

**Supplementary Material**

*for*

**A theoretical study on the environmental oxidation  
of fenpyrazamine fungicide initiated by hydroxyl  
radical in the aqueous phase**

## Table of Content

**Figure S1.** Structure of fenpyrazamine (FPA).

**Figure S2.** Plot of Fukui function for radical attack ( $f^0$ ) describing the possible main reactive sites of FPA.

**Figure S3.** Representation of the HOMO, LUMO, and ESP maps of FPA molecule

**Figure S4.** Plot of the molar fraction (%) of the neutral or protonated forms of FPA as a function of the pH in the aqueous phase.

**Figure S5.** Standard Gibbs free reaction energy ( $\Delta_r G^\circ$ ) and standard reaction enthalpy ( $\Delta_r H^\circ$ ) calculated for the further reactions of C39-Add with  $^3\text{O}_2$ ,  $\text{HO}^\bullet$ ,  $^\bullet\text{NO}$ , and  $^\bullet\text{NO}_2$  at 298 K. Units are in  $\text{kJ mol}^{-1}$ . All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

**Table S1.** Acute and chronic toxicity classification based on European Union and Chinese criteria ( $\text{mg L}^{-1}$ ).

**Table S2.** Cartesian coordinates of the structures involved in the abstraction and the addition reactions

**Table S3.** Standard enthalpy ( $\Delta H^\circ_{0\text{K}}$ ) for MCR and MCP, adiabatic energy barrier ( $E_0$ ) for TS, and standard reaction enthalpy ( $\Delta_r H^\circ_{0\text{K}}$ ) for products (P) at 0 K of the FHT reactions, in addition to their standard activation enthalpy ( $\Delta H^{\circ\ddagger}_{298\text{K}}$ ) and standard reaction enthalpy ( $\Delta_r H^\circ_{298\text{K}}$ ) at 298 K. Units are in  $\text{kJ mol}^{-1}$ . All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

**Table S4.** Standard enthalpy, entropy, and Gibbs free energy of activation, and the ones of reaction for all the FHT reactions at 298 K temperature calculated at the M06-2X/6-31+G(d,p) level of theory (level 1, L1), and at the M06-2X/6-311++G(3df,3pd) level of theory (level 2, L2) in the aqueous phase. Differences of standard Gibbs free energy of activation ( $\Delta\Delta G^{\circ\ddagger}$ ) and reaction ( $\Delta\Delta_r G^\circ$ ) between the level 1 and level 2 are also shown.

**Table S5.** Standard enthalpy ( $\Delta H^\circ_{0K}$ ) for MCR and MCP, adiabatic energy barrier ( $E_0$ ) for TS, and standard reaction enthalpy ( $\Delta_r H^\circ_{0K}$ ) for products (P) at 0 K of the RAF reactions, in addition to their standard activation enthalpy ( $\Delta H^{\ddagger}_{298K}$ ) and standard reaction enthalpy ( $\Delta_r H^\circ_{298K}$ ) at 298 K. Units are in kJ mol<sup>-1</sup>. All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

**Table S6.** Standard enthalpy, entropy, and Gibbs free energy of activation, and the ones of reaction for all the RAF reactions at 298 K temperature calculated at the M06-2X/6-31+G(d,p) level of theory (level 1, L1), and at the M06-2X/6-311++G(3df,3pd) level of theory (level 2, L2) in the aqueous phase. Differences of standard Gibbs free energy of activation ( $\Delta\Delta G^{\ddagger}$ ) and reaction ( $\Delta\Delta_r G^\circ$ ) between the level 1 and level 2 are also shown.

**Table S7.** Apparent rate constants ( $k$ , in M<sup>-1</sup> s<sup>-1</sup>) of all oxidation reactions, with the total FHT, RAF, SET, and the overall rate constants in the temperature range of 283-323 K. (The most favourable pathways are in bold).

**Table S8.** Branching ratio ( $\Gamma$ , %) of all oxidation reactions, with the total FHT, RAF, SET, and the overall branching ratio at the temperature range of 283-323 K. (The most favourable pathways are in bold).

**Table S9.** Tunnelling correction estimated by the Eckart method for formal hydrogen transfer (FHT) at the temperature T from 283 to 333 K.

**Table S10.** Tunnelling correction estimated by the Eckart method for Radical adduct formation (RAF) at the temperature T from 283 to 333 K.

**Table S11.** Cartesian coordinates of all intermediate species involved in the further reactions of H15-Abs product at 298 K.

**Table S12.** Standard enthalpy ( $\Delta_r H^\circ_{298K}$ ), and Gibbs free energy of reaction ( $\Delta_r G^\circ_{298K}$ ) for the O<sub>2</sub>-addition to various carbon atom on the H15-Abs intermediate resulted from the most dominant FHT reaction at H15 hydrogen atom. Calculations were performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory in water.

**Table S13.** Cartesian coordinates of all intermediate species involved in the further reactions of C39-Add product.

## Methodology

The determination of the rate constant follows the formulation introduced by Eyring (Eyring, 1935).

$$k_{TST} = \left( \frac{k_B T}{h} \right) \times \frac{q_{TS}}{\prod q_{R(s)}} \times e^{-E_0/RT} \quad \text{Eq. 1}$$

where  $q_{R(s)}$  and  $q_{TS}$  refer to the functions of total reagent partition and transition state, and  $E_0$  corresponds to the adiabatic vibration barrier, including all energy corrections (ZPE and SOC corrections). Its formula is given below:

$$E_0 = \Delta E^\ddagger + \Delta E_{ZPE} + \Delta E_{SOC} \quad \text{Eq. 2}$$

For a bimolecular reaction:

$$\Delta E_{ZPE} = ZPE_{TS} - ZPE_{Reactant1} - ZPE_{Reactant2} \quad \text{Eq. 3}$$

$$\Delta E_{SOC} = SOC_{TS} - SOC_{Reactant1} - SOC_{Reactant2} \quad \text{Eq. 4}$$

$$\Delta E^\ddagger = E_{TS}^\ddagger - E_{Reactant1}^\ddagger - E_{Reactant2}^\ddagger \quad \text{Eq. 5}$$

where  $E^\ddagger$  is the electronic energy obtained from the frequency calculations without correction. Its unit is Hartree (a Hartree equals 2625.5 kJ mol<sup>-1</sup>).

The kinetics for the abstraction and the addition reactions between FPA and HO• radical was studied using the pre-reactive complexes scheme proposed by Singleton and Cvetanovic (Singleton and Cvetanovic, 1976).

Briefly, a two-step mechanism is considered:



This scheme involved a fast pre-equilibrium between the reactants and the pre-reactive complex (MCR), leading to the hydrogen abstraction/radical addition followed by post-reactive complexes and products. The effective rate  $r$  applied to reactions (R1-R2) for steady-state conditions (the concentration of the intermediates is constant, *i.e.*, the effective rate of product formation is constant and does not depend on time) is defined as follows (Eq. 6):

$$r = r_c = k [\text{HO}^\bullet] [\text{FPA}] \quad \text{Eq. 6}$$

6

where  $k$  is the rate constant for each pathway, and it is calculated by the following equation (Eq. 7):

$$k = \frac{k_c k_a}{k_b + k_c} \quad \text{Eq. 7}$$

The changes in entropy in the reverse reaction (R2) are much more significant than in the reaction (R3). Thus,  $k_b$  is expected to be larger than  $k_c$ , and  $k$  can be written as (Eq. 8):

$$k = \frac{k_c k_a}{k_b} = k_c K_{a,b} \quad \text{Eq. 8}$$

8

where  $K_{a,b}$  is the equilibrium constant for the separated reactants versus the pre-reactive complex (MCR). The equilibrium constant ( $K_{a,b}$ ) of the first step is computed based on basic statistical thermodynamics principles, while  $k_c$  is calculated by the classical TST formula (Evans and Polanyi, 1935) (Eq. 9) (Eq. 10).

$$K_{a,b}(T) = \frac{q_{MCR}(T)}{q_{HO\cdot}(T)q_{FPA}(T)} \exp\left(\frac{E_{FPA} + E_{HO\cdot} - E_{MCR}}{k_B T}\right) \quad \text{Eq. 9}$$

$$k_c(T) = \kappa(T) \times \frac{k_B T}{h} \times \frac{q_{TS}(T)}{q_{MCR}(T)} \times \exp\left(-\frac{E_{TS} - E_{MCR}}{k_B T}\right) \quad \text{Eq. 10}$$

The terms  $q_{HO\cdot}(T)$ ,  $q_{Pesticide}(T)$ ,  $q_{MCR}(T)$ , and  $q_{TS}(T)$  are the total partition functions of the reactants ( $HO\cdot$  and FPA), MCR, and TS at the temperature T (K), respectively.  $E_{HO\cdot}$ ,  $E_{FPA}$ ,  $E_{MCR}$ , and  $E_{TS}$  are the total potential energies at 0 K (including the zero-point energy and SOC corrections) of the  $HO\cdot$  radical, pesticide, MCR, and TS, respectively. The  $\kappa(T)$  is the transmission coefficient used for the tunnelling correction estimated by the Eckart method (Eckart, 1930) at the temperature T.

For the SET (single electron transfer) reaction, the reaction barrier was calculated by Marcus' theory (Marcus, 1956, 1957a, 1957b) as follows (Eq. 11):

$$\Delta G_{SET}^{\ddagger} = \frac{\lambda}{4} \left(1 + \frac{\Delta_r G_{SET}^{\circ}}{\lambda}\right)^2 \quad \text{Eq. 11}$$

$\Delta_r G_{SET}^{\circ}$  is the standard Gibbs free reaction energy calculated from the energy difference between reactants and products. The  $\lambda$  is the nuclear reorganization energy, which is calculated by the below equation (Eq. 12):

$$\lambda = \Delta H_{SET}^{\circ} - \Delta_r G_{SET}^{\circ} \quad \text{Eq. 12}$$

where the  $\Delta H_{SET}^{\circ}$  is the non-adiabatic energy between the reactants and products.

In the aqueous phase, the apparent rate constant ( $k_{app}$ ) is typically including a diffusion limit, especially for the reaction with  $HO\cdot$  radical that has the rate constant close to the diffusion limit of the solution. The  $k_{app}$  was calculated based on the Collins-Kimball (Collins and Kimball, 1949) as follows (Eq. 13):

$$k_{app} = \frac{k_D k}{k_D + k} \quad \text{Eq. 13}$$

where  $k$  is the thermal rate constant, and  $k_D$  is the steady-state Smoluchowski (Smoluchowski, 1918) rate constant for an irreversible bimolecular diffusion-controlled reaction (**Eq. 14**):

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad \text{Eq. 14}$$

where  $R_{AB}$  is the reaction distance,  $N_A$  is the Avogadro number, and  $D_{AB}$  is the mutual diffusion coefficient of reactants. It can be estimated from  $D_A$  and  $D_B$ , according to Truhlar (Truhlar, 1985). The  $D_A$  and  $D_B$  values were calculated from the Stokes-Einstein approach (Einstein, 1905; Stokes, 2009) (**Eq. 15**):

$$D_{A \text{ or } B} = \frac{k_B T}{6\pi\eta a_{A \text{ or } B}} \quad \text{Eq. 15}$$

where  $\eta$  denotes the solvent's viscosity (*i.e.*, the viscosity of water is  $8.91 \times 10^{-4}$  Pa s (Medina *et al.*, 2013)) varied as a function of temperature, and  $a$  is the radius of solute.

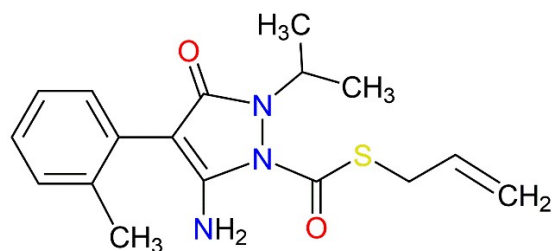
The rate constants were calculated with the GPOP software (Miyoshi, 2022). The total rate constant ( $k_{\text{total}}$ ) of each reaction mechanism was derived by adding up the rate constant ( $k_i$ ) of all individual reactions. The overall rate constant ( $k_{\text{overall}}$ ) (Bentz *et al.*, 2018; Galano and Alvarez-Idaboy, 2013) was obtained by summing up the total rate constant of the three mechanisms (*i.e.*,  $k_{\text{overall}} = k_{\text{total}}(\text{FHT}) + k_{\text{total}}(\text{RAF}) + k_{\text{total}}(\text{SET})$ ).  $k_{\text{total}}(\text{FHT})$  is the total rate constant of the H-abstraction reactions (formal hydrogen transfer),  $k_{\text{total}}(\text{RAF})$  is the total rate constant of the HO $\cdot$ -addition reactions (radical adduct formation), and  $k_{\text{total}}(\text{SET})$  is the total rate constant of the charge transfer reactions (single electron transfer).

The branching ratios for each reaction are determined by dividing their respective apparent rate constants ( $k_i$ ) by the overall rate constant ( $k_{\text{overall}}$ ).

## References

- Bentz, E.N., Lobayan, R.M., Martínez, H., Redondo, P., Largo, A., 2018. Intrinsic Antioxidant Potential of the Aminoindole Structure: A Computational Kinetics Study of Tryptamine. *J. Phys. Chem. B* 122, 6386–6395. <https://doi.org/10.1021/acs.jpcc.8b03807>
- Collins, F.C., Kimball, G.E., 1949. Diffusion-controlled reaction rates. *Journal of Colloid Science* 4, 425–437. [https://doi.org/10.1016/0095-8522\(49\)90023-9](https://doi.org/10.1016/0095-8522(49)90023-9)
- Eckart, C., 1930. The Penetration of a Potential Barrier by Electrons. *Phys. Rev.* 35, 1303–1309. <https://doi.org/10.1103/PhysRev.35.1303>
- Einstein, A., 1905. Zur Elektrodynamik bewegter Körper. *Annalen der Physik* 322, 891–921. <https://doi.org/10.1002/andp.19053221004>
- EU, 1967. General classification and labeling requirements for dangerous substances and preparations. Annex VI of Directive 67/548/EEC. [https://ec.europa.eu/environment/archives/dansub/pdfs/annex6\\_en.pdf](https://ec.europa.eu/environment/archives/dansub/pdfs/annex6_en.pdf) (accessed 6.26.24).
- Evans, M.G., Polanyi, M., 1935. Some applications of the transition state method to the calculation of reaction velocities, especially in solution. *Trans. Faraday Soc.* 31, 875–894. <https://doi.org/10.1039/TF9353100875>
- Eyring, H., 1935. The Activated Complex in Chemical Reactions. *The Journal of Chemical Physics* 3, 107–115. <https://doi.org/10.1063/1.1749604>

- Galano, A., Alvarez-Idaboy, J.R., 2013. A computational methodology for accurate predictions of rate constants in solution: Application to the assessment of primary antioxidant activity. *Journal of Computational Chemistry* 34, 2430–2445. <https://doi.org/10.1002/jcc.23409>
- Marcus, R.A., 1957a. On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. II. Applications to Data on the Rates of Isotopic Exchange Reactions. *The Journal of Chemical Physics* 26, 867–871. <https://doi.org/10.1063/1.1743423>
- Marcus, R.A., 1957b. On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. III. Applications to Data on the Rates of Organic Redox Reactions. *The Journal of Chemical Physics* 26, 872–877. <https://doi.org/10.1063/1.1743424>
- Marcus, R.A., 1956. On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. I. *The Journal of Chemical Physics* 24, 966–978. <https://doi.org/10.1063/1.1742723>
- Medina, M.E., Iuga, C., Alvarez-Idaboy, J.R., 2013. Antioxidant activity of propyl gallate in aqueous and lipid media: a theoretical study. *Phys. Chem. Chem. Phys.* 15, 13137–13146. <https://doi.org/10.1039/C3CP51644J>
- MEE, 2004. Chinese hazard evaluation guideline for the hazard evaluation of new chemical substances (HJ/T 154–2004). Ministry of Ecology and Environment. [https://english.mee.gov.cn/special\\_reports/chemical\\_regulation/newchemicals/200712/t20071217\\_115157.shtml](https://english.mee.gov.cn/special_reports/chemical_regulation/newchemicals/200712/t20071217_115157.shtml) (accessed 6.26.24).
- Miyoshi, A, n.d. GPOP software. Revision 2022.01.20m1. <http://akrmys.com/gpop/>
- Singleton, D.L., Cvetanovic, R.J., 1976. Temperature dependence of the reaction of oxygen atoms with olefins. *J. Am. Chem. Soc.* 98, 6812–6819. <https://doi.org/10.1021/ja00438a006>
- Smoluchowski, M. v, 1918. Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen. *Zeitschrift für Physikalische Chemie* 92U, 129–168. <https://doi.org/10.1515/zpch-1918-9209>
- Stokes, G.G., 2009. *Mathematical and Physical Papers*. Cambridge Core. <https://doi.org/10.1017/CBO9780511702297>
- Truhlar, D.G., 1985. Nearly encounter-controlled reactions: The equivalence of the steady-state and diffusional viewpoints. *Journal of Chemical Education* 62, 104–106. <https://doi.org/10.1021/ed062p104>



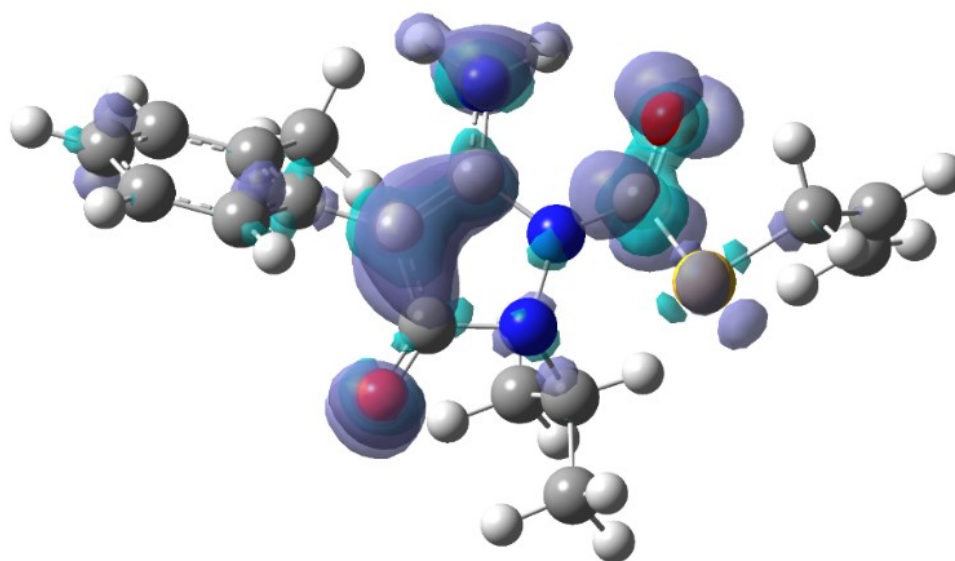
**Figure S1.** Structure of fenpyrazamine (FPA).

**Table S1.** Acute and chronic toxicity classification based on European Union and Chinese criteria ( $\text{mg L}^{-1}$ ).

Classification	Acute toxicity <sup>1</sup>	Chronic toxicity <sup>2</sup>
<b>Not harmful</b>	$\text{LC}_{50} > 100$ or $\text{EC}_{50} > 100$	$\text{ChV} > 10$
<b>Harmful</b>	$10 < \text{LC}_{50} < 100$ or $10 < \text{EC}_{50} < 100$	$1 < \text{ChV} < 10$
<b>Toxic</b>	$1 < \text{LC}_{50} < 10$ or $1 < \text{EC}_{50} < 10$	$0.1 < \text{ChV} < 1$
<b>Very toxic</b>	$\text{LC}_{50} < 1$ or $\text{EC}_{50} < 1$	$\text{ChV} < 0.1$

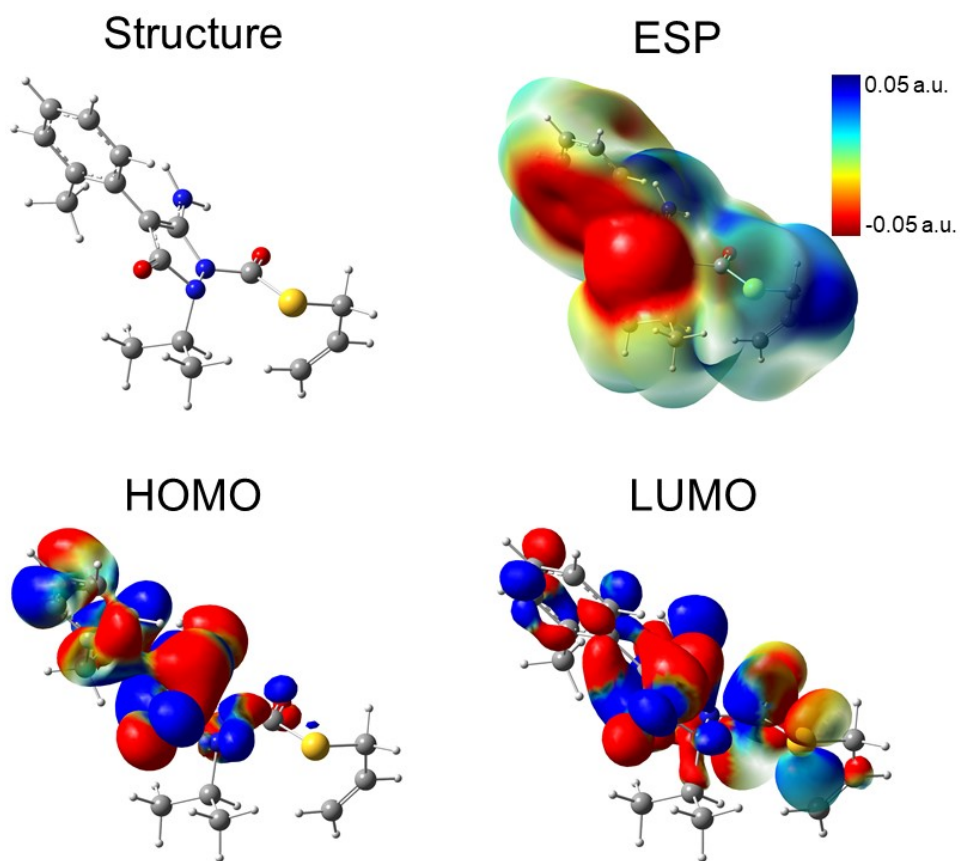
<sup>1</sup>Criteria set by the European Union (described in Annex VI of Directive 67/548/EEC) (EU, 1967).

<sup>2</sup>Criteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154–2004) (MEE, 2004).

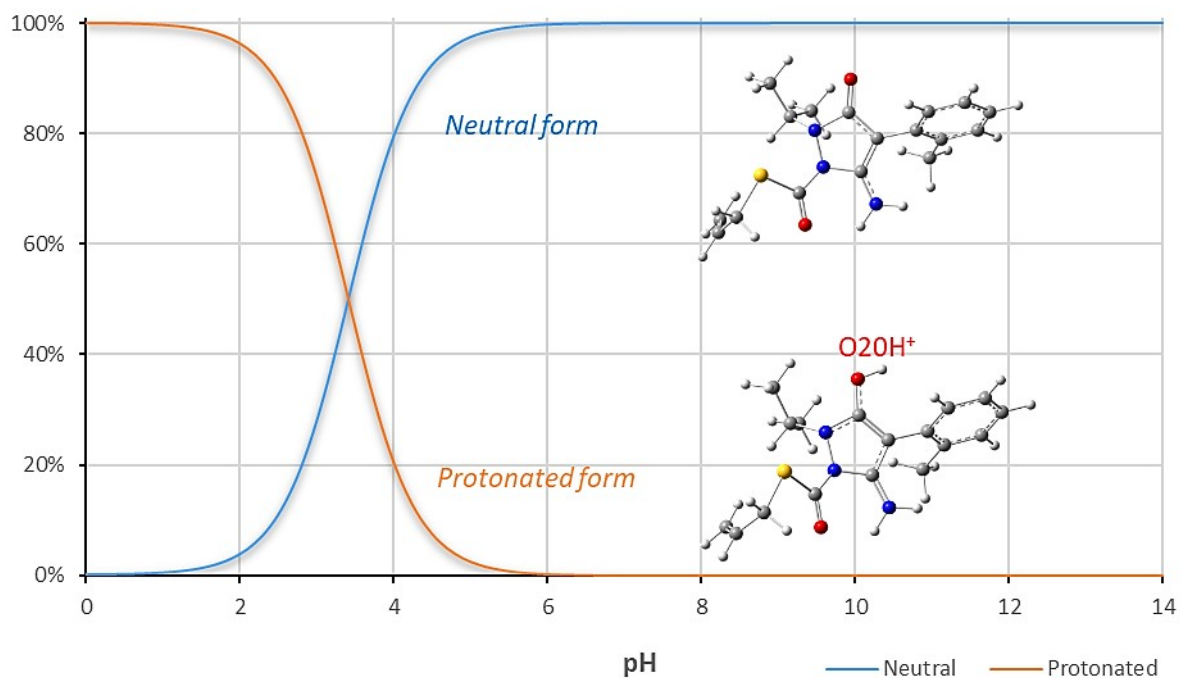


**Figure S2.** Plot of Fukui function for radical attack ( $f^0$ ) describing the possible main reactive sites of FPA.



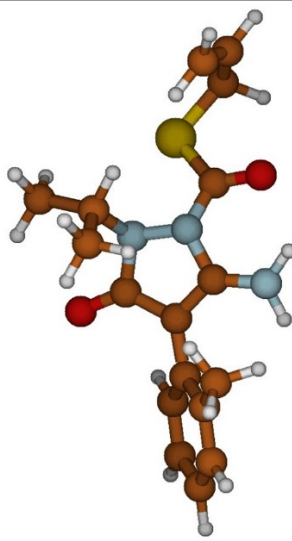


**Figure S3.** Representation of the HOMO, LUMO, and ESP maps of FPA molecule.

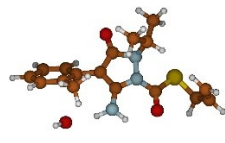
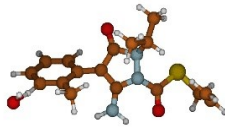
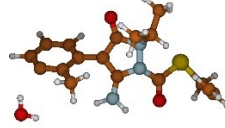
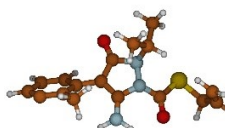


**Figure S4.** Plot of the molar fraction (%) of the neutral or protonated forms of FPA as a function of the pH in the aqueous phase.

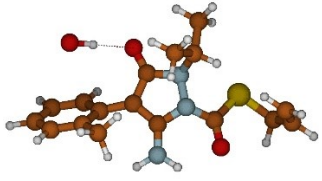
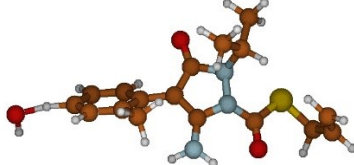
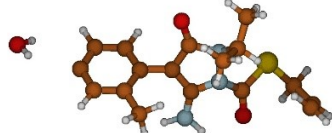
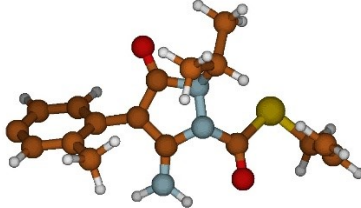
**Table S2.** Cartesian coordinates of the structures involved in the abstraction and the addition reactions.

MAIN MOLECULE								
Fenpyrazamine								
	Coordinates			Unscaled vibrational frequencies (cm <sup>-1</sup> )			Rotational constants (GHz)	Structure
C	-2.870015	-0.217919	-0.292138	26.7156	35.3687	44.9470	0.48750	
C	-3.639880	-0.683934	0.793455	54.4311	66.6066	73.2203	0.14167	
C	-5.017303	-0.860191	0.606583	87.8598	97.1976	114.4062	0.12953	
C	-5.632753	-0.570426	-0.608178	133.9135	144.1414	154.2928		
C	-4.870437	-0.087209	-1.672960	161.8094	186.7865	215.2015		
C	-3.499636	0.083567	-1.510485	222.9496	227.7855	253.4631		
C	-1.417793	0.006625	-0.178666	261.7054	266.0225	279.3888		
C	-3.032678	-0.976238	2.141552	294.4980	303.9958	334.6480		
H	-5.615121	-1.217506	1.441445	360.6353	364.2977	421.7859		
H	-6.703380	-0.712186	-0.720653	442.8102	458.8974	464.2604		
H	-5.339250	0.149829	-2.622920	477.7973	506.4569	533.8859		
H	-2.894943	0.449661	-2.336081	535.4112	543.0103	557.9964		
H	-2.168101	-0.335954	2.340405	573.7922	599.9853	630.6603		
H	-2.697008	-2.016973	2.212352	645.4350	659.4660	692.0356		
H	-3.771872	-0.818509	2.930653	710.7243	728.9700	743.5533		
C	-0.438947	-0.904144	0.169538	773.4618	793.5494	796.9607		
N	0.809533	-0.264620	0.156832	832.8079	875.2893	901.6540		
N	0.639453	1.076878	-0.248184	908.0342	931.1367	941.8259		
C	-0.760814	1.245283	-0.446181	944.7903	961.7032	964.4609		
O	-1.243105	2.344001	-0.751867	981.7514	988.1375	1006.0898		
N	-0.549483	-2.204832	0.430739	1023.1152	1026.4822	1033.6979		
H	0.268872	-2.768672	0.617206	1061.2465	1062.1689	1078.7151		
H	-1.446632	-2.651596	0.291770	1119.7839	1138.4895	1165.8341		
C	1.282759	2.031390	0.721045	1167.4014	1179.8736	1201.0677		
C	0.460634	2.173490	1.996415	1216.7317	1224.8261	1237.1942		
C	1.579047	3.359031	0.042193	1262.4925	1296.6967	1304.5015		
H	2.236272	1.558746	0.970257	1311.5482	1324.4830	1328.8677		
H	1.028572	2.752541	2.729611	1354.2982	1364.1989	1401.3312		
H	0.241530	1.193123	2.433022	1405.6783	1410.0147	1423.3294		
H	-0.482320	2.695021	1.804405	1425.1521	1441.4714	1464.3208		
H	0.664072	3.910506	-0.182180	1469.6009	1476.4691	1477.3631		
H	2.190601	3.965795	0.715993	1483.3390	1491.4150	1493.0242		
H	2.137041	3.205038	-0.885897	1501.1199	1541.8962	1601.8950		
C	1.980032	-0.931953	-0.206183	1624.0701	1648.0052	1681.7404		

O	2.182143	-2.081074	0.142193	1711.9317	1737.7610	1746.0987		
S	3.104000	0.018451	-1.192667	3067.6576	3067.8043	3081.7549		
C	4.491602	-1.151687	-1.203313	3098.4280	3124.0777	3134.6905		
C	5.282238	-1.258157	0.070703	3146.8993	3148.1385	3157.1663		
C	5.038155	-0.651428	1.230424	3158.7986	3159.2385	3173.8264		
H	4.115439	-2.133335	-1.504968	3178.7406	3186.7289	3206.1106		
H	5.135117	-0.795048	-2.014476	3212.4616	3224.6160	3237.9011		
H	6.139694	-1.925118	-0.014946	3266.1728	3585.8116	3717.9866		
H	5.688692	-0.813641	2.084081					
H	4.194649	0.021087	1.372460					

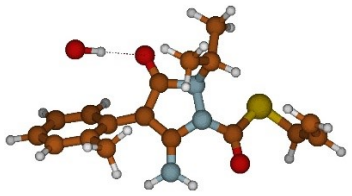
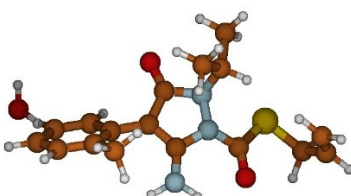
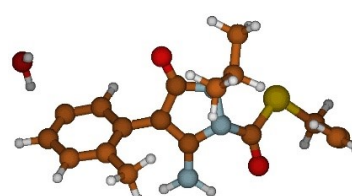
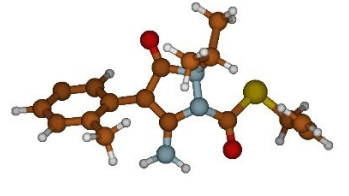
ABSTRACTION REACTION															
H9-Abs															
MCR			TS			MCP			RAD						
															
C	-2.703730	0.115767	-0.275942	C	-2.524313	0.136477	-0.588807	C	-2.543918	0.390624	-0.537979	C	-0.802057	1.233351	-0.436192
C	-3.489550	-0.298374	0.823405	C	-3.387820	-0.517263	0.319196	C	-3.429358	-0.310413	0.316595	C	-1.449881	-0.010495	-0.166289
C	-4.881401	-0.374298	0.657355	C	-4.738932	-0.550056	-0.017901	C	-4.765071	-0.223203	-0.025060	C	-0.463900	-0.916238	0.177882
C	-5.492565	-0.037376	-0.546820	C	-5.282475	0.041570	-1.145226	C	-5.321004	0.477951	-1.067107	N	0.779551	-0.268358	0.158753
C	-4.712582	0.392711	-1.621435	C	-4.417296	0.712846	-2.014435	C	-4.424667	1.189710	-1.878049	N	0.599477	1.072086	-0.245255
C	-3.330100	0.464692	-1.481981	C	-3.055614	0.750347	-1.734895	C	-3.059489	1.136069	-1.612834	C	-2.899999	-0.242259	-0.267151
C	-1.239273	0.236158	-0.179670	C	-1.075808	0.230297	-0.346272	C	-1.091236	0.394510	-0.303341	C	-3.649036	-0.732835	0.830420
C	-2.884282	-0.620728	2.164951	C	-2.905613	-1.138376	1.603455	C	-2.979434	-1.071981	1.536881	C	-5.001404	-0.889082	0.596868
H	-5.488970	-0.691354	1.501482	H	-5.479242	-1.126860	0.701682	H	-5.015039	-3.136679	0.974146	C	-5.689470	-0.600473	-0.557020
H	-6.571969	-0.101552	-0.643702	H	-6.347774	-0.013707	-1.345394	H	-6.389649	0.489896	-1.258029	C	-4.929229	-0.090182	-1.619498
H	-5.177611	0.664419	-2.563958	H	-4.805674	1.192335	-2.907410	H	-4.794878	1.771142	-2.717059	C	-3.555835	0.078799	-1.468289
H	-2.715043	0.787053	-2.317859	H	-2.377773	1.256459	-2.416658	H	-2.365850	1.674328	-2.252504	C	-3.045856	-1.038895	2.177099
H	-2.000918	-0.005699	2.362050	H	-1.991041	-0.656082	1.958596	H	-2.051214	-0.657051	1.939877	N	-0.564551	-2.217298	0.437756
H	-2.574667	-1.670349	2.223829	H	-2.695288	-2.205734	1.474178	H	-2.804220	-2.128664	1.304997	C	1.953335	-0.928629	-0.208770
H	-3.614624	-0.448789	2.959034	H	-3.671004	-1.044930	2.377579	H	-3.749624	-1.028002	2.310678	S	3.065427	0.027059	-1.203072
C	-0.322517	-0.735274	0.181886	C	-0.179630	-0.799531	-0.129603	C	-0.244453	-0.692008	-0.185750	C	4.461220	-1.133262	-1.217747
N	0.965249	-0.177736	0.158740	N	1.100276	-0.259648	0.060177	N	1.060725	-0.232323	0.041138	C	5.258137	-1.231658	0.052994
N	0.884338	1.165835	-0.266217	N	1.039148	1.143458	-0.080511	N	1.065586	1.179019	0.029629	C	5.015011	-0.624348	1.212599
C	-0.501871	1.422848	-0.469502	C	-0.330062	1.448018	-0.322819	C	-0.288060	1.568743	-0.174595	C	1.243879	2.031267	0.718841
O	-0.908754	2.546413	-0.794441	O	-0.724307	2.616068	-0.430431	O	-0.626581	2.758878	-0.171754	C	1.530360	3.358760	0.035579
N	-0.518685	-2.021142	0.457587	N	-0.384230	-2.114680	-0.137494	N	-0.509962	-1.990244	-0.310271	O	-1.292781	2.328820	-0.737383
H	0.266002	-2.627069	0.656864	H	0.388712	-2.758323	-0.030627	H	0.231878	-2.676265	-0.264140	C	0.427894	2.171937	1.998225
H	-1.444455	-2.415277	0.304661	H	-1.286806	-2.463677	-0.433603	H	-1.430452	-2.269669	-0.624454	O	2.164444	-2.075368	0.141469
C	1.584063	2.089826	0.693625	C	1.666169	1.846454	1.093120	C	1.729684	1.741202	1.257454	H	-6.760588	-0.751844	-0.650208
C	0.770897	2.296042	1.965938	C	0.767463	1.794369	2.322740	C	0.833422	1.621110	2.484161	H	-5.410004	0.163289	-2.559600
C	1.960598	3.389740	0.001119	C	2.077482	3.258120	0.706847	C	2.209927	3.159974	0.997482	H	-2.966171	0.461790	-2.296434
H	2.507016	1.562700	0.949025	H	2.573784	1.272719	1.297172	H	2.608387	1.107564	1.402147	H	-2.174414	-0.406880	2.371361
H	1.370833	2.850873	2.692352	H	1.314595	2.181608	3.186492	H	1.402656	1.897716	3.375709	H	-2.725329	-2.084236	2.240953
H	0.494736	1.336011	2.415063	H	0.464916	0.765317	2.544502	H	0.478811	0.592718	2.612135	H	-3.784056	-0.873034	2.964949
H	-0.139972	2.868987	1.765454	H	-0.129702	2.405680	2.183551	H	-0.031452	2.287744	2.409862	H	0.258087	-2.774799	0.624872
H	1.080660	3.993537	-0.228435	H	1.209278	3.900037	0.546762	H	1.374863	3.856282	0.901016	H	-1.458802	-2.671321	0.303428

H	2.608642	3.964809	0.668593	H	2.674443	3.681298	1.519677	H	2.828645	3.478084	1.841386	H	2.200725	1.563133	0.963651
H	2.507253	3.192515	-0.925534	H	2.686642	3.251460	-0.201580	H	2.816601	3.204724	0.088446	H	0.997977	2.753308	2.727890
C	2.089843	-0.923949	-0.193826	C	2.254815	-0.927866	-0.349440	C	2.179216	-0.912038	-0.443849	H	0.214044	1.191281	2.436832
O	2.219604	-2.078216	0.171843	O	2.361205	-2.133973	-0.220280	O	2.228869	-2.128513	-0.431467	H	-0.517585	2.690469	1.810746
S	3.270528	-0.060635	-1.194627	S	3.505157	0.109275	-1.056292	S	3.472903	0.128228	-1.062640	H	0.611568	3.905002	-0.186002
C	4.587287	-1.310082	-1.179816	C	4.822315	-1.131606	-1.198871	C	4.725082	-1.155483	-1.346289	H	2.141723	3.970184	0.705319
C	5.369094	-1.437230	0.097811	C	5.503200	-1.529637	0.080850	C	5.397134	-1.712959	-0.122767	H	2.085073	3.205440	-0.894577
C	5.151964	-0.803230	1.248313	C	5.193594	-1.146928	1.317873	C	5.118692	-1.443323	1.150904	H	4.090686	-2.118067	-1.516022
H	4.155228	-2.274031	-1.463315	H	4.417865	-2.011090	-1.707983	H	4.272048	-1.958227	-1.935030	H	5.098645	-0.773476	-2.032325
H	5.251181	-1.007564	-1.996434	H	5.546412	-0.674378	-1.881412	H	5.465081	-0.668600	-1.990131	H	6.119899	-1.892694	-0.035249
H	6.192188	-2.147566	0.024540	H	6.333663	-2.217609	-0.075196	H	6.191627	-2.420206	-0.359213	H	5.670569	-0.780216	2.063586
H	5.790753	-0.985935	2.106705	H	5.765219	-1.510591	2.165953	H	5.679796	-1.918529	1.949370	H	4.167484	0.042537	1.357196
H	4.343111	-0.086981	1.377739	H	4.372723	-0.465311	1.531202	H	4.334663	-0.748240	1.444380				
O	-3.345586	-2.814154	-0.254688	O	-6.343445	-1.673394	1.594451	O	-5.888269	-2.939750	1.339604				
H	-3.941499	-2.993076	0.500936	H	-6.005294	-1.223853	2.393172	H	-5.924539	-1.972709	1.358970				

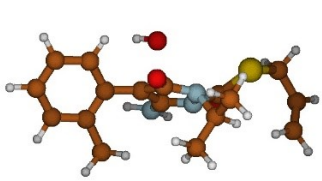
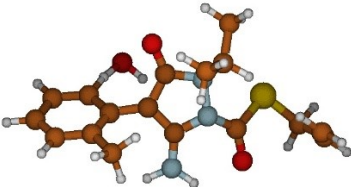
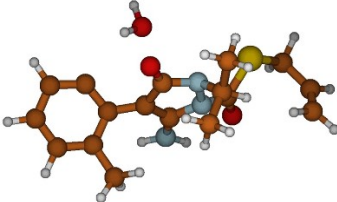
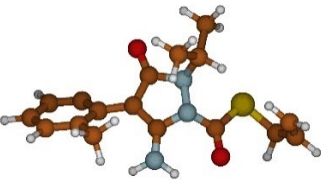
H10-Abs															
MCR	TS	MCP	RAD												
															
C	-2.660561	-0.515283	-0.260649	C	-0.331928	1.298844	-0.427768	C	-0.353163	1.263189	-0.363912	C	-3.531150	0.053589	-1.534804
C	-3.381754	-1.096774	0.801368	C	-1.028335	0.095925	-0.101377	C	-1.011898	0.053264	0.009249	C	-2.909693	-0.237625	-0.308970
C	-4.754117	-1.320892	0.629667	C	-0.075331	-0.845107	0.239337	C	-0.027708	-0.866803	0.315246	C	-3.674305	-0.696200	0.785448
C	-5.412008	-0.967144	-0.545645	N	1.195835	-0.257109	0.167360	N	1.228296	-0.258891	0.175512	C	-5.057932	-0.882619	0.607341
C	-4.698583	-0.372729	-1.586876	N	1.065822	1.078849	-0.269253	N	1.054458	1.068501	-0.272299	C	-5.601119	-0.589171	-0.619786
C	-3.330919	-0.153766	-1.441498	C	-2.491206	-0.068424	-0.158240	C	-2.472695	-0.139523	0.025210	C	-4.906615	-0.116539	-1.711489
C	-1.222203	-0.212301	-0.151145	C	-3.235323	-0.489488	0.963751	C	-3.151402	-0.549408	1.193339	C	-1.458308	-0.007330	-0.193305
C	-2.727803	-1.459810	2.109368	C	-4.627318	-0.614548	0.834983	C	-4.549247	-0.704241	1.139270	C	-0.806931	1.235297	-0.454843
H	-5.315323	-1.766476	1.447186	C	-5.238952	-0.298064	-0.365548	C	-5.186460	-0.427435	-0.045405	N	0.593352	1.073135	-0.252466
H	-6.478278	-1.146181	-0.644441	C	-4.531130	0.134638	-1.477762	C	-4.578331	-0.001506	-1.205761	N	0.768275	-0.268482	0.150633

H	-5.199977	-0.084024	-2.505376	C	-3.147728	0.246140	-1.359076	C	-3.189416	0.136531	-1.151267	C	-0.476723	-0.914449	0.156470
H	-2.762648	0.297682	-2.250945	C	-2.591477	-0.786541	2.292883	C	-2.434315	-0.806430	2.492809	O	-1.294270	2.331884	-0.759903
H	-1.905791	-0.778712	2.349496	N	-0.227083	-2.132649	0.540107	N	-0.144820	-2.152305	0.640207	N	-0.582613	-2.215839	0.415274
H	-2.318673	-2.476002	2.083709	C	2.326728	-0.980282	-0.214141	C	2.352778	-0.968910	-0.246225	C	1.944201	-0.929337	-0.207042
H	-3.459047	-1.422809	2.920294	S	3.455895	-0.099144	-1.256826	S	3.416345	-0.087898	-1.356063	O	2.150269	-2.077678	0.141417
C	-0.177145	-1.079441	0.118916	C	4.801639	-1.317376	-1.270110	C	4.784372	-1.279968	-1.405857	C	1.228473	2.028861	0.721118
N	1.021029	-0.354398	0.145475	C	5.620885	-1.416451	-0.013670	C	5.661101	-1.336030	-0.186068	C	0.400588	2.165287	1.993371
N	0.752473	0.996611	-0.159259	C	5.421846	-0.777309	1.137243	C	5.496796	-0.682555	0.962266	C	-3.063671	-0.973546	2.134317
C	-0.651692	1.078497	-0.323139	C	1.776147	2.033283	0.652355	C	1.792616	2.046853	0.600871	S	3.068050	0.027818	-1.186921
O	-1.212565	2.171459	-0.530232	C	2.095324	3.331109	-0.072093	C	2.047844	3.342441	-0.152457	C	4.463283	-1.133192	-1.188459
N	-0.196163	-2.399272	0.275910	O	-0.779563	2.406722	-0.750678	O	-0.835340	2.359422	-0.677780	C	5.245611	-1.235283	0.091057
H	0.658223	-2.918424	0.428550	C	1.002741	2.239213	1.949180	C	1.084021	2.252622	1.934268	C	4.991144	-0.629085	1.248819
H	-1.064583	-2.893922	0.117338	O	2.493975	-2.127948	0.156702	O	2.557043	-2.107085	0.135485	C	1.521711	3.358812	0.045496
C	1.356348	1.930691	0.855828	H	-5.216559	-0.937570	1.688975	O	-8.114391	-0.421146	-1.449538	H	-5.665633	-1.233362	1.437793
C	0.549574	1.947203	2.148484	H	-6.419549	-0.376626	-0.430570	H	-5.092303	-1.016771	2.027586	H	-5.382874	0.109367	-2.660294
C	1.562042	3.310231	0.251404	H	-5.031945	0.377279	-2.409202	H	-7.638868	-0.352952	-0.609565	H	-2.922931	0.413228	-2.361106
H	2.339958	1.501501	1.061741	H	-2.558936	0.574395	-2.211479	H	-5.130878	0.211876	-2.115777	H	-2.209255	-0.318264	2.327769
H	1.097570	2.512045	2.907414	H	-1.700313	-0.171947	2.450664	H	-2.645606	0.457331	-2.036250	H	-2.712002	-2.008688	2.206553
H	0.393957	0.931015	2.526362	H	-2.287977	-1.836783	2.363818	H	-1.555763	-0.162847	2.596869	H	-3.805376	-0.824205	2.922343
H	-0.424248	2.424753	2.002531	H	-3.296806	-0.594404	3.104628	H	-2.094811	-1.845808	2.561374	H	0.237170	-2.776434	0.605313
H	0.612663	3.816991	0.069013	H	0.576572	-2.722619	0.709805	H	-3.104606	-0.623904	3.335817	H	-1.477510	-2.666111	0.272700
H	2.145120	3.913142	0.953239	H	-1.141823	-2.551408	0.431813	H	0.674339	-2.728828	0.778613	H	2.183020	1.559998	0.973423
H	2.115877	3.244081	-0.689427	H	2.719846	1.532127	0.882760	H	-1.057837	-2.584633	0.580709	H	0.962923	2.746117	2.729471
C	2.234337	-0.912046	-0.265936	H	1.614685	2.817394	2.646766	H	2.757005	1.567016	0.786497	H	0.184544	1.183333	2.427904
O	2.517268	-2.063357	0.008704	H	0.764069	1.279684	2.420328	H	1.718860	2.852615	2.591868	H	-0.544105	2.682577	1.798396
S	3.276109	0.174639	-1.197737	H	0.072822	2.788961	1.772910	H	0.891482	1.294289	2.428360	H	0.605258	3.906221	-0.182773
C	4.745316	-0.887821	-1.288411	H	1.191982	3.906367	-0.283323	H	0.134168	2.780098	1.801049	H	2.126912	3.967593	0.723197
C	5.553663	-1.013938	-0.027509	H	2.747413	3.934666	0.565615	H	1.124302	3.900214	-0.318075	H	2.085148	3.208751	-0.879939
H	5.353047	-0.436244	-2.079503	H	2.618236	3.133573	-1.012256	H	2.723768	3.963420	0.442269	H	5.110175	-0.771614	-1.994775
C	5.270141	-0.511943	1.172473	H	4.384297	-2.293160	-1.534546	H	2.521175	3.144280	-1.118427	H	4.095951	-2.117135	-1.493399
H	4.438037	-1.873881	-1.648084	H	5.435372	-1.005734	-2.107084	H	5.373280	-0.974762	-2.277167	H	6.106752	-1.898253	0.011537
H	6.462537	-1.599694	-0.162392	H	6.456827	-2.109578	-0.104007	H	4.375195	-2.269128	-1.630482	H	5.636878	-0.787941	2.106748
H	5.939455	-0.678120	2.010696	H	6.088218	-0.938544	1.978785	H	6.509576	-2.009797	-0.302206	H	4.143667	0.039577	1.385237
H	4.375717	0.077457	1.363864	H	4.601594	-0.077390	1.283438	H	6.203796	-0.812850	1.775556				
O	-3.935712	2.389365	-0.436370	O	-7.718460	-0.683505	-0.607718	H	4.666547	-0.000418	1.134190				
H	-2.942456	2.304865	-0.449377	H	-7.601465	-1.441533	-1.212260	H	-7.427730	-0.625287	-2.098529				

