Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Theoretical Estimation of Kinetic Parameters for Nucleophilic Substitution Reactions in Solution: An Application of Solution Translational Entropy Model

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S1 Sackur-Tetrode equation

$$S_{trans} = Rln[(\frac{10^{\frac{-15}{2}}}{N_A^4[X]})(\frac{2\pi MRTe^{\frac{5}{3}}}{h^2})^{\frac{3}{2}}]$$

Here, *T*/K is temperature; *M*/g mol^{-1} is the mass of the particle; *[X]*/mol L^{-1} is the concentration of the particles; *h* is Plank's constant.

S2 Experimental values and calculated activation enthalpies, activation entropies, and activation free energies for several SN reactions at the different calculation models displayed in **Fig. 2.**

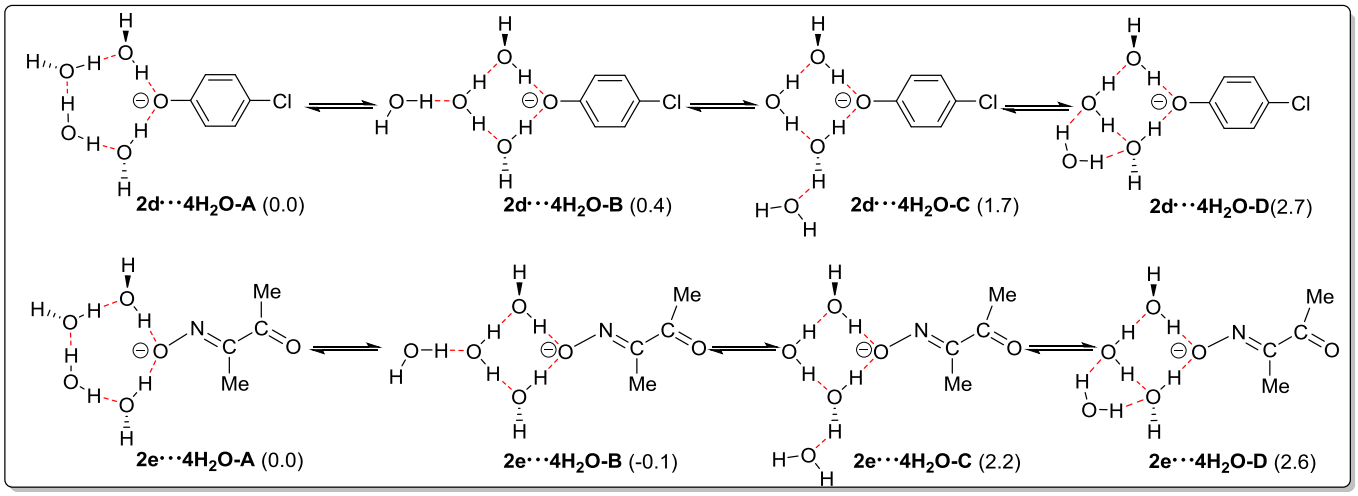
Reaction		$\Delta E_e^{\neq}$	$\Delta H^{\neq}$	$\Delta S^{\neq}$	$\Delta G^{\neq}$
1a+1b (MeOH, 273.15 K)	CAM-B3LYP /DZVP	27.1	27.9	-35.1	38.4
	M062x/DZVP	24.7	26.0	-31.9	35.5
	CAM-B3LYP +IDSCRF/DZVP	18.3	18.9	-19.8	25.1
	CAM-B3LYP +IDSCRF/TZVP	18.3	18.9	-19.4	25.0
	CAM-B3LYP +IDSCRF/6-311++g(d,p)	18.2	18.8	-19.6	24.9
	B3LYP +IDSCRF/DZVP	17.0	17.5	-19.0	23.5
	M062x+IDSCRF/DZVP	16.3	16.8	-19.8	23.0
	ωB97x+IDSCRF/DZVP	19.1	19.7	-19.4	25.7
	ωB97xD+IDSCRF/DZVP	16.8	17.4	-19.9	23.6
	B2PLYP+IDSCRF /DZVP	19.0			
	Exp. [7]		20.3	-19.5	26.4
1ba+2b (MeOH , 293.15 K)	CAM-B3LYP /DZVP	8.8	9.8	-46.9	23.8
	M062x/DZVP	-0.1	0.8	-47.5	15.0
	CAM-B3LYP +IDSCRF/DZVP	6.8	7.7	-22.4	13.8
	CAM-B3LYP +IDSCRF/TZVP	8.6	9.6	-22.3	15.7
	CAM-B3LYP +IDSCRF/6-311++g(d,p)	7.5	8.3	-24.3	15.0
	B3LYP +IDSCRF/DZVP	7.2	8.1	-23.2	14.4
	M062x+IDSCRF/DZVP	-1.5	-0.9	-22.7	5.3
	ωB97x+IDSCRF/DZVP	5.0	5.7	-22.4	11.8
	ωB97xD+IDSCRF/DZVP	0.5	1.4	-22.8	7.7
	B2PLYP+IDSCRF /DZVP	13.1			
	Exp. [9(c)]		11.0	-30.2	19.3
1da+2d (H_2O, 298.15 K)	CAM-B3LYP +IDSCRF/DZVP	3.6	4.2	-23.1	11.0
	CAM-B3LYP +IDSCRF/TZVP	5.3	5.9	-23.9	13.0
	CAM-B3LYP +IDSCRF/6-311++g(d,p)	6.0	6.7	-24.1	13.9

	B3LYP +IDSCRF/DZVP	5.8	6.4	-24.5	13.7
	M062x+IDSCRF/DZVP	-3.9	-3.4	-23.6	3.6
	ωB97x+IDSCRF/DZVP	0.01	0.6	-23.8	7.7
	ωB97xD+IDSCRF/DZVP	-1.7	-1.0	-24.0	6.2
	B2PLYP+IDSCRF /DZVP	8.0			
	Exp. [11]		13.5±1.9	-12.1±6.4	17.1±3.8
1da+2e (H_2O, 298.15 K)	CAM-B3LYP +IDSCRF/DZVP	0.9	1.4	-23.3	8.4
	CAM-B3LYP +IDSCRF/TZVP	2.4	2.9	-24.7	10.3
	CAM-B3LYP +IDSCRF/6311++g(d,p)	3.0	3.6	-24.4	10.8
	B3LYP +IDSCRF/DZVP	2.4	3.0	-23.6	10.0
	M062x+IDSCRF/DZVP	-3.7	-3.2	-24.7	4.2
	ωB97x+IDSCRF/DZVP	-2.1	-1.6	-24.1	5.6
	ωB97xD+IDSCRF/DZVP	-2.9	-2.4	-25.6	5.2
	B2PLYP+IDSCRF /DZVP	5.2			
	Exp. [11]		10.4±0.7	-15.4±2.3	15.0±1.4

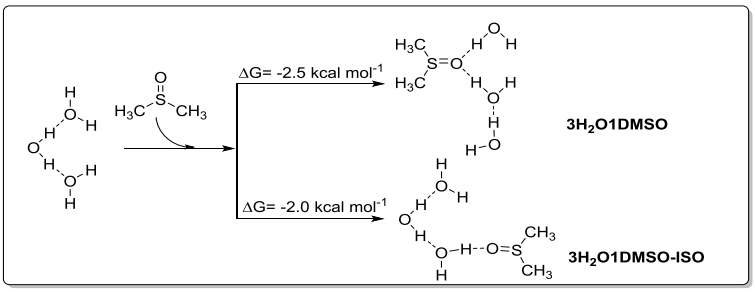
S3 The relative Gibbs free energies (in kcal mol^{-1}) for **TS1s**, **IN1s**, and **TS2s** of some chosen reactions in the article. The relative Gibbs free energies of reactants is zero.

Reactions	**TS1**	**IN1**	**TS2**
1da+2e ··2MeOH	19.3	-7.0	-0.4
1da+2d ··3H_2O	18.9	16.0	18.2
1da+2d ··2H_2O1DMSO	17.2	11.3	15.3
1da+2e ··3H_2O	15.6	12.3	15.3
1da+2e ··2H_2O1DMSO	14.7	9.4	13.7
1db+2d ··3H_2O	17.6	16.6	16.8
1db+2d ··2H_2O1DMSO	15.7	14.4	14.6
1db+2e ··3H_2O	14.9	13.4	13.9
1db+2e ··2H_2O1DMSO	12.7	11.2	11.5
1dc+2b (MeCN)	14.0	—	—
1dc+2c (MeCN)	17.2	—	—
1e+2b (MeCN)	21.1	—	—

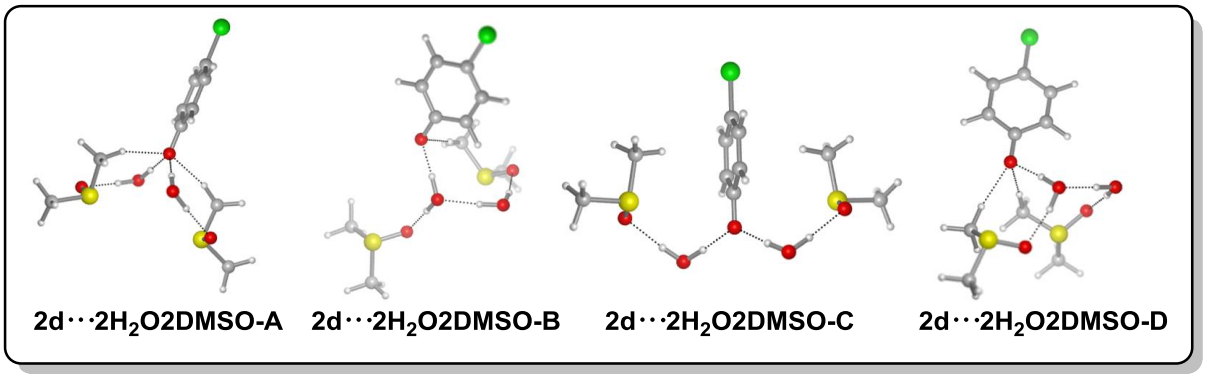
S4 Equilibrium between different complexes involved four H_2O molecules of **2d** and **2e** (values in parentheses are Gibbs free energy in kcal mol^{-1}).



S5 The possible complexes involved three H_2O molecules and one DMSO molecule in DMSO-H_2O mixture.



S6 Comparisons of experimental and calculated activation enthalpies, activation entropies, and activation free energies of **1da+2d** and **1da+2e** reactions involved different explicit water molecules at the CAM-B3LYP+IDSCRF/DZVP level.



Reactions	T	$\Delta H^{\neq}$(exp)	$\Delta H^{\neq}$(l)	$\Delta S^{\neq}$(exp)	$\Delta S^{\neq}$(g)	$\Delta S^{\neq}$(l)	$\Delta G^{\neq}$(l)	$\Delta G^{\neq}$(exp)
1da+2d ··H_2O	298.15 K	13.5±1.9 [11]	6.5	-12.1±6.4	-45.4	-24.0	13.6	17.1±3.8
1da+2d ··2H_2O	298.15 K	13.5±1.9	10.2	-12.1±6.4	-51.3	-27.0	18.2	17.1±3.8

1da+2d ··4H_2O-A	298.15 K	13.5±1.9	16.4	-12.1±6.4	-51.3	-23.2	23.4	17.1±3.8
1da+2d ··4H_2O-B	298.15 K	13.5±1.9	15.0	-12.1±6.4	-43.5	-19.0	20.7	17.1±3.8
1da+2e ··H_2O	298.15 K	10.4±0.7 [11]	2.8	-15.4±2.3	-47.1	-24.7	10.2	15.0±1.4
1da+2e ··2H_2O	298.15 K	10.4±0.7	6.4	-15.4±2.3	-42.8	-22.9	13.3	15.0±1.4
1da+2e ··4H_2O-A	298.15 K	10.4±0.7	13.9	-15.4±2.3	-50.1	-23.6	20.9	15.0±1.4
1da+2e ··4H_2O-B	298.15 K	10.4±0.7	12.6	-15.4±2.3	-42.8	-19.3	18.4	15.0±1.4
1da+2d ··2H_2O2DMSO-A	298.15 K	9.6~8.2 [11]	7.4	-18.4~-15.8	-52.6	-25.0	14.9	15.0~12.9
1da+2d ··2H_2O2DMSO-B	298.15 K	9.6~8.2	6.2	-18.4~-15.8	-51.7	-25.1	13.6	15.0~12.9
1da+2d ··2H_2O2DMSO-C	298.15 K	9.6~8.2	6.6	-18.4~-15.8	-53.6	-24.3	13.9	15.0~12.9
1da+2d ··2H_2O2DMSO-D	298.15 K	9.6~8.2	7.1	-18.4~-15.8	-49.3	-23.5	14.1	15.0~12.9

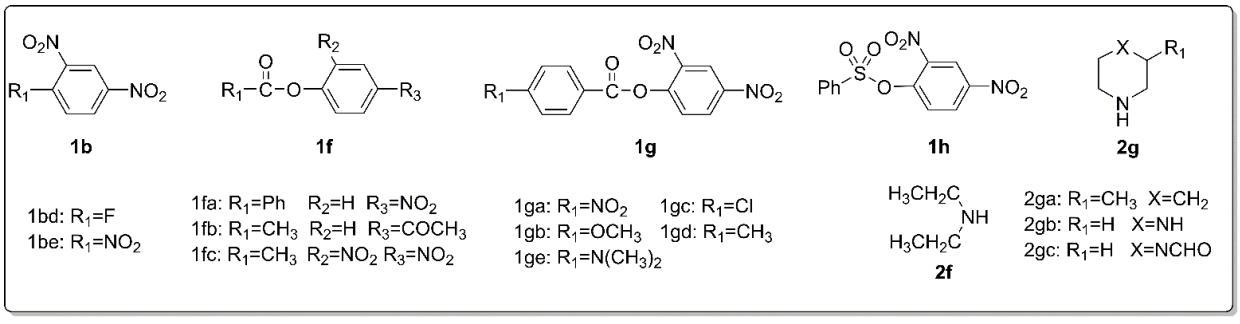
S7 Experimental and calculated activation enthalpies, activation entropies, and activation free energies of SN reactions at the CAM-B3LYP+IDSCRF/DZVP level displayed in **Fig. 4**.

