H	-1.97800	8.56700	-2.81500
H	-3.86800	7.53600	-1.52300
H	0.08600	5.80700	-1.47600

H	-4.79600	5.42400	-0.60500
H	-0.84300	3.71100	-0.55600
H	-3.28200	3.50300	-0.12300
H	4.74900	6.32700	-0.99600
H	3.78100	5.03000	-1.74600
H	3.39600	6.73300	-2.08000
H	9.00900	1.85000	-0.47300
H	9.35600	3.47700	0.14500
H	6.42700	1.25500	-0.81900
H	7.19900	4.53100	1.73900
H	4.18100	2.35900	-0.09700
H	4.60700	4.36800	1.44700
H	-3.61200	-5.10400	-2.58100
H	-3.90100	-3.35300	-2.68200
H	-2.55200	-1.82700	-0.87400
H	-0.23100	-2.08300	0.19300
H	-1.77900	-6.79700	-1.83100
H	0.38600	-7.86200	-1.22700
H	1.78900	-4.15200	0.42300
H	2.16800	-6.54300	-0.11000
H	-9.42600	-1.28300	1.10900
H	-8.44400	-2.67300	-0.63100
H	-7.29300	-2.53100	0.71300
H	-7.04800	-1.59200	-0.78000
H	-7.31800	-0.45000	2.16400
H	-8.50800	0.81500	1.84900
H	-7.25900	1.47300	-0.21100
H	-6.01300	0.26300	0.18500
H	-6.29100	1.63400	1.27000
H	-4.46400	0.47600	-1.78500
H	-2.42500	0.23600	-3.19400
H	-2.85000	1.94100	-2.95600
H	-3.22400	1.13800	-4.49800
H	-6.60900	1.10000	-2.89400
H	-5.71500	1.66500	-4.30800
H	-4.65300	3.43900	-2.95800
H	-5.43700	2.81100	-1.48800
H	-6.41400	3.51700	-2.79000
H	-0.68200	-2.96500	-3.29600
H	2.82500	-0.57000	-3.70600
H	4.45200	-0.45900	-3.00400
H	3.94100	-2.71300	-3.37100
H	1.56400	-3.13300	-1.81200
H	5.23300	-3.24400	2.82700
H	3.43500	-1.54800	2.96800
H	2.51100	-2.43400	1.73200
H	2.84200	-3.18700	3.29900
H	4.36100	-4.34200	0.49200
H	5.49200	-1.29000	1.39800
H	4.05000	-1.02100	-0.32400
H	-4.05800	-2.88800	3.52600
H	-5.53100	-2.01800	2.99500
H	-2.46500	0.56400	0.01900
H	-0.77200	1.32000	-1.58500
H	2.34000	-0.10800	1.02200
H	0.66300	-0.89200	2.60600
H	-4.35200	-1.19900	4.05500
H	-4.77200	-0.40600	-3.28200
H	-9.10300	-0.28800	-0.31500
H	-4.44300	-4.26400	-1.25300
H	9.16600	2.11500	1.27600
H	-1.06900	8.80700	-1.30500
H	3.06600	6.04400	-0.47400
H	-2.84700	2.72200	3.97500
H	6.13800	-2.73600	0.60900
H	0.09700	-4.58000	-3.39900
H	-0.31300	-3.68600	-4.87200
H	-2.02800	-3.39500	3.88000
H	0.01100	-1.20200	4.52300
O	0.90900	-1.31500	4.88200
O	-2.38700	-4.27400	4.09100
Cl	1.82800	2.75400	-0.30600
H	0.97900	-2.27200	4.99000
H	-2.54700	-4.23200	5.04300

d C(4)-O (Asp145): 1.43Å
d C(4)-Cl: 2.4Å
reaction coordinate: 0.97Å
Extrapolated ONIOM energy:
-1624.196731659

C	-1.78665	2.76540	3.74930
C	-0.90703	1.90863	4.43558
C	-1.29721	3.64300	2.76742
C	0.46582	1.92515	4.13225
C	0.07328	3.65362	2.46180
C	0.95281	2.79088	3.13811
C	-1.19044	8.13879	-2.11899
C	-1.73517	6.83275	-1.57192
C	-3.11294	6.69564	-1.31412
C	-0.86880	5.75428	-1.30669
C	-3.62157	5.48852	-0.79975
C	-1.37810	4.54792	-0.79411
C	-2.75394	4.41242	-0.54213
C	3.80201	6.00442	-1.30844
C	8.82542	2.46754	0.35983
C	7.33538	2.77441	0.44867
N	6.74773	3.80679	1.16798
C	6.32433	2.07354	-0.15641
C	5.40702	3.72553	0.99864
N	5.12895	2.68201	0.19683
C	-3.71403	-4.13039	-2.02410
C	-2.39893	-3.88826	-1.35144
C	-1.98826	-2.69688	-0.86630
C	-1.30840	-4.82490	-1.08398
N	-0.72709	-2.82536	-0.31664
C	-0.25290	-4.11133	-0.43860
C	-1.08102	-6.19116	-1.36001
C	0.96188	-4.71508	-0.08965
C	0.13968	-6.80671	-1.01855
C	1.15927	-6.07282	-0.38597
C	-8.65786	-0.75192	0.47737
C	-7.84271	0.21933	1.34734
C	-7.81912	-1.91303	-0.07170
C	-6.78144	1.00303	0.56549
C	-4.53144	0.63081	-2.87892
C	-5.64578	1.62343	-3.24420
C	-3.15221	1.03413	-3.41243
C	-5.48278	2.99668	-2.58266
C	-0.02336	-3.57775	-3.84645

C	1.35200	-2.93680	-3.82430
O	1.84499	-2.56117	-4.88097
N	1.98535	-2.80741	-2.65126
C	3.36582	-2.30177	-2.54665
C	4.11873	-2.82129	-1.28440
O	4.52422	-3.97951	-1.25524
C	3.40982	-0.76935	-2.80768
C	2.94701	0.10209	-1.66782
O	1.62198	0.27893	-1.62801
O	3.73956	0.56176	-0.85631
N	4.32387	-2.02969	-0.22378
C	5.18392	-2.28355	0.93690
C	4.52686	-3.19729	1.98695
O	4.22797	-4.45052	1.42549
C	3.24300	-2.61367	2.56981
C	-4.52692	-1.84552	3.23398
S	-3.69926	-1.25530	1.71933
C	-2.02023	-0.92834	2.34456
O	-1.71204	-1.34294	3.46813
C	-1.06697	-0.25988	1.43894
C	-1.41424	0.43777	0.25698
C	-0.45678	0.84181	-0.65815
C	0.92416	0.61364	-0.42516
C	1.27975	-0.04220	0.78216
C	0.31630	-0.43413	1.69140
H	-1.28418	1.23183	5.18896
H	-1.97106	4.30313	2.24082
H	1.14514	1.26128	4.64885
H	0.45113	4.30710	1.68742
H	2.00020	2.78276	2.87445
H	-0.25875	7.95992	-2.65640
H	-1.91232	8.58378	-2.80433
H	-3.78356	7.52019	-1.50940
H	0.19254	5.84232	-1.49127
H	-4.67964	5.38998	-0.60252
H	-0.70290	3.72899	-0.58602
H	-3.13856	3.48423	-0.14399
H	4.75419	6.35609	-0.91312
H	3.92850	5.01751	-1.75510
H	3.44319	6.69944	-2.06793
H	9.00130	1.68815	-0.38272
H	9.37135	3.36436	0.06509
H	6.41418	1.19785	-0.78991
H	7.23853	4.49366	1.72738
H	4.17975	2.36782	-0.08404
H	4.64316	4.37095	1.42636
H	-3.67686	-5.06554	-2.58294
H	-3.93505	-3.31146	-2.70903
H	-2.57906	-1.78978	-0.89009
H	-0.25877	-2.07231	0.18002
H	-1.85805	-6.77028	-1.83723
H	0.29479	-7.85656	-1.23027
H	1.73629	-4.15842	0.41409
H	2.09075	-6.55397	-0.11360
H	-9.46194	-1.16700	1.08671
H	-8.46935	-2.60369	-0.60961
H	-7.33871	-2.44694	0.74916
H	-7.05947	-1.54181	-0.75907
H	-7.35885	-0.33390	2.15293
H	-8.53202	0.93554	1.79626
H	-7.25016	1.53923	-0.25999
H	-6.02080	0.32678	0.17717
H	-6.30108	1.72205	1.22965
H	-4.47809	0.52867	-1.79435
H	-2.43081	0.24967	-3.18402
H	-2.82284	1.96315	-2.94573
H	-3.19786	1.17128	-4.49351
H	-6.59829	1.20052	-2.92240
H	-5.67930	1.74909	-4.32724
H	-4.59418	3.49815	-2.96593
H	-5.39825	2.88237	-1.50189
H	-6.35435	3.61180	-2.80777
H	-0.71771	-2.94418	-3.30369
H	2.81870	-0.59039	-3.70772
H	4.44936	-0.49902	-3.01114
H	3.91263	-2.74605	-3.38049
H	1.53452	-3.14513	-1.81417
H	5.23543	-3.34637	2.80213
H	3.44655	-1.64503	3.02576
H	2.49213	-2.49930	1.79169
H	2.85738	-3.29001	3.33257
H	4.36571	-4.39022	0.46269
H	5.43527	-1.33614	1.41344
H	3.96853	-1.08724	-0.28981
H	-4.12645	-2.81521	3.53143
H	-5.58348	-1.93333	2.97434
H	-2.46027	0.63018	0.03366
H	-0.74362	1.31582	-1.58935
H	2.32554	-0.21198	1.00148
H	0.63120	-0.92943	2.60343
H	-4.40424	-1.11563	4.03538
H	-4.78951	-0.34304	-3.29731
H	-9.10768	-0.20643	-0.35361
H	-4.49933	-4.19318	-1.27027
H	9.18894	2.12291	1.32856
H	-1.00414	8.82700	-1.29437
H	3.06788	5.93971	-0.50546
H	-2.84042	2.75297	3.97117
H	6.10856	-2.75890	0.60477
H	0.04170	-4.56942	-3.40594
H	-0.35331	-3.66928	-4.87972
H	-2.11507	-3.35864	3.92185
H	-0.00734	-1.21750	4.53145
O	0.89518	-1.36837	4.86439
O	-2.50047	-4.22727	4.12533
Cl	1.95078	2.77517	-0.24113
H	0.93331	-2.32871	4.96121
H	-2.66088	-4.18847	5.07700

2) Water molecules fixed at 90º

d C(4)-O (Asp145): 3.4Å
d C(4)-Cl: 1.76Å
reaction coordinate: -1.64Å
Extrapolated ONIOM energy:
-1624.21286950242

C	-1.85800	3.28300	3.37100
C	-0.99200	3.75100	4.37500
C	-1.76100	3.79300	2.06400
C	-0.02900	4.73200	4.07200
C	-0.79900	4.77300	1.76100
C	0.06600	5.24200	2.76500
C	-0.70100	7.80700	-2.51100
C	-1.08600	6.37100	-2.20900
C	-2.34800	6.08100	-1.65700
C	-0.18400	5.32200	-2.47300
C	-2.70900	4.75100	-1.37700
C	-0.54400	3.99100	-2.19400
C	-1.80800	3.70500	-1.64600
C	4.21800	5.54700	-1.59800
C	9.11600	1.89400	0.18800
C	7.62200	1.68800	0.33000
N	6.83200	2.15800	1.36800
C	6.81300	1.00800	-0.54300
C	5.56300	1.76600	1.12700
N	5.53100	1.07200	-0.02500
C	-3.55700	-4.38800	-2.33900
C	-2.41200	-3.60200	-1.77800
C	-1.97400	-2.40000	-2.22600
C	-1.53200	-3.96000	-0.66800
N	-0.85500	-2.02000	-1.50700
C	-0.55900	-2.93000	-0.51900
C	-1.44100	-5.06100	0.21100
C	0.44900	-2.97900	0.45000
C	-0.42500	-5.12800	1.18400
C	0.51300	-4.08800	1.30900
C	-8.44700	-0.85300	0.04800
C	-7.50100	-0.22900	1.08700
C	-7.75500	-1.89500	-0.84100
C	-6.43000	0.68100	0.47200
C	-4.23100	0.38400	-3.25300
C	-5.53200	1.20200	-3.29300
C	-3.12600	0.96200	-4.14600
C	-5.40100	2.58800	-2.65200
C	0.17700	-3.95400	-4.10500
C	1.51200	-3.24900	-4.01000
O	2.06300	-2.88500	-5.04200
N	2.04400	-3.05900	-2.79900
C	3.38000	-2.49100	-2.58600
C	4.08100	-3.10600	-1.35600
O	4.28000	-4.31600	-1.30100
C	3.32100	-0.94500	-2.60100
C	2.47000	-0.28400	-1.48700
O	1.25000	-0.13600	-1.70500
O	3.09800	0.07200	-0.43200
N	4.49300	-2.31300	-0.36500
C	5.33900	-2.75200	0.75100
C	4.53600	-3.33200	1.92400
O	3.76800	-4.42000	1.48100
C	3.62900	-2.29300	2.58000
C	-4.35800	-2.76800	2.36300
S	-3.52500	-1.47700	1.37600
C	-2.17800	-1.13200	2.50100
O	-2.17500	-1.65900	3.61100
C	-1.12700	-0.17700	2.07700
C	-1.03700	0.34800	0.78100
C	-0.01700	1.22800	0.43500
C	0.90000	1.60000	1.41200
C	0.83300	1.10000	2.71200
C	-0.17500	0.20200	3.03900
H	-1.07000	3.35600	5.37800
H	-2.42300	3.42700	1.29400
H	0.63400	5.09500	4.84500
H	-0.71900	5.16100	0.75400
H	0.80500	5.99500	2.53000
H	0.02800	7.83600	-3.32200
H	-1.58300	8.37300	-2.81100
H	-3.04400	6.88100	-1.44700
H	0.78800	5.53500	-2.89500
H	-3.67900	4.53600	-0.95300
H	0.15100	3.18900	-2.40300
H	-2.08500	2.68300	-1.43100
H	4.97300	6.05100	-0.99500
H	4.39700	4.47200	-1.58700
H	4.26700	5.91400	-2.62300
H	9.48500	1.36000	-0.68900
H	9.33300	2.95600	0.07200
H	7.10800	0.51500	-1.46300
H	7.15000	2.70000	2.16200
H	4.65600	0.66200	-0.40500
H	4.68100	1.95800	1.73400
H	-3.28900	-5.44400	-2.38000
H	-3.79400	-4.03900	-3.34300
H	-2.40800	-1.85000	-3.05000
H	-0.27300	-1.19000	-1.67000
H	-2.15400	-5.86800	0.12400
H	-0.35600	-5.99100	1.83600
H	1.16200	-2.17000	0.52000
H	1.29100	-4.15200	2.05900
H	-9.26400	-1.34400	0.57800
H	-8.49200	-2.34400	-1.50800
H	-7.31500	-2.67700	-0.22200
H	-6.97900	-1.42600	-1.44300
H	-7.01500	-1.02100	1.65800
H	-8.09800	0.36800	1.77800
H	-6.90600	1.47400	-0.10500
H	-5.76800	0.10600	-0.17400
H	-5.83700	1.12900	1.26900
H	-3.87100	0.32600	-2.22500
H	-2.24300	0.32400	-4.10300
H	-2.84600	1.96000	-3.80900
H	-3.47400	1.01800	-5.17800
H	-6.30100	0.64800	-2.75400
H	-5.85900	1.31400	-4.32800
H	-4.72100	3.21200	-3.23200

H	-5.02700	2.49100	-1.63200
H	-6.37900	3.06800	-2.62700
H	-0.57900	-3.22900	-4.39200
H	2.91200	-0.67800	-3.57700
H	4.35500	-0.56800	-2.55100
H	4.00000	-2.78300	-3.43600
H	1.53200	-3.36400	-1.98200
H	5.24000	-3.69300	2.67400
H	4.23300	-1.48800	2.99600
H	2.93600	-1.87800	1.85100
H	3.06200	-2.76500	3.38300
H	3.90200	-4.50600	0.52200
H	5.92200	-1.90700	1.11500
H	4.13800	-1.35900	-0.38700
H	-3.62400	-3.50900	2.68200
H	-5.10200	-3.22200	1.70800
H	-1.74900	0.04400	0.02000
H	0.10200	1.56700	-0.58200
H	1.54700	1.42300	3.46100
H	-0.25400	-0.20200	4.04200
H	-4.83900	-2.32900	3.23800
H	-4.45400	-0.62800	-3.59300
H	-8.87200	-0.06600	-0.57800
H	-4.42900	-4.26400	-1.69700
H	9.62800	1.51400	1.07300
H	-0.26700	8.26100	-1.62000
H	3.22900	5.75200	-1.18700
H	-2.59500	2.53000	3.60300
H	6.03300	-3.51900	0.40200
H	-0.07100	-4.42200	-3.15500
H	0.24800	-4.72000	-4.87500
H	-1.24000	-3.26600	4.13700
H	-2.90800	-1.22000	5.34500
O	-3.22000	-0.92500	6.21400
O	-0.94700	-4.18800	4.10600
Cl	2.13600	2.79700	1.03100
H	-3.14900	-1.71600	6.76200
H	-0.74100	-4.31400	3.16800

d C(4)-O (Asp145): 2.4Å
d C(4)-Cl: 1.76Å
reaction coordinate: -0.63Å
Extrapolated ONIOM energy:
-1624.20017342589

C	-2.23300	2.36400	3.51100
C	-1.05400	2.45100	4.27200
C	-2.41200	3.19900	2.39500
C	-0.05400	3.37400	3.91700
C	-1.41300	4.12200	2.03800
C	-0.23400	4.21000	2.79900
C	-2.35200	7.33100	-2.23100
C	-3.24100	6.28100	-1.59600
C	-4.51300	6.63700	-1.10800
C	-2.79900	4.94800	-1.48300
C	-5.34100	5.66700	-0.51500
C	-3.62800	3.98000	-0.88900
C	-4.89900	4.33800	-0.40600
C	2.95200	6.24900	-1.31600
C	8.55300	3.79100	0.44700
C	7.09800	3.41000	0.32200
N	6.01800	4.14500	0.78700
C	6.62200	2.26000	-0.24500
C	4.90000	3.44400	0.50600
N	5.24800	2.30500	-0.11700
C	-2.32400	-5.19500	-2.27100
C	-1.40300	-4.15500	-1.70600
C	-1.27600	-2.87700	-2.14200
C	-0.45900	-4.29500	-0.60200
N	-0.28600	-2.23700	-1.41600
C	0.23800	-3.06100	-0.44800
C	-0.10200	-5.34600	0.27100
C	1.24200	-2.87600	0.50800
C	0.90500	-5.17200	1.24000
C	1.57700	-3.94300	1.35700
C	-7.90600	-2.92100	0.13500
C	-7.18300	-2.15500	1.25500
C	-6.94600	-3.71600	-0.76000
C	-6.34200	-0.97700	0.74700
C	-4.07600	-0.69100	-3.11500
C	-5.48900	-0.10400	-2.97100
C	-3.13600	0.19200	-3.94600
C	-5.53100	1.19000	-2.15000
C	1.21500	-3.88300	-4.00300
C	2.34000	-2.87900	-3.88200
O	2.78700	-2.36900	-4.90200
N	2.81100	-2.59500	-2.66400
C	3.97900	-1.73500	-2.43800
C	4.81600	-2.19100	-1.22300
O	5.31900	-3.31000	-1.20900
C	3.56200	-0.24600	-2.43800
C	2.60900	0.20800	-1.30900
O	1.37900	0.11300	-1.49200
O	3.16900	0.69000	-0.26000
N	5.01700	-1.35600	-0.20000
C	5.94400	-1.60800	0.90900
C	5.31900	-2.42400	2.04900
O	4.85300	-3.65300	1.55400
C	4.18100	-1.67600	2.74100
C	-3.36900	-3.41000	2.97100
S	-2.97700	-2.41800	1.48900
C	-1.68800	-1.40800	2.19900
O	-1.26700	-1.66800	3.32800
C	-1.14300	-0.31900	1.37700
C	-1.74300	0.12500	0.18800
C	-1.14400	1.11500	-0.57700
C	0.08400	1.63400	-0.16200
C	0.64500	1.28400	1.06700
C	0.04500	0.29100	1.81600
H	-0.92700	1.80600	5.13100
H	-3.32200	3.13200	1.81700
H	0.84800	3.44200	4.50800
H	-1.55600	4.76600	1.18100
H	0.52900	4.92400	2.52600
H	-1.64700	6.86100	-2.91700
H	-2.96100	8.04600	-2.78600
H	-4.85700	7.65900	-1.18800
H	-1.82200	4.66500	-1.84800
H	-6.31700	5.94500	-0.14300
H	-3.28800	2.95900	-0.79700

H	-5.53700	3.59300	0.05000
H	3.80700	6.84900	-1.00800
H	3.29600	5.31000	-1.74900
H	2.37700	6.79800	-2.06300
H	9.13500	3.29700	-0.33200
H	8.66800	4.87000	0.34000
H	7.20100	1.46100	-0.69500
H	6.06600	5.03600	1.26700
H	4.55700	1.57700	-0.37500
H	3.87100	3.70500	0.74600
H	-1.80900	-6.15400	-2.31500
H	-2.63900	-4.91000	-3.27500
H	-1.83800	-2.44200	-2.95700
H	0.04800	-1.27600	-1.54600
H	-0.60600	-6.29700	0.18500
H	1.17800	-5.99200	1.89200
H	1.74200	-1.92100	0.58100
H	2.35900	-3.82600	2.09600
H	-8.60600	-3.62100	0.59300
H	-7.52300	-4.28400	-1.49100
H	-6.36300	-4.41000	-0.15400
H	-6.27300	-3.04400	-1.29000
H	-6.54300	-2.84100	1.81000
H	-7.93400	-1.76300	1.94200
H	-6.97400	-0.28400	0.19200
H	-5.53700	-1.33300	0.10500
H	-5.90300	-0.45400	1.59800
H	-3.64800	-0.84800	-2.12600
H	-2.16400	-0.29000	-4.04200
H	-2.99700	1.16000	-3.46400
H	-3.55600	0.34600	-4.94100
H	-6.11800	-0.84300	-2.47500
H	-5.90700	0.08600	-3.96000
H	-5.02200	1.99300	-2.68400
H	-5.05300	1.03500	-1.18200
H	-6.56900	1.48300	-1.99100
H	0.30900	-3.35700	-4.28900
H	3.08700	-0.07400	-3.40600
H	4.48200	0.35800	-2.40100
H	4.64500	-1.86300	-3.29300
H	2.38800	-3.02900	-1.85500
H	6.09300	-2.62600	2.79000
H	4.56200	-0.75900	3.18900
H	3.40000	-1.42600	2.02700
H	3.76000	-2.30500	3.52600
H	5.00500	-3.66300	0.59400
H	6.28700	-0.65800	1.31700
H	4.44200	-0.51600	-0.19100
H	-2.53700	-4.07500	3.20700
H	-4.26000	-3.99200	2.72900
H	-2.69000	-0.29900	-0.12900
H	-1.58600	1.45300	-1.50600
H	1.58000	1.72700	1.37500
H	0.48600	-0.04200	2.74900
H	-3.56100	-2.74700	3.81600
H	-4.15700	-1.66200	-3.60600
H	-8.47700	-2.22100	-0.47700
H	-3.20200	-5.28600	-1.63000
H	8.93100	3.48300	1.42300
H	-1.80000	7.85700	-1.45100
H	2.31500	6.04300	-0.45600
H	-3.00200	1.65700	3.78600
H	6.81400	-2.15400	0.53900
H	1.07800	-4.41100	-3.06200
H	1.47600	-4.59700	-4.78100
H	-1.93100	-0.87300	4.88200
H	0.12300	-2.68400	4.13400
O	0.81300	-3.30400	4.41400
O	-2.49200	-0.47600	5.56700
Cl	0.74600	3.02200	-1.02900
H	0.88200	-3.89400	3.65200
H	-2.36400	-1.04800	6.33400

d C(4)-O (Asp145): 2.2Å
d C(4)-Cl: 1.78Å
reaction coordinate: -0.42Å
Extrapolated ONIOM energy:
-1624.19149478969

C	-2.15600	2.41300	3.50900
C	-1.00300	2.49400	4.30900
C	-2.27000	3.21300	2.35900
C	0.03600	3.37600	3.96000
C	-1.23400	4.09600	2.00900
C	-0.08100	4.17900	2.81000
C	-2.16700	7.37700	-2.25500
C	-3.05600	6.32800	-1.61900
C	-4.31600	6.69200	-1.10600
C	-2.62600	4.99000	-1.52900
C	-5.14400	5.72300	-0.51100
C	-3.45600	4.02200	-0.93400
C	-4.71500	4.38800	-0.42600
C	3.10900	6.16400	-1.34200
C	8.64800	3.57100	0.42400
C	7.17800	3.25100	0.32600
N	6.13800	4.02300	0.82200
C	6.64600	2.12800	-0.24300
C	4.98800	3.36900	0.55700
N	5.27800	2.22400	-0.08600
C	-2.45400	-5.14700	-2.26000
C	-1.50700	-4.12200	-1.70700
C	-1.35200	-2.85200	-2.15400
C	-0.56700	-4.27200	-0.60000
N	-0.35100	-2.22500	-1.43200
C	0.15300	-3.05100	-0.45400
C	-0.23500	-5.32200	0.28400
C	1.15300	-2.87600	0.50800
C	0.76900	-5.15900	1.25800
C	1.46300	-3.94200	1.36900
C	-7.97400	-2.72600	0.14400
C	-7.23800	-1.97200	1.26300
C	-7.03100	-3.55200	-0.74100
C	-6.36600	-0.81800	0.75300
C	-4.09200	-0.60200	-3.11600
C	-5.49200	0.01400	-2.96400
C	-3.14100	0.25700	-3.95800
C	-5.50200	1.31300	-2.15000
C	1.11600	-3.92900	-3.99800
C	2.24100	-2.92700	-3.87100
O	2.68100	-2.40100	-4.88700