H11-Abs			
MCR	TS	MCP	RAD

			
C -2.660460 -0.515456 -0.260705	C -0.529914 1.206871 0.063578	C -2.547593 -0.420365 0.101180	C -0.783435 1.248914 -0.468285
C -3.381806 -1.097156 0.801096	C -1.118727 -0.093541 0.086813	C -3.149722 -1.377247 0.946074	C -1.445232 0.011406 -0.204744
C -4.754182 -1.321069 0.629223	C -0.082719 -1.008934 0.096752	C -4.534411 -1.582689 0.865191	C -0.471524 -0.901862 0.153924
C -5.411914 -0.966906 -0.546060	N 1.136899 -0.318265 0.115799	C -5.340403 -0.852775 -0.013575	N 0.777089 -0.263356 0.154481
C -4.698309 -0.372355 -1.587075	N 0.887627 1.070598 0.074853	C -4.697500 0.082150 -0.794929	N 0.613388 1.077902 -0.253656
C -3.330637 -0.153592 -1.441536	C -2.566594 -0.357490 0.079206	C -3.348501 0.332590 -0.783892	C -2.894836 -0.209013 -0.337407
C -1.222144 -0.212425 -0.150956	C -3.194440 -1.124337 1.083109	C -1.102538 -0.143800 0.134638	C -3.684610 -0.685275 0.730766
C -2.727963 -1.460605 2.109030	C -4.579775 -1.322689 1.014996	C -2.350406 -2.168117 1.950663	C -5.061393 -0.862761 0.533333
H -5.315510 -1.766796 1.446577	C -5.353179 -0.765112 -0.002431	H -4.993433 -2.318916 1.520762	C -5.678700 -0.563803 -0.685133
H -6.478196 -1.145769 -0.645048	C -4.706437 -0.004127 -0.966124	H -6.412640 -1.016692 -0.057365	C -4.859031 -0.082193 -1.682272
H -5.199542 -0.083309 -2.505540	C -3.341796 0.216304 -0.945082	H -5.995320 1.122996 -2.929920	C -3.504719 0.107672 -1.570348
H -2.762210 0.297944 -2.250841	C -2.422347 -1.712954 2.235526	H -2.889815 1.073661 -1.433255	C -3.094839 -0.988453 2.085096
H -1.906233 -0.779331 2.349626	N -0.127521 -2.337430 0.037017	H -1.486611 -1.601497 2.310570	N -0.585894 -2.201997 0.412874
H -2.318462 -2.476632 2.082920	C 2.284442 -0.816023 -0.501516	H -1.976994 -3.103782 1.520319	C 1.950550 -0.932786 -0.197840
H -3.459363 -1.424264 2.919845	S 3.279230 0.401971 -1.317641	H -2.975912 -2.429726 2.807329	S 3.082709 0.014625 -1.177129
C -0.177026 -1.079470 0.119113	C 4.701949 -0.651688 -1.718472	C -0.057406 -1.030695 -0.044806	C 4.467877 -1.158474 -1.177814
N 1.021068 -0.354359 0.145642	C 5.605790 -1.012360 -0.572821	N 1.155941 -0.338117 0.076544	C 5.250414 -1.265240 0.101163
N 0.752429 0.996631 -0.159075	C 5.440974 -0.719230 0.715382	N 0.891019 1.030722 0.296954	C 5.000940 -0.656286 1.258559
C -0.651751 1.078430 -0.322888	C 1.600618 1.792809 1.186943	C -0.527504 1.147047 0.338794	C 1.249254 2.033263 0.719691
O -1.212782 2.171317 -0.529941	C 1.774376 3.262772 0.840405	O -1.081419 2.228303 0.574444	C 1.556182 3.358087 0.040179
N -0.196090 -2.399264 0.276896	O -1.073292 2.318683 0.084391	N -0.089004 -2.326000 -0.347396	O -1.260921 2.346923 -0.782064
H 0.658787 -2.918514 0.426580	C 0.918488 1.566104 2.530757	H 0.766267 -2.840480 -0.510758	C 0.413876 2.181116 1.985714
H -1.064065 -2.894033 0.116176	O 2.551891 -2.003498 -0.465867	H -0.980305 -2.750640 -0.569190	O 2.147990 -2.081312 0.154422
C 1.356302 1.930743 0.855962	H -5.063847 -1.910266 1.790974	C 1.621378 1.546372 1.507924	H -5.666490 -1.226707 1.360381
C 0.549525 1.947228 2.148614	H -6.427105 -0.918385 -0.031266	C 0.972227 1.065789 2.800336	H -6.747726 -0.698518 -0.818115
C 1.561857 3.310287 0.251506	H -5.342417 0.464701 -1.850744	C 1.769687 3.057619 1.434764	H -2.899347 0.478442 -2.393364
H 2.339950 1.501627 1.061852	H -2.859501 0.813381 -1.713810	H 2.617550 1.103649 1.429429	H -2.227374 -0.356162 2.295644
H 1.097488 2.512112 2.907535	H -1.563451 -1.089744 2.501339	H 1.611032 1.333255 3.646375	H -2.770262 -2.032502 2.156338
H 0.393953 0.931038 2.526506	H -2.044471 -2.712587 1.994315	H 0.849153 -0.022531 2.797333	H -3.841231 -0.825632 2.866173

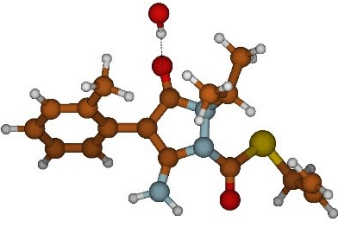
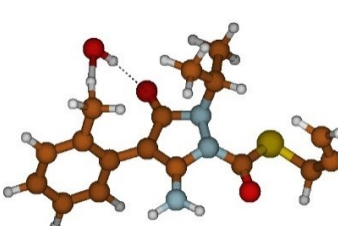
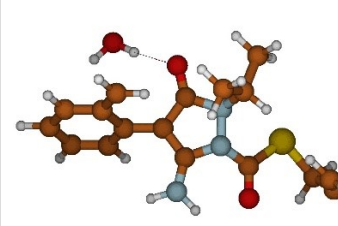
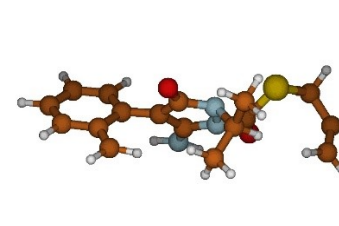
H	-0.424323	2.424719	2.002638	H	-3.068154	-1.810112	3.111225	H	-0.006334	1.533017	2.949568	H	0.230537	-2.766106	0.607525
H	0.612431	3.816948	0.069074	H	0.722595	-2.883703	-0.007311	H	0.811406	3.562777	1.569246	H	-1.480569	-2.649582	0.260946
H	2.144851	3.913267	0.953351	H	-1.020772	-2.785448	-0.122024	H	2.444072	3.379871	2.233198	H	2.198717	1.558440	0.980053
H	2.115732	3.244179	-0.689305	H	2.591702	1.332921	1.214141	H	2.199828	3.361159	0.476037	H	0.975917	2.759667	2.723810
C	2.234395	-0.911918	-0.265916	H	1.543788	1.979344	3.326786	C	2.289099	-0.693845	-0.655702	H	0.186244	1.202515	2.421927
O	2.517328	-2.063290	0.008486	H	0.780648	0.497302	2.726457	O	2.568714	-1.862589	-0.852307	H	-0.524903	2.705803	1.782181
S	3.276062	0.174925	-1.197607	H	-0.056450	2.062264	2.569194	S	3.247248	0.670920	-1.254143	H	0.644957	3.910736	-0.196302
C	4.745237	-0.887553	-1.288669	H	0.822948	3.797334	0.862339	C	4.661048	-0.267676	-1.898380	H	2.161148	3.965630	0.719183
C	5.553684	-1.013982	-0.027860	H	2.441618	3.717036	1.578373	C	5.610890	-0.825890	-0.875776	H	2.124489	3.200098	-0.880931
C	5.270266	-0.512244	1.172255	H	2.224619	3.379162	-0.149586	C	5.489268	-0.790143	0.449527	H	4.091399	-2.139601	-1.480776
H	4.437883	-1.873511	-1.648553	H	4.337600	-1.553382	-2.218853	H	4.283354	-1.064052	-2.545993	H	5.117022	-0.804069	-1.985478
H	5.352902	-0.435782	-2.079700	H	5.257486	-0.075951	-2.466115	H	5.182876	0.446176	-2.544320	H	6.106555	-1.934635	0.021596
H	6.462542	-1.599715	-0.162947	H	6.478749	-1.585436	-0.884141	H	6.477982	-1.312591	-1.321457	H	5.645845	-0.819141	2.116356
H	5.939644	-0.678620	2.010387	H	6.170663	-1.042726	1.451001	H	6.248345	-1.236144	1.084446	H	4.158457	0.018722	1.394671
H	4.375870	0.077134	1.363849	H	4.587482	-0.152868	1.082449	H	4.643134	-0.320191	0.946661				
O	-3.935889	2.389602	-0.435916	O	-6.071860	1.229915	-2.680842	O	-6.306191	2.025252	-2.774049				
H	-2.942665	2.304672	-0.449350	H	-6.098604	2.042244	-2.139768	H	-6.073821	2.202047	-1.852321				

H12-Abs															
MCR			TS			MCP			RAD						
															
C	2.832352	-0.247888	0.194439	C	-0.681852	1.233344	-0.036498	C	-0.725410	1.253658	-0.138234	C	-3.549770	0.220791	-1.434638
C	3.521735	-0.535498	-1.002950	C	-1.317102	-0.043505	0.038894	C	-1.379521	0.000491	0.065016	C	-2.879722	-0.198762	-0.296534
C	4.913595	-0.679375	-0.944749	C	-0.320519	-0.987784	0.194916	C	-0.394775	-0.939080	0.304207	C	-3.675098	-0.769738	0.726406
C	5.616814	-0.523992	0.246618	N	0.920245	-0.336697	0.242623	N	0.852801	-0.297815	0.317451	C	-5.053461	-0.905436	0.504942
C	4.932145	-0.203015	1.419087	N	0.725017	1.051420	0.074588	N	0.675196	1.071624	0.026207	C	-5.663077	-0.477729	-0.672328
C	3.548855	-0.065977	1.388176	C	-2.768565	-0.262920	-0.060616	C	-2.829708	-0.206206	-0.060797	C	-4.895358	0.118248	-1.684177
C	1.372147	-0.057215	0.214038	C	-3.513895	-0.893581	0.960306	C	-3.623830	-0.825921	0.933695	C	-1.428405	0.009131	-0.179658
C	2.828112	-0.654424	-2.336690	C	-4.895874	-1.043691	0.786343	C	-5.001635	-0.955124	0.705317	C	-0.773083	1.255134	-0.419369

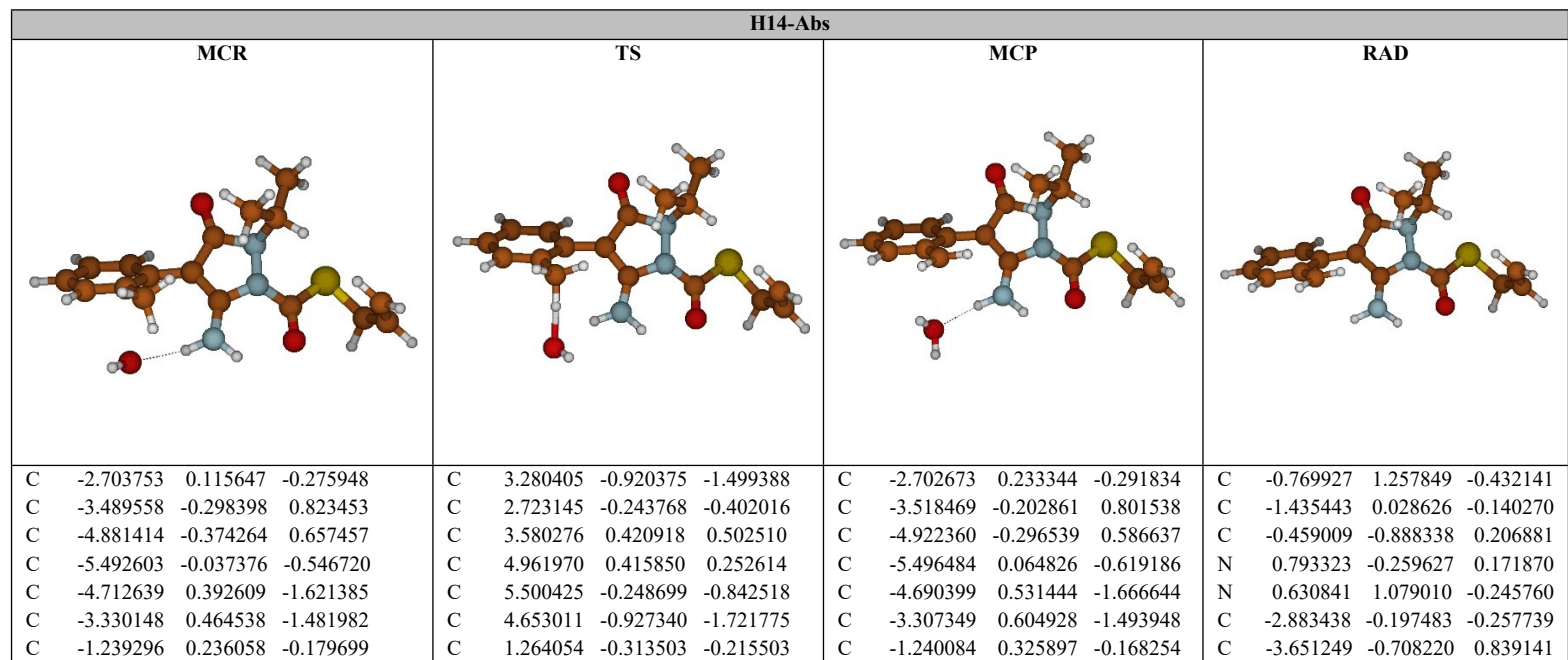


H	5.451654	-0.900506	-1.862923	C	-5.551237	-0.576101	-0.349596	C	-5.611689	-0.476249	-0.452026	N	0.625609	1.082364	-0.224268
H	6.696333	-0.639212	0.256561	C	-4.826466	0.064688	-1.359314	C	-4.845446	0.164830	-1.437193	N	0.797658	-0.269841	0.142174
H	5.469967	-0.063819	2.351433	C	-3.462489	0.203336	-1.179145	C	-3.501059	0.259396	-1.180178	C	-0.448003	-0.914194	0.132533
H	3.003978	0.175473	2.295718	C	-2.858674	-1.390801	2.222364	C	-3.027872	-1.323518	2.224698	O	-1.257756	2.357979	-0.702118
H	1.963390	0.012593	-2.407137	N	-0.411741	-2.314087	0.241593	N	-0.497579	-2.258338	0.448027	N	-0.552276	-2.224205	0.343909
H	2.477598	-1.675682	-2.519780	C	2.079890	-0.918502	-0.273629	C	2.014067	-0.929470	-0.133004	C	1.973011	-0.922717	-0.234220
H	3.523209	-0.399354	-3.139763	S	3.144583	0.195288	-1.147095	S	3.106706	0.104317	-1.068579	O	2.178165	-2.079450	0.085583
C	0.379479	-0.891138	-0.333862	C	4.549147	-0.927684	-1.395162	C	4.499842	-1.051483	-1.209316	C	1.269413	2.013844	0.767039
N	-0.838012	-0.218375	-0.299272	C	5.395281	-1.211878	-0.185663	C	5.324845	-1.253243	0.030877	C	0.444711	2.130606	2.043221
N	-0.656050	1.075560	0.239174	C	5.186623	-0.805084	1.064718	C	5.101350	-0.753577	1.244462	C	-3.084500	-1.206070	2.042041
C	0.720284	1.201547	0.521018	C	1.404037	1.840239	1.161558	C	1.337104	1.950204	1.052713	S	3.095965	0.056418	-1.192381
O	1.228834	2.245797	0.918775	C	1.656979	3.267134	0.702182	C	1.619923	3.325229	0.469330	C	4.487851	-1.108323	-1.229044
N	0.493093	-2.135982	-0.744455	O	-1.187444	2.358839	-0.128158	O	-1.213451	2.366296	-0.373517	C	5.275415	-1.244118	0.044047
H	-0.313935	-2.657604	-1.065353	C	0.638810	1.754217	2.476859	C	0.536531	1.996713	2.348670	C	5.025157	-0.669034	1.218421
H	1.389733	-2.600323	-0.652889	O	2.307503	-2.104748	-0.121347	O	2.227171	-2.102413	0.113995	C	1.569148	3.354826	0.116711
C	-1.276170	2.141069	-0.622061	H	-5.468143	-1.529050	1.572554	O	-0.770635	0.319271	-3.147528	H	-5.662451	-1.343250	1.291362
C	-0.425616	2.426694	-1.853604	H	-6.624537	-0.704480	-0.451539	H	-5.609939	-1.430679	1.470000	H	-6.735035	-0.593557	-0.803615
C	-1.575693	3.379503	0.207200	H	-5.314449	0.436616	-2.254265	H	-6.683161	-0.589093	-0.589310	H	-5.347224	0.471577	-2.605739
H	-2.226181	1.705135	-0.942103	H	-2.839618	0.740327	-2.042503	H	-5.296583	0.555566	-2.343774	H	-2.202718	-0.612886	2.301540
H	-0.971687	3.099383	-2.520333	H	-2.006475	-0.764914	2.503328	H	-0.865083	0.343255	-4.108978	H	-2.781600	-2.258596	2.013950
H	-0.208795	1.504420	-2.402813	H	-2.491471	-2.416043	2.101212	H	-2.149939	-0.737194	2.511518	H	-3.824182	-1.099071	2.839065
H	0.518367	2.908135	-1.580041	H	-3.577513	-1.394335	3.044927	H	-2.716267	-2.370635	2.142437	H	0.272843	-2.789639	0.494197
H	-0.660148	3.890998	0.510312	H	0.417231	-2.890180	0.304511	H	-3.766300	-1.263374	3.027719	H	-1.439573	-2.675465	0.163027
H	-2.169657	4.068342	-0.399818	H	-1.311242	-2.745165	0.070930	H	0.330054	-2.832426	0.542230	H	2.221391	1.533813	1.007462
H	-2.151339	3.120752	1.100342	H	2.372306	1.348532	1.286304	H	-1.389745	-2.698454	0.263218	H	1.014228	2.688608	2.791315
C	-2.023079	-0.906772	0.014188	H	1.235049	2.209953	3.271940	H	2.294709	1.460387	1.247638	H	0.217869	1.141548	2.455695
O	-2.229115	-2.016204	-0.435865	H	0.445719	0.711459	2.750694	H	1.116626	2.520086	3.113459	H	-0.494284	2.662599	1.860895
S	-3.125344	-0.033984	1.084356	H	-0.315134	2.287343	2.415732	H	0.322366	0.986784	2.714621	H	0.655040	3.910324	-0.101335
C	-4.530465	-1.180612	0.997525	H	0.727723	3.832918	0.613801	H	-0.408617	2.531277	2.210190	H	2.176647	3.948080	0.805993
C	-5.325481	-1.161596	-0.278007	H	2.293160	3.762743	1.440969	H	0.700052	3.888935	0.302627	H	2.132174	3.219650	-0.811260
C	-5.067245	-0.469916	-1.385846	H	2.173723	3.279399	-0.261775	H	2.241675	3.882057	1.176069	H	4.115521	-2.083172	-1.556378
H	-4.167768	-2.190315	1.210118	H	4.177419	-1.859279	-1.831025	H	2.161949	3.242149	-0.477058	H	5.132163	-0.729007	-2.029202
H	-5.165338	-0.886952	1.840007	H	5.151418	-0.434945	-2.165627	H	4.120473	-2.008742	-1.577984	H	6.136103	-1.904783	-0.056530
H	-6.199091	-1.811905	-0.243556	H	6.262957	-1.831755	-0.409855	H	5.119802	-0.627279	-2.006123	H	5.673866	-0.850497	2.069587
H	-5.723039	-0.546031	-2.247432	H	5.875688	-1.082367	1.856234	H	6.189388	-1.895905	-0.133255	H	4.178188	-0.004185	1.375283
H	-4.208192	0.191654	-1.476525	H	4.335616	-0.187515	1.344610	H	5.775297	-0.977922	2.065244				
O	0.592157	-0.823002	2.180307	O	-2.052953	1.115268	-3.059147	H	4.252323	-0.109532	1.464225				
H	1.297618	-1.490950	2.205314	H	-1.288800	0.538248	-2.861152	H	-1.560287	0.768251	-2.812284				

H13-Abs			
MCR	TS	MCP	RAD

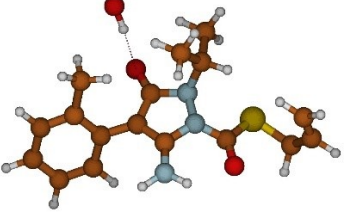
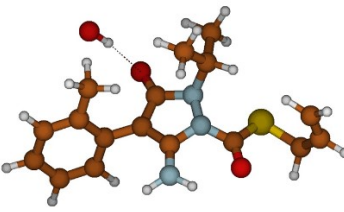
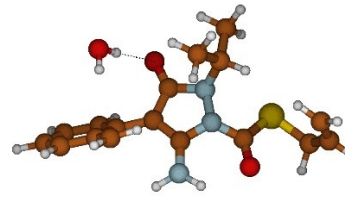
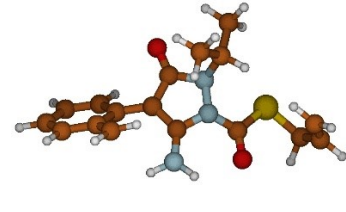
			
C -2.692997 -0.872891 -0.112973	C -0.689427 0.757713 -0.737226	C -2.618349 -0.706635 0.086500	C -0.809872 1.006694 -0.663347
C -3.729769 -0.081113 0.421077	C -1.227695 -0.414402 -0.144301	C -3.590684 0.041509 0.825362	C -1.425043 -0.135085 -0.066796
C -5.043327 -0.561102 0.339799	C -0.171520 -1.096798 0.432478	C -4.953325 -0.353693 0.716765	C -0.414832 -0.889214 0.500203
C -5.338510 -1.792740 -0.238644	N 1.006655 -0.369259 0.231795	C -5.331966 -1.443983 -0.048281	N 0.812153 -0.243337 0.295078
C -4.308611 -2.579164 -0.755606	N 0.714954 0.788211 -0.521124	C -4.365835 -2.187653 -0.738400	N 0.597225 0.927643 -0.462549
C -2.998587 -2.114474 -0.694265	C -2.644168 -0.835414 -0.152509	C -3.023614 -1.807582 -0.668199	C -2.858123 -0.475557 -0.105637
C -1.283112 -0.436650 -0.070703	C -3.616925 -0.129731 0.588157	C -1.199598 -0.307546 0.091752	C -3.840091 0.411267 0.443388
C -3.475154 1.250546 1.078347	C -4.949864 -0.560543 0.529012	C -3.241078 1.140557 1.638346	C -5.208551 0.039225 0.326758
H -5.845725 0.045108 0.753098	C -5.318500 -1.673570 -0.221351	H -5.700581 0.219383 1.259194	C -5.587679 -1.156124 -0.258749
H -6.366739 -2.138830 -0.281341	C -4.350278 -2.383126 -0.932489	H -6.379343 -1.723097 -0.109924	C -4.615353 -2.029731 -0.762642
H -4.523483 -3.541480 -1.209481	C -3.023244 -1.960093 -0.896674	H -4.656330 -3.044104 -1.337838	C -3.266229 -1.676284 -0.688129
H -2.193770 -2.712501 -1.115506	C -3.260533 1.044413 1.434826	H -2.275625 -2.363949 -1.228080	C -3.493340 1.605383 1.110181
H -3.601110 2.068573 0.359513	N -0.175262 -2.265795 1.066445	H -4.355345 1.062551 -1.530678	N -0.486179 -2.058290 1.133144
H -2.462489 1.316375 1.484879	C 2.247174 -0.989830 0.072631	H -2.209304 1.435526 1.784720	C 1.998151 -0.957353 0.110362
H -4.189105 1.414541 1.889609	S 3.306833 -0.235263 -1.129108	H -4.013916 1.690245 2.163485	S 3.075805 -0.304292 -1.134909
C -0.219881 -1.144808 0.466716	C 4.808445 -1.199094 -0.794838	C -0.124388 -1.071103 0.509245	C 4.493505 -1.401895 -0.851716
N 0.959094 -0.415432 0.276180	C 5.549562 -0.858614 0.467802	N 1.055796 -0.339940 0.324036	C 5.322847 -1.117825 0.369159
N 0.660844 0.773784 -0.421831	C 5.187289 0.003713 1.415245	N 0.741538 0.901576 -0.268937	C 5.094767 -0.205675 1.311784
C -0.745077 0.756943 -0.620111	C 1.240882 2.032841 0.145343	C -0.672204 0.924882 -0.386751	C 1.246739 2.129492 0.166147
O -1.329225 1.695748 -1.193022	C 1.409371 3.148559 -0.873268	O -1.266529 1.924156 -0.827619	C 1.519590 3.191762 -0.886561
N -0.213423 -2.334829 1.058591	O -1.263886 1.677537 -1.347383	N -0.109831 -2.309891 0.993846	O -1.325740 1.965286 -1.254331
H 0.646623 -2.744127 1.398230	C 0.381765 2.434287 1.338526	H 0.759675 -2.763920 1.238570	C 0.443474 2.649865 1.352123
H -1.073245 -2.866913 1.093321	O 2.542316 -1.974916 0.723704	H -0.974026 -2.836108 1.004114	O 2.238884 -1.953226 0.767661
C 1.222999 1.981488 0.279778	H -5.701222 -0.016546 1.095563	C 1.370713 2.056709 0.461674	H -5.960522 0.713650 0.727647
C 0.423455 2.325322 1.529950	H -6.356474 -1.990600 -0.245472	C 0.608423 2.400727 1.735303	H -6.639678 -1.416274 -0.325050
C 1.361432 3.146738 -0.687194	H -4.626021 -3.256059 -1.515649	C 1.542171 3.241941 -0.474704	H -4.905072 -2.968608 -1.223035
H 2.227460 1.672034 0.579657	H -2.263832 -2.500103 -1.456403	H 2.364288 1.693708 0.735299	H -2.513028 -2.339828 -1.106512
H 0.954213 3.095760 2.096096	H -3.319256 2.012921 0.812372	H 1.191643 3.115438 2.322214	H -2.460833 1.889480 1.271914
H 0.305115 1.448265 2.175156	H -2.240362 1.008048 1.822795	H 0.445049 1.507997 2.348717	H -4.271874 2.248950 1.503834

H	-0.566848	2.713192	1.272482	H	-3.978263	1.205801	2.242202	H	-0.359477	2.857002	1.505313	H	0.346648	-2.512151	1.483242
H	0.390654	3.561477	-0.968415	H	0.683185	-2.674203	1.411408	H	0.580213	3.677327	-0.751804	H	-1.373981	-2.541866	1.164609
H	1.939820	3.935124	-0.197338	H	-1.030285	-2.807236	1.075132	H	2.131769	4.007997	0.036892	H	2.207877	1.757455	0.530124
H	1.891760	2.841460	-1.593736	H	2.232671	1.746864	0.504552	H	2.073534	2.946382	-1.383820	H	1.032111	3.401268	1.885430
C	2.189117	-1.040621	0.054009	H	0.876888	3.242841	1.883155	C	2.263492	-0.961498	-0.005791	H	0.207658	1.840838	2.052018
O	2.493318	-2.054677	0.653846	H	0.245705	1.593010	2.026606	O	2.580629	-2.020699	0.502759	H	-0.489205	3.117687	1.021827
S	3.219167	-0.246702	-1.148267	H	-0.602005	2.791131	1.014863	S	3.247464	-0.094500	-1.195479	H	0.593411	3.630587	-1.262546
C	4.714531	-1.249119	-0.915752	H	0.444492	3.522256	-1.221533	C	4.735849	-1.130592	-1.111562	H	2.118818	3.986914	-0.433908
C	5.506158	-0.985584	0.334579	H	1.947472	3.973855	-0.398461	C	5.592677	-0.967643	0.112685	H	2.080129	2.771977	-1.726692
C	5.190914	-0.170254	1.338723	H	1.990728	2.806892	-1.734388	C	5.336489	-0.229176	1.190380	H	4.134973	-2.434965	-0.840445
H	4.438548	-2.305497	-0.980589	H	4.551208	-2.261886	-0.814845	H	4.438374	-2.175744	-1.235928	H	5.104164	-1.287735	-1.753297
H	5.323610	-1.025522	-1.797888	H	5.445199	-1.009910	-1.665357	H	5.303517	-0.853339	-2.005979	H	6.197015	-1.763481	0.448703
H	6.431639	-1.558913	0.380204	H	6.480504	-1.414305	0.576928	H	6.512696	-1.549762	0.068157	H	5.774504	-0.100229	2.151456
H	5.851281	-0.070396	2.194371	H	5.814659	0.158216	2.287449	H	6.039100	-0.199322	2.017240	H	4.236694	0.462729	1.283699
H	4.278716	0.422838	1.347226	H	4.267959	0.583164	1.360030	H	4.432296	0.367965	1.289217				
O	-2.167728	4.152963	-0.310554	O	-3.218760	3.208466	-0.105350	O	-3.829162	1.733443	-1.986861				
H	-1.821579	3.264648	-0.586403	H	-2.508074	2.767382	-0.630988	H	-2.972293	1.747094	-1.516191				

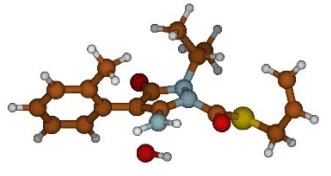
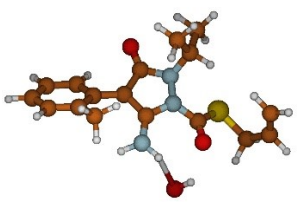
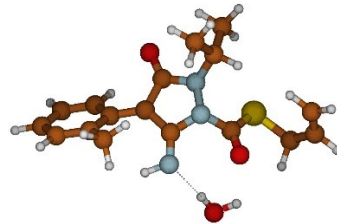
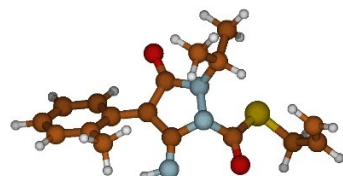


C	-2.884246	-0.620698	2.164984	C	0.521490	-1.535007	-0.211557	C	-2.983303	-0.525206	2.067654	C	-5.039520	-0.940641	0.625441
H	-5.488972	-0.691243	1.501619	N	-0.859623	-1.236022	-0.048028	H	-5.545083	-0.647947	1.405349	C	-5.648038	-0.635666	-0.578679
H	-6.572014	-0.101511	-0.643560	N	-0.935141	0.168287	0.062458	H	-6.571536	-0.009496	-0.751107	C	-4.893323	-0.092150	-1.627784
H	-5.177689	0.664294	-2.563905	O	0.351106	0.715825	-0.063777	H	-5.134383	0.820916	-2.613542	C	-3.523340	0.113021	-1.459134
H	-2.715109	0.786838	-2.317896	C	0.925845	-2.702990	-0.275765	H	-2.678055	0.942948	-2.313045	C	-3.091329	-0.947617	2.112277
H	-2.000996	-0.005506	2.362101	N	0.530421	2.032747	-0.102333	H	-1.931035	-0.401986	2.293427	N	-0.577227	-2.184908	0.480253
H	-2.574400	-1.670256	2.223804	C	-2.073112	0.819098	-0.414321	H	-3.717489	-2.930311	0.856449	C	1.955798	-0.940625	-0.192001
H	-3.614605	-0.448978	2.959092	O	-2.201451	2.025004	-0.306111	H	-3.641139	-0.862451	2.860814	S	3.079846	-0.009483	-1.196447
C	-0.322516	-0.735330	0.181923	C	-1.542505	-1.918708	1.106610	C	-0.346256	-0.681920	0.156609	C	4.457781	-1.191003	-1.205153
N	0.965238	-0.177756	0.158759	C	-0.709565	-1.835126	2.380067	N	0.954175	-0.153441	0.148314	C	5.257181	-1.290412	0.063933
N	0.884300	1.165780	-0.266303	C	3.074283	1.135871	1.707946	N	0.905758	1.206263	-0.227909	C	5.025076	-0.671505	1.219682
C	-0.501918	1.422746	-0.469596	S	-3.274266	-0.241633	-1.172487	C	-0.474819	1.502677	-0.419977	C	1.289091	2.037451	0.710224
O	-0.908827	2.546265	-0.794659	C	-4.591891	0.984853	-1.407125	O	-0.854192	2.645793	-0.709123	C	1.589454	3.356660	0.017065
N	-0.518634	-2.021198	0.457657	C	-5.347462	1.394831	-0.173945	N	-0.570629	-1.970304	0.388075	O	-1.244410	2.356451	-0.748142
H	0.266047	-2.627092	0.657064	C	-5.108516	1.029073	1.083715	H	0.201304	-2.590041	0.594705	C	0.477644	2.197287	1.990242
H	-1.444385	-2.415374	0.304755	C	-1.927490	-3.340513	0.730822	H	-1.513413	-2.350375	0.279825	O	2.150706	-2.087573	0.167024
C	1.584008	2.089855	0.693475	H	5.617102	0.934404	0.948121	C	1.623460	2.076190	0.769015	H	-5.624260	-1.346976	1.446418
C	0.770883	2.296071	1.965815	H	6.573172	-0.243869	-1.008251	C	0.812520	2.249559	2.047671	H	-6.711259	-0.813107	-0.708196
C	1.960447	3.389764	0.000909	H	5.059689	-1.453502	-2.579730	C	2.029419	3.394655	0.130345	H	-5.365797	0.154078	-2.573120
H	2.507003	1.562794	0.948854	H	2.617323	-1.437586	-2.187206	H	2.534825	1.520138	1.003823	H	-2.931210	0.508275	-2.280280
H	1.370818	2.850964	2.692183	H	2.093708	0.797476	2.049902	H	1.423996	2.758806	2.797440	H	-2.061292	-0.702313	2.341306
H	0.494795	1.336042	2.414988	H	2.962658	2.243654	1.438188	H	0.510725	1.279142	2.456327	H	-3.712155	-1.343630	2.907741
H	-0.140028	2.868957	1.765348	H	3.795155	1.124847	2.528064	H	-0.083254	2.852799	1.869108	H	0.233696	-2.749023	0.695300
H	1.080469	3.993503	-0.228643	H	-0.242382	2.657294	0.085960	H	1.164026	4.028684	-0.071168	H	-1.488653	-2.617785	0.405332
H	2.608476	3.964893	0.668347	H	1.465883	2.419066	-0.173969	H	2.692106	3.925386	0.819850	H	2.240841	1.559644	0.956283
H	2.507090	3.192537	-0.925750	H	-2.462321	-1.346519	1.251387	H	2.569884	3.223698	-0.805115	H	1.057157	2.774807	2.715499
C	2.089868	-0.923956	-0.193725	H	-1.301560	-2.202577	3.222644	C	2.062880	-0.911687	-0.225214	H	0.250318	1.222452	2.435127
O	2.219695	-2.078171	0.172073	H	-0.420072	-0.800405	2.593003	O	2.168877	-2.078947	0.105639	H	-0.460673	2.728129	1.801150
S	3.270576	-0.060650	-1.194509	H	0.194166	-2.447784	2.303951	S	3.261434	-0.043537	-1.201115	H	0.676385	3.911688	-0.206341
C	4.587360	-1.310066	-1.179589	H	-1.050343	-3.982876	0.633835	C	4.552984	-1.318972	-1.222238	H	2.209153	3.965722	0.681296
C	5.369148	-1.437114	0.098060	H	-2.567153	-3.747277	1.519208	C	5.332880	-1.495738	0.050660	H	2.140345	3.190555	-0.913156
C	5.152001	-0.803031	1.248512	H	-2.485922	-3.356961	-0.209539	C	5.129227	-0.887316	1.217335	H	4.071239	-2.172633	-1.493559
H	4.155334	-2.274044	-1.463039	H	-4.166895	1.860685	-1.905701	H	4.101800	-2.266242	-1.530911	H	5.097834	-0.848332	-2.025017
H	5.251261	-1.007578	-1.996213	H	-5.272900	0.511807	-2.122542	H	5.222163	-1.007722	-2.031256	H	6.109878	-1.963437	-0.021683
H	6.192247	-2.147451	0.024853	H	-6.171619	2.075205	-0.386647	H	6.141156	-2.220690	-0.041922	H	5.680692	-0.829770	2.070186
H	5.790780	-0.985673	2.106925	H	-5.730645	1.399591	1.892388	H	5.764216	-1.105166	2.070329	H	4.186838	0.007647	1.361364
H	4.343144	-0.086777	1.377880	H	-4.297696	0.355297	1.353057	H	4.335136	-0.158248	1.365422				
O	-3.345533	-2.813840	-0.255350	O	2.901324	3.662021	0.800647	O	-3.200470	-3.248987	0.102925				
H	-3.941235	-2.993076	0.500369	H	2.365822	4.079100	1.504668	H	-3.134806	-4.205419	0.227129				

H15-Abs

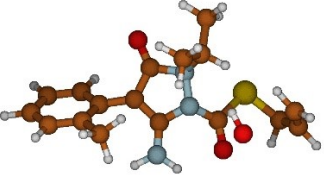
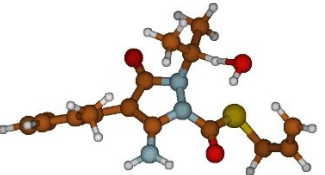
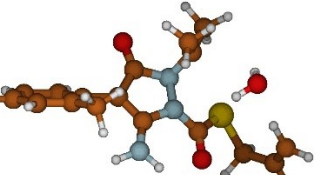
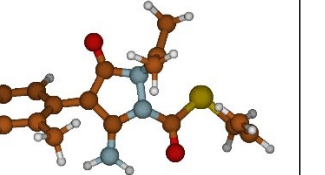
	MCR	TS	MCP	RAD
				
C	-2.998648 -2.114475 -0.694306	C -3.023388 -1.959990 -0.896618	C -3.295802 -0.476419 -1.576571	C -0.459140 -0.888314 0.206752
C	-2.693007 -0.872853 -0.113094	C -2.644208 -0.835303 -0.152520	C -2.667278 -0.577895 -0.335250	C -1.435498 0.028711 -0.140426
C	-3.729723 -0.081102 0.421097	C -3.616865 -0.129570 0.588230	C -3.435068 -0.938726 0.819362	C -0.769899 1.257985 -0.431926
C	-5.043285 -0.561124 0.340014	C -4.949832 -0.560308 0.529187	C -4.811782 -1.247339 0.630412	N 0.630769 1.079019 -0.245429
C	-5.338512 -1.792798 -0.238317	C -5.318582 -1.673324 -0.221139	C -5.409739 -1.151400 -0.613350	N 0.793177 -0.259600 0.172260
C	-4.308658 -2.579217 -0.755395	C -4.350449 -2.382953 -0.932326	C -4.656118 -0.751525 -1.725744	C -2.883508 -0.197357 -0.257786
C	-1.283134 -0.436579 -0.071000	C -1.227721 -0.414344 -0.144431	C -1.237654 -0.249482 -0.227080	C -3.523571 0.113423 -1.459015
C	-0.745041 0.757002 -0.620403	C -0.689390 0.757649 -0.737509	C -0.650067 0.979564 -0.639181	C -4.893579 -0.091752 -1.627534
N	0.660863 0.773837 -0.422030	N 0.715024 0.788064 -0.521477	N 0.750441 0.924902 -0.417566	C -5.648116 -0.635579 -0.578472
N	0.959069 -0.415475 0.275824	N 1.006652 -0.369397 0.231493	N 0.994821 -0.340802 0.156754	C -5.039427 -0.940821 0.625499
C	-0.219917 -1.144788 0.466395	C -0.171562 -1.096806 0.432308	C -0.209634 -1.048631 0.246802	C -3.651144 -0.708382 0.839087
O	-1.329187 1.695689 -1.193483	O -1.263795 1.677455 -1.347749	O -1.197974 2.009891 -1.068995	C -3.091069 -0.948092 2.112098
N	-0.213518 -2.334658 1.058632	N -0.175420 -2.265801 1.066251	N -0.249613 -2.306606 0.673559	O -1.244318 2.356689 -0.747721
C	2.189066 -1.040676 0.053650	C 2.247152 -0.990027 0.072526	C 2.213950 -0.974463 -0.093969	C 1.289359 2.037569 0.710136
O	2.493181 -2.054805 0.653430	O 2.542209 -1.974999 0.723814	O 2.474040 -2.051984 0.408695	C 1.589802 3.356552 0.016577
C	1.222953 1.981407 0.279763	C 1.240944 2.032657 0.145083	C 1.318744 2.035566 0.426689	C 1.955713 -0.940725 -0.191464
C	0.423389 2.324913 1.530027	C 0.382043 2.433755 1.338539	C 0.465170 2.287683 1.663894	S 3.079459 -0.010057 -1.196697
C	-3.475000 1.250518 1.078419	C -3.260318 1.044508 1.434928	C -2.888256 -0.938350 2.120714	C 4.457552 -1.191414 -1.205306
S	3.219408 -0.246499 -1.148199	S 3.306927 -0.235759 -1.129301	S 3.299658 -0.092965 -1.179963	C 5.257227 -1.290406 0.063639
C	4.714750 -1.248921 -0.915543	C 4.808595 -1.199269 -0.794359	C 4.760948 -1.155838 -1.006832	C 5.025465 -0.671084 1.219231
C	5.506183 -0.985463 0.334921	C 5.549277 -0.858257 0.468394	C 5.519723 -1.037184 0.285262	N -0.577236 -2.185352 0.477836
C	5.190448 -0.170676 1.339352	C 5.186709 0.004531 1.415306	C 5.197494 -0.307447 1.351184	O 2.150714 -2.087387 0.168277
C	1.361327 3.146827 -0.686995	C 1.409013 3.148629 -0.873321	C 1.544422 3.280375 -0.415898	C 0.478197 2.197864 1.990282
H	-5.845647 0.045076 0.753398	H -5.701118 -0.016271 1.095794	H -5.397170 -1.538571 1.498423	H -5.624047 -1.347422 1.446431
H	-6.366737 -2.138922 -0.280820	H -6.356575 -1.990295 -0.245182	H -6.465171 -1.379831 -0.725163	H -6.711346 -0.813044 -0.707876
H	-4.523572 -3.541565 -1.209184	H -4.626282 -3.255883 -1.515446	H -5.122067 -0.666940 -2.702010	H -5.366186 0.154694 -2.572746
H	-2.193884 -2.712460 -1.115707	H -2.264043 -2.500052 -1.456388	H -2.704478 -0.185278 -2.440686	H -2.931554 0.508899 -2.280134
H	-2.462300 1.316200 1.484890	H -2.240207 1.007899 1.823035	H -1.865966 -0.635344 2.313466	H -2.061093 -0.702577 2.341204

H	-4.188831	1.414436	1.889805	H	-3.978129	1.206050	2.242202	H	-3.508298	-1.215041	2.965754	H	-3.711787	-1.344421	2.907490
H	-3.600954	2.068635	0.359712	H	-3.318707	2.013060	0.812501	H	-3.306569	1.692644	1.324236	H	0.232258	-2.748186	0.701141
H	0.646900	-2.744698	1.396450	H	0.682933	-2.674245	1.411402	H	0.588493	-2.782393	0.979575	H	-1.489650	-2.617040	0.408338
H	-1.073055	-2.867278	1.092179	H	-1.030584	-2.807017	1.075109	H	-1.129957	-2.804909	0.639714	H	2.241079	1.559676	0.956144
H	2.227424	1.671982	0.579649	H	2.232869	1.746760	0.503979	H	2.294616	1.659164	0.743046	H	1.057925	2.775478	2.715294
H	0.954069	3.095276	2.096344	H	0.877172	3.242275	1.883214	H	0.986947	2.983596	2.326299	H	0.250806	1.223167	2.435434
H	0.305176	1.447676	2.175014	H	0.246234	1.592335	2.026493	H	0.290174	1.358090	2.216537	H	-0.460067	2.728799	1.801225
H	-0.566978	2.712718	1.272722	H	-0.601842	2.790531	1.015140	H	-0.500988	2.727839	1.396627	H	0.676771	3.911686	-0.206728
H	0.390507	3.561210	-0.968608	H	0.443993	3.522503	-1.221005	H	0.601228	3.740669	-0.715707	H	2.209791	3.965662	0.680492
H	1.939194	3.935388	-0.196817	H	1.947411	3.973745	-0.398539	H	2.107441	4.004902	0.179268	H	2.140414	3.190113	-0.913749
H	1.892138	2.841834	-1.593353	H	1.989922	2.807169	-1.734824	H	2.125560	3.043933	-1.311809	H	4.071142	-2.173182	-1.493411
H	4.438749	-2.305292	-0.980477	H	4.551536	-2.262107	-0.814112	H	4.459145	-2.192317	-1.182144	H	5.097420	-0.848847	-2.025365
H	5.323947	-1.025294	-1.797584	H	5.445559	-1.010243	-1.664758	H	5.402210	-0.865244	-1.845578	H	6.109792	-1.963614	-0.021901
H	6.431928	-1.558375	0.380415	H	6.480159	-1.413935	0.578102	H	6.425026	-1.643313	0.303946	H	5.681309	-0.829103	2.069605
H	5.850665	-0.070839	2.195118	H	5.813784	0.159411	2.287656	H	5.832092	-0.309025	2.231819	H	4.187349	0.008225	1.360903
H	4.277989	0.422016	1.347974	H	4.267420	0.583999	1.359508	H	4.304202	0.312877	1.386770				
O	-2.167737	4.153276	-0.310244	O	-3.218036	3.208724	-0.105022	O	-3.347793	2.482784	0.767347				
H	-1.821360	3.265084	-0.586057	H	-2.507661	2.767483	-0.630958	H	-2.661031	2.343026	0.088747				