Reactions	T	$\Delta H^{\neq}$(exp)	$\Delta H^{\neq}$(l)	$\Delta S^{\neq}$(exp)	$\Delta S^{\neq}$(g)	$\Delta S^{\neq}$(l)	$\Delta G^{\neq}$(g)	$\Delta G^{\neq}$(l)	$\Delta G^{\neq}$(exp)
1ba+2b ··MeOH	273.15 K	11.0 [9(c)]	12.6	-30.2	-47.8	-24.4	25.6	19.3	19.3
1ba+2b ··2MeOH	273.15 K	11.0 [9(c)]	11.3	-30.2	-54.5	-28.4	26.2	19.1	19.3
1bb+2b ··2MeOH	273.15 K	11.2 [9(c)]	11.8	-29.5	-54.6	-28.7	26.7	19.6	19.8
1bc+2b ··2MeOH	273.15 K	11.4 [9(c)]	9.5	-29.3	-57.1	-31.4	25.1	18.1	19.4
1ca+2b ··2MeOH [b]	293.15 K	14.8 [8(c)]	16.1	-29.0	-44.7	-24.1	29.3	23.2	23.3
1cb+2b ··2MeOH	293.15 K	15.3 [8(c)]	17.1	-28.0	-46.5	-25.3	30.7	24.5	23.5
1cc+2b ··2MeOH	293.15 K	12.9 [8(b)]	13.8	-30.0	-48.0	-26.7	28.8	21.6	21.7
1cd+2b ··2MeOH	293.15 K	14.9 [8(a)]	15.0	-25.0	-47.2	-25.2	28.8	22.3	22.2
1ce+2b ··2MeOH	293.15 K	14.4 [8(d)]	15.8	-27.2	-51.0	-26.7	30.7	23.6	22.3
1cf+2b ··2MeOH	293.15 K	11.7 [8(a)]	12.5	-28.5	-51.6	-28.2	27.6	20.7	19.9
1cg+2b ··2MeOH	293.15 K	13.8 [8(a)]	13.8	-30.5	-56.9	-30.7	30.5	22.8	22.6
1da+2d ··3H_2O	298.15 K	13.5±1.9 [11]	13.2	-12.1±6.4	-44.1	-18.8	26.4	18.9	17.1±3.8
1da+2e ··3H_2O	298.15 K	10.4±0.7 [11]	10.7	-15.4±2.3	-37.9	-16.4	22.0	15.6	15.0±1.4
1db+2d ··3H_2O	298.15 K	12.3 [10]	10.8	-18.1	-47.7	-22.5	25.1	17.6	17.7
1db+2e ··3H_2O	298.15 K	8.0 [10]	7.1	-23.5	-47.6	-23.6	21.3	14.1	15.0

S8 Experimental and calculated activation enthalpies, activation entropies, and activation free energies of SN reactions at the B3LYP+IDSCRF/DZVP level displayed in **Fig. 4**

Reactions	**T**	$\Delta H^{\neq}$**(exp)**	$\Delta H^{\neq}$**(l)**	$\Delta S^{\neq}$**(exp)**	$\Delta S^{\neq}$**(g)**	$\Delta S^{\neq}$**(l)**	$\Delta G^{\neq}$**(g)**	$\Delta G^{\neq}$**(l)**	$\Delta G^{\neq}$**(exp)**
1ba+2b ··2MeOH	273.15 K	11.0 [9(c)]	12.4	-30.2	-53.1	-28.5	26.9	20.2	19.3
1bb+2b ··2MeOH	273.15 K	11.2 [9(c)]	12.5	-29.5	-52.1	-27.6	26.7	20.0	19.8
1bc+2b ··2MeOH	273.15 K	11.4 [9(c)]	10.9	-29.3	-59.8	-31.8	27.2	19.6	19.4
1ca+2b ··2MeOH	293.15 K	14.8 [8(c)]	15.0	-29.0	-45.1	-24.0	28.2	22.1	23.3
1cb+2b ··2MeOH	293.15 K	15.3 [8(c)]	15.7	-28.0	-46.5	-24.0	28.8	22.7	23.5
1cc+2b ··2MeOH	293.15 K	12.9 [8(b)]	13.1	-30.0	-46.7	-26.5	26.8	20.9	21.7
1cd+2b ··2MeOH	293.15 K	14.9 [8(a)]	16.3	-25.0	-48.0	-25.6	30.3	22.8	22.2
1ce+2b ··2MeOH	293.15 K	14.4 [8(d)]	16.9	-27.2	-45.8	-24.4	30.3	24.0	22.3
1cf+2b ··2MeOH	293.15 K	11.7 [8(a)]	16.1	-28.5	-54.8	-29.9	32.2	24.9	19.9
1cg+2b ··2MeOH	293.15 K	13.8 [8(a)]	13.9	-30.5	-51.3	-28.9	29.0	22.4	22.6
1da+2d ··3H_2O	298.15 K	13.5±1.9 [11]	16.1	-12.1±6.4	-41.9	-18.6	28.6	21.7	17.1±3.8
1da+2e ··3H_2O	298.15 K	10.4±0.7[11]	12.9	-15.4±2.3	-41.6	-17.7	25.3	18.1	15.0±1.4
1db+2d ··3H_2O	298.15 K	12.3 [10]	13.3	-18.1	-48.3	-23.7	27.7	20.4	17.7
1db+2e ··3H_2O	298.15 K	8.0 [10]	9.2	-23.5	-47.1	-24.7	23.3	16.6	15.0

S9 Experimental and calculated activation free energies and rate constants for all the SN reactions studied at the CAM-B3LYP+IDSCRF/DZVP level.



Reaction	T	$\Delta G^{\neq}$(g) kcal mol^{-1}	$\Delta G^{\neq}$(l) kcal mol^{-1}	$\Delta G^{\neq}$(exp) kcal mol^{-1}	k(g) L mol^{-1} s^{-1}	k(1) L mol^{-1} s^{-1}	k(exp) L mol^{-1} s^{-1}	ln[k(g)/L mol^{-1} s^{-1}]	ln[k(l)/L mol^{-1} s^{-1}]	ln[k(exp)/ L mol^{-1} s^{-1}]
1a+2a (MeOH)	313.15k	29.5	25.1	26.4 [7]	1.7×10^{-8}	2.0×10^{-5}	2.5×10^{-6}	-17.9	-10.8	-12.9
1ba+2b ··2MeOH	273.15 K	26.2	19.1	19.3 [9(c)]	6.2×10^{-9}	3.0×10^{-3}	2.0×10^{-3}	-18.9	-5.8	-6.2
1bb+2b ··2MeOH	273.15 K	26.7	19.6	19.8 [9(c)]	2.5×10^{-9}	1.2×10^{-3}	2.0×10^{-3}	-19.8	-6.7	-6.2
1bc+2b ··2MeOH	273.15 K	25.1	18.1	19.4 [9(c)]	4.7×10^{-8}	1.9×10^{-2}	1.4×10^{-3}	-16.9	-4.0	-6.6

1ca+2b ··2MeOH	293.15 K	29.3	23.2	23.3 [8(c)]	8.8×10^{-10}	3.1×10^{-5}	2.6×10^{-5}	-20.9	-10.4	-10.6
1cb+2b ··2MeOH	293.15 K	30.7	24.5	23.5 [8(c)]	8.7×10^{-11}	3.3×10^{-6}	1.8×10^{-5}	-23.3	-12.6	-10.9
1cc+2b ··2MeOH	293.15 K	28.8	21.6	21.7 [8(b)]	9.7×10^{-9}	4.8×10^{-4}	4.0×10^{-4}	-18.4	-7.6	-7.8
1cd+2b ··2MeOH	293.15 K	28.8	22.3	22.2 [8(a)]	2.1×10^{-9}	1.4×10^{-4}	1.7×10^{-4}	-20.0	-8.8	-8.7
1ce+2b ··2MeOH	293.15 K	30.7	23.6	22.3 [8(d)]	7.9×10^{-11}	1.6×10^{-5}	1.4×10^{-4}	-23.3	-11.1	-8.8
1cf+2b ··2MeOH	293.15 K	27.6	20.7	19.9 [8(a)]	1.6×10^{-8}	2.3×10^{-3}	8.9×10^{-3}	-17.9	-6.1	-4.7
1cg+2b ··2MeOH	293.15 K	30.5	22.8	22.6 [8(a)]	1.1×10^{-10}	6.1×10^{-5}	8.7×10^{-5}	-22.9	-9.7	-9.4
1da+2d ··3H_2O	298.15 K	26.4	18.9	17.1±3.8 [13]	2.8×10^{-7}	8.7×10^{-2}	1.5	-15.1	-2.4	0.4
1da+2e ··3H_2O	298.15 K	22.0	15.6	15.0±1.4 [11]	4.6×10^{-4}	2.3×10^{1}	4.9×10^{1}	-7.7	3.1	3.9
1db+2d ··3H_2O	298.15 K	25.1	17.6	17.7 [10]	2.5×10^{-6}	7.8×10^{-1}	6.8×10^{-1}	-12.9	-0.2	-0.4
1db+2e ··3H_2O	298.15 K	21.3	14.1	15.0 [10]	1.5×10^{-3}	2.8×10^{2}	6.6×10^{1}	-6.5	5.6	4.2
1bb+2b (MeCN)	298.15 K	21.8	15.1	17.8	6.5×10^{-4}	5.3×10^{1}	5.8×10^{-1} [9(a)]	-7.3	4.0	-0.5
1ba+2c (MeCN)	298.15 K	23.3	16.4	19.3	5.2×10^{-5}	5.9	4.1×10^{-2} [9(a)]	-9.9	1.8	-3.2
1bb+2c (MeCN)	298.15 K	23.8	16.8	19.3	2.2×10^{-5}	3.0	4.2×10^{-2} [9(a)]	-10.7	1.1	-3.2
1dc+2b (MeCN)	298.15 K	20.4	14.0	14.1	6.9×10^{-3}	3.4×10^{2}	2.9×10^{2} [12(b)]	-5.0	5.8	5.7
1dc+2c (MeCN)	298.15 K	23.5	17.2	15.6	3.7×10^{-5}	1.5	2.2×10^{1} [12(b)]	-10.2	0.4	3.1
1e+2b (MeCN)	298.15 K	28.4	21.1	23.3	9.5×10^{-9}	2.0×10^{-3}	5.3×10^{-5} [12(c)]	-18.5	-6.2	-9.8
1ba+2b ··2H_2O	298.15K	25.2	18.1	19.3	2.1×10^{-6}	3.3×10^{-1}	4.3×10^{-2} [9(a)]	-13.1	-1.1	-3.1
1ba+2f (MeCN)	298.15 K	26.4	19.7	20.7	2.8×10^{-7}	2.2×10^{-2}	4.2×10^{-3} [9(a)]	-15.1	-3.8	-5.5
1ba+2f ··2H_2O	298.15 K	31.4	24.2	22.2	6.0×10^{-11}	1.1×10^{-5}	3.4×10^{-4} [9(a)]	-23.5	-11.4	-8.0
1bb+2b ··2H_2O	298.15 K	25.7	18.6	19.3	9.0×10^{-7}	1.4×10^{-1}	4.7×10^{-2} [9(a)]	-13.9	-2.0	-3.1
1bb+2f (MeCN)	298.15 K	26.8	20.3	20.5	1.4×10^{-7}	8.2×10^{-3}	5.6×10^{-3} [9(a)]	-15.8	-4.8	-5.2
1bb+2f ··2H_2O	298.15 K	32.4	25.1	22.0	1.1×10^{-11}	2.9×10^{-6}	4.6×10^{-4} [9(a)]	-25.2	-12.8	-7.7
1bd+2b ··2MeOH	273.15 K	21.3	14.4	15.7	5.2×10^{-5}	1.7×10^{1}	1.5 [9(c)]	-9.9	2.8	0.4
1bd+2b ··2H_2O	298.15 K	21.9	14.4	16.2	5.5×10^{-4}	1.7×10^{2}	8.2 [9(a)]	-7.5	5.1	2.1