N	2.72300	-2.66300	-2.65300
C	3.90800	-1.82900	-2.42900
C	4.73600	-2.30700	-1.21500
O	5.18200	-3.45000	-1.19200
C	3.52200	-0.33200	-2.43500
C	2.60800	0.16400	-1.29600
O	1.36700	0.14300	-1.47100
O	3.19200	0.61400	-0.25300
N	4.98800	-1.47100	-0.20500
C	5.90500	-1.75900	0.90400
C	5.24400	-2.53400	2.05200
O	4.73400	-3.75200	1.57200
C	4.13200	-1.73400	2.72800
C	-3.49800	-3.27800	2.99100
S	-3.03300	-2.34300	1.49300
C	-1.74700	-1.33300	2.21600
O	-1.36900	-1.56900	3.36600
C	-1.15700	-0.29000	1.37700
C	-1.71800	0.13600	0.16000
C	-1.06800	1.06800	-0.63100
C	0.19400	1.53100	-0.23200
C	0.69000	1.24200	1.04700
C	0.03800	0.30600	1.82200
H	-0.92500	1.87400	5.19200
H	-3.15900	3.14900	1.75000
H	0.91800	3.43900	4.58100
H	-1.32700	4.71200	1.12500
H	0.71100	4.86200	2.54200
H	-1.47600	6.90700	-2.95700
H	-2.77700	8.10200	-2.79500
H	-4.65000	7.71700	-1.16800
H	-1.65800	4.70000	-1.91300
H	-6.11100	6.00600	-0.11900
H	-3.12400	2.99800	-0.86000
H	-5.35300	3.64500	0.03200
H	3.94800	6.73000	-0.93900
H	3.46500	5.22400	-1.76300
H	2.62500	6.74700	-2.12600
H	9.19100	3.07400	-0.38100
H	8.80400	4.64700	0.33900
H	7.18500	1.31200	-0.71300
H	6.23100	4.90500	1.31000
H	4.56200	1.52300	-0.34000
H	3.97600	3.67000	0.82200
H	-1.96200	-6.11900	-2.29300
H	-2.76200	-4.86600	-3.26700
H	-1.90700	-2.41300	-2.97100
H	-0.01200	-1.26700	-1.56000
H	-0.75700	-6.26400	0.20400
H	1.02100	-5.97700	1.92000
H	1.67000	-1.93000	0.58100
H	2.23900	-3.83200	2.11400
H	-8.69400	-3.40500	0.60300
H	-7.61800	-4.10900	-1.47200
H	-6.46900	-4.25700	-0.12700
H	-6.33800	-2.90000	-1.27100
H	-6.61700	-2.67100	1.82500
H	-7.98200	-1.55800	1.94400
H	-6.98000	-0.11100	0.19400
H	-5.57000	-1.19600	0.11200
H	-5.91500	-0.30300	1.60200
H	-3.66000	-0.76400	-2.13000
H	-2.18000	-0.24600	-4.06000
H	-2.97800	1.22400	-3.48300
H	-3.56600	0.41400	-4.95100
H	-6.13100	-0.71000	-2.45800
H	-5.91400	0.20600	-3.95100
H	-4.98000	2.10200	-2.69200
H	-5.02000	1.15200	-1.18500
H	-6.53200	1.62900	-1.98400
H	0.21400	-3.40400	-4.30000
H	3.03800	-0.15600	-3.39700
H	4.45600	0.25100	-2.41400
H	4.57000	-1.97300	-3.28400
H	2.30600	-3.10900	-1.84700
H	6.00600	-2.75500	2.80000
H	4.54300	-0.82400	3.16000
H	3.36100	-1.47000	2.00700
H	3.68600	-2.33400	3.52200
H	4.87700	-3.77500	0.61100
H	6.29500	-0.82400	1.30200
H	4.45200	-0.60600	-0.19800
H	-2.69300	-3.95800	3.27300
H	-4.39700	-3.84300	2.74000
H	-2.68100	-0.25400	-0.15100
H	-1.48600	1.39600	-1.57500
H	1.62200	1.68000	1.36900
H	0.43800	0.01000	2.78500
H	-3.69500	-2.58600	3.81100
H	-4.19800	-1.57400	-3.60100
H	-8.52400	-2.01600	-0.47600
H	-3.33300	-5.20900	-1.61800
H	9.03600	3.22500	1.38300
H	-1.59900	7.88900	-1.47900
H	2.38700	5.96000	-0.55100
H	-2.95400	1.73700	3.77800
H	6.74600	-2.35000	0.53700
H	0.96600	-4.45000	-3.05600
H	1.38500	-4.64900	-4.76800
H	-2.02600	-0.76000	4.90000
H	0.00000	-2.61200	4.15300
O	0.67800	-3.25500	4.41000
O	-2.55600	-0.36600	5.61100
Cl	0.85800	2.94700	-1.07600
H	0.72100	-3.83100	3.63600
H	-2.42500	-0.96400	6.35700

d C(4)-O (Asp145): 2.0Å
d C(4)-Cl: 1.80Å
reaction coordinate: -0.2Å
Extrapolated ONIOM energy:
-1624.18044549713

C	-2.05300	2.48000	3.50400
C	-0.92800	2.55200	4.34300
C	-2.09800	3.23900	2.32300
C	0.15300	3.38500	4.00100
C	-1.02000	4.07300	1.97800
C	0.10600	4.14700	2.81800
C	-1.92800	7.42100	-2.29700

C	-2.82300	6.38100	-1.65500	H	-1.05900	4.65400	1.06700
C	-4.06800	6.76100	-1.11800	H	0.93100	4.79100	2.55400
C	-2.41400	5.03500	-1.58400	H	-1.25500	6.94700	-3.01200
C	-4.90200	5.80000	-0.51700	H	-2.53400	8.16000	-2.82100
C	-3.24900	4.07600	-0.98400	H	-4.38600	7.79200	-1.16500
C	-4.49300	4.45800	-0.45100	H	-1.45700	4.73300	-1.98700
C	3.30800	6.04000	-1.39100	H	-5.85700	6.09600	-0.10600
C	8.76300	3.27500	0.37500	H	-2.93200	3.04500	-0.92600
C	7.27200	3.06700	0.32500	H	-5.13400	3.72100	0.01300
N	6.30800	3.89200	0.88300	H	4.16400	6.57800	-0.98500
C	6.64300	2.00300	-0.25800	H	3.62800	5.07400	-1.78100
C	5.10500	3.32900	0.64300	H	2.86500	6.62400	-2.19900
N	5.29300	2.18900	-0.04600	H	9.23600	2.79000	-0.48000
C	-2.62700	-5.08500	-2.23600	H	8.99400	4.34000	0.34600
C	-1.64700	-4.08400	-1.70200	H	7.10600	1.16700	-0.77100
C	-1.46100	-2.82300	-2.16200	H	6.48200	4.74900	1.39500
C	-0.70700	-4.24700	-0.59600	H	4.53600	1.53500	-0.30300
N	-0.44400	-2.21400	-1.44900	H	4.13000	3.69300	0.95800
C	0.04100	-3.04100	-0.46200	H	-2.16800	-6.07400	-2.25200
C	-0.40000	-5.29600	0.29700	H	-2.92700	-4.81200	-3.24800
C	1.04000	-2.87800	0.50300	H	-2.01200	-2.37700	-2.97900
C	0.60300	-5.14500	1.27400	H	-0.10300	-1.25800	-1.57500
C	1.32100	-3.94100	1.37700	H	-0.94600	-6.22500	0.22800
C	-8.05900	-2.47200	0.16900	H	0.83300	-5.96100	1.94700
C	-7.30200	-1.73500	1.28600	H	1.57400	-1.94200	0.57300
C	-7.14100	-3.33700	-0.70400	H	2.09100	-3.83900	2.13000
C	-6.38800	-0.61600	0.77200	H	-8.80400	-3.12200	0.62900
C	-4.11800	-0.49400	-3.11100	H	-7.74300	-3.87800	-1.43400
C	-5.50200	0.15800	-2.96900	H	-6.60600	-4.05500	-0.08200
C	-3.13900	0.34000	-3.94700	H	-6.42200	-2.71400	-1.23600
C	-5.48300	1.46100	-2.16200	H	-6.70800	-2.45100	1.85600
C	0.97600	-3.99500	-3.98900	H	-8.03400	-1.29100	1.96100
C	2.10900	-3.00400	-3.86000	H	-6.97400	0.10900	0.20700
O	2.54600	-2.46800	-4.87200	H	-5.60400	-1.02600	0.13600
N	2.60400	-2.76400	-2.64400	H	-5.92200	-0.11200	1.61900
C	3.81500	-1.97000	-2.42300	H	-3.69700	-0.66500	-2.12100
C	4.61700	-2.47300	-1.20300	H	-2.19000	-0.18800	-4.04200
O	4.97400	-3.64700	-1.15100	H	-2.95400	1.30300	-3.47000
C	3.48300	-0.46100	-2.45200	H	-3.55200	0.50800	-4.94200
C	2.62700	0.10400	-1.30800	H	-6.16200	-0.54700	-2.46400
O	1.37500	0.16900	-1.47900	H	-5.91400	0.35600	-3.96000
O	3.23600	0.53000	-0.28200	H	-4.94300	2.23600	-2.70700
N	4.94500	-1.63100	-0.22100	H	-5.00600	1.29500	-1.19600
C	5.84700	-1.95900	0.88900	H	-6.50600	1.80100	-2.00000
C	5.14400	-2.66300	2.05900	H	0.08100	-3.46400	-4.30300
O	4.58700	-3.87300	1.61600	H	2.98700	-0.28400	-3.40800
C	4.06300	-1.79400	2.69900	H	4.43600	0.08700	-2.45900
C	-3.64500	-3.11000	3.01900	H	4.47400	-2.14800	-3.27500
S	-3.10400	-2.24500	1.50400	H	2.19300	-3.21800	-1.83900
C	-1.80700	-1.24600	2.23300	H	5.89100	-2.89100	2.81900
O	-1.46500	-1.46500	3.40100	H	4.51000	-0.88600	3.10100
C	-1.16600	-0.25800	1.37900	H	3.30500	-1.52500	1.96600
C	-1.68500	0.16300	0.14000	H	3.59000	-2.34600	3.51200
C	-0.97500	1.02300	-0.67600	H	4.69300	-3.91500	0.65000
C	0.33400	1.40400	-0.30000	H	6.30100	-1.04400	1.26600
C	0.76800	1.16200	1.02300	H	4.48100	-0.72700	-0.23400
C	0.05200	0.30100	1.82100	H	-2.87800	-3.81300	3.34400
H	-0.90300	1.96300	5.25000	H	-4.56100	-3.64500	2.76300
H	-2.96500	3.17900	1.68300	H	-2.67100	-0.17100	-0.16500
H	1.01400	3.44100	4.65200	H	-1.36900	1.35200	-1.62900

H	1.70500	1.58100	1.35600
H	0.41400	0.03600	2.80800
H	-3.83300	-2.38600	3.81300
H	-4.24500	-1.46300	-3.59600
H	-8.58000	-1.74700	-0.45800
H	-3.50700	-5.10700	-1.59200
H	9.16300	2.84400	1.29400
H	-1.34000	7.91900	-1.52500
H	2.56300	5.88900	-0.60900
H	-2.88400	1.84200	3.76700
H	6.64500	-2.61300	0.53100
H	0.81100	-4.50800	-3.04500
H	1.24400	-4.72400	-4.75100
H	-2.10800	-0.63600	4.91500
H	-0.13000	-2.54900	4.16900
O	0.53200	-3.21500	4.40900
O	-2.60600	-0.23800	5.64900
Cl	0.99200	2.88200	-1.09300
H	0.53500	-3.79000	3.63200
H	-2.48600	-0.86400	6.37300

d C(4)-O (Asp145): 1.9Å
d C(4)-Cl: 1.82Å
reaction coordinate: -0.07Å
Extrapolated ONIOM energy:
-1624.17497541097

C	-1.92300	2.54100	3.49200
C	-0.79900	2.55100	4.33600
C	-1.91200	3.28200	2.29800
C	0.33600	3.30500	3.98700
C	-0.77800	4.03600	1.94700
C	0.34600	4.04800	2.79200
C	-1.63900	7.47600	-2.33200
C	-2.55400	6.45600	-1.68600
C	-3.79000	6.86300	-1.14800
C	-2.17300	5.10200	-1.61000
C	-4.64300	5.92300	-0.54200
C	-3.02700	4.16200	-1.00500
C	-4.26100	4.57200	-0.47100
C	3.53900	5.88100	-1.44600
C	8.88300	2.89800	0.30500
C	7.37600	2.87000	0.33800
N	6.54900	3.77500	0.98700
C	6.59200	1.91700	-0.24700
C	5.27500	3.36900	0.79800
N	5.28500	2.24800	0.05200
C	-2.85800	-4.99100	-2.21700
C	-1.83400	-4.02700	-1.69900
C	-1.60400	-2.77800	-2.17100
C	-0.89600	-4.21800	-0.59700
N	-0.56100	-2.20200	-1.46700
C	-0.10200	-3.04000	-0.47700
C	-0.62700	-5.26900	0.30600
C	0.90500	-2.90600	0.48500
C	0.38000	-5.14500	1.28200
C	1.14200	-3.96800	1.37300
C	-8.16400	-2.14400	0.20400
C	-7.39500	-1.42400	1.32400
C	-7.26600	-3.04600	-0.65300
C	-6.43700	-0.34200	0.81100
C	-4.16000	-0.34500	-3.10300
C	-5.51500	0.36600	-2.96100
C	-3.13900	0.45700	-3.92000
C	-5.44100	1.66300	-2.14700
C	0.77900	-4.05800	-3.99200
C	1.95000	-3.11400	-3.87300
O	2.41400	-2.60900	-4.88900
N	2.44900	-2.88000	-2.65800
C	3.70300	-2.15700	-2.44300
C	4.45400	-2.68500	-1.20100
O	4.67700	-3.88800	-1.09200
C	3.46500	-0.63200	-2.51100
C	2.69200	0.02600	-1.36400
O	1.43200	0.15000	-1.50300
O	3.35200	0.46000	-0.38200
N	4.88100	-1.83800	-0.26400
C	5.75500	-2.20800	0.85400
C	5.00200	-2.80600	2.05200
O	4.38900	-4.00800	1.66900
C	3.96300	-1.85000	2.63500
C	-3.80700	-2.92000	3.03800
S	-3.19700	-2.11900	1.51400
C	-1.85300	-1.17600	2.24300
O	-1.53600	-1.40400	3.41800
C	-1.14900	-0.24200	1.38600
C	-1.62900	0.20700	0.13900
C	-0.85700	1.00300	-0.68300
C	0.48700	1.29500	-0.31700
C	0.89300	1.02100	1.01600
C	0.11000	0.23000	1.82000
H	-0.81700	1.97600	5.25200
H	-2.77700	3.26800	1.65400
H	1.19600	3.31200	4.64100
H	-0.77400	4.60100	1.02600
H	1.21300	4.63100	2.52100
H	-0.97400	6.98500	-3.04400
H	-2.23100	8.22300	-2.86200
H	-4.08700	7.90100	-1.19800
H	-1.22300	4.77900	-2.01200
H	-5.59000	6.23900	-0.12900
H	-2.73100	3.12500	-0.94400
H	-4.91700	3.85200	-0.00200
H	4.40800	6.40400	-1.04800
H	3.82800	4.88500	-1.78200
H	3.13500	6.44100	-2.29000
H	9.24300	2.45000	-0.62200
H	9.24100	3.92700	0.35800
H	6.92100	1.05700	-0.82000
H	6.85400	4.58000	1.52100
H	4.46000	1.68100	-0.19900
H	4.37300	3.83300	1.18900
H	-2.44700	-6.00100	-2.20900
H	-3.14000	-4.72500	-3.23600
H	-2.14700	-2.31700	-2.98500
H	-0.20400	-1.25300	-1.59000
H	-1.20900	-6.17700	0.24800
H	0.57700	-5.96100	1.96600
H	1.47300	-1.99100	0.54600
H	1.91000	-3.88400	2.13000

H	-8.93500	-2.76500	0.66100
H	-7.87800	-3.57400	-1.38500
H	-6.76200	-3.77700	-0.01900
H	-6.52100	-2.45100	-1.18100
H	-6.83300	-2.15500	1.90700
H	-8.12000	-0.94900	1.98600
H	-6.99100	0.39800	0.23200
H	-5.66000	-0.78500	0.18800
H	-5.96300	0.15300	1.65900
H	-3.75400	-0.54800	-2.11300
H	-2.21700	-0.11600	-4.02400
H	-2.90900	1.39800	-3.42200
H	-3.54100	0.66600	-4.91200
H	-6.20600	-0.31200	-2.46000
H	-5.91600	0.58700	-3.95100
H	-4.86900	2.41600	-2.68900
H	-4.97100	1.47200	-1.18200
H	-6.44900	2.04500	-1.98300
H	-0.09500	-3.49400	-4.30400
H	2.95300	-0.45200	-3.45700
H	4.44900	-0.14600	-2.56000
H	4.35800	-2.39600	-3.28200
H	2.01800	-3.30800	-1.84900
H	5.72900	-3.03200	2.83300
H	4.45300	-0.94700	2.99500
H	3.22600	-1.58000	1.88100
H	3.45400	-2.33400	3.46900
H	4.43800	-4.07300	0.69900
H	6.29000	-1.32400	1.19800
H	4.52900	-0.88500	-0.32300
H	-3.09000	-3.66600	3.38200
H	-4.75400	-3.39800	2.78500
H	-2.63700	-0.05300	-0.16800
H	-1.23000	1.36000	-1.63600
H	1.85600	1.37400	1.35300
H	0.45000	-0.04900	2.81100
H	-3.95100	-2.17100	3.81900
H	-4.32700	-1.30000	-3.60300
H	-8.65400	-1.40800	-0.43500
H	-3.74000	-4.95700	-1.57700
H	9.27900	2.33400	1.15000
H	-1.04300	7.96700	-1.56300
H	2.77400	5.79600	-0.67400
H	-2.79600	1.96400	3.75900
H	6.49100	-2.94100	0.51700
H	0.59800	-4.56100	-3.04500
H	1.01400	-4.80000	-4.75200
H	-2.13600	-0.52400	4.91400
H	-0.28000	-2.56300	4.18900
O	0.35900	-3.25900	4.40900
O	-2.61400	-0.12100	5.65900
Cl	1.17000	2.82500	-1.03800
H	0.33900	-3.81300	3.61700
H	-2.52400	-0.77100	6.36600

d C(4)-O (Asp145): 1.85Å
d C(4)-Cl: 1.84Å
reaction coordinate: -0.01Å
Extrapolated ONIOM energy:
-1624.17265062581

C	-1.86200	2.55900	3.49000
C	-0.73500	2.51400	4.33000
C	-1.82000	3.30000	2.29800
C	0.43400	3.21300	3.97600
C	-0.65300	3.99900	1.94200
C	0.47400	3.95600	2.78200
C	-1.50300	7.50900	-2.33600
C	-2.42400	6.49600	-1.68700
C	-3.65800	6.91100	-1.15200
C	-2.04900	5.14000	-1.60800
C	-4.51500	5.97700	-0.54300
C	-2.90800	4.20600	-1.00100
C	-4.14100	4.62400	-0.46800
C	3.64300	5.81000	-1.45900
C	8.92900	2.71900	0.28200
C	7.42200	2.77300	0.34700
N	6.65900	3.70700	1.03100
C	6.57300	1.87800	-0.23900
C	5.36000	3.37600	0.86100
N	5.29300	2.27200	0.09300
C	-2.97500	-4.93000	-2.21600
C	-1.92800	-3.99200	-1.70200
C	-1.67700	-2.74600	-2.16900
C	-0.99000	-4.20600	-0.60400
N	-0.61900	-2.19400	-1.46800
C	-0.17200	-3.04500	-0.48400
C	-0.74100	-5.26500	0.29500
C	0.84000	-2.93600	0.47500
C	0.27000	-5.16400	1.27000
C	1.05600	-4.00200	1.36200
C	-8.21700	-1.97500	0.21400
C	-7.44000	-1.26400	1.33300
C	-7.33100	-2.89300	-0.63800
C	-6.46200	-0.20000	0.81900
C	-4.18400	-0.25800	-3.10100
C	-5.52300	0.48400	-2.96200
C	-3.13700	0.52600	-3.90100
C	-5.42300	1.77500	-2.14200
C	0.67600	-4.07100	-3.99800
C	1.86800	-3.15200	-3.88300
O	2.34500	-2.66500	-4.90000
N	2.36900	-2.92400	-2.66800
C	3.64500	-2.24200	-2.45500
C	4.36700	-2.78000	-1.20200
O	4.52600	-3.99000	-1.06600
C	3.46100	-0.71000	-2.54600
C	2.73600	-0.00200	-1.40000
O	1.47200	0.14700	-1.52000
O	3.42600	0.44100	-0.44800
N	4.83800	-1.93500	-0.28300
C	5.69800	-2.32300	0.83800
C	4.92900	-2.87300	2.04800
O	4.29400	-4.07100	1.69200
C	3.90800	-1.88200	2.60600
C	-3.89100	-2.81900	3.04300

S	-3.24900	-2.05100	1.51500
C	-1.87900	-1.14000	2.24500
O	-1.57800	-1.37200	3.42500
C	-1.13900	-0.23800	1.38900
C	-1.59600	0.23200	0.13900
C	-0.78900	0.98900	-0.68500
C	0.57000	1.23000	-0.32200
C	0.96500	0.92400	1.01200
C	0.14300	0.17600	1.81700
H	-0.77600	1.93900	5.24500
H	-2.68800	3.32900	1.65800
H	1.29600	3.17600	4.62600
H	-0.62500	4.56400	1.02100
H	1.36700	4.49500	2.50600
H	-0.83500	7.01300	-3.04000
H	-2.09100	8.25400	-2.87300
H	-3.95000	7.95000	-1.20600
H	-1.10100	4.81000	-2.00800
H	-5.46200	6.29900	-0.13200
H	-2.61700	3.16800	-0.93500
H	-4.80000	3.90900	0.00400
H	4.53000	6.31800	-1.08200
H	3.90300	4.80100	-1.78000
H	3.24200	6.36400	-2.30800
H	9.24400	2.27800	-0.66500
H	9.34400	3.72500	0.35500
H	6.84100	1.01300	-0.83700
H	7.01800	4.48300	1.57500
H	4.43800	1.75000	-0.16100
H	4.49500	3.88300	1.28100
H	-2.58800	-5.94900	-2.21100
H	-3.25500	-4.65700	-3.23400
H	-2.21600	-2.26900	-2.97600
H	-0.25600	-1.24700	-1.58200
H	-1.34200	-6.16000	0.23600
H	0.45000	-5.98400	1.95300
H	1.42700	-2.03200	0.53600
H	1.82400	-3.93400	2.12100
H	-8.99900	-2.58300	0.67200
H	-7.95000	-3.41500	-1.36900
H	-6.83900	-3.62900	-0.00100
H	-6.57800	-2.31100	-1.16700
H	-6.89200	-2.00100	1.92100
H	-8.15800	-0.77300	1.99100
H	-7.00100	0.54600	0.23500
H	-5.69100	-0.65800	0.20100
H	-5.98300	0.29100	1.66700
H	-3.79200	-0.48000	-2.10900
H	-2.23000	-0.06800	-4.00600
H	-2.88500	1.45500	-3.38900
H	-3.52600	0.75900	-4.89300
H	-6.23300	-0.18100	-2.46800
H	-5.91300	0.71800	-3.95300
H	-4.83400	2.51800	-2.67900
H	-4.95800	1.56900	-1.17700
H	-6.42200	2.17700	-1.97700
H	-0.18800	-3.48800	-4.30400
H	2.94100	-0.52700	-3.48800
H	4.46100	-0.26200	-2.61900
H	4.29600	-2.51500	-3.28700
H	1.92600	-3.33700	-1.85800
H	5.64900	-3.09600	2.83600
H	4.41800	-0.98300	2.94900
H	3.18200	-1.61100	1.84400
H	3.38600	-2.33800	3.44700
H	4.31300	-4.14400	0.72100
H	6.26700	-1.45400	1.16700
H	4.54500	-0.96500	-0.36800
H	-3.19700	-3.58100	3.39900
H	-4.84900	-3.27400	2.78700
H	-2.61400	0.01600	-0.17100
H	-1.14800	1.36200	-1.63600
H	1.94600	1.22700	1.34800
H	0.47200	-0.12000	2.80800
H	-4.02000	-2.06000	3.81600
H	-4.37000	-1.20400	-3.61100
H	-8.69500	-1.23300	-0.42700
H	-3.85400	-4.87600	-1.57300
H	9.31100	2.11100	1.10300
H	-0.91100	8.00400	-1.56600
H	2.88700	5.75900	-0.67600
H	-2.76000	2.02300	3.75900
H	6.40600	-3.08700	0.51000
H	0.49000	-4.57400	-3.05200
H	0.89200	-4.81600	-4.76200
H	-2.15700	-0.48600	4.92000
H	-0.36100	-2.57700	4.17500
O	0.26200	-3.28800	4.39300
O	-2.61200	-0.07100	5.67200
Cl	1.26900	2.80100	-0.98800
H	0.23300	-3.83700	3.59800
H	-2.53700	-0.72900	6.37400

d C(4)-O (Asp145): 1.8Å
d C(4)-Cl: 1.87Å
reaction coordinate: 0.07Å
Extrapolated ONIOM energy:
-1624.17075427738

C	-1.81882	2.55662	3.49663
C	-0.68221	2.44703	4.31684
C	-1.76242	3.31653	2.31655
C	0.51181	3.09755	3.95557
C	-0.57047	3.96712	1.95304
C	0.56677	3.85762	2.77280
C	-1.40983	7.54729	-2.30691
C	-2.33389	6.53183	-1.66574
C	-3.57394	6.94467	-1.14242
C	-1.95661	5.17729	-1.58015
C	-4.43432	6.00956	-0.53979
C	-2.81884	4.24238	-0.97961
C	-4.05667	4.65846	-0.45816
C	3.71228	5.76990	-1.44552
C	8.95554	2.59554	0.27466
C	7.45201	2.70799	0.36094
N	6.73421	3.67119	1.05383
C	6.56023	1.84744	-0.21427
C	5.42076	3.39199	0.90012
N	5.29958	2.29123	0.13357
C	-3.06349	-4.86922	-2.23010

C	-1.99766	-3.95729	-1.71085	H	6.78439	0.97329	-0.81585
C	-1.72894	-2.71042	-2.16385	H	7.13031	4.43361	1.59136
C	-1.05923	-4.20118	-0.62044	H	4.42620	1.80000	-0.11789
N	-0.66013	-2.18482	-1.46109	H	4.58239	3.93535	1.32896
C	-0.22095	-3.05626	-0.49060	H	-2.69735	-5.89607	-2.23263
C	-0.82644	-5.27409	0.26693	H	-3.33798	-4.58348	-3.24577
C	0.79657	-2.97566	0.46489	H	-2.26583	-2.21455	-2.96084
C	0.18850	-5.20072	1.24013	H	-0.29598	-1.23724	-1.55717
C	0.99511	-4.05438	1.34164	H	-1.44414	-6.15748	0.20123
C	-8.25775	-1.84781	0.22014	H	0.35471	-6.03020	1.91539
C	-7.47548	-1.14091	1.33944	H	1.39946	-2.08419	0.53339
C	-7.37791	-2.77189	-0.63166	H	1.76457	-4.00657	2.10042
C	-6.48735	-0.08722	0.82480	H	-9.04385	-2.44996	0.67784
C	-4.20578	-0.17733	-3.09573	H	-8.00060	-3.29028	-1.36130
C	-5.53233	0.58689	-2.96464	H	-6.88941	-3.50981	0.00574
C	-3.13492	0.59574	-3.87595	H	-6.62146	-2.19502	-1.16207
C	-5.41556	1.87116	-2.13618	H	-6.93576	-1.88229	1.92972
C	0.59703	-4.05767	-4.01597	H	-8.19091	-0.64314	1.99518
C	1.80236	-3.15645	-3.90003	H	-7.01864	0.66144	0.23662
O	2.28719	-2.67550	-4.91706	H	-5.71737	-0.55410	0.21141
N	2.30706	-2.93713	-2.68572	H	-6.00750	0.40236	1.67275
C	3.59971	-2.28520	-2.47437	H	-3.82819	-0.41475	-2.10110
C	4.30349	-2.83470	-1.21529	H	-2.23962	-0.01623	-3.98138
O	4.42282	-4.04848	-1.06827	H	-2.86906	1.51206	-3.34898
C	3.45668	-0.75028	-2.57833	H	-3.51062	0.84946	-4.86805
C	2.77530	-0.00903	-1.42975	H	-6.25762	-0.06750	-2.48029
O	1.50677	0.16083	-1.53206	H	-5.90961	0.83431	-3.95776
O	3.48817	0.43543	-0.50037	H	-4.81188	2.60781	-2.66604
N	4.80160	-1.99726	-0.30441	H	-4.95876	1.65192	-1.17071
C	5.65228	-2.40040	0.81820	H	-6.40956	2.28870	-1.97391
C	4.87495	-2.92957	2.03186	H	-0.26069	-3.45972	-4.31066
O	4.22630	-4.12335	1.68448	H	2.92627	-0.56086	-3.51312
C	3.86685	-1.92187	2.58193	H	4.46613	-0.33082	-2.67152
C	-3.94928	-2.75490	3.03872	H	4.24508	-2.58170	-3.30302
S	-3.28863	-2.00072	1.51164	H	1.85926	-3.34392	-1.87543
C	-1.89288	-1.12715	2.24486	H	5.59112	-3.15599	2.82220
O	-1.59807	-1.37753	3.42274	H	4.38863	-1.02989	2.92508
C	-1.12597	-0.24424	1.39425	H	3.14820	-1.64191	1.81588
C	-1.56374	0.25038	0.14622	H	3.33337	-2.36777	3.42235
C	-0.72886	0.97459	-0.67782	H	4.23020	-4.19629	0.71365
C	0.64265	1.17111	-0.31854	H	6.24073	-1.54353	1.14314
C	1.02966	0.82483	1.01228	H	4.54941	-1.01741	-0.40201
C	0.17571	0.11306	1.81669	H	-3.27466	-3.53499	3.39294
H	-0.73417	1.85955	5.22337	H	-4.91881	-3.18534	2.78247
H	-2.63829	3.39607	1.69190	H	-2.58967	0.07664	-0.16506
H	1.38189	3.00930	4.58963	H	-1.07709	1.36859	-1.62550
H	-0.53028	4.54472	1.04009	H	2.02406	1.07979	1.34758
H	1.48026	4.35706	2.48877	H	0.49855	-0.20711	2.80187
H	-0.73018	7.05092	-3.00007	H	-4.05948	-1.99427	3.81300
H	-1.99478	8.28586	-2.85581	H	-4.40224	-1.11543	-3.61640
H	-3.86803	7.98295	-1.20067	H	-8.72977	-1.10270	-0.42199
H	-1.00351	4.84927	-1.97074	H	-3.94088	-4.80163	-1.58630
H	-5.38517	6.33025	-0.13743	H	9.32433	1.97171	1.08991
H	-2.52543	3.20496	-0.90949	H	-0.83056	8.04945	-1.53196
H	-4.71801	3.94250	0.00946	H	2.96733	5.73358	-0.65032
H	4.61265	6.26682	-1.08565	H	-2.73681	2.05781	3.76962
H	3.95216	4.75572	-1.76559	H	6.34305	-3.18054	0.49202
H	3.30592	6.32565	-2.29103	H	0.41044	-4.56609	-3.07280
H	9.23990	2.14348	-0.67662	H	0.79700	-4.79853	-4.78744
H	9.41070	3.58408	0.34297	H	-2.15365	-0.48739	4.91948