H22-Abs															
MCR			TS			MCP			RAD						
															
C	-3.624818	-0.075868	-1.346962	C	3.633618	-0.422876	-1.301796	C	-3.525704	0.338483	-1.423361	C	-0.465202	-1.018116	0.321086
C	-2.829124	-0.283075	-0.210127	C	2.945779	0.104768	-0.170747	C	-2.932275	-0.081306	-0.211266	C	-1.428761	-0.034388	-0.103389
C	-3.439102	-0.549820	1.034784	C	3.671742	0.813813	0.836261	C	-3.727859	-0.678458	0.799102	C	-0.707180	1.216255	-0.332906
C	-4.835163	-0.657901	1.075958	C	5.032656	1.021476	0.627891	C	-5.084455	-0.875686	0.528534	N	0.631636	0.997283	-0.037670
C	-5.618186	-0.481558	-0.061139	C	5.681329	0.550022	-0.513308	C	-5.653192	-0.499389	-0.686087	N	0.795365	-0.340859	0.386686
C	-5.010201	-0.174971	-1.278387	C	4.979496	-0.183509	-1.479975	C	-4.871825	0.117959	-1.666497	C	-2.858537	-0.184235	-0.272859
C	-1.366428	-0.117390	-0.325552	C	1.543356	-0.136124	-0.102480	C	-1.514330	0.146461	-0.059219	C	-3.421193	0.333924	-1.459930
C	-0.733346	1.171231	-0.563296	C	0.886853	-1.388848	-0.511085	C	-0.835400	1.392270	-0.416061	C	-4.776072	0.199366	-1.719804

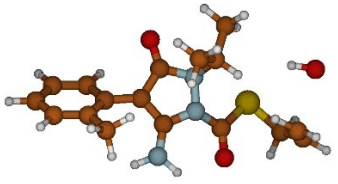
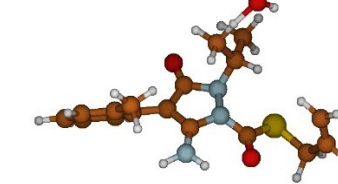
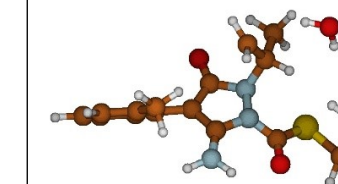
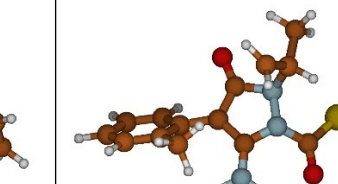
N	0.643429	1.060960	-0.272922	N	-0.485528	-1.263622	-0.262367	N	0.509247	1.245056	-0.109724	C	-5.594953	-0.430090	-0.778916
N	0.840960	-0.249293	0.219545	N	-0.690177	0.018186	0.288635	N	0.710318	-0.021549	0.485012	C	-5.053600	-0.903800	0.413639
C	-0.365408	-0.943710	0.224189	C	0.481369	0.730838	0.323030	C	-0.508895	-0.760538	0.432898	C	-3.689537	-0.793830	0.698857
O	-1.261371	2.221713	-0.912910	O	1.413479	-2.420899	-0.894839	O	-1.340200	2.436864	-0.820940	C	-3.190554	-1.252072	2.046612
N	-0.460958	-2.206607	0.581969	N	0.545095	2.019997	0.535109	N	-0.560646	-2.023777	0.658471	O	-1.177345	2.312088	-0.628937
C	2.055244	-0.900590	-0.058721	C	-1.948974	0.653651	0.121222	C	1.920172	-0.679385	0.179648	C	1.367447	1.998478	0.799783
O	2.268607	-2.014925	0.374848	O	-2.208529	1.630970	0.786738	O	2.267950	-1.656532	0.804879	C	1.718329	3.232295	-0.017475
C	1.232713	2.106615	0.634874	C	-1.158274	-2.363823	0.516893	C	1.240523	2.365313	0.561527	C	1.956068	-0.997500	-0.057390
C	0.364049	2.328433	1.866615	C	-0.347948	-2.737387	1.751040	C	0.476104	2.850201	1.788059	S	2.933936	-0.075952	-1.224454
C	-2.661966	-0.685102	2.320501	C	3.068113	1.247023	2.146226	C	-3.202225	-1.033951	2.167383	C	4.347103	-1.209388	-1.334660
S	3.177049	0.021540	-1.066196	S	-2.976007	-0.060064	-1.112632	S	2.833809	0.017351	-1.171221	C	5.294150	-1.208716	-0.167137
C	4.600367	-1.100855	-0.958736	C	-4.400423	1.054311	-0.931534	C	4.286340	-1.069637	-1.099794	C	5.164819	-0.548974	0.982041
C	5.348624	-1.100272	0.344866	C	-5.271089	0.828044	0.271634	C	5.260522	-0.807867	0.014504	N	-0.576032	-2.280554	0.515222
C	5.044562	-0.433337	1.456198	C	-5.084738	-0.049072	1.255189	C	5.143920	0.075280	1.003763	O	2.245051	-2.106856	0.334275
C	1.516421	3.379495	-0.146276	C	-1.456406	-3.540492	-0.397037	C	1.553812	3.474729	-0.431121	C	0.584286	2.316899	2.068117
H	-5.311443	-0.865404	2.030695	H	5.602884	1.540655	1.392704	H	-5.709029	-1.317507	1.300220	H	-5.704668	-1.354987	1.157588
H	-6.698373	-0.567502	0.006879	H	6.743069	0.736223	-0.640486	H	-6.710641	-0.671659	-0.861098	H	-6.659010	-0.535527	-0.966539
H	-5.609269	-0.015893	-2.169352	H	5.487617	-0.556657	-2.362233	H	-5.311428	0.424015	-2.609866	H	-5.192829	0.582698	-2.645158
H	-3.139858	0.153439	-2.289029	H	3.070793	-0.967695	-2.051181	H	-2.902896	0.805409	-2.179710	H	-2.770368	0.811199	-2.185926
H	-1.799028	-0.012366	2.348624	H	2.163360	0.690778	2.398950	H	-2.313007	-0.458407	2.433931	H	-2.272492	-0.740674	2.344514
H	-2.293336	-1.705963	2.465450	H	2.831858	2.316297	2.140542	H	-2.953874	-2.098277	2.236831	H	-3.000773	-2.330548	2.058538
H	-3.307217	-0.446521	3.168956	H	3.797255	1.086583	2.943736	H	-3.974021	-0.834526	2.914620	H	-3.953534	-1.051946	2.802737
H	0.341367	-2.717947	0.930415	H	-0.300488	2.586087	0.614019	H	0.730081	-3.328847	-0.099200	H	-1.545832	-2.558568	0.351013
H	-1.352767	-2.676722	0.471610	H	1.421942	2.503732	0.367159	H	-1.514293	-2.357363	0.506064	H	2.294719	1.487774	1.071165
H	2.187596	1.678663	0.950310	H	-2.106942	-1.924102	0.833968	H	2.183457	1.916438	0.883995	H	1.200592	2.935027	2.726342
H	0.885936	2.995559	2.557866	H	-0.939841	-3.414211	2.372435	H	1.094420	3.566052	2.336122	H	0.321228	1.398937	2.603524
H	0.171791	1.383352	2.385157	H	-0.106755	-1.849815	2.345327	H	0.241354	2.015047	2.455358	H	-0.331370	2.869448	1.837263
H	-0.592034	2.790070	1.601204	H	0.580229	-3.247317	1.477225	H	-0.453779	3.349619	1.500833	H	0.829265	3.816714	-0.261470
H	0.594620	3.884712	-0.440701	H	-0.540320	-4.041268	-0.716059	H	0.650231	4.006103	-0.735540	H	2.391168	3.858953	0.574375
H	2.091388	4.056510	0.491471	H	-2.067111	-4.258830	0.156361	H	2.228074	4.188222	0.050355	H	2.228767	2.956087	-0.944128
H	2.105756	3.163982	-1.041942	H	-2.014659	-3.218360	-1.280265	H	2.049802	3.076429	-1.320409	H	3.969222	-2.218959	-1.519938
H	4.265078	-2.110819	-1.210932	H	-4.030699	2.084225	-0.959564	H	3.941733	-2.107995	-1.073500	H	4.873498	-0.896007	-2.242277
H	5.258895	-0.771879	-1.769422	H	-4.976112	0.896398	-1.849418	H	4.777962	-0.922406	-2.067248	H	6.165702	-1.843463	-0.325143
H	6.230376	-1.740190	0.327650	H	-6.138869	1.486404	0.294151	H	6.143513	-1.444454	-0.034846	H	5.921876	-0.635772	1.755134
H	5.670947	-0.519756	2.338402	H	-5.792596	-0.114799	2.075281	H	5.922728	0.167941	1.754163	H	4.313757	0.095255	1.193251
H	4.175061	0.216605	1.530096	H	-4.234019	-0.726892	1.281425	H	4.281976	0.731858	1.101775				
O	-0.991196	-0.776474	-2.347860	O	-1.442027	3.722015	-1.266947	O	1.241203	-3.958091	-0.641765				
H	-0.070031	-1.082459	-2.289762	H	-2.062357	3.384094	-0.609778	H	2.141230	-3.606214	-0.619086				

H27-Abs			
MCR	TS	MCP	RAD

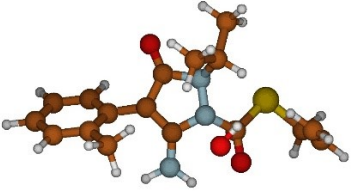
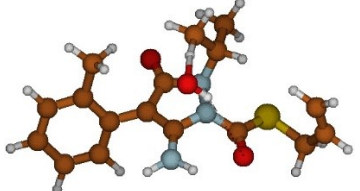
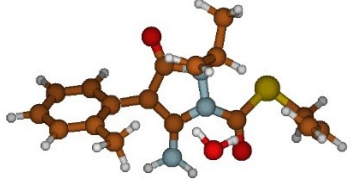
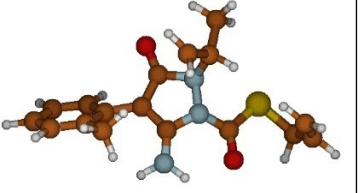
															
C	-3.033707	-0.148594	-0.319625	C	-3.591784	-0.412851	-1.527453	C	-3.083698	-0.267687	-0.260498	C	-0.826374	1.345543	-0.251577
C	-3.715618	-0.823127	0.714063	C	-2.997130	-0.334490	-0.258240	C	-3.803381	-0.574860	0.912720	C	-1.481212	0.080788	-0.209358
C	-5.103158	-0.982504	0.603861	C	-3.795618	-0.467206	0.896328	C	-5.183678	-0.791658	0.809204	C	-0.495781	-0.889731	-0.146200
C	-5.812404	-0.477498	-0.482647	C	-5.166309	-0.706816	0.733691	C	-5.849813	-0.691683	-0.409331	N	0.755268	-0.270036	-0.115687
C	-5.136477	0.210427	-1.491716	C	-5.747687	-0.795323	-0.528459	C	-5.137119	-0.362564	-1.563483	N	0.585611	1.125306	-0.242405
C	-3.757203	0.368736	-1.406023	C	-4.957022	-0.639231	-1.667925	C	-3.764110	-0.155477	-1.483574	C	-2.942423	-0.107596	-0.247924
C	-1.577461	0.072279	-0.275393	C	-1.549887	-0.068223	-0.176267	C	-1.632178	-0.014610	-0.238675	C	-3.632816	-0.808855	0.761912
C	-3.003346	-1.355180	1.930999	C	-0.894770	1.043013	-0.784526	C	-3.141046	-0.654565	2.264161	C	-5.024880	-0.929075	0.656670
H	-5.633104	-1.500424	1.399422	N	0.504304	0.970489	-0.482249	H	-5.743051	-1.027652	1.711103	C	-5.729648	-0.361337	-0.401181
H	-6.888444	-0.612110	-0.537033	N	0.673090	-0.191326	0.300625	H	-6.921390	-0.860255	-0.456343	C	-5.044498	0.352146	-1.386146
H	-5.678558	0.615836	-2.340334	C	-0.578071	-0.815365	0.461550	H	-5.645895	-0.272864	-2.518169	C	-3.661395	0.472652	-1.305521
H	-3.219518	0.893943	-2.191068	O	-1.365673	1.990330	-1.422217	H	-3.197404	0.091192	-2.377593	C	-2.927561	-1.410161	1.950394
H	-2.132876	-0.743255	2.185994	N	-0.689723	-1.976913	1.098657	H	-2.290429	0.029924	2.335760	N	-0.616806	-2.214825	-0.172968
H	-2.651742	-2.380906	1.772574	C	1.817545	-0.971935	0.054237	H	-2.770164	-1.664735	2.470098	C	1.950991	-0.874500	-0.468266
H	-3.680950	-1.371407	2.788003	O	2.038485	-1.971899	0.709242	H	-3.857173	-0.403402	3.050174	S	3.181089	0.218355	-1.128839
C	-0.574815	-0.873661	-0.176432	C	1.044890	2.183145	0.196878	C	-0.629915	-0.851000	0.220426	C	4.571308	-0.947671	-1.151965
N	0.666382	-0.223613	-0.156721	C	0.189431	2.635850	1.367069	N	0.611810	-0.212279	0.082202	C	5.177813	-1.265515	0.186886
N	0.470327	1.170073	-0.272925	C	-3.223212	-0.339125	2.284543	N	0.410620	1.040181	-0.543524	C	4.771872	-0.840731	1.381924
C	-0.943869	1.348425	-0.347619	S	2.839597	-0.400788	-1.272016	C	-1.004045	1.168360	-0.722018	C	1.353197	1.901786	0.699994
O	-1.448709	2.476878	-0.409030	C	4.051171	-1.757449	-1.275476	O	-1.489100	2.213150	-1.172582	C	1.751638	3.262310	0.257109
N	-0.665204	-2.201372	-0.157738	C	5.122579	-1.731157	-0.223601	N	-0.726428	-2.092929	0.686916	O	-1.290479	2.493026	-0.245162
H	0.165431	-2.778166	-0.141191	C	5.261290	-0.854259	0.768087	H	0.101271	-2.624635	0.921022	C	1.218018	1.556550	2.143858
H	-1.570559	-2.626918	-0.309607	C	1.393772	3.269517	-0.796320	H	-1.622969	-2.559565	0.632329	O	2.114345	-2.075049	-0.325753
C	1.146755	1.910906	0.851572	O	3.174998	1.748653	1.609517	C	1.023741	2.144208	0.168662	H	-5.561542	-1.467023	1.434268
C	0.409049	1.724146	2.172110	H	-5.786560	-0.808302	1.620762	C	0.480463	2.437157	1.528056	H	-6.809105	-0.466875	-0.451750
C	1.358362	3.369582	0.480022	H	-6.814224	-0.976044	-0.622116	C	1.599391	3.227331	-0.670262	H	-5.582549	0.806720	-2.212083
H	2.130656	1.441148	0.929374	H	-5.399149	-0.698323	-2.657546	H	3.303271	1.620010	1.685534	H	-3.116736	1.017591	-2.072149
H	1.008019	2.148879	2.982362	H	-2.964880	-0.300283	-2.408050	H	1.162949	3.082306	2.086577	H	-2.026966	-0.846833	2.211687
H	0.250367	0.661253	2.387907	H	-2.847587	-1.299948	2.653702	H	0.308933	1.520360	2.102864	H	-2.625490	-2.445156	1.754585
H	-0.560969	2.231729	2.160528	H	-3.993428	0.000386	2.981121	H	-0.483101	2.965793	1.444310	H	-3.593409	-1.423816	2.816639



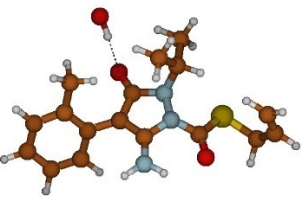
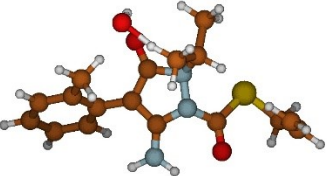
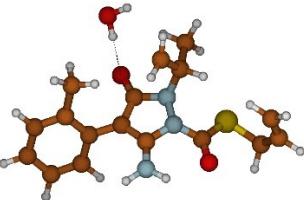
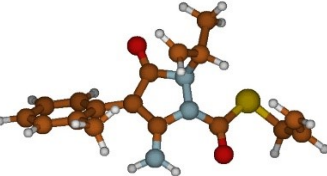
H	0.417652	3.922598	0.460189	H	-2.391329	0.371417	2.310727	H	0.829699	3.965074	-0.945796	H	0.196663	-2.813824	-0.129967
H	2.010460	3.826386	1.229868	H	0.125615	-2.446527	1.469692	H	2.373508	3.763454	-0.111133	H	-1.535464	-2.616045	-0.307914
H	1.842813	3.456152	-0.496789	H	-1.576378	-2.464256	1.067745	H	2.032255	2.831808	-1.592307	H	2.032712	2.005428	2.718111
C	1.828254	-0.796920	-0.662399	H	2.055815	1.849286	0.650524	C	1.787011	-0.917658	-0.190520	H	1.227231	0.474277	2.309263
O	2.038893	-1.992225	-0.558233	H	0.704992	3.433159	1.907874	O	1.976047	-2.026777	0.275230	H	0.270102	1.947308	2.549689
S	2.940614	0.337201	-1.454420	H	0.003726	1.808951	2.060310	S	2.933424	-0.082391	-1.252048	H	0.986605	4.012314	0.508481
C	4.359659	-0.786935	-1.595257	H	-0.771098	3.025756	1.012193	C	4.108959	-1.447531	-1.509984	H	2.675031	3.562647	0.764338
C	5.109398	-1.050387	-0.318451	H	0.488802	3.719970	-1.213316	C	5.122477	-1.710114	-0.434155	H	1.913632	3.294909	-0.823442
C	4.966550	-0.423586	0.850585	H	1.960084	4.050252	-0.280887	C	5.207967	-1.121948	0.756177	H	4.254314	-1.862948	-1.659277
H	4.017624	-1.723369	-2.041608	H	2.001445	2.871531	-1.613223	H	3.529244	-2.351259	-1.720303	H	5.314357	-0.466218	-1.796344
H	5.020161	-0.307906	-2.326526	H	3.499451	-2.701216	-1.236755	H	4.618788	-1.175894	-2.440377	H	6.040926	-1.927015	0.117855
H	5.855809	-1.838462	-0.413839	H	4.505264	-1.698471	-2.270333	H	5.841674	-2.481191	-0.709607	H	5.297783	-1.145041	2.281428
H	5.589846	-0.691571	1.697718	H	5.839778	-2.545006	-0.328970	H	5.991513	-1.400883	1.454138	H	3.915559	-0.180605	1.509099
H	4.253516	0.385967	0.993746	H	6.085489	-0.943738	1.469212	H	4.509734	-0.351822	1.073977				
O	2.857391	-1.340177	2.439410	H	4.569651	-0.027349	0.912049	O	3.240697	1.121378	2.512736				
H	2.403578	-0.492694	2.249632	H	2.799670	1.010380	2.131293	H	2.494637	0.521450	2.372851				

H28-Abs															
MCR				TS				MCP				RAD			
															
C	-0.945255	1.193250	-0.460594	C	-0.841785	0.776593	-1.007629	C	-0.929675	0.904179	-0.944546	C	-3.530329	0.071840	-1.506225
C	-1.685531	0.003476	-0.182716	C	-1.544903	-0.198124	-0.239744	C	-1.638992	-0.115698	-0.246035	C	-2.867765	-0.217946	-0.303753
C	-0.768796	-0.976044	0.147775	C	-0.596779	-0.958483	0.418732	C	-0.695432	-0.950122	0.323373	C	-3.605609	-0.669689	0.809878
N	0.521346	-0.426136	0.115622	N	0.680485	-0.468102	0.111701	N	0.584605	-0.469451	0.018314	C	-4.987428	-0.847391	0.665513
N	0.440697	0.924124	-0.286112	N	0.560927	0.605359	-0.796360	N	0.473269	0.677521	-0.797047	C	-5.636829	-0.570722	-0.535205
C	-3.151784	-0.113774	-0.271039	C	-3.011043	-0.341314	-0.200919	C	-3.106959	-0.221864	-0.172479	C	-4.905914	-0.099656	-1.626708
C	-3.932505	-0.543046	0.821825	C	-3.732723	-0.277872	1.008838	C	-3.790425	-0.209148	1.060664	C	-1.413534	0.005773	-0.223147
C	-5.322169	-0.618039	0.659005	C	-5.126555	-0.412016	0.960665	C	-5.188121	-0.302962	1.048460	C	-0.766779	1.254190	-0.455301
C	-5.937726	-0.264201	-0.538598	C	-5.802542	-0.585594	-0.244088	C	-5.903546	-0.387718	-0.143287	N	0.640447	1.091377	-0.262110

C	-5.162665	0.182657	-1.610069	C	-5.085964	-0.623410	-1.441314	C	-5.223992	-0.374946	-1.362334	N	0.814929	-0.262548	0.098406
C	-3.780546	0.253097	-1.471875	C	-3.700476	-0.503836	-1.413209	C	-3.835266	-0.293939	-1.370262	C	-0.428978	-0.908660	0.099526
C	-3.323324	-0.899411	2.153465	C	-3.056439	-0.051355	2.336543	C	-3.064553	-0.078334	2.374917	O	-1.255832	2.359106	-0.721782
N	-0.960557	-2.267570	0.408148	N	-0.761143	-2.032000	1.187192	N	-0.869224	-2.076410	1.009749	N	-0.534066	-2.214675	0.329971
C	1.639240	-1.167447	-0.264111	C	1.802030	-1.293621	0.039868	C	1.694790	-1.297980	-0.115284	C	1.997985	-0.908006	-0.254165
S	2.787650	-0.287595	-1.289968	S	2.944546	-0.885980	-1.251632	S	2.842244	-0.807727	-1.374679	O	2.198789	-2.069365	0.053183
C	4.183935	-1.441573	-1.200141	C	4.285846	-2.013384	-0.777161	C	4.198071	-1.935963	-0.946543	C	1.241267	2.016599	0.788065
C	4.956038	-1.444416	0.088817	C	5.089384	-1.619500	0.430680	C	4.982655	-1.589213	0.288362	C	0.400349	2.070115	2.018705
C	4.586469	-0.929973	1.265383	C	4.879822	-0.587863	1.245826	C	4.717496	-0.634817	1.178372	C	-2.952495	-0.939817	2.140856
C	1.174961	1.832232	0.663037	C	1.296546	1.825764	-0.312231	C	1.244120	1.845634	-0.206011	S	3.144816	0.091513	-1.163323
C	1.605371	3.104991	-0.047604	C	1.615066	2.754700	-1.471928	C	1.564568	2.868567	-1.283496	C	4.547365	-1.060595	-1.167659
O	-1.349798	2.324975	-0.757797	O	-1.278489	1.688566	-1.720425	O	-1.359187	1.892700	-1.552771	C	5.293101	-1.207248	0.129248
C	0.374583	2.084197	1.935116	C	0.535102	2.501829	0.814199	C	0.547247	2.423023	0.980505	C	4.995455	-0.656618	1.304290
O	1.786864	-2.321576	0.092673	O	1.954637	-2.215449	0.820612	O	1.840019	-2.276629	0.595482	C	1.516139	3.383237	0.179208
H	-5.928411	-0.946440	1.499615	H	-5.687518	-0.361733	1.890615	H	-5.720196	-0.291924	1.996459	H	-5.561607	-1.193968	1.521139
H	-7.017589	-0.327565	-0.632445	H	-6.884120	-0.680968	-0.249624	H	-6.987094	-0.453887	-0.121007	H	-6.710287	-0.713005	-0.615394
H	-5.630812	0.468809	-2.546750	H	-5.601661	-0.750044	-2.388091	H	-5.770876	-0.432370	-2.298256	H	-5.402375	0.127810	-2.564886
H	-3.166768	0.589422	-2.303366	H	-3.131502	-0.542383	-2.338377	H	-3.294520	-0.293068	-2.313049	H	-2.948926	0.428992	-2.352246
H	-2.415578	-0.320548	2.348112	H	-2.152254	0.555210	2.228481	H	-2.159793	0.529438	2.273112	H	-2.126554	-0.245407	2.327684
H	-3.055269	-1.960746	2.200936	H	-2.765440	-0.998339	2.804867	H	-2.762978	-1.056782	2.765379	H	-2.545007	-1.955784	2.189975
H	-4.037417	-0.707921	2.958041	H	-3.736646	0.456637	3.024373	H	-3.714456	0.385112	3.120999	H	-3.682086	-0.839828	2.947898
H	-0.177076	-2.883335	0.581224	H	0.035060	-2.526270	1.567256	H	-0.077590	-2.615683	1.333833	H	0.284665	-2.779095	0.512767
H	-1.884665	-2.657802	0.275751	H	-1.687434	-2.430701	1.270505	H	-1.804202	-2.454382	1.091843	H	-1.434383	-2.658158	0.200424
H	2.075668	1.272598	0.927749	H	2.237914	1.438049	0.085538	H	2.182565	1.388265	0.120636	H	2.198647	1.546393	1.027440
H	1.000711	2.618594	2.654650	H	1.232247	3.309180	1.286590	H	2.819074	3.180252	1.764957	H	0.490449	1.304510	2.780257
H	0.060281	1.139935	2.392739	H	0.294365	1.823151	1.637664	H	0.500413	1.863373	1.908380	H	-0.363187	2.833058	2.125790
H	-0.511830	2.693166	1.733415	H	-0.349025	3.049267	0.476119	H	-0.022026	3.341721	0.890672	H	0.591882	3.927858	-0.020399
H	0.748958	3.732405	-0.303318	H	0.713187	3.219013	-1.874310	H	0.670240	3.402229	-1.609573	H	2.114226	3.964329	0.886591
H	2.261916	3.672246	0.618559	H	2.280854	3.545615	-1.114445	H	2.271376	3.594869	-0.871414	H	2.080073	3.283349	-0.752454
H	2.159148	2.870611	-0.961630	H	2.124179	2.210542	-2.272209	H	2.027849	2.385399	-2.148014	H	4.195603	-2.034322	-1.520119
H	3.828370	-2.448808	-1.438662	H	3.868555	-3.016304	-0.649924	H	3.799061	-2.951958	-0.876306	H	5.214844	-0.664991	-1.940492
H	4.837439	-1.132241	-2.021767	H	4.930835	-2.047041	-1.661357	H	4.851986	-1.911393	-1.824247	H	6.165398	-1.855166	0.047327
H	5.918625	-1.948509	0.010633	H	5.924069	-2.292932	0.623477	H	5.853723	-2.227805	0.432326	H	5.617367	-0.845253	2.173719
H	5.240907	-1.010412	2.127473	H	5.536690	-0.413450	2.092182	H	5.363888	-0.486406	2.037726	H	4.135375	-0.004977	1.444320
H	3.629212	-0.437714	1.424431	H	4.061000	0.114600	1.104109	H	3.856984	0.025082	1.090102				
O	5.318237	1.447020	0.294774	O	2.240194	4.207670	1.771135	O	3.756629	2.987145	1.909693				
H	4.347165	1.573632	0.267232	H	2.923778	3.976405	1.111595	H	3.988517	2.364018	1.207706				

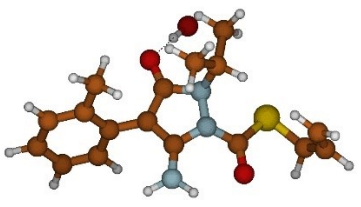
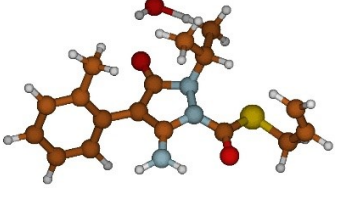
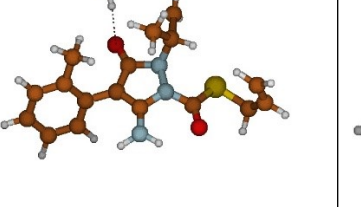
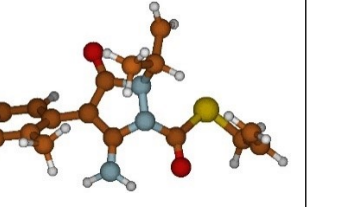
H29-Abs															
MCR				TS				MCP				RAD			
															
C	-2.948172	-0.123828	-0.383508	C	-5.613158	-1.130368	-0.159091	C	-0.863683	1.440491	-0.257625	C	-3.530026	0.072264	-1.506222
C	-3.659350	-0.803501	0.627052	C	-5.134522	0.049460	0.410060	C	-1.487806	0.169127	-0.398536	C	-2.867706	-0.217889	-0.303684
C	-5.044277	-0.955434	0.479593	C	-3.773548	0.371970	0.385953	C	-0.480992	-0.778498	-0.436949	C	-3.605794	-0.669991	0.809630
C	-5.722906	-0.438646	-0.620862	C	-2.883427	-0.519010	-0.248382	N	0.751954	-0.135553	-0.292276	C	-4.987588	-0.847675	0.664905
C	-5.018147	0.254372	-1.606488	C	-3.369560	-1.705855	-0.812685	N	0.555108	1.257895	-0.180656	C	-5.636730	-0.570629	-0.535851
C	-3.640933	0.405835	-1.483881	C	-4.726988	-2.017765	-0.767680	C	-2.942675	-0.059473	-0.433852	C	-4.905574	-0.099194	-1.627048
C	-1.492821	0.088740	-0.298647	C	-1.438376	-0.221357	-0.306345	C	-3.578795	-0.851252	0.545531	C	-1.413492	0.005815	-0.222776
C	-2.981417	-1.350126	1.857432	C	-0.827001	0.880857	-0.968869	C	-4.967000	-1.017625	0.467188	C	-0.766716	1.254273	-0.454838
H	-5.596961	-1.477453	1.256826	N	0.588190	0.805135	-0.781941	C	-5.719265	-0.406572	-0.533616	N	0.640424	1.091479	-0.261569
H	-6.797715	-0.568139	-0.704360	N	0.800219	-0.336345	0.020629	C	-5.088242	0.397294	-1.483642	N	0.814933	-0.262389	0.099147
H	-5.536199	0.669001	-2.465595	C	-0.427052	-0.956809	0.281427	C	-3.707552	0.564317	-1.430353	C	-0.428959	-0.908547	0.100072
H	-3.080827	0.934585	-2.250650	C	1.227157	2.032538	-0.196640	C	-2.810683	-1.493906	1.672680	O	-1.255798	2.359181	-0.721345
H	-2.107422	-0.752790	2.134495	C	1.488594	3.063252	-1.288261	N	-0.565507	-2.086953	-0.658245	N	-0.533935	-2.214602	0.330306
H	-2.641526	-2.380447	1.702865	C	2.001087	-1.034581	-0.059717	C	1.948894	-0.641581	-0.775226	C	1.997887	-0.907975	-0.253739
H	-3.677904	-1.359664	2.699281	O	2.220989	-1.987583	0.666858	S	3.134338	0.581490	-1.271850	O	2.198787	-2.069189	0.054033
C	-0.500683	-0.863236	-0.166300	O	-1.341949	1.812485	-1.600879	C	4.560861	-0.521680	-1.481548	C	1.241524	2.016904	0.788162
N	0.745972	-0.220185	-0.095421	N	-0.504456	-2.092005	0.971413	C	5.170599	-1.065565	-0.219340	C	0.400709	2.070961	2.018870
N	0.558541	1.173477	-0.217948	C	-3.276909	1.630579	1.047467	C	4.746190	-0.894829	1.031318	C	-2.953036	-0.940625	-2.140687
C	-0.848540	1.361709	-0.346658	C	0.429828	2.610708	0.956562	C	1.168498	1.795621	1.092526	S	3.144409	0.091182	-1.163628
O	-1.341978	2.493826	-0.425379	S	3.138653	-0.432122	-1.276926	C	1.427263	3.295181	0.949903	C	4.546712	-1.061212	-1.168108
N	-0.596812	-2.189745	-0.167180	C	4.579777	-1.428070	-0.800173	O	-1.371458	2.562767	-0.139662	C	5.292767	-1.207907	0.128612
H	0.224698	-2.771557	-0.073266	C	5.274920	-1.024902	0.470394	C	0.360651	1.456880	2.303374	C	4.996226	-0.656228	1.303435
H	-1.501096	-2.613601	-0.328505	C	4.892056	-0.103243	1.351765	O	2.146128	-1.843012	-0.838126	C	1.516581	3.383327	0.178901
C	1.208469	1.930971	0.910995	H	2.192772	1.692537	0.184874	H	-5.463785	-1.625842	1.218928	H	-5.561943	-1.194541	1.520297
C	0.364435	1.896150	2.180313	H	0.971551	3.426850	1.439206	H	-6.795162	-0.549474	-0.565141	H	-6.710169	-0.712896	-0.616324

C	1.556757	3.341340	0.463737	H	-0.581311	2.924487	0.681744	H	-5.665429	0.885967	-2.262348	H	-5.401839	0.128567	-2.565259
H	2.140525	1.390128	1.096647	H	0.291076	1.805848	1.795275	H	-3.203096	1.180070	-2.170368	H	-2.948449	0.429692	-2.352005
H	0.958403	2.276526	3.015968	H	2.037751	2.606202	-2.116391	H	-1.992439	-0.850979	2.015239	H	-2.126123	-0.247339	2.327352
H	0.055793	0.873218	2.419784	H	2.096482	3.870346	-0.871070	H	-2.370383	-2.450250	1.368469	H	-2.547063	-1.957189	2.190128
H	-0.528029	2.521094	2.080675	H	0.559187	3.489204	-1.669604	H	-3.474467	-1.692862	2.517237	H	-3.682496	-0.839381	2.947700
H	0.658935	3.937003	0.285870	H	-2.671010	-2.383677	-1.297583	H	0.252635	-2.678439	-0.603390	H	0.284635	-2.778814	0.514415
H	2.139786	3.825681	1.252271	H	-1.401197	-2.554555	1.044880	H	-1.477808	-2.495189	-0.815536	H	-1.434321	-2.658100	0.201359
H	2.157346	3.323811	-0.450031	H	0.323403	-2.528319	1.353968	H	2.137448	1.297746	1.166646	H	2.198842	1.546629	1.027625
C	1.910547	-0.791482	-0.613127	H	-5.826605	0.732098	0.896461	H	0.876652	1.213788	3.224847	H	0.490691	1.305573	2.780656
O	2.106268	-1.990925	-0.555655	H	-4.066327	2.083451	1.651552	H	0.395206	-1.097782	2.367984	H	-0.362964	2.833829	2.125544
S	3.048792	0.362648	-1.332042	H	-2.418793	1.418913	1.694793	H	-0.684776	1.743397	2.360587	H	0.592412	3.928115	-0.020653
C	4.462138	-0.762498	-1.512292	H	-2.947645	2.366544	0.306477	H	0.494585	3.859952	0.915201	H	2.114951	3.964462	0.886008
C	5.167383	-1.142187	-0.239648	H	-5.088004	-2.941083	-1.209647	H	2.007329	3.631515	1.813398	H	2.080293	3.283088	-0.752859
C	4.846266	-0.787663	1.003137	H	-6.674361	-1.357175	-0.120737	H	2.004361	3.495318	0.041874	H	4.194663	-2.034907	-1.520355
H	4.131050	-1.656775	-2.047318	H	4.277650	-2.478299	-0.755743	H	4.274792	-1.338225	-2.150416	H	5.214093	-0.665848	-1.941154
H	5.148839	-0.229378	-2.178197	H	5.264145	-1.329613	-1.649185	H	5.294232	0.087998	-2.019549	H	6.164422	-1.856696	0.046699
H	6.028541	-1.788584	-0.406814	H	6.188602	-1.590382	0.651540	H	6.056749	-1.672122	-0.404609	H	5.618403	-0.844875	2.172673
H	5.437883	-1.133161	1.845106	H	5.486784	0.089237	2.239197	H	5.279620	-1.349613	1.860090	H	4.136845	-0.003678	1.443463
H	3.998091	-0.143401	1.226349	H	3.987016	0.488678	1.228777	H	3.868551	-0.300197	1.277898				
O	1.328113	-1.371963	2.309648	O	0.361267	0.816175	2.837442	O	1.047261	-1.813734	2.403479				
H	1.961496	-0.633888	2.431118	H	1.132995	0.332147	2.479257	H	1.851877	-1.422078	2.034279				

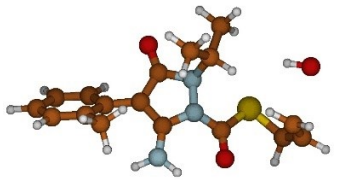
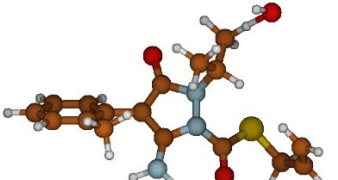
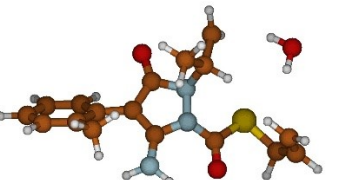
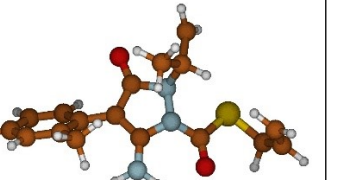
H30-Abs															
MCR			TS			MCP			RAD						
															
C	-5.339014	-1.792012	-0.238136	C	-5.413477	-1.675034	-0.235014	C	-5.359373	-1.784111	-0.217473	C	-0.393773	-0.924834	0.389509
C	-5.043470	-0.560373	0.340121	C	-5.097941	-0.428936	0.301159	C	-5.049574	-0.550557	0.349926	C	-1.404348	-0.165134	-0.166995
C	-3.729787	-0.080663	0.421152	C	-3.776076	0.028763	0.369848	C	-3.732402	-0.078265	0.411977	C	-0.795598	0.989272	-0.736698
C	-2.693265	-0.872714	-0.113006	C	-2.752853	-0.800493	-0.131680	C	-2.707246	-0.880335	-0.129567	N	0.616339	0.922378	-0.523124

C	-2.999233	-2.114295	-0.694115	C	-3.078171	-2.056505	-0.668387	C	-3.027255	-2.123210	-0.699546	N	0.830759	-0.268178	0.205140
C	-4.309359	-2.578713	-0.755175	C	-4.396799	-2.498594	-0.718929	C	-4.341042	-2.580021	-0.742251	C	-2.846582	-0.481309	-0.160609
C	-1.283319	-0.436716	-0.071026	C	-1.335141	-0.389881	-0.092691	C	-1.294159	-0.454518	-0.098326	C	-3.760508	0.356761	0.511528
C	-0.745151	0.756895	-0.620240	C	-0.759708	0.760032	-0.701182	C	-0.749625	0.739576	-0.644872	C	-5.118076	0.020529	0.482169
N	0.660703	0.773563	-0.421936	N	0.645416	0.739770	-0.487243	N	0.660612	0.742934	-0.442220	C	-5.570995	-1.123290	-0.174975
N	0.958862	-0.415800	0.275793	N	0.898774	-0.395588	0.310973	N	0.945975	-0.440878	0.271032	C	-4.661783	-1.959618	-0.820490
C	-0.220127	-1.145137	0.466207	C	-0.304101	-1.084316	0.514876	C	-0.239672	-1.164066	0.451185	C	-3.307241	-1.632210	-0.813625
C	1.223251	1.981089	0.279503	C	1.275235	1.978000	0.074222	C	1.221921	1.959970	0.243082	C	-3.293523	1.570671	1.271625
C	1.361928	3.146243	-0.687540	C	1.539265	2.990346	-1.029510	C	1.445898	3.082619	-0.761330	O	-1.311775	1.955932	-1.312185
C	2.189010	-1.040868	0.054105	C	2.110224	-1.078270	0.148810	C	2.175723	-1.072924	0.068278	C	1.206172	2.130309	0.188943
O	2.493255	-2.054583	0.654478	O	2.382792	-2.037089	0.845651	O	2.469867	-2.082125	0.681117	C	0.361754	2.565940	1.338224
O	-1.329368	1.695721	-1.193123	O	-1.307926	1.686985	-1.322343	O	-1.322489	1.687700	-1.206616	C	2.031766	-0.956160	0.042453
N	-0.213562	-2.335837	1.056609	N	-0.341323	-2.235610	1.179802	N	-0.243344	-2.351059	1.050025	S	3.162796	-0.217548	-1.105130
C	-3.474749	1.250932	1.078420	C	-3.489625	1.377853	0.974561	C	-3.458277	1.257194	1.053361	C	4.591243	-1.291921	-0.788094
C	0.424042	2.325092	1.529858	C	0.504468	2.543886	1.253060	C	0.399684	2.354968	1.422989	C	5.328613	-1.059041	0.500904
S	3.219207	-0.247325	-1.148314	S	3.160244	-0.443850	-1.127741	S	3.223391	-0.291591	-1.127339	C	4.999592	-0.226423	1.486237
C	4.714613	-1.249543	-0.915199	C	4.615625	-1.479665	-0.805051	C	4.715224	-1.290851	-0.860945	N	-0.466795	-2.105026	1.001312
C	5.506157	-0.985323	0.335032	C	5.438526	-1.116143	0.398949	C	5.487784	-1.011703	0.397890	C	1.483525	3.236816	-0.816433
C	5.190930	-0.169317	1.338633	C	5.180521	-0.177174	1.306796	C	5.159425	-0.181510	1.385500	O	2.258144	-1.982481	0.657707
H	2.227648	1.671398	0.579329	H	2.244097	1.640626	0.457118	H	2.211987	1.634244	0.592259	H	2.163783	1.761108	0.568852
H	0.955066	3.095448	2.095861	H	1.117879	3.244257	1.824762	H	0.488427	3.363216	1.811046	H	-0.250672	3.457578	1.266050
H	-0.566284	2.713084	1.272709	H	-0.395406	3.198942	0.889670	H	-1.064603	4.590441	0.257187	H	0.324257	1.971586	2.243975
H	0.305758	1.448030	2.175071	H	0.082373	1.776271	1.909009	H	-0.023731	1.588750	2.065251	H	2.067311	2.854846	-1.658291
H	1.892425	2.840841	-1.593942	H	2.161511	2.548892	-1.812524	H	2.083239	2.737935	-1.580064	H	2.060886	4.021961	-0.320462
H	1.940213	3.934687	-0.197663	H	2.070490	3.845131	-0.601515	H	1.949155	3.909243	-0.252349	H	0.558413	3.675178	-1.194734
H	0.391246	3.560988	-0.969075	H	0.608410	3.348115	-1.472549	H	0.504535	3.449318	-1.173067	H	-2.590492	-2.269060	-1.326691
H	-2.194637	-2.712512	-1.115499	H	-2.281518	-2.684607	-1.060461	H	-2.230958	-2.728994	-1.125921	H	-1.352555	-2.593935	1.005292
H	-1.074252	-2.866262	1.094725	H	-1.214292	-2.745316	1.220779	H	-1.105393	-2.879767	1.078918	H	0.366577	-2.570457	1.334410
H	0.645492	-2.743156	1.401043	H	0.498162	-2.640583	1.571848	H	0.611395	-2.760420	1.402642	H	-5.828340	0.662491	0.996940
H	-5.845658	0.046053	0.753509	H	-5.890511	0.205788	0.689765	H	-5.843242	0.062804	0.769414	H	-4.111991	1.991887	1.859713
H	-4.188906	1.415329	1.889429	H	-4.236547	1.620313	1.734749	H	-4.190848	1.457056	1.839514	H	-2.472765	1.313926	1.950080
H	-2.462228	1.316230	1.485387	H	-2.497341	1.412310	1.434269	H	-2.455840	1.301481	1.489160	H	-2.920711	2.347716	0.596177
H	-3.599939	2.068993	0.359508	H	-3.524842	2.162020	0.211147	H	-3.531500	2.064232	0.317114	H	-5.002399	-2.854776	-1.331303
H	-4.524510	-3.541024	-1.208929	H	-4.628110	-3.472735	-1.138197	H	-4.567416	-3.543794	-1.187375	H	-6.630282	-1.361956	-0.176368
H	-6.367313	-2.137922	-0.280590	H	-6.447752	-2.003615	-0.269660	H	-6.390135	-2.124162	-0.245060	H	4.264676	-2.333269	-0.860306
H	4.438706	-2.305969	-0.979552	H	4.291776	-2.522666	-0.747915	H	4.440140	-2.347941	-0.917001	H	5.256783	-1.108467	-1.637816
H	5.323713	-1.026329	-1.797421	H	5.218764	-1.383390	-1.713647	H	5.337461	-1.077845	-1.736469	H	6.223633	-1.673355	0.595354
H	6.431576	-1.558718	0.381069	H	6.336319	-1.725488	0.498839	H	6.411264	-1.586083	0.465587	H	5.618560	-0.153528	2.374937
H	5.851251	-0.068958	2.194258	H	5.859560	-0.014246	2.137769	H	5.807094	-0.071161	2.249516	H	4.116074	0.407334	1.446748
H	4.278785	0.423860	1.346700	H	4.298586	0.458058	1.258090	H	4.248810	0.413861	1.372082				
O	-2.166647	4.153471	-0.310301	O	-1.404362	4.019722	0.306055	O	-1.898129	4.252866	-0.096515				
H	-1.820169	3.265288	-0.586159	H	-1.579436	3.353363	-0.396148	H	-1.683008	3.355005	-0.409966				



H31-Abs															
MCR				TS				MCP				RAD			
															
C	-0.399416	-1.164636	0.327624	C	-5.510063	-1.460989	-0.268148	C	-5.389639	-1.691031	-0.205897	C	-0.384820	-0.898432	0.422903
C	-1.408254	-0.286892	-0.036201	C	-5.100915	-0.347448	0.464770	C	-5.017800	-0.533109	0.476694	C	-1.395713	-0.155476	-0.157332
C	-0.787279	0.955240	-0.321432	C	-3.753226	0.019146	0.546809	C	-3.684710	-0.112514	0.530503	C	-0.785684	0.976552	-0.770318
N	0.613563	0.839853	-0.120525	C	-2.803539	-0.757879	-0.148536	C	-2.711414	-0.880986	-0.141299	N	0.625068	0.908648	-0.558463
N	0.825343	-0.489283	0.300869	C	-3.220290	-1.879285	-0.878461	C	-3.090509	-2.046326	-0.820947	N	0.840606	-0.252302	0.213415
C	-2.847420	-0.599351	-0.143259	C	-4.565565	-2.236837	-0.938292	C	-4.421553	-2.457143	-0.852984	C	-2.836077	-0.482020	-0.150641
C	-3.791955	0.071883	0.660006	C	-1.369606	-0.408840	-0.106725	C	-1.291653	-0.475506	-0.125815	C	-3.764059	0.370455	0.482503
C	-5.144111	-0.254776	0.510441	C	-0.782893	0.795408	-0.579291	C	-0.752713	0.726985	-0.656608	C	-5.117961	0.019524	0.454744
C	-5.562062	-1.231002	-0.393333	N	0.623838	0.744392	-0.367502	N	0.656527	0.734448	-0.450836	C	-5.554370	-1.151250	-0.164707
C	-4.622508	-1.905818	-1.171204	N	0.868135	-0.499075	0.254872	N	0.948788	-0.463961	0.231899	C	-4.631554	-2.000635	-0.772926
C	-3.272795	-1.583969	-1.045415	C	-0.341638	-1.192822	0.386398	C	-0.232812	-1.196040	0.399530	C	-3.280403	-1.659866	-0.766349
C	-3.365573	1.098660	1.676089	C	1.221865	1.877409	0.418045	C	1.190712	1.937276	0.273526	C	-3.316535	1.617553	1.198482
O	-1.300257	2.035040	-0.679123	C	1.528392	3.064546	-0.469596	C	1.311245	3.076345	-0.671772	O	-1.298882	1.923959	-1.380813
C	1.225682	1.826689	0.840850	C	2.076486	-1.154756	0.006250	C	2.185242	-1.078124	0.021961	C	1.219282	2.134112	0.088189
C	0.396722	1.955045	2.112879	O	2.332670	-2.218267	0.539327	O	2.483342	-2.102656	0.607090	C	0.418484	2.587561	1.305060
C	2.020842	-1.126221	-0.042365	O	-1.324856	1.786472	-1.095720	O	-1.329499	1.678133	-1.209578	C	2.039500	-0.949959	0.070616
S	3.116887	-0.158812	-1.041829	N	-0.388945	-2.420210	0.895989	N	-0.232309	-2.399957	0.964026	S	3.153027	-0.280347	-1.134840
C	4.546375	-1.277136	-1.013938	C	-3.337859	1.201473	1.382647	C	-3.306633	1.117047	1.314240	C	4.590600	-1.324744	-0.763844
C	5.325815	-1.327923	0.270375	C	0.387162	2.226641	1.644402	C	0.379080	2.261484	1.526675	C	5.340246	-0.998367	0.497525
C	5.048057	-0.706449	1.414592	S	3.156862	-0.319984	-1.122039	S	3.236280	-0.250870	-1.139844	C	5.025833	-0.089427	1.418201
N	-0.480204	-2.455178	0.633998	C	4.613662	-1.385096	-0.926160	C	4.738795	-1.235628	-0.879718	N	-0.458599	-2.058744	1.071239
C	1.477337	3.160820	0.156685	C	5.383817	-1.229597	0.355268	C	5.488521	-0.981296	0.398108	C	1.392869	3.191395	-0.938645
O	2.253114	-2.261208	0.329182	C	5.069853	-0.472387	1.404347	C	5.132574	-0.185481	1.404370	O	2.272108	-1.941663	0.737532
O	0.125801	3.319663	-2.597723	H	2.187708	1.488182	0.755611	H	2.197686	1.632791	0.595202	H	2.207915	1.797866	0.431690
H	2.193869	1.386681	1.092160	H	0.922599	2.966490	2.245570	H	0.880344	3.060140	2.079940	H	0.973784	3.371297	1.826986