1bd+2f (MeCN)	298.15 K	21.6	14.9	16.7	9.1×10^{-4}	7.4×10^{1}	3.5 [9(a)]	-7.0	4.3	1.3
1bd+2f ··$2H_2O$	298.15 K	26.1	19.0	17.9	4.6×10^{-7}	7.3×10^{-2}	5.0×10^{-1} [9(a)]	-14.6	-2.6	-0.7
1be+2b ··2MeOH	273.15 K	22.8	15.2	16.4	3.3×10^{-6}	3.9	4.0×10^{-1} [9(c)]	-12.6	1.4	-0.9
1fa+2d ··$3H_2O$	298.15 K	27.2	20.0	18.3	7.2×10^{-8}	1.3×10^{-2}	2.5×10^{-1} [16(b)]	-16.5	-4.3	-1.4
1fa+2e ··$3H_2O$	298.15 K	24.1	17.0	15.6	1.3×10^{-5}	2.1	2.3×10^{1} [16(b)]	-11.2	0.7	3.1
1fb+2d ··$3H_2O$	298.15 K	27.1	20.4	18.5	8.5×10^{-8}	6.9×10^{-3}	1.7×10^{-1} [16(c)]	-16.3	-5.0	-1.8
1fb+2e ··$3H_2O$	298.15 K	23.0	16.7	15.6	8.6×10^{-5}	3.6	2.4×10^{1} [16(c)]	-9.4	1.3	3.2
1fc+2d ··$3H_2O$	298.15 K	22.1	15.6	16.0	3.9×10^{-4}	2.3×10^{1}	1.2×10^{1} [16(c)]	-7.9	3.1	2.5
1fc+2e ··$3H_2O$	298.15 K	19.2	12.9	13.6	5.2×10^{-2}	2.2×10^{3}	6.2×10^{2} [16(c)]	-3.0	7.7	6.4
1ga+2b (MeCN)	298.15 K	19.5	12.9	12.7	3.0×10^{-2}	2.2×10^{3}	3.2×10^{3} [12(b)]	-3.4	7.7	8.0
1ga+2c (MeCN)	298.15 K	22.8	15.6	14.6	1.2×10^{-4}	2.3×10^{1}	1.3×10^{2} [12(b)]	-9.0	3.1	4.9
1gb+2b (MeCN)	298.15 K	21.3	15.2	14.9	1.5×10^{-3}	4.5×10^{1}	6.9×10^{1} [12(b)]	-6.5	3.8	4.2
1gb+2c (MeCN)	298.15 K	24.2	18.0	16.4	1.1×10^{-5}	4×10^{-1}	5.7 [12(b)]	-11.4	-0.9	1.7
1gc+2b (MeCN)	298.15 K	19.8	13.8	13.7	1.9×10^{-2}	4.4×10^{2}	5.2×10^{2} [12(b)]	-4.0	6.1	6.2
1gc+2c (MeCN)	298.15 K	23.9	17.4	15.3	1.9×10^{-5}	1.1	3.6×10^{1} [12(b)]	-10.9	0.1	3.6
1gd+2b (MeCN)	298.15 K	20.2	14.3	14.4	9.7×10^{-3}	2.0×10^{2}	1.6×10^{2} [12(b)]	-4.6	5.3	5.1
1gd+2c (MeCN)	298.15 K	23.7	17.4	16.0	2.6×10^{-5}	1.1	1.3×10^{1} [12(b)]	-10.5	0.1	2.5
1ge+2b (MeCN)	298.15 K	22.4	16.6	16.2	2.4×10^{-4}	4.2	9.0 [12(b)]	-8.3	1.4	2.2
1ge+2c (MeCN)	298.15 K	25.3	19.3	17.6	1.8×10^{-6}	4.4×10^{-2}	8.3×10^{-1} [12(b)]	-13.2	-3.1	-0.2
1h+2c (MeCN)	298.15 K	21.4	14.9	17.4	1.3×10^{-3}	7.4×10^{1}	1.0 [12(c)]	-6.7	4.3	9.9
1h+2ga (MeCN)	298.15 K	19.6	13.2	15.8	2.7×10^{-2}	1.3×10^{3}	1.5×10^{1} [12(c)]	-3.6	7.2	2.7
1h+2gb (MeCN)	298.15 K	19.5	12.8	15.8	3.2×10^{-2}	2.5×10^{3}	1.6×10^{1} [12(c)]	-3.4	7.8	2.8
1h+2gc (MeCN)	298.15 K	22.6	16.7	17.2	1.7×10^{-4}	3.5	1.6 [12(c)]	-8.7	1.3	0.5

S10 The optimized geometries for the transition states and minima of the reactions studied in **Fig.1** and **Fig.4**, obtained with CAM-B3LYP+IDSCRF/DZVP.

Species	Cartesian coordinates			Species	Cartesian coordinates		
1a	C	-1.15563	0.78878	0.00001	**2a**	C	-0.22708	-1.11020	-0.00000
(MeOH)	C	0.02410	-0.16428	0.00001	(MeOH)	C	-1.50307	-0.60655	-0.00003
	H	-1.18214	1.41712	0.88929		C	-0.19268	1.08452	0.00003
	C	1.35048	0.60178	0.00000		N	0.60613	-0.01509	0.00006
	H	-0.02958	-0.81329	0.88006		H	0.15502	-2.12275	-0.00001
	H	-0.02959	-0.81330	-0.88004		H	-2.43574	-1.15735	-0.00004
	H	1.39468	1.25774	-0.87844		H	0.21538	2.08933	0.00006
	H	1.39468	1.25774	0.87843		C	2.05933	-0.03285	-0.00004
	C	2.56563	-0.32598	0.00000		H	2.42625	0.99407	0.00074
	C	3.89682	0.42521	-0.00001		H	2.43631	-0.54149	0.88990
	H	2.52058	-0.98338	-0.87776		H	2.43626	-0.54013	-0.89078
	H	2.52059	-0.98336	0.87778		N	-1.47315	0.77046	-0.00001
	C	5.10688	-0.50779	0.00000					
	H	3.94115	1.08226	-0.87709					
	H	3.94116	1.08229	0.87704					
	H	6.04552	0.05469	-0.00002					
	H	5.10678	-1.15488	0.88349					
	H	5.10677	-1.15492	-0.88346					
	H	-1.18215	1.41710	-0.88929					
	Br	-2.87848	-0.17735	0.00003					
TS_{aa}	C	0.02962	-1.15837	-0.26849	**P_{aa}**	C	-0.64638	-0.62648	1.37036
(MeOH)	C	-0.81201	-0.05743	-0.85395	(MeOH)	C	-1.08997	0.82924	1.25538
	H	0.50310	-1.88983	-0.90356		H	-1.49528	-1.28260	1.57407
	C	-1.35372	0.91358	0.19048		C	-2.16464	1.08193	0.19904
	H	-0.20592	0.47849	-1.59070		H	-1.46737	1.11887	2.24250
	H	-1.63022	-0.51320	-1.41499		H	-0.21368	1.45894	1.06262
	H	-1.94880	0.35241	0.92033		H	-1.78545	0.81002	-0.79360
	H	-0.51315	1.35589	0.73900		H	-3.02542	0.42889	0.39305
	C	-2.20572	2.02450	-0.42089		C	-2.62954	2.53793	0.17139
	C	-2.75073	3.00598	0.61629		C	-3.70264	2.80734	-0.88307
	H	-3.04400	1.57851	-0.97190		H	-1.76704	3.19090	-0.01413
	H	-1.61120	2.57526	-1.16174		H	-3.01602	2.81429	1.16082
	C	-3.60343	4.11342	-0.00102		C	-4.16466	4.26355	-0.90281
	H	-3.34464	2.45620	1.35657		H	-3.31515	2.53272	-1.87171
	H	-1.91330	3.45235	1.16638		H	-4.56316	2.15275	-0.69856
	H	-3.98021	4.80110	0.76231		H	-4.93181	4.42896	-1.66534
	H	-3.02573	4.70110	-0.72236		H	-4.58749	4.55684	0.06386
	H	-4.46753	3.69784	-0.53015		H	-3.33046	4.93969	-1.11764
	H	0.21804	-1.22015	0.79045		H	0.07221	-0.75037	2.18308

	Br	-1.72240	-2.87727	0.18629		Br	4.25586	0.63305	0.84667
	C	3.80898	0.87568	-0.98538		C	0.31466	-2.09288	-1.81422
	C	2.57313	0.44669	-1.38678		C	-0.61823	-1.87277	-0.84985
	C	2.74138	-0.01717	0.71352		C	1.25820	-0.90482	-0.21090
	N	3.90235	0.57382	0.35477		N	1.47747	-1.47914	-1.39387
	H	4.61416	1.35753	-1.52419		H	0.25045	-2.63045	-2.75080
	H	2.12610	0.50229	-2.37142		H	-1.65221	-2.18347	-0.78350
	H	2.54097	-0.36224	1.72146		H	2.01312	-0.35447	0.35286
	C	5.03953	0.84882	1.22255		C	2.75327	-1.46360	-2.11188
	H	4.81787	0.48082	2.22434		H	3.10194	-2.48771	-2.25146
	H	5.93003	0.34171	0.84694		H	2.61569	-0.98410	-3.08192
	H	5.22544	1.92325	1.27145		H	3.47504	-0.90212	-1.51752
	N	1.91639	-0.10691	-0.31316		N	-0.00863	-1.13135	0.14270
1ba (MeOH)	C	1.34711	0.44805	-0.07947	**1bb** (MeOH)	C	-0.83231	-0.39880	-0.02497
	C	-0.64872	-1.47031	0.04431		C	1.92269	-0.69602	0.02794
	C	-0.00098	0.81721	0.00525		C	0.01084	0.71668	0.00709
	C	1.67038	-0.90854	-0.09766		C	-0.25952	-1.67023	-0.03261
	C	0.67748	-1.87504	-0.04605		C	1.11832	-1.82836	0.00476
	C	-1.00686	-0.13400	0.08454		C	1.39124	0.58193	0.01588
	N	-0.43527	2.22007	0.01570		N	-0.49784	2.09498	0.03306
	H	2.71411	-1.20306	-0.14874		H	-0.90120	-2.54471	-0.07212
	H	0.92950	-2.92984	-0.06879		H	1.56268	-2.81791	0.00826
	H	-2.04550	0.16736	0.16447		H	2.03185	1.45691	0.02472
	N	-1.70717	-2.48331	0.10667		N	3.38099	-0.84978	0.05839
	O	0.13584	3.00750	-0.72700		O	-1.46204	2.34124	0.74507
	O	-1.37059	2.50774	0.75552		O	0.10164	2.92225	-0.64588
	O	-2.86849	-2.09609	0.18493		O	4.06505	0.16823	0.07756
	O	-1.37088	-3.66227	0.07744		O	3.83461	-1.98907	0.06254
	Cl	2.64094	1.58953	-0.09686		Br	-2.71291	-0.28799	-0.14270
1bc (MeOH)	C	-0.81004	-0.93149	-0.15560	**2b** ··2MeOH (MeOH)	C	-3.75464	-0.76377	0.16967
	C	1.77090	-0.16115	0.46569		H	-4.66240	-1.37196	0.21248
	C	-0.44652	0.41851	-0.14201		H	-3.68904	-0.18516	1.10178
	C	0.14911	-1.88541	0.16326		H	-3.85767	-0.05767	-0.66622
	C	1.45641	-1.50907	0.45789		O	-2.64967	-1.63439	0.00151
	C	0.83459	0.82341	0.18384		H	-1.82341	-1.07781	-0.03391
	N	-1.38641	1.49272	-0.49775		C	2.79575	-2.42871	0.45903
	H	-0.13265	-2.93287	0.20245		H	3.62001	-3.06203	0.11212
	H	2.21029	-2.25214	0.69526		H	3.21180	-1.50475	0.86356
	H	1.09988	1.87529	0.20640		H	2.25185	-2.94965	1.25527
	N	3.14506	0.25413	0.79337		O	1.93245	-2.05815	-0.61712