H	-0.42294	-2.62425	4.15615
O	0.18990	-3.34933	4.35725
O	-2.59704	-0.07280	5.67909
Cl	1.35225	2.79202	-0.91965
H	0.15577	-3.87587	3.54737
H	-2.53470	-0.74224	6.37087

d C(4)-O (Asp145): 1.75Å
d C(4)-Cl: 1.92Å
reaction coordinate: 0.17Å
Extrapolated ONIOM energy:
-1624.16978185218

C	-1.69600	2.56900	3.61700
C	-0.53400	2.29900	4.36100
C	-1.61900	3.35800	2.45700
C	0.70700	2.81200	3.94200
C	-0.38000	3.87300	2.03700
C	0.78300	3.59800	2.77800
C	-1.20100	7.79600	-1.99200
C	-2.10200	6.69700	-1.46300
C	-3.40600	7.00600	-1.03100
C	-1.63900	5.36900	-1.38800
C	-4.24300	5.99400	-0.52800
C	-2.47800	4.35800	-0.88400
C	-3.77800	4.67000	-0.45200
C	3.85900	5.79200	-1.27200
C	8.99800	2.36200	0.26000
C	7.50600	2.57800	0.37200
N	6.86500	3.54900	1.12500
C	6.54800	1.81800	-0.23800
C	5.53200	3.37400	0.97400
N	5.32500	2.32900	0.14900
C	-3.34600	-4.54300	-2.27000
C	-2.16100	-3.90100	-1.62400
C	-1.77700	-2.61200	-1.77200
C	-1.22100	-4.49600	-0.68000
N	-0.64200	-2.38000	-1.01800
C	-0.27700	-3.49800	-0.30000
C	-1.08000	-5.77400	-0.09900
C	0.74600	-3.75000	0.62100
C	-0.04800	-6.04200	0.82000
C	0.86200	-5.03400	1.18000
C	-8.37700	-1.39800	0.36000
C	-7.42500	-0.77500	1.39400
C	-7.65400	-2.29000	-0.65800
C	-6.46600	0.26400	0.79800
C	-4.31400	0.21600	-2.97100
C	-5.64700	0.95600	-3.16300
C	-3.12100	0.93900	-3.60700
C	-5.71100	2.29900	-2.42700
C	0.31500	-3.82000	-4.09100
C	1.60100	-3.03500	-4.00100
O	2.10800	-2.59400	-5.02500
N	2.14300	-2.86900	-2.79600
C	3.48300	-2.31700	-2.60100
C	4.13500	-2.89200	-1.32500
O	4.09200	-4.10100	-1.11000
C	3.45400	-0.77600	-2.72200
C	2.86200	0.01100	-1.55800
O	1.58600	0.19900	-1.60200
O	3.62800	0.45100	-0.67600
N	4.75000	-2.07800	-0.46700
C	5.50800	-2.51500	0.70500
C	4.63000	-2.86400	1.91600
O	3.89100	-4.01900	1.63000
C	3.68300	-1.73800	2.32100
C	-3.98100	-2.64300	3.06600
S	-3.39800	-1.78700	1.56200
C	-1.86500	-1.11200	2.23900
O	-1.52700	-1.47800	3.37400
C	-1.05200	-0.26200	1.39600
C	-1.47200	0.30600	0.17000
C	-0.59800	0.97300	-0.66000
C	0.79000	1.08500	-0.31900
C	1.18400	0.62800	0.97700
C	0.29200	-0.04000	1.78100
H	-0.59800	1.69400	5.25500
H	-2.51300	3.56700	1.89000
H	1.59600	2.59500	4.51500
H	-0.32100	4.47200	1.14000
H	1.73200	3.98700	2.44400
H	-0.43500	7.37200	-2.64200
H	-1.78900	8.51500	-2.56300
H	-3.76700	8.02400	-1.08300
H	-0.63800	5.11900	-1.70900
H	-5.24300	6.23600	-0.19400
H	-2.11500	3.34200	-0.81500
H	-4.41900	3.89600	-0.05500
H	4.78400	6.22000	-0.88800
H	4.05100	4.79700	-1.67300
H	3.46900	6.42900	-2.06700
H	9.23700	1.90900	-0.70300
H	9.52200	3.31500	0.33900
H	6.70000	0.96300	-0.88900
H	7.31900	4.25100	1.69800
H	4.42200	1.90400	-0.12500
H	4.74000	3.95200	1.44300
H	-3.10600	-5.57200	-2.53600
H	-3.62300	-3.99400	-3.17100
H	-2.29200	-1.87500	-2.37400
H	-0.22300	-1.46000	-0.90200
H	-1.78300	-6.55300	-0.35700
H	0.04700	-7.02600	1.26000
H	1.43400	-2.96900	0.90400
H	1.65000	-5.25100	1.89200
H	-9.10900	-2.00800	0.89100
H	-8.39000	-2.75900	-1.31200
H	-7.09400	-3.06800	-0.13800
H	-6.97300	-1.69600	-1.26600
H	-6.84500	-1.56300	1.87500
H	-8.02600	-0.28200	2.15900
H	-7.03500	1.05100	0.30200
H	-5.79300	-0.20700	0.08200
H	-5.87000	0.70500	1.59800
H	-4.12700	0.07800	-1.90600
H	-2.22300	0.33000	-3.50200
H	-2.95300	1.89700	-3.11400
H	-3.31200	1.10900	-4.66700
H	-6.44800	0.32100	-2.78400

H	-5.82100	1.12200	-4.22700
H	-4.99700	3.00200	-2.85600
H	-5.48800	2.15300	-1.37100
H	-6.71400	2.71700	-2.52400
H	-0.51600	-3.12400	-4.15800
H	2.91200	-0.55500	-3.64300
H	4.48700	-0.43200	-2.84600
H	4.10300	-2.67600	-3.42400
H	1.68200	-3.25700	-1.98400
H	5.28300	-3.08300	2.76200
H	4.25700	-0.85600	2.60400
H	3.02100	-1.48600	1.49600
H	3.08200	-2.06200	3.17100
H	3.89400	-4.14800	0.66500
H	6.19000	-1.72000	1.00300
H	4.62300	-1.08100	-0.62000
H	-3.32100	-3.48000	3.29600
H	-4.98700	-3.00500	2.84900
H	-2.51300	0.21800	-0.13100
H	-0.92900	1.39900	-1.59900
H	2.20400	0.78600	1.29400
H	0.61700	-0.43100	2.73900
H	-3.99500	-1.95200	3.90900
H	-4.40200	-0.77100	-3.42900
H	-8.91100	-0.60600	-0.16700
H	-4.18400	-4.53700	-1.57200
H	9.33400	1.69800	1.05800
H	-0.72200	8.30500	-1.15500
H	3.12200	5.72600	-0.47200
H	-2.65000	2.17400	3.93400
H	6.10400	-3.39400	0.45100
H	0.20700	-4.46500	-3.22200
H	0.34600	-4.43100	-4.99100
H	-1.85400	-0.68200	4.99600
H	-0.47400	-2.94800	3.85600
O	0.10100	-3.72100	3.97000
O	-2.17600	-0.31800	5.83800
Cl	1.53900	2.79100	-0.78200
H	0.10000	-4.12200	3.09000
H	-2.08400	-1.05700	6.45200

d C(4)-O (Asp145): 1.58Å
d C(4)-Cl: 1.9Å
reaction coordinate: 0.31Å
Extrapolated ONIOM energy:
-1624.17103996769

C	-1.67700	2.72900	3.77400
C	-1.32200	1.75900	4.72700
C	-0.68200	3.33700	2.98900
C	0.02600	1.39500	4.89300
C	0.66600	2.97200	3.15200
C	1.02100	2.00100	4.10600
C	-0.63300	8.06300	-2.58600
C	-1.30900	7.09600	-1.63400
C	-2.52700	7.44800	-1.02100
C	-0.72300	5.84700	-1.35100
C	-3.15700	6.55600	-0.13400
C	-1.35400	4.95600	-0.46400
C	-2.57100	5.30900	0.14400
C	4.20200	5.65300	-1.61400
C	8.96700	1.87100	0.26300
C	7.51000	2.26500	0.38900
N	6.99800	3.32300	1.12600
C	6.45900	1.61200	-0.19000
C	5.65100	3.30500	0.99300
N	5.30800	2.27400	0.19600
C	-3.92100	-4.01500	-2.12500
C	-2.62400	-3.69900	-1.46000
C	-2.19900	-2.45900	-1.13800
C	-1.58200	-4.61400	-1.00600
N	-0.95800	-2.53800	-0.53900
C	-0.53200	-3.84000	-0.43100
C	-1.40300	-6.01400	-1.03700
C	0.62900	-4.41900	0.09000
C	-0.23400	-6.60700	-0.52100
C	0.78000	-5.81300	0.04300
C	-8.68300	-0.25200	0.17200
C	-7.68700	0.49300	1.07700
C	-8.04100	-1.41400	-0.59700
C	-6.60000	1.25200	0.30600
C	-4.42500	0.75500	-3.15400
C	-4.64000	2.27600	-3.16400
C	-3.08500	0.31800	-3.75700
C	-3.68600	3.03300	-2.23400
C	-0.17500	-3.75600	-3.89800
C	1.17300	-3.06400	-3.84200
O	1.69100	-2.67900	-4.88300
N	1.75800	-2.91300	-2.65000
C	3.14500	-2.45300	-2.49700
C	3.81000	-3.02900	-1.21900
O	3.92200	-4.24600	-1.09600
C	3.25300	-0.92200	-2.72700
C	2.82200	0.00500	-1.60600
O	1.55600	0.33000	-1.60300
O	3.65800	0.42100	-0.79000
N	4.25600	-2.22300	-0.25000
C	5.02600	-2.62200	0.93300
C	4.18200	-3.27200	2.04200
O	3.67100	-4.49900	1.59300
C	3.03200	-2.38800	2.51700
C	-4.36300	-2.34000	2.63900
S	-3.78600	-1.01800	1.51900
C	-2.05100	-0.95800	2.07700
O	-1.74300	-1.66200	3.04800
C	-1.12200	-0.15100	1.32000
C	-1.44800	0.60500	0.16000
C	-0.49100	1.19000	-0.62600
C	0.92500	1.06200	-0.32700
C	1.23400	0.37300	0.91000
C	0.25000	-0.20100	1.67300
H	-2.08400	1.28800	5.33200
H	-0.95200	4.08300	2.25600
H	0.28700	0.63900	5.62300
H	1.42400	3.42900	2.53300
H	2.05400	1.70900	4.22900
H	0.01400	7.52000	-3.27600
H	-1.38500	8.60400	-3.16100
H	-2.98100	8.40600	-1.23000
H	0.21200	5.56300	-1.81400

H	-4.09300	6.83000	0.33300
H	-0.90200	3.99700	-0.25200
H	-3.05800	4.62100	0.82100
H	5.18500	5.92500	-1.23100
H	4.20100	4.60500	-1.91600
H	3.96500	6.27500	-2.47700
H	9.12800	1.33900	-0.67600
H	9.59800	2.76000	0.27500
H	6.49400	0.73100	-0.82300
H	7.54100	3.97800	1.67600
H	4.36200	1.95400	-0.07300
H	4.94100	3.98600	1.45500
H	-3.83100	-4.94600	-2.68500
H	-4.19400	-3.21000	-2.80800
H	-2.76400	-1.54800	-1.29500
H	-0.49900	-1.72900	-0.12500
H	-2.18100	-6.63800	-1.45400
H	-0.11600	-7.68300	-0.54100
H	1.39400	-3.80900	0.54000
H	1.67100	-6.27500	0.45400
H	-9.48200	-0.65300	0.79700
H	-8.81300	-1.94900	-1.15100
H	-7.56500	-2.10300	0.10100
H	-7.30000	-1.03900	-1.30200
H	-7.21400	-0.21800	1.75600
H	-8.24500	1.21300	1.67700
H	-7.05900	1.94900	-0.39600
H	-5.96400	0.55300	-0.23600
H	-5.98200	1.81100	1.01000
H	-4.49100	0.38600	-2.13000
H	-3.05000	-0.77000	-3.81000
H	-2.25800	0.66800	-3.14000
H	-2.98200	0.72400	-4.76400
H	-5.66200	2.47900	-2.84000
H	-4.52400	2.65300	-4.18100
H	-2.65900	2.93400	-2.58300
H	-3.76700	2.64400	-1.21800
H	-3.95200	4.09000	-2.23100
H	-0.93400	-3.07700	-3.52300
H	2.68300	-0.71200	-3.63300
H	4.30600	-0.69600	-2.92500
H	3.70700	-2.90400	-3.31600
H	1.29000	-3.27100	-1.83000
H	4.83200	-3.47000	2.89400
H	3.42600	-1.45900	2.92900
H	2.36300	-2.16200	1.69200
H	2.47200	-2.91300	3.29200
H	3.74400	-4.51800	0.62200
H	5.51300	-1.74200	1.35200
H	4.11200	-1.22900	-0.38500
H	-3.74100	-3.22700	2.51500
H	-5.39600	-2.55400	2.35700
H	-2.48900	0.71600	-0.13400
H	-0.76200	1.74600	-1.51600
H	2.27000	0.32600	1.22100
H	0.51400	-0.73000	2.58300
H	-4.31600	-2.00600	3.67500
H	-5.22700	0.29500	-3.73200
H	-9.12500	0.45000	-0.53700
H	-4.69800	-4.12400	-1.36800
H	9.24500	1.22000	1.09200
H	-0.03500	8.77400	-2.01600
H	3.44800	5.80800	-0.84200
H	-2.71400	3.00500	3.65000
H	5.80100	-3.33200	0.63800
H	-0.13500	-4.67000	-3.31100
H	-0.39800	-4.00700	-4.93300
H	-1.66000	-1.37500	4.97200
H	-1.03900	-3.52200	2.87600
O	-0.77800	-4.45600	2.85100
O	-1.68100	-1.31200	5.94200
Cl	1.79700	2.74500	-0.45300
H	-0.60100	-4.63700	1.91800
H	-1.72100	-2.23500	6.22100

d C(4)-O (Asp145): 1.54Å
d C(4)-Cl: 1.95Å
reaction coordinate: 0.41Å
Extrapolated ONIOM energy:
-1624.17298763639

C	-1.69400	2.72800	3.77800
C	-1.35400	1.76200	4.74100
C	-0.68900	3.30400	2.98000
C	-0.01300	1.37100	4.90600
C	0.65200	2.91200	3.14200
C	0.99000	1.94600	4.10600
C	-0.62400	8.08400	-2.57400
C	-1.28500	7.09600	-1.63300
C	-2.51100	7.42100	-1.02000
C	-0.67800	5.85500	-1.36000
C	-3.12800	6.51000	-0.14400
C	-1.29500	4.94400	-0.48300
C	-2.52100	5.27100	0.12400
C	4.20600	5.66400	-1.59500
C	8.96000	1.87200	0.28700
C	7.50500	2.27700	0.41300
N	7.00000	3.33600	1.15400
C	6.44700	1.63800	-0.17200
C	5.65400	3.33200	1.01800
N	5.30200	2.30900	0.21600
C	-3.93400	-3.98900	-2.12900
C	-2.63500	-3.69000	-1.45800
C	-2.20300	-2.45600	-1.11900
C	-1.59600	-4.61600	-1.01900
N	-0.96200	-2.55000	-0.52100
C	-0.54100	-3.85500	-0.43400
C	-1.42300	-6.01600	-1.07200
C	0.62000	-4.44800	0.07200
C	-0.25500	-6.62200	-0.56900
C	0.76500	-5.84200	0.00300
C	-8.69400	-0.21900	0.16200
C	-7.70500	0.54000	1.06400
C	-8.04000	-1.37800	-0.60100
C	-6.62400	1.30500	0.29000
C	-4.42800	0.78400	-3.15500
C	-4.60800	2.30900	-3.18300
C	-3.10500	0.30800	-3.76800
C	-3.62800	3.05600	-2.27400
C	-0.18400	-3.73500	-3.89500

C	1.16700	-3.04800	-3.83700
O	1.68500	-2.66300	-4.87800
N	1.75500	-2.89900	-2.64600
C	3.14600	-2.44500	-2.49700
C	3.81800	-3.02200	-1.22200
O	3.97000	-4.23600	-1.12100
C	3.26600	-0.91600	-2.73900
C	2.85100	0.01200	-1.61800
O	1.57600	0.33100	-1.60200
O	3.68700	0.42900	-0.80800
N	4.22500	-2.22200	-0.23000
C	5.01000	-2.61500	0.94600
C	4.18800	-3.31500	2.04200
O	3.69600	-4.53900	1.56200
C	3.02400	-2.46900	2.55100
C	-4.39100	-2.28700	2.66500
S	-3.80100	-0.99500	1.51800
C	-2.06800	-0.92900	2.08900
O	-1.77000	-1.62600	3.06800
C	-1.12600	-0.14100	1.32600
C	-1.43600	0.60800	0.15800
C	-0.46600	1.14100	-0.65000
C	0.94800	0.98600	-0.35700
C	1.24500	0.27800	0.87400
C	0.24900	-0.24100	1.66100
H	-2.12300	1.31500	5.35600
H	-0.94500	4.04500	2.23900
H	0.23600	0.62100	5.64400
H	1.41600	3.34400	2.51300
H	2.01700	1.63300	4.22700
H	0.03200	7.55900	-3.26900
H	-1.38400	8.62000	-3.14300
H	-2.98100	8.37300	-1.22200
H	0.26300	5.59200	-1.82100
H	-4.07000	6.76200	0.32200
H	-0.82700	3.99100	-0.27900
H	-2.99800	4.56700	0.79200
H	5.19800	5.91200	-1.21900
H	4.18000	4.62100	-1.91100
H	3.97100	6.30300	-2.44700
H	9.11400	1.32300	-0.64300
H	9.59600	2.75800	0.28000
H	6.47600	0.76100	-0.80900
H	7.54800	3.98400	1.70800
H	4.35100	2.00600	-0.05700
H	4.94900	4.01900	1.48100
H	-3.86000	-4.92900	-2.67500
H	-4.18500	-3.18800	-2.82600
H	-2.76200	-1.54000	-1.26500
H	-0.49900	-1.74900	-0.09600
H	-2.20500	-6.63000	-1.49600
H	-0.14200	-7.69800	-0.60600
H	1.39100	-3.84900	0.52900
H	1.65500	-6.31300	0.40400
H	-9.48900	-0.62500	0.78900
H	-8.80600	-1.92300	-1.15300
H	-7.55700	-2.05900	0.10100
H	-7.30200	-0.99900	-1.30700
H	-7.22500	-0.16300	1.74700
H	-8.26900	1.25800	1.66000
H	-7.08800	1.99100	-0.41900
H	-5.98000	0.60800	-0.24400
H	-6.01400	1.87500	0.99100
H	-4.49100	0.42800	-2.12600
H	-3.09100	-0.78100	-3.79800
H	-2.26300	0.65400	-3.16900
H	-3.00800	0.69200	-4.78400
H	-5.62100	2.53900	-2.85200
H	-4.49500	2.66900	-4.20600
H	-2.60500	2.92400	-2.62700
H	-3.71300	2.68800	-1.25100
H	-3.86500	4.12000	-2.28900
H	-0.94100	-3.05600	-3.51300
H	2.68900	-0.70500	-3.64200
H	4.31800	-0.70000	-2.94600
H	3.70200	-2.90400	-3.31800
H	1.28500	-3.25100	-1.82400
H	4.84900	-3.52400	2.88300
H	3.40100	-1.54200	2.98200
H	2.34100	-2.23900	1.73900
H	2.48400	-3.02500	3.31800
H	3.78500	-4.53900	0.59200
H	5.46700	-1.72600	1.38200
H	4.05800	-1.23100	-0.34800
H	-3.78900	-3.18900	2.54800
H	-5.43100	-2.48400	2.39900
H	-2.47400	0.74600	-0.13200
H	-0.72800	1.68200	-1.55200
H	2.28200	0.18400	1.17000
H	0.50500	-0.78000	2.56800
H	-4.32300	-1.93800	3.69500
H	-5.24600	0.33300	-3.71800
H	-9.14200	0.47500	-0.55000
H	-4.71900	-4.07000	-1.37700
H	9.23800	1.23400	1.12700
H	-0.03700	8.79800	-1.99500
H	3.46300	5.82300	-0.81300
H	-2.72500	3.02400	3.65500
H	5.80900	-3.29200	0.63900
H	-0.14500	-4.65400	-3.31500
H	-0.41000	-3.97700	-4.93200
H	-1.68400	-1.34900	4.99400
H	-1.07400	-3.49200	2.87500
O	-0.80600	-4.42300	2.85200
O	-1.72000	-1.30400	5.96400
Cl	1.83100	2.72400	-0.40300
H	-0.65300	-4.61300	1.91700
H	-1.76300	-2.23100	6.22500

d C(4)-O (Asp145): 1.51Å
d C(4)-Cl: 2.0Å
reaction coordinate: 0.49Å
Extrapolated ONIOM energy:
-1624.17451030842

C	-1.77100	2.64900	3.82500
C	-1.31200	1.72300	4.77800
C	-0.85900	3.27100	2.95400
C	0.05700	1.41600	4.85900
C	0.51100	2.96500	3.03600

C	0.97000	2.03700	3.98800	H	-1.20800	3.98300	2.22200
C	-1.03100	8.10600	-2.42200	H	0.39900	0.69400	5.58900
C	-1.65600	6.98800	-1.60800	H	1.20600	3.43300	2.35500
C	-2.96300	7.13000	-1.10300	H	2.02000	1.79000	4.04500
C	-0.93300	5.80800	-1.34300	H	-0.25100	7.70600	-3.07000
C	-3.54400	6.10000	-0.34000	H	-1.79200	8.58400	-3.03900
C	-1.51500	4.77900	-0.58000	H	-3.52300	8.03300	-1.29900
C	-2.81900	4.92500	-0.07700	H	0.07200	5.68400	-1.72100
C	3.92100	5.92100	-1.50800	H	-4.54800	6.21400	0.04500
C	8.87500	2.35200	0.29500	H	-0.95500	3.87700	-0.37700
C	7.39900	2.67800	0.40700	H	-3.26400	4.13300	0.50800
N	6.83100	3.70600	1.14600	H	4.90900	6.19700	-1.14000
C	6.38100	1.98800	-0.19100	H	3.93600	4.89300	-1.87200
C	5.48800	3.63300	0.99600	H	3.63800	6.58600	-2.32400
N	5.19700	2.59700	0.18600	H	9.05700	1.74700	-0.59500
C	-3.72900	-4.12200	-2.08700	H	9.45600	3.27200	0.21800
C	-2.42900	-3.83300	-1.41000	H	6.46100	1.11600	-0.83200
C	-2.02700	-2.61300	-0.99600	H	7.33800	4.38000	1.70800
C	-1.35300	-4.75300	-1.05100	H	4.26400	2.25000	-0.09700
N	-0.77600	-2.70600	-0.41700	H	4.74300	4.28100	1.45300
C	-0.31100	-4.00000	-0.43200	H	-3.64900	-5.04500	-2.66100
C	-1.13600	-6.13900	-1.20900	H	-3.98700	-3.30300	-2.75800
C	0.87900	-4.58800	0.01100	H	-2.61600	-1.70800	-1.08200
C	0.06200	-6.73900	-0.77200	H	-0.32700	-1.91500	0.04100
C	1.06700	-5.96700	-0.16300	H	-1.90500	-6.74700	-1.66300
C	-8.65200	-0.62100	0.28400	H	0.21000	-7.80400	-0.89100
C	-7.62500	0.00100	1.24500	H	1.64100	-4.00200	0.49900
C	-8.02100	-1.59200	-0.72200	H	1.98000	-6.43500	0.18600
C	-6.62200	0.93300	0.55400	H	-9.38700	-1.16800	0.87500
C	-4.46900	0.63000	-3.05500	H	-8.81000	-2.06100	-1.31200
C	-5.37400	1.87200	-3.01800	H	-7.46500	-2.36700	-0.19300
C	-3.12800	0.87200	-3.75500	H	-7.35200	-1.05800	-1.39600
C	-4.83200	2.99300	-2.12400	H	-7.08000	-0.79300	1.75700
C	-0.01100	-3.66100	-3.87900	H	-8.16500	0.57900	1.99500
C	1.32900	-2.95400	-3.83900	H	-7.15300	1.71700	0.01300
O	1.82700	-2.56100	-4.88700	H	-5.99700	0.37000	-0.13900
N	1.93000	-2.79400	-2.65500	H	-5.97900	1.39300	1.30500
C	3.30600	-2.29200	-2.52300	H	-4.28500	0.28700	-2.03600
C	4.00900	-2.82600	-1.24400	H	-2.55200	-0.05300	-3.76900
O	4.22800	-4.02900	-1.14000	H	-2.55600	1.63400	-3.22600
C	3.36700	-0.76100	-2.77900	H	-3.30000	1.20100	-4.78100
C	2.90200	0.14700	-1.66500	H	-6.35000	1.57200	-2.63400
O	1.60300	0.37700	-1.64400	H	-5.51000	2.25300	-4.03100
O	3.71000	0.61800	-0.86000	H	-3.90700	3.39500	-2.53700
N	4.36600	-2.00000	-0.25400	H	-4.64600	2.61300	-1.11900
C	5.16100	-2.33400	0.93400	H	-5.56600	3.79800	-2.06900
C	4.37800	-3.10400	2.01300	H	-0.76200	-3.02000	-3.42800
O	4.02700	-4.37600	1.53400	H	2.78900	-0.58100	-3.68800
C	3.11800	-2.38000	2.47800	H	4.41100	-0.50300	-2.97800
C	-4.20900	-2.46800	2.77200	H	3.87100	-2.73900	-3.34300
S	-3.71500	-1.16600	1.59300	H	1.47700	-3.15400	-1.82700
C	-1.97500	-0.99700	2.12600	H	5.03000	-3.23800	2.87700
O	-1.62300	-1.65200	3.11600	H	3.38200	-1.41100	2.90000
C	-1.07600	-0.19500	1.32300	H	2.43300	-2.24000	1.64400
C	-1.42500	0.51100	0.13900	H	2.62100	-2.97900	3.24200
C	-0.48200	1.04400	-0.70100	H	4.09000	-4.36000	0.56200
C	0.93700	0.95400	-0.41700	H	5.53500	-1.41400	1.38100
C	1.27500	0.26900	0.81400	H	4.14700	-1.02100	-0.38100
C	0.30700	-0.25100	1.63400	H	-3.56100	-3.33700	2.65700
H	-2.01200	1.24300	5.44800	H	-5.24100	-2.72700	2.53000