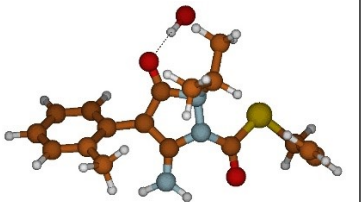
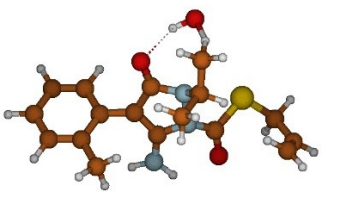
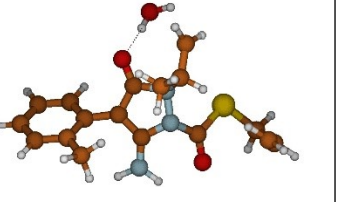
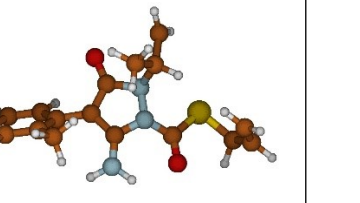
H	0.950552	2.549062	2.844918	H	-0.578666	2.652248	1.355429	H	-0.629651	2.599081	1.270239	H	-0.553970	2.991979	1.008438
H	-0.555211	2.457869	1.913406	H	0.216833	1.338826	2.261842	H	0.308596	1.383850	2.177309	H	0.263766	1.755872	1.999842
H	0.194917	0.972742	2.553314	H	1.901067	2.784675	-1.457158	H	1.547608	2.897101	-1.713923	H	1.822381	2.945487	-1.902733
H	2.008892	3.023351	-0.790377	H	2.222042	3.744519	0.031136	H	1.441651	4.071793	-0.263985	H	1.222991	4.228795	-0.678257
H	2.099877	3.774758	0.813800	H	0.584228	3.726576	-0.650473	H	-1.004278	4.665239	0.066126	H	-2.553564	-2.307639	-1.250798
H	0.546235	3.702519	-0.026605	H	-2.476704	-2.467733	-1.410871	H	-2.329171	-2.627495	-1.335968	H	-1.345569	-2.544772	1.096226
H	-2.532708	-2.092508	-1.658794	H	-1.266104	-2.923935	0.868010	H	-1.089577	-2.937531	0.963554	H	0.373278	-2.510233	1.426715
H	-1.373286	-2.921750	0.540128	H	0.452673	-2.891323	1.199456	H	0.626818	-2.822440	1.289541	H	-5.838488	0.672615	0.940428
H	0.345899	-2.988906	0.868754	H	-5.838719	0.246475	0.998133	H	-5.773664	0.053968	0.992020	H	-4.140062	2.043997	1.775622
H	-5.878581	0.259079	1.125260	H	-4.169744	1.541485	2.003553	H	-4.154566	1.468603	1.906382	H	-2.488168	1.399704	1.880908
H	-4.198982	1.355197	2.333930	H	-2.497945	0.942402	2.035788	H	-2.472140	0.906082	1.991501	H	-2.962426	2.377149	0.493956
H	-2.540177	0.722001	2.289266	H	-3.012850	2.039277	0.756569	H	-2.988046	1.930908	0.654101	H	-4.959099	-2.916512	-1.254717
H	-3.015940	2.016946	1.193187	H	-4.871776	-3.108035	-1.508773	H	-4.698698	-3.362008	-1.384649	H	-6.611210	-1.400481	-0.165980
H	-4.936167	-2.670405	-1.874885	H	-6.562834	-1.723637	-0.309681	H	-6.431753	-1.995225	-0.226406	H	4.268512	-2.369785	-0.759152
H	-6.618106	-1.466823	-0.483971	H	4.304694	-2.424986	-1.065309	H	4.480549	-2.294666	-0.969233	H	5.245263	-1.197924	-1.632234
H	4.209834	-2.277867	-1.299091	H	5.249474	-1.125711	-1.779087	H	5.370399	-0.989050	-1.739573	H	6.232984	-1.608715	0.631246
H	5.185399	-0.913226	-1.825451	H	6.289865	-1.834266	0.382468	H	6.419533	-1.543663	0.463582	H	5.654261	0.047732	2.292548
H	6.207639	-1.964925	0.207367	H	5.712162	-0.450200	2.279094	H	5.765203	-0.090933	2.281314	H	4.145841	0.545697	1.338843
H	5.695428	-0.827329	2.277452	H	4.176272	0.147968	1.431958	H	4.213139	0.396339	1.394093				
H	4.179787	-0.061881	1.535279	O	-0.636516	4.447699	-0.796198	O	-1.742039	4.373613	-0.485544				
H	-0.416303	2.865719	-1.893226	H	-1.119513	3.595351	-0.895790	H	-1.526336	3.448887	-0.708420				

H32-Abs															
MCR				TS				MCP				RAD			
															
C	-3.151767	-0.113698	-0.271130	C	-0.826105	0.987467	-0.707722	C	-3.136528	-0.095711	-0.265668	C	-0.755400	1.258837	-0.462154
C	-3.932531	-0.542591	0.821861	C	-1.586289	-0.110395	-0.206619	C	-3.914818	-0.469541	0.848964	C	-1.403891	0.016516	-0.196492
C	-5.322174	-0.617766	0.658972	C	-0.685168	-1.035240	0.287439	C	-5.306798	-0.527396	0.700018	C	-0.418482	-0.891497	0.144710
C	-5.937665	-0.264456	-0.538827	N	0.617242	-0.533760	0.141370	C	-5.926329	-0.208944	-0.505462	N	0.826699	-0.246563	0.129907
C	-5.162569	0.182055	-1.610409	N	0.558396	0.719262	-0.504489	C	-5.153133	0.184400	-1.598990	N	0.648386	1.094466	-0.268547

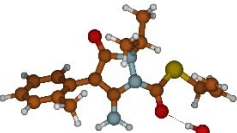
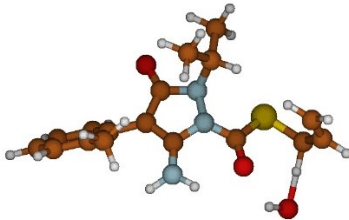
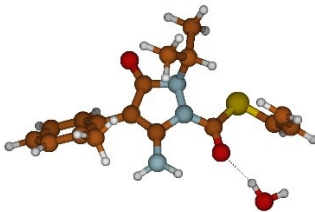
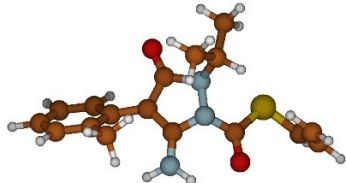


C	-3.780459	0.252667	-1.472143	C	-3.056465	-0.202873	-0.247097	C	-3.768884	0.236627	-1.474492	C	-2.856107	-0.214192	-0.297660
C	-1.685519	0.003589	-0.182701	C	-3.823008	-0.396951	0.920573	C	-1.667626	-0.003294	-0.193611	C	-3.613655	-0.678759	0.797168
C	-3.323374	-0.898375	2.153663	C	-5.217185	-0.462464	0.798980	C	-3.299259	-0.784411	2.188066	C	-4.991987	-0.861136	0.623968
H	-5.928454	-0.945886	1.499663	C	-5.850376	-0.322096	-0.433099	H	-5.911243	-0.813422	1.557223	C	-5.619713	-0.578442	-0.586254
H	-7.017514	-0.327958	-0.632743	C	-5.088856	-0.105227	-1.582516	H	-7.007813	-0.257992	-0.588552	C	-4.869462	-0.096177	-1.659927
H	-5.630682	0.467799	-2.547231	C	-3.702541	-0.049286	-1.484169	H	-5.624432	0.442882	-2.542099	C	-3.497806	0.080653	-1.511070
H	-3.166647	0.588730	-2.303714	C	-3.191711	-0.513078	2.284065	H	-3.156605	0.530586	-2.322972	C	-2.991629	-0.962057	2.140409
H	-2.415990	-0.318947	2.348341	N	-0.906924	-2.251085	0.780099	H	-2.385014	-0.207031	2.355476	N	-0.521895	-2.192998	0.400457
H	-3.054672	-1.959537	2.201367	C	1.709940	-1.366548	-0.104791	H	-3.039516	-1.845625	2.270924	C	2.004841	-0.902467	-0.226792
H	-4.037710	-0.707167	2.958087	S	2.887122	-0.728446	-1.265115	H	-4.005652	-0.558377	2.990412	S	3.129073	0.065959	-1.196148
C	-0.768946	-0.975961	0.148126	C	4.166163	-1.999738	-1.058957	C	-0.767020	-0.988930	0.166706	C	4.534581	-1.082381	-1.185704
N	0.521283	-0.426201	0.115932	C	4.977055	-1.926967	0.204647	N	0.534009	-0.468626	0.104261	C	5.304451	-1.179521	0.101771
N	0.440800	0.924018	-0.286059	C	4.821647	-1.081630	1.221433	N	0.476391	0.864287	-0.351484	C	5.033093	-0.577155	1.257727
C	-0.945102	1.193236	-0.460729	C	1.306736	1.773276	0.261205	C	-0.907806	1.158944	-0.521489	C	1.255146	2.056419	0.722152
O	-1.349522	2.324910	-0.758272	C	1.631094	2.934265	-0.657705	O	-1.288406	2.290428	-0.849396	C	1.441647	3.376112	0.070179
N	-0.960793	-2.267400	0.408848	O	-1.206012	2.058066	-1.199081	N	-0.986056	-2.263835	0.478726	O	-1.239875	2.359209	-0.756908
H	-0.177280	-2.883129	0.581934	C	0.567890	2.188687	1.526905	H	-0.214515	-2.890475	0.666212	C	0.455473	2.117360	2.019763
H	-1.884894	-2.657649	0.276434	O	1.814294	-2.444851	0.450597	H	-1.920223	-2.637164	0.369823	O	2.213266	-2.051987	0.115841
C	1.175068	1.832177	0.663062	H	-5.812228	-0.610552	1.696721	C	1.209122	1.806254	0.566974	H	-5.580649	-1.217258	1.465791
C	0.374299	2.084962	1.934759	H	-6.933291	-0.371522	-0.494547	C	0.461147	2.029236	1.877318	H	-6.690763	-0.724854	-0.688195
C	1.606306	3.104481	-0.047891	H	-5.570721	0.014333	-2.547856	C	1.520261	3.059072	-0.168470	H	-5.348230	0.135585	-2.606206
H	2.075364	1.272193	0.928456	H	-3.099516	0.108570	-2.374444	H	2.147115	1.278287	0.793090	H	-2.902122	0.446065	-2.343490
H	1.000439	2.619293	2.654330	H	-2.273593	0.078321	2.352354	H	1.094236	2.606430	2.556366	H	-2.134424	-0.309445	2.331600
H	0.059412	1.141006	2.392613	H	-2.933429	-1.551552	2.519733	H	0.227242	1.073088	2.355853	H	-2.640637	-1.997837	2.209237
H	-0.511763	2.694275	1.732546	H	-3.887008	-0.166934	3.052491	H	-0.467047	2.584835	1.714143	H	-3.726400	-0.813835	2.935417
H	0.750214	3.732018	-0.304400	H	-0.139239	-2.843913	1.065985	H	1.407888	4.019345	0.319863	H	0.298222	-2.752534	0.592304
H	2.262595	3.671886	0.618388	H	-1.844486	-2.628876	0.735994	H	3.911965	2.927808	0.169842	H	-1.419247	-2.642536	0.271633
H	2.160550	2.869525	-0.961488	H	2.248177	1.291273	0.538796	H	1.857871	3.016067	-1.197689	H	2.239298	1.619340	0.943186
C	1.639135	-1.167637	-0.263676	H	1.206936	2.847498	2.121593	C	1.636059	-1.248486	-0.245479	H	1.006542	2.713309	2.751914
O	1.786707	-2.321722	0.093309	H	0.320802	1.314109	2.137545	O	1.744748	-2.396943	0.143411	H	0.310896	1.114620	2.433959
S	2.787467	-0.287981	-1.289707	H	-0.353761	2.728092	1.287167	S	2.822739	-0.429816	-1.276864	H	-0.521826	2.583198	1.860915
C	4.183714	-1.442011	-1.200001	H	0.801278	3.625479	-0.809113	C	4.147422	-1.666882	-1.189385	H	1.240434	4.285976	0.621826
C	4.955999	-1.444778	0.088849	H	2.469726	3.548775	-0.138798	C	4.912273	-1.731397	0.103227	H	1.889862	3.435340	-0.914697
C	4.586882	-0.929670	1.265260	H	2.066250	2.615996	-1.608371	C	4.632325	-1.112292	1.248775	H	4.179308	-2.069098	-1.495868
H	3.828122	-2.449260	-1.438410	H	3.697852	-2.982866	-1.159402	H	3.728648	-2.646559	-1.437793	H	5.186325	-0.713634	-1.984831
H	4.837091	-1.132694	-2.021737	H	4.817131	-1.867392	-1.929478	H	4.821198	-1.393182	-2.007506	H	6.171991	-1.835001	0.030228
H	5.918318	-1.949388	0.010698	H	5.767363	-2.676055	0.246543	H	5.783116	-2.384146	0.049576	H	5.671435	-0.731894	2.121913
H	5.241415	-1.010055	2.127283	H	5.477628	-1.132216	2.084771	H	5.267852	-1.249479	2.117974	H	4.178772	0.084351	1.386781
H	3.629888	-0.436881	1.424235	H	4.047639	-0.316941	1.233171	H	3.768705	-0.460149	1.370613				
O	5.317733	1.447518	0.293751	O	3.411954	4.235685	0.716885	O	4.769678	2.525024	0.370312				
H	4.346567	1.573600	0.267045	H	2.772729	4.432177	1.429497	H	4.551393	1.646997	0.711892				



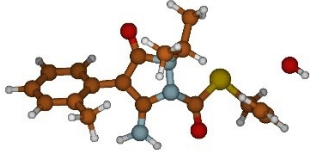
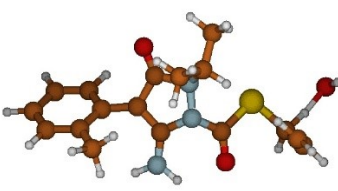
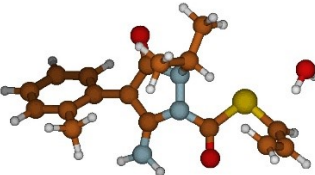
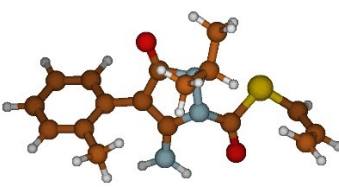
H33-Abs															
MCR				TS				MCP				RAD			
															
C	-2.875545	-0.314133	-0.280280	C	-0.769726	1.147187	-0.090487	C	-2.856480	-0.335521	-0.282297	C	-0.755414	1.258162	-0.463147
C	-3.649525	-1.080735	0.614593	C	-1.453593	-0.099332	-0.136123	C	-3.622356	-1.164879	0.562218	C	-1.403791	0.015989	-0.196661
C	-5.026559	-1.187365	0.380535	C	-0.492654	-1.090144	-0.025134	C	-4.998790	-1.269001	0.322704	C	-0.418357	-0.891648	0.145402
C	-5.636627	-0.544515	-0.693441	N	0.766767	-0.493815	0.126458	C	-5.616325	-0.564302	-0.707102	N	0.826785	-0.246561	0.130469
C	-4.869380	0.231663	-1.563399	N	0.622407	0.907347	0.089295	C	-4.857496	0.273762	-1.525678	N	0.648374	1.094179	-0.268961
C	-3.498492	0.340543	-1.354406	C	-2.908730	-0.260539	-0.304419	C	-3.487505	0.381549	-1.311166	C	-2.855987	-0.214858	-0.297875
C	-1.422955	-0.140205	-0.098887	C	-3.689222	-0.961146	0.637971	C	-1.404950	-0.159475	-0.093959	C	-3.613678	-0.677671	0.797623
C	-3.043730	-1.764887	1.813077	C	-5.068650	-1.061810	0.416235	C	-3.010927	-1.918620	1.715260	C	-4.991987	-0.860123	0.624598
H	-5.628425	-1.775697	1.068639	C	-5.674674	-0.475074	-0.691851	H	-5.594390	-1.905667	0.972226	C	-5.619559	-0.579147	-0.586145
H	-6.707355	-0.641316	-0.845472	C	-4.900827	0.237213	-1.609247	H	-6.686302	-0.661226	-0.864248	C	-4.869175	-0.098607	-1.660463
H	-5.334172	0.743697	-2.400083	C	-3.527338	0.338610	-1.412731	H	-5.328233	0.834564	-2.327026	C	-3.497476	0.078285	-1.511755
H	-2.889605	0.934258	-2.031102	C	-3.086323	-1.579895	1.872907	H	-2.884953	1.023158	-1.948764	C	-2.991449	-0.958650	2.141231
H	-2.201150	-1.194851	2.216301	N	-0.629253	-2.409519	-0.107893	H	-2.157830	-1.380414	2.139306	N	-0.521682	-2.192941	0.402336
H	-2.674588	-2.765013	1.559814	C	1.931541	-1.066405	-0.386488	H	-2.656582	-2.907833	1.404526	C	2.005021	-0.902464	-0.226138
H	-3.792718	-1.882746	2.599751	S	3.081330	0.087541	-1.083322	H	-3.752843	-2.070630	2.502839	S	3.128967	0.065726	-1.196027
C	-0.443570	-1.119131	-0.039004	C	4.461436	-1.058321	-1.361900	C	-0.417038	-1.130400	-0.093288	C	4.534510	-1.082508	-1.185467
N	0.803038	-0.506733	0.137610	C	5.223060	-1.491447	-0.140384	N	0.825368	-0.518988	0.120120	C	5.304969	-1.178791	0.101713
N	0.634881	0.892965	0.155934	C	4.948563	-1.207803	1.131147	N	0.644599	0.875842	0.217606	C	5.033323	-0.576863	1.257818
C	-0.758651	1.109946	0.006747	C	1.238208	1.547253	1.302765	C	-0.755050	1.091455	0.093691	C	1.254579	2.056852	0.721468
O	-1.239734	2.260584	0.027688	C	1.317830	3.056785	1.155298	O	-1.245382	2.228613	0.206439	C	1.440620	3.376378	0.068994
N	-0.556863	-2.434939	-0.183696	O	-1.215723	2.305048	-0.146218	N	-0.516848	-2.437517	-0.312034	O	-1.239999	2.358261	-0.758716
H	0.259456	-3.032264	-0.164575	C	0.495773	1.158837	2.578860	H	0.305985	-3.025834	-0.325589	C	0.454769	2.117885	2.018949
H	-1.456100	-2.820214	-0.442858	O	2.108148	-2.269963	-0.346161	H	-1.411560	-2.817721	-0.593161	O	2.213751	-2.051785	0.116972
C	1.269238	1.506385	1.378427	H	-5.675482	-1.599317	1.140630	C	1.257206	1.433092	1.487281	H	-5.580802	-1.214899	1.466876
C	0.446428	1.227030	2.630017	H	-6.747353	-0.565487	-0.833764	C	0.435281	1.063652	2.715836	H	-6.690619	-0.725580	-0.687953
C	1.543375	2.985984	1.160766	H	-5.362512	0.705556	-2.472856	C	1.487956	2.891733	1.331600	H	-5.347836	0.131830	-2.607120

H	2.230163	0.992847	1.464307	H	-2.913389	0.881941	-2.126181	H	2.228419	0.926357	1.546379	H	-2.901675	0.442440	-2.344642
H	1.003813	1.560378	3.509498	H	-2.238945	-0.993459	2.241514	H	0.988591	1.347220	3.614854	H	-2.137254	-0.302223	2.333021
H	0.246306	0.155936	2.739470	H	-2.723965	-2.595262	1.676876	H	0.253096	-0.015139	2.752212	H	-2.635684	-1.992774	2.210189
H	-0.506186	1.765900	2.603921	H	-3.834745	-1.647515	2.666000	H	-0.524795	1.588402	2.721965	H	-3.727398	-0.813835	2.935763
H	0.622506	3.573806	1.175726	H	0.175726	-3.020056	-0.057195	H	1.029820	3.598294	2.012898	H	0.298691	-2.752356	0.593518
H	2.184488	3.341504	1.972383	H	-1.535769	-2.790314	-0.347748	H	2.174335	3.249260	0.572384	H	-1.418818	-2.642764	0.272943
H	2.064619	3.153749	0.212756	H	2.253722	1.147184	1.336106	H	0.830608	4.459873	-0.985324	H	2.238921	1.620323	0.942712
C	1.976631	-1.036351	-0.404739	H	1.023912	1.569989	3.443393	C	2.004418	-1.005412	-0.448035	H	1.005476	2.714330	2.750972
O	2.174679	-2.236931	-0.414473	H	0.450475	0.070955	2.690489	O	2.212635	-2.201442	-0.533231	H	0.310581	1.115239	2.433518
S	3.098352	0.166259	-1.061236	H	-0.522098	1.562713	2.574169	S	3.122667	0.244947	-1.017636	H	-0.522717	2.583243	1.859851
C	4.487197	-0.944786	-1.424479	H	0.402054	3.568156	1.453780	C	4.522928	-0.830789	-1.439050	H	1.237759	4.286443	0.619713
C	5.280922	-1.428056	-0.243048	H	2.182429	3.465420	1.682513	C	5.311702	-1.382401	-0.284546	H	1.889201	3.435321	-0.915727
C	5.032550	-1.210480	1.046704	H	1.476427	3.351937	0.022940	C	5.049819	-1.253232	1.014381	H	4.179154	-2.069447	-1.494857
H	4.111098	-1.790907	-2.006842	H	4.086106	-1.928153	-1.908614	H	4.157359	-1.641157	-2.076413	H	5.185937	-0.714249	-1.985076
H	5.128026	-0.359468	-2.092166	H	5.124780	-0.516531	-2.044184	H	5.164000	-0.200164	-2.063770	H	6.173225	-1.833297	0.029870
H	6.144835	-2.027753	-0.528333	H	6.085720	-2.114073	-0.376011	H	6.184378	-1.953258	-0.600658	H	5.672107	-0.731037	2.121781
H	5.686343	-1.621150	1.809685	H	5.579946	-1.587571	1.928263	H	5.701466	-1.706759	1.754590	H	4.178423	0.083814	1.387254
H	4.183428	-0.622257	1.388749	H	4.099120	-0.594189	1.424416	H	4.191562	-0.697668	1.386826				
O	0.198663	4.073549	-1.400527	O	1.054713	3.718956	-1.261441	O	-0.055589	4.261743	-1.313294				
H	-0.352484	3.429313	-0.875332	H	0.147975	3.363179	-1.124378	H	-0.394288	3.563245	-0.720121				

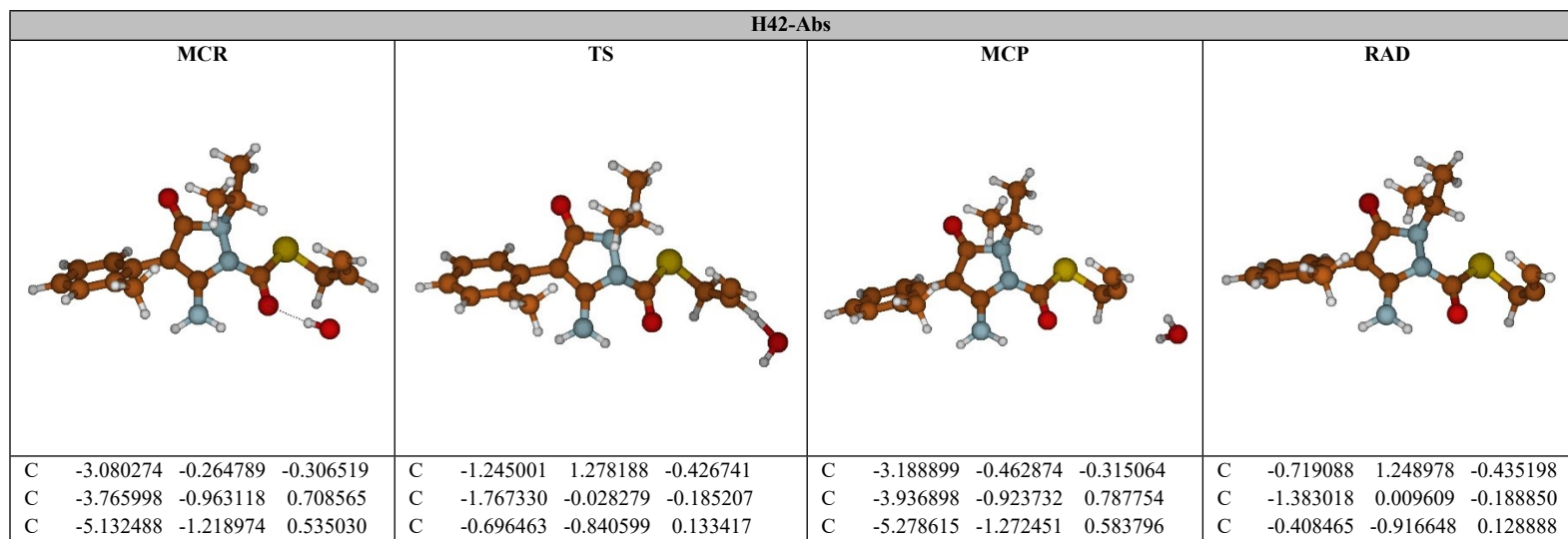
H40-Abs															
MCR				TS				MCP				RAD			
															
C	-3.080274	-0.264935	-0.306491	C	-1.029947	1.240085	-0.635352	C	-3.020751	-0.368254	-0.280457	C	-0.734371	1.252643	-0.419612
C	-3.766111	-0.963042	0.708671	C	-1.593937	0.018021	-0.158197	C	-3.750016	-0.833775	0.832847	C	-1.389746	0.006395	-0.184115
C	-5.132571	-1.218943	0.535034	C	-0.558355	-0.730068	0.366587	C	-5.096447	-1.176448	0.651052	C	-0.410423	-0.912076	0.140318
C	-5.818492	-0.786818	-0.596926	N	0.635796	0.001317	0.256249	C	-5.721935	-1.050410	-0.586260	N	0.837866	-0.269908	0.143862
C	-5.140305	-0.076205	-1.588634	N	0.373452	1.232172	-0.382685	C	-5.001921	-0.567505	-1.680248	N	0.666770	1.082124	-0.223745

C	-3.780950	0.177933	-1.439785	C	-3.019425	-0.342900	-0.258550	C	-3.661333	-0.232433	-1.522677	C	-2.842154	-0.215541	-0.301368
C	-1.646266	0.056341	-0.197311	C	-3.786852	-0.675861	0.876341	C	-1.604934	0.027262	-0.175959	C	-3.610229	-0.708339	0.773597
C	-3.081053	-1.418923	1.971266	C	-5.138662	-0.996918	0.695320	C	-3.135119	-0.953965	2.203673	C	-4.987972	-0.879576	0.584610
H	-5.665872	-1.754865	1.316289	C	-5.732543	-0.975295	-0.563705	H	-5.663200	-1.533545	1.507372	C	-5.605201	-0.559979	-0.621736
H	-6.879036	-0.995370	-0.700370	C	-4.974322	-0.622420	-1.681237	H	-6.768597	-1.318422	-0.694079	C	-4.844510	-0.050745	-1.675488
H	-5.664923	0.272542	-2.472674	C	-3.627819	-0.311644	-1.523630	H	-5.479755	-0.457173	-2.648673	C	-3.473439	0.115936	-1.511009
H	-3.241145	0.721359	-2.210845	C	-3.205347	-0.676637	2.266918	H	-3.088698	0.135030	-2.370142	C	-3.000868	-1.034695	2.112865
H	-2.273227	-0.738602	2.257301	N	-0.568265	-1.967190	0.856633	H	-2.345538	-0.212347	2.357123	N	-0.517545	-2.219232	0.366716
H	-2.645324	-2.417313	1.852502	C	1.865480	-0.611120	0.050123	H	-2.694205	-1.945022	2.359097	C	2.008941	-0.926863	-0.225852
H	-3.799589	-1.471967	2.792649	S	2.935844	0.245974	-1.081092	H	-3.898624	-0.813551	2.972711	S	3.129608	0.070879	-1.204573
C	-0.588314	-0.813541	-0.019534	C	4.438160	-0.715570	-0.835440	C	-0.536311	-0.730122	0.261268	C	4.545055	-0.974214	-1.223773
N	0.605758	-0.076300	0.034859	C	5.157397	-0.587670	0.465373	N	0.632379	0.047741	0.197326	C	5.288482	-1.306707	-0.095005
N	0.317732	1.293929	-0.143685	C	4.773774	0.117631	1.529889	N	0.318145	1.322416	-0.321382	C	5.028040	-0.913356	1.200785
C	-1.098527	1.372221	-0.283730	C	0.894920	2.391638	0.424558	C	-1.089032	1.304906	-0.551235	C	1.303714	2.010295	0.775666
O	-1.676203	2.459777	-0.403718	C	1.085351	3.612258	-0.461309	O	-1.687088	2.306095	-0.963111	C	1.598913	3.357130	0.135476
N	-0.585871	-2.143136	0.040307	O	-1.587695	2.219478	-1.145056	N	-0.500003	-2.005304	0.640484	O	-1.217996	2.357616	-0.697212
H	0.281541	-2.658401	0.110169	C	0.023325	2.661098	1.645060	H	0.374402	-2.452936	0.880644	C	0.476451	2.114055	2.051361
H	-1.447989	-2.637150	-0.150978	O	2.153482	-1.656923	0.604752	H	-1.334648	-2.566522	0.528938	O	2.218494	-2.078804	0.096938
C	0.907887	2.127759	0.963082	H	-5.734728	-1.252524	1.567888	C	0.811158	2.421435	0.582939	H	-5.584565	-1.257246	1.411349
C	0.118042	1.981164	2.258073	H	-6.784158	-1.223374	-0.671042	C	-0.051202	2.548612	1.832936	H	-6.676033	-0.698748	-0.735964
C	1.066809	3.571262	0.513675	H	-5.426817	-0.594458	-2.667553	C	0.946077	3.722664	-0.191396	H	-5.314793	0.209512	-2.618612
H	1.906401	1.709026	1.112361	H	-3.025616	-0.045790	-2.388395	H	1.812291	2.097476	0.878716	H	-2.869937	0.502234	-2.328220
H	0.656166	2.482355	3.067132	H	-2.401761	0.059123	2.366675	H	0.419768	3.251452	2.525451	H	-2.135733	-0.399901	2.326357
H	0.000376	0.926650	2.529685	H	-2.790491	-1.657050	2.526761	H	-0.150636	1.584020	2.342175	H	-2.665696	-2.077084	2.156913
H	-0.872906	2.437994	2.171585	H	-3.981667	-0.446952	3.000725	H	-1.049531	2.925603	1.589118	H	-3.738717	-0.896464	2.906882
H	0.101542	4.070025	0.409108	H	0.284736	-2.413125	1.166448	H	-0.028559	4.135262	-0.458384	H	0.300302	-2.785926	0.546505
H	1.650929	4.107127	1.267213	H	-1.421044	-2.508118	0.790307	H	1.467087	4.449314	0.438380	H	-1.414293	-2.664366	0.219760
H	1.600346	3.625827	-0.439599	H	1.880799	2.061752	0.762704	H	1.531121	3.574250	-1.103576	H	2.257638	1.533254	1.014763
C	1.812948	-0.574525	-0.439821	H	0.509480	3.408891	2.277366	C	1.876846	-0.502988	-0.075982	H	1.040349	2.673961	2.802315
O	2.109160	-1.749843	-0.284390	H	-0.114347	1.751069	2.238714	O	2.199840	-1.586128	0.377667	H	0.258518	1.121342	2.459737
S	2.828651	0.606154	-1.276250	H	-0.958750	3.046217	1.352770	S	2.912307	0.504496	-1.130170	H	-0.467272	2.638248	1.870696
C	4.310343	-0.416141	-1.512186	O	0.129679	4.033591	-0.778327	C	4.442222	-0.352824	-0.994529	H	0.683307	3.911712	-0.078189
C	5.205981	-0.576063	-0.316668	H	1.625095	4.373635	0.108886	C	5.167525	-0.487855	0.187932	H	2.204938	3.946769	0.829149
C	4.938062	-0.238202	0.947789	H	1.675196	3.362630	-1.347929	C	4.801773	-0.019138	1.430642	H	2.162255	3.230690	-0.793568
H	4.002708	-1.393006	-1.898332	H	4.194894	-1.828641	-1.019595	H	4.878406	-3.298090	-0.817969	H	4.852490	-1.304799	-2.209296
H	4.854494	0.086790	-2.317838	H	5.087694	-0.464049	-1.680620	H	4.836523	-0.723183	-1.934078	H	6.150281	-1.946354	-0.275225
H	6.164913	-1.033815	-0.556104	H	6.089089	-1.150684	0.497154	H	6.106385	-1.031311	0.097471	H	5.669693	-1.237022	2.011424
H	5.672473	-0.404662	1.729180	H	5.388152	0.139484	2.424272	H	5.439773	-0.188467	2.289689	H	4.195824	-0.261439	1.450426
H	3.997366	0.222795	1.242353	H	3.855086	0.700226	1.546914	H	3.887143	0.544792	1.590154				
O	4.439683	-2.891077	0.952473	O	3.844579	-3.278684	-1.051806	O	4.015935	-3.646198	-0.556777				
H	3.634650	-2.564169	0.494906	H	3.148976	-3.190255	-0.367656	H	3.509437	-2.867666	-0.271923				



H41-Abs															
MCR				TS				MCP				RAD			
															
C	-3.187201	-0.153664	-0.293213	C	-1.016934	1.241579	-0.370342	C	-3.183242	-0.087814	-0.289231	C	-0.734258	1.252689	-0.419571
C	-3.972224	-0.595562	0.791505	C	-1.702565	0.004177	-0.175752	C	-3.966860	-0.554145	0.786277	C	-1.389713	0.006472	-0.184186
C	-5.355205	-0.721840	0.605291	C	-0.763678	-0.917676	0.244926	C	-5.356474	-0.618870	0.618966	C	-0.410485	-0.912001	0.140429
C	-5.960773	-0.406152	-0.607998	N	0.485301	-0.286025	0.349016	C	-5.969102	-0.219851	-0.565847	N	0.837868	-0.269947	0.143989
C	-5.182496	0.053341	-1.671753	N	0.359837	1.061852	-0.050243	C	-5.191101	0.263374	-1.619290	N	0.666876	1.082125	-0.223642
C	-3.806362	0.174561	-1.509981	C	-3.141356	-0.205296	-0.416656	C	-3.808960	0.324447	-1.476798	C	-2.842103	-0.215514	-0.301508
C	-1.727507	0.015723	-0.180031	C	-4.004679	-0.684889	0.589751	C	-1.716750	0.021062	-0.194232	C	-3.610157	-0.708394	0.773452
C	-3.374114	-0.912933	2.137935	C	-5.363029	-0.840738	0.283554	C	-3.360591	-0.961466	2.104671	C	-4.987884	-0.879757	0.584426
H	-5.964768	-1.060405	1.439452	C	-5.870910	-0.518598	-0.972081	H	-5.964937	-0.976110	1.446128	C	-5.605127	-0.560047	-0.621877
H	-7.035841	-0.509189	-0.720198	C	-5.016346	-0.023363	-1.958353	H	-7.048995	-0.276609	-0.663508	C	-4.844482	-0.050561	-1.675542
H	-5.643282	0.310144	-2.620504	C	-3.662627	0.127807	-1.677270	H	-5.656975	0.584889	-2.545553	C	-3.473424	0.116175	-1.511062
H	-3.189622	0.521466	-2.334946	C	-3.516834	-1.012705	1.977512	H	-3.192788	0.688971	-2.294520	C	-3.000878	-1.034613	2.112798
H	-2.491747	-0.298452	2.340260	N	-0.900182	-2.220498	0.480456	H	-2.448552	-0.396603	2.319413	N	-0.517499	-2.219181	0.366957
H	-3.067657	-1.962900	2.203167	C	1.676344	-0.954163	0.072492	H	-3.100751	-2.025880	2.114750	C	2.008975	-0.926895	-0.225974
H	-4.108705	-0.738576	2.927811	S	2.878268	0.013952	-0.807296	H	-4.073422	-0.792953	2.915487	S	3.129517	0.071189	-1.204623
C	-0.783778	-0.932026	0.166501	C	4.244159	-1.168386	-0.732954	C	-0.805176	-0.974859	0.097469	C	4.545244	-0.973607	-1.224046
N	0.488097	-0.340209	0.153967	C	4.959014	-1.322161	0.563401	N	0.487744	-0.429067	0.088537	C	5.288355	-1.306609	-0.095366
N	0.368918	1.008092	-0.246340	C	4.712118	-0.658647	1.694790	N	0.415455	0.939253	-0.250167	C	5.027843	-0.914018	1.200732
C	-1.023985	1.229200	-0.445778	C	0.917410	1.997441	0.988875	C	-0.971734	1.217851	-0.422286	C	1.303667	2.010097	0.775999
O	-1.463570	2.345661	-0.750850	C	1.279707	3.333870	0.361343	O	-1.372451	2.360361	-0.677488	C	1.598661	3.357233	0.136309
N	-0.941849	-2.227785	0.428223	O	-1.462665	2.346408	-0.705769	N	-1.005768	-2.274113	0.307249	O	-1.217736	2.357586	-0.697617
H	-0.142725	-2.821253	0.606624	C	-0.015785	2.125224	2.186943	H	-0.226637	-2.903080	0.449322	C	0.476418	2.113297	2.051753
H	-1.852723	-2.643757	0.283055	O	1.851478	-2.108049	0.416094	H	-1.932838	-2.651240	0.158066	O	2.218351	-2.078869	0.096469
C	1.044068	1.933681	0.729669	H	-6.032688	-1.207709	1.057438	C	1.129098	1.796603	0.761960	H	-5.584462	-1.257568	1.411110
C	0.225058	2.097116	2.004439	H	-6.929734	-0.644417	-1.177029	C	0.323249	1.933631	2.048023	H	-6.675944	-0.698888	-0.736161

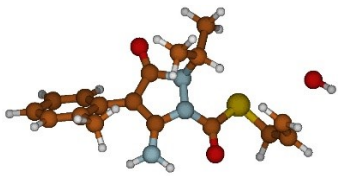
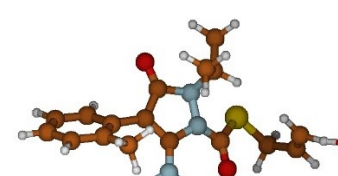
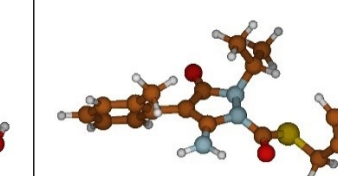
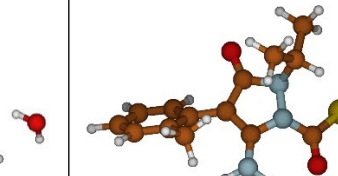
C	1.387647	3.254131	0.059405	H	-5.400445	0.238686	-2.939250	C	1.516839	3.131213	0.146280	H	-5.314809	0.209873	-2.618595
H	1.980104	1.426356	0.977384	H	-2.986998	0.503813	-2.441014	H	2.048201	1.246825	0.980925	H	-2.869963	0.502725	-2.328185
H	0.810818	2.653224	2.741355	H	-2.669386	-0.383147	2.264806	H	0.932549	2.437093	2.803418	H	-2.135718	-0.399858	2.326277
H	-0.027833	1.122668	2.435929	H	-3.193533	-2.057061	2.051529	H	0.038585	0.951181	2.439804	H	-2.665798	-2.077026	2.157065
H	-0.699425	2.651091	1.813280	H	-4.320317	-0.868230	2.703799	H	-0.582181	2.527187	1.887063	H	-3.738775	-0.896215	2.906742
H	0.492632	3.838184	-0.162992	H	-0.102992	-2.789273	0.732697	H	0.642884	3.756728	-0.044769	H	0.300524	-2.785602	0.546881
H	2.018538	3.835151	0.738052	H	-1.781420	-2.663960	0.255698	H	2.172429	3.658763	0.844957	H	-1.414234	-2.664452	0.220499
H	1.941785	3.086487	-0.868630	H	1.842611	1.514998	1.314982	H	2.060069	2.983168	-0.791589	H	2.257702	1.533150	1.014850
C	1.632182	-1.049030	-0.213233	H	0.486858	2.689261	2.977245	C	1.604739	-1.163112	-0.295890	H	1.039979	2.673477	2.802757
O	1.792923	-2.206441	0.129804	H	-0.279257	1.139991	2.586383	O	1.731412	-2.333552	0.002550	H	0.259042	1.120444	2.460077
S	2.790481	-0.133787	-1.193189	H	-0.934382	2.656359	1.918431	S	2.793067	-0.228098	-1.258281	H	-0.467597	2.636979	1.871104
C	4.135333	-1.351312	-1.207032	H	0.391045	3.896716	0.069777	C	4.171550	-1.317642	-1.211161	H	0.683076	3.912337	-0.076091
C	4.923138	-1.484809	0.063918	H	1.834872	3.923689	1.096244	C	4.828838	-1.707854	-0.046691	H	2.205615	3.946190	0.829756
C	4.670455	-0.902166	1.241217	H	1.914621	3.191977	-0.517950	C	4.506463	-1.334396	1.241487	H	2.161068	3.231182	-0.793354
H	3.725962	-2.320901	-1.505269	H	3.949911	-2.126827	-1.169152	H	4.536141	-1.627979	-2.183719	H	4.852959	-1.303628	-2.209664
H	4.792077	-1.019480	-2.017670	H	4.981274	-0.736813	-1.517397	H	5.899625	1.133806	-0.699089	H	6.150294	-1.946047	-0.275674
H	5.780578	-2.150655	-0.028573	H	5.754543	-2.065475	0.535120	H	5.678361	-2.372326	-0.191300	H	5.669745	-1.237952	2.011066
H	5.313666	-1.088728	2.095638	H	5.298775	-0.856230	2.586215	H	5.087176	-1.701737	2.079268	H	4.195468	-0.262534	1.450980
H	3.823135	-0.237514	1.393717	H	3.922453	0.085227	1.773887	H	3.681799	-0.661745	1.462446				
O	6.031869	0.908510	-0.072648	O	5.859837	0.105928	-2.342931	O	5.814258	1.600683	0.143222				
H	6.735995	0.595550	0.527505	H	6.313951	0.552731	-1.600560	H	5.588701	0.905734	0.777643				