	O	-1.43966	2.46180	0.24658		H	1.53927	-2.85740	-1.01266
	O	-2.01687	1.36066	-1.53804		C	0.77355	1.86725	-1.26204
	O	3.39163	1.45430	0.79554		C	-0.42596	0.91918	-1.19768
	O	3.95942	-0.62559	1.04416		C	-0.14688	0.62632	1.20513
	S	-2.51170	-1.54019	-0.37101		C	1.06059	1.56644	1.22025
	O	-2.50162	-2.87927	0.21944		C	0.97422	2.58083	0.07718
	O	-3.40508	-0.51548	0.16732		H	-1.34794	1.50202	-1.07512
	C	-2.77958	-1.71545	-2.11980		H	-0.52684	0.35675	-2.13113
	C	-2.15039	-2.76552	-2.78824		H	1.67306	1.28902	-1.50861
	C	-3.65086	-0.84182	-2.76353		H	0.62847	2.59306	-2.07013
	C	-2.39183	-2.92788	-4.14827		H	-1.05653	1.19542	1.43624
	H	-1.49402	-3.45243	-2.26072		H	-0.04939	-0.14377	1.97680
	C	-3.89225	-1.02594	-4.12211		H	1.12015	2.07663	2.18823
	H	-4.13098	-0.04008	-2.21237		H	1.97847	0.97364	1.11514
	C	-3.26086	-2.06031	-4.81148		H	0.12819	3.25712	0.25725
	H	-1.90854	-3.73756	-4.68760		H	1.87414	3.20414	0.04885
	H	-4.57377	-0.35824	-4.64160		N	-0.35200	-0.04269	-0.08799
	H	-3.45019	-2.19532	-5.87320		H	0.43220	-0.67869	-0.25679
2b (MeOH)	C	-1.87431	1.26709	-0.04769	**2b** ··MeOH (MeOH)	C	3.34206	-0.27727	-0.72752
	C	-0.34516	1.20107	0.01824		H	4.43277	-0.24325	-0.79470
	C	-0.38562	-1.22083	0.18348		H	3.01979	-1.30594	-0.94090
	C	-1.91625	-1.24433	0.12365		H	2.93250	0.38055	-1.50672
	C	-2.44754	-0.02531	-0.63494		O	2.97023	0.14022	0.57484
	H	0.06108	1.17890	-1.00141		H	1.97837	0.11513	0.63292
	H	0.05952	2.09727	0.49970		C	-1.92096	1.26561	-0.04994
	H	-2.27102	1.41738	0.96503		C	-0.39183	1.24000	-0.01959
	H	-2.18468	2.13382	-0.64275		C	-0.37331	-1.19159	0.16864
	H	0.01885	-1.35084	-0.82880		C	-1.90194	-1.24469	0.14501
	H	-0.00985	-2.05631	0.78309		C	-2.47643	-0.04508	-0.61269
	H	-2.25658	-2.17304	-0.34894		H	-0.00270	1.21133	-1.04488
	H	-2.31545	-1.24247	1.14649		H	0.00530	2.14649	0.44707
	H	-2.15550	-0.10221	-1.69068		H	-2.29720	1.41682	0.97011
	H	-3.54238	-0.00553	-0.61319		H	-2.26349	2.11943	-0.64498
	N	0.17123	0.02377	0.72550		H	0.01537	-1.31484	-0.84976
	H	-0.09285	0.09530	1.70907		H	0.03725	-2.00950	0.76843
						H	-2.23099	-2.18516	-0.31066
						H	-2.27679	-1.24222	1.17669
						H	-2.20812	-0.12549	-1.67417
						H	-3.57024	-0.04951	-0.56383
						N	0.15981	0.07636	0.69353

				H	-0.09306	0.15056	1.68132
TS1$_{bab}$ (MeOH)	N	3.46150	-1.31273	-0.99321	**IN1$_{bab}$** (MeOH)	N	-4.18884	-0.30800	0.96147
	C	2.23020	-1.05061	-0.29796		C	-2.75303	-0.35911	0.64824
	C	2.16068	-0.00221	0.64498		C	-1.98043	-1.38342	1.16659
	C	1.13362	-1.85594	-0.53057		C	-2.21691	0.62231	-0.16744
	C	-0.05932	-1.59694	0.13172		C	-0.86718	0.56204	-0.47177
	H	1.18781	-2.68319	-1.22845		H	-2.83616	1.41286	-0.57604
	H	3.04679	0.58341	0.86529		H	-2.42448	-2.14664	1.79679
	C	0.99405	0.23921	1.31234		C	-0.62182	-1.40906	0.87380
	C	-0.20727	-0.49204	1.03121		C	-0.04173	-0.44243	0.06082
	N	-1.18090	-2.44301	-0.19037		N	-0.39677	1.57367	-1.43193
	H	0.95902	0.99669	2.08825		H	-0.02380	-2.20528	1.30114
	O	4.43010	-0.58395	-0.75853		O	-4.64350	-1.18739	1.68318
	O	3.50288	-2.25019	-1.79536		O	-4.84442	0.61006	0.48328
	O	-0.96412	-3.55929	-0.66619		O	-0.94897	2.66232	-1.42143
	O	-2.31745	-1.99813	-0.00177		O	0.48374	1.24149	-2.21792
	C	-2.29245	3.19414	-0.03640		C	3.71026	-0.81084	0.67922
	C	-1.40811	2.18128	0.69257		C	2.22612	-0.93329	0.99550
	C	-1.02620	0.94083	-1.37805		C	1.73611	-1.32793	-1.41076
	C	-1.89230	1.92430	-2.16671		C	3.21277	-1.20050	-1.74783
	C	-1.89628	3.30439	-1.50883		C	4.09119	-1.60914	-0.56659
	H	-0.37029	2.53188	0.70009		H	1.97011	-1.97150	1.20914
	H	-1.72918	2.05197	1.72857		H	1.93650	-0.29862	1.83341
	H	-3.34080	2.88309	0.04679		H	3.96069	0.24576	0.55404
	H	-2.20587	4.16274	0.46602		H	4.25485	-1.17410	1.55574
	H	0.02412	1.25338	-1.40429		H	1.47018	-2.35575	-1.14712
	H	-1.09011	-0.06001	-1.81111		H	1.10062	-0.99212	-2.22624
	H	-1.51660	1.98021	-3.19318		H	3.40562	-1.83315	-2.61900
	H	-2.91591	1.53464	-2.22183		H	3.42715	-0.16887	-2.04761
	H	-0.89599	3.74846	-1.58513		H	3.96891	-2.68174	-0.37398
	H	-2.58123	3.97391	-2.03766		H	5.14493	-1.44589	-0.80722
	N	-1.41960	0.86297	0.03702		N	1.40224	-0.48165	-0.19627
	H	-2.34390	0.43030	0.12188		H	1.71597	0.53060	-0.32378
	Cl	-1.28118	-0.66236	2.43299		Cl	2.16028	2.41046	0.30966
TS2$_{bab}$ (MeOH)	N	4.02872	1.60730	-0.17346	**P$_{bab}$** (MeOH)	N	-4.66557	-1.27503	-0.64846
	C	2.87205	0.72304	0.02027		C	-3.36741	-0.73765	-0.25958
	C	2.88996	-0.55650	-0.50332		C	-2.95903	0.50503	-0.73100
	C	1.78697	1.19553	0.73415		C	-2.55222	-1.48756	0.56902
	C	0.68818	0.36735	0.90962		C	-1.31287	-0.97563	0.91855
	H	1.78473	2.19729	1.14587		H	-2.85654	-2.46942	0.91250

H	3.75183	-0.92193	-1.05206	H	-3.60291	1.08155	-1.38682
C	1.78749	-1.38146	-0.31198	C	-1.73546	1.02036	-0.33899
C	0.66125	-0.94769	0.38539	C	-0.86985	0.31209	0.51583
N	-0.41300	0.98400	1.67116	N	-0.46944	-1.90834	1.67235
H	1.86184	-2.38613	-0.72462	H	-1.47337	2.00457	-0.71897
O	4.98111	1.16644	-0.80602	O	-5.36452	-0.60298	-1.40271
O	3.97534	2.73385	0.30779	O	-4.99646	-2.37198	-0.20276
O	-0.15355	1.95733	2.36330	O	-1.00913	-2.63976	2.49174
O	-1.53841	0.50013	1.56975	O	0.73614	-1.94470	1.41850
C	-1.58554	-4.00681	-0.07582	C	2.14375	2.55714	0.67655
C	-0.35842	-3.12316	-0.25899	C	0.71206	2.16219	0.32896
C	-0.62353	-2.25144	2.01707	C	0.51768	0.92783	2.41789
C	-1.85399	-3.11569	2.24060	C	1.94746	1.27165	2.80844
C	-1.80467	-4.37948	1.38751	C	2.37882	2.59538	2.18351
H	0.53888	-3.66901	0.03769	H	0.02136	2.94498	0.67201
H	-0.23659	-2.83395	-1.30328	H	0.59688	2.10021	-0.75429
H	-2.47809	-3.51425	-0.47278	H	2.84911	1.85425	0.21546
H	-1.42613	-4.89991	-0.68689	H	2.34237	3.53319	0.22413
H	0.28815	-2.79646	2.28311	H	-0.16809	1.69700	2.80222
H	-0.67394	-1.35236	2.62409	H	0.23048	-0.01478	2.87702
H	-1.89110	-3.36178	3.30594	H	2.00348	1.31912	3.90021
H	-2.75607	-2.53522	2.02018	H	2.61560	0.46252	2.49025
H	-0.98414	-5.02024	1.73071	H	1.79373	3.41198	2.62328
H	-2.72858	-4.95318	1.49927	H	3.43051	2.80193	2.40214
N	-0.47163	-1.85952	0.56148	N	0.35213	0.86131	0.93869
H	-1.43100	-1.32870	0.07129	H	1.69264	-0.39819	-0.10377
C	-3.43144	-0.25912	-3.03634	C	3.28387	-1.17590	-2.99838
C	-2.43007	-1.06329	-2.21076	C	2.46360	-0.29515	-2.06725
C	-3.83342	-0.84305	-0.20620	C	3.55569	-1.35951	-0.07982
C	-4.86940	-0.03613	-0.98470	C	4.38267	-2.24470	-1.00043
C	-4.84587	-0.39772	-2.47084	C	4.61324	-1.57865	-2.35798
H	-2.65032	-2.13253	-2.29318	H	2.97630	0.64649	-1.85647
H	-1.41001	-0.90607	-2.57308	H	1.47410	-0.07372	-2.47228
H	-3.13206	0.79635	-3.03543	H	2.70287	-2.06881	-3.25808
H	-3.39134	-0.59996	-4.07566	H	3.44791	-0.62366	-3.92750
H	-4.09338	-1.90678	-0.22935	H	4.07423	-0.42388	0.14519
H	-3.79780	-0.53194	0.84044	H	3.29979	-1.85552	0.85734
H	-5.85937	-0.21816	-0.55472	H	5.33234	-2.45605	-0.50170
H	-4.65938	1.03331	-0.85870	H	3.87278	-3.20645	-1.13237
H	-5.18972	-1.43165	-2.59973	H	5.24277	-0.69034	-2.22915