H	-2.47100	0.60600	-0.14200
H	-0.77100	1.53800	-1.62100
H	2.31900	0.20300	1.09100
H	0.59300	-0.76700	2.54500
H	-4.14100	-2.09700	3.79500
H	-4.99600	-0.16300	-3.58800
H	-9.17200	0.17200	-0.25600
H	-4.51100	-4.23200	-1.33500
H	9.19600	1.79300	1.17500
H	-0.59600	8.84400	-1.74800
H	3.18900	6.00700	-0.70400
H	-2.82400	2.87900	3.76600
H	6.01700	-2.94300	0.63800
H	0.07000	-4.61000	-3.35300
H	-0.27800	-3.85100	-4.91700
H	-1.48500	-1.36800	5.04800
H	-0.87500	-3.48200	2.89700
O	-0.53700	-4.39000	2.85600
O	-1.49800	-1.33700	6.01800
Cl	1.73400	2.78900	-0.43500
H	-0.48300	-4.59100	1.91200
H	-1.49100	-2.26900	6.26900

d C(4)-O (Asp145): 1.49Å
d C(4)-Cl: 2.05Å
reaction coordinate: 0.56Å
Extrapolated ONIOM energy:
-1624.17665813141

C	-1.78200	2.63500	3.82500
C	-1.35500	1.69700	4.78100
C	-0.84600	3.24100	2.96900
C	0.00800	1.36300	4.88000
C	0.51700	2.90700	3.06800
C	0.94400	1.96800	4.02400
C	-0.99500	8.11700	-2.42100
C	-1.60800	6.99400	-1.60400
C	-2.91900	7.12000	-1.10600
C	-0.86900	5.82600	-1.33000
C	-3.48900	6.08500	-0.34100
C	-1.44000	4.79200	-0.56500
C	-2.74900	4.92200	-0.06900
C	3.94500	5.90700	-1.49700
C	8.87700	2.31200	0.31300
C	7.40200	2.65200	0.42200
N	6.84400	3.69000	1.15600
C	6.37700	1.97000	-0.17300
C	5.50000	3.63000	1.00500
N	5.19800	2.59300	0.20000
C	-3.75000	-4.09900	-2.11500
C	-2.45200	-3.80000	-1.43800
C	-2.05200	-2.57300	-1.04000
C	-1.37800	-4.71400	-1.06100
N	-0.80200	-2.65800	-0.45900
C	-0.33700	-3.95100	-0.45200
C	-1.16000	-6.10300	-1.19500
C	0.85200	-4.53100	0.00300
C	0.03700	-6.69500	-0.74500
C	1.04100	-5.91300	-0.14700
C	-8.66300	-0.57900	0.24800
C	-7.64900	0.03000	1.23100
C	-8.01800	-1.53600	-0.76200
C	-6.63600	0.97100	0.56700
C	-4.46600	0.65800	-3.07700
C	-5.35200	1.91100	-3.01100
C	-3.11700	0.89900	-3.76400
C	-4.79400	3.00400	-2.09200
C	-0.02500	-3.65200	-3.89600
C	1.31800	-2.94900	-3.84900
O	1.81800	-2.55300	-4.89500
N	1.92000	-2.79400	-2.66300
C	3.29800	-2.29400	-2.53200
C	4.01100	-2.83500	-1.26000
O	4.28300	-4.03000	-1.18700
C	3.36400	-0.76300	-2.78700
C	2.91400	0.14100	-1.66400
O	1.61400	0.38000	-1.63800
O	3.72600	0.59800	-0.85700
N	4.32200	-2.02600	-0.24000
C	5.14000	-2.35800	0.93400
C	4.38500	-3.16600	2.00400
O	4.00500	-4.41500	1.48600
C	3.14600	-2.44900	2.53400
C	-4.24800	-2.44500	2.74700
S	-3.73300	-1.14900	1.57000
C	-1.99900	-0.98900	2.12000
O	-1.66000	-1.65200	3.10800
C	-1.08300	-0.19000	1.32800
C	-1.41900	0.53300	0.15200
C	-0.46200	1.04300	-0.69100
C	0.95100	0.91400	-0.41000
C	1.27700	0.20700	0.80700
C	0.29800	-0.28800	1.63300
H	-2.07200	1.22900	5.44100
H	-1.17100	3.96100	2.23400
H	0.32600	0.63400	5.61300
H	1.23000	3.36300	2.39800
H	1.98800	1.70100	4.09400
H	-0.21400	7.72300	-3.07100
H	-1.76100	8.58800	-3.03700
H	-3.49100	8.01400	-1.30900
H	0.13900	5.71500	-1.70200
H	-4.49600	6.18600	0.03900
H	-0.86800	3.90000	-0.35500
H	-3.18500	4.12600	0.51900
H	4.93900	6.18000	-1.14600
H	3.95100	4.87900	-1.86200
H	3.65000	6.57400	-2.30800
H	9.05300	1.69800	-0.57200
H	9.46600	3.22600	0.22700
H	6.44800	1.09400	-0.81000
H	7.35600	4.36200	1.71500
H	4.25900	2.25800	-0.08000
H	4.76000	4.28600	1.45700
H	-3.66700	-5.03000	-2.67600
H	-4.00700	-3.28900	-2.79800
H	-2.64100	-1.66900	-1.13900
H	-0.35200	-1.86200	-0.01100
H	-1.92800	-6.71800	-1.64100
H	0.18500	-7.76300	-0.84500

H	1.61400	-3.93600	0.48100
H	1.95300	-6.37500	0.21200
H	-9.40600	-1.13500	0.82300
H	-8.79800	-1.99800	-1.36900
H	-7.46900	-2.31800	-0.23600
H	-7.34000	-0.99300	-1.41900
H	-7.11200	-0.77000	1.74200
H	-8.20000	0.59800	1.98200
H	-7.15900	1.76200	0.02800
H	-6.00100	0.41600	-0.12400
H	-6.00400	1.42000	1.33300
H	-4.29200	0.28500	-2.06700
H	-2.55800	-0.03600	-3.80600
H	-2.53400	1.63200	-3.20800
H	-3.27900	1.26400	-4.77900
H	-6.33300	1.61700	-2.63500
H	-5.48300	2.31700	-4.01500
H	-3.86400	3.40200	-2.49700
H	-4.61200	2.59700	-1.09600
H	-5.51700	3.81700	-2.01600
H	-0.77800	-3.00400	-3.45800
H	2.77900	-0.57800	-3.69000
H	4.40800	-0.51100	-2.99200
H	3.85900	-2.74100	-3.35600
H	1.46600	-3.15500	-1.83700
H	5.06200	-3.33900	2.84200
H	3.43100	-1.49900	2.98400
H	2.43800	-2.27300	1.72800
H	2.66700	-3.07200	3.29100
H	4.11200	-4.38600	0.51800
H	5.49700	-1.43600	1.39200
H	4.06800	-1.05300	-0.33900
H	-3.60400	-3.31900	2.63800
H	-5.28000	-2.69700	2.49600
H	-2.46300	0.65700	-0.12600
H	-0.74000	1.54600	-1.60900
H	2.32100	0.10300	1.07500
H	0.57500	-0.82300	2.53500
H	-4.18600	-2.07400	3.77000
H	-5.00100	-0.11300	-3.63300
H	-9.17600	0.22000	-0.28800
H	-4.53400	-4.20100	-1.36400
H	9.19400	1.75900	1.19800
H	-0.56500	8.85900	-1.74900
H	3.22700	5.99400	-0.68100
H	-2.82900	2.88700	3.75300
H	6.00600	-2.94200	0.61800
H	0.04700	-4.59700	-3.36200
H	-0.28200	-3.85000	-4.93400
H	-1.53700	-1.39100	5.04700
H	-0.90000	-3.48600	2.88500
O	-0.57700	-4.39900	2.83800
O	-1.55800	-1.36900	6.01800
Cl	1.79200	2.78300	-0.37100
H	-0.49400	-4.58500	1.89400
H	-1.55100	-2.30300	6.25900

d C(4)-O (Asp145): 1.48Å
d C(4)-Cl: 2.1Å
reaction coordinate: 0.62Å
Extrapolated ONIOM energy:
-1624.17883487548

C	-1.77500	2.56700	3.87200
C	-1.35800	1.60400	4.80800
C	-0.83200	3.18400	3.03200
C	0.00100	1.25700	4.90300
C	0.52700	2.83700	3.12800
C	0.94400	1.87300	4.06300
C	-1.01400	8.14900	-2.30300
C	-1.60800	6.98000	-1.53900
C	-2.95200	7.02000	-1.12200
C	-0.81800	5.85400	-1.23200
C	-3.50500	5.94300	-0.40500
C	-1.37100	4.77800	-0.51400
C	-2.71400	4.82100	-0.10000
C	3.93100	5.92900	-1.43300
C	8.87200	2.31100	0.30400
C	7.39800	2.65400	0.42900
N	6.85000	3.69200	1.16900
C	6.36400	1.97700	-0.15800
C	5.50400	3.63800	1.03000
N	5.19000	2.60400	0.22700
C	-3.76300	-4.07100	-2.16000
C	-2.46600	-3.73800	-1.49700
C	-2.07000	-2.49500	-1.14800
C	-1.39000	-4.63400	-1.08200
N	-0.81800	-2.55400	-0.57000
C	-0.35100	-3.84400	-0.50500
C	-1.17000	-6.02600	-1.15300
C	0.83900	-4.40100	-0.02500
C	0.02600	-6.59600	-0.67400
C	1.02900	-5.78800	-0.11000
C	-8.66700	-0.58800	0.27500
C	-7.65600	0.01700	1.26200
C	-8.01400	-1.51100	-0.76200
C	-6.66500	0.99000	0.61100
C	-4.48500	0.69900	-3.05000
C	-5.43200	1.90900	-3.06600
C	-3.10800	0.99100	-3.65800
C	-4.97500	3.05500	-2.15600
C	-0.04600	-3.59700	-3.95100
C	1.29900	-2.89300	-3.89600
O	1.79100	-2.47900	-4.93900
N	1.91100	-2.75600	-2.71200
C	3.28900	-2.25000	-2.58600
C	4.03200	-2.80700	-1.33700
O	4.39300	-3.98100	-1.32600
C	3.34600	-0.71400	-2.81900
C	2.91900	0.16700	-1.67000
O	1.61700	0.41300	-1.62300
O	3.74000	0.59500	-0.86000
N	4.28000	-2.03700	-0.26900
C	5.13900	-2.36900	0.87400
C	4.44300	-3.25000	1.92700
O	4.00700	-4.45100	1.34300
C	3.25200	-2.55800	2.58300
C	-4.26000	-2.45900	2.74900

S	-3.73100	-1.17400	1.56600
C	-1.99700	-1.02700	2.12200
O	-1.65700	-1.71800	3.08900
C	-1.07300	-0.20900	1.35000
C	-1.40500	0.55300	0.19900
C	-0.44300	1.05900	-0.64400
C	0.96400	0.88400	-0.38200
C	1.28900	0.13800	0.80600
C	0.30700	-0.35200	1.63500
H	-2.08100	1.12800	5.45600
H	-1.14900	3.92400	2.31200
H	0.31200	0.50900	5.62100
H	1.24700	3.30400	2.47200
H	1.98700	1.59700	4.13000
H	-0.17300	7.81200	-2.90900
H	-1.76800	8.58500	-2.95800
H	-3.56400	7.88100	-1.35000
H	0.21600	5.80900	-1.54100
H	-4.53700	5.97800	-0.08700
H	-0.75900	3.91900	-0.27700
H	-3.13500	3.99300	0.45200
H	4.93600	6.19100	-1.10600
H	3.91800	4.90400	-1.80400
H	3.62000	6.60400	-2.23000
H	9.02300	1.60500	-0.51400
H	9.44800	3.21400	0.09800
H	6.42400	1.10300	-0.79800
H	7.37000	4.36300	1.72300
H	4.24400	2.28300	-0.04700
H	4.77000	4.29800	1.48700
H	-3.66800	-5.01000	-2.70500
H	-4.03800	-3.27900	-2.85700
H	-2.66100	-1.59500	-1.28000
H	-0.36900	-1.74300	-0.14700
H	-1.93600	-6.66300	-1.57200
H	0.17500	-7.66700	-0.72500
H	1.60000	-3.78200	0.42500
H	1.94100	-6.23300	0.27100
H	-9.39600	-1.16800	0.84200
H	-8.79100	-1.97300	-1.37200
H	-7.44800	-2.29500	-0.25700
H	-7.35100	-0.94200	-1.41200
H	-7.10100	-0.78500	1.75100
H	-8.21000	0.56000	2.02900
H	-7.20600	1.78100	0.09100
H	-6.02500	0.46100	-0.09500
H	-6.03700	1.43500	1.38200
H	-4.35500	0.35600	-2.02300
H	-2.50500	0.08400	-3.64800
H	-2.59600	1.76100	-3.08200
H	-3.22400	1.33100	-4.68800
H	-6.41500	1.57600	-2.72800
H	-5.53300	2.27900	-4.08700
H	-4.04900	3.49000	-2.53100
H	-4.82000	2.68700	-1.14100
H	-5.74200	3.83000	-2.13900
H	-0.80600	-2.93700	-3.54400
H	2.74200	-0.51600	-3.70700
H	4.38500	-0.45700	-3.04000
H	3.84000	-2.67800	-3.42600
H	1.46300	-3.12700	-1.88700
H	5.16800	-3.49100	2.70400
H	3.58100	-1.64900	3.08600
H	2.50300	-2.30800	1.83700
H	2.80500	-3.23000	3.31700
H	4.18400	-4.40400	0.38700
H	5.46900	-1.45000	1.35800
H	3.96200	-1.07900	-0.31600
H	-3.66000	-3.35900	2.61100
H	-5.31000	-2.66400	2.53100
H	-2.44900	0.70600	-0.06500
H	-0.71800	1.58800	-1.54900
H	2.33300	-0.00700	1.05400
H	0.58100	-0.92600	2.51400
H	-4.14700	-2.10000	3.77200
H	-4.94800	-0.10800	-3.62000
H	-9.19800	0.21500	-0.24000
H	-4.54100	-4.17100	-1.40200
H	9.22500	1.86000	1.23200
H	-0.66900	8.90500	-1.59700
H	3.23600	6.01600	-0.59700
H	-2.81900	2.83100	3.80300
H	6.02100	-2.90400	0.51800
H	0.01300	-4.52800	-3.39300
H	-0.28400	-3.82000	-4.98900
H	-1.52900	-1.50000	5.02800
H	-0.90900	-3.57500	2.83000
O	-0.55600	-4.47700	2.79200
O	-1.57100	-1.48700	5.99800
Cl	1.85600	2.78200	-0.26100
H	-0.41800	-4.64900	1.85100
H	-1.55100	-2.42200	6.23300

d C(4)-O (Asp145): 1.46Å
d C(4)-Cl: 2.2Å
reaction coordinate: 0.74Å
Extrapolated ONIOM energy:
-1624.18339082675

C	-1.77700	2.55300	3.88400
C	-1.39300	1.58000	4.82300
C	-0.81000	3.15000	3.05600
C	-0.04400	1.20100	4.93300
C	0.53900	2.77100	3.16700
C	0.92300	1.79600	4.10400
C	-0.96000	8.17200	-2.27900
C	-1.53600	6.98700	-1.52600
C	-2.88800	6.99200	-1.13200
C	-0.72300	5.88200	-1.20500
C	-3.42400	5.89900	-0.42500
C	-1.26000	4.79100	-0.49800
C	-2.61000	4.79800	-0.10700
C	3.96600	5.91100	-1.41100
C	8.87900	2.25000	0.31800
C	7.40700	2.61200	0.44200
N	6.87400	3.66600	1.17100
C	6.36100	1.94400	-0.13600
C	5.52800	3.63000	1.03500
N	5.19700	2.59200	0.24400
C	-3.80100	-4.02800	-2.18800

C	-2.50400	-3.69400	-1.52500	H	6.40800	1.06300	-0.76700
C	-2.10100	-2.44900	-1.19000	H	7.40300	4.33600	1.71600
C	-1.43400	-4.59100	-1.09400	H	4.24000	2.29400	-0.02200
N	-0.84900	-2.50900	-0.61100	H	4.80100	4.30400	1.48200
C	-0.39100	-3.80100	-0.52600	H	-3.71000	-4.97400	-2.72000
C	-1.22400	-5.98600	-1.14400	H	-4.06900	-3.24200	-2.89500
C	0.79400	-4.35800	-0.03500	H	-2.68500	-1.54700	-1.33500
C	-0.03300	-6.55700	-0.65300	H	-0.39200	-1.69800	-0.20000
C	0.97400	-5.74800	-0.09900	H	-1.99300	-6.62300	-1.55600
C	-8.68200	-0.51700	0.25400	H	0.10900	-7.63000	-0.68900
C	-7.67000	0.09000	1.24000	H	1.55900	-3.73700	0.40600
C	-8.03300	-1.45900	-0.76700	H	1.88300	-6.19400	0.29000
C	-6.66800	1.04600	0.58200	H	-9.41900	-1.08400	0.82500
C	-4.48600	0.75100	-3.06000	H	-8.81100	-1.92100	-1.37600
C	-5.41900	1.97200	-3.07800	H	-7.47600	-2.24200	-0.25000
C	-3.10000	1.03000	-3.65300	H	-7.36100	-0.90400	-1.42100
C	-4.95300	3.11000	-2.16200	H	-7.12500	-0.71100	1.74000
C	-0.07800	-3.57500	-3.97100	H	-8.22400	0.64600	1.99800
C	1.27400	-2.88200	-3.91100	H	-7.19900	1.83700	0.05100
O	1.76700	-2.46400	-4.95100	H	-6.03000	0.50400	-0.11500
N	1.89100	-2.75800	-2.72700	H	-6.03900	1.49500	1.35100
C	3.27400	-2.25900	-2.60400	H	-4.37100	0.40000	-2.03400
C	4.02800	-2.82500	-1.36300	H	-2.50900	0.11400	-3.64800
O	4.44000	-3.98100	-1.38400	H	-2.58100	1.78600	-3.06400
C	3.34000	-0.72200	-2.83100	H	-3.20100	1.38300	-4.68000
C	2.93400	0.15000	-1.67000	H	-6.40700	1.65000	-2.74600
O	1.63000	0.41000	-1.61700	H	-5.50900	2.34600	-4.09800
O	3.75900	0.55300	-0.85500	H	-4.02200	3.53700	-2.53400
N	4.23200	-2.08000	-0.26800	H	-4.80400	2.73800	-1.14900
C	5.11000	-2.40500	0.86500	H	-5.71200	3.89300	-2.14500
C	4.44600	-3.33100	1.90000	H	-0.83600	-2.90400	-3.57800
O	3.98600	-4.50500	1.28000	H	2.72900	-0.51300	-3.71100
C	3.27600	-2.66500	2.62000	H	4.38000	-0.47200	-3.06100
C	-4.31100	-2.40800	2.74400	H	3.81800	-2.68500	-3.44900
S	-3.75200	-1.14600	1.55000	H	1.44300	-3.12900	-1.90200
C	-2.02600	-1.01000	2.12500	H	5.19400	-3.60400	2.64400
O	-1.70000	-1.70600	3.09100	H	3.62200	-1.77900	3.15100
C	-1.07900	-0.20200	1.35900	H	2.50600	-2.38300	1.90700
C	-1.39500	0.58300	0.22100	H	2.84900	-3.36700	3.33700
C	-0.41900	1.05500	-0.63000	H	4.20600	-4.45000	0.33300
C	0.97300	0.81800	-0.38100	H	5.41300	-1.48500	1.36600
C	1.28700	0.05700	0.79200	H	3.88000	-1.13300	-0.28800
C	0.29600	-0.39800	1.63300	H	-3.73300	-3.32300	2.61200
H	-2.13400	1.11900	5.46300	H	-5.36600	-2.58900	2.52700
H	-1.10100	3.89800	2.33300	H	-2.43500	0.77500	-0.03200
H	0.24400	0.44700	5.65400	H	-0.68100	1.59500	-1.53300
H	1.27800	3.22300	2.52100	H	2.32700	-0.13400	1.02400
H	1.95900	1.49800	4.18300	H	0.55600	-0.99200	2.50300
H	-0.09700	7.85900	-2.86600	H	-4.18800	-2.04300	3.76300
H	-1.71300	8.58500	-2.95200	H	-4.95300	-0.04700	-3.63900
H	-3.51800	7.83700	-1.37000	H	-9.20300	0.28300	-0.27300
H	0.31700	5.86400	-1.49600	H	-4.58100	-4.11400	-1.43100
H	-4.46300	5.90800	-0.12400	H	9.23300	1.82300	1.25700
H	-0.62800	3.94900	-0.25100	H	-0.65300	8.93800	-1.56700
H	-3.01800	3.95900	0.43700	H	3.27900	5.99200	-0.56800
H	4.97400	6.17700	-1.09300	H	-2.81400	2.84400	3.80300
H	3.95600	4.88700	-1.78600	H	6.00600	-2.90400	0.49300
H	3.64400	6.58700	-2.20300	H	-0.03300	-4.50200	-3.40500
H	9.01600	1.51700	-0.47900	H	-0.30800	-3.80500	-5.01000
H	9.46200	3.14000	0.08100	H	-1.57200	-1.52300	5.04100

H	-0.95200	-3.57400	2.81500
O	-0.60400	-4.47700	2.77800
O	-1.63100	-1.51900	6.01000
Cl	1.95100	2.77800	-0.17600
H	-0.45600	-4.64700	1.83800
H	-1.60800	-2.45600	6.23800

d C(4)-O (Asp145): 1.44Å
d C(4)-Cl: 2.3Å
reaction coordinate: 0.86Å
Extrapolated ONIOM energy:
-1624.18829791416

C	-1.78900	2.67000	3.79000
C	-1.57600	1.71700	4.80200
C	-0.70300	3.12600	3.02100
C	-0.28200	1.22200	5.04300
C	0.58900	2.62600	3.25900
C	0.80100	1.67400	4.27000
C	-0.57100	8.14400	-2.55700
C	-1.16700	7.09900	-1.63400
C	-2.44100	7.30200	-1.07100
C	-0.44800	5.92800	-1.32400
C	-2.99600	6.34000	-0.20700
C	-1.00200	4.96600	-0.46100
C	-2.27600	5.17200	0.09800
C	4.23000	5.68600	-1.53400
C	8.93600	1.85000	0.38100
C	7.48400	2.29200	0.49200
N	7.00800	3.40000	1.17900
C	6.40300	1.65700	-0.06000
C	5.66100	3.42900	1.04200
N	5.27500	2.38000	0.29300
C	-3.96300	-3.91100	-2.23900
C	-2.67200	-3.59900	-1.55400
C	-2.23600	-2.35900	-1.24000
C	-1.64300	-4.51900	-1.07500
N	-0.99900	-2.44500	-0.63200
C	-0.58800	-3.74900	-0.50300
C	-1.47900	-5.92100	-1.08500
C	0.56700	-4.33200	0.03100
C	-0.32000	-6.51800	-0.55000
C	0.70100	-5.72800	0.00700
C	-8.72700	-0.12600	0.01800
C	-7.80100	0.73200	0.89500
C	-8.03100	-1.36900	-0.55200
C	-6.66000	1.40100	0.11800
C	-4.41300	0.87200	-3.23800
C	-4.58400	2.39700	-3.19500
C	-3.04100	0.42300	-3.75500
C	-3.70500	3.08000	-2.14300
C	-0.18900	-3.66800	-3.95600
C	1.17300	-2.99600	-3.87200
O	1.69100	-2.59200	-4.90600
N	1.77500	-2.87500	-2.67900
C	3.17100	-2.41700	-2.53800
C	3.89400	-3.00400	-1.28700
O	4.28900	-4.16600	-1.31100
C	3.29400	-0.88400	-2.77600
C	2.92800	0.01100	-1.61800
O	1.63700	0.34600	-1.58400
O	3.76000	0.36700	-0.79300
N	4.08900	-2.27300	-0.18100
C	4.95000	-2.61500	0.95900
C	4.25900	-3.53000	1.98500
O	3.74000	-4.67200	1.35100
C	3.12700	-2.82600	2.73000
C	-4.56000	-2.11200	2.64300
S	-3.85700	-0.94400	1.43000
C	-2.16500	-0.87800	2.09400
O	-1.91300	-1.58500	3.07100
C	-1.14800	-0.12600	1.35200
C	-1.40100	0.68800	0.22200
C	-0.38400	1.09000	-0.62200
C	0.97200	0.73600	-0.36400
C	1.23200	-0.03700	0.80500
C	0.20400	-0.42200	1.64200
H	-2.40500	1.36000	5.39900
H	-0.85400	3.86000	2.24400
H	-0.12300	0.49000	5.82400
H	1.41600	2.96900	2.65400
H	1.79300	1.28600	4.45000
H	0.15200	7.68000	-3.22900
H	-1.35900	8.60600	-3.15200
H	-2.99700	8.20100	-1.30000
H	0.53400	5.76000	-1.74200
H	-3.97400	6.50000	0.22300
H	-0.44100	4.07100	-0.22700
H	-2.70400	4.43000	0.75700
H	5.19200	6.01200	-1.14100
H	4.29700	4.64800	-1.86200
H	3.95000	6.31400	-2.38000
H	9.03100	1.06800	-0.37300
H	9.56000	2.69700	0.09200
H	6.40300	0.75200	-0.65800
H	7.57100	4.06400	1.69700
H	4.30000	2.13500	0.03800
H	4.96900	4.15800	1.45800
H	-3.88000	-4.86000	-2.76800
H	-4.20400	-3.12200	-2.95300
H	-2.78600	-1.44200	-1.41800
H	-0.52100	-1.64000	-0.23400
H	-2.26000	-6.54300	-1.49800
H	-0.21500	-7.59600	-0.55400
H	1.34200	-3.72500	0.47300
H	1.58300	-6.19500	0.42900
H	-9.57100	-0.45400	0.62700
H	-8.75900	-1.97200	-1.09500
H	-7.61200	-1.96500	0.25900
H	-7.23600	-1.07800	-1.23900
H	-7.37800	0.11500	1.68900
H	-8.40100	1.51600	1.36000
H	-7.06600	1.99800	-0.69900
H	-5.98400	0.64700	-0.28200
H	-6.09800	2.05100	0.78900
H	-4.57200	0.45900	-2.24100
H	-3.02700	-0.66200	-3.85100
H	-2.25700	0.72800	-3.06400
H	-2.85200	0.86700	-4.73400
H	-5.62700	2.61800	-2.96300