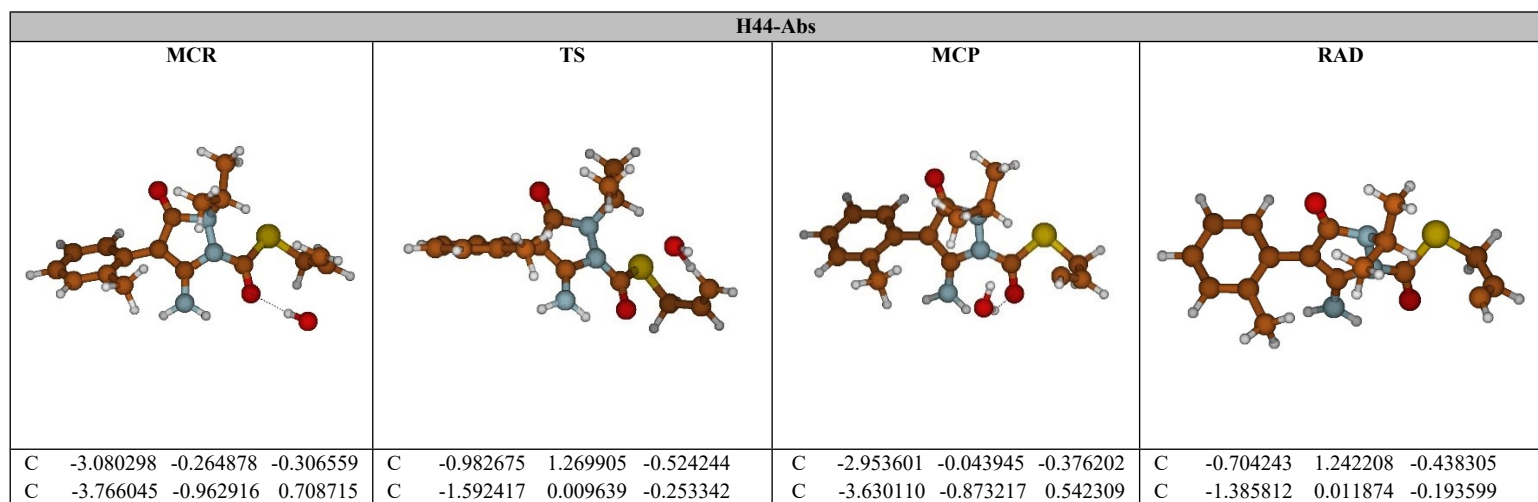


C	-5.818556	-0.786570	-0.596723	N	0.477861	-0.073032	0.132654	C	-5.882195	-1.156390	-0.665309	N	0.844742	-0.285994	0.119085
C	-5.140487	-0.075709	-1.588341	N	0.167301	1.252706	-0.240057	C	-5.144059	-0.677810	-1.749120	N	0.682352	1.066630	-0.251614
C	-3.781116	0.178367	-1.439610	C	-3.189569	-0.398301	-0.291344	C	-3.807681	-0.337178	-1.569424	C	-2.838425	-0.199972	-0.289543
C	-1.646241	0.056419	-0.197506	C	-3.889419	-0.985674	0.782731	C	-1.776389	-0.062662	-0.188123	C	-3.598839	-0.679626	0.796776
C	-3.080913	-1.419361	1.971029	C	-5.243815	-1.297406	0.604496	C	-3.347126	-1.031929	2.170540	C	-4.979971	-0.840075	0.623957
H	-5.665687	-1.755077	1.316232	C	-5.905535	-1.024255	-0.589539	H	-5.859512	-1.626048	1.432071	C	-5.607622	-0.522124	-0.577500
H	-6.879115	-0.995091	-0.700085	C	-5.214737	-0.420764	-1.641672	H	-6.925822	-1.428731	-0.790310	C	-4.854245	-0.025733	-1.642546
H	-5.665217	0.273283	-2.472219	C	-3.866736	-0.114542	-1.488375	H	-5.604566	-0.575137	-2.726744	C	-3.480030	0.130000	-1.494103
H	-3.241411	0.721968	-2.210615	C	-3.234685	-1.266096	2.110832	H	-3.221110	0.026706	-2.408876	C	-2.976972	-1.002666	2.131066
H	-2.271917	-0.740141	2.256329	N	-0.667463	-2.152136	0.359506	H	-2.564551	-0.284986	2.333761	N	-0.525354	-2.222060	0.360326
H	-2.646837	-2.418510	1.852555	C	1.710078	-0.604174	-0.241837	H	-2.903415	-2.019330	2.340489	C	2.008408	-0.950917	-0.263614
H	-3.799103	-1.470885	2.792817	S	2.726555	0.486509	-1.205015	H	-4.125681	-0.891019	2.924245	S	3.133714	0.021743	-1.231110
C	-0.588325	-0.813563	-0.019821	C	4.235561	-0.526383	-1.219867	C	-0.713324	-0.812091	0.277699	C	4.553328	-1.154568	-1.209555
N	0.605792	-0.076408	0.034715	C	4.981822	-0.553726	0.075835	N	0.452892	-0.032991	0.230150	C	5.203634	-1.243357	0.099651
N	0.317856	1.293893	-0.143727	C	4.701316	-0.052379	1.269481	N	0.146319	1.231638	-0.316663	C	5.075097	-0.816751	1.333238
C	-1.098449	1.372260	-0.283780	C	0.711797	2.248348	0.749001	C	-1.255621	1.211111	-0.569571	C	1.335427	1.991503	0.740524
O	-1.676027	2.459868	-0.403703	C	0.866351	3.612535	0.095934	O	-1.847760	2.207282	-1.003739	C	1.637431	3.333981	0.094479
N	-0.585943	-2.143146	0.039646	O	-1.841910	2.327103	-0.701712	N	-0.680297	-2.083323	0.671900	O	-1.195209	2.357255	-0.713075
H	0.281327	-2.658536	0.110240	C	-0.115931	2.279708	2.028206	H	0.193132	-2.525195	0.926410	C	0.519245	2.105963	2.022397
H	-1.448238	-2.637139	-0.150837	O	2.036426	-1.731933	0.078633	H	-1.508998	-2.650119	0.545793	O	2.208550	-2.108684	0.054022
C	0.907880	2.127411	0.963382	H	-5.787433	-1.748920	1.430680	C	0.632045	2.346724	0.570181	H	-5.570735	-1.207601	1.459398
C	0.117895	1.980450	2.258234	H	-6.957409	-1.271984	-0.695144	C	-0.247792	2.504294	1.804485	H	-6.680800	-0.652238	-0.679195
C	1.066887	3.571042	0.514428	H	-5.720765	-0.195157	-2.575191	C	0.785535	3.630936	-0.228698	H	-5.332660	0.233118	-2.581969
H	1.906376	1.708622	1.112630	H	-3.317167	0.345937	-2.305083	H	1.627113	2.023448	0.887097	H	-2.882189	0.506181	-2.320157
H	0.655965	2.481355	3.067506	H	-2.439653	-0.546292	2.327060	H	0.216691	3.218086	2.490164	H	-2.107514	-0.369870	2.332761
H	0.000134	0.925860	2.529514	H	-2.790184	-2.267317	2.134808	H	-0.360617	1.550426	2.330888	H	-2.644475	-2.045841	2.176253
H	-0.873018	2.437370	2.171800	H	-3.974795	-1.218806	2.913295	H	-1.240129	2.881687	1.538006	H	-3.706053	-0.858523	2.932073
H	0.101657	4.069894	0.409943	H	0.208165	-2.631662	0.520806	H	-0.182670	4.041911	-0.520523	H	0.289588	-2.795165	0.532929
H	1.650962	4.106654	1.268184	H	-1.510315	-2.688618	0.199181	H	1.299354	4.368652	0.394113	H	-1.427891	-2.659283	0.225783
H	1.600514	3.625877	-0.438780	H	1.710111	1.872622	0.987509	H	1.384859	3.460851	-1.127774	H	2.286807	1.506376	0.973596
C	1.812994	-0.574637	-0.440078	H	0.393224	2.898449	2.772038	C	1.704878	-0.587315	-0.027900	H	1.093796	2.663356	2.767131
O	2.109196	-1.749949	-0.284656	H	-0.232815	1.273419	2.444627	O	2.030456	-1.661413	0.442765	H	0.296469	1.116328	2.435596
S	2.828578	0.606155	-1.276456	H	-1.107642	2.706464	1.848613	S	2.745738	0.391572	-1.080876	H	-0.421538	2.637443	1.847788
C	4.310475	-0.415878	-1.512223	H	-0.101805	4.068887	-0.118523	C	4.292109	-0.586558	-0.868009	H	0.724865	3.895202	-0.114998
C	5.205987	-0.575649	-0.316553	H	1.411547	4.267126	0.781794	C	4.889429	-0.425194	0.460450	H	2.252675	3.920886	0.782345
C	4.937729	-0.238014	0.947895	H	1.436397	3.536084	-0.834488	C	4.666906	0.131654	1.626450	H	2.193603	3.200212	-0.837869
H	4.003067	-1.392822	-1.898322	H	3.979383	-1.541011	-1.536619	H	4.073760	-1.635105	-1.086054	H	4.198677	-2.130254	-1.550200
H	4.854655	0.087171	-2.317769	H	4.857060	-0.084705	-2.005010	H	4.957330	-0.205025	-1.648667	H	5.237510	-0.755996	-1.964721
H	6.165058	-1.033117	-0.555945	H	5.985188	-1.142781	-0.031916	H	6.953984	-1.608484	-0.074143	H	5.779929	-1.094107	2.113792
H	5.672004	-0.404393	1.729430	H	5.376588	-0.200854	2.106599	H	5.372530	0.041219	2.449179	H	4.246236	-0.162283	1.624867
H	3.996883	0.222780	1.242294	H	3.796862	0.527416	1.452932	H	3.756367	0.710278	1.815962				
O	4.439793	-2.890880	0.952756	O	7.027123	-2.085711	-0.027485	O	7.354879	-2.226517	-0.702316				

H	3.635071	-2.564405	0.494332	H	6.517351	-2.848090	0.309968	H	6.643320	-2.432520	-1.323281
---	----------	-----------	----------	---	----------	-----------	----------	---	----------	-----------	-----------

H43-Abs															
MCR			TS			MCP			RAD						
															
C	-3.185922	-0.153258	-0.293775	C	-1.174919	1.307941	-0.305069	C	-3.253105	-0.294284	-0.189212	C	-0.713323	1.237626	-0.450021
C	-3.973292	-0.593752	0.789771	C	-1.770324	0.018657	-0.158177	C	-3.881890	-1.039073	0.829745	C	-1.380517	0.005328	-0.177456
C	-5.355882	-0.720273	0.600706	C	-0.739264	-0.891732	-0.029722	C	-5.257961	-1.281070	0.726022	C	-0.410279	-0.909523	0.183691
C	-5.958829	-0.406128	-0.614267	N	0.484685	-0.206658	-0.063366	C	-6.007601	-0.790504	-0.339789	N	0.842830	-0.278774	0.173075
C	-5.178236	0.052030	-1.676918	N	0.241922	1.170109	-0.257114	C	-5.385384	-0.033444	-1.333784	N	0.684647	1.060887	-0.242674
C	-3.802471	0.173428	-1.512310	C	-3.220214	-0.244486	-0.175729	C	-4.017876	0.207743	-1.254515	C	-2.833506	-0.209803	-0.299186
C	-1.726394	0.015962	-0.178018	C	-3.874408	-0.892460	0.892114	C	-1.812448	0.013036	-0.153240	C	-3.613923	-0.662564	0.784370
C	-3.378266	-0.909506	2.137961	C	-5.257995	-1.094122	0.802202	C	-3.125851	-1.560170	2.024749	C	-4.991305	-0.830253	0.589421
H	-5.967242	-1.057801	1.433974	C	-5.990194	-0.656260	-0.298016	H	-5.747163	-1.853318	1.510382	C	-5.596436	-0.544670	-0.631494
H	-7.033650	-0.509315	-0.728667	C	-5.342059	0.005390	-1.342300	H	-7.073721	-0.990058	-0.389652	C	-4.823452	-0.074628	-1.694499
H	-5.636948	0.307639	-2.626995	C	-3.967168	0.204983	-1.276577	H	-5.959738	0.361236	-2.166101	C	-3.452597	0.087501	-1.523931
H	-3.183947	0.519250	-2.336394	C	-3.137758	-1.354195	2.123198	H	-3.521370	0.786778	-2.028729	C	-3.017649	-0.949337	2.138503
H	-2.494973	-0.296512	2.340665	N	-0.787735	-2.219230	0.055349	H	-2.291135	-0.903962	2.288812	N	-0.530327	-2.207202	0.455033
H	-3.074311	-1.960033	2.205940	C	1.632850	-0.768420	-0.619754	H	-2.714241	-2.557666	1.834487	C	2.009595	-0.955738	-0.182399
H	-4.113934	-0.731924	2.926123	S	2.630309	0.358879	-1.558055	H	-3.792212	-1.641034	2.886852	S	3.136393	-0.018955	-1.179826
C	-0.783562	-0.931578	0.171590	C	4.050786	-0.733033	-1.842442	C	-0.753980	-0.872234	-0.084131	C	4.530500	-1.178577	-1.147583
N	0.488679	-0.340454	0.159494	C	4.948855	-0.973132	-0.658299	N	0.448193	-0.149877	-0.068082	C	5.286956	-1.249696	0.161501
N	0.370583	1.007049	-0.243744	C	4.759037	-0.550590	0.581785	N	0.164056	1.228917	-0.169399	C	4.981443	-0.651239	1.288872
C	-1.021942	1.228657	-0.444905	C	0.944939	2.005542	0.778904	C	-1.256465	1.326718	-0.212115	C	1.329862	2.016616	0.724193
O	-1.460576	2.344884	-0.752259	C	1.143806	3.424079	0.269656	O	-1.827743	2.424646	-0.242912	C	1.638017	3.338367	0.039303
N	-0.942455	-2.226741	0.435710	O	-1.713571	2.417961	-0.406991	N	-0.762094	-2.203482	-0.088814	O	-1.185902	2.337388	-0.766466
H	-0.143732	-2.820143	0.616146	C	0.237538	1.939255	2.127219	H	0.103140	-2.727169	-0.098789	C	0.502409	2.171348	1.994574
H	-1.853307	-2.642728	0.290508	O	1.901818	-1.944690	-0.458592	H	-1.638724	-2.681797	-0.251346	O	2.206516	-2.102505	0.175796
C	1.046087	1.934099	0.730525	H	-5.766472	-1.591847	1.624212	C	0.840767	2.011300	0.924093	H	-5.597282	-1.177281	1.422729

C	0.226717	2.100574	2.004651	H	-7.062503	-0.822446	-0.336228	C	0.139307	1.823933	2.264032	H	-6.667294	-0.679396	-0.750249
C	1.390650	3.253024	0.057760	H	-5.902148	0.358312	-2.202605	C	0.990641	3.469400	0.520884	H	-5.284118	0.159042	-2.649267
H	1.981744	1.426582	0.979431	H	-3.451093	0.710163	-2.088770	H	1.840711	1.573969	0.987387	H	-2.839781	0.443458	-2.347962
H	0.812523	2.657730	2.740736	H	-2.275761	-0.715917	2.338978	H	0.740042	2.283725	3.053412	H	-2.151365	-0.311960	2.339338
H	-0.027040	1.127139	2.437909	H	-2.769689	-2.379905	2.007563	H	0.022127	0.760948	2.500630	H	-2.687419	-1.991145	2.218126
H	-0.697304	2.654802	1.811980	H	-3.804896	-1.343113	2.988485	H	-0.847195	2.298171	2.264529	H	-3.761551	-0.783127	2.921408
H	0.496048	3.837209	-0.165971	H	0.060312	-2.769470	0.085223	H	0.028131	3.983787	0.500779	H	0.283574	-2.774588	0.650279
H	2.021753	3.834970	0.735417	H	-1.680712	-2.679620	-0.064549	H	1.631965	3.968232	1.253057	H	-1.428885	-2.650189	0.313134
H	1.944894	3.083231	-0.869819	H	1.929272	1.540224	0.877188	H	1.459795	3.555072	-0.463444	H	2.279068	1.538586	0.980447
C	1.632182	-1.050709	-0.207284	H	0.854885	2.431785	2.883315	C	1.615730	-0.638862	-0.652065	H	1.070300	2.751178	2.727189
O	1.792565	-2.207450	0.138191	H	0.082363	0.900498	2.438060	O	1.920003	-1.814452	-0.563431	H	0.274885	1.195010	2.435867
S	2.789683	-0.138163	-1.190474	H	-0.731116	2.447535	2.092077	S	2.578884	0.573940	-1.515687	H	-0.436265	2.697667	1.794672
C	4.131734	-1.358646	-1.207938	H	0.197779	3.964293	0.200985	C	4.046755	-0.443536	-1.830266	H	0.727701	3.894575	-0.192282
C	4.925506	-1.490264	0.059386	H	1.794922	3.956869	0.968491	C	4.922888	-0.711458	-0.626335	H	2.250467	3.944874	0.712523
C	4.679673	-0.904382	1.236479	H	1.622583	3.420135	-0.713807	C	4.677049	-0.387097	0.621486	H	2.199173	3.175526	-0.885352
H	3.718621	-2.328022	-1.501760	H	3.692659	-1.684684	-2.244018	H	3.737315	-1.385767	-2.290136	H	4.175189	-2.171652	-1.435165
H	4.785193	-1.030366	-2.022661	H	4.619078	-0.240431	-2.637979	H	4.613864	0.116752	-2.580010	H	5.197990	-0.826697	-1.940405
H	5.782773	-2.156024	-0.036199	H	5.828535	-1.572961	-0.891907	H	5.845810	-1.242961	-0.871279	H	6.172404	-1.887745	0.114275
H	5.327305	-1.088795	2.087949	H	5.557006	-0.867192	1.397779	H	6.540565	-1.224457	1.837251	H	4.221185	0.009154	1.688080
H	3.832540	-0.240159	1.392090	H	3.953260	0.066623	0.973960	H	3.916846	0.104972	1.215634				
O	6.003185	0.936478	-0.060551	O	6.680623	-1.012095	2.128422	O	7.458535	-1.512557	1.725996				
H	6.782503	0.517938	0.353427	H	7.182675	-0.254369	1.771665	H	7.602139	-1.480881	0.770756				

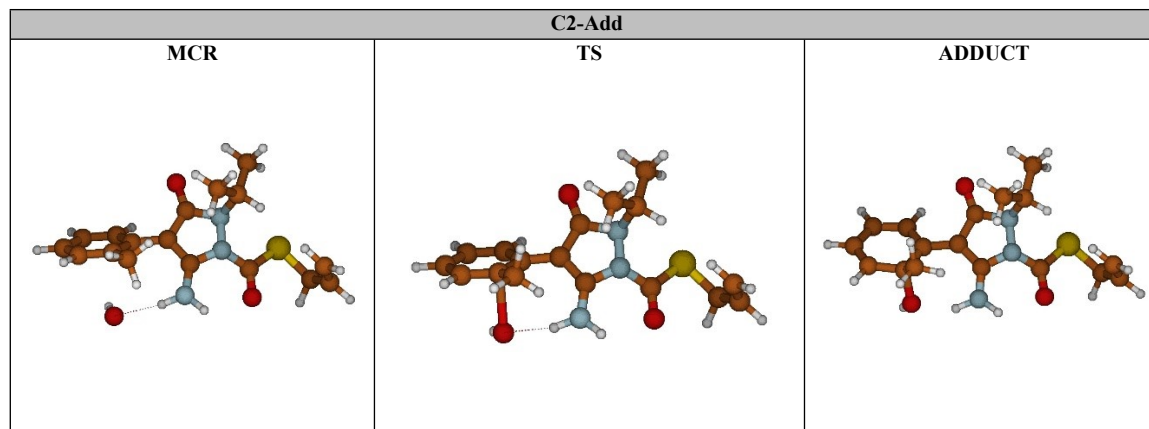


C	-5.132532	-1.218792	0.535230	C	-0.574210	-0.883124	0.021382	C	-5.019697	-1.004591	0.422637	C	-0.422834	-0.931175	0.111419
C	-5.818565	-0.786688	-0.596667	N	0.654134	-0.210663	-0.039781	C	-5.735514	-0.326210	-0.560464	N	0.838006	-0.319924	0.093218
C	-5.140470	-0.076127	-1.588475	N	0.431955	1.139207	-0.395038	C	-5.064497	0.512036	-1.452144	N	0.694846	1.035887	-0.270886
C	-3.781091	0.177972	-1.439787	C	-3.042602	-0.249827	-0.295253	C	-3.683264	0.646564	-1.356880	C	-2.844627	-0.175915	-0.286633
C	-1.646271	0.056379	-0.197520	C	-3.741597	-0.749935	0.822639	C	-1.495758	0.159453	-0.309764	C	-3.605012	-0.658059	0.798569
C	-3.080923	-1.418800	1.971283	C	-5.121890	-0.959896	0.706328	C	-2.909086	-1.599582	1.648890	C	-4.989094	-0.799040	0.631973
H	-5.665765	-1.754665	1.316567	C	-5.808230	-0.669754	-0.469867	H	-5.545954	-1.641441	1.129367	C	-5.619587	-0.459344	-0.561957
H	-6.879125	-0.995221	-0.699992	C	-5.116349	-0.152009	-1.565936	H	-6.812990	-0.444110	-0.624447	C	-4.865991	0.039820	-1.625637
H	-5.665185	0.272623	-2.472457	C	-3.743478	0.052005	-1.473796	H	-5.611800	1.052243	-2.218329	C	-3.489139	0.176173	-1.483542
H	-3.241355	0.721368	-2.210916	C	-3.054597	-1.043766	2.131454	H	-3.149303	1.288753	-2.052356	C	-2.980396	-1.004693	2.125699
H	-2.272449	-0.739039	2.256785	N	-0.643975	-2.191205	0.260430	H	-2.037553	-1.037113	1.997715	N	-0.556681	-2.236693	0.335111
H	-2.646108	-2.417626	1.852804	C	1.834181	-0.838863	-0.423952	H	-2.556236	-2.583513	1.319714	C	1.997748	-0.999532	-0.271817
H	-3.799242	-1.470892	2.792920	S	2.974269	0.186701	-1.312519	H	-3.581266	-1.760834	2.494996	S	3.129977	-0.061461	-1.262947
C	-0.588349	-0.813588	-0.019768	C	4.301248	-1.029216	-1.546806	C	-0.497909	-0.795985	-0.365643	C	4.572773	-1.149198	-1.086043
N	0.605741	-0.076433	0.034801	C	5.184963	-1.326362	-0.370615	N	0.743778	-0.159915	-0.249031	C	5.199780	-1.117601	0.283672
N	0.317802	1.293845	-0.143740	C	5.031958	-1.023345	0.908529	N	0.557640	1.233141	-0.133597	C	4.745513	-0.464648	1.329009
C	-1.098482	1.372205	-0.283836	C	1.073696	2.083394	0.586973	C	-0.855864	1.427962	-0.177349	C	1.377134	1.942986	0.717983
O	-1.676071	2.459816	-0.403846	C	1.220072	3.470759	-0.018318	O	-1.354062	2.554278	-0.054421	C	1.696082	3.283115	0.075731
N	-0.585968	-2.143172	0.039627	O	-1.510496	2.359521	-0.783054	N	-0.590536	-2.105720	-0.580885	O	-1.165294	2.360309	-0.704315
H	0.281248	-2.658579	0.110688	C	0.344062	2.079240	1.924410	H	0.230268	-2.696305	-0.569711	C	0.577061	2.065450	2.009277
H	-1.448301	-2.637154	-0.150711	O	2.044405	-2.010661	-0.163967	H	-1.501441	-2.508433	-0.757696	O	2.185215	-2.152347	0.073223
C	0.907886	2.127514	0.963194	H	-5.664976	-1.344106	1.566243	C	1.234403	1.764769	1.105210	H	-5.579646	-1.168713	1.466632
C	0.117964	1.980766	2.258112	H	-6.879330	-0.838126	-0.527714	C	0.466036	1.394088	2.368396	H	-6.694879	-0.574759	-0.658932
C	1.066896	3.571083	0.514017	H	-5.640932	0.085867	-2.486085	C	1.486963	3.257009	0.969617	H	-5.346417	0.315465	-2.559251
H	1.906383	1.708740	1.112463	H	-3.193002	0.444702	-2.324693	H	2.202456	1.255296	1.122494	H	-2.891297	0.553824	-2.308931
H	0.656002	2.481918	3.067254	H	-2.207750	-0.371473	2.299479	H	1.070980	1.645279	3.243951	H	-2.095713	-0.392907	2.325658
H	0.000329	0.926227	2.529639	H	-2.672448	-2.070314	2.161915	H	0.251521	0.320040	2.399728	H	-2.671122	-2.055387	2.160612
H	-0.872998	2.437564	2.171598	H	-3.757905	-0.932777	2.960252	H	-0.478224	1.944094	2.435026	H	-3.700274	-0.850550	2.933177
H	0.101679	4.070005	0.409730	H	0.196311	-2.742729	0.370145	H	0.555508	3.825957	0.993397	H	0.251011	-2.820334	0.506775
H	1.651228	4.106736	1.267544	H	-1.538083	-2.653039	0.154130	H	2.111149	3.582297	1.806764	H	-1.465801	-2.661128	0.205011
H	1.600267	3.625759	-0.439343	H	2.074032	1.676404	0.738170	H	2.015324	3.478910	0.037986	H	2.322582	1.438150	0.937689
C	1.812967	-0.574687	-0.439935	H	0.918902	2.660751	2.650772	C	1.917089	-0.657661	-0.791959	H	1.169625	2.607985	2.750894
O	2.109178	-1.749981	-0.284398	H	0.240264	1.059816	2.312219	O	2.136257	-1.859698	-0.819024	H	0.340359	1.077789	2.419532
S	2.828554	0.606037	-1.276386	H	-0.650949	2.528420	1.836525	S	3.033854	0.564583	-1.418563	H	-0.355648	2.614998	1.847638
C	4.310399	-0.416044	-1.512245	H	0.259123	3.978808	-0.112741	C	4.511260	-0.484944	-1.532562	H	0.791095	3.860819	-0.121885
C	5.206031	-0.575765	-0.316683	H	1.861608	4.065811	0.637997	C	5.099747	-0.870931	-0.199962	H	2.328041	3.856108	0.760217
C	4.937988	-0.237956	0.947767	H	1.692138	3.418085	-1.003766	C	4.566021	-0.658331	0.981535	H	2.240541	3.144095	-0.862691
H	4.002954	-1.392997	-1.898295	H	3.859979	-1.955001	-1.927747	H	4.278970	-1.372658	-2.126799	H	4.293140	-2.168980	-1.362879
H	4.854490	0.086952	-2.317892	H	4.906256	-0.608630	-2.355702	H	5.230256	0.110938	-2.102707	H	5.284864	-0.790306	-1.835603
H	6.165033	-1.033392	-0.556081	H	6.081819	-1.889086	-0.642296	H	6.062818	-1.387504	-0.268127	H	6.113660	-1.713903	0.374610
H	5.672374	-0.404351	1.729194	H	5.717021	-1.290761	1.707008	H	4.824979	-0.859472	2.012206	H	5.037538	-0.322000	2.360706
H	3.997251	0.223004	1.242256	H	4.077693	-0.414609	1.306632	H	2.008320	-1.207960	2.249400				

O	4.439862	-2.890703	0.952984	O	3.091665	0.049141	2.075590	O	1.760822	-2.138567	2.149121
H	3.635042	-2.564376	0.494631	H	3.359740	-0.373665	2.914226	H	1.952937	-2.337332	1.219616

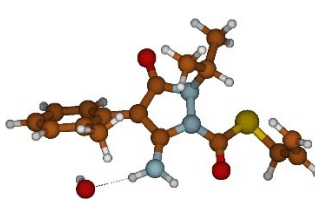
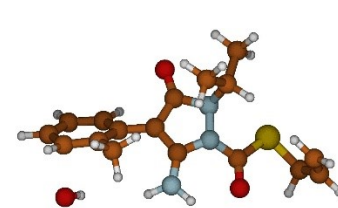
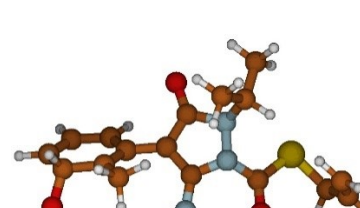
ADDITION REACTION											
MCR			C1-Add			ADDUCT					
MCR			TS			ADDUCT					
C	-0.541303	1.357243	-0.510758	C	-0.632981	1.202886	-0.497151	C	-0.821169	0.812270	-0.499469
C	-1.253727	0.174602	-0.143723	C	-1.260443	-0.045913	-0.198650	C	-1.249563	-0.505035	-0.167967
C	-0.314503	-0.753148	0.268734	C	-0.263639	-0.916133	0.212991	C	-0.144883	-1.193577	0.293693
N	0.962045	-0.173483	0.197589	N	0.965564	-0.240127	0.182788	N	0.978620	-0.350099	0.206193
N	0.850047	1.139132	-0.307680	N	0.766162	1.077614	-0.278016	N	0.585414	0.904400	-0.305303
C	-2.719282	0.040543	-0.211348	C	-2.720831	-0.237856	-0.270662	C	-2.700159	-0.935800	-0.220146
C	-3.494198	-0.297564	0.921266	C	-3.502659	-0.476389	0.914203	C	-3.487759	-0.234749	0.876001
C	-4.887832	-0.359277	0.782348	C	-4.885306	-0.337587	0.839178	C	-4.578105	0.535716	0.573826
C	-5.513912	-0.080763	-0.430323	C	-5.512801	0.087600	-0.333713	C	-5.034617	0.718800	-0.753609
C	-4.746796	0.274388	-1.541842	C	-4.756004	0.397500	-1.473773	C	-4.361988	0.076876	-1.825519
C	-3.362877	0.332193	-1.427693	C	-3.384229	0.261632	-1.434923	C	-3.262396	-0.691982	-1.597314
C	-2.870216	-0.587584	2.259706	C	-2.851682	-0.900841	2.194426	C	-3.005333	-0.426169	2.281219
N	-0.479456	-2.021278	0.638172	N	-0.341943	-2.198867	0.548413	N	-0.022498	-2.438914	0.750843
C	2.096361	-0.918885	-0.126626	C	2.157710	-0.889469	-0.146180	C	2.244230	-0.838103	-0.120930
S	3.250263	-0.092113	-1.187267	S	3.253827	0.047336	-1.175849	S	3.186505	0.203413	-1.202738
C	4.588363	-1.316983	-1.123814	C	4.678881	-1.075838	-1.127538	C	4.752407	-0.713392	-1.144055
C	5.387997	-1.365652	0.148107	C	5.468520	-1.094624	0.151419	C	5.560215	-0.571345	0.115604
C	5.169879	-0.684351	1.270985	C	5.198625	-0.445575	1.282153	C	5.224879	0.083255	1.225387
C	1.545806	2.135920	0.579169	C	1.379494	2.088230	0.652952	C	1.051661	2.028786	0.579060
C	1.893624	3.390913	-0.205204	C	1.657666	3.389258	-0.082727	C	1.100366	3.333413	-0.200296
O	-0.974365	2.451542	-0.894815	O	-1.139614	2.280172	-0.835902	O	-1.491862	1.791831	-0.854471

C	0.743927	2.416057	1.844460	C	0.541089	2.270450	1.912482	C	0.224148	2.117191	1.856116
O	2.251978	-2.048180	0.301532	O	2.393673	-2.013447	0.256934	O	2.643502	-1.901752	0.317356
H	-5.486564	-0.619307	1.651481	H	-5.481461	-0.545038	1.723093	H	-5.114485	1.020158	1.386500
H	-6.595758	-0.132616	-0.505253	H	-6.592897	0.193889	-0.355818	H	-5.905127	1.335153	-0.947172
H	-5.223768	0.498526	-2.490695	H	-5.245096	0.746462	-2.376947	H	-4.729834	0.204208	-2.839609
H	-2.756087	0.597227	-2.289330	H	-2.778998	0.497888	-2.304843	H	-2.735236	-1.185235	-2.409947
H	-1.968430	0.010714	2.420889	H	-1.947746	-0.316790	2.395396	H	-2.002649	-0.000004	2.413220
H	-2.585441	-1.642813	2.341890	H	-2.556752	-1.955639	2.145024	H	-2.934077	-1.490045	2.534103
H	-3.580428	-0.375387	3.062155	H	-3.544007	-0.784454	3.030349	H	-3.680907	0.055938	2.991343
H	0.326291	-2.603035	0.827232	H	0.497879	-2.726812	0.744927	H	0.889695	-2.813845	0.972570
H	-1.381658	-2.454038	0.462002	H	-1.217240	-2.664678	0.321767	H	-0.831007	-3.042220	0.676577
H	2.479401	1.640779	0.858549	H	2.339080	1.645876	0.932962	H	2.076392	1.755332	0.843824
H	1.344696	3.025245	2.525184	H	1.089091	2.894532	2.623547	H	0.674379	2.852735	2.528327
H	0.485489	1.484514	2.359357	H	0.338733	1.306354	2.391394	H	0.200019	1.152568	2.374216
H	-0.176584	2.963020	1.617564	H	-0.410699	2.761949	1.688128	H	-0.802765	2.431316	1.642808
H	1.000458	3.959939	-0.469981	H	0.735062	3.913265	-0.339164	H	0.099603	3.700201	-0.435317
H	2.534519	4.023483	0.415533	H	2.252208	4.036953	0.567804	H	1.608204	4.084967	0.410822
H	2.438297	3.139180	-1.119770	H	2.226600	3.203852	-0.998306	H	1.660996	3.209672	-1.131315
H	4.169779	-2.301438	-1.351859	H	4.336928	-2.082914	-1.382452	H	4.545245	-1.767301	-1.350262
H	5.237015	-1.046175	-1.963434	H	5.313168	-0.737048	-1.953529	H	5.320384	-0.328610	-1.997612
H	6.226181	-2.060144	0.097396	H	6.350159	-1.732763	0.097712	H	6.519117	-1.086595	0.066479
H	5.823217	-0.812585	2.128285	H	5.852214	-0.544694	2.143106	H	5.900325	0.109690	2.074707
H	4.346927	0.019354	1.378287	H	4.330809	0.201378	1.392730	H	4.279166	0.611224	1.329158
O	-3.074237	-2.713996	-0.714621	O	-2.735242	-2.244862	-0.872915	O	-2.686470	-2.362356	0.025527
H	-3.945081	-2.512069	-0.313204	H	-3.695741	-2.378184	-0.797450	H	-3.605240	-2.670340	0.011371



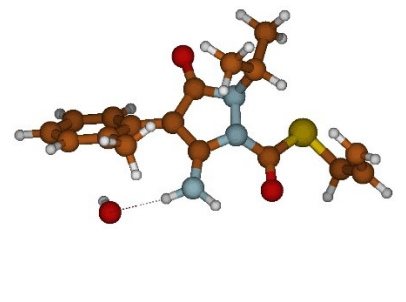
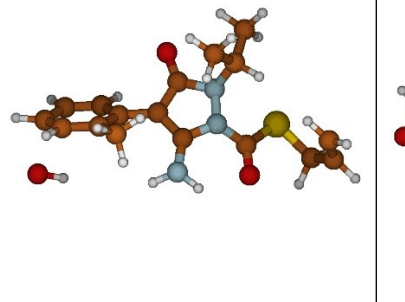
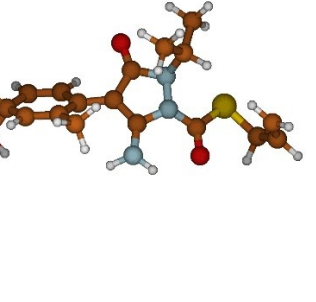
C	-0.492849	1.436132	-0.479683	C	-0.508260	1.413422	-0.453989	C	-0.536438	1.353814	-0.414851
C	-1.237511	0.258702	-0.176708	C	-1.237198	0.216133	-0.186225	C	-1.243058	0.108900	-0.259783
C	-0.328180	-0.717419	0.189053	C	-0.311703	-0.761989	0.146581	C	-0.278766	-0.849441	0.059571
N	0.963652	-0.170687	0.159903	N	0.968907	-0.192978	0.138819	N	0.980132	-0.234601	0.101966
N	0.892357	1.170016	-0.276979	N	0.879241	1.162053	-0.246949	N	0.851359	1.134120	-0.204230
C	-2.701314	0.132687	-0.273489	C	-2.692176	0.072700	-0.326365	C	-2.689552	-0.014563	-0.395517
C	-3.325742	0.429865	-1.493298	C	-3.296881	0.443932	-1.528584	C	-3.355739	0.793793	-1.303596
C	-4.706729	0.323764	-1.638324	C	-4.680111	0.358831	-1.695473	C	-4.752712	0.828156	-1.402061
C	-5.483699	-0.086519	-0.554430	C	-5.486410	-0.103388	-0.651435	C	-5.547290	0.030160	-0.528812
C	-4.873065	-0.370614	0.664510	C	-4.903075	-0.466693	0.552800	C	-4.960397	-0.795843	0.372919
C	-3.484349	-0.260899	0.834922	C	-3.500887	-0.402732	0.749697	C	-3.471104	-0.971574	0.496945
C	-2.876028	-0.534188	2.185635	C	-2.945669	-0.543491	2.141113	C	-3.055130	-0.846061	1.963564
N	-0.537952	-2.000059	0.469878	N	-0.506423	-2.056142	0.362569	N	-0.399370	-2.157416	0.240179
C	2.081331	-0.929505	-0.187237	C	2.102268	-0.920854	-0.224776	C	2.149722	-0.897994	-0.271063
S	3.268964	-0.084759	-1.195478	S	3.283458	-0.020964	-1.192106	S	3.308775	0.093456	-1.174472
C	4.574681	-1.345599	-1.171960	C	4.607118	-1.263233	-1.204464	C	4.679976	-1.094908	-1.225993
C	5.356795	-1.469560	0.105767	C	5.381872	-1.421401	0.074001	C	5.445424	-1.282914	0.053956
C	5.144153	-0.827559	1.252652	C	5.158407	-0.814935	1.238045	C	5.185377	-0.741235	1.242037
C	1.600630	2.097043	0.673534	C	1.560412	2.061949	0.749476	C	1.495345	1.997320	0.848527
C	1.984597	3.388177	-0.031263	C	1.930946	3.386874	0.102967	C	1.847878	3.361629	0.278232
O	-0.892262	2.559179	-0.816341	O	-0.920799	2.538918	-0.761714	O	-0.972140	2.490609	-0.624112
C	0.791702	2.320239	1.945696	C	0.731897	2.220116	2.018749	C	0.644596	2.069353	2.111229
O	2.200528	-2.081946	0.187666	O	2.236525	-2.083516	0.109918	O	2.330569	-2.068042	0.012691
O	-3.429139	-2.855438	-0.033090	O	-3.339698	-2.596914	0.284656	O	-3.172748	-2.353682	0.133488
H	-5.478980	-0.674398	1.514414	H	-5.519876	-0.814395	1.376780	H	-5.555369	-1.418753	1.036769
H	-6.560717	-0.178393	-0.655398	H	-6.561759	-0.172196	-0.778399	H	-6.630259	0.084544	-0.591814
H	-5.171411	0.554102	-2.591955	H	-5.125839	0.647914	-2.642082	H	-5.226808	1.466194	-2.139367
H	-2.711557	0.735163	-2.336269	H	-2.673459	0.797724	-2.344690	H	-2.770456	1.427680	-1.961643
H	-2.017766	0.117916	2.374678	H	-2.708496	0.449377	2.540182	H	-3.229000	0.175562	2.311240
H	-2.526465	-1.569430	2.265540	H	-2.031376	-1.138770	2.172963	H	-1.997209	-1.085599	2.100323
H	-3.616827	-0.375126	2.972626	H	-3.683956	-1.009069	2.797332	H	-3.652609	-1.531904	2.571036
H	0.238583	-2.613153	0.678605	H	0.267572	-2.660736	0.602098	H	0.405541	-2.718115	0.484309
H	-1.470222	-2.383267	0.328633	H	-1.464116	-2.413375	0.298512	H	-1.334804	-2.558312	0.172138
H	2.520459	1.565751	0.931614	H	2.485845	1.535450	0.997135	H	2.428552	1.479486	1.084141
H	1.396971	2.877661	2.665681	H	1.320460	2.752955	2.770420	H	1.212667	2.568225	2.900977
H	0.510194	1.366235	2.404200	H	0.455035	1.244180	2.431982	H	0.379554	1.066503	2.463707
H	-0.115748	2.897500	1.741991	H	-0.179769	2.795043	1.827173	H	-0.274206	2.638234	1.938424
H	1.108126	3.995232	-0.265478	H	1.047600	3.989884	-0.115427	H	0.956085	3.958101	0.077743
H	2.636910	3.965348	0.630210	H	2.566864	3.945827	0.795322	H	2.462553	3.895394	1.008669
H	2.529011	3.179015	-0.956620	H	2.488441	3.225053	-0.824058	H	2.422315	3.259484	-0.646997
H	4.133792	-2.307932	-1.447318	H	4.181689	-2.221089	-1.516996	H	4.295430	-2.052683	-1.587772
H	5.240237	-1.055510	-1.991671	H	5.274050	-0.934674	-2.008497	H	5.343118	-0.703846	-2.004829

H	6.175492	-2.185329	0.036185	H	6.205643	-2.129509	-0.011992	H	6.296992	-1.954166	-0.053978
H	5.782348	-1.009048	2.111740	H	5.792512	-1.017956	2.095342	H	5.817234	-0.960039	2.097099
H	4.339773	-0.105615	1.378332	H	4.348357	-0.102408	1.379940	H	4.346941	-0.067450	1.406601
H	-3.651588	-2.478316	-0.909844	H	-3.684340	-2.543683	-0.626010	H	-3.495746	-2.501187	-0.768984

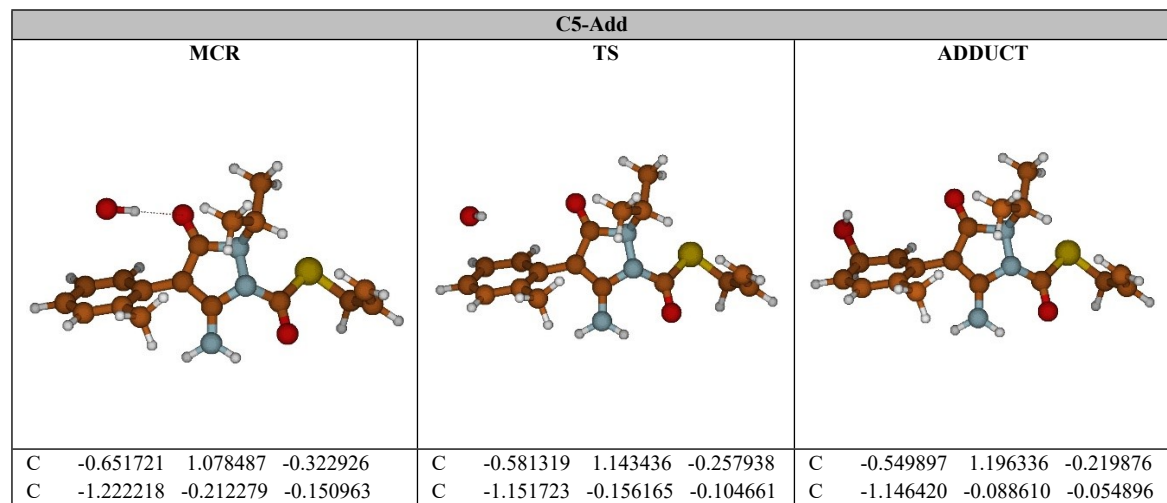
C3-Add											
MCR				TS				ADDUCT			
											
C	-2.701260	0.132331	-0.273898	C	-2.631871	0.176239	-0.295481	C	-2.602807	0.123233	-0.348867
C	-3.325667	0.428678	-1.493908	C	-3.240570	0.555654	-1.505282	C	-3.177459	0.596418	-1.566938
C	-4.706684	0.322652	-1.638808	C	-4.625626	0.488057	-1.683227	C	-4.573103	0.520937	-1.787183
C	-5.483669	-0.086696	-0.554578	C	-5.422022	0.014288	-0.654257	C	-5.400353	-0.016545	-0.846636
C	-4.873037	-0.370018	0.664551	C	-4.827366	-0.409010	0.555919	C	-4.884843	-0.552895	0.450339
C	-3.484304	-0.260389	0.834819	C	-3.429920	-0.263754	0.771099	C	-3.396981	-0.400822	0.645645
C	-1.237458	0.258381	-0.177162	C	-1.168353	0.277052	-0.180747	C	-1.139714	0.234371	-0.201611
C	-2.875788	-0.532737	2.185628	C	-2.868316	-0.625137	2.114276	C	-2.880757	-0.851078	1.978491
H	-5.478962	-0.673101	1.514698	H	-5.459889	-0.620595	1.411598	H	-5.392871	-0.048361	1.285999
H	-6.560706	-0.178474	-0.655417	H	-6.498775	-0.055769	-0.769486	H	-6.471639	-0.086977	-1.012436
H	-5.171361	0.552372	-2.592589	H	-5.065867	0.800948	-2.624125	H	-4.979929	0.889097	-2.724512
H	-2.711472	0.733304	-2.337116	H	-2.609611	0.905264	-2.318002	H	-2.525936	1.002458	-2.333381
H	-2.018570	0.120745	2.374709	H	-1.936125	-0.091446	2.318340	H	-1.907104	-0.410191	2.208516
H	-2.524539	-1.567401	2.265597	H	-2.659290	-1.700293	2.172761	H	-2.775073	-1.942488	2.022615
H	-3.616916	-0.374819	2.972537	H	-3.590640	-0.392321	2.900557	H	-3.589870	-0.571166	2.765312
C	-0.328074	-0.717579	0.188858	C	-0.278266	-0.727533	0.147881	C	-0.237868	-0.772955	0.081806
N	0.963720	-0.170730	0.159641	N	1.022135	-0.204193	0.143655	N	1.056115	-0.232557	0.118240
N	0.892321	1.169982	-0.277229	N	0.976287	1.154485	-0.237445	N	0.993970	1.144121	-0.188614
C	-0.492913	1.435879	-0.480166	C	-0.402293	1.453949	-0.432603	C	-0.387872	1.433705	-0.378073
O	-0.892441	2.558802	-0.817048	O	-0.783067	2.594920	-0.724398	O	-0.781672	2.585113	-0.607204
N	-0.537719	-2.000166	0.470014	N	-0.510319	-2.016383	0.386614	N	-0.451835	-2.075641	0.257032



H	0.238900	-2.613152	0.678756	H	0.254619	-2.657633	0.550445	H	0.322643	-2.714142	0.381276
H	-1.469971	-2.383517	0.328938	H	-1.442603	-2.379101	0.229291	H	-1.379747	-2.440552	0.083917
C	1.600160	2.097024	0.673653	C	1.698830	2.028864	0.752087	C	1.695803	1.973910	0.852973
C	0.791024	2.319550	1.945799	C	0.890789	2.211577	2.031167	C	0.871541	2.085555	2.129988
C	1.983788	3.388509	-0.030682	C	2.105032	3.342209	0.103186	C	2.097762	3.321439	0.275293
H	2.520147	1.565972	0.931658	H	2.609509	1.472350	0.988167	H	2.608796	1.414720	1.072767
H	1.395940	2.877171	2.665930	H	1.503879	2.727007	2.775360	H	1.473139	2.563961	2.907528
H	0.509991	1.365322	2.404123	H	0.590978	1.244128	2.448028	H	0.571747	1.096092	2.491822
H	-0.116711	2.896377	1.742124	H	-0.005676	2.813053	1.850166	H	-0.025961	2.691289	1.970119
H	1.107213	3.995628	-0.264343	H	1.239807	3.975504	-0.101367	H	1.228915	3.955068	0.087841
H	2.636258	3.965426	0.630859	H	2.769174	3.877133	0.787975	H	2.745663	3.829468	0.995248
H	2.527941	3.179832	-0.956302	H	2.643870	3.164117	-0.831852	H	2.652589	3.194361	-0.658766
C	2.081460	-0.929423	-0.187423	C	2.128973	-0.969008	-0.226720	C	2.177613	-0.960400	-0.278137
O	2.200710	-2.081906	0.187357	O	2.225450	-2.136013	0.107122	O	2.284978	-2.144313	-0.013111
S	3.269205	-0.084463	-1.195415	S	3.333578	-0.109349	-1.200511	S	3.388784	-0.030440	-1.177440
C	4.575026	-1.345185	-1.171876	C	4.621173	-1.388982	-1.210999	C	4.692761	-1.291851	-1.237676
C	5.356884	-1.469325	0.105993	C	5.394295	-1.562918	0.066417	C	5.444350	-1.531126	0.042023
C	5.144125	-0.827326	1.252857	C	5.186739	-0.949645	1.229840	C	5.207218	-0.990534	1.235404
H	4.134316	-2.307510	-1.447541	H	4.168242	-2.335857	-1.518280	H	4.257798	-2.224649	-1.607457
H	5.240746	-1.054849	-1.991374	H	5.294909	-1.082682	-2.018061	H	5.377311	-0.931240	-2.012622
H	6.175509	-2.185190	0.036531	H	6.201026	-2.290352	-0.019727	H	6.262057	-2.242439	-0.070995
H	5.782157	-1.008912	2.112047	H	5.817127	-1.166178	2.086562	H	5.824578	-1.249501	2.089820
H	4.339796	-0.105303	1.378413	H	4.394165	-0.217721	1.371812	H	4.402399	-0.278175	1.405210
O	-3.429000	-2.855514	-0.031090	O	-4.767690	-2.492003	0.185320	O	-5.281704	-1.934367	0.621678
H	-3.651061	-2.479140	-0.908260	H	-4.157709	-2.423971	-0.571452	H	-4.892343	-2.440685	-0.107344

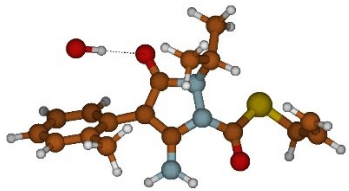
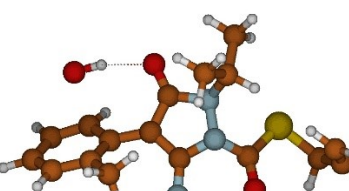
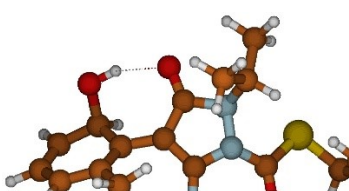
C4-Add												
MCR				TS				ADDUCT				
												