	H	-5.54079	0.23817	-3.02746		H	5.15447	-2.25930	-3.02013
	N	-2.46790	-0.70350	-0.77032		N	2.26266	-0.98312	-0.74683
	H	-2.21155	0.28664	-0.69442		H	1.70282	-1.83751	-0.88858
	Cl	2.67857	-4.47149	-1.61827		Cl	-1.31902	3.95218	-2.28085
TS1$_{bab}$ $\cdot\cdot$MeOH	N	3.45533	-1.26366	-1.00067	**TS1$_{bab}$**$\cdot\cdot$2MeOH	N	3.62045	-1.06636	-1.18656
	C	2.22831	-1.01147	-0.29655		C	2.35324	-0.90276	-0.52520
	C	2.15267	0.03504	0.64958		C	2.22980	-0.01293	0.56375
	C	1.13919	-1.82889	-0.52771		C	1.27563	-1.65924	-0.94093
	C	-0.05479	-1.58394	0.13632		C	0.04644	-1.50639	-0.31251
	H	1.20072	-2.65459	-1.22677		H	1.37427	-2.36947	-1.75311
	H	3.03196	0.62913	0.88224		H	3.09636	0.52868	0.93260
	C	0.98202	0.26177	1.31619		C	1.02232	0.12358	1.18953
	C	-0.21257	-0.47982	1.03526		C	-0.15503	-0.54959	0.73166
	N	-1.16822	-2.44097	-0.18555		N	-1.04201	-2.30681	-0.81775
	H	0.93978	1.01658	2.09449		H	0.93797	0.75173	2.07002
	O	4.42454	-0.52899	-0.77529		O	4.58376	-0.40515	-0.78238
	O	3.49898	-2.19675	-1.80635		O	3.70095	-1.85447	-2.13171
	O	-0.94086	-3.55473	-0.66227		O	-0.77833	-3.32495	-1.46115
	O	-2.30888	-2.00709	0.00389		O	-2.19559	-1.92207	-0.60780
	C	-2.32594	3.18607	-0.04687		C	-4.94143	0.07481	-1.16464
	C	-1.43264	2.18236	0.68382		H	-5.92847	-0.37200	-1.00176
	C	-1.04967	0.93449	-1.38182		H	-5.07613	1.08921	-1.54327
	C	-1.92577	1.90767	-2.17218		H	-4.39616	-0.51639	-1.90876
	C	-1.93668	3.29110	-1.52155		O	-4.21107	0.17927	0.05910
	H	-0.39696	2.53925	0.68662		H	-4.05717	-0.71502	0.41396
	H	-1.74949	2.05594	1.72150		C	-2.02018	3.37371	0.03099
	H	-3.37203	2.86905	0.04220		C	-1.23791	2.21788	0.65838
	H	-2.24338	4.15782	0.45010		C	-0.84890	1.21666	-1.53200
	H	-0.00170	1.25436	-1.41320		C	-1.60634	2.35127	-2.22590
	H	-1.10785	-0.06882	-1.80991		C	-1.54793	3.63621	-1.39923
	H	-1.55468	1.96078	-3.20049		H	-0.18219	2.49653	0.75506
	H	-2.94679	1.51044	-2.22109		H	-1.61770	1.98563	1.65650
	H	-0.93984	3.74169	-1.60446		H	-3.08810	3.12598	0.03314
	H	-2.62849	3.95302	-2.05102		H	-1.89559	4.26587	0.65326
	N	-1.43773	0.86085	0.03483		H	0.22145	1.45230	-1.49001
	H	-2.35899	0.42277	0.12435		H	-0.96322	0.28378	-2.08997
	C	5.22739	2.57683	0.33589		H	-1.17934	2.50605	-3.22202
	H	4.89306	3.51286	0.78663		H	-2.65070	2.05005	-2.37019
	H	6.27040	2.69376	0.01814		H	-0.51669	4.01061	-1.37978
	H	4.60943	2.36698	-0.54514		H	-2.15854	4.41535	-1.86578

	O	5.09070	1.56214	1.32806		N	-1.30604	0.99584	-0.15476
	H	5.33548	0.70847	0.92957		H	-2.26955	0.63789	-0.14883
	Cl	-1.28620	-0.65697	2.43596		C	5.28688	2.53245	0.72734
						H	4.90579	3.41321	1.24704
						H	6.34761	2.69161	0.49927
						H	4.73624	2.40899	-0.21263
						O	5.09799	1.41891	1.59740
						H	5.38665	0.61356	1.13292
						Cl	-1.32627	-0.88234	2.01407
TS1$_{bbb}$ $\cdot\cdot$2MeOH	N	-4.00341	-0.88999	-0.34136	**TS1$_{bbb}$**$\cdot\cdot$2MeOH	N	-3.44399	-1.63592	1.71291
	C	-2.57057	-0.98485	-0.44373		C	-2.27894	-1.12829	1.02573
	C	-1.94165	-0.89501	-1.70344		C	-2.35770	-0.77114	-0.33364
	C	-1.82790	-1.20250	0.69963		C	-1.08776	-1.02548	1.71014
	C	-0.44384	-1.28755	0.61138		C	0.03571	-0.53238	1.05515
	H	-2.30828	-1.30222	1.66561		H	-1.01210	-1.31652	2.75092
	H	-2.53330	-0.78535	-2.60819		H	-3.28451	-0.90350	-0.88595
	C	-0.58007	-0.99919	-1.78698		C	-1.24170	-0.30294	-0.97542
	C	0.24640	-1.11807	-0.62682		C	-0.00186	-0.07540	-0.29981
	N	0.26962	-1.47590	1.85186		N	1.23301	-0.40483	1.84465
	H	-0.10244	-1.00083	-2.76079		H	-1.28800	-0.10315	-2.03888
	O	-4.65546	-0.71193	-1.37616		O	-4.50075	-1.72361	1.08215
	O	-4.52765	-0.98624	0.77068		O	-3.33825	-1.95652	2.89748
	O	-0.33698	-1.94154	2.81901		O	1.28750	-0.93274	2.95548
	O	1.45435	-1.13519	1.89896		O	2.15725	0.25554	1.36040
	C	4.04486	1.20134	2.14518		C	3.51326	3.26146	1.59488
	H	4.96841	0.89736	2.65013		H	4.60464	3.35845	1.56248
	H	4.13885	2.24626	1.84561		H	3.09089	4.20572	1.94284
	H	3.20374	1.10209	2.84033		H	3.24177	2.46661	2.29738
	O	3.83183	0.44239	0.95267		O	2.97642	3.01583	0.29532
	H	3.72983	-0.49730	1.18871		H	3.29632	2.15753	-0.03239
	C	2.17124	2.68931	-1.75829		C	-0.29695	4.17955	-1.40772
	C	1.55690	1.28864	-1.81084		C	-0.27434	2.65165	-1.48822
	C	0.27643	1.71030	0.22081		C	-0.63500	2.46605	0.91917
	C	0.84038	3.12949	0.32577		C	-0.67024	3.98896	1.06477
	C	1.23335	3.66735	-1.05039		C	-1.14489	4.65243	-0.22777
	H	0.64956	1.30753	-2.42566		H	-1.28212	2.27736	-1.70126
	H	2.25196	0.57428	-2.25905		H	0.38609	2.31679	-2.29071
	H	3.13000	2.64041	-1.22891		H	0.72996	4.54660	-1.29986
	H	2.38416	3.02200	-2.77941		H	-0.68423	4.57508	-2.35226
	H	-0.66963	1.72453	-0.33405		H	-1.65083	2.07897	0.77576

	H	0.07332	1.30643	1.21583		H	-0.22646	2.00977	1.82419
	H	0.09321	3.77395	0.80012		H	-1.32537	4.24721	1.90291
	H	1.71691	3.11953	0.98433		H	0.33417	4.34683	1.31825
	H	0.33047	3.81068	-1.65729		H	-2.19671	4.39565	-0.40611
	H	1.70792	4.64860	-0.95279		H	-1.09596	5.74170	-0.13519
	N	1.18452	0.79413	-0.47891		N	0.17525	2.03483	-0.22881
	H	2.03336	0.63648	0.07852		H	1.15970	2.27399	-0.05922
	C	-4.12896	0.97321	-4.28736		C	-6.04005	-0.12786	-1.51390
	H	-3.39831	1.40836	-4.97129		H	-5.90044	0.60988	-2.30582
	H	-5.13319	1.27337	-4.60951		H	-7.11023	-0.34974	-1.42602
	H	-3.94823	1.36448	-3.27910		H	-5.68580	0.29592	-0.56686
	O	-3.96095	-0.44161	-4.34102		O	-5.29263	-1.28470	-1.88472
	H	-4.57731	-0.85079	-3.70825		H	-5.37119	-1.94618	-1.17453
	Br	1.88473	-2.09893	-0.95958		S	1.45434	-0.30606	-1.47431
						O	0.82790	-0.52190	-2.78411
						O	2.44679	0.76708	-1.38446
						C	2.19166	-1.84317	-0.95858
						C	1.49364	-3.02693	-1.19792
						C	3.46060	-1.83451	-0.38598
						C	2.08266	-4.23300	-0.83305
						H	0.51433	-3.01100	-1.66825
						C	4.04084	-3.05089	-0.03548
						H	3.98146	-0.89704	-0.22269
						C	3.35219	-4.24330	-0.25345
						H	1.55307	-5.16512	-1.00857
						H	5.03231	-3.06488	0.40840
						H	3.80941	-5.18907	0.02544
1ca (MeOH)	C	-1.45349	0.21002	0.00022	**1cb** (MeOH)	C	-0.83303	0.29497	0.00005
	C	-0.95638	1.48610	0.00019		C	-0.29306	1.55353	0.00021
	C	0.46078	1.49546	0.00005		C	1.12422	1.51494	0.00008
	C	0.96934	0.22672	0.00002		C	1.58850	0.22914	0.00000
	S	-0.23538	-1.01329	-0.00070		S	0.34022	-0.96661	-0.00038
	H	-1.57915	2.37422	0.00044		H	-0.88250	2.46395	0.00045
	H	1.07797	2.38739	0.00023		H	1.77122	2.38557	0.00023
	N	2.35248	-0.12298	0.00025		Br	-2.66202	-0.12219	0.00018
	O	2.63592	-1.32456	0.00018		N	2.95970	-0.16719	0.00011
	O	3.18251	0.78463	0.00065		O	3.20213	-1.37777	0.00014
	Cl	-3.11298	-0.22847	0.00049		O	3.82004	0.71196	0.00042
1cc (MeOH)	C	-1.23502	-0.54715	-0.18941	**1cd** (MeOH)	C	0.19775	0.42059	-0.00001
	C	-1.37399	0.54169	-1.01422		C	-1.07722	-0.09942	-0.00005

	C -2.69877 1.03721 -0.99194 C -3.50325 0.30748 -0.15937 S -2.68563 -0.99759 0.63514 H -0.57107 0.95950 -1.61155 H -3.05355 1.88420 -1.56924 N -4.88718 0.52546 0.07135 O -5.46659 -0.24406 0.84697 O -5.43772 1.46402 -0.50684 O -0.15553 -1.33331 0.02438 C 1.11627 -0.78528 0.02243 C 1.39468 0.43149 0.64202 C 2.11503 -1.55711 -0.56441 C 2.70380 0.89085 0.66074 H 0.60558 1.00987 1.11257 C 3.42485 -1.10099 -0.54239 H 1.85695 -2.50306 -1.03086 C 3.69881 0.12009 0.06652 H 2.95341 1.83154 1.13855 H 4.22316 -1.67862 -0.99453 N 5.07663 0.60610 0.08833 O 5.94752 -0.09439 -0.42351 O 5.30113 1.69271 0.61758		C -2.09842 0.89980 -0.00003 C -1.57690 2.15206 0.00000 S 0.14918 2.13995 0.00008 H -3.15674 0.67017 -0.00006 H -2.10731 3.09695 0.00002 N -1.40895 -1.50220 -0.00010 O -2.60485 -1.79653 0.00004 O -0.50099 -2.33076 0.00010 Cl 1.71492 -0.36712 -0.00002
1ce (MeOH)	C -0.19789 -0.42170 0.00001 C 1.07569 0.09960 0.00002 C 2.09977 -0.89691 0.00001 C 1.58080 -2.15070 -0.00001 S -0.14469 -2.13795 0.00001 H 3.15750 -0.66473 0.00002 H 2.11371 -3.09428 -0.00002 Br -1.86883 0.41865 0.00001 N 1.41018 1.50320 0.00005 O 2.60668 1.79499 -0.00006 O 0.50444 2.33364 -0.00001	**1cf** (MeOH)	C -0.46740 0.90678 0.11713 C -1.05371 0.72959 1.35230 C -2.43132 0.40146 1.29832 C -2.86822 0.33633 0.00792 S -1.63049 0.67389 -1.12575 H -3.04378 0.22390 2.17420 S 1.17515 1.40452 -0.41916 O 1.04241 1.43708 -1.87976 O 1.57831 2.61937 0.28103 C 2.26916 0.06964 0.00759 C 2.14795 -1.13642 -0.68164 C 3.25372 0.27988 0.96810 C 3.03548 -2.16487 -0.38363 H 1.38399 -1.27148 -1.44279 C 4.14246 -0.75505 1.24618 H 3.32033 1.23217 1.48364 C 4.03011 -1.97271 0.57661 H 2.95553 -3.11327 -0.90728