H	-4.36000	2.81500	-4.17800
H	-2.65100	2.94800	-2.38400
H	-3.91200	2.66400	-1.15700
H	-3.92900	4.14700	-2.13100
H	-0.94600	-2.97400	-3.60500
H	2.68900	-0.65800	-3.65500
H	4.34200	-0.67800	-3.01100
H	3.71100	-2.86600	-3.37500
H	1.30600	-3.23100	-1.85900
H	5.00300	-3.84800	2.71600
H	3.51800	-1.96700	3.27400
H	2.36300	-2.49500	2.03100
H	2.67600	-3.52200	3.43900
H	3.99900	-4.63700	0.41400
H	5.26900	-1.70300	1.46300
H	3.75500	-1.32000	-0.20200
H	-4.08600	-3.08800	2.53800
H	-5.62600	-2.18100	2.42200
H	-2.42200	0.95800	-0.03200
H	-0.59600	1.65500	-1.52200
H	2.25300	-0.30700	1.03900
H	0.41200	-1.03800	2.51000
H	-4.40200	-1.73900	3.65600
H	-5.17800	0.46100	-3.89900
H	-9.11500	0.47900	-0.80300
H	-4.75800	-3.98100	-1.49700
H	9.27700	1.46000	1.34100
H	-0.07100	8.90900	-1.96300
H	3.46700	5.76600	-0.75900
H	-2.78300	3.05300	3.60800
H	5.83800	-3.13300	0.59300
H	-0.17900	-4.57900	-3.36100
H	-0.39100	-3.92500	-4.99400
H	-1.84400	-1.39000	5.02500
H	-1.24500	-3.50400	2.83000
O	-0.90200	-4.41000	2.81900
O	-1.98100	-1.40000	5.98500
Cl	2.10700	2.71600	-0.08000
H	-0.73800	-4.60100	1.88600
H	-1.98900	-2.34100	6.19900

d C(4)-O (Asp145): 1.43Å
d C(4)-Cl: 2.4Å
reaction coordinate: 0.97Å
Extrapolated ONIOM energy:
-1624.19222661431

C	-1.77200	2.56600	3.87100
C	-1.47600	1.60200	4.85200
C	-0.74300	3.08300	3.06400
C	-0.15300	1.15600	5.02400
C	0.57800	2.63500	3.23500
C	0.87400	1.67100	4.21500
C	-0.76800	8.18100	-2.33700
C	-1.33600	7.01900	-1.54400
C	-2.67800	7.04700	-1.11600
C	-0.52600	5.91300	-1.21900
C	-3.20600	5.97600	-0.37100
C	-1.05500	4.84300	-0.47500
C	-2.39400	4.87400	-0.05000
C	4.09900	5.81000	-1.42800
C	8.91300	2.04100	0.34400
C	7.45300	2.45100	0.46500
N	6.95700	3.54100	1.16800
C	6.38200	1.80500	-0.09500
C	5.61000	3.54700	1.03400
N	5.24200	2.50300	0.27100
C	-3.88800	-3.95000	-2.24200
C	-2.59400	-3.61400	-1.57400
C	-2.17000	-2.36500	-1.28000
C	-1.54900	-4.51600	-1.09600
N	-0.92600	-2.42900	-0.68500
C	-0.49700	-3.72700	-0.54400
C	-1.36800	-5.91600	-1.09000
C	0.67100	-4.28900	-0.01800
C	-0.19600	-6.49300	-0.56200
C	0.82100	-5.68400	-0.02700
C	-8.70500	-0.32400	0.15700
C	-7.70000	0.28400	1.14900
C	-8.06400	-1.32900	-0.80800
C	-6.64200	1.17600	0.48700
C	-4.45700	0.84100	-3.12900
C	-5.24100	2.16100	-3.06500
C	-3.06300	0.98600	-3.74900
C	-4.63100	3.18500	-2.10100
C	-0.14300	-3.58600	-3.99900
C	1.21600	-2.90500	-3.92300
O	1.71500	-2.48000	-4.95800
N	1.83400	-2.79800	-2.73800
C	3.22600	-2.32200	-2.60800
C	3.97400	-2.91000	-1.37200
O	4.40300	-4.06000	-1.41900
C	3.32300	-0.78400	-2.82700
C	2.94100	0.08300	-1.65400
O	1.63800	0.38200	-1.61100
O	3.76400	0.44400	-0.82500
N	4.15500	-2.19200	-0.25500
C	5.03500	-2.52500	0.87300
C	4.37900	-3.47300	1.89200
O	3.86900	-4.61200	1.24400
C	3.24800	-2.80600	2.67000
C	-4.43800	-2.26100	2.70900
S	-3.80000	-1.06200	1.49000
C	-2.10100	-0.94100	2.12400
O	-1.81100	-1.62800	3.10400
C	-1.11000	-0.16700	1.36100
C	-1.39500	0.64300	0.23700
C	-0.39500	1.05300	-0.62800
C	0.96100	0.70500	-0.39400
C	1.25800	-0.04800	0.77300
C	0.25000	-0.44200	1.63100
H	-2.26200	1.20200	5.47800
H	-0.96200	3.82500	2.31000
H	0.07000	0.41500	5.78000
H	1.36400	3.02700	2.60500
H	1.88900	1.32300	4.34200
H	0.07500	7.84500	-2.94100
H	-1.53400	8.58900	-2.99700
H	-3.30400	7.89400	-1.35600
H	0.50700	5.87700	-1.53400

H	-4.23600	6.00300	-0.04300
H	-0.42300	4.00200	-0.22600
H	-2.79800	4.05100	0.52300
H	5.09600	6.09800	-1.09600
H	4.11700	4.78900	-1.81100
H	3.76800	6.48500	-2.21700
H	9.01600	1.23800	-0.38800
H	9.51200	2.89200	0.02000
H	6.39600	0.90900	-0.70600
H	7.50900	4.20900	1.69300
H	4.26700	2.25200	0.01800
H	4.90300	4.25600	1.45900
H	-3.79900	-4.90600	-2.75800
H	-4.14500	-3.17500	-2.96500
H	-2.73200	-1.45700	-1.46700
H	-0.45200	-1.61600	-0.30100
H	-2.14500	-6.55200	-1.48800
H	-0.07700	-7.56900	-0.55500
H	1.44500	-3.66800	0.40600
H	1.71500	-6.13500	0.39000
H	-9.48000	-0.83900	0.72600
H	-8.84100	-1.78300	-1.42300
H	-7.55500	-2.11200	-0.24500
H	-7.35100	-0.82600	-1.46100
H	-7.20000	-0.51800	1.69500
H	-8.25300	0.88800	1.86900
H	-7.12700	1.96800	-0.08400
H	-6.00800	0.58500	-0.17300
H	-6.01600	1.62600	1.25800
H	-4.36000	0.43000	-2.12300
H	-2.58700	0.00800	-3.81100
H	-2.44300	1.64200	-3.13900
H	-3.14600	1.40400	-4.75300
H	-6.25500	1.93900	-2.73000
H	-5.30100	2.59700	-4.06300
H	-3.65900	3.51600	-2.46700
H	-4.51700	2.74500	-1.11100
H	-5.28900	4.05200	-2.03200
H	-0.90400	-2.89600	-3.64900
H	2.71300	-0.55600	-3.70300
H	4.36700	-0.55600	-3.05900
H	3.76200	-2.75200	-3.45700
H	1.38000	-3.17000	-1.91600
H	5.14200	-3.79200	2.60300
H	3.63300	-1.95200	3.22500
H	2.46600	-2.47500	1.99200
H	2.82300	-3.52400	3.37200
H	4.13300	-4.56500	0.30800
H	5.33300	-1.61100	1.38700
H	3.79500	-1.24900	-0.25900
H	-3.90100	-3.20600	2.61300
H	-5.49500	-2.40000	2.48000
H	-2.42400	0.90200	0.00100
H	-0.62900	1.60800	-1.52800
H	2.28600	-0.30400	0.98900
H	0.48100	-1.05200	2.49700
H	-4.31300	-1.87300	3.72000
H	-5.02800	0.13200	-3.73000
H	-9.17900	0.47500	-0.41600
H	-4.67500	-4.01800	-1.49100
H	9.27700	1.68800	1.31000
H	-0.43200	8.95800	-1.65000
H	3.40000	5.86400	-0.59200
H	-2.78800	2.91000	3.74300
H	5.93400	-3.01200	0.49200
H	-0.12500	-4.49500	-3.40200
H	-0.34600	-3.84700	-5.03600
H	-1.69900	-1.47400	5.07600
H	-1.07200	-3.52200	2.82200
O	-0.72500	-4.42600	2.79300
O	-1.79700	-1.50000	6.04000
Cl	2.11800	2.78100	-0.06600
H	-0.57400	-4.60500	1.85500
H	-1.78000	-2.44400	6.23900

3) Water molecules fixed to the position in the PDB file.

d C(4)-O (Asp145): 3.4Å
d C(4)-Cl: 1.76Å
reaction coordinate: -1.64Å
Extrapolated ONIOM energy:
-1624.21423134269

C	-2.89100	1.71100	3.62400
C	-1.80700	2.58300	3.42200
C	-4.07200	1.87000	2.87600
C	-1.90200	3.61400	2.47000
C	-4.16700	2.90200	1.92300
C	-3.08100	3.77200	1.72000
C	-3.64000	6.93100	-1.30200
C	-4.51300	5.69100	-1.29800
C	-5.80800	5.75200	-0.74900
C	-4.04200	4.47900	-1.83900
C	-6.63100	4.61200	-0.74900
C	-4.86600	3.33900	-1.83900
C	-6.16200	3.40600	-1.29700
C	1.82600	6.79300	-0.80100
C	7.89300	5.31300	0.43600
C	6.67200	4.43100	0.54700
N	5.89000	4.26200	1.67900
C	6.14800	3.65900	-0.45500
C	4.90200	3.39800	1.36500
N	5.04200	3.02600	0.08100
C	-1.36900	-5.35700	-2.17600
C	-0.57000	-4.23700	-1.57300
C	-0.67700	-2.92400	-1.88700
C	0.49800	-4.31600	-0.57800
N	0.26500	-2.19400	-1.18500
C	1.02000	-3.00500	-0.37000
C	1.11000	-5.36800	0.13700
C	2.10700	-2.74800	0.47500

C	2.19800	-5.12300	0.99700
C	2.70300	-3.82100	1.15800
C	-7.07300	-4.27900	0.72500
C	-6.42400	-3.15600	1.55300
C	-6.06000	-5.06200	-0.11900
C	-5.83800	-2.02200	0.70200
C	-3.95800	-1.21200	-2.60600
C	-5.37300	-1.38000	-3.18100
C	-3.04000	-0.35400	-3.48600
C	-6.21800	-0.10400	-3.09300
C	1.73800	-3.32600	-4.03900
C	2.81400	-2.26300	-3.97200
O	3.18100	-1.73100	-5.01400
N	3.32000	-1.94000	-2.77700
C	4.35700	-0.91400	-2.59700
C	5.31900	-1.22400	-1.43000
O	6.14100	-2.13000	-1.53500
C	3.71600	0.49100	-2.53800
C	2.68200	0.70100	-1.40600
O	1.52000	0.31000	-1.60100
O	3.12300	1.27700	-0.34000
N	5.28500	-0.47600	-0.32200
C	6.33600	-0.49000	0.70300
C	6.15500	-1.58100	1.76700
O	5.92100	-2.83000	1.16800
C	5.01000	-1.24000	2.70900
C	-2.23200	-4.09300	3.21800
S	-2.22700	-2.95300	1.79400
C	-1.28900	-1.61500	2.48900
O	-0.79200	-1.70500	3.61200
C	-1.11100	-0.45200	1.59700
C	-2.10400	-0.04500	0.69500
C	-1.88800	1.04900	-0.13600
C	-0.66000	1.70200	-0.08200
C	0.34700	1.30600	0.79600
C	0.11100	0.23800	1.65000
H	-0.90300	2.45100	3.99900
H	-4.90400	1.20000	3.03700
H	-1.06700	4.28100	2.30700
H	-5.07100	3.03200	1.34600
H	-3.15400	4.56200	0.98700
H	-2.68600	6.72400	-1.78700
H	-4.14700	7.73200	-1.84000
H	-6.17400	6.68000	-0.33200
H	-3.04800	4.41900	-2.26000
H	-7.62700	4.66600	-0.33200
H	-4.50600	2.41400	-2.26300
H	-6.80000	2.53300	-1.30200
H	2.54900	7.49800	-0.39200
H	2.34800	5.93400	-1.22300
H	1.24300	7.28200	-1.58100
H	8.16200	5.44700	-0.61300
H	7.68600	6.29100	0.87200
H	6.51700	3.55800	-1.46900
H	6.03400	4.70900	2.57700
H	4.39000	2.35800	-0.37300
H	4.10300	3.03700	2.01000
H	-0.73300	-6.23300	-2.30500
H	-1.76300	-5.05400	-3.14700
H	-1.36100	-2.51500	-2.61700
H	0.44500	-1.18900	-1.28500
H	0.74500	-6.37700	0.00600
H	2.66700	-5.94300	1.52500
H	2.48000	-1.73800	0.57800
H	3.55900	-3.65900	1.80200
H	-7.56000	-4.97300	1.41100
H	-6.56900	-5.89100	-0.61300
H	-5.27200	-5.46100	0.52100
H	-5.62100	-4.41800	-0.88000
H	-5.63600	-3.57600	2.17900
H	-7.18500	-2.73100	2.20800
H	-6.60500	-1.61500	0.04400
H	-5.00200	-2.39000	0.10800
H	-5.47600	-1.22900	1.35800
H	-4.02300	-0.76600	-1.61300
H	-2.05800	-0.26800	-3.01900
H	-3.45100	0.64800	-3.60300
H	-2.93200	-0.81200	-4.47000
H	-5.88100	-2.16200	-2.61600
H	-5.30900	-1.70100	-4.22200
H	-5.78300	0.68400	-3.70600
H	-6.27800	0.22700	-2.05600
H	-7.22500	-0.31400	-3.45500
H	0.77500	-2.83600	-4.14500
H	3.22100	0.62700	-3.50100
H	4.52700	1.23300	-2.46100
H	4.98900	-0.92600	-3.48700
H	2.95800	-2.39700	-1.95100
H	7.07200	-1.64600	2.35300
H	5.23900	-0.32900	3.25900
H	4.09300	-1.09400	2.14000
H	4.87000	-2.05600	3.41900
H	6.06300	-2.72700	0.21000
H	6.37500	0.47900	1.19900
H	4.52200	0.19400	-0.25000
H	-1.21100	-4.39100	3.45800
H	-2.81300	-4.96500	2.91400
H	-3.06200	-0.55400	0.67500
H	-2.66300	1.40300	-0.80500
H	1.33000	1.75400	0.73500
H	0.89300	-0.12100	2.31200
H	-2.69100	-3.62000	4.08600
H	-3.52100	-2.20400	-2.50300
H	-7.83600	-3.85400	0.07100
H	-2.19700	-5.60800	-1.51300
H	8.72900	4.85100	0.96100
H	-3.45500	7.24700	-0.27500
H	1.15800	6.45400	-0.00900
H	-2.81000	0.91800	4.35300
H	7.30000	-0.65700	0.21800
H	1.76900	-3.94400	-3.14500
H	1.92300	-3.94800	-4.91200
H	-0.98400	-0.60900	5.26100
H	1.11000	-1.88000	3.85000
O	2.03900	-1.93500	3.58100
O	-1.25500	-0.14600	6.07000
Cl	-0.39800	3.09500	-1.12000
H	2.00300	-2.51300	2.80400
H	-1.21000	-0.82800	6.75000

d C(4)-O (Asp145): 2.4Å
d C(4)-Cl: 1.76Å
reaction coordinate: -0.64Å
Extrapolated ONIOM energy:
-1624.20216139364

C	-2.33200	2.47900	3.40800
C	-1.18800	2.94400	4.08200
C	-2.69900	3.05100	2.17700
C	-0.41100	3.97600	3.52500
C	-1.92400	4.08500	1.62100
C	-0.78000	4.54700	2.29400
C	-2.51800	7.20300	-2.34300
C	-3.34900	6.08300	-1.75000
C	-4.40600	6.38000	-0.86900
C	-3.06600	4.74100	-2.07000
C	-5.18300	5.34400	-0.32000
C	-3.84500	3.70500	-1.52200
C	-4.90500	4.00600	-0.65000
C	2.82500	6.25000	-1.51600
C	8.51100	3.95100	0.19100
C	7.06500	3.51600	0.17200
N	6.00300	4.18700	0.75900
C	6.58200	2.37300	-0.40600
C	4.89000	3.45700	0.53900
N	5.22200	2.35900	-0.16300
C	-2.23800	-5.31700	-2.04800
C	-1.31200	-4.27000	-1.49800
C	-1.22300	-2.98300	-1.91100
C	-0.31800	-4.41400	-0.43700
N	-0.22600	-2.33300	-1.20300
C	0.35700	-3.16700	-0.27900
C	0.10200	-5.47900	0.38900
C	1.40000	-2.98400	0.63600
C	1.15100	-5.30800	1.31300
C	1.80400	-4.06900	1.43200
C	-7.81200	-3.08800	0.41700
C	-6.98300	-2.20800	1.36800
C	-6.94400	-3.96700	-0.49300
C	-6.19300	-1.10500	0.65200
C	-4.09800	-0.87300	-2.97400
C	-5.57700	-0.51000	-3.18000
C	-3.13800	-0.02200	-3.81400
C	-5.94600	0.88500	-2.66200
C	1.23700	-3.98400	-3.89100
C	2.31600	-2.92600	-3.80600
O	2.71000	-2.40400	-4.84200
N	2.80800	-2.60900	-2.60400
C	3.94700	-1.70000	-2.42100
C	4.85200	-2.11600	-1.24000
O	5.43200	-3.19700	-1.26500
C	3.47400	-0.22700	-2.41000
C	2.55900	0.20900	-1.24200
O	1.32600	0.06900	-1.36500
O	3.15000	0.72800	-0.22900
N	5.02800	-1.28700	-0.20800
C	6.02200	-1.48300	0.85400
C	5.52300	-2.37300	2.00100
O	5.08700	-3.61000	1.49900
C	4.40000	-1.70900	2.79200
C	-3.35900	-3.42800	3.10900
S	-2.86600	-2.45200	1.65000
C	-1.77500	-1.28400	2.44000
O	-1.49200	-1.40800	3.63400
C	-1.19700	-0.25200	1.56700
C	-1.79900	0.14700	0.36200
C	-1.19700	1.10100	-0.44400
C	0.04100	1.62100	-0.06200
C	0.62000	1.29400	1.16500
C	0.01500	0.34300	1.96500
H	-0.91100	2.50400	5.03000
H	-3.57500	2.69400	1.65700
H	0.46400	4.33200	4.05000
H	-2.20800	4.52600	0.67600
H	-0.18800	5.34100	1.86300
H	-2.12900	6.90400	-3.31700
H	-3.13000	8.09600	-2.46800
H	-4.62700	7.40700	-0.61300
H	-2.25000	4.50300	-2.73800
H	-5.99600	5.57700	0.35400
H	-3.62800	2.67800	-1.76800
H	-5.50600	3.21200	-0.22900
H	3.62100	6.92000	-1.19200
H	3.25000	5.29800	-1.83600
H	2.28900	6.70200	-2.35100
H	9.05300	3.47700	-0.62900
H	8.57700	5.03300	0.07500
H	7.14800	1.61800	-0.94100
H	6.05900	5.05700	1.27400
H	4.53200	1.62300	-0.40200
H	3.87600	3.66800	0.87300
H	-1.70700	-6.26500	-2.13600
H	-2.60100	-5.01600	-3.03100
H	-1.82100	-2.54100	-2.69500
H	0.07900	-1.36200	-1.33000
H	-0.38400	-6.43900	0.30100
H	1.47200	-6.13700	1.93000
H	1.88500	-2.02000	0.70800
H	2.62200	-3.96600	2.13400
H	-8.44700	-3.74000	1.01900
H	-7.58900	-4.61600	-1.08600
H	-6.27900	-4.58500	0.11200
H	-6.35400	-3.34900	-1.16800
H	-6.29300	-2.83500	1.93400
H	-7.66500	-1.73300	2.07400
H	-6.87200	-0.48000	0.07200
H	-5.44400	-1.54300	-0.00700
H	-5.68500	-0.48700	1.39300
H	-3.84400	-0.76900	-1.92000
H	-2.11100	-0.34500	-3.64400
H	-3.21800	1.02900	-3.53800
H	-3.37500	-0.13200	-4.87300
H	-6.18500	-1.24200	-2.64800
H	-5.82200	-0.57500	-4.24100
H	-5.45300	1.65300	-3.25800
H	-5.64800	0.98600	-1.61800
H	-7.02400	1.02400	-2.73800
H	0.29500	-3.50100	-4.13800
H	2.94800	-0.08200	-3.35600
H	4.37200	0.40900	-2.42100
H	4.58500	-1.80300	-3.30000

H	2.42600	-3.05300	-1.77900
H	6.35600	-2.55400	2.68100
H	4.75900	-0.78500	3.24100
H	3.55700	-1.48400	2.14200
H	4.07100	-2.38100	3.58500
H	5.21900	-3.60000	0.53600
H	6.30600	-0.51600	1.26800
H	4.41400	-0.47700	-0.16900
H	-2.48500	-3.90800	3.54800
H	-4.05900	-4.18500	2.75000
H	-2.75900	-0.26900	0.07700
H	-1.65100	1.41900	-1.37400
H	1.57800	1.71600	1.43100
H	0.49400	0.00300	2.87700
H	-3.84200	-2.79200	3.85200
H	-3.96600	-1.91900	-3.25400
H	-8.45600	-2.45600	-0.19600
H	-3.08500	-5.44000	-1.37200
H	8.97100	3.66000	1.13600
H	-1.68500	7.42700	-1.67600
H	2.13000	6.08000	-0.69400
H	-2.92500	1.68300	3.83600
H	6.91500	-1.94900	0.43200
H	1.15900	-4.51900	-2.94700
H	1.50100	-4.68300	-4.68100
H	-1.67300	-0.28000	5.18300
H	0.30800	-2.03800	4.10200
O	1.24000	-2.23800	3.93200
O	-1.92000	0.23600	5.96700
Cl	0.69400	2.98000	-0.97800
H	1.20400	-2.72700	3.09800
H	-1.87000	-0.40300	6.68800

d C(4)-O (Asp145): 2.2Å
d C(4)-Cl: 1.77Å
reaction coordinate: -0.42Å
Extrapolated ONIOM energy:
-1624.19315271269

C	-2.26900	2.53900	3.38100
C	-1.18400	3.00300	4.14600
C	-2.52100	3.09700	2.11500
C	-0.35100	4.02100	3.64800
C	-1.69000	4.11700	1.61700
C	-0.60500	4.57800	2.38200
C	-2.38100	7.19400	-2.47400
C	-3.23400	6.11200	-1.84300
C	-4.37200	6.46300	-1.09200
C	-2.89000	4.75400	-1.99500
C	-5.16600	5.46300	-0.50200
C	-3.68600	3.75600	-1.40400
C	-4.82500	4.10900	-0.66100
C	2.94200	6.16500	-1.61100
C	8.58300	3.79400	0.14800
C	7.12800	3.39500	0.19200
N	6.12400	4.04100	0.89700
C	6.58000	2.31200	-0.43900
C	4.98000	3.35500	0.69400
N	5.23800	2.30900	-0.11100
C	-2.30500	-5.32500	-2.03500
C	-1.37400	-4.27200	-1.50500
C	-1.27100	-2.99500	-1.94800
C	-0.39500	-4.39600	-0.42700
N	-0.27900	-2.33500	-1.24400
C	0.28300	-3.14900	-0.28800
C	0.00400	-5.44200	0.43200
C	1.30800	-2.94600	0.64400
C	1.03500	-5.25200	1.37200
C	1.69000	-4.01300	1.47600
C	-7.85300	-2.97800	0.37800
C	-7.05900	-2.13800	1.39200
C	-6.95400	-3.84300	-0.51500
C	-6.24000	-1.01300	0.74900
C	-4.08800	-0.86200	-3.02100
C	-5.55400	-0.40500	-3.09000
C	-3.13800	0.01600	-3.84500
C	-5.80100	0.96500	-2.44900
C	1.19900	-4.06900	-3.87700
C	2.26400	-2.99800	-3.78700
O	2.65400	-2.46500	-4.82000
N	2.75200	-2.68400	-2.58300
C	3.90100	-1.79000	-2.39700
C	4.78700	-2.21800	-1.20700
O	5.29600	-3.33600	-1.19500
C	3.45000	-0.31200	-2.40600
C	2.56300	0.16800	-1.23700
O	1.31800	0.08600	-1.36000
O	3.16700	0.67100	-0.23200
N	5.02500	-1.36500	-0.20800
C	6.00300	-1.59100	0.86200
C	5.44500	-2.40500	2.03800
O	4.97100	-3.64500	1.58000
C	4.33300	-1.66400	2.77500
C	-3.47300	-3.32000	3.09900
S	-2.90400	-2.40700	1.62700
C	-1.83300	-1.21600	2.42000
O	-1.59100	-1.31100	3.62600
C	-1.22000	-0.22700	1.53000
C	-1.77300	0.11800	0.28300
C	-1.12700	1.01000	-0.55500
C	0.12700	1.50900	-0.17700
C	0.63000	1.27600	1.11100
C	-0.01900	0.38500	1.94100
H	-0.99400	2.57300	5.12000
H	-3.35100	2.74000	1.52400
H	0.47700	4.37600	4.24400
H	-1.88600	4.54800	0.64500
H	0.02800	5.36400	1.99600
H	-1.86800	6.80100	-3.35300
H	-3.00800	8.03200	-2.77900
H	-4.63900	7.50200	-0.96600
H	-2.01200	4.47600	-2.56000
H	-6.04000	5.73600	0.07300
H	-3.41900	2.71600	-1.51600
H	-5.43700	3.34200	-0.20700
H	3.71500	6.83600	-1.23700
H	3.37600	5.18900	-1.83000
H	2.51200	6.58000	-2.52300
H	9.04800	3.40700	-0.75900
H	8.67200	4.88100	0.15200