C	-0.493070	1.436291	-0.480263	C	-0.398106	1.360353	-0.488917	C	-0.392594	1.327301	-0.430717	
C	-1.237579	0.258822	-0.177378	C	-1.139590	0.207652	-0.074896	C	-1.112901	0.136324	-0.086469	
C	-0.328081	-0.717490	0.187642	C	-0.216349	-0.747519	0.319691	C	-0.164894	-0.819961	0.249380	
N	0.963621	-0.170750	0.158169	N	1.072372	-0.210069	0.202982	N	1.111526	-0.247405	0.172511	
N	0.892323	1.170235	-0.277762	N	0.988575	1.099374	-0.314749	N	0.999603	1.088337	-0.268282	
C	-2.701348	0.132500	-0.274236	C	-2.600681	0.107902	-0.110266	C	-2.564122	0.013123	-0.131444	
C	-3.325855	0.428936	-1.494104	C	-3.261614	0.478345	-1.301910	C	-3.243961	0.456526	-1.312566	
C	-4.706927	0.322796	-1.638863	C	-4.636462	0.410883	-1.405699	C	-4.591908	0.375538	-1.446254	
C	-5.483765	-0.086959	-0.554761	C	-5.397264	-0.067897	-0.313480	C	-5.462472	-0.198046	-0.373813	
C	-4.872942	-0.370580	0.664263	C	-4.739655	-0.358885	0.900381	C	-4.699265	-0.543766	0.865783	
C	-3.484259	-0.260536	0.834513	C	-3.355644	-0.292249	1.021338	C	-3.340180	-0.470753	0.979675	
C	-2.875590	-0.532329	2.185379	C	-2.714676	-0.588588	2.352594	C	-2.677977	-0.831182	2.287574	
N	-0.537804	-2.000301	0.467537	N	-0.406170	-2.011157	0.685937	N	-0.326973	-2.110652	0.525319	
C	2.081622	-0.929176	-0.188123	C	2.176616	-0.994926	-0.137547	C	2.237141	-0.983286	-0.202159	
S	3.269947	-0.083893	-1.195151	S	3.327276	-0.219312	-1.237949	S	3.375384	-0.118654	-1.248266	
C	4.575482	-1.344895	-1.171622	C	4.627969	-1.484742	-1.189644	C	4.712799	-1.346107	-1.247753	
C	5.357175	-1.469315	0.106309	C	5.459015	-1.537780	0.061692	C	5.526556	-1.441565	0.012537	
C	5.143914	-0.827912	1.253412	C	5.289385	-0.834742	1.179459	C	5.326441	-0.794471	1.158806	
C	1.599883	2.096514	0.674147	C	1.738706	2.085591	0.540036	C	1.721422	2.038489	0.649716	
C	1.983795	3.388557	-0.028988	C	2.106060	3.317149	-0.271856	C	2.061642	3.326764	-0.081911	
O	-0.892544	2.559356	-0.816741	O	-0.805895	2.459963	-0.879099	O	-0.823526	2.438987	-0.757161	
C	0.790344	2.318014	1.946218	C	0.977776	2.408912	1.820183	C	0.946937	2.263747	1.942644	
O	2.200780	-2.081738	0.186537	O	2.306132	-2.121667	0.304512	O	2.393293	-2.129930	0.176493	
O	-3.429452	-2.855722	-0.028030	O	-5.654234	-2.079042	-1.025679	O	-6.193303	-1.348218	-0.868474	

H	-5.478775	-0.673921	1.514378	H	-5.331946	-0.647804	1.764500	H	-5.289748	-0.872933	1.718093
H	-6.560851	-0.178795	-0.655348	H	-6.478118	0.007574	-0.331344	H	-6.263860	0.510838	-0.125178
H	-5.171674	0.552499	-2.592618	H	-5.134189	0.687187	-2.329441	H	-5.079696	0.696093	-2.362662
H	-2.711820	0.733875	-2.337314	H	-2.666351	0.806431	-2.148758	H	-2.642655	0.845833	-2.130257
H	-2.019845	0.122948	2.374983	H	-1.805804	0.002017	2.500314	H	-1.839240	-0.162128	2.504867
H	-2.522081	-1.566233	2.265078	H	-2.443248	-1.645395	2.445295	H	-2.288977	-1.853803	2.280316
H	-3.617305	-0.376326	2.972113	H	-3.413312	-0.359547	3.160619	H	-3.399551	-0.759330	3.104368
H	0.238563	-2.613358	0.676966	H	0.382062	-2.613291	0.885625	H	0.472792	-2.708747	0.686748
H	-1.470527	-2.383107	0.328012	H	-1.330175	-2.413448	0.594731	H	-1.242212	-2.523246	0.398673
H	2.519796	1.565270	0.932006	H	2.662425	1.563936	0.803371	H	2.656634	1.524461	0.886072
H	1.395134	2.874833	2.667073	H	1.615933	3.004604	2.478383	H	1.566398	2.834992	2.639269
H	0.508962	1.363424	2.403577	H	0.699221	1.493207	2.352733	H	0.690392	1.310813	2.417834
H	-0.117218	2.895208	1.742786	H	0.071999	2.985536	1.608137	H	0.027150	2.828338	1.760545
H	1.107329	3.995809	-0.262692	H	1.224733	3.909671	-0.524285	H	1.167184	3.913038	-0.300503
H	2.635836	3.964990	0.633399	H	2.780484	3.938504	0.324124	H	2.719339	3.925230	0.554813
H	2.528525	3.180614	-0.954434	H	2.621089	3.035307	-1.194770	H	2.585715	3.115869	-1.018501
H	4.134528	-2.307092	-1.447371	H	4.172569	-2.458761	-1.390394	H	4.290069	-2.320963	-1.507005
H	5.241311	-1.054670	-1.991060	H	5.261738	-1.247665	-2.050459	H	5.351701	-1.044444	-2.084438
H	6.176066	-2.184858	0.036691	H	6.275814	-2.256378	-0.000551	H	6.359137	-2.139654	-0.070299
H	5.781778	-1.009668	2.112690	H	5.961171	-0.969104	2.021402	H	5.988693	-0.954239	2.003875
H	4.339335	-0.106182	1.379077	H	4.489545	-0.106394	1.297169	H	4.509598	-0.089114	1.297762
H	-3.650270	-2.481844	-0.906590	H	-4.696453	-2.245005	-1.083223	H	-5.541789	-2.029181	-1.094012

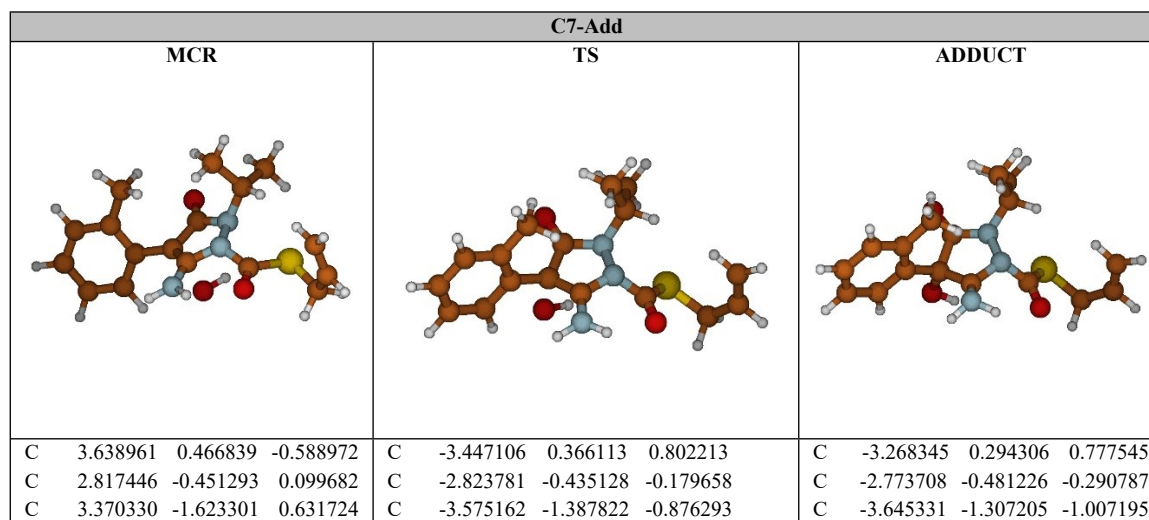


C	-0.177196	-1.079403	0.119296	C	-0.109279	-1.035062	0.119613	C	-0.121058	-0.989840	0.153892
N	1.021002	-0.354377	0.145881	N	1.095293	-0.317733	0.143628	N	1.101548	-0.302673	0.148781
N	0.752472	0.996612	-0.159076	N	0.831293	1.044438	-0.117125	N	0.864299	1.065658	-0.105439
C	-2.660575	-0.515322	-0.260564	C	-2.591657	-0.449852	-0.196484	C	-2.596186	-0.361762	-0.111417
C	-3.330749	-0.154421	-1.441703	C	-3.280025	-0.059706	-1.343693	C	-3.285880	-0.018686	-1.244820
C	-4.698372	-0.373524	-1.587166	C	-4.674174	-0.248185	-1.461463	C	-4.765822	-0.173448	-1.393620
C	-5.411928	-0.967404	-0.545714	C	-5.353851	-0.950438	-0.436436	C	-5.396895	-0.825672	-0.204260
C	-4.754218	-1.320537	0.629881	C	-4.673238	-1.330537	0.704101	C	-4.683245	-1.154647	0.905484
C	-3.381878	-1.096307	0.801641	C	-3.297541	-1.074407	0.861174	C	-3.278295	-0.930022	1.014980
C	-2.728035	-1.458780	2.109856	C	-2.621603	-1.468494	2.142993	C	-2.573151	-1.283566	2.288587
N	-0.196189	-2.399187	0.276649	N	-0.131352	-2.359903	0.245893	N	-0.173780	-2.313032	0.289373
C	2.234254	-0.912067	-0.265739	C	2.294525	-0.869353	-0.310252	C	2.276289	-0.881987	-0.331401
S	3.275871	0.174605	-1.197755	S	3.329938	0.244145	-1.218652	S	3.321687	0.211940	-1.253264
C	4.744973	-0.887969	-1.288816	C	4.786352	-0.827753	-1.379377	C	4.751117	-0.890946	-1.443567
C	5.553693	-1.014070	-0.028129	C	5.617257	-1.012467	-0.140549	C	5.598675	-1.100201	-0.219980
C	5.270462	-0.512218	1.171986	C	5.362315	-0.555207	1.083475	C	5.371802	-0.648023	1.011432
C	1.356308	1.930728	0.856029	C	1.450491	1.938708	0.922897	C	1.517744	1.939826	0.930876
C	1.561952	3.310283	0.251629	C	1.653330	3.338531	0.365606	C	1.737214	3.340488	0.382008
O	-1.212548	2.171483	-0.530013	O	-1.142732	2.233084	-0.431197	O	-1.085807	2.300423	-0.385253
C	0.549510	1.947200	2.148661	C	0.661020	1.913541	2.226231	C	0.750711	1.918239	2.247759
O	2.517198	-2.063369	0.008890	O	2.575275	-2.032398	-0.084249	O	2.532812	-2.053042	-0.117467
H	-5.315532	-1.765707	1.447550	H	-5.203454	-1.828878	1.510892	H	-5.192912	-1.596603	1.758751
H	-6.478170	-1.146541	-0.644635	H	-6.415125	-1.152794	-0.538325	H	-6.467705	-1.003685	-0.249747
H	-5.199690	-0.085308	-2.505861	H	-5.156313	-0.085319	-2.417975	H	-4.986315	-0.753809	-2.300351
H	-2.762342	0.296685	-2.251248	H	-2.738566	0.421307	-2.153256	H	-2.753667	0.411957	-2.089655
H	-1.906020	-0.777612	2.349756	H	-1.783565	-0.805760	2.376636	H	-1.706096	-0.640284	2.465825
H	-2.318961	-2.475012	2.084636	H	-2.228674	-2.490186	2.078657	H	-2.213416	-2.321190	2.270344
H	-3.459340	-1.421413	2.920710	H	-3.334929	-1.445536	2.969920	H	-3.255376	-1.195912	3.138375
H	0.658285	-2.918326	0.428892	H	0.727214	-2.885303	0.345124	H	0.669882	-2.859914	0.396604
H	-1.064680	-2.893851	0.118485	H	-1.000152	-2.848356	0.071125	H	-1.063999	-2.778184	0.166969
H	2.339939	1.501557	1.061903	H	2.435502	1.500280	1.101799	H	2.497450	1.481931	1.089402
H	1.097413	2.512187	2.907550	H	1.219144	2.452697	2.996444	H	1.329673	2.444855	3.011268
H	0.394031	0.931026	2.526624	H	0.508855	0.885669	2.572704	H	0.589955	0.890677	2.591180
H	-0.424375	2.424609	2.002650	H	-0.314066	2.396446	2.108682	H	-0.219309	2.415717	2.149989
H	0.612578	3.817121	0.069429	H	0.703306	3.854067	0.213092	H	0.794772	3.875725	0.252280
H	2.145194	3.913107	0.953403	H	2.246920	3.915098	1.080712	H	2.355687	3.898996	1.090359
H	2.115627	3.244152	-0.689299	H	2.194937	3.304032	-0.584033	H	2.259706	3.303864	-0.578225
H	4.437496	-1.874042	-1.648289	H	4.462850	-1.795513	-1.772988	H	4.400345	-1.849550	-1.836246
H	5.352526	-0.436562	-2.080134	H	5.383690	-0.349951	-2.162948	H	5.345689	-0.422303	-2.234736
H	6.462596	-1.599718	-0.163282	H	6.516736	-1.602024	-0.315925	H	6.484356	-1.704519	-0.414347
H	5.940034	-0.678435	2.009995	H	6.045200	-0.761159	1.901693	H	6.063749	-0.872522	1.817050
H	4.376066	0.077107	1.363717	H	4.478181	0.035343	1.314665	H	4.502106	-0.043769	1.261181

O	-3.934855	2.389490	-0.438302	O	-5.272632	1.713475	-0.957106	O	-5.389028	1.104645	-1.671585
H	-2.941523	2.304744	-0.450802	H	-4.817906	1.719090	-0.096051	H	-5.230067	1.676726	-0.905695

			C6-Add								
MCR				TS				ADDUCT			
											
C	-3.381779	-1.096275	0.801825	C	-3.362532	-1.097061	0.797882	C	-3.373503	-1.060900	0.821916
C	-2.660584	-0.515333	-0.260501	C	-2.678447	-0.357970	-0.181320	C	-2.695752	-0.263174	-0.085093
C	-3.330896	-0.154450	-1.441543	C	-3.402639	0.157074	-1.299083	C	-3.444871	0.433181	-1.206519
C	-4.698566	-0.373502	-1.586823	C	-4.736606	-0.258452	-1.534219	C	-4.764346	-0.198109	-1.524333
C	-5.412012	-0.967274	-0.545252	C	-5.387589	-1.030871	-0.592159	C	-5.367607	-1.045910	-0.650308
C	-4.754149	-1.320402	0.630271	C	-4.710320	-1.416494	0.571716	C	-4.716894	-1.425442	0.554870
C	-1.222215	-0.212288	-0.151094	C	-1.242523	-0.073152	-0.085852	C	-1.259245	-0.009560	-0.002643
C	-0.651791	1.078528	-0.322961	C	-0.615993	1.196655	-0.272355	C	-0.602157	1.243210	-0.208217
N	0.752441	0.996655	-0.159303	N	0.786497	1.046748	-0.127800	N	0.798063	1.064938	-0.088684
N	1.021031	-0.354394	0.145160	N	1.001256	-0.317521	0.155396	N	0.988971	-0.305829	0.180548
C	-0.177096	-1.079424	0.118768	C	-0.225218	-0.990057	0.142005	C	-0.252118	-0.950807	0.188647
O	-1.212674	2.171555	-0.529793	O	-1.124027	2.311724	-0.468027	O	-1.087212	2.370560	-0.407123
N	-0.196130	-2.399238	0.275960	N	-0.294150	-2.311346	0.258498	N	-0.347498	-2.271919	0.287165
C	2.234376	-0.911972	-0.266166	C	2.185012	-0.919889	-0.281173	C	2.149789	-0.927680	-0.288144
O	2.517247	-2.063338	0.008307	O	2.423553	-2.085398	-0.025082	O	2.368376	-2.101727	-0.053233
C	1.356323	1.930532	0.855990	C	1.444150	1.943511	0.887731	C	1.488877	1.939449	0.924783
C	0.549609	1.946646	2.148692	C	0.651857	1.990221	2.188558	C	0.719487	1.984296	2.239283
C	-2.727719	-1.458838	2.109896	C	-2.718736	-1.540269	2.086930	C	-2.753444	-1.567378	2.102092
S	3.276227	0.174857	-1.197719	S	3.257774	0.135020	-1.213450	S	3.226591	0.116908	-1.227885
C	4.745454	-0.887574	-1.288486	C	4.679877	-0.987018	-1.338504	C	4.622922	-1.031822	-1.394237
C	5.553804	-1.013832	-0.027592	C	5.497947	-1.164961	-0.090187	C	5.461616	-1.241995	-0.164733
C	5.270091	-0.512295	1.172537	C	5.252519	-0.666446	1.119571	C	5.246058	-0.759697	1.057213
C	1.561877	3.310243	0.251930	C	1.709164	3.315556	0.289564	C	1.764712	3.313956	0.337565
O	-3.935942	2.389036	-0.438601	O	-3.929534	2.026050	-0.584178	O	-3.736120	1.807906	-0.848867

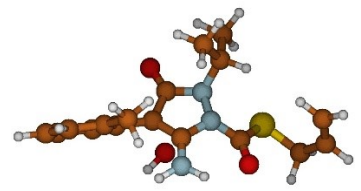
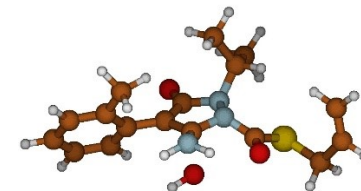
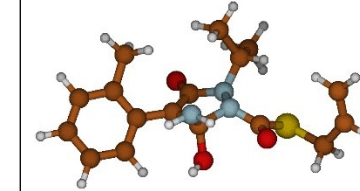
H	-5.315381	-1.765522	1.448024	H	-5.239815	-1.985498	1.331828	H	-5.243675	-2.041541	1.277400
H	-6.478293	-1.146288	-0.643968	H	-6.420382	-1.328892	-0.740031	H	-6.358558	-1.437617	-0.861076
H	-5.199959	-0.085314	-2.505486	H	-5.243694	0.079523	-2.431931	H	-5.257321	0.120098	-2.438247
H	-2.762590	0.296553	-2.251215	H	-2.838784	0.604496	-2.111372	H	-2.809739	0.450460	-2.102960
H	-2.317890	-2.474748	2.084204	H	-2.378843	-2.580266	2.034029	H	-2.474784	-2.624738	2.032177
H	-3.459041	-1.422351	2.920771	H	-3.445488	-1.478396	2.900916	H	-3.480558	-1.480364	2.914578
H	-1.906175	-0.777192	2.350082	H	-1.857542	-0.917514	2.343486	H	-1.861786	-0.998282	2.377084
H	0.658374	-2.918417	0.427886	H	0.544914	-2.866955	0.363767	H	0.482625	-2.848049	0.341943
H	-1.064511	-2.893883	0.117105	H	-1.179201	-2.770086	0.085326	H	-1.246042	-2.704917	0.116024
H	2.339990	1.501389	1.061738	H	2.407798	1.466015	1.081328	H	2.447733	1.443901	1.095787
H	1.097617	2.511306	2.907745	H	1.234873	2.521208	2.945779	H	1.322925	2.498348	2.992149
H	0.394079	0.930346	2.526310	H	0.449126	0.980194	2.560795	H	0.506936	0.973733	2.604476
H	-0.424254	2.424174	2.002918	H	-0.298055	2.517050	2.055916	H	-0.224207	2.527172	2.127643
H	0.612466	3.816936	0.069525	H	0.782409	3.865990	0.117420	H	0.843702	3.881032	0.190415
H	2.144779	3.913034	0.954013	H	2.324774	3.887099	0.989858	H	2.402985	3.866951	1.032438
H	2.115867	3.244401	-0.688833	H	2.251807	3.228971	-0.656137	H	2.287314	3.230108	-0.619589
H	4.438170	-1.873607	-1.648233	H	4.326640	-1.953933	-1.707862	H	4.243253	-1.986939	-1.768112
H	5.353202	-0.435955	-2.079536	H	5.296135	-0.549717	-2.131044	H	5.232170	-0.596978	-2.193488
H	6.462840	-1.599310	-0.162592	H	6.378360	-1.788146	-0.244662	H	6.329369	-1.875724	-0.345677
H	5.939415	-0.678583	2.010729	H	5.924563	-0.872520	1.946673	H	5.929747	-0.989062	1.868473
H	4.375529	0.076841	1.364089	H	4.387252	-0.041257	1.330305	H	4.394206	-0.125415	1.293765
H	-2.942680	2.304352	-0.450738	H	-2.985915	2.275867	-0.488181	H	-2.870011	2.233336	-0.681310



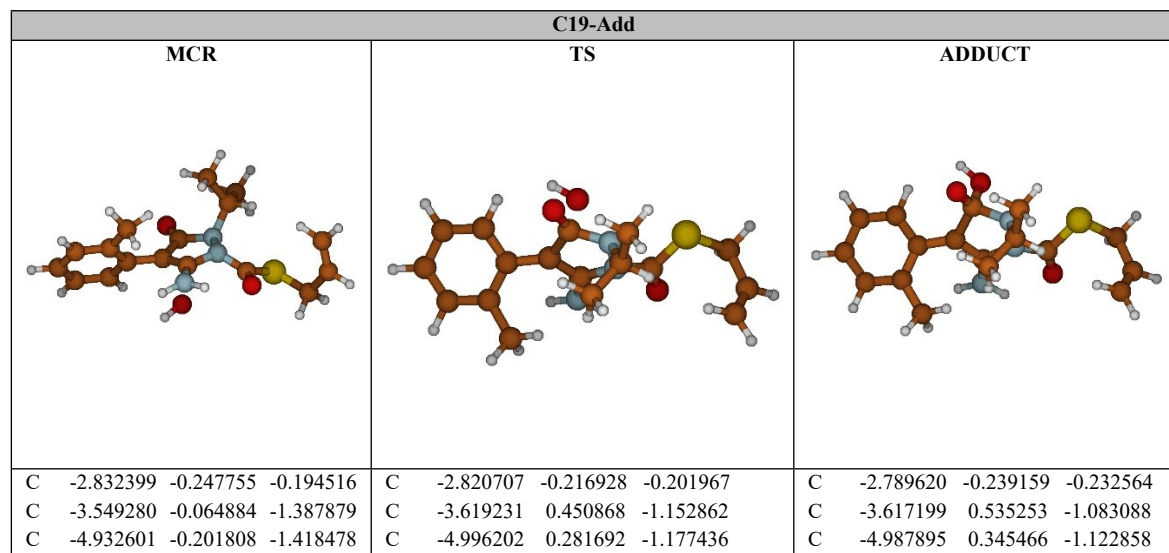
C	4.734065	-1.883328	0.518742	C	-4.939765	-1.538924	-0.634397	C	-5.001362	-1.369982	-0.689075
C	5.556963	-0.965862	-0.131284	C	-5.565817	-0.735747	0.314492	C	-5.498248	-0.604614	0.361455
C	5.007267	0.190850	-0.681046	C	-4.818327	0.202178	1.024053	C	-4.631289	0.213838	1.082414
C	1.361818	-0.204304	0.201464	C	-1.351732	-0.293788	-0.403715	C	-1.292438	-0.486527	-0.642664
C	0.739483	0.987023	0.753738	C	-0.727398	0.976526	-0.812444	C	-0.687413	0.920962	-0.843814
N	-0.633707	0.955668	0.437939	N	0.622883	0.937229	-0.456423	N	0.550599	0.953226	-0.278314
N	-0.828991	-0.146749	-0.424591	N	0.806561	-0.187618	0.378806	N	0.771354	-0.195726	0.523006
C	0.377169	-0.820544	-0.594478	C	-0.409028	-0.877971	0.471695	C	-0.401495	-1.023505	0.420742
O	1.259520	1.893517	1.399090	O	-1.258748	1.927639	-1.379137	O	-1.225498	1.852167	-1.432715
N	0.494555	-1.893666	-1.345756	N	-0.556113	-1.967787	1.207001	N	-0.781654	-1.789497	1.496696
C	-2.025397	-0.883585	-0.304126	C	2.006315	-0.920423	0.275912	C	1.970468	-0.911432	0.295644
O	-2.243878	-1.821166	-1.042999	O	2.205897	-1.865237	1.011977	O	2.195696	-1.912577	0.945710
C	-1.281953	2.214182	-0.060221	C	1.318347	2.178595	0.010312	C	1.279829	2.198695	0.089022
C	-0.453287	2.877472	-1.152857	C	0.521387	2.913027	1.080126	C	0.505356	3.030007	1.103714
C	3.078610	1.701511	-1.246059	C	-2.683291	1.377989	1.616417	C	-2.403911	1.227180	1.585962
S	-3.102512	-0.340275	0.985831	S	3.124286	-0.371175	-0.978927	S	3.049063	-0.285604	-0.962853
C	-4.503803	-1.439050	0.630546	C	4.522961	-1.456032	-0.573841	C	4.444524	-1.418700	-0.709035
C	-5.338691	-1.085742	-0.568264	C	5.309601	-1.092443	0.654162	C	5.297550	-1.156410	0.500367
C	-5.120486	-0.115697	-1.453462	C	5.056116	-0.116722	1.523678	C	5.103712	-0.241046	1.447529
C	-1.591573	3.138938	1.106648	C	1.667549	3.056182	-1.182575	C	1.642467	2.994638	-1.159043
O	0.700023	-1.437919	1.894244	O	-1.079797	-1.252117	-2.041887	O	-1.138514	-1.179816	-1.895930
H	5.646807	0.893662	-1.208531	H	-5.301755	0.820543	1.775616	H	-5.013544	0.809103	1.907508
H	6.622547	-1.153725	-0.221854	H	-6.628619	-0.841414	0.510076	H	-6.551073	-0.644776	0.623581
H	5.148053	-2.794288	0.939106	H	-5.505395	-2.282320	-1.187210	H	-5.658914	-2.017581	-1.260403
H	2.719934	-2.324310	1.142891	H	-3.085888	-2.010483	-1.613806	H	-3.260857	-1.908916	-1.821186
H	2.833705	2.471769	-0.507943	H	-2.358587	2.220992	0.998681	H	-2.219247	2.156043	1.037348
H	2.160493	1.473923	-1.797813	H	-1.788038	0.939376	2.070353	H	-1.434567	0.789956	1.841551
H	3.805890	2.120564	-1.944860	H	-3.312875	1.770863	2.417707	H	-2.906362	1.489263	2.519841
H	-0.300839	-2.273601	-1.845642	H	0.206998	-2.333142	1.763488	H	-0.007139	-2.222225	1.992742
H	1.382070	-2.384292	-1.361929	H	-1.426065	-2.484272	1.140543	H	-1.515400	-2.456986	1.275657
H	-2.228117	1.875390	-0.490826	H	2.248003	1.815705	0.455519	H	2.201444	1.846654	0.558337
H	-1.027720	3.699462	-1.588492	H	1.140214	3.715186	1.491632	H	1.132099	3.870588	1.414780
H	-0.215018	2.165508	-1.949729	H	0.245562	2.238476	1.896245	H	0.254410	2.440398	1.989384
H	0.478603	3.284740	-0.749220	H	-0.385174	3.358980	0.662082	H	-0.412335	3.431144	0.664868
H	-0.679012	3.545142	1.547390	H	0.770547	3.474389	-1.644116	H	0.758805	3.453644	-1.606916
H	-2.197085	3.971996	0.739199	H	2.293933	3.882725	-0.836169	H	2.335433	3.790281	-0.872601
H	-2.157655	2.614162	1.881342	H	2.223944	2.491666	-1.935798	H	2.130484	2.363676	-1.906279
H	-4.128174	-2.463120	0.550316	H	4.154951	-2.483557	-0.505415	H	4.059274	-2.442046	-0.693548
H	-5.113482	-1.393548	1.538746	H	5.164228	-1.405103	-1.459854	H	5.043836	-1.316689	-1.619516
H	-6.206842	-1.733591	-0.685547	H	6.173877	-1.737498	0.809601	H	6.156976	-1.823016	0.566397
H	-5.803408	0.035165	-2.283497	H	5.706680	0.040713	2.378126	H	5.796920	-0.153182	2.278149
H	-4.268671	0.557815	-1.386428	H	4.206800	0.555389	1.420069	H	4.260823	0.446909	1.431851



H	0.018269	-0.851328	2.263551	H	-0.149246	-1.057130	-2.238670	H	-0.213826	-1.460662	-1.978833
---	----------	-----------	----------	---	-----------	-----------	-----------	---	-----------	-----------	-----------

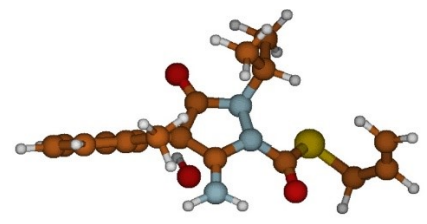
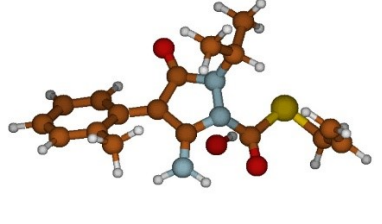
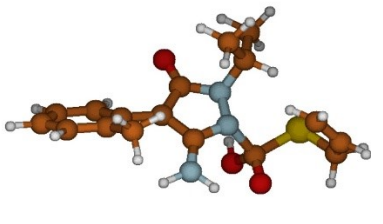
C16-Add											
MCR			TS			ADDUCT					
											
C	-3.549080	-0.064219	-1.387835	C	-3.453210	-0.055293	-1.447255	C	-3.312256	-1.646319	-0.665605
C	-2.832447	-0.247497	-0.194380	C	-2.843741	-0.199258	-0.188625	C	-2.844331	-0.412783	-0.173600
C	-3.521765	-0.536402	1.002757	C	-3.622712	-0.497354	0.947649	C	-3.760855	0.538391	0.333447
C	-4.913611	-0.680335	0.944463	C	-4.999290	-0.682806	0.770051	C	-5.123048	0.225404	0.292524
C	-5.616922	-0.523680	-0.246686	C	-5.596025	-0.566578	-0.482003	C	-5.582510	-0.984353	-0.223708
C	-4.932363	-0.201329	-1.418830	C	-4.821371	-0.242724	-1.597842	C	-4.672751	-1.928430	-0.699166
C	-1.372250	-0.056835	-0.213921	C	-1.397790	0.020585	-0.101836	C	-1.409622	-0.150073	-0.168430
C	-0.379542	-0.891317	0.333153	C	-0.381705	-0.872628	0.340567	C	-0.376321	-1.066608	0.429451
N	0.837981	-0.218686	0.298750	N	0.839419	-0.170816	0.357997	N	0.854891	-0.235751	0.320376
N	0.656131	1.075617	-0.238862	N	0.651975	1.106154	-0.232489	N	0.614070	0.946238	-0.428136
C	-0.720231	1.201877	-0.520521	C	-0.720928	1.238973	-0.504047	C	-0.751000	1.016248	-0.715818
N	-0.493160	-2.136466	0.742836	N	-0.526848	-2.013662	1.014710	N	-0.666273	-1.375558	1.795012
O	-1.228643	2.246388	-0.917814	O	-1.225545	2.269659	-0.942876	O	-1.268780	1.953256	-1.323673
C	1.276290	2.140555	0.623089	C	1.295346	2.203666	0.569240	C	1.258932	2.171586	0.152251
C	0.425609	2.425717	1.854655	C	0.457825	2.562769	1.790754	C	0.417893	2.767444	1.275470
C	2.023101	-0.906869	-0.014836	C	1.998650	-0.879689	-0.006025	C	2.051062	-0.899057	0.123834
O	2.229135	-2.016482	0.434806	O	2.192697	-2.001308	0.419716	O	2.329186	-1.892274	0.775976
C	-2.828177	-0.656704	2.336389	C	-3.038913	-0.579812	2.335190	C	-3.319828	1.833198	0.966377
C	1.576237	3.379351	-0.205477	C	1.605943	3.396280	-0.320984	C	1.579605	3.174879	-0.945132
S	3.125488	-0.033519	-1.084410	S	3.104117	-0.015448	-1.080717	S	3.123432	-0.209694	-1.119476
C	4.530751	-1.180006	-0.997881	C	4.480110	-1.198953	-1.044563	C	4.573705	-1.262687	-0.836979
C	5.325406	-1.161670	0.277887	C	5.301842	-1.226470	0.213752	C	5.398830	-0.947991	0.379403
C	5.066960	-0.470504	1.385992	C	5.084478	-0.550873	1.340160	C	5.144774	-0.039964	1.319538
O	-0.592411	-0.821750	-2.180904	O	-0.297321	-1.322199	-1.622025	O	-0.193477	-2.194849	-0.408550
H	-5.451646	-0.902486	1.862405	H	-5.610584	-0.906813	1.640439	H	-5.833402	0.944107	0.692380

H	-6.696437	-0.638945	-0.256663	H	-6.666492	-0.715291	-0.585613	H	-6.647571	-1.194010	-0.241808
H	-5.470225	-0.061082	-2.350993	H	-5.279956	-0.138334	-2.575765	H	-5.018674	-2.877471	-1.095526
H	-3.004367	0.178431	-2.295166	H	-2.834353	0.188776	-2.306352	H	-2.601030	-2.368917	-1.051290
H	-2.478173	-1.678282	2.518660	H	-2.812519	-1.615610	2.609264	H	-2.385336	1.711917	1.522321
H	-3.523164	-0.401931	3.139653	H	-3.759059	-0.199603	3.063896	H	-4.087095	2.188132	1.658099
H	-1.963132	0.009828	2.407410	H	-2.117975	0.002456	2.426513	H	-3.157895	2.610028	0.213295
H	0.313840	-2.658286	1.063472	H	0.298391	-2.589287	1.143087	H	0.066626	-1.979047	2.167027
H	-1.389836	-2.600696	0.651100	H	-1.409188	-2.499110	0.892468	H	-1.555312	-1.873574	1.844543
H	2.226139	1.704252	0.943104	H	2.240861	1.769226	0.903072	H	2.199147	1.805194	0.570487
H	0.971793	3.097839	2.521865	H	1.023394	3.248656	2.427011	H	0.990437	3.555564	1.772151
H	0.208425	1.503183	2.403291	H	0.219050	1.669247	2.377263	H	0.163603	2.006345	2.020240
H	-0.518180	2.907609	1.581239	H	-0.474649	3.056442	1.500008	H	-0.505611	3.208424	0.887719
H	0.660853	3.891170	-0.508534	H	0.694748	3.903111	-0.644557	H	0.670339	3.609027	-1.365962
H	2.170210	4.067782	0.401996	H	2.210777	4.106986	0.249014	H	2.179613	3.982117	-0.515804
H	2.152017	3.120923	-1.098627	H	2.174000	3.087797	-1.203145	H	2.154123	2.705795	-1.748584
H	4.168256	-2.189627	-1.211183	H	4.086053	-2.194560	-1.268028	H	4.246627	-2.305983	-0.816689
H	5.165838	-0.885734	-1.839990	H	5.105646	-0.906932	-1.894579	H	5.179858	-1.137353	-1.740161
H	6.198976	-1.812034	0.243357	H	6.157084	-1.898516	0.148484	H	6.293909	-1.564540	0.458968
H	5.722552	-0.547096	2.247692	H	5.755335	-0.661346	2.186310	H	5.823223	0.091023	2.156710
H	4.207948	0.191095	1.476809	H	4.244767	0.130407	1.461132	H	4.264729	0.599055	1.290613
H	-1.298592	-1.488915	-2.206215	H	-1.112730	-1.830480	-1.763597	H	-0.603142	-2.967607	0.008957

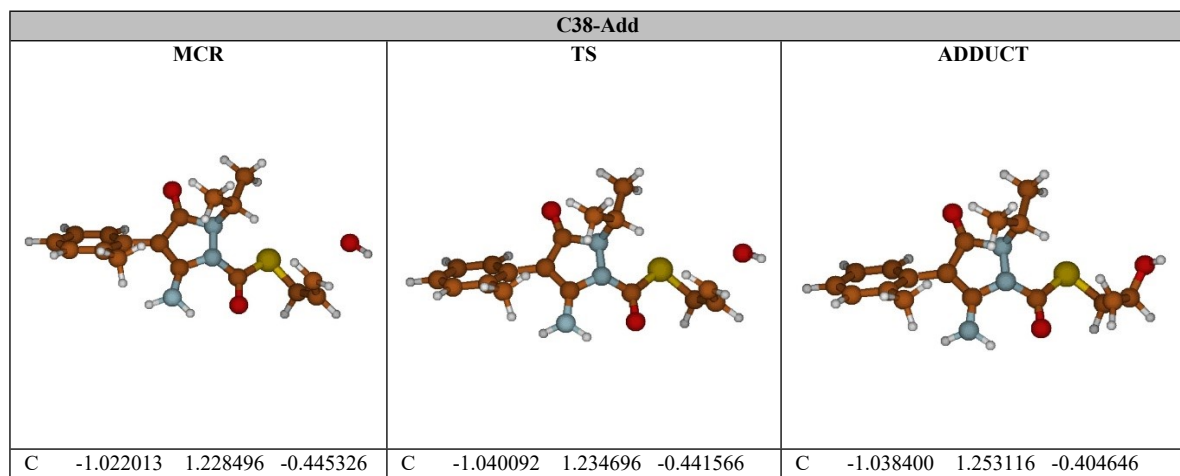


C	-5.616937	-0.523600	-0.246051	C	-5.604771	-0.547841	-0.234177	C	-5.573995	-0.606175	-0.284246
C	-4.913363	-0.679867	0.944993	C	-4.829044	-1.175297	0.735418	C	-4.779726	-1.341857	0.589897
C	-3.521488	-0.536091	1.002887	C	-3.438616	-1.023504	0.784458	C	-3.391572	-1.182447	0.645029
C	-1.372172	-0.057241	-0.214426	C	-1.381026	0.004461	-0.231653	C	-1.370393	0.011738	-0.296512
C	-2.827573	-0.656038	2.336389	C	-2.689796	-1.671410	1.922917	C	-2.636169	-1.978398	1.679304
H	-5.451185	-0.901589	1.863164	H	-5.308493	-1.787300	1.494866	H	-5.244660	-2.052472	1.267956
H	-6.696468	-0.638739	-0.255718	H	-6.680951	-0.689770	-0.242000	H	-6.648257	-0.761498	-0.298835
H	-5.470642	-0.061874	-2.350585	H	-5.589852	0.793770	-1.927562	H	-5.597286	0.935353	-1.799360
H	-3.004786	0.177335	-2.295451	H	-3.151976	1.098796	-1.886566	H	-3.164263	1.270727	-1.737703
H	-1.962180	0.010097	2.406828	H	-1.773343	-1.133641	2.177701	H	-1.706383	-1.498281	1.985839
H	-2.478052	-1.677711	2.519075	H	-2.424085	-2.708928	1.694262	H	-2.398155	-2.983785	1.315310
H	-3.522194	-0.400510	3.139732	H	-3.326981	-1.691162	2.810156	H	-3.261124	-2.099765	2.567193
C	-0.379456	-0.891432	0.333048	C	-0.332760	-0.943975	-0.081483	C	-0.298960	-0.926296	-0.246897
N	0.837976	-0.218635	0.298738	N	0.866092	-0.264420	-0.010977	N	0.886163	-0.228283	-0.158715
N	0.656023	1.075576	-0.239064	N	0.685289	1.135347	-0.090313	N	0.687838	1.166389	-0.011969
C	-0.720332	1.201655	-0.520827	C	-0.707281	1.296074	-0.476077	C	-0.704325	1.386745	-0.601274
O	-1.228881	2.246077	-0.918137	O	-1.227599	2.413935	-0.524643	O	-1.319192	2.453568	-0.206727
N	-0.492969	-2.136509	0.742963	N	-0.420869	-2.252025	-0.120623	N	-0.357404	-2.228244	-0.408797
H	0.314087	-2.658220	1.063648	H	0.408263	-2.831895	-0.038163	H	0.491897	-2.785513	-0.422173
H	-1.389586	-2.600859	0.651249	H	-1.321473	-2.683540	-0.297846	H	-1.250451	-2.669758	-0.599170
C	1.276089	2.140699	0.622713	C	1.046070	1.780851	1.220909	C	0.901201	1.544609	1.418551
C	0.425413	2.425925	1.854259	C	0.054627	1.478706	2.339907	C	-0.110949	0.971335	2.408328
C	1.575847	3.379411	-0.206055	C	1.278746	3.270790	1.021410	C	1.063693	3.053528	1.556099
H	2.226024	1.704585	0.942736	H	2.007112	1.322170	1.475422	H	1.875615	1.097983	1.650722
H	0.971504	3.098223	2.521366	H	0.433540	1.904322	3.273296	H	0.162623	1.294555	3.417381
H	0.208368	1.503442	2.403032	H	-0.065275	0.400922	2.490592	H	-0.096095	-0.122759	2.404775
H	-0.518455	2.907637	1.580797	H	-0.926382	1.921697	2.137742	H	-1.128308	1.318098	2.202048
H	0.660383	3.890973	-0.509299	H	0.344329	3.805430	0.840499	H	0.107676	3.573188	1.479656
H	2.169616	4.068081	0.401346	H	1.736396	3.676175	1.928220	H	1.498378	3.269990	2.536390
H	2.151772	3.120922	-1.099093	H	1.957773	3.448922	0.182730	H	1.739528	3.443155	0.789082
C	2.023118	-0.906839	-0.014733	C	2.090214	-0.817182	-0.389816	C	2.130576	-0.726246	-0.525731
O	2.229102	-2.016394	0.435067	O	2.283107	-2.017097	-0.322548	O	2.332410	-1.924484	-0.626375
S	3.125581	-0.033647	-1.084368	S	3.277018	0.367083	-0.949495	S	3.339988	0.529532	-0.823967
C	4.530872	-1.180057	-0.997555	C	4.699735	-0.752778	-1.091099	C	4.765495	-0.559046	-1.109121
C	5.325480	-1.161424	0.278232	C	5.337232	-1.184268	0.200206	C	5.369354	-1.200386	0.109272
C	5.067040	-0.469878	1.386104	C	4.922903	-0.921225	1.437786	C	4.917642	-1.149440	1.360663
H	4.168461	-2.189743	-1.210695	H	4.400421	-1.623988	-1.680783	H	4.483305	-1.319917	-1.842816
H	5.165981	-0.885916	-1.839698	H	5.421151	-0.192961	-1.695230	H	5.503241	0.089005	-1.593492
H	6.198978	-1.811893	0.243934	H	6.233464	-1.785951	0.051640	H	6.273676	-1.766989	-0.111280
H	5.722555	-0.546271	2.247879	H	5.474042	-1.296691	2.294245	H	5.446066	-1.661925	2.158414
H	4.208058	0.191800	1.476646	H	4.033977	-0.328475	1.643859	H	4.018318	-0.601926	1.635348
O	-0.592821	-0.821978	-2.180979	O	-0.432026	0.553067	-2.279780	O	-0.417096	1.361737	-2.029797

H	-1.297511	-1.490745	-2.205709	H	-1.275949	0.723007	-2.724660	H	-1.153243	1.829088	-2.451355
---	-----------	-----------	-----------	---	-----------	----------	-----------	---	-----------	----------	-----------

C34-Add											
MCR			TS			ADDUCT					
											
C	-3.575502	-0.060424	-1.377307	C	-3.518465	0.414688	-1.290826	C	-3.648006	0.622354	-1.074487
C	-2.833913	-0.256092	-0.201583	C	-2.883492	-0.124203	-0.138850	C	-2.883787	-0.109425	-0.128384
C	-3.501124	-0.541791	1.008995	C	-3.656374	-0.798977	0.850469	C	-3.535426	-0.975126	0.795179
C	-4.895334	-0.673579	0.980192	C	-5.019200	-0.962366	0.607809	C	-4.918538	-1.116991	0.687478
C	-5.622930	-0.505019	-0.194267	C	-5.620975	-0.479716	-0.553405	C	-5.652882	-0.435445	-0.281960
C	-4.960256	-0.183514	-1.379223	C	-4.868636	0.220050	-1.504913	C	-5.015958	0.445312	-1.163495
C	-1.373143	-0.074319	-0.247208	C	-1.470493	0.066431	-0.038539	C	-1.466423	0.090895	-0.147598
C	-0.377529	-0.906544	0.303768	C	-0.442332	-0.845377	0.367758	C	-0.388996	-0.858654	-0.040675
N	0.834098	-0.226733	0.286803	N	0.774172	-0.202843	0.337961	N	0.810713	-0.221783	-0.041026
N	0.650703	1.069825	-0.242008	N	0.590566	1.125593	-0.102816	N	0.576968	1.171601	-0.195663
C	-0.724277	1.191060	-0.533363	C	-0.760895	1.309882	-0.385438	C	-0.796996	1.387782	-0.313472
N	-0.487169	-2.159570	0.683521	N	-0.567351	-2.123340	0.604413	N	-0.513215	-2.167677	-0.092041
O	-1.235145	2.237752	-0.925503	O	-1.254486	2.374298	-0.729995	O	-1.324186	2.490380	-0.403589
C	1.261631	2.133051	0.628354	C	1.271728	2.148462	0.762351	C	1.291052	2.023673	0.815940
C	0.399340	2.413344	1.852835	C	0.440079	2.455725	2.001695	C	0.556248	2.014280	2.151881
C	2.029505	-0.905089	-0.013530	C	1.865638	-0.942060	-0.278271	C	1.877633	-0.850176	-1.095434
O	2.240603	-2.010856	0.442151	O	2.098848	-2.068071	0.123693	O	2.039462	-2.090559	-0.876652
C	-2.782502	-0.672721	2.328479	C	-3.098533	-1.244922	2.177333	C	-2.821368	-1.658698	1.932681
C	1.566784	3.374134	-0.194882	C	1.617791	3.384969	-0.051627	C	1.539315	3.421303	0.270815
S	3.129650	-0.026091	-1.079826	S	3.101590	0.105563	-1.055897	S	3.444912	0.210795	-0.964078
C	4.543567	-1.161205	-0.982547	C	4.509504	-1.035044	-0.949337	C	4.612078	-1.008718	-0.297843
C	5.331319	-1.131935	0.297295	C	5.157274	-1.185139	0.398929	C	4.550137	-1.314123	1.171636
C	5.062761	-0.437237	1.400767	C	4.755513	-0.659732	1.554561	C	3.595948	-0.962831	2.032350