				H	4.92094	-0.60931	1.98978
				H	4.72398	-2.77841	0.80181
				H	-3.86810	0.10461	-0.34197
				N	-0.36215	0.84497	2.61800
				O	-1.03532	0.77955	3.64251
				O	0.85596	0.99569	2.59470
1cg (MeOH)	C	1.07863	-0.46405	0.49302	**TS1$_{cab}$**$\cdot\cdot$2MeOH	C	0.32458	-1.53942	-0.42707
	C	1.59257	0.53514	1.28782		C	0.11033	-1.96937	0.90872
	C	2.85328	1.02833	0.83451		C	-1.18482	-1.75292	1.33422
	C	3.26556	0.38923	-0.28973		C	-2.01426	-1.25098	0.32993
	S	2.14334	-0.81608	-0.81390		S	-1.18218	-1.09751	-1.20616
	H	3.40411	1.81458	1.33623		H	0.90912	-2.37867	1.51692
	O	-0.03258	-1.21694	0.65948		H	-1.54453	-1.94761	2.33942
	C	-1.27389	-0.72441	0.31159		N	-3.32392	-0.87668	0.45415
	C	-1.45664	0.48711	-0.34992		O	-3.89296	-0.36191	-0.55348
	C	-2.35003	-1.54514	0.64843		O	-3.92497	-1.03838	1.53724
	C	-2.74588	0.88521	-0.67812		C	-3.15856	2.77213	0.67366
	H	-0.61416	1.11929	-0.61241		H	-2.60504	3.68300	0.91023
	C	-3.63485	-1.14844	0.32078		H	-4.22643	3.01770	0.61965
	H	-2.16514	-2.48258	1.16408		H	-3.00536	2.05038	1.48603
	C	-3.81693	0.06582	-0.33953		O	-2.66384	2.28661	-0.56895
	H	-2.91824	1.82357	-1.19322		H	-3.13680	1.45994	-0.77694
	H	-4.48867	-1.76729	0.57252		C	4.51068	-0.40250	2.14617
	N	-5.16854	0.48793	-0.68645		H	5.60181	-0.40218	2.05272
	O	-6.10447	-0.25097	-0.38436		H	4.17946	0.60817	2.38878
	O	-5.31310	1.56332	-1.26596		H	4.21497	-1.07648	2.95724
	H	4.17842	0.55116	-0.85035		O	3.88380	-0.76010	0.91157
	N	0.95301	1.03289	2.47451		H	4.15708	-1.65642	0.64185
	O	1.57023	1.85380	3.15259		C	2.34278	2.27836	-1.37988
	O	-0.17167	0.61687	2.75386		C	1.59304	0.95227	-1.53770
						C	0.67042	1.14574	0.71261
						C	1.40326	2.46969	0.94074
						C	1.63353	3.19638	-0.38452
						H	0.60982	1.13170	-1.98890
						H	2.14535	0.27290	-2.19024
						H	3.36327	2.07263	-1.03515
						H	2.42653	2.75564	-2.36171
						H	-0.33038	1.34576	0.31187
						H	0.56192	0.59388	1.64947
						H	0.81461	3.08637	1.62766

			H 2.36524 2.27505 1.43090 H 0.66662 3.50697 -0.79934 H 2.21864 4.10723 -0.22396 N 1.37112 0.28342 -0.24837 H 2.26224 -0.04225 0.14775 Cl 1.53122 -2.32893 -1.41967
TS1$_{cbb}$ $\cdot\cdot$2MeOH	0.40589 -1.23317 -0.09422 C 0.12487 -1.61511 1.24278 C -1.23019 -1.69241 1.49854 C -2.01453 -1.47057 0.36556 S -1.04350 -1.21724 -1.07306 H 0.90818 -1.77779 1.97423 H -1.66292 -1.90457 2.47093 N -3.38035 -1.42106 0.30622 O -3.91707 -1.12553 -0.80198 O -4.06323 -1.65724 1.32510 C -4.10657 2.13324 0.24619 H -3.84703 3.17310 0.45448 H -5.19344 2.06523 0.11363 H -3.82027 1.52272 1.11207 O -3.40499 1.74928 -0.93068 H -3.61686 0.81529 -1.11253 Br 2.01030 -1.85755 -0.94067 C 4.65716 0.21428 1.49280 H 5.17241 -0.24728 2.34182 H 4.58967 -0.51354 0.68374 H 5.23120 1.08067 1.14678 O 3.31605 0.57553 1.83561 H 3.32088 1.21795 2.56938 C 1.60242 2.90342 -1.14351 C 1.20789 1.42922 -1.27433 C -0.02672 1.51666 0.82560 C 0.34398 2.98778 1.02726 C 0.57505 3.67721 -0.31758 H 0.27792 1.34163 -1.84879 H 1.98290 0.86868 -1.80080 H 2.58814 2.96878 -0.66729 H 1.70247 3.33208 -2.14599 H -0.98256 1.44797 0.29283 H -0.13097 1.00680 1.78628	**TS1$_{ccb}$**$\cdot\cdot$2MeOH	C -5.36964 -1.87812 -0.26329 H -6.10513 -1.07158 -0.28577 H -5.90030 -2.83597 -0.32810 H -4.83711 -1.83630 0.69551 O -4.49375 -1.68249 -1.36754 H -3.82894 -2.39454 -1.35093 C -0.57963 4.44926 2.44569 H 0.03490 5.34860 2.55984 H -1.54815 4.73720 2.03440 H -0.73392 3.98779 3.42707 O 0.00857 3.53254 1.51910 H 0.88769 3.25384 1.83546 C -2.42401 3.11391 -1.79125 C -1.47134 1.93912 -1.55093 C -2.76640 1.21536 0.38748 C -3.75070 2.37404 0.21190 C -3.82205 2.80576 -1.25373 H -1.79783 1.07226 -2.13915 H -0.45418 2.18998 -1.85904 H -2.02324 4.00599 -1.29458 H -2.45752 3.33306 -2.86366 H -3.13931 0.33470 -0.14983 H -2.65919 0.94964 1.44267 H -4.73619 2.06508 0.57576 H -3.43187 3.22006 0.83351 H -4.27032 1.99871 -1.84672 H -4.47292 3.67893 -1.36320 N -1.43583 1.52939 -0.14221 H -0.97704 2.24946 0.42840 C -0.10614 -0.09588 0.19468 C -0.21990 -0.38531 1.57337 C -0.97177 -1.52134 1.81647 C -1.36483 -2.17454 0.65013 S -0.76416 -1.39062 -0.79582

	H	-0.45734	3.48117	1.58680		H	0.20539	0.26050	2.33395
	H	1.25084	3.05286	1.64078		H	-1.24020	-1.88635	2.80246
	H	-0.37306	3.72581	-0.86735		N	-2.16917	-3.28514	0.56543
	H	0.90836	4.70858	-0.16596		O	-2.50252	-3.69123	-0.58309
	N	0.97944	0.79763	0.03229		O	-2.55395	-3.85773	1.60410
	H	1.85624	0.72987	0.56534		O	0.90138	0.67457	-0.33663
						C	2.21418	0.27177	-0.27184
						C	3.12797	1.22017	-0.74247
						C	2.64331	-0.97041	0.19771
						C	4.48056	0.93271	-0.74251
						H	2.75894	2.17534	-1.10376
						C	4.00262	-1.25809	0.19818
						H	1.94318	-1.71244	0.56049
						C	4.90380	-0.30864	-0.26866
						H	5.20289	1.65656	-1.10259
						H	4.35929	-2.21689	0.55757
						N	6.32727	-0.61870	-0.26458
						O	6.68487	-1.71709	0.15920
						O	7.10984	0.23253	-0.68550
TS1$_{cdb}$ $\cdot\cdot$2MeOH	C	0.36441	3.12351	1.34054	**TS1$_{ceb}$**$\cdot\cdot$2MeOH	C	-0.94537	2.93752	-1.65298
	C	0.21306	1.63127	1.64769		C	-0.42597	1.50045	-1.74816
	C	0.85129	2.52384	-1.05134		C	-1.81147	2.41049	0.64624
	C	1.30511	3.34581	0.15577		C	-2.14890	3.02259	-0.71394
	H	1.17239	1.21954	1.97881		H	-1.18397	0.86002	-2.21174
	H	-0.51759	1.46975	2.44428		H	0.47732	1.45277	-2.36123
	H	-0.62269	3.54638	1.11853		H	-0.14059	3.58729	-1.28894
	H	0.73626	3.63226	2.23585		H	-1.20754	3.28504	-2.65752
	H	1.57233	2.60522	-1.87109		H	-2.69586	2.38172	1.29086
	H	-0.10488	2.90845	-1.42697		H	-1.06338	3.02859	1.15723
	H	2.32184	3.04366	0.43483		H	-2.99473	2.48079	-1.15477
	H	1.34694	4.40883	-0.10118		H	-2.46502	4.06352	-0.59488
	N	-0.21672	0.87033	0.46527		N	-0.11657	0.94095	-0.42455
	H	-1.16576	1.16556	0.20020		H	0.66886	1.45886	-0.00928
	C	-0.43981	-1.16518	0.86862		C	0.58162	-1.02847	-0.53389
	C	-0.40966	-1.84787	-0.37513		C	0.40697	-1.61193	0.74570
	C	0.83199	-2.53254	-0.62884		C	-0.69276	-2.54057	0.81489
	S	0.99808	-1.61707	1.77879		S	-0.49094	-1.84449	-1.66027
	H	1.04584	-3.01982	-1.57232		H	-1.00857	-3.00070	1.74333
	C	1.68148	-2.47885	0.41357		C	-1.27846	-2.74615	-0.37927
	H	2.68225	-2.88691	0.48944		H	-2.12981	-3.37370	-0.61448

	N	-1.43654	-1.82862	-1.30864		N	1.16491	-1.29679	1.86582
	O	-1.32665	-2.52158	-2.33838		O	0.97132	-1.92889	2.92198
	O	-2.45060	-1.11846	-1.10799		O	2.02324	-0.38538	1.80042
	C	0.69457	1.04931	-0.67534		C	-1.27120	0.98819	0.48507
	H	1.66885	0.63381	-0.39815		H	-2.05255	0.33853	0.07696
	H	0.30466	0.47280	-1.51855		H	-0.96250	0.58037	1.45130
	C	-3.35705	2.35762	-1.47095		C	2.01676	3.21652	2.03249
	H	-4.41547	2.22942	-1.72382		H	2.97123	3.35840	2.55164
	H	-3.18546	3.40163	-1.20431		H	1.69200	4.17715	1.62968
	H	-2.74755	2.11139	-2.34815		H	1.26839	2.86248	2.75099
	O	-2.99722	1.56697	-0.33874		O	2.15670	2.32074	0.93048
	H	-3.10083	0.62590	-0.56712		H	2.40386	1.44265	1.27087
	C	4.18102	-0.04581	-1.80347		C	-4.41838	-0.77356	1.45645
	H	3.98866	0.82556	-2.43174		H	-4.52974	0.21565	1.90385
	H	5.16285	-0.45676	-2.06783		H	-5.27000	-1.39278	1.76325
	H	3.41159	-0.80096	-2.00404		H	-3.49335	-1.22751	1.83138
	O	4.14293	0.40222	-0.45004		O	-4.38216	-0.58827	0.04328
	H	4.31803	-0.34880	0.14438		H	-4.29160	-1.45336	-0.39393
	Cl	-1.88672	-0.98519	1.84432		Br	2.30337	-0.59910	-1.28182
TS1$_{cfb}$ $\cdot\cdot$2MeOH	C	-3.18558	1.64673	-1.96791	**TS1$_{cgb}$**$\cdot\cdot$2MeOH	C	-3.13704	2.35306	-1.98222
	C	-1.95042	0.75024	-1.85347		C	-2.08551	1.24892	-1.84181
	C	-3.67044	1.21078	0.45172		C	-4.13862	1.59578	0.19771
	C	-4.25865	1.24208	-0.95845		C	-4.42866	1.97398	-1.25608
	H	-2.20476	-0.27905	-2.12809		H	-2.42698	0.34383	-2.35667
	H	-1.16199	1.09416	-2.52451		H	-1.13489	1.55242	-2.28799
	H	-2.88777	2.68800	-1.79889		H	-2.73583	3.28501	-1.56604
	H	-3.56621	1.58365	-2.99248		H	-3.32567	2.53274	-3.04579
	H	-4.40384	0.83693	1.17338		H	-5.04590	1.23682	0.69466
	H	-3.39807	2.22503	0.76593		H	-3.79933	2.47998	0.75166
	H	-4.64438	0.24695	-1.21012		H	-4.89540	1.12099	-1.76414
	H	-5.10378	1.93589	-1.00385		H	-5.14508	2.80035	-1.29913
	N	-1.41617	0.72451	-0.47826		N	-1.83833	0.89943	-0.43679
	H	-1.06131	1.65751	-0.22816		H	-1.39368	1.69914	0.03000
	C	0.14645	-0.57385	-0.23390		C	-0.34681	-0.58493	-0.24811
	C	0.32358	-0.83330	1.15198		C	-0.45638	-1.13653	1.05069
	C	-0.07549	-2.14967	1.56986		C	-1.08044	-2.43303	1.07473
	S	-0.30803	-2.09488	-0.99960		S	-0.80726	-1.81600	-1.42236
	H	-0.07423	-2.45818	2.60835		H	-1.31949	-2.95188	1.99501
	C	-0.45801	-2.92235	0.53646		C	-1.32916	-2.91319	-0.15927
	H	-0.81935	-3.94382	0.55296		H	-1.79810	-3.85137	-0.43072