H	7.09100	1.58900	-1.06500
H	6.23500	4.86700	1.47200
H	4.52200	1.60700	-0.36800
H	3.99600	3.56500	1.10900
H	-1.78400	-6.28100	-2.08500
H	-2.64900	-5.05000	-3.03300
H	-1.86100	-2.56800	-2.74700
H	0.02500	-1.36500	-1.37800
H	-0.48600	-6.40100	0.36000
H	1.33800	-6.06600	2.01800
H	1.79300	-1.98200	0.70600
H	2.49100	-3.89400	2.19400
H	-8.52500	-3.63800	0.92800
H	-7.57700	-4.46000	-1.16300
H	-6.33300	-4.49200	0.10200
H	-6.31700	-3.21500	-1.13700
H	-6.39300	-2.78900	1.96000
H	-7.76600	-1.68700	2.09000
H	-6.89800	-0.35600	0.17900
H	-5.47600	-1.42600	0.09000
H	-5.74800	-0.43200	1.53100
H	-3.76200	-0.87300	-1.98200
H	-2.12400	-0.37900	-3.78400
H	-3.13400	1.03600	-3.46200
H	-3.45400	0.02700	-4.88800
H	-6.16500	-1.14100	-2.56700
H	-5.87700	-0.37600	-4.13200
H	-5.32000	1.74800	-3.03400
H	-5.41100	0.97700	-1.43100
H	-6.87300	1.16300	-2.42100
H	0.25800	-3.60200	-4.15400
H	2.91800	-0.17100	-3.34900
H	4.35700	0.31100	-2.43300
H	4.54500	-1.91000	-3.27100
H	2.37600	-3.13700	-1.76100
H	6.25700	-2.58900	2.74200
H	4.71800	-0.73100	3.18300
H	3.50800	-1.44400	2.10100
H	3.96800	-2.28400	3.59400
H	5.07900	-3.66500	0.61400
H	6.34900	-0.63200	1.24300
H	4.45100	-0.52600	-0.18900
H	-2.61800	-3.74700	3.62400
H	-4.12300	-4.11700	2.73500
H	-2.73400	-0.29200	-0.00800
H	-1.54500	1.28500	-1.51500
H	1.57100	1.71900	1.40000
H	0.41100	0.11000	2.89700
H	-4.02600	-2.66300	3.77200
H	-4.03300	-1.88200	-3.40400
H	-8.45900	-2.31900	-0.24700
H	-3.16300	-5.41600	-1.36900
H	9.10200	3.38600	1.01600
H	-1.64200	7.54000	-1.75100
H	2.15800	6.05400	-0.86200
H	-2.90500	1.75200	3.76500
H	6.86400	-2.12800	0.45900
H	1.10500	-4.58800	-2.92600
H	1.49000	-4.77800	-4.64900
H	-1.88800	-0.23300	5.19700
H	0.21900	-1.91300	4.12400
O	1.14700	-2.14400	3.96700
O	-2.03700	0.31000	5.98800
Cl	0.76600	2.89300	-1.08600
H	1.10000	-2.64900	3.14300
H	-1.90700	-0.30500	6.71800

d C(4)-O (Asp145): 2.0Å
d C(4)-Cl: 1.80Å
reaction coordinate: -0.20Å
Extrapolated ONIOM energy:
-1624.18198859436

C	-2.28700	2.69200	3.33500
C	-1.42800	3.33700	4.24200
C	-2.32100	3.10300	1.99100
C	-0.60700	4.39400	3.80800
C	-1.50000	4.15800	1.55500
C	-0.64400	4.80500	2.46300
C	-2.27300	7.14400	-2.70700
C	-3.08500	6.07900	-1.99800
C	-4.19200	6.44700	-1.21000
C	-2.73300	4.72100	-2.11400
C	-4.94900	5.46300	-0.54900
C	-3.49100	3.73700	-1.45400
C	-4.60000	4.10700	-0.67300
C	3.02900	6.06800	-1.77600
C	8.62400	3.67000	0.09000
C	7.16100	3.32000	0.19500
N	6.21900	3.96100	0.98400
C	6.54500	2.28900	-0.45900
C	5.04200	3.32400	0.80800
N	5.22300	2.31300	-0.06100
C	-2.36900	-5.35800	-1.93400
C	-1.42400	-4.30200	-1.43900
C	-1.31400	-3.03800	-1.91600
C	-0.44300	-4.40500	-0.36200
N	-0.31700	-2.36600	-1.23000
C	0.23900	-3.15700	-0.25200
C	-0.04800	-5.43300	0.52000
C	1.26000	-2.93600	0.68000
C	0.98000	-5.22500	1.45900
C	1.63500	-3.98400	1.53800
C	-7.90300	-2.87400	0.37300
C	-7.14400	-2.02500	1.40700
C	-6.97600	-3.76300	-0.46500
C	-6.29200	-0.91400	0.78100
C	-4.08500	-0.90000	-3.05200
C	-5.53300	-0.38400	-3.05200
C	-3.14100	-0.06000	-3.92200
C	-5.69400	0.99200	-2.39700
C	1.16500	-4.19800	-3.78100
C	2.22600	-3.12500	-3.70500
O	2.61400	-2.60100	-4.74200
N	2.71600	-2.80000	-2.50500
C	3.87600	-1.92000	-2.33600
C	4.74000	-2.32600	-1.12200
O	5.21500	-3.45700	-1.06400
C	3.44900	-0.43600	-2.40800
C	2.58200	0.12000	-1.26700

O	1.32600	0.09400	-1.41200
O	3.18100	0.63200	-0.27500
N	4.99600	-1.44400	-0.15300
C	5.96700	-1.65900	0.92700
C	5.39100	-2.42400	2.12700
O	4.91200	-3.67700	1.71000
C	4.27900	-1.64700	2.82600
C	-3.59700	-3.14500	3.14800
S	-2.95600	-2.33600	1.64400
C	-1.86900	-1.12900	2.40300
O	-1.64500	-1.18000	3.61800
C	-1.22900	-0.20100	1.48000
C	-1.74500	0.08300	0.19900
C	-1.06200	0.89700	-0.68200
C	0.22500	1.36700	-0.33100
C	0.66100	1.24100	1.00700
C	-0.03000	0.42800	1.87700
H	-1.40400	3.01600	5.27400
H	-2.97400	2.60200	1.29200
H	0.04600	4.89100	4.51100
H	-1.52900	4.47200	0.52000
H	-0.02100	5.62100	2.12600
H	-1.80500	6.72500	-3.59800
H	-2.92100	7.96900	-3.00500
H	-4.46600	7.48800	-1.11100
H	-1.87700	4.42900	-2.70700
H	-5.79800	5.74900	0.05600
H	-3.21800	2.69600	-1.54000
H	-5.18100	3.35200	-0.16200
H	3.78400	6.75100	-1.38700
H	3.46100	5.07500	-1.90600
H	2.67000	6.43400	-2.73800
H	9.01000	3.36600	-0.88400
H	8.76000	4.74700	0.19900
H	6.99900	1.58300	-1.14600
H	6.38900	4.75400	1.59200
H	4.48200	1.64400	-0.32600
H	4.09100	3.54800	1.28800
H	-1.85600	-6.31900	-1.97300
H	-2.72800	-5.10100	-2.93100
H	-1.90700	-2.62800	-2.72200
H	-0.03000	-1.39600	-1.38000
H	-0.54300	-6.39100	0.47000
H	1.27800	-6.02400	2.12500
H	1.74500	-1.97100	0.72800
H	2.42900	-3.85000	2.26100
H	-8.60500	-3.51700	0.90500
H	-7.57700	-4.38300	-1.13100
H	-6.39100	-4.41000	0.19000
H	-6.30300	-3.15300	-1.06600
H	-6.50600	-2.67200	2.01000
H	-7.87500	-1.55900	2.06900
H	-6.92300	-0.25900	0.18000
H	-5.50900	-1.34100	0.15600
H	-5.82500	-0.32800	1.57300
H	-3.71100	-0.92300	-2.02900
H	-2.14300	-0.49700	-3.91100
H	-3.07900	0.95900	-3.54100
H	-3.50800	-0.03600	-4.94900
H	-6.14900	-1.09700	-2.50300
H	-5.90200	-0.33800	-4.07800
H	-5.20600	1.75700	-3.00200
H	-5.25700	0.98300	-1.39800
H	-6.75400	1.23400	-2.32000
H	0.22500	-3.74000	-4.07900
H	2.92300	-0.32500	-3.35700
H	4.36600	0.16900	-2.45600
H	4.52700	-2.08300	-3.19600
H	2.34300	-3.24500	-1.67700
H	6.19400	-2.58800	2.84500
H	4.66700	-0.70200	3.20100
H	3.45900	-1.44900	2.13800
H	3.90400	-2.23300	3.66600
H	5.01200	-3.72700	0.74400
H	6.33200	-0.69600	1.28000
H	4.45800	-0.58200	-0.17200
H	-2.76900	-3.52800	3.74300
H	-4.22800	-3.96800	2.81000
H	-2.71600	-0.31200	-0.08200
H	-1.45900	1.12700	-1.66300
H	1.58900	1.70600	1.30200
H	0.36300	0.22900	2.86800
H	-4.18500	-2.44600	3.74500
H	-4.08800	-1.92100	-3.43500
H	-8.47400	-2.22000	-0.28800
H	-3.21800	-5.43000	-1.25300
H	9.18200	3.15500	0.87200
H	-1.50000	7.51700	-2.03500
H	2.19300	6.01100	-1.07800
H	-2.91700	1.87900	3.67100
H	6.81800	-2.22500	0.54400
H	1.06100	-4.69700	-2.82000
H	1.46500	-4.92400	-4.53400
H	-1.83300	-0.00300	5.12700
H	0.15300	-1.79400	4.12800
O	1.07300	-2.05500	3.96800
O	-2.07100	0.50400	5.92100
Cl	0.81500	2.80500	-1.23500
H	1.00200	-2.58800	3.16400
H	-2.17200	-0.17200	6.60000

d C(4)-O (Asp145): 1.9Å
d C(4)-Cl: 1.82Å
reaction coordinate: -0.08Å
Extrapolated ONIOM energy:
-1624.17636916582

C	-2.28300	2.82700	3.27800
C	-1.59400	3.56600	4.25600
C	-2.15300	3.17100	1.92100
C	-0.78200	4.65100	3.87900
C	-1.33900	4.25300	1.54200
C	-0.65600	4.99600	2.52100
C	-2.07900	7.11000	-2.90900
C	-2.88600	6.08000	-2.14400
C	-4.00300	6.48200	-1.38800
C	-2.51900	4.72100	-2.17700
C	-4.75400	5.53100	-0.67400
C	-3.27200	3.77000	-1.46500
C	-4.38900	4.17400	-0.71400

C	3.18700	5.93100	-1.89900	H	-5.61000	5.84300	-0.09100
C	8.70500	3.44400	0.07500	H	-2.98700	2.73000	-1.48700
C	7.21800	3.22700	0.20800	H	-4.96500	3.44500	-0.16100
N	6.34700	3.95800	1.00100	H	3.96600	6.59800	-1.53300
C	6.50400	2.24600	-0.42100	H	3.58400	4.92100	-2.00400
C	5.11700	3.42100	0.85500	H	2.83500	6.28200	-2.86900
N	5.19600	2.38700	-0.00300	H	9.04000	3.12600	-0.91300
C	-2.47500	-5.36800	-1.87700	H	8.94300	4.50000	0.20300
C	-1.51300	-4.31900	-1.40500	H	6.88400	1.49300	-1.10200
C	-1.37600	-3.07200	-1.91600	H	6.59700	4.73900	1.59700
C	-0.54500	-4.41000	-0.31600	H	4.41400	1.76300	-0.25400
N	-0.37500	-2.39800	-1.23800	H	4.20100	3.73400	1.35100
C	0.15600	-3.17100	-0.23100	H	-1.99000	-6.34400	-1.86100
C	-0.17900	-5.41900	0.60000	H	-2.80200	-5.14500	-2.89300
C	1.16400	-2.93900	0.71200	H	-1.95700	-2.67400	-2.73600
C	0.83700	-5.20100	1.54900	H	-0.08700	-1.43200	-1.40000
C	1.50800	-3.96700	1.60600	H	-0.69000	-6.37100	0.57000
C	-7.97300	-2.70800	0.31900	H	1.11000	-5.98500	2.24300
C	-7.26900	-1.85900	1.39000	H	1.66100	-1.98000	0.74400
C	-7.00600	-3.61600	-0.45200	H	2.28800	-3.82400	2.34100
C	-6.37200	-0.76000	0.80800	H	-8.71400	-3.33800	0.81200
C	-4.07500	-0.89600	-3.10600	H	-7.57200	-4.23300	-1.15100
C	-5.48800	-0.29700	-3.02900	H	-6.47300	-4.26600	0.24300
C	-3.12000	-0.08500	-3.99000	H	-6.28800	-3.02000	-1.01300
C	-5.53900	1.06700	-2.33100	H	-6.67300	-2.50700	2.03300
C	1.10300	-4.32900	-3.71000	H	-8.03300	-1.38200	2.00500
C	2.18600	-3.27800	-3.64500	H	-6.96200	-0.10000	0.17200
O	2.60200	-2.78900	-4.68800	H	-5.56100	-1.19700	0.22700
N	2.66300	-2.93700	-2.44600	H	-5.94200	-0.17600	1.62200
C	3.85000	-2.09700	-2.27900	H	-3.66200	-0.97100	-2.10000
C	4.66000	-2.49500	-1.02600	H	-2.15000	-0.58200	-4.03800
O	5.03700	-3.65600	-0.89100	H	-2.97800	0.91500	-3.58100
C	3.48200	-0.60300	-2.41800	H	-3.52800	-0.00500	-4.99900
C	2.64900	0.04400	-1.30500	H	-6.12200	-0.98800	-2.47300
O	1.38500	0.06000	-1.45600	H	-5.89700	-0.19900	-4.03600
O	3.26200	0.57900	-0.34300	H	-5.03100	1.81900	-2.93500
N	4.97800	-1.57900	-0.11000	H	-5.06300	1.00300	-1.35100
C	5.91500	-1.80400	0.99500	H	-6.57800	1.36900	-2.20200
C	5.27600	-2.46300	2.22500	H	0.17800	-3.85900	-4.03200
O	4.77000	-3.72500	1.87700	H	2.95900	-0.51200	-3.37100
C	4.17300	-1.60500	2.83800	H	4.42100	-0.03700	-2.49200
C	-3.76800	-2.96900	3.13900	H	4.51600	-2.31700	-3.11400
S	-3.02700	-2.25900	1.63100	H	2.26900	-3.35500	-1.61300
C	-1.91600	-1.06200	2.38200	H	6.05300	-2.60500	2.97700
O	-1.72300	-1.08600	3.60400	H	4.58200	-0.64800	3.15600
C	-1.22500	-0.19200	1.44700	H	3.37700	-1.43200	2.11700
C	-1.70000	0.07800	0.14500	H	3.76000	-2.11900	3.70700
C	-0.96400	0.82800	-0.74800	H	4.83700	-3.81800	0.91100
C	0.34800	1.25000	-0.39800	H	6.34000	-0.85000	1.30300
C	0.74700	1.13900	0.96200	H	4.51800	-0.67600	-0.19300
C	-0.00100	0.39500	1.84200	H	-2.97900	-3.29600	3.81600
H	-1.69400	3.29300	5.29800	H	-4.36400	-3.82500	2.81700
H	-2.67600	2.59900	1.17000	H	-2.68400	-0.27600	-0.14400
H	-0.26000	5.22000	4.63600	H	-1.33800	1.05100	-1.74000
H	-1.24300	4.51400	0.49700	H	1.68800	1.57200	1.26500
H	-0.03800	5.83300	2.22900	H	0.36400	0.21400	2.84700
H	-1.59300	6.64300	-3.76600	H	-4.40500	-2.24100	3.64300
H	-2.73400	7.90500	-3.26600	H	-4.15300	-1.90300	-3.51600
H	-4.28800	7.52400	-1.35200	H	-8.49400	-2.05400	-0.38200
H	-1.65600	4.40300	-2.74500	H	-3.34200	-5.38600	-1.21500

H	9.22900	2.86200	0.83400
H	-1.32000	7.53500	-2.25200
H	2.35300	5.92100	-1.19700
H	-2.91000	1.99600	3.57000
H	6.73200	-2.44400	0.65500
H	0.97600	-4.80500	-2.74000
H	1.39700	-5.07900	-4.44200
H	-1.89700	0.15200	5.07300
H	0.04200	-1.73600	4.17300
O	0.95400	-2.03800	4.03600
O	-2.14500	0.67100	5.85600
Cl	0.93800	2.73900	-1.26400
H	0.87300	-2.58500	3.24200
H	-2.34400	-0.00300	6.51600

d C(4)-O (Asp145): 1.85Å
d C(4)-Cl: 1.84Å
reaction coordinate: -0.01Å
Extrapolated ONIOM energy:
-1624.17400433495

C	-2.11400	3.02400	3.24600
C	-1.49800	3.80100	4.24300
C	-1.81800	3.26000	1.89300
C	-0.59500	4.81900	3.88700
C	-0.91300	4.27500	1.53400
C	-0.30500	5.05800	2.53100
C	-1.59600	7.26000	-2.97400
C	-2.41100	6.25600	-2.18400
C	-3.51100	6.69000	-1.41900
C	-2.06900	4.89000	-2.20200
C	-4.26900	5.76300	-0.68100
C	-2.83000	3.96400	-1.46600
C	-3.92900	4.40000	-0.70500
C	3.56800	5.70800	-1.94100
C	8.88600	2.83800	0.06300
C	7.38800	2.84300	0.26000
N	6.67500	3.61800	1.16300
C	6.50100	2.04500	-0.40500
C	5.37000	3.28800	1.04500
N	5.24900	2.33900	0.09700
C	-2.89500	-5.15200	-1.89200
C	-1.81900	-4.27000	-1.33600
C	-1.51300	-3.01700	-1.75100
C	-0.91300	-4.55700	-0.23000
N	-0.44900	-2.53100	-1.01100
C	-0.06000	-3.43000	-0.04100
C	-0.73000	-5.65900	0.63100
C	0.92300	-3.39500	0.95700
C	0.25500	-5.63600	1.63600
C	1.07800	-4.51000	1.80000
C	-8.19300	-2.09300	0.27400
C	-7.44400	-1.27800	1.34100
C	-7.27800	-3.05300	-0.49700
C	-6.47600	-0.24300	0.75500
C	-4.16400	-0.58200	-3.14400
C	-5.50000	0.17400	-3.07800
C	-3.10100	0.13400	-3.98800
C	-5.40600	1.52000	-2.35100
C	0.75500	-4.38300	-3.71700
C	1.96300	-3.48300	-3.67900
O	2.46100	-3.10300	-4.73200
N	2.44700	-3.15100	-2.48500
C	3.71900	-2.45200	-2.31200
C	4.38500	-2.85000	-0.98000
O	4.40900	-4.03000	-0.63500
C	3.53000	-0.93800	-2.55000
C	2.81200	-0.13900	-1.46100
O	1.53500	-0.07700	-1.53900
O	3.51600	0.44100	-0.60100
N	4.94700	-1.91400	-0.21600
C	5.72200	-2.19100	0.99400
C	4.85300	-2.40400	2.24200
O	4.12100	-3.58800	2.08800
C	3.90400	-1.24000	2.52100
C	-4.04500	-2.58300	3.12500
S	-3.23200	-1.99600	1.60200
C	-1.95300	-0.95800	2.33400
O	-1.75900	-1.00300	3.55500
C	-1.14600	-0.19800	1.39700
C	-1.57000	0.13600	0.09200
C	-0.74300	0.79400	-0.79200
C	0.60900	1.08000	-0.43200
C	0.99300	0.86300	0.92400
C	0.15000	0.21000	1.79200
H	-1.72100	3.60500	5.28300
H	-2.28500	2.65800	1.12900
H	-0.12800	5.41700	4.65700
H	-0.69200	4.45400	0.49100
H	0.38200	5.84500	2.25400
H	-1.12500	6.77000	-3.82700
H	-2.24100	8.05900	-3.33800
H	-3.77600	7.73700	-1.39500
H	-1.22000	4.54700	-2.77600
H	-5.11000	6.09900	-0.09100
H	-2.56400	2.91800	-1.47500
H	-4.50900	3.69000	-0.13200
H	4.39100	6.32000	-1.57200
H	3.89900	4.67600	-2.05600
H	3.23500	6.09000	-2.90600
H	9.12400	2.56600	-0.96600
H	9.29400	3.82900	0.26700
H	6.72400	1.30600	-1.16700
H	7.07000	4.29300	1.80800
H	4.38700	1.83600	-0.17400
H	4.54000	3.68600	1.62500
H	-2.52300	-6.17300	-1.97700
H	-3.19900	-4.79600	-2.87600
H	-2.02200	-2.48300	-2.54200
H	-0.06200	-1.59100	-1.10100
H	-1.36200	-6.52800	0.52000
H	0.38400	-6.48800	2.29100
H	1.54800	-2.52300	1.07600
H	1.83100	-4.51400	2.57800
H	-8.96600	-2.68100	0.77000
H	-7.87800	-3.64600	-1.18800
H	-6.77300	-3.72400	0.20000
H	-6.53500	-2.49700	-1.06600
H	-6.89300	-1.95600	1.99400
H	-8.18000	-0.74900	1.94700

H	-7.01800	0.44200	0.10200
H	-5.68600	-0.73600	0.18900
H	-6.02000	0.32600	1.56600
H	-3.78400	-0.72800	-2.13300
H	-2.19900	-0.47500	-4.03700
H	-2.84900	1.09600	-3.54400
H	-3.47800	0.29300	-4.99900
H	-6.22000	-0.45100	-2.54800
H	-5.87600	0.33800	-4.08900
H	-4.80400	2.22000	-2.93000
H	-4.95800	1.38200	-1.36600
H	-6.40600	1.93700	-2.23200
H	-0.11500	-3.78900	-3.98200
H	2.99900	-0.84500	-3.49900
H	4.52500	-0.49400	-2.67500
H	4.39500	-2.80600	-3.09100
H	1.99600	-3.49300	-1.64700
H	5.51200	-2.52200	3.10200
H	4.47500	-0.32400	2.66500
H	3.21000	-1.10500	1.69400
H	3.33500	-1.45100	3.42600
H	4.15300	-3.84000	1.14800
H	6.38900	-1.35200	1.18700
H	4.73100	-0.95000	-0.45600
H	-3.30700	-3.04400	3.78100
H	-4.78400	-3.32400	2.81500
H	-2.58700	-0.09500	-0.21200
H	-1.08200	1.06600	-1.78400
H	1.98700	1.15500	1.23100
H	0.49300	-0.04100	2.79000
H	-4.53600	-1.76100	3.64800
H	-4.34600	-1.56400	-3.58200
H	-8.68000	-1.41500	-0.42800
H	-3.75500	-5.13700	-1.22200
H	9.34200	2.11300	0.73800
H	-0.82400	7.68400	-2.33200
H	2.73800	5.74500	-1.23400
H	-2.81500	2.24800	3.52300
H	6.33400	-3.08300	0.84600
H	0.61200	-4.86600	-2.75200
H	0.91600	-5.14300	-4.47800
H	-1.74200	0.31700	4.98300
H	-0.12900	-1.92200	4.13300
O	0.75500	-2.31600	4.06800
O	-1.94000	0.86600	5.76000
Cl	1.28100	2.61700	-1.19700
H	0.67800	-2.88500	3.28900
H	-2.14200	0.21600	6.44300

d C(4)-O (Asp145): 1.8Å
d C(4)-Cl: 1.87Å
reaction coordinate: 0.07Å
Extrapolated ONIOM energy:
-1624.17244030062

C	-2.12400	3.07400	3.23600
C	-1.57700	3.88900	4.24300
C	-1.75600	3.27800	1.89500
C	-0.67400	4.91500	3.90900
C	-0.85100	4.30100	1.55800
C	-0.31400	5.12300	2.56500
C	-1.53600	7.26100	-3.02100
C	-2.33700	6.25800	-2.21600
C	-3.44900	6.68600	-1.46600
C	-1.97000	4.89900	-2.20600
C	-4.19300	5.76100	-0.71300
C	-2.71700	3.97300	-1.45500
C	-3.82800	4.40400	-0.70800
C	3.61000	5.67300	-1.95700
C	8.89500	2.77000	0.08600
C	7.39600	2.81500	0.27000
N	6.69400	3.62800	1.14700
C	6.49400	2.02500	-0.38600
C	5.38200	3.32800	1.02500
N	5.24500	2.36000	0.09800
C	-2.94200	-5.13400	-1.88200
C	-1.85300	-4.27400	-1.32000
C	-1.53600	-3.02000	-1.71900
C	-0.94600	-4.58600	-0.22000
N	-0.46800	-2.55300	-0.97300
C	-0.08500	-3.46800	-0.01600
C	-0.77200	-5.70100	0.62600
C	0.89600	-3.45200	0.98400
C	0.21200	-5.69800	1.63200
C	1.04300	-4.57900	1.81200
C	-8.22400	-2.02000	0.24400
C	-7.48500	-1.20800	1.32000
C	-7.30300	-2.98300	-0.51700
C	-6.50600	-0.17700	0.74600
C	-4.16700	-0.55900	-3.16400
C	-5.48100	0.23400	-3.08100
C	-3.08900	0.13500	-4.00400
C	-5.34200	1.56600	-2.33500
C	0.72200	-4.40400	-3.69500
C	1.93800	-3.51400	-3.65800
O	2.44700	-3.14800	-4.71100
N	2.42000	-3.17700	-2.46400
C	3.70300	-2.49800	-2.29100
C	4.35000	-2.89000	-0.94700
O	4.34500	-4.06400	-0.58400
C	3.54700	-0.98500	-2.55700
C	2.85000	-0.15100	-1.48500
O	1.57000	-0.07200	-1.56900
O	3.55900	0.43300	-0.63600
N	4.92600	-1.95400	-0.19200
C	5.68600	-2.22800	1.02800
C	4.80500	-2.41800	2.27100
O	4.06800	-3.60100	2.12900
C	3.85800	-1.24600	2.52100
C	-4.12300	-2.48900	3.11500
S	-3.26900	-1.95700	1.59400
C	-1.96300	-0.94200	2.32100
O	-1.76800	-0.98400	3.54300
C	-1.13900	-0.20800	1.38100
C	-1.54700	0.12500	0.06900
C	-0.69800	0.74700	-0.82000
C	0.66100	1.01400	-0.45800
C	1.03500	0.78400	0.90100
C	0.16900	0.16700	1.77200
H	-1.85300	3.71500	5.27500

H	-2.16900	2.64700	1.12400
H	-0.26200	5.54200	4.68600
H	-0.57600	4.45500	0.52400
H	0.37200	5.91500	2.30400
H	-1.04900	6.76400	-3.86100
H	-2.19400	8.04000	-3.40700
H	-3.73300	7.72900	-1.46400
H	-1.11200	4.56100	-2.76900
H	-5.04300	6.09300	-0.13300
H	-2.43100	2.93200	-1.44300
H	-4.39700	3.69500	-0.12300
H	4.45700	6.23700	-1.56700
H	3.90000	4.63300	-2.11100
H	3.29300	6.10300	-2.90600
H	9.13500	2.46100	-0.93200
H	9.32500	3.75600	0.26400
H	6.70500	1.26300	-1.12800
H	7.09900	4.30800	1.78000
H	4.37600	1.86900	-0.17100
H	4.55700	3.75900	1.58900
H	-2.59200	-6.16300	-1.96100
H	-3.22800	-4.77500	-2.87100
H	-2.04400	-2.46900	-2.49900
H	-0.08900	-1.60900	-1.04300
H	-1.41100	-6.56200	0.50400
H	0.33400	-6.55900	2.27600
H	1.52700	-2.58700	1.11600
H	1.79500	-4.59700	2.59100
H	-9.00500	-2.60700	0.73100
H	-7.89600	-3.57400	-1.21400
H	-6.80700	-3.65400	0.18500
H	-6.55200	-2.42700	-1.07700
H	-6.94600	-1.88800	1.98000
H	-8.22800	-0.67600	1.91700
H	-7.03700	0.51000	0.08600
H	-5.71100	-0.67300	0.19100
H	-6.06000	0.39100	1.56300
H	-3.78700	-0.72900	-2.15600
H	-2.20500	-0.50000	-4.06700
H	-2.80500	1.08400	-3.55000
H	-3.46600	0.31900	-5.01100
H	-6.21600	-0.37600	-2.55600
H	-5.85500	0.42400	-4.08800
H	-4.72100	2.25600	-2.90600
H	-4.89600	1.40100	-1.35400
H	-6.32900	2.01300	-2.20700
H	-0.14500	-3.80100	-3.95100
H	3.01800	-0.89800	-3.50800
H	4.55100	-0.56500	-2.68900
H	4.37900	-2.87900	-3.05900
H	1.96100	-3.50800	-1.62600
H	5.45500	-2.52500	3.13900
H	4.43100	-0.33000	2.65400
H	3.17100	-1.12500	1.68600
H	3.28100	-1.44000	3.42600
H	4.09500	-3.86100	1.19100
H	6.36200	-1.39600	1.21800
H	4.74000	-0.98900	-0.45200
H	-3.38400	-2.81500	3.84600
H	-4.76900	-3.32300	2.83500
H	-2.56700	-0.08400	-0.23900
H	-1.02700	1.01500	-1.81700
H	2.03400	1.05300	1.21200
H	0.50500	-0.08600	2.77300
H	-4.72200	-1.67900	3.53400
H	-4.38100	-1.53100	-3.61200
H	-8.70100	-1.34000	-0.46400
H	-3.80800	-5.09700	-1.22100
H	9.32900	2.05500	0.78700
H	-0.77700	7.71400	-2.38200
H	2.78300	5.71600	-1.24800
H	-2.82500	2.29300	3.49600
H	6.28800	-3.12900	0.89400
H	0.58100	-4.89100	-2.73200
H	0.87200	-5.16100	-4.46100
H	-1.72100	0.35800	4.95000
H	-0.16100	-1.93500	4.12400
O	0.71600	-2.34700	4.06900
O	-1.90600	0.91300	5.72500
Cl	1.32200	2.60600	-1.18100
H	0.63100	-2.93000	3.30100
H	-2.12000	0.26900	6.41000

d C(4)-O (Asp145): 1.75Å
d C(4)-Cl: 1.90Å
reaction coordinate: 0.15Å
Extrapolated ONIOM energy:
-1624.17146125904