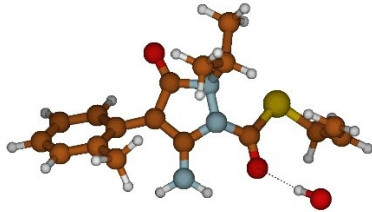
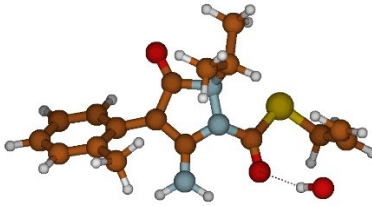
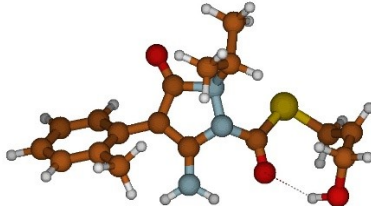
O	-0.649048	-0.989183	-2.167768	O	0.639066	-1.280801	-2.046768	O	1.286222	-0.578572	-2.351969
H	-5.415057	-0.894639	1.908892	H	-5.625907	-1.457317	1.360786	H	-5.432291	-1.759227	1.397287
H	-6.703442	-0.610242	-0.181637	H	-6.684698	-0.630915	-0.707999	H	-6.727820	-0.575900	-0.337284
H	-5.516305	-0.033408	-2.299089	H	-5.338895	0.604644	-2.403235	H	-5.587440	0.984774	-1.911000
H	-3.052354	0.180143	-2.297510	H	-2.916236	0.935730	-2.027245	H	-3.135896	1.288249	-1.760675
H	-1.916243	-0.006629	2.389022	H	-2.171718	-0.730033	2.438123	H	-1.888011	-1.158616	2.200621
H	-2.429072	-1.695564	2.496176	H	-2.914385	-2.324374	2.189729	H	-2.597992	-2.703598	1.694221
H	-3.462346	-0.423883	3.146408	H	-3.831616	-1.038113	2.960633	H	-3.468895	-1.661809	2.812618
H	0.314563	-2.679332	1.020638	H	0.262790	-2.690208	0.763089	H	0.336656	-2.717284	-0.220899
H	-1.383030	-2.623496	0.581472	H	-1.463800	-2.579519	0.468837	H	-1.423659	-2.584186	-0.247925
H	2.209205	1.697327	0.955921	H	2.199152	1.658110	1.064461	H	2.254674	1.531400	0.933043
H	0.937354	3.086995	2.525111	H	1.024891	3.083500	2.679139	H	1.179842	2.497486	2.909033
H	0.181437	1.489369	2.398676	H	0.172654	1.535651	2.532235	H	0.356581	0.987593	2.478898
H	-0.544089	2.891663	1.572075	H	-0.475678	2.995299	1.741495	H	-0.392170	2.557904	2.093918
H	0.653148	3.884537	-0.505527	H	0.720933	3.934584	-0.344795	H	0.611712	3.986286	0.159958
H	2.153684	4.062631	0.419315	H	2.238370	4.042421	0.563469	H	2.185682	3.956410	0.972471
H	2.151343	3.118522	-1.083121	H	2.181208	3.116963	-0.949541	H	2.045962	3.375483	-0.697583
H	4.190020	-2.174324	-1.194221	H	4.198016	-2.010767	-1.334381	H	4.500899	-1.934457	-0.871291
H	5.180645	-0.864596	-1.822321	H	5.233209	-0.632902	-1.666215	H	5.600088	-0.605889	-0.545272
H	6.209213	-1.776788	0.270107	H	6.048489	-1.812416	0.378185	H	5.391560	-1.910664	1.526457
H	5.714399	-0.505549	2.266145	H	5.310804	-0.845663	2.468664	H	3.653240	-1.257731	3.075908
H	4.199002	0.219154	1.484112	H	3.869880	-0.032107	1.630351	H	2.729003	-0.384286	1.723117
H	-0.871568	-0.223517	-2.723341	H	1.219165	-0.946867	-2.741965	H	1.192263	0.377898	-2.489265



C	-1.726375	0.015807	-0.178191	C	-1.726628	0.010827	-0.178777	C	-1.716671	0.016684	-0.184123
C	-0.783503	-0.931582	0.171792	C	-0.770873	-0.922452	0.173607	C	-0.753744	-0.922616	0.132202
N	0.488701	-0.340386	0.159621	N	0.492361	-0.311647	0.166387	N	0.504327	-0.303624	0.146106
N	0.370548	1.007019	-0.244044	N	0.355244	1.034479	-0.235530	N	0.357619	1.053870	-0.210981
C	-3.185923	-0.153523	-0.293863	C	-3.183247	-0.179338	-0.299304	C	-3.172292	-0.178631	-0.308132
C	-3.802523	0.172459	-1.512543	C	-3.799979	0.137584	-1.520265	C	-3.794257	0.180181	-1.514959
C	-5.178318	0.051020	-1.676983	C	-5.173667	-0.001018	-1.688885	C	-5.167292	0.038854	-1.686130
C	-5.958849	-0.406452	-0.614011	C	-5.951806	-0.466833	-0.627801	C	-5.940045	-0.472150	-0.641985
C	-5.355843	-0.719910	0.601122	C	-5.348755	-0.771686	0.589513	C	-5.332204	-0.818667	0.561653
C	-3.973242	-0.593340	0.790015	C	-3.968430	-0.627908	0.782541	C	-3.952385	-0.673197	0.757351
C	-3.378034	-0.908302	2.138301	C	-3.373494	-0.934327	2.132916	C	-3.353659	-1.027986	2.094231
N	-0.942367	-2.226616	0.436462	N	-0.910444	-2.220155	0.435145	N	-0.886708	-2.230341	0.344481
C	1.632203	-1.050701	-0.207119	C	1.647390	-1.003151	-0.197716	C	1.670060	-0.977835	-0.220711
S	2.789619	-0.138301	-1.190556	S	2.792416	-0.069497	-1.177776	S	2.806140	-0.016878	-1.182717
C	4.131776	-1.358711	-1.207850	C	4.146743	-1.274630	-1.209953	C	4.219882	-1.162065	-1.178048
C	4.925606	-1.489912	0.059464	C	4.974693	-1.374392	0.035802	C	5.189688	-0.941106	-0.012482
O	6.003273	0.935675	-0.060172	O	6.023689	0.608347	-0.125521	O	5.772561	0.348886	-0.205329
C	1.045942	1.934233	0.730178	C	1.012372	1.970149	0.743322	C	1.016848	1.961862	0.791435
C	1.390418	3.253127	0.057302	C	1.340125	3.295110	0.074025	C	1.341050	3.305484	0.158659
O	-1.460671	2.344563	-0.753123	O	-1.494992	2.344244	-0.748822	O	-1.501499	2.370667	-0.670465
C	0.226445	2.100826	2.004202	C	0.185317	2.122181	2.014267	C	0.193669	2.077287	2.068876
O	1.792658	-2.207359	0.138593	O	1.828063	-2.156494	0.148610	O	1.846517	-2.138231	0.105575
C	4.679883	-0.903591	1.236418	C	4.672209	-0.878713	1.256098	C	4.564346	-1.060217	1.332852
H	-5.967176	-1.056905	1.434622	H	-5.958497	-1.115272	1.421489	H	-5.937783	-1.197559	1.381288
H	-7.033686	-0.509639	-0.728270	H	-7.024971	-0.583148	-0.745157	H	-7.012661	-0.591261	-0.761554
H	-5.637089	0.306087	-2.627177	H	-5.632596	0.247558	-2.640718	H	-5.629884	0.320048	-2.627061
H	-3.184041	0.517783	-2.336867	H	-3.183268	0.490063	-2.342888	H	-3.181679	0.567489	-2.324926
H	-2.495491	-0.294222	2.341030	H	-2.499612	-0.308770	2.338093	H	-2.475295	-0.414944	2.316842
H	-3.072757	-1.958430	2.206399	H	-3.054911	-1.980435	2.202461	H	-3.041760	-2.077969	2.127115
H	-4.113999	-0.731549	2.926367	H	-4.114170	-0.766775	2.918575	H	-4.090294	-0.882487	2.888107
H	-0.143618	-2.819975	0.616996	H	-0.104713	-2.801240	0.624018	H	-0.078150	-2.813287	0.514181
H	-1.853213	-2.642656	0.291375	H	-1.815395	-2.649028	0.290463	H	-1.790447	-2.657268	0.187469
H	1.981613	1.426782	0.979166	H	1.954405	1.476310	0.995647	H	1.960205	1.462085	1.026087
H	0.812130	2.658214	2.740212	H	0.760026	2.686419	2.753697	H	0.770583	2.620016	2.822583
H	-0.027213	1.127454	2.437650	H	-0.055927	1.144352	2.444788	H	-0.046415	1.087370	2.471650
H	-0.697635	2.654908	1.811375	H	-0.745888	2.663275	1.818891	H	-0.738223	2.623500	1.892098
H	0.495825	3.837443	-0.166141	H	0.437964	3.866426	-0.152568	H	0.437378	3.880406	-0.052394
H	2.021795	3.834990	0.734777	H	1.959685	3.885204	0.755251	H	1.959149	3.878687	0.855512
H	1.944366	3.083295	-0.870444	H	1.900712	3.135149	-0.851481	H	1.901922	3.171756	-0.770842
H	3.718710	-2.328180	-1.501453	H	3.735844	-2.256773	-1.462008	H	3.839651	-2.184428	-1.173477
H	4.785196	-1.030592	-2.022669	H	4.776881	-0.963191	-2.047654	H	4.740065	-0.983940	-2.123188
H	5.782853	-2.155723	-0.035909	H	5.851977	-2.009182	-0.074203	H	5.962690	-1.714698	-0.125152



H	3.832804	-0.239309	1.391922	H	3.791359	-0.266867	1.432407	H	4.069403	-0.201788	1.775282
H	5.327691	-1.087658	2.087821	H	5.322566	-1.074652	2.102167	H	4.495002	-2.025524	1.818589
H	6.782873	0.517901	0.354018	H	6.754398	0.388410	0.480065	H	6.373414	0.519949	0.533519

C39-Add											
MCR	TS	ADDUCT									
											
C	-3.766086	-0.962500	0.708935	C	-3.780269	-0.936037	0.705847	C	-3.766224	-1.003179	0.704741
C	-3.080233	-0.264990	-0.306649	C	-3.088443	-0.233443	-0.302126	C	-3.090156	-0.289072	-0.305925
C	-3.780926	0.177469	-1.440064	C	-3.788462	0.242225	-1.422387	C	-3.797030	0.150005	-1.436891
C	-5.140352	-0.076518	-1.588663	C	-5.153351	0.016035	-1.565896	C	-5.152422	-0.123342	-1.587956
C	-5.818552	-0.786525	-0.596550	C	-5.837880	-0.698882	-0.581703	C	-5.820437	-0.849922	-0.600950
C	-5.132598	-1.218233	0.535568	C	-5.152454	-1.163222	0.537766	C	-5.128601	-1.278532	0.528746
C	-1.646186	0.056219	-0.197608	C	-1.647883	0.059013	-0.198108	C	-1.661216	0.052881	-0.194062
C	-1.098427	1.372065	-0.283826	C	-1.075672	1.365802	-0.263135	C	-1.132617	1.376633	-0.274081
N	0.317870	1.293729	-0.143808	N	0.340348	1.257468	-0.139052	N	0.283374	1.317781	-0.133555
N	0.605837	-0.076570	0.034623	N	0.603198	-0.121274	0.008897	N	0.592024	-0.048161	0.043564
C	-0.588262	-0.813736	-0.019922	C	-0.605400	-0.834220	-0.047608	C	-0.590210	-0.801898	-0.017661
O	-1.676051	2.459655	-0.403798	O	-1.633170	2.466461	-0.355305	O	-1.726169	2.456766	-0.390336
N	-0.585843	-2.143332	0.039552	N	-0.627018	-2.164403	-0.013735	N	-0.569853	-2.131953	0.035456
C	1.812995	-0.574775	-0.440346	C	1.793270	-0.632760	-0.493852	C	1.810788	-0.530840	-0.426287
O	2.109237	-1.750073	-0.284972	O	2.075338	-1.813720	-0.365576	O	2.119270	-1.701522	-0.257602
C	0.907997	2.127299	0.963196	C	0.957914	2.055597	0.978985	C	0.864606	2.159619	0.970796
C	0.118204	1.980281	2.258159	C	0.180577	1.893054	2.279564	C	0.076571	2.006809	2.266272
C	-3.080898	-1.417822	1.971658	C	-3.094498	-1.426932	1.954824	C	-3.075523	-1.455913	1.965392
S	2.828507	0.606045	-1.276769	S	2.818807	0.546362	-1.325839	S	2.809119	0.656638	-1.270773
C	4.310432	-0.415977	-1.512392	C	4.272004	-0.506132	-1.600225	C	4.376989	-0.342245	-1.429845
C	5.205808	-0.575695	-0.316649	C	5.211502	-0.663458	-0.443655	C	5.199492	-0.287909	-0.205370
C	4.937497	-0.238011	0.947780	C	4.992432	-0.320422	0.843783	C	4.925477	-1.167562	0.968841
C	1.066803	3.570945	0.514207	C	1.136901	3.506132	0.560999	C	1.008355	3.604030	0.519248
H	-5.665930	-1.753677	1.317126	H	-5.690365	-1.702625	1.313446	H	-5.654243	-1.826877	1.306576

H	-6.879144	-0.994939	-0.699785	H	-6.902792	-0.886001	-0.681179	H	-6.877733	-1.073552	-0.706153
H	-5.665008	0.271908	-2.472809	H	-5.677327	0.389874	-2.439999	H	-5.681769	0.222889	-2.470172
H	-3.241106	0.720477	-2.211410	H	-3.243823	0.789033	-2.187657	H	-3.265006	0.705811	-2.204522
H	-2.273896	-0.736632	2.257976	H	-2.274470	-0.764676	2.248507	H	-2.279700	-0.763984	2.257223
H	-2.643996	-2.415698	1.852890	H	-2.674824	-2.429299	1.813752	H	-2.622613	-2.445886	1.840811
H	-3.799597	-1.471774	2.792834	H	-3.808497	-1.485124	2.779794	H	-3.794394	-1.526493	2.785164
H	0.281484	-2.658676	0.109830	H	0.231074	-2.697056	0.039700	H	0.304641	-2.634841	0.106504
H	-1.448099	-2.637297	-0.151215	H	-1.500219	-2.639368	-0.202797	H	-1.424223	-2.636878	-0.161703
H	1.906553	1.708598	1.112284	H	1.950702	1.616270	1.106930	H	1.867192	1.751223	1.119653
H	0.656246	2.481390	3.067326	H	0.737634	2.364248	3.093811	H	0.609979	2.513726	3.074916
H	0.000708	0.925695	2.529555	H	0.045389	0.834770	2.527239	H	-0.030929	0.951383	2.538724
H	-0.872815	2.436981	2.171780	H	-0.802151	2.370924	2.215861	H	-0.918814	2.453852	2.179772
H	0.101516	4.069731	0.409935	H	0.179645	4.024667	0.482597	H	0.037875	4.092122	0.412326
H	1.651014	4.106590	1.267833	H	1.741552	4.013298	1.318174	H	1.585512	4.147846	1.272499
H	1.600217	3.625819	-0.439118	H	1.657641	3.573778	-0.398498	H	1.542552	3.662352	-0.433427
H	4.003103	-1.392932	-1.898531	H	3.935484	-1.483968	-1.959648	H	4.076764	-1.352787	-1.714913
H	4.854666	0.087060	-2.317917	H	4.800173	-0.030162	-2.432841	H	4.874829	0.132088	-2.277895
H	6.164903	-1.033223	-0.555877	H	6.156379	-1.133377	-0.710970	H	5.815330	0.591310	-0.043855
H	5.671781	-0.404358	1.729313	H	5.785999	-0.416369	1.575599	H	5.781251	-1.148181	1.648395
H	3.996669	0.222831	1.242163	H	4.085049	0.188467	1.159571	H	4.055917	-0.792585	1.537510
O	4.439486	-2.890090	0.954422	O	4.362365	-2.403532	1.363309	O	4.707559	-2.532396	0.616332
H	3.634877	-2.564301	0.495336	H	3.593138	-2.369413	0.761393	H	3.820535	-2.592577	0.229459

**Table S3.** Standard enthalpy ( $\Delta H^\circ_{0K}$ ) for MCR and MCP, adiabatic energy barrier ( $E_0$ ) for TS, and standard reaction enthalpy ( $\Delta_r H^\circ_{0K}$ ) for products (P) at 0 K of the FHT reactions, in addition to their standard activation enthalpy ( $\Delta H^{\ddagger}_{298K}$ ) and standard reaction enthalpy ( $\Delta_r H^\circ_{298K}$ ) at 298 K. Units are in  $\text{kJ mol}^{-1}$ . All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

Positions	MCR	TS	MCP	P	$\Delta H^{\ddagger}_{298K}$	$\Delta_r H^\circ_{298K}$
H9	-17.99	15.00	-43.81	-36.58	11.93	-36.06
H10	-26.54	17.14	-39.29	-35.82	14.51	-35.13
H11	-26.53	16.64	-38.63	-34.61	14.18	-34.09
H12	-24.97	13.50	-46.26	-36.24	10.69	-35.59
H13	-19.67	-10.87	-145.27	-125.17	-15.15	-125.20
H14	-17.98	-0.12	-136.73	-125.65	-3.73	-125.49
H15	-19.65	-10.86	-144.79	-125.67	-15.15	-125.49
H22	-21.39	12.72	-103.97	-94.46	8.56	-94.65
H23	-3.61	50.18	-98.77	-92.50	46.23	-93.16
H27	-12.54	6.54	-109.70	-109.29	2.99	-107.23
H28	-14.71	10.06	-87.11	-79.85	6.15	-77.65
H29	-12.02	3.96	-92.53	-79.85	0.11	-77.64
H30	-19.66	-1.50	-99.19	-82.72	-6.38	-80.51
H31	-22.20	-1.99	-102.02	-85.34	-6.35	-83.21
H32	-14.71	8.39	-94.00	-83.46	5.01	-81.82
H33	-20.19	7.96	-97.65	-83.50	2.77	-81.84
H40	-19.80	-0.78	-153.40	-141.58	-4.56	-140.99
H41	-14.51	8.23	-147.88	-141.59	5.07	-140.99
H42	-19.81	12.34	-64.25	-59.80	9.29	-58.61
H43	-14.11	17.87	-45.81	-40.08	14.97	-39.29
H44	-19.82	14.83	-59.17	-44.85	11.83	-44.03

**Table S4.** Standard enthalpy, entropy, and Gibbs free energy of activation, and the ones of reaction for all the FHT reactions at 298 K temperature calculated at the M06-2X/6-31+G(d,p) level of theory (level 1, L1), and at the M06-2X/6-311++G(3df,3pd) level of theory (level 2, L2) in the aqueous phase. Differences of standard Gibbs free energy of activation ( $\Delta\Delta G^{\ddagger}$ ) and reaction ( $\Delta\Delta_r G^\circ$ ) between the level 1 and level 2 are also shown.

	Level	$\Delta H^{\ddagger}_{298K}$	$\Delta S^{\ddagger}_{298K}$	$\Delta G^{\ddagger}_{298K}$	$\Delta_r H^{\circ}_{298K}$	$\Delta_r S^{\circ}_{298K}$	$\Delta_r G^{\circ}_{298K}$	$\Delta\Delta G^{\ddagger}$	$\Delta\Delta_r G^\circ$
<b>H9</b>	L1	13.44	-129.34	52.00	-31.67	9.59	-34.53		
	L2	11.93	-129.34	50.49	-36.06	9.59	-38.92	-1.52	-4.39
<b>H10</b>	L1	15.79	-123.53	52.62	-30.87	11.57	-34.31		
	L2	14.51	-123.53	51.34	-35.13	11.57	-38.58	-1.27	-4.26
<b>H11</b>	L1	15.39	-120.12	51.20	-29.81	9.47	-32.64		
	L2	14.18	-120.12	50.00	-34.09	9.47	-36.92	-1.21	-4.28
<b>H12</b>	L1	11.66	-126.59	49.40	-30.98	11.67	-34.46		
	L2	10.69	-126.59	48.43	-35.59	11.67	-39.07	-0.97	-4.61
<b>H13</b>	L1	-15.44	-136.86	25.36	-119.93	0.42	-120.05		
	L2	-15.15	-136.86	25.65	-125.20	0.42	-125.33	0.29	-5.27
<b>H14</b>	L1	-3.56	-133.88	36.36	-120.19	4.59	-121.56		
	L2	-3.73	-133.88	36.19	-125.49	4.59	-126.86	-0.16	-5.30
<b>H15</b>	L1	-15.44	-137.15	25.45	-120.19	4.75	-121.61		
	L2	-15.15	-137.15	25.74	-125.49	4.75	-126.91	0.29	-5.30
<b>H22</b>	L1	11.27	-129.58	49.90	-87.00	15.57	-91.64		
	L2	8.56	-129.58	47.19	-94.65	15.57	-99.29	-2.71	-7.64
<b>H23</b>	L1	47.19	-126.81	85.00	-91.57	7.62	-93.84		
	L2	46.23	-126.81	84.03	-93.16	7.62	-95.43	-0.97	-1.60
<b>H27</b>	L1	2.51	-136.55	43.22	-102.21	32.23	-111.82		
	L2	2.99	-136.55	43.70	-107.23	32.23	-116.85	0.48	-5.03
<b>H28</b>	L1	7.37	-131.68	46.63	-73.67	24.74	-81.04		
	L2	6.15	-131.68	45.41	-77.65	24.74	-85.02	-1.22	-3.98
<b>H29</b>	L1	-0.48	-139.32	41.06	-73.66	24.77	-81.05		
	L2	0.11	-139.32	41.64	-77.64	24.77	-85.03	0.59	-3.98
<b>H30</b>	L1	-5.26	-150.47	39.61	-76.34	22.13	-82.94		
	L2	-6.38	-150.47	38.48	-80.51	22.13	-87.11	-1.13	-4.17
<b>H31</b>	L1	-5.65	-140.53	36.25	-78.60	25.69	-86.26		
	L2	-6.35	-140.53	35.55	-83.21	25.69	-90.87	-0.71	-4.61
<b>H32</b>	L1	6.15	-124.43	43.24	-77.14	18.24	-82.58		
	L2	5.01	-124.43	42.11	-81.82	18.24	-87.25	-1.13	-4.67
<b>H33</b>	L1	3.23	-149.76	47.88	-77.17	18.48	-82.68		
	L2	2.77	-149.76	47.42	-81.84	18.48	-87.35	-0.46	-4.67
<b>H40</b>	L1	-4.12	-133.91	35.81	-136.57	11.88	-140.11		

	L2	-4.56	-133.91	35.37	-140.99	11.88	-144.53	-0.44	-4.42
<b>H41</b>	L1	6.07	-129.15	44.58	-136.57	11.97	-140.13		
	L2	5.07	-129.15	43.58	-140.99	11.97	-144.56	-1.00	-4.42
<b>H42</b>	L1	10.56	-125.62	48.02	-54.32	17.23	-59.46		
	L2	9.29	-125.62	46.74	-58.61	17.23	-63.74	-1.27	-4.28
<b>H43</b>	L1	16.51	-125.36	53.89	-35.04	12.58	-38.79		
	L2	14.97	-125.36	52.35	-39.29	12.58	-43.04	-1.54	-4.25
<b>H44</b>	L1	11.60	-133.72	51.47	-40.12	12.01	-43.70		
	L2	11.83	-133.72	51.70	-44.03	12.01	-47.61	0.23	-3.92

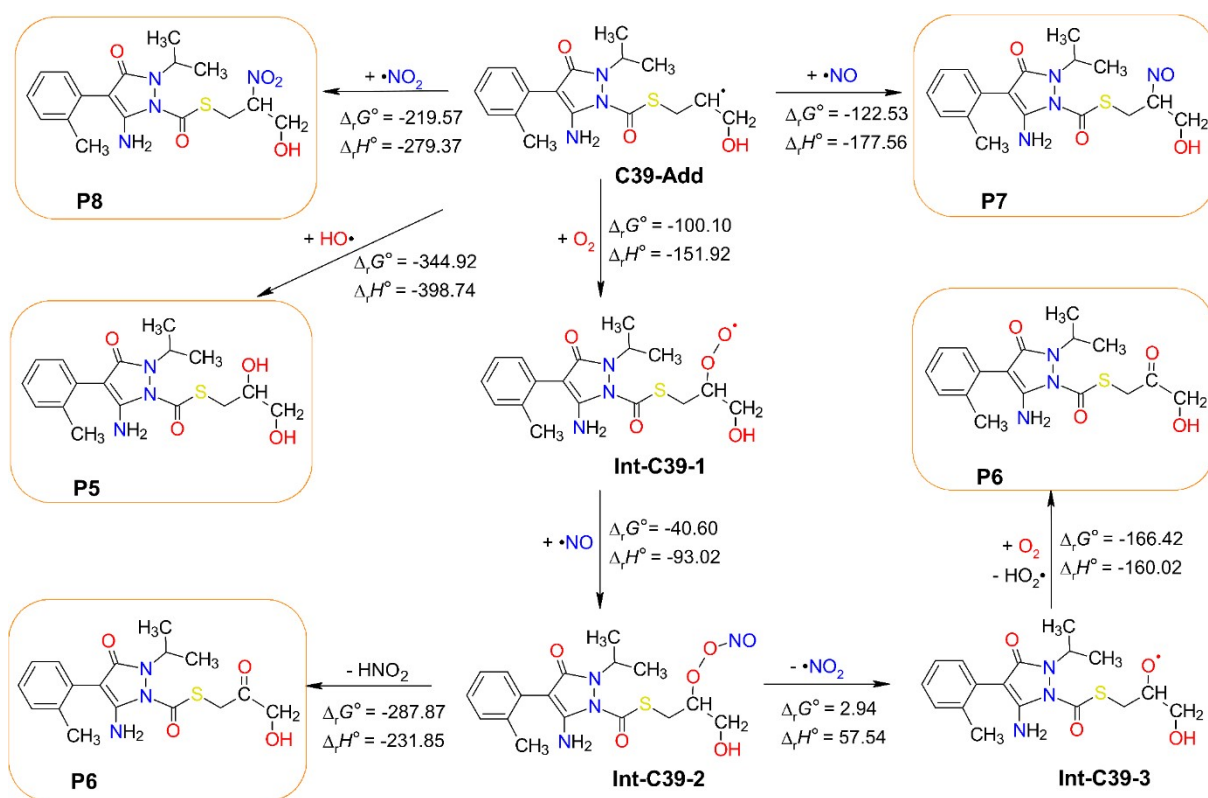
**Table S5.** Standard enthalpy ( $\Delta H^\circ_{0K}$ ) for MCR and MCP, adiabatic energy barrier ( $E_0$ ) for TS, and standard reaction enthalpy ( $\Delta_r H^\circ_{0K}$ ) for products (P) at 0 K of the RAF reactions, in addition to their standard activation enthalpy ( $\Delta H^{\circ\ddagger}_{298K}$ ) and standard reaction enthalpy ( $\Delta_r H^\circ_{298K}$ ) at 298 K. Units are in  $\text{kJ mol}^{-1}$ . All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

Positions	MCR	TS	P	$\Delta H^{\circ\ddagger}_{298K}$	$\Delta_r H^\circ_{298K}$
C1	-17.93	-1.21	-66.36	-5.89	-70.74
C2	-20.13	-10.24	-85.26	-14.94	-91.04
C3	-20.13	-3.17	-74.29	-6.66	-78.53
C4	-20.12	0.66	-73.41	-3.09	-78.16
C5	-26.54	0.35	-68.88	-2.67	-72.90
C6	-26.55	-2.81	-76.66	-7.99	-82.62
C7	-22.43	-18.31	-48.91	-23.41	-54.29
C16	-24.96	-7.87	-89.99	-13.49	-95.38
C19	-25.02	6.05	-32.21	0.02	-38.38
C34	-22.83	32.79	-43.11	27.61	-48.45
C38	-14.11	-9.83	-128.50	-13.56	-132.79
C39	-19.81	-14.64	-135.40	-18.93	-140.60

**Table S6:** Standard enthalpy, entropy, and Gibbs free energy of activation, and the ones of reaction for all the RAF reactions at 298 K temperature calculated at the M06-2X/6-31+G(d,p) level of theory (level 1, L1), and at the M06-2X/6-311++G(3df,3pd) level of theory (level 2, L2) in the aqueous phase. Differences of standard Gibbs free energy of activation ( $\Delta\Delta G^{\ddagger}$ ) and reaction ( $\Delta\Delta_r G^\circ$ ) between the level 1 and level 2 are also shown.

	Level	$\Delta H^{\ddagger}_{298K}$	$\Delta S^{\ddagger}_{298K}$	$\Delta G^{\ddagger}_{298K}$	$\Delta_r H^\circ_{298K}$	$\Delta_r S^\circ_{298K}$	$\Delta_r G^\circ_{298K}$	$\Delta\Delta G^{\ddagger}$	$\Delta\Delta_r G^\circ$
<b>C1</b>	L1	-7.12	-149.41	37.43	-71.46	-139.17	-29.97		
	L2	-5.89	-149.41	38.65	-70.74	-139.17	-29.24	1.23	0.72
<b>C2</b>	L1	-15.41	-150.79	29.55	-91.27	-156.81	-44.51		
	L2	-14.94	-150.79	30.02	-91.04	-156.81	-44.29	0.47	0.22
<b>C3</b>	L1	-5.80	-135.64	34.64	-75.80	-140.29	-33.98		
	L2	-6.66	-135.64	33.79	-78.53	-140.29	-36.71	-0.86	-2.73
<b>C4</b>	L1	-2.39	-136.66	38.35	-75.60	-145.51	-32.21		
	L2	-3.09	-136.66	37.65	-78.16	-145.51	-34.78	-0.70	-2.56
<b>C5</b>	L1	-2.22	-126.10	35.38	-70.86	-138.08	-29.70		
	L2	-2.67	-126.10	34.93	-72.90	-138.08	-31.73	-0.45	-2.03
<b>C6</b>	L1	-6.31	-134.72	33.86	-77.44	-142.81	-34.86		
	L2	-6.86	-134.72	33.31	-79.59	-142.81	-37.01	-0.55	-2.15
<b>C7</b>	L1	-25.73	-152.42	19.71	-59.52	-147.46	-15.56		
	L2	-23.39	-152.42	22.06	-55.86	-147.46	-11.90	2.34	3.66
<b>C16</b>	L1	-14.46	-159.39	33.07	-100.32	-151.82	-55.06		
	L2	-13.49	-159.39	34.03	-95.38	-151.82	-50.11	0.96	4.94
<b>C19</b>	L1	-1.23	-164.01	47.67	-45.47	-164.10	3.45		
	L2	0.02	-164.01	48.92	-38.38	-164.10	10.55	1.25	7.09
<b>C34</b>	L1	24.50	-154.31	70.50	-58.43	-152.81	-12.87		
	L2	27.61	-154.31	73.62	-48.45	-152.81	-2.89	3.12	9.99
<b>C38</b>	L1	-14.20	-130.52	24.71	-134.58	-141.43	-92.41		
	L2	-13.56	-130.52	25.35	-132.79	-141.43	-90.63	0.64	1.79
<b>C39</b>	L1	-20.11	-134.93	20.12	-141.86	-143.94	-98.94		
	L2	-18.93	-134.93	21.30	-140.60	-143.94	-97.69	1.18	1.26





**Figure S5.** Standard Gibbs free reaction energy ( $\Delta_r G^\circ$ ) and standard reaction enthalpy ( $\Delta_r H^\circ$ ) calculated for the further reactions of C39-Add with  $^3\text{O}_2$ ,  $\text{HO}\cdot$ ,  $\cdot\text{NO}$ , and  $\cdot\text{NO}_2$  at 298 K. Units are in  $\text{kJ mol}^{-1}$ . All calculations are performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory.

**Table S7.** Apparent rate constants ( $k$ , in  $M^{-1} s^{-1}$ ) of all oxidation reactions, with the total FHT, RAF, SET, and the overall rate constants in the temperature range of 283-323 K. (The most favourable pathways are in bold).

T (K)	H9-Abs	H10-Abs	H11-Abs	H12-Abs	H13-Abs	H14-Abs	H15-Abs	H22-Abs	H23-Abs	H27-Abs	H28-Abs	H29-Abs
283	1.00×10 <sup>6</sup>	8.54×10 <sup>5</sup>	1.50×10 <sup>6</sup>	4.03×10 <sup>6</sup>	<b>1.45×10<sup>9</sup></b>	2.79×10 <sup>8</sup>	<b>1.70×10<sup>9</sup></b>	1.23×10 <sup>8</sup>	1.40	1.66×10 <sup>7</sup>	8.26×10 <sup>6</sup>	4.14×10 <sup>7</sup>
288	1.08×10 <sup>6</sup>	9.29×10 <sup>5</sup>	1.63×10 <sup>6</sup>	4.21×10 <sup>6</sup>	<b>1.66×10<sup>9</sup></b>	2.79×10 <sup>8</sup>	<b>1.95×10<sup>9</sup></b>	1.18×10 <sup>8</sup>	1.86	1.70×10 <sup>7</sup>	8.59×10 <sup>6</sup>	4.14×10 <sup>7</sup>
293	1.17×10 <sup>6</sup>	1.01×10 <sup>6</sup>	1.77×10 <sup>6</sup>	4.40×10 <sup>6</sup>	<b>1.88×10<sup>9</sup></b>	2.79×10 <sup>8</sup>	<b>2.20×10<sup>9</sup></b>	1.13×10 <sup>8</sup>	2.47	1.73×10 <sup>7</sup>	8.93×10 <sup>6</sup>	4.15×10 <sup>7</sup>
298	1.26×10 <sup>6</sup>	1.10×10 <sup>6</sup>	1.92×10 <sup>6</sup>	4.61×10 <sup>6</sup>	<b>2.11×10<sup>9</sup></b>	2.78×10 <sup>8</sup>	<b>2.45×10<sup>9</sup></b>	1.08×10 <sup>8</sup>	3.24	1.77×10 <sup>7</sup>	9.29×10 <sup>6</sup>	4.16×10 <sup>7</sup>
303	1.36×10 <sup>6</sup>	1.19×10 <sup>6</sup>	2.07×10 <sup>6</sup>	4.83×10 <sup>6</sup>	<b>2.34×10<sup>9</sup></b>	2.77×10 <sup>8</sup>	<b>2.70×10<sup>9</sup></b>	1.03×10 <sup>8</sup>	4.24	1.81×10 <sup>7</sup>	9.67×10 <sup>6</sup>	4.17×10 <sup>7</sup>
308	1.46×10 <sup>6</sup>	1.29×10 <sup>6</sup>	2.25×10 <sup>6</sup>	5.06×10 <sup>6</sup>	<b>2.56×10<sup>9</sup></b>	2.75×10 <sup>8</sup>	<b>2.94×10<sup>9</sup></b>	9.88×10 <sup>7</sup>	5.52	1.84×10 <sup>7</sup>	1.01×10 <sup>7</sup>	4.18×10 <sup>7</sup>
313	1.57×10 <sup>6</sup>	1.40×10 <sup>6</sup>	2.43×10 <sup>6</sup>	5.31×10 <sup>6</sup>	<b>2.78×10<sup>9</sup></b>	2.74×10 <sup>8</sup>	<b>3.18×10<sup>9</sup></b>	9.49×10 <sup>7</sup>	7.14	1.89×10 <sup>7</sup>	1.05×10 <sup>7</sup>	4.20×10 <sup>7</sup>
318	1.69×10 <sup>6</sup>	1.52×10 <sup>6</sup>	2.62×10 <sup>6</sup>	5.57×10 <sup>6</sup>	<b>2.99×10<sup>9</sup></b>	2.72×10 <sup>8</sup>	<b>3.39×10<sup>9</sup></b>	9.14×10 <sup>7</sup>	9.18	1.93×10 <sup>7</sup>	1.09×10 <sup>7</sup>	4.22×10 <sup>7</sup>
323	1.81×10 <sup>6</sup>	1.64×10 <sup>6</sup>	2.83×10 <sup>6</sup>	5.85×10 <sup>6</sup>	<b>3.18×10<sup>9</sup></b>	2.70×10 <sup>8</sup>	<b>3.59×10<sup>9</sup></b>	8.83×10 <sup>7</sup>	1.17×10 <sup>1</sup>	1.97×10 <sup>7</sup>	1.13×10 <sup>7</sup>	4.25×10 <sup>7</sup>

T (K)	H30-Abs	H31-Abs	H32-Abs	H33-Abs	H40-Abs	H41-Abs	H42-Abs	H43-Abs	H44-Abs	C1-Add	C2-Add	C3-Add
283	1.62×10 <sup>8</sup>	<b>4.17×10<sup>8</sup></b>	2.67×10 <sup>7</sup>	5.77×10 <sup>6</sup>	<b>4.55×10<sup>8</sup></b>	2.38×10 <sup>7</sup>	4.28×10 <sup>6</sup>	6.70×10 <sup>5</sup>	1.47×10 <sup>6</sup>	5.38×10 <sup>7</sup>	8.70×10 <sup>8</sup>	3.32×10 <sup>8</sup>
288	1.56×10 <sup>8</sup>	<b>4.14×10<sup>8</sup></b>	2.77×10 <sup>7</sup>	5.76×10 <sup>6</sup>	<b>4.58×10<sup>8</sup></b>	2.43×10 <sup>7</sup>	4.55×10 <sup>6</sup>	7.28×10 <sup>5</sup>	1.53×10 <sup>6</sup>	5.36×10 <sup>7</sup>	9.10×10 <sup>8</sup>	3.38×10 <sup>8</sup>
293	1.51×10 <sup>8</sup>	<b>4.09×10<sup>8</sup></b>	2.88×10 <sup>7</sup>	5.76×10 <sup>6</sup>	<b>4.58×10<sup>8</sup></b>	2.48×10 <sup>7</sup>	4.85×10 <sup>6</sup>	7.90×10 <sup>5</sup>	1.59×10 <sup>6</sup>	5.34×10 <sup>7</sup>	9.37×10 <sup>8</sup>	3.43×10 <sup>8</sup>
298	1.45×10 <sup>8</sup>	<b>4.03×10<sup>8</sup></b>	3.00×10 <sup>7</sup>	5.77×10 <sup>6</sup>	<b>4.55×10<sup>8</sup></b>	2.54×10 <sup>7</sup>	5.15×10 <sup>6</sup>	8.57×10 <sup>5</sup>	1.66×10 <sup>6</sup>	5.32×10 <sup>7</sup>	9.53×10 <sup>8</sup>	3.46×10 <sup>8</sup>
303	1.40×10 <sup>8</sup>	<b>3.96×10<sup>8</sup></b>	3.11×10 <sup>7</sup>	5.78×10 <sup>6</sup>	<b>4.52×10<sup>8</sup></b>	2.60×10 <sup>7</sup>	5.48×10 <sup>6</sup>	9.29×10 <sup>5</sup>	1.73×10 <sup>6</sup>	5.29×10 <sup>7</sup>	9.58×10 <sup>8</sup>	3.48×10 <sup>8</sup>
308	1.36×10 <sup>8</sup>	<b>3.88×10<sup>8</sup></b>	3.23×10 <sup>7</sup>	5.81×10 <sup>6</sup>	<b>4.48×10<sup>8</sup></b>	2.66×10 <sup>7</sup>	5.82×10 <sup>6</sup>	1.01×10 <sup>6</sup>	1.81×10 <sup>6</sup>	5.27×10 <sup>7</sup>	9.54×10 <sup>8</sup>	3.49×10 <sup>8</sup>
313	1.31×10 <sup>8</sup>	<b>3.79×10<sup>8</sup></b>	3.35×10 <sup>7</sup>	5.84×10 <sup>6</sup>	<b>4.43×10<sup>8</sup></b>	2.73×10 <sup>7</sup>	6.18×10 <sup>6</sup>	1.09×10 <sup>6</sup>	1.89×10 <sup>6</sup>	5.25×10 <sup>7</sup>	9.43×10 <sup>8</sup>	3.50×10 <sup>8</sup>
318	1.27×10 <sup>8</sup>	<b>3.71×10<sup>8</sup></b>	3.48×10 <sup>7</sup>	5.88×10 <sup>6</sup>	<b>4.38×10<sup>8</sup></b>	2.80×10 <sup>7</sup>	6.55×10 <sup>6</sup>	1.18×10 <sup>6</sup>	1.98×10 <sup>6</sup>	5.23×10 <sup>7</sup>	9.27×10 <sup>8</sup>	3.51×10 <sup>8</sup>
323	1.23×10 <sup>8</sup>	<b>3.63×10<sup>8</sup></b>	3.61×10 <sup>7</sup>	5.93×10 <sup>6</sup>	<b>4.32×10<sup>8</sup></b>	2.87×10 <sup>7</sup>	6.94×10 <sup>6</sup>	1.27×10 <sup>6</sup>	2.08×10 <sup>6</sup>	5.21×10 <sup>7</sup>	9.07×10 <sup>8</sup>	3.51×10 <sup>8</sup>

T (K)	C4-Add	C5-Add	C6-Add	C7-Add	C16-Add	C19-Add	C34-Add	C38-Add	C39-Add	FHT	RAF	SET	Overall
283	8.04×10 <sup>7</sup>	2.14×10 <sup>8</sup>	1.26×10 <sup>8</sup>	<b>1.29×10<sup>9</sup></b>	2.60×10 <sup>8</sup>	8.62×10 <sup>5</sup>	2.19×10 <sup>1</sup>	<b>1.39×10<sup>9</sup></b>	<b>1.51×10<sup>9</sup></b>	4.73×10 <sup>9</sup>	6.12×10 <sup>9</sup>	1.27×10 <sup>9</sup>	1.21×10 <sup>10</sup>
288	8.16×10 <sup>7</sup>	2.21×10 <sup>8</sup>	1.24×10 <sup>8</sup>	<b>1.49×10<sup>9</sup></b>	2.55×10 <sup>8</sup>	8.89×10 <sup>5</sup>	2.77×10 <sup>1</sup>	<b>1.58×10<sup>9</sup></b>	<b>1.75×10<sup>9</sup></b>	5.17×10 <sup>9</sup>	6.80×10 <sup>9</sup>	1.55×10 <sup>9</sup>	1.35×10 <sup>10</sup>
293	8.28×10 <sup>7</sup>	2.27×10 <sup>8</sup>	1.22×10 <sup>8</sup>	<b>1.71×10<sup>9</sup></b>	2.49×10 <sup>8</sup>	9.16×10 <sup>5</sup>	3.48×10 <sup>1</sup>	<b>1.77×10<sup>9</sup></b>	<b>2.00×10<sup>9</sup></b>	5.63×10 <sup>9</sup>	7.50×10 <sup>9</sup>	1.93×10 <sup>9</sup>	1.51×10 <sup>10</sup>
298	8.40×10 <sup>7</sup>	2.33×10 <sup>8</sup>	1.20×10 <sup>8</sup>	<b>1.94×10<sup>9</sup></b>	2.43×10 <sup>8</sup>	9.44×10 <sup>5</sup>	4.34×10 <sup>1</sup>	<b>1.97×10<sup>9</sup></b>	<b>2.28×10<sup>9</sup></b>	6.09×10 <sup>9</sup>	8.21×10 <sup>9</sup>	2.35×10 <sup>9</sup>	1.67×10 <sup>10</sup>
303	8.51×10 <sup>7</sup>	2.38×10 <sup>8</sup>	1.18×10 <sup>8</sup>	<b>2.17×10<sup>9</sup></b>	2.36×10 <sup>8</sup>	9.71×10 <sup>5</sup>	5.37×10 <sup>1</sup>	<b>2.16×10<sup>9</sup></b>	<b>2.56×10<sup>9</sup></b>	6.55×10 <sup>9</sup>	8.93×10 <sup>9</sup>	2.85×10 <sup>9</sup>	1.83×10 <sup>10</sup>
308	8.62×10 <sup>7</sup>	2.44×10 <sup>8</sup>	1.15×10 <sup>8</sup>	<b>2.42×10<sup>9</sup></b>	2.29×10 <sup>8</sup>	1.00×10 <sup>6</sup>	6.60×10 <sup>1</sup>	<b>2.35×10<sup>9</sup></b>	<b>2.86×10<sup>9</sup></b>	7.00×10 <sup>9</sup>	9.66×10 <sup>9</sup>	3.44×10 <sup>9</sup>	2.01×10 <sup>10</sup>
313	8.72×10 <sup>7</sup>	2.49×10 <sup>8</sup>	1.13×10 <sup>8</sup>	<b>2.66×10<sup>9</sup></b>	2.22×10 <sup>8</sup>	1.03×10 <sup>6</sup>	8.07×10 <sup>1</sup>	<b>2.53×10<sup>9</sup></b>	<b>3.17×10<sup>9</sup></b>	7.44×10 <sup>9</sup>	1.04×10 <sup>10</sup>	4.09×10 <sup>9</sup>	2.19×10 <sup>10</sup>
318	8.83×10 <sup>7</sup>	2.54×10 <sup>8</sup>	1.11×10 <sup>8</sup>	<b>2.91×10<sup>9</sup></b>	2.15×10 <sup>8</sup>	1.06×10 <sup>6</sup>	9.81×10 <sup>1</sup>	<b>2.70×10<sup>9</sup></b>	<b>3.48×10<sup>9</sup></b>	7.84×10 <sup>9</sup>	1.11×10 <sup>10</sup>	4.83×10 <sup>9</sup>	2.38×10 <sup>10</sup>
323	8.94×10 <sup>7</sup>	2.59×10 <sup>8</sup>	1.09×10 <sup>8</sup>	<b>3.15×10<sup>9</sup></b>	2.08×10 <sup>8</sup>	1.09×10 <sup>6</sup>	1.19×10 <sup>2</sup>	<b>2.85×10<sup>9</sup></b>	<b>3.80×10<sup>9</sup></b>	8.22×10 <sup>9</sup>	1.18×10 <sup>10</sup>	5.63×10 <sup>9</sup>	2.56×10 <sup>10</sup>

**Table S8.** Branching ratio ( $\Gamma$ , %) of all oxidation reactions, with the total FHT, RAF, SET, and the overall branching ratio at the temperature range of 283-323 K. (The most favourable pathways are in bold).

T (K)	H9-Abs	H10-Abs	H11-Abs	H12-Abs	H13-Abs	H14-Abs	H15-Abs	H22-Abs	H23-Abs	H27-Abs	H28-Abs	H29-Abs
283	0.01	0.01	0.01	0.03	<b>11.96</b>	2.30	<b>14.06</b>	1.02	0.00	0.14	0.07	0.34
288	0.01	0.01	0.01	0.03	<b>12.28</b>	2.07	<b>14.39</b>	0.87	0.00	0.13	0.06	0.31
293	0.01	0.01	0.01	0.03	<b>12.50</b>	1.85	<b>14.59</b>	0.75	0.00	0.12	0.06	0.28
298	0.01	0.01	0.01	0.03	<b>12.66</b>	1.67	<b>14.70</b>	0.65	0.00	0.11	0.06	0.25
303	0.01	0.01	0.01	0.03	<b>12.74</b>	1.51	<b>14.73</b>	0.56	0.00	0.10	0.05	0.23
308	0.01	0.01	0.01	0.03	<b>12.74</b>	1.37	<b>14.65</b>	0.49	0.00	0.09	0.05	0.21
313	0.01	0.01	0.01	0.02	<b>12.69</b>	1.25	<b>14.50</b>	0.43	0.00	0.09	0.05	0.19
318	0.01	0.01	0.01	0.02	<b>12.58</b>	1.14	<b>14.28</b>	0.38	0.00	0.08	0.05	0.18
323	0.01	0.01	0.01	0.02	<b>12.43</b>	1.06	<b>14.01</b>	0.34	0.00	0.08	0.04	0.17

T (K)	H30-Abs	H31-Abs	H32-Abs	H33-Abs	H40-Abs	H41-Abs	H42-Abs	H43-Abs	H44-Abs	C1-Add	C2-Add	C3-Add
283	1.34	<b>3.44</b>	0.22	0.05	<b>3.76</b>	0.20	0.04	0.01	0.01	0.44	7.18	2.74
288	1.15	<b>3.06</b>	0.21	0.04	<b>3.38</b>	0.18	0.03	0.01	0.01	0.40	6.73	2.50
293	1.00	<b>2.72</b>	0.19	0.04	<b>3.04</b>	0.16	0.03	0.01	0.01	0.35	6.22	2.27
298	0.87	<b>2.42</b>	0.18	0.03	<b>2.73</b>	0.15	0.03	0.01	0.01	0.32	5.72	2.08
303	0.77	<b>2.16</b>	0.17	0.03	<b>2.47</b>	0.14	0.03	0.01	0.01	0.29	5.22	1.90
308	0.67	<b>1.93</b>	0.16	0.03	<b>2.23</b>	0.13	0.03	0.01	0.01	0.26	4.75	1.74
313	0.60	<b>1.73</b>	0.15	0.03	<b>2.02</b>	0.12	0.03	0.00	0.01	0.24	4.31	1.60
318	0.54	<b>1.56</b>	0.15	0.02	<b>1.84</b>	0.12	0.03	0.00	0.01	0.22	3.90	1.48
323	0.48	<b>1.42</b>	0.14	0.02	<b>1.69</b>	0.11	0.03	0.00	0.01	0.20	3.54	1.37

T (K)	C4-Add	C5-Add	C6-Add	C7-Add	C16-Add	C19-Add	C34-Add	C38-Add	C39-Add	FHT	RAF	SET	Overall
283	0.66	1.77	1.04	<b>10.65</b>	2.15	0.01	0.00	<b>11.47</b>	<b>12.45</b>	39.00	50.55	10.45	100.00
288	0.60	1.63	0.92	<b>11.03</b>	1.89	0.01	0.00	<b>11.68</b>	<b>12.91</b>	38.24	50.29	11.47	100.00
293	0.55	1.51	0.81	<b>11.35</b>	1.66	0.01	0.00	<b>11.78</b>	<b>13.30</b>	37.39	49.81	12.80	100.00
298	0.50	1.40	0.72	<b>11.62</b>	1.46	0.01	0.00	<b>11.82</b>	<b>13.66</b>	36.58	49.29	14.13	100.00
303	0.46	1.30	0.64	<b>11.85</b>	1.29	0.01	0.00	<b>11.79</b>	<b>13.97</b>	35.74	48.71	15.54	100.00
308	0.43	1.21	0.57	<b>12.02</b>	1.14	0.00	0.00	<b>11.68</b>	<b>14.23</b>	34.85	48.04	17.12	100.00
313	0.40	1.14	0.52	<b>12.15</b>	1.01	0.00	0.00	<b>11.54</b>	<b>14.46</b>	33.95	47.36	18.69	100.00
318	0.37	1.07	0.47	<b>12.24</b>	0.90	0.00	0.00	<b>11.35</b>	<b>14.65</b>	33.01	46.65	20.34	100.00
323	0.35	1.01	0.43	<b>12.29</b>	0.81	0.00	0.00	<b>11.14</b>	<b>14.82</b>	32.07	45.95	21.98	100.00

**Table S9.** Tunnelling correction estimated by the Eckart method for formal hydrogen transfer (FHT) at the temperature  $T$  from 283 to 333 K.