	N	0.74473	0.13174	2.05810		N	-0.04029	-0.49139	2.20950
	O	0.88450	-0.17226	3.25748		O	-0.18796	-1.06437	3.30301
	O	0.96373	1.28859	1.63528		O	0.48642	0.64514	2.13451
	C	-2.43459	0.31201	0.50455		C	-3.06472	0.50854	0.27020
	H	-2.72042	-0.72060	0.28077		H	-3.43899	-0.41277	-0.18934
	H	-1.98157	0.33908	1.49811		H	-2.80490	0.28584	1.30932
	C	-0.94097	3.99006	1.66393		C	-0.72637	3.97759	1.89005
	H	-0.32866	4.86001	1.92840		H	0.11708	4.43788	2.41692
	H	-1.98577	4.30199	1.61670		H	-1.29725	4.76254	1.39149
	H	-0.82813	3.22389	2.43833		H	-1.37425	3.47898	2.62025
	O	-0.59349	3.48560	0.37498		O	-0.27637	3.07502	0.88076
	H	0.31708	3.14237	0.39805		H	0.19940	2.34055	1.30901
	C	-4.51144	-2.80375	1.35555		C	-5.40685	-2.44688	0.57080
	H	-5.13539	-1.96672	1.67355		H	-6.00585	-1.58866	0.88018
	H	-5.04891	-3.73720	1.56164		H	-6.00490	-3.35634	0.70511
	H	-3.58185	-2.79062	1.93730		H	-4.51888	-2.50527	1.21165
	O	-4.26617	-2.63203	-0.03864		O	-5.06038	-2.23973	-0.79665
	H	-3.71795	-3.36770	-0.36461		H	-4.52564	-2.98964	-1.11202
	S	1.34322	0.37946	-1.29045		O	0.57544	0.34753	-0.65341
	O	1.21700	-0.22647	-2.62153		C	1.92391	0.10724	-0.54292
	O	1.12909	1.82257	-1.18383		C	2.72749	1.22355	-0.79266
	C	2.93991	-0.03772	-0.62686		C	2.48584	-1.13279	-0.23719
	C	3.48856	-1.27984	-0.94645		C	4.10404	1.10638	-0.73506
	C	3.61852	0.89417	0.15432		H	2.25449	2.17259	-1.02593
	C	4.74913	-1.59760	-0.45194		C	3.86890	-1.24885	-0.17586
	H	2.94815	-1.97908	-1.57757		H	1.87156	-2.00573	-0.05258
	C	4.88236	0.56272	0.63595		C	4.66074	-0.13389	-0.42397
	H	3.16806	1.85544	0.37489		H	4.74352	1.96141	-0.92316
	C	5.44193	-0.67893	0.33796		H	4.32912	-2.20198	0.05940
	H	5.19336	-2.56011	-0.68946		N	6.11007	-0.26494	-0.35989
	H	5.43017	1.27787	1.24321		O	6.58574	-1.36403	-0.07714
	H	6.42835	-0.93137	0.71829		O	6.79582	0.73010	-0.59200
1da (H_2O)	C	3.62612	-1.61121	0.85938	**1db** (H_2O)	C	-2.94375	-0.69197	1.24193
	C	2.52951	-0.76730	0.97074		C	-1.58850	-0.97847	1.32768
	C	2.43592	0.33080	0.12383		C	-0.78268	-0.78282	0.21050
	C	3.41087	0.62228	-0.82297		C	-1.29539	-0.31147	-0.99264
	C	4.50937	-0.21860	-0.93824		C	-2.65117	-0.02465	-1.08535
	C	4.59625	-1.32319	-0.09604		C	-3.45211	-0.21863	0.03545
	H	3.73154	-2.47735	1.50282		H	-3.59928	-0.83451	2.09359
	H	1.75216	-0.95425	1.70565		H	-1.15708	-1.35546	2.25036

	H	3.30675	1.49684	-1.45826		H	-0.63615	-0.17688	-1.84526
	H	5.28857	-0.02245	-1.66605		H	-3.08228	0.34305	-2.00962
	O	1.38447	1.22257	0.29805		O	0.56253	-1.13122	0.26353
	N	5.75319	-2.21100	-0.21535		N	-4.88079	0.08208	-0.05819
	O	6.60445	-1.94529	-1.06112		O	-5.31844	0.49578	-1.12964
	O	5.82019	-3.18184	0.53534		O	-5.57787	-0.09279	0.93891
	C	0.22483	1.07781	-0.38438		C	1.42951	-0.26272	0.86409
	C	-0.72531	2.15248	-0.01852		C	2.82508	-0.80902	0.84143
	C	-1.99754	2.20165	-0.60635		H	2.85298	-1.76942	1.36135
	C	-0.36663	3.13408	0.91916		H	3.13565	-0.98323	-0.19134
	C	-2.89096	3.20901	-0.26476		H	3.50181	-0.10441	1.32117
	H	-2.27896	1.44519	-1.33144		O	1.07606	0.79396	1.33264
	C	-1.26447	4.14054	1.25790					
	H	0.61331	3.10927	1.38208					
	C	-2.52732	4.18119	0.66806					
	H	-3.87414	3.23733	-0.72656					
	H	-0.97761	4.89572	1.98467					
	H	-3.22751	4.96893	0.93443					
	S	-0.04230	-0.13443	-1.45539					
2d (H_2O)	C	3.42827	1.15664	0.07574	**2e** (H_2O)	C	-1.09816	0.04840	-0.00441
	C	4.86077	1.09095	0.07644		O	-1.88496	1.01771	-0.01596
	C	5.52023	2.36431	0.07566		C	0.33835	0.22815	0.00159
	C	4.82527	3.56712	0.07458		N	1.08961	-0.86728	0.01386
	C	3.43121	3.56725	0.07414		O	2.37003	-0.69179	0.01903
	C	2.73419	2.35994	0.07471		C	-1.69295	-1.34758	0.00328
	H	2.87576	0.21892	0.07609		H	-2.33054	-1.45862	-0.87890
	H	6.60858	2.37387	0.07593		H	-0.93726	-2.12998	0.01303
	H	5.36800	4.50989	0.07408		H	-2.33939	-1.44522	0.88059
	H	1.64636	2.36141	0.07430		C	0.94161	1.60280	-0.00601
	O	5.50503	-0.02507	0.07706		H	1.58809	1.74119	-0.87976
	Cl	2.54618	5.10029	0.07274		H	0.15542	2.35822	-0.01589
						H	1.57914	1.75470	0.87206
$TS1_{dab}$	C	-4.93593	-1.63663	0.98052	**$IN1_{dab}$**	C	2.88860	2.01948	-1.25422
	C	-4.07997	-0.56555	1.19235		C	1.55801	1.67732	-1.11982
	C	-2.82814	-0.54349	0.57589		C	1.16409	0.63877	-0.25436
	C	-2.41972	-1.58283	-0.26383		C	2.13847	-0.05321	0.48520
	C	-3.27026	-2.65534	-0.47649		C	3.47425	0.28826	0.34865
	C	-4.51691	-2.67212	0.14970		C	3.84474	1.31805	-0.51531
	H	-5.91100	-1.67404	1.45274		H	3.19236	2.81906	-1.92038
	H	-4.37023	0.25989	1.83542		H	0.79121	2.20325	-1.68086

	H	-1.45104	-1.51169	-0.74150		H	1.85056	-0.83765	1.17019
	H	-2.98000	-3.47223	-1.12767		H	4.23392	-0.24134	0.91287
	O	-2.08254	0.58890	0.76231		O	-0.15413	0.38761	-0.24302
	N	-5.40803	-3.80016	-0.07688		N	5.24102	1.66668	-0.64890
	O	-5.02344	-4.71406	-0.80743		O	6.07449	1.03919	0.01076
	O	-6.51132	-3.79591	0.47066		O	5.55078	2.58033	-1.41901
	C	-0.74768	0.55916	1.11177		C	-0.78748	-0.58222	0.66173
	C	-0.24650	1.96296	1.22653		C	-0.36704	-1.98989	0.21497
	C	1.03696	2.21539	1.72085		C	-0.11455	-3.01301	1.12636
	C	-1.04590	3.05026	0.84698		C	-0.27177	-2.26648	-1.15411
	C	1.51174	3.51977	1.83475		C	0.23732	-4.28842	0.68280
	H	1.65725	1.37922	2.02373		H	-0.18725	-2.79235	2.18613
	C	-0.57290	4.35368	0.96629		C	0.08222	-3.53688	-1.59980
	H	-2.04290	2.87522	0.45948		H	-0.47291	-1.48025	-1.87555
	C	0.70969	4.59607	1.45978		C	0.33923	-4.55501	-0.68068
	H	2.51321	3.69500	2.21993		H	0.43373	-5.07547	1.40685
	H	-1.20920	5.18518	0.67319		H	0.15739	-3.73363	-2.66650
	H	1.07811	5.61470	1.55300		H	0.61686	-5.54768	-1.02662
	S	-0.12239	-0.71128	2.02180		S	-0.61632	-0.16625	2.38308
	O	-0.13235	0.35677	-0.81861		C	-3.98431	0.66854	-0.02761
	C	1.14103	0.08533	-1.00802		C	-4.73022	-0.54843	-0.48221
	C	2.07387	1.10425	-1.32617		H	-4.29397	-0.93823	-1.40640
	C	1.64551	-1.23509	-0.90816		H	-4.65137	-1.34137	0.26620
	C	3.41586	0.82287	-1.55315		H	-5.77822	-0.30599	-0.65169
	H	1.71349	2.12668	-1.40019		N	-2.74614	0.69296	0.31232
	C	2.98957	-1.52171	-1.13117		O	-2.16336	-0.53746	0.17669
	H	0.95653	-2.03807	-0.66568		C	-4.68541	1.99018	0.05464
	C	3.86740	-0.49136	-1.45219		O	-5.87692	2.05925	-0.22326
	H	4.10966	1.62039	-1.80633		C	-3.90320	3.21048	0.46728
	H	3.35198	-2.54393	-1.05863		H	-4.58289	4.05964	0.53942
	Cl	5.56916	-0.85270	-1.74338		H	-3.39936	3.04431	1.42161
						H	-3.12308	3.42217	-0.26851
$TS2_{dab}$	C	3.31788	0.14379	1.21655	**P_{dab}**	C	2.43617	-0.15880	-1.47642
	C	2.08654	0.58412	0.77065		C	2.30228	-1.57810	-1.07615
	C	1.37857	-0.11912	-0.23800		C	1.65984	-2.49134	-1.92398
	C	1.96669	-1.29951	-0.76444		C	2.82702	-2.02920	0.14544
	C	3.19717	-1.74331	-0.32486		C	1.54286	-3.82644	-1.55772
	C	3.87072	-1.01956	0.66830		H	1.24846	-2.14493	-2.86647
	H	3.86133	0.68732	1.98167		C	2.71575	-3.36875	0.50297
	H	1.64287	1.48744	1.17433		H	3.33351	-1.33617	0.80820