C	-2.14200	3.12500	3.22900
C	-1.68100	3.98500	4.24000
C	-1.69700	3.29800	1.90700
C	-0.78800	5.02700	3.92800
C	-0.80300	4.33700	1.59200
C	-0.35200	5.20500	2.60200
C	-1.49900	7.25600	-3.07100
C	-2.27800	6.25300	-2.24500
C	-3.39500	6.67200	-1.49700
C	-1.88400	4.90100	-2.21200
C	-4.11600	5.74500	-0.72300
C	-2.60900	3.97400	-1.44100
C	-3.72400	4.39600	-0.69600
C	3.63500	5.64600	-1.98000
C	8.89700	2.72600	0.09600
C	7.39700	2.80100	0.27100
N	6.70500	3.63400	1.13800
C	6.48400	2.02300	-0.38300
C	5.38800	3.35700	1.01200
N	5.23800	2.38400	0.09200
C	-2.97700	-5.12400	-1.86600
C	-1.87700	-4.28300	-1.29800
C	-1.55600	-3.02600	-1.68300
C	-0.96800	-4.61300	-0.20600
N	-0.48400	-2.57400	-0.93500
C	-0.10200	-3.50100	0.01000
C	-0.79600	-5.73900	0.62700
C	0.87900	-3.50000	1.01000
C	0.18900	-5.75000	1.63200
C	1.02300	-4.63600	1.82500
C	-8.24900	-1.97100	0.22500

C	-7.49800	-1.15100	1.28800
C	-7.33600	-2.94000	-0.53700
C	-6.51500	-0.13300	0.69700
C	-4.17300	-0.55100	-3.17700
C	-5.45900	0.28600	-3.09500
C	-3.07500	0.10400	-4.02500
C	-5.27600	1.61600	-2.35500
C	0.69800	-4.42500	-3.67000
C	1.91700	-3.53800	-3.63600
O	2.43100	-3.18100	-4.68900
N	2.39600	-3.19200	-2.44300
C	3.68800	-2.52900	-2.27200
C	4.32200	-2.91400	-0.91900
O	4.30400	-4.08500	-0.54700
C	3.55800	-1.01700	-2.56200
C	2.88000	-0.15400	-1.50400
O	1.59500	-0.06200	-1.59800
O	3.58900	0.43100	-0.66200
N	4.90300	-1.97800	-0.16800
C	5.65800	-2.24900	1.05600
C	4.77500	-2.43800	2.29800
O	4.04300	-3.62500	2.16100
C	3.82300	-1.26900	2.54000
C	-4.16400	-2.42700	3.11600
S	-3.29700	-1.92600	1.59100
C	-1.97200	-0.92700	2.31100
O	-1.77700	-0.96800	3.53300
C	-1.13600	-0.21300	1.36800
C	-1.53100	0.11500	0.05000
C	-0.66300	0.69700	-0.84800
C	0.70100	0.95100	-0.48500
C	1.06800	0.71000	0.87800
C	0.18200	0.13200	1.75500
H	-2.01300	3.83400	5.25800
H	-2.04400	2.63200	1.13200
H	-0.44000	5.68800	4.70900
H	-0.47100	4.46800	0.57200
H	0.32600	6.01000	2.35900
H	-1.01800	6.75500	-3.91100
H	-2.17200	8.02300	-3.45600
H	-3.69900	7.70900	-1.51200
H	-1.02200	4.56900	-2.77200
H	-4.97000	6.07100	-0.14500
H	-2.30100	2.94000	-1.41200
H	-4.27500	3.68700	-0.09400
H	4.50300	6.17200	-1.58500
H	3.88900	4.60200	-2.16400
H	3.32300	6.11100	-2.91600
H	9.13700	2.40200	-0.91700
H	9.34400	3.70600	0.26600
H	6.68400	1.25100	-1.11800
H	7.11900	4.31200	1.76800
H	4.36400	1.90400	-0.17900
H	4.56900	3.80800	1.56800
H	-2.64900	-6.16200	-1.92600
H	-3.24000	-4.77200	-2.86300
H	-2.06600	-2.46200	-2.45200
H	-0.11700	-1.62500	-0.98500
H	-1.43900	-6.59600	0.49700
H	0.30800	-6.61900	2.26600
H	1.51200	-2.63700	1.15300
H	1.77400	-4.66400	2.60500
H	-9.02500	-2.55200	0.72400
H	-7.93800	-3.53800	-1.22200
H	-6.83200	-3.60500	0.16500
H	-6.59300	-2.39000	-1.11300
H	-6.96000	-1.82800	1.95200
H	-8.23300	-0.60800	1.88300
H	-7.04300	0.54800	0.02900
H	-5.72300	-0.64200	0.14800
H	-6.06300	0.44300	1.50600
H	-3.79500	-0.72800	-2.17000
H	-2.21300	-0.56000	-4.08800
H	-2.75900	1.04500	-3.57500
H	-3.45000	0.29600	-5.03100
H	-6.21300	-0.29800	-2.56600
H	-5.83000	0.48400	-4.10200
H	-4.63200	2.28200	-2.93000
H	-4.83400	1.44100	-1.37400
H	-6.24600	2.09600	-2.22800
H	-0.16900	-3.81900	-3.91800
H	3.03100	-0.93600	-3.51500
H	4.56900	-0.61700	-2.70000
H	4.36200	-2.93100	-3.03000
H	1.93200	-3.51400	-1.60500
H	5.42300	-2.53800	3.16800
H	4.39200	-0.34900	2.66900
H	3.13900	-1.15700	1.70200
H	3.24400	-1.46000	3.44400
H	4.06300	-3.88300	1.22200
H	6.33300	-1.41600	1.24700
H	4.73800	-1.01300	-0.44000
H	-3.42900	-2.74000	3.85700
H	-4.81000	-3.26400	2.84800
H	-2.55400	-0.07600	-0.26100
H	-0.98300	0.95400	-1.85100
H	2.07300	0.95700	1.19000
H	0.51200	-0.12100	2.75700
H	-4.76300	-1.60700	3.51600
H	-4.41900	-1.51700	-3.62000
H	-8.73100	-1.29500	-0.48300
H	-3.85100	-5.05900	-1.21800
H	9.31400	2.01100	0.80700
H	-0.73800	7.72500	-2.44700
H	2.81500	5.69800	-1.26300
H	-2.83700	2.33200	3.47000
H	6.26200	-3.14900	0.92600
H	0.56100	-4.91700	-2.70900
H	0.84100	-5.17800	-4.44200
H	-1.71500	0.39200	4.91700
H	-0.18800	-1.94000	4.11900
O	0.68200	-2.36700	4.07300
O	-1.88700	0.95200	5.69300
Cl	1.35100	2.60600	-1.16700
H	0.58700	-2.96800	3.32100
H	-2.09900	0.31100	6.38200

d C(4)-O (Asp145): 1.56Å
d C(4)-Cl: 1.82Å
reaction coordinate: 0.34Å
Extrapolated ONIOM energy:
-1624.17132569867

C	-1.70700	2.92900	3.75300
C	-1.05900	2.15100	4.72600
C	-0.95700	3.57100	2.75300
C	0.33900	2.00100	4.69200
C	0.44100	3.42500	2.72000
C	1.08900	2.63500	3.68700
C	-1.04900	8.04400	-2.60100
C	-1.73500	6.94500	-1.81400
C	-3.07400	7.09900	-1.40900
C	-1.03600	5.76900	-1.47600
C	-3.71400	6.08300	-0.67400
C	-1.67500	4.75600	-0.74000
C	-3.01400	4.91100	-0.34000
C	3.90100	5.84900	-1.69700
C	8.85600	2.30000	0.14000
C	7.37900	2.59900	0.28400
N	6.80800	3.60600	1.04900
C	6.36600	1.89700	-0.30500
C	5.46400	3.50900	0.92300
N	5.18000	2.47800	0.10300
C	-3.83400	-4.14400	-1.83200
C	-2.50800	-3.96200	-1.16400
C	-2.05100	-2.79900	-0.65400
C	-1.45000	-4.94200	-0.93300
N	-0.79500	-2.98500	-0.11300
C	-0.36500	-4.28200	-0.28100
C	-1.27700	-6.31000	-1.24200
C	0.82400	-4.94100	0.05300
C	-0.08000	-6.97900	-0.92000
C	0.96900	-6.29800	-0.27400
C	-8.69100	-0.52900	0.50300
C	-7.72500	0.46600	1.16700
C	-8.02900	-1.87000	0.16000
C	-6.61100	0.95500	0.23300
C	-4.55300	0.58000	-2.94000
C	-4.43500	1.94600	-3.63300
C	-3.52600	-0.44500	-3.43400
C	-3.12000	2.66900	-3.32400
C	-0.14200	-3.77100	-3.69600
C	1.21600	-3.10700	-3.70600
O	1.71600	-2.77400	-4.77400
N	1.82500	-2.91900	-2.53300
C	3.20500	-2.43300	-2.42300
C	3.88500	-2.91900	-1.11700
O	4.02100	-4.12300	-0.92100
C	3.27500	-0.91400	-2.72600
C	2.78900	0.03200	-1.64900
O	1.49300	0.23300	-1.62600
O	3.60100	0.56100	-0.87900
N	4.31400	-2.04300	-0.20300
C	5.11700	-2.33300	0.98800
C	4.34000	-3.01500	2.12600
O	4.03700	-4.33700	1.76600
C	3.06000	-2.27900	2.50200
C	-4.38800	-2.00100	3.17700
S	-3.73800	-1.07200	1.75000
C	-2.01900	-0.81000	2.33300
O	-1.71300	-1.28700	3.43700
C	-1.12300	-0.13400	1.43300
C	-1.50500	0.46300	0.19700
C	-0.59700	0.97300	-0.68800
C	0.83400	0.96300	-0.41400
C	1.20300	0.37800	0.86600
C	0.26600	-0.12500	1.72800
H	-1.63500	1.66200	5.49900
H	-1.45500	4.17300	2.00900
H	0.82800	1.38700	5.43700
H	1.01100	3.90900	1.94100
H	2.16100	2.50600	3.65500
H	-0.24300	7.62500	-3.20600
H	-1.76700	8.53200	-3.26100
H	-3.61600	8.00000	-1.66100
H	-0.00800	5.63700	-1.78000
H	-4.74300	6.20500	-0.36700
H	-1.13700	3.85300	-0.48400
H	-3.50500	4.12800	0.22200
H	4.90400	6.10600	-1.35700
H	3.86900	4.79900	-1.99000
H	3.63900	6.47000	-2.55400
H	9.04400	1.80300	-0.81300
H	9.43200	3.22500	0.17300
H	6.45100	1.03600	-0.95900
H	7.31400	4.27900	1.61300
H	4.25200	2.10800	-0.16700
H	4.71800	4.13300	1.40700
H	-3.72300	-4.00600	-2.90700
H	-4.54800	-3.41900	-1.44200
H	-2.60900	-1.87100	-0.64900
H	-0.30400	-2.27400	0.42700
H	-2.07800	-6.84700	-1.72900
H	0.03600	-8.02800	-1.15800
H	1.61400	-4.42100	0.57600
H	1.88200	-6.81900	-0.01600
H	-9.51400	-0.72000	1.19300
H	-8.78400	-2.55600	-0.22700
H	-7.58100	-2.30400	1.05400
H	-7.26100	-1.73100	-0.60100
H	-7.27600	0.00500	2.04800
H	-8.29900	1.33300	1.49500
H	-7.04400	1.40100	-0.66300
H	-5.96500	0.12400	-0.04800
H	-6.01000	1.70500	0.74900
H	-4.43400	0.71100	-1.86400
H	-3.73000	-1.40900	-2.97100
H	-2.51700	-0.13200	-3.16300
H	-3.59700	-0.54800	-4.51800
H	-5.25800	2.57500	-3.29000
H	-4.53200	1.81800	-4.71200
H	-2.28100	2.13800	-3.77300
H	-2.97900	2.72700	-2.24600
H	-3.15500	3.67900	-3.73400
H	-0.83900	-3.14100	-3.15400
H	2.71200	-0.76200	-3.64900
H	4.32300	-0.66200	-2.91700
H	3.76900	-2.91700	-3.22200

H	1.36700	-3.23500	-1.69100
H	4.98400	-3.04600	3.00500
H	3.28700	-1.24900	2.76900
H	2.35400	-2.29800	1.67200
H	2.60500	-2.77600	3.35900
H	3.97100	-4.37200	0.79400
H	5.52200	-1.39900	1.37500
H	4.13600	-1.06500	-0.39600
H	-3.93700	-2.99200	3.22900
H	-5.46400	-2.09000	3.02200
H	-2.55800	0.52000	-0.06800
H	-0.91600	1.40800	-1.62800
H	2.25200	0.37400	1.13600
H	0.58600	-0.56100	2.66800
H	-4.18200	-1.45900	4.10000
H	-5.55300	0.18500	-3.12600
H	-9.10400	-0.08700	-0.40500
H	-4.20600	-5.15000	-1.63500
H	9.17900	1.64500	0.95100
H	-0.63600	8.78000	-1.91100
H	3.18400	6.02300	-0.89500
H	-2.78100	3.03200	3.77800
H	5.95300	-2.98000	0.71600
H	-0.05000	-4.75300	-3.24000
H	-0.48500	-3.88600	-4.72300
H	-1.02200	-0.80800	5.29000
H	-0.60400	-2.87600	3.16700
O	0.05100	-3.48400	2.78700
O	-0.78700	-0.72500	6.23000
Cl	1.55500	2.70600	-0.64300
H	-0.47200	-4.12100	2.28400
H	-0.86600	-1.62800	6.55800

d C(4)-O (Asp145): 1.51Å
d C(4)-Cl: 1.95Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.17360761363

C	-1.66000	2.97100	3.76100
C	-0.97600	2.14600	4.66800
C	-0.95100	3.64900	2.75400
C	0.41500	1.98000	4.55900
C	0.44100	3.48800	2.64700
C	1.12400	2.64800	3.54500
C	-0.92800	8.10800	-2.50800
C	-1.62100	6.97500	-1.77500
C	-2.98100	7.09100	-1.42600
C	-0.91200	5.80800	-1.43000
C	-3.62800	6.04600	-0.74100
C	-1.55800	4.76500	-0.74300
C	-2.91600	4.88200	-0.39900
C	3.98600	5.82100	-1.63300
C	8.88400	2.17400	0.16600
C	7.41000	2.50400	0.29800
N	6.85400	3.52300	1.05800
C	6.38600	1.82300	-0.29800
C	5.50900	3.45400	0.92200
N	5.20800	2.42900	0.10100
C	-3.92100	-4.03600	-1.81300
C	-2.58700	-3.90000	-1.15100
C	-2.09800	-2.75700	-0.62400
C	-1.55200	-4.91000	-0.94300
N	-0.84200	-2.98300	-0.09700
C	-0.44600	-4.28700	-0.28900
C	-1.41600	-6.27600	-1.27400
C	0.72900	-4.98100	0.02600
C	-0.23300	-6.97900	-0.97200
C	0.83700	-6.33600	-0.32400
C	-8.70900	-0.35400	0.56000
C	-7.65500	0.54100	1.23400
C	-8.14800	-1.70900	0.11100
C	-6.55700	1.02100	0.27700
C	-4.56200	0.70800	-2.88700
C	-4.38700	2.03200	-3.64700
C	-3.62000	-0.40000	-3.37200
C	-3.01400	2.67800	-3.43300
C	-0.22800	-3.71400	-3.68600
C	1.15200	-3.09600	-3.70000
O	1.65800	-2.78200	-4.77100
N	1.77200	-2.92600	-2.53000
C	3.16500	-2.47500	-2.42800
C	3.84300	-2.97200	-1.12400
O	3.98800	-4.17800	-0.94400
C	3.27200	-0.96000	-2.74000
C	2.80900	-0.00600	-1.66300
O	1.51000	0.20700	-1.62900
O	3.62900	0.51100	-0.89600
N	4.25900	-2.10600	-0.19400
C	5.06700	-2.39900	0.99400
C	4.30100	-3.11200	2.12000
O	4.00900	-4.43000	1.73700
C	3.01400	-2.39800	2.51500
C	-4.41500	-1.91200	3.21900
S	-3.76200	-0.99000	1.78900
C	-2.02700	-0.78300	2.34700
O	-1.71800	-1.27600	3.44300
C	-1.11700	-0.12800	1.44100
C	-1.48500	0.48200	0.20800
C	-0.56300	0.94600	-0.68900
C	0.86600	0.88800	-0.42300
C	1.22400	0.27700	0.84600
C	0.27400	-0.18100	1.72100
H	-1.52300	1.63400	5.44700
H	-1.47700	4.29000	2.06300
H	0.93100	1.33000	5.25300
H	0.98000	3.99900	1.86300
H	2.19100	2.50800	3.45300
H	-0.07800	7.72300	-3.07300
H	-1.62400	8.58200	-3.20000
H	-3.53100	7.98400	-1.68300
H	0.13200	5.70500	-1.69100
H	-4.67200	6.13800	-0.47600
H	-1.01100	3.87000	-0.48100
H	-3.41200	4.07700	0.12600
H	5.02100	5.99900	-1.34400
H	3.86200	4.78200	-1.94000
H	3.72400	6.47500	-2.46500
H	9.06400	1.64900	-0.77300
H	9.47500	3.09100	0.17400

H	6.45800	0.95800	-0.94900
H	7.36900	4.18700	1.62400
H	4.27300	2.08100	-0.17400
H	4.77200	4.09500	1.39800
H	-3.81500	-3.87300	-2.88500
H	-4.61800	-3.30600	-1.39900
H	-2.63400	-1.81700	-0.60100
H	-0.33100	-2.29300	0.45100
H	-2.23300	-6.78500	-1.76400
H	-0.14500	-8.02700	-1.22600
H	1.53700	-4.48900	0.55000
H	1.73900	-6.88300	-0.08100
H	-9.51200	-0.53600	1.27500
H	-8.95900	-2.32300	-0.28100
H	-7.69200	-2.22200	0.95800
H	-7.40400	-1.57100	-0.67400
H	-7.19700	0.00100	2.06300
H	-8.16000	1.41800	1.64000
H	-7.00200	1.54700	-0.56800
H	-5.97800	0.17200	-0.08500
H	-5.88700	1.69900	0.80700
H	-4.39100	0.87900	-1.82400
H	-3.86600	-1.32700	-2.85700
H	-2.58400	-0.14000	-3.15100
H	-3.74000	-0.54600	-4.44600
H	-5.15100	2.72800	-3.29800
H	-4.54300	1.86400	-4.71400
H	-2.23300	2.07200	-3.89200
H	-2.81700	2.77600	-2.36600
H	-3.00400	3.66800	-3.88900
H	-0.89800	-3.07100	-3.12200
H	2.70900	-0.79800	-3.66200
H	4.32400	-0.73200	-2.93300
H	3.71200	-2.97700	-3.22800
H	1.30600	-3.22000	-1.68500
H	4.94800	-3.15300	2.99700
H	3.23200	-1.37100	2.80600
H	2.30800	-2.40500	1.68600
H	2.56600	-2.91900	3.36100
H	3.94300	-4.44900	0.76500
H	5.45500	-1.46300	1.39400
H	4.08200	-1.12700	-0.37800
H	-3.99000	-2.91500	3.25800
H	-5.49600	-1.97100	3.08100
H	-2.53700	0.57700	-0.05100
H	-0.87200	1.38200	-1.63200
H	2.27400	0.21900	1.10200
H	0.58500	-0.63800	2.65400
H	-4.18100	-1.38200	4.14300
H	-5.59100	0.36900	-3.01700
H	-9.13200	0.16600	-0.30100
H	-4.31400	-5.03800	-1.63900
H	9.19300	1.53700	0.99600
H	-0.57700	8.84500	-1.78700
H	3.32600	6.03100	-0.79100
H	-2.73000	3.08300	3.84200
H	5.91400	-3.02700	0.71200
H	-0.16400	-4.70700	-3.24900
H	-0.58800	-3.79800	-4.70900
H	-0.99100	-0.81900	5.28600
H	-0.66200	-2.90800	3.16500
O	-0.02100	-3.53200	2.78600
O	-0.73100	-0.72300	6.21800
Cl	1.63200	2.67300	-0.59900
H	-0.55800	-4.14900	2.27300
H	-0.82800	-1.61700	6.56800

d C(4)-O (Asp145): 1.51Å
d C(4)-Cl: 2.0Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.17532435285

C	-1.90600	2.75400	3.73600
C	-1.09600	1.98800	4.58900
C	-1.32400	3.53400	2.72300
C	0.30000	1.98300	4.41900
C	0.07200	3.53700	2.55700
C	0.88300	2.75500	3.39900
C	-1.74000	7.97300	-2.45300
C	-2.27700	6.71800	-1.78900
C	-3.64700	6.61400	-1.48200
C	-1.41000	5.65600	-1.46600
C	-4.14800	5.45500	-0.85900
C	-1.91100	4.49800	-0.84300
C	-3.28000	4.39700	-0.54000
C	3.39000	6.20900	-1.61400
C	8.65200	3.08300	0.13800
C	7.15100	3.25600	0.27100
N	6.49100	4.21300	1.03000
C	6.20000	2.47200	-0.32300
C	5.16100	4.00500	0.89400
N	4.96600	2.95400	0.07500
C	-3.44000	-4.42200	-1.84000
C	-2.12100	-4.15600	-1.18600
C	-1.75200	-2.97100	-0.65600
C	-0.98500	-5.05300	-0.98600
N	-0.47400	-3.06500	-0.13900
C	0.05500	-4.32000	-0.33800
C	-0.70800	-6.39700	-1.31900
C	1.30000	-4.88500	-0.03500
C	0.54500	-6.97300	-1.02800
C	1.54700	-6.22100	-0.38800
C	-8.57700	-1.28000	0.58000
C	-7.61700	-0.58100	1.55700
C	-7.85200	-2.15900	-0.44700
C	-6.72100	0.47200	0.89200
C	-4.58000	0.23600	-2.87500
C	-5.83100	1.10600	-3.07600
C	-3.30800	0.84600	-3.47400
C	-5.77300	2.44700	-2.33500
C	0.19000	-3.70000	-3.72400
C	1.50900	-2.96100	-3.74200
O	1.97800	-2.59900	-4.81500
N	2.12000	-2.73700	-2.57500
C	3.46100	-2.14500	-2.48300
C	4.20700	-2.57100	-1.18900
O	4.53800	-3.74400	-1.04500
C	3.40700	-0.62600	-2.79600
C	2.86400	0.26900	-1.70700

O	1.54600	0.34000	-1.65300
O	3.63300	0.85900	-0.94500
N	4.48200	-1.68100	-0.22800
C	5.34000	-1.87100	0.94500
C	4.70200	-2.71700	2.06000
O	4.56800	-4.04800	1.63500
C	3.34500	-2.18800	2.50500
C	-4.22100	-2.30500	3.23400
S	-3.58500	-1.40300	1.78500
C	-1.86600	-1.04000	2.34500
O	-1.48900	-1.50300	3.43100
C	-1.02500	-0.29900	1.43400
C	-1.45400	0.30600	0.21900
C	-0.57700	0.84700	-0.68400
C	0.85200	0.89000	-0.43500
C	1.27300	0.27800	0.80900
C	0.37100	-0.25900	1.69200
H	-1.54900	1.39900	5.37400
H	-1.94700	4.12800	2.07100
H	0.91400	1.37700	5.07100
H	0.51500	4.12900	1.77000
H	1.95300	2.73800	3.25700
H	-0.83000	7.74400	-3.00700
H	-2.48200	8.37300	-3.14500
H	-4.31900	7.42500	-1.72200
H	-0.35500	5.72100	-1.69300
H	-5.20100	5.37900	-0.62600
H	-1.24300	3.68700	-0.59200
H	-3.66000	3.50600	-0.05900
H	4.42400	6.44900	-1.36900
H	3.31600	5.16400	-1.91700
H	3.05400	6.84500	-2.43300
H	8.88300	2.53800	-0.77800
H	9.13800	4.05800	0.09900
H	6.36000	1.61900	-0.97500
H	6.93400	4.92800	1.59500
H	4.06900	2.51600	-0.19900
H	4.36000	4.56700	1.36900
H	-3.42400	-5.39800	-2.32500
H	-3.64200	-3.65400	-2.58700
H	-2.38300	-2.09200	-0.62700
H	-0.03300	-2.32400	0.40400
H	-1.47000	-6.99100	-1.80300
H	0.74000	-8.00600	-1.28500
H	2.05700	-4.31300	0.48300
H	2.50400	-6.67100	-0.15300
H	-9.25300	-1.91200	1.15600
H	-8.58900	-2.68800	-1.05200
H	-7.22400	-2.88900	0.06600
H	-7.23500	-1.54600	-1.10400
H	-6.99000	-1.32900	2.04400
H	-8.21200	-0.08600	2.32500
H	-7.33600	1.21100	0.37800
H	-6.04600	-0.00100	0.18000
H	-6.12600	0.97300	1.65600
H	-4.42600	0.06500	-1.80900
H	-2.48100	0.14500	-3.35900
H	-3.05500	1.77500	-2.96200
H	-3.45700	1.04800	-4.53600
H	-6.69500	0.55100	-2.70800
H	-5.97700	1.29100	-4.14100
H	-4.99200	3.07800	-2.75900
H	-5.57200	2.28100	-1.27700
H	-6.72900	2.95900	-2.44000
H	-0.52900	-3.12700	-3.14800
H	2.82000	-0.52200	-3.71000
H	4.42800	-0.29100	-2.99900
H	4.04700	-2.58600	-3.29100
H	1.68800	-3.07200	-1.72800
H	5.37100	-2.70400	2.92100
H	3.43800	-1.15500	2.83600
H	2.62800	-2.25100	1.68900
H	2.98300	-2.79500	3.33600
H	4.52100	-4.04800	0.66200
H	5.58700	-0.89600	1.36300
H	4.16300	-0.73500	-0.38600
H	-3.38800	-2.41900	3.93100
H	-4.58300	-3.28400	2.91800
H	-2.51400	0.33200	-0.02300
H	-0.92900	1.27300	-1.61600
H	2.32900	0.28200	1.04600
H	0.73100	-0.71900	2.60600
H	-5.02700	-1.73900	3.70300
H	-4.75500	-0.73000	-3.35000
H	-9.17300	-0.53000	0.05700
H	-4.22800	-4.40800	-1.08600
H	9.03400	2.52200	0.99200
H	-1.52000	8.72000	-1.69000
H	2.75500	6.37800	-0.74400
H	-2.97600	2.74200	3.86500
H	6.26800	-2.35900	0.64100
H	0.34700	-4.68900	-3.30000
H	-0.17000	-3.80500	-4.74600
H	-0.77800	-0.96600	5.26500
H	-0.28700	-3.04500	3.13500
O	0.42500	-3.58500	2.75600
O	-0.51100	-0.83000	6.18900
Cl	1.46700	2.79100	-0.54200
H	-0.03000	-4.24000	2.21200
H	-0.51400	-1.72200	6.55600

d C(4)-O (Asp145): 1.49Å
d C(4)-Cl: 2.05Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.17754902454