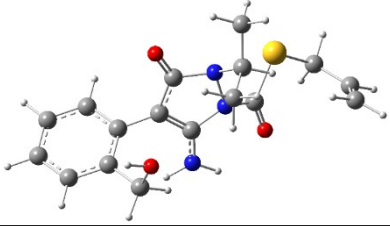
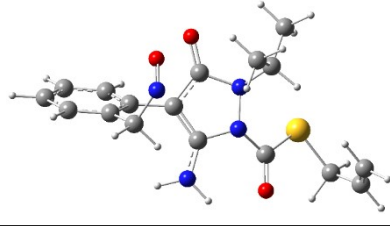
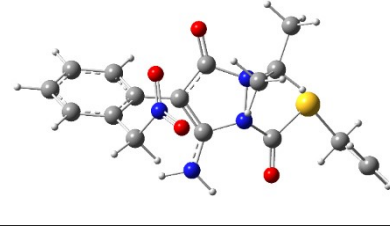
T (K)	H9-Abs	H10-Abs	H11-Abs	H12-Abs	H13-Abs	H14-Abs	H15-Abs	H22-Abs	H23-Abs	H27-Abs	
283	3.27	4.17	4.23	5.60	2.19	2.40	2.19	114.45	7.22	2.92	
288	3.13	3.93	3.99	5.22	2.14	2.32	2.14	96.51	6.60	2.81	
293	2.99	3.72	3.78	4.88	2.09	2.25	2.09	82.06	6.07	2.71	
298	2.88	3.54	3.59	4.59	2.04	2.19	2.04	70.32	5.61	2.62	
303	2.77	3.38	3.42	4.33	2.00	2.13	2.00	60.72	5.22	2.53	
308	2.67	3.23	3.27	4.10	1.95	2.08	1.95	52.79	4.88	2.46	
313	2.58	3.09	3.13	3.90	1.92	2.03	1.92	46.21	4.58	2.39	
318	2.50	2.97	3.01	3.71	1.88	1.99	1.88	40.69	4.32	2.32	
323	2.43	2.86	2.90	3.55	1.84	1.94	1.84	36.05	4.09	2.26	
328	2.36	2.76	2.79	3.40	1.81	1.90	1.81	32.12	3.88	2.20	
333	2.29	2.67	2.70	3.26	1.78	1.87	1.78	28.76	3.69	2.15	

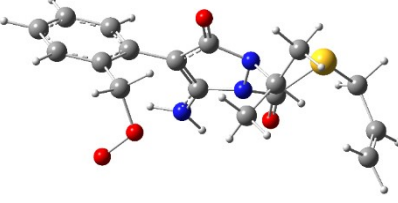
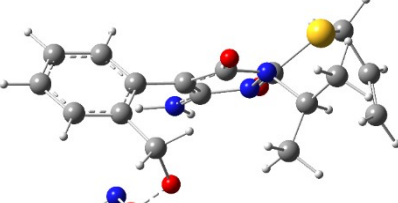
T (K)	H28-Abs	H29-Abs	H30-Abs	H31-Abs	H32-Abs	H33-Abs	H40-Abs	H41-Abs	H42-Abs	H43-Abs	H44-Abs
283	3.05	3.03	3.07	2.89	2.60	4.51	3.12	4.18	2.92	4.95	7.84
288	2.92	2.91	2.95	2.78	2.51	4.25	3.00	3.97	2.80	4.65	7.21
293	2.81	2.81	2.84	2.68	2.43	4.02	2.88	3.77	2.70	4.38	6.66
298	2.71	2.71	2.74	2.59	2.35	3.82	2.78	3.60	2.60	4.14	6.19
303	2.61	2.62	2.65	2.50	2.28	3.64	2.68	3.44	2.51	3.93	5.77
308	2.53	2.54	2.57	2.43	2.22	3.47	2.59	3.29	2.43	3.74	5.41
313	2.45	2.47	2.49	2.36	2.16	3.33	2.51	3.16	2.36	3.57	5.08
318	2.38	2.40	2.42	2.29	2.11	3.19	2.44	3.05	2.29	3.42	4.80
323	2.31	2.34	2.35	2.23	2.06	3.07	2.37	2.94	2.23	3.28	4.54
328	2.25	2.28	2.29	2.18	2.01	2.96	2.31	2.84	2.17	3.15	4.31
333	2.20	2.22	2.24	2.13	1.97	2.86	2.25	2.75	2.12	3.04	4.10

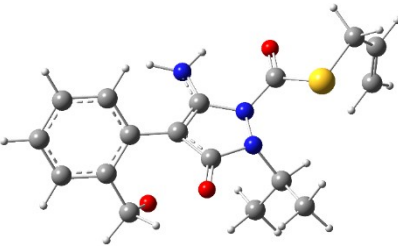
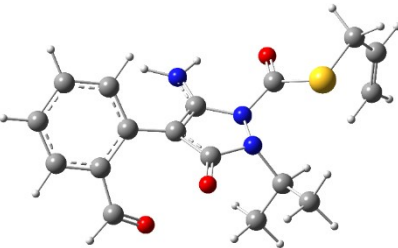
**Table S10.** Tunnelling correction estimated by the Eckart method for Radical adduct formation (RAF) at the temperature  $T$  from 283 to 333 K.

<b>T (K)</b>	<b>C1-Add</b>	<b>C2-Add</b>	<b>C3-Add</b>	<b>C4-Add</b>	<b>C5-Add</b>	<b>C6-Add</b>	<b>C7-Add</b>	<b>C16-Add</b>	<b>C19-Add</b>	<b>C34-Add</b>	<b>C38-Add</b>	<b>C39-Add</b>
<b>283</b>	1.05	1.08	1.11	1.13	1.12	1.22	1.09	1.22	1.16	1.13	1.04	1.11
<b>288</b>	1.05	1.07	1.11	1.13	1.12	1.21	1.08	1.21	1.15	1.13	1.04	1.11
<b>293</b>	1.05	1.07	1.11	1.12	1.12	1.21	1.08	1.20	1.15	1.12	1.04	1.11
<b>298</b>	1.04	1.07	1.10	1.12	1.11	1.20	1.08	1.20	1.14	1.12	1.04	1.10
<b>303</b>	1.04	1.07	1.10	1.11	1.11	1.19	1.08	1.19	1.14	1.12	1.04	1.10
<b>308</b>	1.04	1.06	1.10	1.11	1.10	1.18	1.07	1.18	1.13	1.11	1.03	1.10
<b>313</b>	1.04	1.06	1.09	1.11	1.10	1.18	1.07	1.18	1.13	1.11	1.03	1.09
<b>318</b>	1.04	1.06	1.09	1.10	1.10	1.17	1.07	1.17	1.12	1.10	1.03	1.09
<b>323</b>	1.04	1.06	1.09	1.10	1.09	1.17	1.07	1.17	1.12	1.10	1.03	1.09
<b>328</b>	1.04	1.06	1.08	1.10	1.09	1.16	1.07	1.16	1.12	1.10	1.03	1.08
<b>333</b>	1.04	1.05	1.08	1.09	1.09	1.16	1.06	1.16	1.11	1.09	1.03	1.08

**Table S11.** Cartesian coordinates of all intermediate species involved in the further reactions of H15-Abs product at 298K.

P1-OH-pathway				P3-NO-pathway				P4-NO <sub>2</sub> -pathway			
											
0 1				0 1				0 1			
C	-3.54915400	-0.45679700	0.71072000	C	-3.47299300	-0.59111800	0.65588000	C	3.38917100	-0.53935600	-0.63975900
C	-2.71677600	-0.46011000	-0.42580400	C	-2.62039100	-0.59662500	-0.46435100	C	2.49066100	-0.93023500	0.37018500
C	-3.26849700	-0.74143900	-1.68103900	C	-3.14950400	-0.89182600	-1.72659400	C	2.96543400	-1.68825900	1.44513800
C	-4.62568700	-1.03170900	-1.81616600	C	-4.50127700	-1.19266900	-1.88244000	C	4.30461400	-2.07199600	1.51048400
C	-5.44501300	-1.05230800	-0.68889600	C	-5.34111500	-1.20605600	-0.76986400	C	5.18570700	-1.70159900	0.49654200
C	-4.90406900	-0.76344300	0.56404900	C	-4.82510400	-0.90173600	0.48887300	C	4.72626900	-0.93206800	-0.57167800
C	-1.27566400	-0.15210700	-0.32399100	C	-1.18815900	-0.26102000	-0.34593700	C	1.07491900	-0.51227600	0.34111600
C	-0.29719900	-0.90975900	0.28678200	C	-0.20653000	-0.96127100	0.32424100	C	0.08933600	-0.92063600	-0.53556400
N	0.93861300	-0.26331700	0.14431200	N	1.01888700	-0.29728400	0.16657500	N	-1.11815900	-0.30103300	-0.18558300
N	0.75980400	0.91929200	-0.60654900	N	0.82998500	0.82549100	-0.66793500	N	-0.91456100	0.49984100	0.95930200
C	-0.63630400	0.99292500	-0.88166600	C	-0.56012500	0.86476200	-0.95924200	C	0.46825200	0.38224600	1.27371000
N	-0.40300300	-2.09068400	0.89305200	N	-0.29893400	-2.10808500	0.99718800	N	0.16405400	-1.78483700	-1.54591200
O	-1.13153600	1.95961600	-1.47703100	O	-1.06596800	1.78842300	-1.61085900	O	0.98632500	1.02440500	2.19579100
C	1.35254000	2.11290000	0.09238300	C	1.43088500	2.07301000	-0.08373700	C	-1.43299300	1.89705500	0.75347500
C	0.48334200	2.56857800	1.25832000	C	0.56540500	2.64550700	-0.08379200	C	-0.52144600	2.69627000	-0.16900800
C	2.13274400	-0.97292100	0.01419200	C	2.22547800	-0.99807500	0.08930900	C	-2.34702800	-0.94650000	-0.34632500
O	2.33264200	-1.98824200	0.65588200	O	2.44363000	-1.94938100	0.81673100	O	-2.57365800	-1.62520100	-1.33092100
C	-3.02122000	-0.03975900	2.06340300	C	-2.97723400	-0.18870900	2.01066400	C	2.93397200	0.32414700	-1.77441100
C	1.64895900	3.21905200	-0.90741700	C	1.73855800	3.07564100	-1.18452400	C	-1.68888700	2.57406500	2.09025200
S	3.28996400	-0.28280000	-1.13635100	S	3.36209400	-0.39757100	-1.12886200	S	-3.49762300	-0.69685900	0.97703500
C	4.68815300	-1.38751500	-0.79011000	C	4.79041700	-1.42390800	-0.67908500	C	-4.93676300	-1.51190300	0.22864000
C	5.42454400	-1.14871500	0.49830500	C	5.51890800	-1.03402400	0.57666800	C	-5.63575800	-0.75570900	-0.86628900
C	5.11822300	-0.28033300	1.45975500	C	5.18929500	-0.08016600	1.44513300	C	-5.27255600	0.40325100	-1.41143800
H	-5.54246900	-0.76289000	1.44403800	H	-5.47863200	-0.89568400	1.35716200	H	5.41071500	-0.62365000	-1.35696600
H	-6.50104700	-1.28531800	-0.78370600	H	-6.39396000	-1.44568000	-0.88051600	H	6.22779500	-2.00133000	0.53929800
H	-5.03742700	-1.24833600	-2.79697600	H	-4.89412800	-1.42148100	-2.86816100	H	4.65571000	-2.66336400	2.35027800
H	-2.62129400	-0.73814700	-2.55404600	H	-2.48784800	-0.88759300	-2.58852700	H	2.27357400	-1.97994400	2.23022500
H	-2.06041100	-0.50947000	2.28613700	H	-2.03645100	-0.66752500	2.30922700	H	2.02323700	-0.01485700	-2.27208300
H	-3.73363100	-0.33456900	2.84132400	H	-3.69703900	-0.42711900	2.79983900	H	3.71175700	0.45854800	-2.52941900
H	0.41110100	-2.56262500	1.26261300	H	0.52236300	-2.54607200	1.39269700	H	-0.66043200	-2.03782100	-2.07429300
H	-1.29513700	-2.56818800	0.86557900	H	-1.16827400	-2.62487900	0.94836500	H	1.01900500	-2.31376600	-1.66579000
H	2.30512000	1.74905200	0.48558000	H	2.37933000	1.74048900	0.34572700	H	-2.39646300	1.75536400	0.25730500
H	1.02023300	3.32737100	1.83408200	H	1.10909600	3.45148200	1.53218700	H	-1.00108400	3.64630600	-0.42021400
H	0.25414900	1.73157600	1.92695500	H	0.33306900	1.87746000	1.77730100	H	-0.33908800	2.15162100	-1.10169600
H	-0.45482700	3.00700700	0.90430400	H	-0.37029900	3.05471600	0.63908200	H	0.43829400	2.91287700	0.31155700
H	0.73274100	3.66611900	-1.29736100	H	0.82630100	3.48387400	-1.62338400	H	-0.75796200	2.80760000	2.61000500
H	2.22472900	3.99970500	-0.40213700	H	2.31303100	3.90083700	-0.75422900	H	-2.22488400	3.50974400	1.90758500
H	2.24259700	2.83883500	-1.74374100	H	2.33685800	2.61363800	-1.97505300	H	-2.30721200	1.94256400	2.73469100
H	4.33466700	-2.42109000	-0.84411700	H	4.46605100	-2.46699300	-0.62652200	H	-4.63104400	-2.50159100	-0.12227000
H	5.36266400	-1.23792000	-1.63953200	H	5.46003500	-1.34229500	-1.54167400	H	-5.62043900	-1.67025400	1.06922500
H	6.29757600	-1.79039400	0.61414400	H	6.40858700	-1.63700600	0.75626300	H	-6.53260100	-1.25966500	-1.22555600
H	5.73367600	-0.20579600	2.35074300	H	5.80280500	0.10108600	2.32205800	H	-5.86528800	0.84893100	-2.20405100
H	4.25667500	0.38123000	1.39766300	H	4.31118500	0.54996100	1.31896100	H	-4.38552100	0.94670300	-1.09251300
O	-2.78351300	1.36985300	2.12232700	N	-2.69478200	1.26050600	2.20403300	N	2.60679300	1.73507200	-1.33164800
H	-3.63128200	1.82254700	2.00798800	O	-2.78025700	1.93536200	1.21428600	O	2.88009600	2.09498500	-0.20211800
								O	2.08218300	2.45499200	-2.16542900

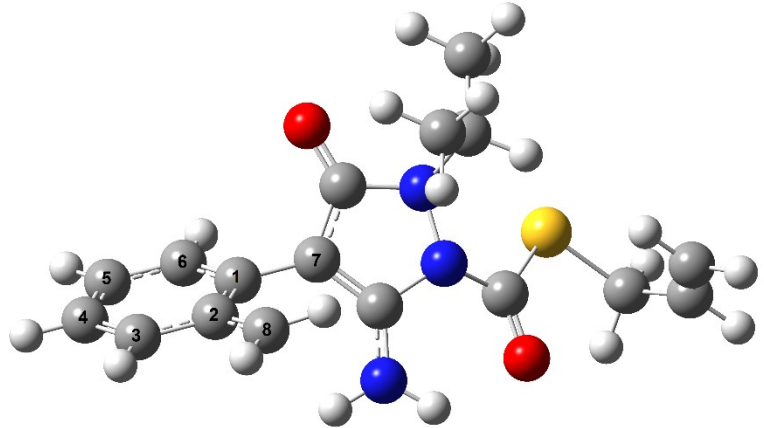
Int-H15-1-O <sub>2</sub> -pathway				Int-H15-2-O <sub>2</sub> -pathway			
							
0 2				0 1			
C	-3.57444100	0.19407700	-0.02797700	C	-0.10680400	-1.15995800	1.07060500
C	-2.56888100	-0.67691100	-0.48893500	C	-0.82269800	0.02730900	0.74155000
C	-2.93582900	-1.92236500	-1.01022400	C	0.06930500	0.88348000	0.12250100
C	-4.27727600	-2.29691000	-1.08970600	N	1.31960600	0.25774900	0.03887000
C	-5.26980200	-1.42346700	-0.65119500	N	1.24626000	-1.01400600	0.64733200
C	-4.91418700	-0.18452400	-0.11772100	C	-2.24000300	0.31049400	1.04091000
C	-1.14331400	-0.29959000	-0.41290500	C	-3.27279200	-0.48847200	0.51227900
C	-0.17169000	-0.92343400	0.34513200	C	-4.60101400	-0.18692000	0.81745500
N	1.05306600	-0.27537300	0.14045500	C	-4.92186200	0.90053000	1.62999600
N	0.87633200	0.76768300	-0.79456200	C	-3.90343200	1.70329700	2.13899200
C	-0.51053900	0.76611100	-1.11681400	C	-2.57233000	1.40455400	1.84852900
N	-0.27895500	-1.97979300	1.14760400	C	-2.97704200	-1.61073600	-0.44632400
O	-1.00407900	1.61406600	-1.87313500	O	-2.41462200	-1.12822500	-1.68641500
C	1.43349700	2.06938000	-0.28596800	O	-3.39185700	-0.33956600	-2.32144900
C	0.53098300	2.69068000	0.77308700	N	-0.11710700	2.12540700	-0.31497100
C	2.26671900	-0.96517500	0.16505800	C	2.51437500	0.97546400	0.11193500
O	2.46763400	-1.84999000	0.97658200	S	3.80597800	0.17821900	1.02603400
C	-3.21623100	1.50929600	0.60259000	C	5.14567600	1.34522700	0.65392800
C	1.73680800	3.00490200	-1.44520600	C	5.72685100	1.27239200	-0.73041500
S	3.43969900	-0.45440300	-1.06003200	C	5.31809100	0.51137000	-1.74351300
C	4.85755300	-1.43076500	-0.48441600	C	1.76429100	-2.09283200	-0.26566400
C	5.54194700	-0.94026300	0.76085600	C	2.19114300	-3.30901000	0.54032800
C	5.17983200	0.07622700	1.54078800	O	-0.50952900	-2.20227900	1.60525900
H	-5.68153300	0.49501400	0.24277200	C	0.76725300	-2.41864000	-1.37118900
H	-6.31575200	-1.70611700	-0.71440400	O	2.62539200	2.06505300	-0.41947400
H	-4.54327400	-3.26596300	-1.50008500	H	-5.39113100	-0.80460200	0.39834300
H	-2.15973700	-2.59541900	-1.36521400	H	-5.96015700	1.12327800	1.85420300
H	-2.52410200	2.10222900	0.00208200	H	-4.14015000	2.55638600	2.76708600
H	-4.10328200	2.09534900	0.85027700	H	-1.77569100	2.01936900	2.25977400
H	0.53269300	-2.36115800	1.61504000	H	-2.19778400	-2.28707700	-0.08498900
H	-1.15353900	-2.48856200	1.16465600	H	-3.88015800	-2.18336900	-0.67380300
H	2.38186100	1.79231600	0.18144100	H	0.62358200	2.62940800	-0.78334200
H	1.03967200	3.54749500	1.22335600	H	-1.02983700	2.54875000	-0.20839300
H	0.30732300	1.97102600	1.56747400	H	2.65834900	-1.65604100	-0.71791200
H	-0.40919100	3.04255600	0.33617900	H	1.23686600	-3.09139300	-2.09401300
H	0.82350700	3.36588500	-1.92156100	H	0.45891900	-1.51104900	-1.90088000
H	2.28865700	3.86739400	-1.06085600	H	-0.12185300	-2.91563200	-0.96931800
H	2.35566500	2.50597500	-2.19648900	H	1.33397200	-3.82430600	0.97786500
H	4.53776400	-2.46958800	-0.36290200	H	2.70733400	-4.00514100	-0.12685800
H	5.55560800	-1.41025800	-1.32792400	H	2.87953100	-3.02289400	1.34073300
H	6.42723900	-1.52206500	1.01614300	H	4.79325100	2.35786600	0.86975900
H	5.76260800	0.32893400	2.42100800	H	5.91634900	1.11226200	1.39606500
H	4.30436100	0.68905700	1.33595000	H	6.57277100	1.94440000	-0.87241700
O	-2.48212600	1.30503400	1.85298300	H	5.82439000	0.55321300	-2.70274000
O	-3.20714400	0.70777900	2.75112200	H	4.47754500	-0.17418600	-1.65792600
				N	-3.03982400	1.00622200	-2.09806200
				O	-3.83667600	1.69831100	-2.60684400

Int-H15-3-O <sub>2</sub> -pathway				P2-O <sub>2</sub> -pathway			
							
0 2				0 1			
C	-3.13313200	-1.86145200	-0.76670000	C	-3.01847900	-1.93345000	-0.56933000
C	-2.73003200	-0.62667100	-0.24459900	C	-2.72347400	-0.64357500	-0.11068000
C	-3.70396200	0.26228000	0.24906600	C	-3.80453100	0.21362400	0.19749700
C	-5.05257400	-0.08892200	0.18147700	C	-5.12223800	-0.21914000	0.00018200
C	-5.44624200	-1.31778700	-0.34934700	C	-5.39574500	-1.50579800	-0.45113900
C	-4.48275100	-2.21004000	-0.81520400	C	-4.33487700	-2.36703000	-0.72503300
C	-1.29857300	-0.26761400	-0.21719200	C	-1.31306300	-0.23004100	-0.03115400
C	-0.69725600	0.83870200	-0.88418400	C	-0.73073400	0.89807000	-0.68882800
N	0.70528300	0.81798500	-0.63770700	N	0.67425200	0.85810800	-0.49598500
N	0.92583900	-0.28603200	0.21420900	N	0.92314000	-0.24639400	0.34601700
C	-0.28953100	-0.94343900	0.44245900	C	-0.28699300	-0.91528000	0.58835300
O	-1.22631100	1.73408500	-1.55756700	O	-1.27634200	1.80576000	-1.32837800
N	-0.35893700	-2.05097000	1.17653100	N	-0.32271500	-2.03591200	1.30758900
C	2.13534500	-0.97798200	0.12552500	C	2.11886400	-0.95599000	0.18410200
O	2.37609100	-1.91557900	0.86356800	O	2.39347600	-1.89146900	0.91203700
C	1.29036300	2.08254300	-0.06959400	C	1.34080300	2.11315300	-0.01042700
C	0.44053400	2.62951800	1.07077700	C	0.57017100	2.76020600	1.13333600
C	-3.29518800	1.56347100	0.89426600	C	-3.67189300	1.55040400	0.81360100
O	-2.47395600	1.41522100	2.00009600	O	-2.66323700	2.00979800	1.32370900
S	3.24132700	-0.38727300	-1.12587400	S	3.15086000	-0.39102800	-1.13959100
C	4.68644300	-1.39660300	-0.69177900	C	4.59407000	-1.44233800	-0.81261000
C	5.44010300	-0.98203000	0.54090900	C	5.45033100	-1.05359800	0.35994300
C	5.12231000	-0.01776500	1.40226700	C	5.22114400	-0.08918800	1.24867300
C	1.53844200	3.09482400	-1.17631600	C	1.59056100	3.05954500	-1.17410500
H	-5.79932200	0.60286500	0.56291000	H	-5.93684100	0.46366400	0.22831500
H	-6.49916500	-1.57852500	-0.38995200	H	-6.42114000	-1.83208600	-0.58832400
H	-4.77824300	-3.17095200	-1.22458500	H	-4.52709300	-3.37384000	-1.08253800
H	-2.38004000	-2.54542400	-1.15017500	H	-2.20150400	-2.59896800	-0.83566900
H	-2.75705500	2.22900000	0.19174600	H	-4.60857400	2.13530500	0.82914800
H	-4.17439600	2.14988500	1.21191100	H	0.52350900	-2.43372800	1.69230300
H	0.47327200	-2.46213700	1.57797500	H	-1.19460900	-2.54266200	1.38318600
H	-1.23599000	-2.55451100	1.21161100	H	2.30936700	1.77527600	0.36644600
H	2.25977500	1.77484600	0.33087200	H	1.18029500	3.55362500	1.57363400
H	0.96922000	3.45705700	1.55173900	H	0.34192100	2.02910600	1.91624800
H	0.25583100	1.85792100	1.82594800	H	-0.36498300	3.20181400	0.77801500
H	-0.52111400	3.00376900	0.70415600	H	0.65581000	3.46185700	-1.56990800
H	0.60352900	3.48660300	-1.58112400	H	2.20244500	3.89443000	-0.82085100
H	2.11081300	3.92977600	-0.76228000	H	2.12853500	2.55286200	-1.98036500
H	2.11807700	2.64854000	-1.98943600	H	4.25428300	-2.47716500	-0.71327900
H	4.37073900	-2.44094200	-0.61575000	H	5.17852200	-1.38741800	-1.73673500
H	5.33605000	-1.32441900	-1.57029800	H	6.34541200	-1.66776000	0.45452500
H	6.33874300	-1.57494400	0.70901300	H	5.92085000	0.09026800	2.05885000
H	5.75406800	0.18178300	2.26209800	H	4.34262200	0.55110600	1.20389700
H	4.23629700	0.60327200	1.28663100				



**Table S12.** Standard enthalpy ( $\Delta_r H^\circ_{298K}$ ), and Gibbs free energy of reaction ( $\Delta_r G^\circ_{298K}$ ) for the  $O_2$ -addition to various carbon atom on the H15-Abs intermediate resulted from the most dominant FHT reaction at H15 hydrogen atom. Calculations were performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory in water.

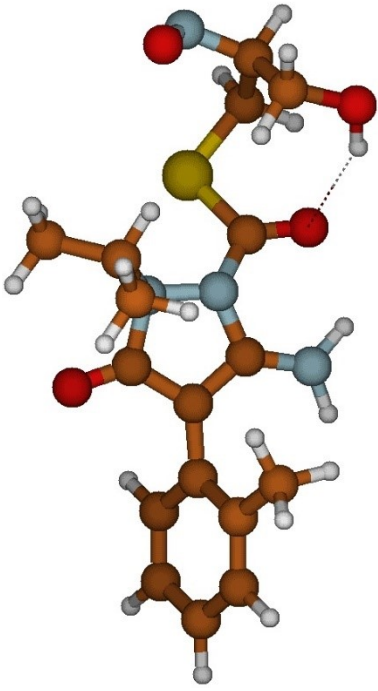
Position	$\Delta_r H^\circ_{298K}$	$\Delta_r G^\circ_{298K}$
Int-H15-C1	36.0	81.5
Int-H15-C2	1.4	54.7
Int-H15-C3	9.7	54.3
Int-H15-C4	246.9	287.7
Int-H15-C5	6.5	51.3
Int-H15-C6	9.7	54.6
Int-H15-C7	49.7	102.1
<b>Int-H15-C8</b>	<b>-115.3</b>	<b>-72.3</b>



**H15-Abs radical structure**

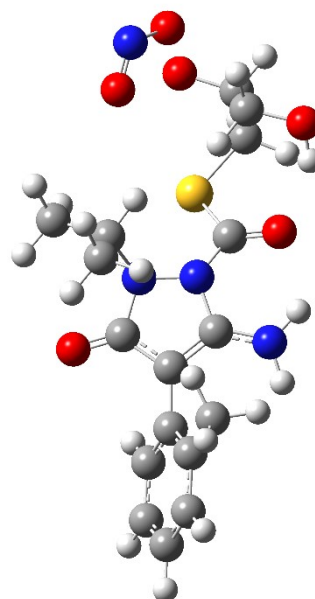
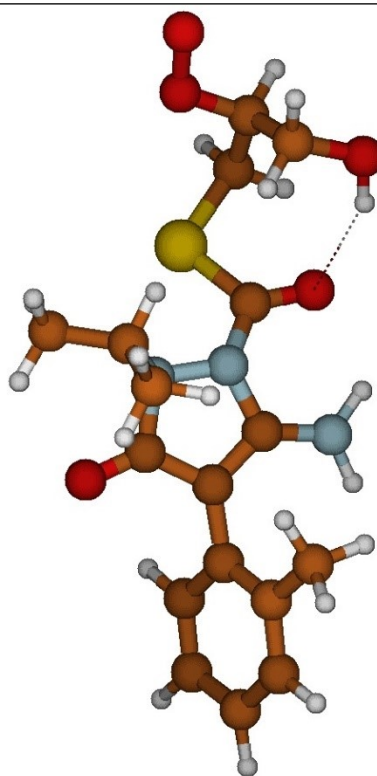
**Table S13.** Cartesian coordinates of all intermediate species involved in the further reactions of C39-Add product.

P5					Structures
6	0	-0.894394	-0.855481	-0.053614	
6	0	-1.917147	0.060437	-0.204061	
6	0	-1.316579	1.354199	-0.272290	
7	0	0.096924	1.215450	-0.151272	
7	0	0.328531	-0.168570	-0.000262	
6	0	-3.364084	-0.200424	-0.302872	
6	0	-4.067963	-0.885614	0.708784	
6	0	-5.445412	-1.082695	0.545658	
6	0	-6.124288	-0.604894	-0.572093	
6	0	-5.427510	0.093368	-1.559680	
6	0	-4.057439	0.289270	-1.421278	
6	0	-3.389417	-1.390124	1.956329	
8	0	-1.850251	2.466702	-0.364744	
6	0	0.733073	2.001811	0.965235	
6	0	0.944592	3.446854	0.543767	
6	0	1.516773	-0.710814	-0.468968	
16	0	2.575430	0.435330	-1.309663	
6	0	4.073808	-0.589425	-1.465854	
6	0	5.026093	-0.468048	-0.274604	
6	0	4.508964	-1.087731	1.022608	
8	0	4.287233	-2.482848	0.899431	
7	0	-0.945533	-2.184861	-0.020638	
8	0	1.770205	-1.895518	-0.312081	
6	0	-0.046711	1.859321	2.266709	
1	0	-5.992390	-1.608945	1.324036	
1	0	-7.193424	-0.768528	-0.667604	
1	0	-5.946140	0.477864	-2.432338	
1	0	-3.503539	0.823039	-2.189092	
1	0	-2.548107	-0.751429	2.241699	
1	0	-3.001435	-2.405613	1.818304	
1	0	-4.099736	-1.422329	2.785922	
1	0	-0.100856	-2.737336	0.043023	
1	0	-1.830486	-2.640425	-0.202545	
1	0	1.716271	1.541197	1.093627	
1	0	0.521393	2.320165	3.079254	
1	0	-0.204601	0.804814	2.517115	
1	0	-1.018856	2.358313	2.202933	
1	0	-0.000864	3.986161	0.462319	
1	0	1.559036	3.942514	1.300699	
1	0	1.468402	3.500094	-0.414974	
1	0	3.783514	-1.625685	-1.652657	
1	0	4.567910	-0.206089	-2.361910	

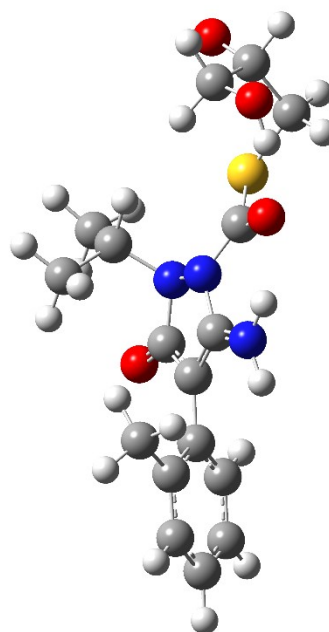
1	0	5.945511	-0.990638	-0.559385	
1	0	5.271743	-0.946142	1.792278	
1	0	3.596532	-0.571227	1.358669	
1	0	3.442218	-2.611601	0.440988	
8	0	5.399647	0.883929	-0.046631	
1	0	4.632742	1.374229	0.288993	
<b>P7</b>					
6	0	-1.075852	-0.889797	-0.083166	
6	0	-2.066837	0.063679	-0.211259	
6	0	-1.419359	1.333018	-0.309691	
7	0	-0.008850	1.141381	-0.229299	
7	0	0.172852	-0.249383	-0.071704	
6	0	-3.524977	-0.141429	-0.267876	
6	0	-4.226776	-0.799977	0.762626	
6	0	-5.614870	-0.943378	0.637054	
6	0	-6.305374	-0.438089	-0.461164	
6	0	-5.609458	0.234126	-1.467319	
6	0	-4.229640	0.376309	-1.366672	
6	0	-3.536660	-1.331935	1.992330	
8	0	-1.912128	2.464379	-0.396291	
6	0	0.688660	1.912653	0.861889	
6	0	0.949725	3.341880	0.415321	
6	0	1.329686	-0.839981	-0.554822	
16	0	2.409066	0.259935	-1.433902	
6	0	3.891552	-0.793533	-1.520448	
6	0	4.808850	-0.665053	-0.298951	
6	0	4.231414	-1.155807	1.022453	
8	0	4.022878	-2.559149	0.990116	
7	0	-1.174560	-2.216091	-0.040595	
8	0	1.551364	-2.028491	-0.382587	
6	0	-0.062925	1.818081	2.184286	
1	0	-6.160129	-1.449109	1.430097	
1	0	-7.382268	-0.560056	-0.527118	
1	0	-6.136502	0.639859	-2.325196	
1	0	-3.676780	0.889060	-2.149370	
1	0	-2.654538	-0.737140	2.247395	
1	0	-3.208070	-2.367675	1.850293	
1	0	-4.221693	-1.321512	2.843516	
1	0	-0.350466	-2.799712	0.014018	
1	0	-2.081119	-2.640080	-0.189272	
1	0	1.655131	1.413114	0.971737	
1	0	0.546458	2.260622	2.976842	
1	0	-0.260616	0.774008	2.449960	
1	0	-1.013350	2.359194	2.140562	
1	0	0.024865	3.916760	0.340036	
1	0	1.595915	3.823823	1.154556	

1	0	1.459620	3.359789	-0.552229	
1	0	3.588121	-1.833779	-1.653381	
1	0	4.417393	-0.474463	-2.423092	
1	0	5.713013	-1.238360	-0.540993	
1	0	4.953162	-0.956155	1.818004	
1	0	3.305309	-0.626167	1.280581	
1	0	3.192108	-2.729953	0.519711	
7	0	5.270338	0.743190	-0.268874	
8	0	4.958881	1.338349	0.730203	
<b>P8</b>					
6	0	-1.345672	-0.880758	-0.052223	
6	0	-2.328278	0.078061	-0.201979	
6	0	-1.675523	1.347028	-0.243888	
7	0	-0.269854	1.150337	-0.098092	
7	0	-0.096567	-0.244511	0.032352	
6	0	-3.783459	-0.123481	-0.318304	
6	0	-4.523510	-0.790937	0.679366	
6	0	-5.905957	-0.931822	0.501143	
6	0	-6.554474	-0.415701	-0.617646	
6	0	-5.821217	0.265170	-1.590807	
6	0	-4.445855	0.405472	-1.437499	
6	0	-3.877439	-1.334689	1.927673	
8	0	-2.161614	2.480954	-0.331500	
6	0	0.368101	1.892796	1.047961	
6	0	0.652316	3.332582	0.651967	
6	0	1.074168	-0.824487	-0.432688	
16	0	2.205026	0.308869	-1.196240	
6	0	3.605460	-0.818541	-1.481274	
6	0	4.629606	-0.865748	-0.361726	
6	0	4.123851	-1.395354	0.988575	
8	0	3.767529	-2.757057	0.863066	
7	0	-1.451085	-2.206855	-0.045404	
8	0	1.273878	-2.023498	-0.308776	
6	0	-0.451955	1.767433	2.326083	
1	0	-6.480760	-1.444299	1.268583	
1	0	-7.628231	-0.536092	-0.725034	
1	0	-6.315830	0.679242	-2.463864	
1	0	-3.863839	0.925087	-2.194100	
1	0	-3.016465	-0.730672	2.229474	
1	0	-3.525293	-2.362048	1.781603	
1	0	-4.597235	-1.350313	2.749538	
1	0	-0.632123	-2.795345	0.028862	
1	0	-2.352880	-2.622857	-0.239364	
1	0	1.325802	1.387631	1.197075	
1	0	0.113782	2.193420	3.159040	
1	0	-0.660483	0.717493	2.557929	
1	0	-1.400167	2.308045	2.244496	
1	0	-0.267511	3.911229	0.548792	
1	0	1.263006	3.793605	1.433361	
1	0	1.207008	3.375333	-0.289830	
1	0	3.222145	-1.827260	-1.648195	
1	0	4.068564	-0.478065	-2.407862	
1	0	5.472238	-1.487502	-0.684427	
1	0	4.929843	-1.334683	1.719208	
1	0	3.280848	-0.791141	1.349545	
1	0	2.883861	-2.807578	0.464510	
7	0	5.258129	0.497069	-0.153977	
8	0	5.991536	0.632352	0.810552	
8	0	5.024664	1.382303	-0.957348	
<b>Int-C39-1</b>					

6	0	-1.144060	-0.856181	-0.023934
6	0	-2.156176	0.066423	-0.201477
6	0	-1.541774	1.351702	-0.299703
7	0	-0.129628	1.201863	-0.164142
7	0	0.086589	-0.180869	0.018948
6	0	-3.605700	-0.181786	-0.297585
6	0	-4.319562	-0.829349	0.731693
6	0	-5.698431	-1.017237	0.569808
6	0	-6.368834	-0.566270	-0.564097
6	0	-5.661967	0.095175	-1.569647
6	0	-4.290387	0.281363	-1.432439
6	0	-3.649999	-1.304190	1.995654
8	0	-2.062852	2.466548	-0.424276
6	0	0.501578	2.005995	0.943055
6	0	0.734258	3.438406	0.490618
6	0	1.266391	-0.744215	-0.445209
16	0	2.346782	0.386248	-1.281135
6	0	3.777859	-0.709809	-1.532208
6	0	4.794805	-0.700208	-0.403945
6	0	4.300203	-1.182596	0.959133
8	0	4.020735	-2.569011	0.925440
7	0	-1.209390	-2.183482	0.042955
8	0	1.505675	-1.930454	-0.280551
6	0	-0.295419	1.902499	2.237813
1	0	-6.253118	-1.514716	1.361505
1	0	-7.439240	-0.722086	-0.658463
1	0	-6.173988	0.458426	-2.455213
1	0	-3.728645	0.786420	-2.213838
1	0	-2.802555	-0.666623	2.264921
1	0	-3.273100	-2.327578	1.888659
1	0	-4.362916	-1.304173	2.823654
1	0	-0.370779	-2.743357	0.120237
1	0	-2.098881	-2.633908	-0.129815
1	0	1.476989	1.536485	1.094448
1	0	0.267656	2.377422	3.045717
1	0	-0.466676	0.855978	2.511692
1	0	-1.261673	2.409278	2.150219
1	0	-0.204489	3.984953	0.383467
1	0	1.343647	3.945812	1.243791
1	0	1.271216	3.463697	-0.461964
1	0	3.424197	-1.729537	-1.699426
1	0	4.246875	-0.356700	-2.453337
1	0	5.668407	-1.283197	-0.710510
1	0	5.099796	-1.025803	1.686671
1	0	3.425567	-0.602419	1.281826
1	0	3.148935	-2.690982	0.517321
8	0	5.233615	0.682604	-0.267875
8	0	6.355895	0.780528	0.381899
<b>Int-C39-2</b>				
6	0	-4.656006	0.364978	-1.313482
6	0	-3.931598	-0.046866	-0.183248
6	0	-4.621740	-0.495048	0.961804
6	0	-6.021413	-0.542674	0.919842
6	0	-6.732600	-0.144332	-0.208797
6	0	-6.045967	0.320521	-1.331664
6	0	-2.461428	0.044303	-0.221776
6	0	-1.538617	-0.958521	0.004903
7	0	-0.248072	-0.427983	-0.133737
7	0	-0.334623	0.933259	-0.494022
6	0	-1.726455	1.228880	-0.535203
7	0	-1.730710	-2.252924	0.247861
8	0	-2.134925	2.374259	-0.765085
6	0	0.494345	1.797096	0.420436
6	0	-0.186109	2.006668	1.767523
6	0	0.839135	-1.174531	-0.562108
8	0	0.994015	-2.329272	-0.193848
6	0	-3.905616	-0.902115	2.223910
6	0	0.875760	3.092915	-0.275295
16	0	1.930224	-0.319143	-1.664994
6	0	3.372412	-1.427205	-1.574504
6	0	4.322932	-1.088734	-0.432270
8	0	4.680222	0.286458	-0.685022
8	0	5.639319	0.703866	0.254708
6	0	3.741659	-1.277643	0.969158
8	0	3.485800	-2.649429	1.213105



1	0	-6.557651	-0.885301	1.801370	
1	0	-7.817541	-0.187438	-0.208857	
1	0	-6.588631	0.640902	-2.215548	
1	0	-4.111209	0.715023	-2.186310	
1	0	-2.970928	-0.348298	2.352724	
1	0	-3.659385	-1.969871	2.218385	
1	0	-4.541518	-0.719062	3.093393	
1	0	-0.948769	-2.883301	0.365472	
1	0	-2.671355	-2.622292	0.199941	
1	0	1.408688	1.220233	0.579246	
1	0	0.512816	2.498996	2.449339	
1	0	-0.477599	1.049041	2.212473	
1	0	-1.074444	2.638525	1.671663	
1	0	0.006048	3.732042	-0.441148	
1	0	1.585022	3.633071	0.358790	
1	0	1.356759	2.889747	-1.236555	
1	0	3.037248	-2.463439	-1.494393	
1	0	3.885758	-1.307980	-2.531348	
1	0	5.219005	-1.711358	-0.538342	
1	0	4.479181	-0.960538	1.710668	
1	0	2.838404	-0.668656	1.109378	
1	0	2.644334	-2.882516	0.789806	
7	0	5.110655	1.622439	1.186114	
8	0	3.969227	1.837751	1.071250	
<b>Int-C39-3</b>					
6	0	-4.029995	0.235570	-1.444277	
6	0	-3.338445	-0.224710	-0.312413	
6	0	-4.039895	-0.904253	0.704828	
6	0	-5.412745	-1.125396	0.534157	
6	0	-6.089695	-0.676739	-0.596767	
6	0	-5.395740	0.016031	-1.590181	
6	0	-1.896243	0.058708	-0.205860	
6	0	-0.862574	-0.840795	-0.032546	
7	0	0.350458	-0.136443	0.025883	
7	0	0.101245	1.242362	-0.144028	
6	0	-1.312991	1.359425	-0.285809	
7	0	-0.897439	-2.170098	0.018825	
8	0	-1.860630	2.462849	-0.400960	
6	0	0.707552	2.050122	0.974049	
6	0	-0.092691	1.913586	2.263702	
6	0	1.548709	-0.667437	-0.431579	
8	0	1.809657	-1.850830	-0.272689	
6	0	-3.363966	-1.377751	1.965917	
6	0	0.907709	3.492562	0.538208	
16	0	2.610384	0.490265	-1.249468	
6	0	4.080346	-0.559393	-1.476591	
6	0	5.065824	-0.460967	-0.313471	
8	0	5.489649	0.831853	-0.078910	
6	0	4.591404	-1.093071	1.015685	
8	0	4.342471	-2.475976	0.867129	
1	0	-5.957819	-1.647372	1.316735	
1	0	-7.155326	-0.858712	-0.698103	
1	0	-5.913172	0.377630	-2.473280	
1	0	-3.478109	0.764925	-2.216576	
1	0	-2.535432	-0.721132	2.247974	
1	0	-2.958696	-2.388944	1.847512	
1	0	-4.080753	-1.408083	2.790000	
1	0	-0.045989	-2.710698	0.092482	
1	0	-1.774417	-2.638703	-0.168551	
1	0	1.693397	1.603004	1.125041	
1	0	0.454931	2.393053	3.079521	
1	0	-0.240096	0.860348	2.525537	
1	0	-1.070439	2.397948	2.176796	
1	0	-0.043218	4.018079	0.433388	
1	0	1.502077	4.005944	1.299316	
1	0	1.447428	3.540992	-0.411913	
1	0	3.765222	-1.588766	-1.660083	
1	0	4.553671	-0.177793	-2.384134	
1	0	5.986032	-1.013845	-0.590598	
1	0	5.391471	-0.970734	1.747810	
1	0	3.700311	-0.565929	1.381220	
1	0	3.464388	-2.582301	0.467763	
<b>P6</b>					



6	0	-3.873343	-0.265634	-1.510702
6	0	-3.204390	-0.460432	-0.291535
6	0	-3.881222	-1.068509	0.785641
6	0	-5.202857	-1.490158	0.589155
6	0	-5.855777	-1.304975	-0.626426
6	0	-5.189643	-0.680740	-1.682317
6	0	-1.816481	0.019889	-0.169476
6	0	-0.693517	-0.699017	0.189237
7	0	0.420859	0.156483	0.176868
7	0	0.017506	1.444747	-0.234880
6	0	-1.390502	1.355604	-0.443869
7	0	-0.564001	-1.995627	0.458960
8	0	-2.059310	2.346456	-0.760178
6	0	0.462828	2.500885	0.742270
6	0	-0.377526	2.480193	2.013229
6	0	1.686989	-0.284478	-0.180817
8	0	2.107056	-1.375690	0.171656
6	0	-3.235890	-1.258071	2.134323
6	0	0.500551	3.862554	0.067168
16	0	2.637558	0.852011	-1.151775
6	0	4.133220	-0.170629	-1.223566
6	0	4.657855	-0.524029	0.157765
8	0	4.796773	0.324393	1.020509
6	0	5.073086	-1.956871	0.441279
8	0	4.543069	-2.916031	-0.447510
1	0	-5.728663	-1.958516	1.417470
1	0	-6.882368	-1.637678	-0.746259
1	0	-5.689744	-0.523385	-2.632848
1	0	-3.342258	0.211787	-2.329907
1	0	-2.512290	-0.465588	2.347743
1	0	-2.705287	-2.214870	2.194017
1	0	-3.995579	-1.256985	2.919660
1	0	0.343832	-2.399440	0.647945
1	0	-1.359402	-2.603155	0.309999
1	0	1.488298	2.219221	0.995228
1	0	0.065851	3.156342	2.749128
1	0	-0.407856	1.475636	2.448511
1	0	-1.401612	2.812731	1.816222
1	0	-0.503116	4.228321	-0.156997
1	0	0.983191	4.572619	0.744606
1	0	1.079303	3.822716	-0.860189
1	0	3.949167	-1.056806	-1.828215
1	0	4.887130	0.449717	-1.719903
1	0	6.164415	-1.996705	0.353466
1	0	4.806421	-2.167141	1.483481
1	0	3.578108	-2.906718	-0.355354