C	-1.91700	2.75200	3.73400
C	-1.11300	1.96100	4.57000
C	-1.33000	3.54300	2.73200
C	0.28200	1.94300	4.39400
C	0.06500	3.53200	2.56100
C	0.87100	2.72600	3.38500
C	-1.72500	7.98900	-2.44100
C	-2.24500	6.72400	-1.78300
C	-3.61500	6.59700	-1.48300
C	-1.36300	5.67400	-1.45700
C	-4.10100	5.43000	-0.86600
C	-1.85000	4.50800	-0.84000
C	-3.21800	4.38400	-0.54500

C	3.39900	6.20900	-1.59500	H	-5.15400	5.33700	-0.63800
C	8.64900	3.06600	0.16100	H	-1.16900	3.70700	-0.58800
C	7.14700	3.24800	0.28500	H	-3.58700	3.48600	-0.06900
N	6.49000	4.21800	1.02900	H	4.44700	6.41600	-1.37900
C	6.19400	2.46400	-0.30400	H	3.28400	5.16600	-1.89100
C	5.15800	4.01700	0.89000	H	3.06200	6.85200	-2.40900
N	4.96000	2.95800	0.08200	H	8.88000	2.46500	-0.72000
C	-3.45900	-4.40300	-1.85200	H	9.13600	4.03700	0.06100
C	-2.14200	-4.13500	-1.19400	H	6.35000	1.60300	-0.94600
C	-1.76900	-2.94700	-0.67100	H	6.93400	4.93700	1.58800
C	-1.00800	-5.03300	-0.99000	H	4.05800	2.52800	-0.19100
N	-0.49200	-3.04300	-0.15200	H	4.35800	4.59000	1.35200
C	0.03500	-4.30000	-0.34600	H	-3.67300	-5.47100	-1.82400
C	-0.73300	-6.37900	-1.32100	H	-3.42400	-4.06700	-2.88800
C	1.27900	-4.86700	-0.04200	H	-2.39600	-2.06500	-0.64800
C	0.51800	-6.95600	-1.02800	H	-0.04700	-2.29900	0.38200
C	1.52200	-6.20500	-0.39100	H	-1.49700	-6.97100	-1.80400
C	-8.59200	-1.25000	0.56400	H	0.71100	-7.99000	-1.28200
C	-7.62900	-0.56400	1.54700	H	2.03900	-4.29500	0.47200
C	-7.87000	-2.12400	-0.47000	H	2.47800	-6.65700	-0.15600
C	-6.72900	0.49000	0.89200	H	-9.27100	-1.88500	1.13500
C	-4.58500	0.26000	-2.88100	H	-8.60900	-2.64500	-1.08000
C	-5.82900	1.13900	-3.08500	H	-7.24600	-2.86100	0.03700
C	-3.30200	0.86700	-3.46100	H	-7.25100	-1.50800	-1.12200
C	-5.76600	2.47500	-2.33500	H	-7.00600	-1.31900	2.02900
C	0.17600	-3.68800	-3.72800	H	-8.22300	-0.07300	2.31900
C	1.50300	-2.95900	-3.74300	H	-7.34100	1.23700	0.38400
O	1.97400	-2.60000	-4.81600	H	-6.05600	0.02200	0.17500
N	2.11700	-2.73900	-2.57600	H	-6.13200	0.98200	1.65900
C	3.46000	-2.15000	-2.48700	H	-4.44200	0.07800	-1.81500
C	4.21800	-2.57700	-1.19800	H	-2.48100	0.16000	-3.34500
O	4.59500	-3.73900	-1.08000	H	-3.04900	1.78900	-2.93700
C	3.41100	-0.63100	-2.80300	H	-3.44000	1.08200	-4.52200
C	2.87800	0.26300	-1.71000	H	-6.69900	0.58800	-2.72800
O	1.55800	0.34000	-1.65200	H	-5.96400	1.33300	-4.15000
O	3.65100	0.84200	-0.94500	H	-4.98000	3.10500	-2.75100
N	4.45300	-1.70100	-0.21300	H	-5.57300	2.30100	-1.27700
C	5.32300	-1.88100	0.95400	H	-6.72000	2.99400	-2.44200
C	4.71000	-2.75900	2.05700	H	-0.53900	-3.10900	-3.15300
O	4.57900	-4.08200	1.60300	H	2.81800	-0.52500	-3.71400
C	3.35400	-2.25300	2.53400	H	4.43200	-0.30100	-3.01100
C	-4.25200	-2.27800	3.23000	H	4.04200	-2.59200	-3.29800
S	-3.60300	-1.38900	1.77800	H	1.68300	-3.07000	-1.72800
C	-1.88400	-1.03500	2.34400	H	5.39100	-2.76100	2.90900
O	-1.51200	-1.50100	3.42900	H	3.44300	-1.22800	2.89100
C	-1.02900	-0.30000	1.43500	H	2.62800	-2.29900	1.72400
C	-1.44800	0.32200	0.22600	H	3.00600	-2.88500	3.35100
C	-0.55800	0.84200	-0.67900	H	4.55800	-4.06300	0.62900
C	0.86700	0.84800	-0.43300	H	5.54500	-0.90400	1.38300
C	1.28000	0.21400	0.79900	H	4.10100	-0.76400	-0.35000
C	0.36800	-0.30000	1.68700	H	-3.42200	-2.39900	3.92900
H	-1.57000	1.36500	5.34700	H	-4.62600	-3.25300	2.91600
H	-1.94800	4.15700	2.09300	H	-2.50700	0.37300	-0.01300
H	0.89200	1.32000	5.03400	H	-0.90100	1.27700	-1.61100
H	0.51300	4.13300	1.78300	H	2.33800	0.18200	1.02900
H	1.94000	2.69900	3.23700	H	0.72000	-0.78000	2.59300
H	-0.80600	7.77600	-2.98800	H	-5.05200	-1.70000	3.69500
H	-2.46800	8.37700	-3.13800	H	-4.76000	-0.70100	-3.36700
H	-4.29800	7.39900	-1.72500	H	-9.18500	-0.49400	0.04700
H	-0.30900	5.75700	-1.67800	H	-4.25000	-3.86800	-1.32400

H	9.03300	2.55900	1.04700
H	-1.52200	8.73800	-1.67500
H	2.79300	6.40200	-0.71000
H	-2.98600	2.75000	3.86600
H	6.26200	-2.33900	0.63900
H	0.32400	-4.67800	-3.30500
H	-0.18300	-3.78800	-4.75100
H	-0.79500	-0.98900	5.27400
H	-0.31900	-3.06700	3.13300
O	0.40200	-3.59900	2.76000
O	-0.53500	-0.85300	6.20000
Cl	1.52300	2.78900	-0.48800
H	-0.04100	-4.24200	2.19100
H	-0.53900	-1.74600	6.56500

d C(4)-O (Asp145): 1.48Å
d C(4)-Cl: 2.1Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.17977366553

C	-1.92800	2.74700	3.73400
C	-1.13400	1.93500	4.56000
C	-1.33100	3.54500	2.74400
C	0.26100	1.90300	4.38500
C	0.06300	3.51900	2.57300
C	0.85900	2.69100	3.38600
C	-1.71600	8.00300	-2.43100
C	-2.21900	6.72900	-1.77600
C	-3.58800	6.58100	-1.48200
C	-1.32200	5.69400	-1.44800
C	-4.05800	5.40500	-0.86800
C	-1.79200	4.51900	-0.83400
C	-3.16000	4.37200	-0.54500
C	3.40300	6.21100	-1.58100
C	8.64400	3.05400	0.17800
C	7.14100	3.24300	0.29700
N	6.48600	4.22100	1.03300
C	6.18400	2.45900	-0.28900
C	5.15400	4.02600	0.89100
N	4.95100	2.96300	0.09100
C	-3.47700	-4.38600	-1.86500
C	-2.15900	-4.11600	-1.20800
C	-1.78600	-2.92700	-0.68900
C	-1.02600	-5.01600	-0.99500
N	-0.50800	-3.02000	-0.17000
C	0.01700	-4.27900	-0.35500
C	-0.75400	-6.36500	-1.31200
C	1.26100	-4.84500	-0.04700
C	0.49600	-6.94200	-1.01400
C	1.50100	-6.18600	-0.38400
C	-8.60600	-1.22700	0.54800
C	-7.64700	-0.54100	1.53400
C	-7.88100	-2.10200	-0.48300
C	-6.74300	0.51200	0.88100
C	-4.59100	0.28100	-2.88800
C	-5.82800	1.17000	-3.09000
C	-3.30200	0.88100	-3.46200
C	-5.75600	2.50300	-2.33500
C	0.16300	-3.67600	-3.73500
C	1.49600	-2.95600	-3.74700
O	1.96800	-2.59800	-4.81900
N	2.11400	-2.74000	-2.58000
C	3.46000	-2.15100	-2.49500
C	4.23100	-2.57800	-1.21300
O	4.66200	-3.72300	-1.12200
C	3.41100	-0.63200	-2.81200
C	2.89000	0.25900	-1.71200
O	1.56700	0.34200	-1.65000
O	3.66700	0.82500	-0.94400
N	4.42300	-1.72000	-0.20200
C	5.30600	-1.88700	0.95700
C	4.72300	-2.79900	2.04900
O	4.59000	-4.11000	1.56300
C	3.37200	-2.31500	2.56200
C	-4.27900	-2.25900	3.22200
S	-3.61900	-1.37800	1.77000
C	-1.90100	-1.03200	2.34100
O	-1.53400	-1.50200	3.42400
C	-1.03400	-0.30100	1.43400
C	-1.44300	0.33800	0.23300
C	-0.54100	0.84200	-0.67300
C	0.88000	0.81000	-0.42900
C	1.28400	0.15800	0.79000
C	0.36300	-0.33800	1.68300
H	-1.59800	1.33400	5.32900
H	-1.94200	4.17400	2.11300
H	0.86400	1.26400	5.01600
H	0.51800	4.12400	1.80300
H	1.92700	2.65400	3.23600
H	-0.79100	7.80500	-2.97400
H	-2.46200	8.37900	-3.13200
H	-4.28200	7.37200	-1.72600
H	-0.26800	5.79300	-1.66300
H	-5.11000	5.29600	-0.64500
H	-1.09900	3.72900	-0.57900
H	-3.51700	3.46800	-0.07200
H	4.45700	6.40400	-1.38500
H	3.26700	5.16700	-1.86500
H	3.06200	6.85100	-2.39500
H	8.87200	2.41700	-0.67800
H	9.13100	4.02000	0.03600
H	6.33800	1.59300	-0.92400
H	6.93200	4.94200	1.58700
H	4.04500	2.54100	-0.18100
H	4.35400	4.60600	1.34600
H	-3.42400	-5.31600	-2.43200
H	-3.72600	-3.56800	-2.54100
H	-2.41300	-2.04400	-0.67100
H	-0.06100	-2.27100	0.35500
H	-1.51900	-6.96000	-1.79000
H	0.68700	-7.97900	-1.25800
H	2.02200	-4.27100	0.46200
H	2.45600	-6.63800	-0.14400
H	-9.28800	-1.86100	1.11700
H	-8.61900	-2.62300	-1.09400
H	-7.25900	-2.83900	0.02700
H	-7.26000	-1.48700	-1.13300
H	-7.02600	-1.29500	2.01900
H	-8.24200	-0.04800	2.30300

H	-7.35200	1.25900	0.37000
H	-6.06800	0.04200	0.16700
H	-6.14800	1.00400	1.65000
H	-4.45200	0.09100	-1.82300
H	-2.48600	0.16800	-3.34500
H	-3.04400	1.79900	-2.93300
H	-3.43500	1.10100	-4.52200
H	-6.70200	0.62400	-2.73500
H	-5.96100	1.36900	-4.15400
H	-4.96600	3.12900	-2.75000
H	-5.56100	2.32300	-1.27800
H	-6.70600	3.02800	-2.43700
H	-0.55100	-3.09000	-3.16500
H	2.81200	-0.52400	-3.71800
H	4.43100	-0.30500	-3.02700
H	4.03600	-2.59300	-3.31000
H	1.68000	-3.06800	-1.73100
H	5.42000	-2.81700	2.88800
H	3.46100	-1.30100	2.94900
H	2.63400	-2.34100	1.76300
H	3.03900	-2.97300	3.36500
H	4.60300	-4.07300	0.59000
H	5.50200	-0.91000	1.39900
H	4.03400	-0.79500	-0.31500
H	-3.45000	-2.39400	3.92000
H	-4.66800	-3.22800	2.90600
H	-2.50200	0.41300	-0.00300
H	-0.87700	1.28600	-1.60300
H	2.34200	0.09400	1.01400
H	0.70800	-0.83700	2.58100
H	-5.07000	-1.67000	3.68900
H	-4.77300	-0.67600	-3.38000
H	-9.19700	-0.47100	0.02900
H	-4.25000	-4.47300	-1.10200
H	9.02900	2.58400	1.08300
H	-1.53000	8.75500	-1.66500
H	2.81600	6.42200	-0.68700
H	-2.99700	2.75600	3.86600
H	6.25600	-2.31400	0.63100
H	0.30200	-4.66600	-3.30900
H	-0.19200	-3.77700	-4.75900
H	-0.82600	-1.00600	5.28400
H	-0.34500	-3.09300	3.13000
O	0.38600	-3.61600	2.76400
O	-0.55800	-0.87800	6.20800
Cl	1.57800	2.79000	-0.43100
H	-0.04000	-4.24400	2.16600
H	-0.51800	-1.77600	6.55600

d C(4)-O (Asp145): 1.46Å
d C(4)-Cl: 2.2Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.18439125996

C	-1.93500	2.74400	3.73900
C	-1.14800	1.91000	4.55000
C	-1.33200	3.54600	2.75700
C	0.24400	1.85800	4.36500
C	0.06000	3.50200	2.57800
C	0.84800	2.65100	3.37300
C	-1.68100	8.02700	-2.40100
C	-2.16100	6.74000	-1.75600
C	-3.52800	6.56400	-1.46400
C	-1.24600	5.71900	-1.43300
C	-3.97700	5.37600	-0.86000
C	-1.69600	4.53100	-0.82900
C	-3.06100	4.35700	-0.54300
C	3.42600	6.20300	-1.54900
C	8.64600	3.01000	0.20800
C	7.14300	3.21500	0.31900
N	6.49600	4.20500	1.04600
C	6.17800	2.44100	-0.26700
C	5.16200	4.02700	0.89900
N	4.94800	2.96200	0.10300
C	-3.51400	-4.35300	-1.87900
C	-2.19600	-4.08700	-1.21900
C	-1.81600	-2.89800	-0.70500
C	-1.07000	-4.99200	-1.00100
N	-0.54000	-2.99700	-0.18600
C	-0.02200	-4.25900	-0.36400
C	-0.80600	-6.34400	-1.31200
C	1.21800	-4.83100	-0.05300
C	0.44100	-6.92800	-1.01000
C	1.45100	-6.17600	-0.38300
C	-8.62900	-1.17300	0.53700
C	-7.71600	-0.39200	1.49700
C	-7.85600	-2.11900	-0.39000
C	-6.79400	0.60900	0.79100
C	-4.60000	0.32300	-2.88800
C	-5.81400	1.23800	-3.11500
C	-3.29200	0.88400	-3.45900
C	-5.71500	2.58100	-2.38200
C	0.13200	-3.65800	-3.74000
C	1.47500	-2.95400	-3.74900
O	1.94900	-2.59900	-4.82200
N	2.10000	-2.74700	-2.58300
C	3.45200	-2.16700	-2.50200
C	4.23300	-2.59600	-1.22500
O	4.70700	-3.72600	-1.15900
C	3.41500	-0.64700	-2.82200
C	2.91300	0.24500	-1.71400
O	1.58600	0.34300	-1.65300
O	3.69400	0.78900	-0.94000
N	4.38700	-1.75900	-0.19000
C	5.27800	-1.91500	0.96600
C	4.71600	-2.85700	2.04300
O	4.57800	-4.15600	1.52600
C	3.37000	-2.39200	2.58600
C	-4.22000	-2.31400	3.20600
S	-3.64500	-1.35700	1.76600
C	-1.93200	-1.01500	2.32300
O	-1.57900	-1.50000	3.40300
C	-1.04200	-0.28700	1.42400
C	-1.43400	0.37200	0.23000
C	-0.51400	0.84600	-0.67800
C	0.89600	0.75100	-0.43700
C	1.28600	0.08800	0.77200
C	0.35100	-0.37400	1.67200
H	-1.61700	1.30700	5.31400

H	-1.93600	4.19500	2.13800
H	0.84300	1.20300	4.98500
H	0.52100	4.11100	1.81300
H	1.91500	2.60000	3.21400
H	-0.75200	7.85000	-2.94400
H	-2.43200	8.39400	-3.10000
H	-4.23600	7.34500	-1.70300
H	-0.19300	5.83800	-1.64500
H	-5.02700	5.24700	-0.63700
H	-0.98700	3.75300	-0.57800
H	-3.40100	3.44300	-0.07700
H	4.47200	6.42300	-1.33900
H	3.32400	5.16100	-1.85500
H	3.07200	6.84900	-2.35200
H	8.86800	2.31000	-0.60000
H	9.13600	3.96000	-0.00600
H	6.32200	1.57000	-0.89800
H	6.94700	4.92500	1.59700
H	4.03100	2.56200	-0.16800
H	4.36500	4.61900	1.34300
H	-3.45600	-5.27100	-2.46500
H	-3.77300	-3.52300	-2.53600
H	-2.43700	-2.01000	-0.69200
H	-0.08500	-2.24600	0.33100
H	-1.57300	-6.93800	-1.78800
H	0.62500	-7.96700	-1.25000
H	1.98400	-4.26100	0.45400
H	2.40200	-6.63300	-0.14100
H	-9.32500	-1.76700	1.13200
H	-8.56400	-2.70100	-0.98100
H	-7.24300	-2.80000	0.20100
H	-7.22000	-1.55000	-1.06800
H	-7.11000	-1.09300	2.07200
H	-8.34700	0.16000	2.19500
H	-7.38600	1.30100	0.19100
H	-6.08400	0.08500	0.15100
H	-6.23600	1.17500	1.53800
H	-4.47500	0.14700	-1.81900
H	-2.49400	0.15400	-3.32500
H	-3.01700	1.80300	-2.94100
H	-3.41100	1.09100	-4.52300
H	-6.70400	0.71900	-2.75600
H	-5.93500	1.42200	-4.18300
H	-4.90700	3.18100	-2.80100
H	-5.53200	2.41600	-1.32000
H	-6.65100	3.12700	-2.50100
H	-0.57600	-3.06400	-3.17100
H	2.81000	-0.53400	-3.72300
H	4.43800	-0.33100	-3.04300
H	4.02000	-2.61400	-3.32000
H	1.66500	-3.07100	-1.73300
H	5.42500	-2.89200	2.87200
H	3.46000	-1.38900	3.00100
H	2.62300	-2.39600	1.79400
H	3.04600	-3.07500	3.37200
H	4.62600	-4.10100	0.55500
H	5.45000	-0.93900	1.41900
H	3.96800	-0.84500	-0.28400
H	-3.64500	-3.23600	3.30300
H	-5.26900	-2.54700	3.01900
H	-2.49100	0.48000	-0.00400
H	-0.83400	1.29800	-1.61000
H	2.34100	-0.02000	0.98900
H	0.68000	-0.89300	2.56500
H	-4.12100	-1.72400	4.11700
H	-4.80000	-0.63600	-3.36700
H	-9.20900	-0.47100	-0.06500
H	-4.28500	-4.46300	-1.11500
H	9.03300	2.60500	1.14400
H	-1.51000	8.77700	-1.62900
H	2.82500	6.37500	-0.65600
H	-3.00300	2.76700	3.87600
H	6.23800	-2.31400	0.63300
H	0.25900	-4.65000	-3.31500
H	-0.22200	-3.75400	-4.76500
H	-0.87900	-1.03800	5.29000
H	-0.39800	-3.11700	3.12300
O	0.33600	-3.64200	2.77000
O	-0.62000	-0.91200	6.21700
Cl	1.67900	2.80600	-0.36500
H	-0.07500	-4.24800	2.14000
H	-0.58300	-1.81100	6.56500

d C(4)-O (Asp145): 1.43Å
d C(4)-Cl: 2.4Å
reaction coordinate: 0.44Å
Extrapolated ONIOM energy:
-1624.19342627587

C	-1.92400	2.74700	3.73900
C	-1.17600	1.88100	4.55300
C	-1.28200	3.53700	2.77100
C	0.21700	1.78500	4.38500
C	0.11000	3.44700	2.60900
C	0.85900	2.56400	3.40700
C	-1.57100	8.05500	-2.40400
C	-2.03600	6.76300	-1.75800
C	-3.40000	6.57100	-1.46500
C	-1.10800	5.75300	-1.43400
C	-3.83400	5.37800	-0.85900
C	-1.54300	4.56000	-0.82800
C	-2.90600	4.37000	-0.54300
C	3.50600	6.15800	-1.53500
C	8.67400	2.88900	0.23800
C	7.17300	3.13100	0.33500
N	6.54600	4.15600	1.02900
C	6.19100	2.36600	-0.24000
C	5.20900	4.00900	0.87500
N	4.97300	2.93000	0.10700
C	-3.58200	-4.29900	-1.90300
C	-2.26300	-4.04800	-1.23700
C	-1.86900	-2.86100	-0.72400
C	-1.15000	-4.96800	-1.00800
N	-0.59700	-2.97800	-0.19700
C	-0.09600	-4.24800	-0.36800
C	-0.90300	-6.32500	-1.31200
C	1.13400	-4.83600	-0.04700
C	0.33300	-6.92400	-1.00000
C	1.35000	-6.18400	-0.37000
C	-8.66000	-1.04900	0.49700

C	-7.74700	-0.26900	1.45800
C	-7.88900	-2.01500	-0.41100
C	-6.80500	0.71200	0.75100
C	-4.59700	0.39300	-2.91100
C	-5.78700	1.34200	-3.12500
C	-3.27400	0.92800	-3.47200
C	-5.64900	2.67600	-2.38100
C	0.08200	-3.65300	-3.75000
C	1.43700	-2.96900	-3.75100
O	1.91700	-2.61900	-4.82200
N	2.06700	-2.77500	-2.58500
C	3.42900	-2.21300	-2.50500
C	4.21500	-2.65200	-1.23200
O	4.72900	-3.76600	-1.19300
C	3.41400	-0.69100	-2.82400
C	2.93000	0.19900	-1.70800
O	1.59700	0.32300	-1.65900
O	3.71000	0.71200	-0.91800
N	4.33600	-1.83900	-0.17400
C	5.23400	-1.98800	0.97800
C	4.68800	-2.95200	2.04400
O	4.51400	-4.23500	1.49600
C	3.36100	-2.48200	2.62900
C	-4.29400	-2.22000	3.19700
S	-3.68400	-1.30500	1.74500
C	-1.98100	-0.96700	2.32200
O	-1.64500	-1.43300	3.41200
C	-1.06200	-0.26200	1.41700
C	-1.43600	0.41200	0.23000
C	-0.49500	0.83500	-0.69100
C	0.89300	0.64500	-0.45900
C	1.27300	0.00600	0.75100
C	0.32300	-0.40400	1.66600
H	-1.67300	1.28800	5.30700
H	-1.85500	4.21200	2.15100
H	0.78700	1.10800	5.00700
H	0.60100	4.04600	1.85500
H	1.92600	2.48200	3.25800
H	-0.63800	7.88900	-2.94300
H	-2.32500	8.41000	-3.10700
H	-4.11700	7.34300	-1.70500
H	-0.05600	5.88400	-1.64500
H	-4.88300	5.23700	-0.63600
H	-0.82300	3.79300	-0.57700
H	-3.23500	3.45300	-0.07500
H	4.45900	6.55600	-1.18800
H	3.64800	5.15000	-1.92800
H	3.10800	6.79800	-2.32200
H	8.87800	2.09200	-0.47700
H	9.17400	3.79900	-0.09600
H	6.31600	1.47700	-0.84900
H	7.00900	4.88100	1.56300
H	4.03700	2.56700	-0.15800
H	4.41900	4.63100	1.29000
H	-3.53100	-5.21800	-2.48800
H	-3.82600	-3.46600	-2.56300
H	-2.47700	-1.96500	-0.71900
H	-0.13200	-2.23400	0.32200
H	-1.67600	-6.90900	-1.79100
H	0.50400	-7.96700	-1.23500
H	1.90600	-4.27400	0.46100
H	2.29300	-6.65400	-0.12100
H	-9.37000	-1.62700	1.09000
H	-8.59800	-2.59400	-1.00400
H	-7.29100	-2.69800	0.19300
H	-7.23900	-1.46200	-1.08800
H	-7.15700	-0.97200	2.04700
H	-8.37900	0.29800	2.14300
H	-7.38200	1.40400	0.13700
H	-6.09600	0.17300	0.12500
H	-6.24800	1.27900	1.49800
H	-4.47800	0.19900	-1.84400
H	-2.49600	0.17500	-3.34900
H	-2.97500	1.83200	-2.94100
H	-3.38600	1.15400	-4.53300
H	-6.68900	0.84400	-2.76900
H	-5.90600	1.53900	-4.19200
H	-4.83100	3.25900	-2.80200
H	-5.46200	2.49600	-1.32300
H	-6.57300	3.24500	-2.48700
H	-0.62000	-3.04700	-3.18600
H	2.80800	-0.56600	-3.72300
H	4.44100	-0.39100	-3.04600
H	3.98800	-2.66600	-3.32700
H	1.62700	-3.09100	-1.73400
H	5.41500	-3.01900	2.85300
H	3.47500	-1.49200	3.06800
H	2.59700	-2.45400	1.85400
H	3.04300	-3.18100	3.40400
H	4.61500	-4.16600	0.53000
H	5.39100	-1.01400	1.44100
H	3.89400	-0.93500	-0.25000
H	-3.73400	-3.14700	3.32400
H	-5.34400	-2.44300	2.99900
H	-2.48800	0.57100	0.00600
H	-0.79600	1.29200	-1.62600
H	2.32300	-0.14600	0.96200
H	0.63400	-0.92700	2.56300
H	-4.20100	-1.61100	4.09600
H	-4.82200	-0.55400	-3.40300
H	-9.22400	-0.34700	-0.11900
H	-4.35800	-4.39800	-1.14300
H	9.06300	2.59800	1.21400
H	-1.41300	8.80900	-1.63300
H	2.79700	6.12000	-0.70800
H	-2.99100	2.80800	3.86200
H	6.19800	-2.36800	0.63800
H	0.19000	-4.64700	-3.32100
H	-0.26800	-3.74600	-4.77600
H	-0.93600	-1.05100	5.32900
H	-0.48100	-3.10300	3.13400
O	0.27000	-3.59400	2.76800
O	-0.70900	-0.93600	6.26500
Cl	1.82700	2.85000	-0.29900
H	-0.12300	-4.23300	2.16100
H	-0.69800	-1.83700	6.60900