	H	1.42519	-1.84421	-1.53203		C	2.07216	-4.26947	-0.34475
	H	3.64673	-2.64101	-0.73480		H	1.03626	-4.52437	-2.21879
	O	0.22159	0.31129	-0.68251		H	3.13379	-3.71054	1.44598
	N	5.15329	-1.47668	1.12812		H	1.98258	-5.31507	-0.06124
	O	5.63331	-2.50634	0.63641		C	3.47303	4.03937	0.29385
	O	5.74138	-0.82866	2.00356		O	3.35990	4.79714	1.24276
	C	-1.30859	-0.16128	0.28633		C	4.07926	4.46545	-1.01397
	C	-1.43693	-1.56157	-0.25313		H	4.31230	5.52900	-0.96781
	C	-1.06756	-2.66052	0.52494		H	4.99056	3.89320	-1.20696
	C	-1.90125	-1.78736	-1.55685		H	3.39616	4.26030	-1.84103
	C	-1.16198	-3.95607	0.01880		C	2.98730	2.61239	0.44603
	H	-0.71249	-2.49055	1.53558		N	3.10808	1.90835	-0.61621
	C	-2.00386	-3.08039	-2.05928		O	2.69230	0.59412	-0.37472
	H	-2.17767	-0.94656	-2.18247		C	2.43032	2.15336	1.75554
	C	-1.63311	-4.17317	-1.27376		H	3.08654	1.39839	2.19786
	H	-0.86832	-4.79840	0.64025		H	2.34342	2.99613	2.43893
	H	-2.37032	-3.23663	-3.07094		H	1.45250	1.68919	1.60909
	H	-1.71137	-5.18342	-1.66784		S	2.27723	0.43569	-2.99048
	S	-1.09604	0.14785	1.94156					
	C	-2.99026	2.63553	-0.84415					
	C	-4.03605	2.02595	-1.72562					
	H	-3.56924	1.55300	-2.59444					
	H	-4.57802	1.24490	-1.18676					
	H	-4.73239	2.79097	-2.06537					
	N	-2.07910	1.99089	-0.21173					
	O	-2.16366	0.64278	-0.47256					
	C	-2.95436	4.12528	-0.64533					
	O	-3.80597	4.81938	-1.18406					
	C	-1.86632	4.72410	0.20553					
	H	-2.03763	5.79649	0.29843					
	H	-1.84215	4.25467	1.19110					
	H	-0.89083	4.54300	-0.25355					
$TS1_{dae}$	C	3.18618	0.36732	0.08710	**$IN1_{dae}$**	C	-3.55826	-1.32167	0.07400
	C	1.83290	0.09196	-0.02730		C	-2.34180	-0.67692	0.22405
	C	1.40023	-1.23275	0.04735		C	-2.27379	0.71980	0.08794
	C	2.29900	-2.28241	0.22167		C	-3.44480	1.44634	-0.19676
	C	3.65608	-2.01184	0.33486		C	-4.65847	0.80426	-0.34807
	C	4.07969	-0.68804	0.26924		C	-4.70812	-0.58426	-0.20994
	H	3.55331	1.38591	0.03024		H	-3.62126	-2.39951	0.17466
	H	1.09761	0.87351	-0.18043		H	-1.44958	-1.24081	0.44720

	H	1.92802	-3.30186	0.26826		H	-3.37377	2.52542	-0.29580
	H	4.37563	-2.81068	0.47375		H	-5.56041	1.36419	-0.56786
	O	0.08069	-1.56514	-0.15617		O	-1.16229	1.47412	0.17763
	N	5.50319	-0.39647	0.38879		N	-5.97189	-1.26832	-0.36492
	O	6.28305	-1.33704	0.53805		O	-6.97839	-0.60062	-0.62024
	O	5.86603	0.77843	0.33553		O	-6.00117	-2.49574	-0.23701
	C	-0.91015	-1.12936	0.68418		C	0.12389	0.98218	0.64477
	C	-2.22760	-1.65040	0.22624		C	1.04991	2.18466	0.41381
	C	-3.39150	-1.33802	0.93730		C	2.06067	2.52374	1.30987
	C	-2.32798	-2.45853	-0.91385		C	0.92505	2.92764	-0.76766
	C	-4.62751	-1.82070	0.51835		C	2.92923	3.58296	1.03976
	H	-3.31565	-0.71250	1.81924		H	2.15498	1.94863	2.22463
	C	-3.56463	-2.94785	-1.32675		C	1.78475	3.98808	-1.03804
	H	-1.43600	-2.70978	-1.47648		H	0.14839	2.67129	-1.48109
	C	-4.72040	-2.62970	-0.61437		C	2.79470	4.32110	-0.13309
	H	-5.52310	-1.56580	1.07950		H	3.71309	3.83084	1.75153
	H	-3.62544	-3.58050	-2.20877		H	1.66900	4.55579	-1.95825
	H	-5.68572	-3.01083	-0.93825		H	3.46854	5.14824	-0.34291
	S	-0.58741	-0.65665	2.25313		S	0.07196	0.32337	2.30025
	C	-2.15862	2.64297	-0.61046		O	0.44058	-0.00577	-0.40613
	C	-1.44997	2.95263	-1.89666		C	1.62407	-0.70150	-0.33560
	H	-0.36404	2.93420	-1.75567		C	2.76347	-0.20709	-0.97245
	H	-1.67622	2.19539	-2.65473		C	1.66615	-1.95161	0.28462
	H	-1.74771	3.93391	-2.26605		C	3.94228	-0.94985	-0.98350
	N	-1.97514	1.51679	0.03997		H	2.72342	0.75835	-1.46603
	O	-1.15051	0.67404	-0.49670		C	2.83920	-2.70168	0.27482
	C	-3.09768	3.60083	-0.02945		H	0.77696	-2.33119	0.77453
	O	-3.31355	4.69644	-0.57051		C	3.96858	-2.19019	-0.35615
	C	-3.84251	3.26084	1.24440		H	4.82803	-0.56720	-1.48224
	H	-3.72713	4.08964	1.94792		H	2.87220	-3.67643	0.75292
	H	-4.90832	3.18256	1.00872		Cl	5.44935	-3.13356	-0.37140
	H	-3.50474	2.33063	1.69585					
$TS2_{dae}$	C	-3.79219	0.99692	0.60646	**P_{dae}**	C	-1.56922	0.93510	-1.00171
	C	-2.41587	0.94097	0.55801		C	-1.23997	2.37519	-0.87487
	C	-1.74711	0.40629	-0.58107		C	-0.22311	2.94183	-1.65640
	C	-2.55747	-0.07595	-1.65296		C	-1.94106	3.18981	0.02840
	C	-3.93045	-0.01829	-1.60205		C	0.08601	4.29120	-1.53811
	C	-4.55816	0.52106	-0.46751		H	0.32145	2.31627	-2.35583
	H	-4.29320	1.40986	1.47544		C	-1.62834	4.54012	0.14359
	H	-1.83344	1.29781	1.39583		H	-2.72984	2.76608	0.63944

	H -2.05478 -0.48924 -2.52287 H -4.53217 -0.38482 -2.42660 O -0.45500 0.33899 -0.71648 N -5.98168 0.58447 -0.40740 O -6.64503 0.16100 -1.36720 O -6.52323 1.06119 0.60249 C 0.83103 0.69236 0.59757 C 0.72087 2.19978 0.60354 C 0.40228 2.89969 1.76667 C 0.96654 2.91922 -0.57312 C 0.32404 4.29264 1.75865 H 0.22124 2.34362 2.68071 C 0.88842 4.30753 -0.58298 H 1.21044 2.38309 -1.48384 C 0.56584 5.00179 0.58512 H 0.07597 4.82266 2.67486 H 1.07779 4.85205 -1.50477 H 0.50507 6.08728 0.57759 S 0.51542 -0.25007 1.98497 O 1.89206 0.36990 -0.22384 C 2.35354 -0.93023 -0.34085 C 1.56977 -1.94889 -0.87744 C 3.68243 -1.16119 -0.00306 C 2.12109 -3.21295 -1.06205 H 0.53923 -1.74297 -1.13990 C 4.24012 -2.42440 -0.19065 H 4.27813 -0.35093 0.40735 C 3.45046 -3.43993 -0.71620 H 1.51948 -4.01566 -1.47856 H 5.27714 -2.61180 0.07170 Cl 4.14194 -5.03444 -0.95472		C -0.61539 5.09444 -0.63802 H 0.87618 4.71900 -2.14919 H -2.17715 5.16187 0.84582 H -0.37254 6.15009 -0.54642 C -4.14232 -1.05257 -0.89294 C -3.06299 -0.69905 -0.09598 C -2.52293 -1.57493 0.83482 C -3.06880 -2.84921 0.96277 C -4.14495 -3.21197 0.15843 C -4.68968 -2.32644 -0.76654 H -4.55080 -0.34123 -1.60506 H -1.68479 -1.26558 1.45271 H -2.66092 -3.55012 1.68491 H -5.53444 -2.62328 -1.38087 Cl -4.83317 -4.81286 0.31958 O -2.57173 0.60712 -0.16154 S -0.84028 -0.13667 -2.00882
2d ··3H_2O	C 1.19432 -0.89711 0.78635 C 2.04627 0.05260 0.16456 C 1.41939 1.01589 -0.66812 C 0.04279 1.02939 -0.86409 C -0.75617 0.07933 -0.23364 C -0.18254 -0.88415 0.59138 H 1.63971 -1.65264 1.42945 H 2.04125 1.75961 -1.16081 H -0.40838 1.78015 -1.50805	**2e** ··3H_2O	O -1.48919 2.04126 -0.14229 H -1.02185 1.16431 -0.09651 H -1.08128 2.59699 0.54503 O -3.06736 -1.58685 0.36512 H -2.12173 -1.25947 0.23301 O -4.09730 1.04428 0.40302 H -3.24597 1.49714 0.22488 H -3.29455 -2.08239 -0.44095 H -3.86179 0.09078 0.40585

	H	-0.80906	-1.62520	1.08151		C	2.56073	-1.76789	-0.68185
	Cl	-2.50347	0.09614	-0.48185		O	3.71917	-1.37337	-0.86047
	O	3.34728	0.03693	0.34688		C	2.24856	-3.24707	-0.77222
	H	4.06890	-0.70980	1.61716		H	3.17462	-3.78895	-0.96909
	O	4.64002	-1.06736	2.36383		H	1.79491	-3.60740	0.15319
	H	4.13135	-0.92153	3.18064		H	1.53024	-3.44114	-1.57192
	O	6.66287	0.87620	1.95813		C	1.47639	-0.82103	-0.38522
	H	5.41616	1.88311	-1.00371		C	1.75263	0.64985	-0.28510
	H	6.03778	0.15758	2.19575		H	2.81764	0.84155	-0.41581
	H	6.21049	1.34519	1.22383		H	1.19582	1.20893	-1.04405
	O	5.06848	1.98463	-0.10037		H	1.43480	1.03616	0.68906
	H	4.35004	1.28805	-0.00224		N	0.29505	-1.34849	-0.21425
						O	-0.69265	-0.51448	0.05267
TS1$_{dab}$ $\cdot\cdot 3H_2O$	C	3.47640	-1.62506	-0.53403	**TS1$_{dae}$**$\cdot\cdot 3H_2O$	C	-3.55194	2.49797	-0.37008
	C	2.28779	-0.91981	-0.43856		C	-2.22661	2.38790	0.02627
	C	2.31745	0.47769	-0.45309		C	-1.58646	1.15037	-0.02828
	C	3.52875	1.16600	-0.55362		C	-2.25471	0.01125	-0.48298
	C	4.72091	0.46462	-0.64828		C	-3.57866	0.11544	-0.87798
	C	4.67930	-0.92724	-0.64104		C	-4.21182	1.35655	-0.81552
	H	3.47850	-2.70919	-0.51922		H	-4.06887	3.45016	-0.33327
	H	1.33767	-1.42507	-0.33526		H	-1.67818	3.25499	0.38213
	H	3.52075	2.25196	-0.55913		H	-1.72321	-0.93127	-0.52318
	H	5.66908	0.98364	-0.73046		H	-4.11989	-0.75213	-1.23847
	O	1.20670	1.25484	-0.28353		O	-0.25131	1.13989	0.28662
	N	5.92426	-1.67226	-0.74145		N	-5.60332	1.46302	-1.23308
	O	6.98016	-1.04307	-0.82378		O	-6.17828	0.44528	-1.61940
	O	5.87364	-2.90301	-0.74020		O	-6.14734	2.56637	-1.18287
	C	0.00274	1.01508	-0.93213		C	0.28653	0.27084	1.21164
	C	-0.96937	2.08581	-0.52751		C	1.75014	0.53953	1.34752
	C	-2.19191	2.21505	-1.19276		C	2.49819	-0.13055	2.32059
	C	-0.68222	2.96093	0.52866		C	2.39933	1.44648	0.50019
	C	-3.10697	3.19532	-0.81587		C	3.86339	0.10704	2.45219
	H	-2.41493	1.54583	-2.01626		H	1.99668	-0.83640	2.97235
	C	-1.59455	3.94482	0.89994		C	3.76429	1.68595	0.63556
	H	0.25771	2.87510	1.06052		H	1.84002	1.96377	-0.26992
	C	-2.81271	4.06688	0.23108		C	4.50271	1.01909	1.61269
	H	-4.05298	3.27902	-1.34504		H	4.43084	-0.42184	3.21398
	H	-1.35199	4.62061	1.71670		H	4.25220	2.39554	-0.02790
	H	-3.52411	4.83570	0.52242		H	5.56845	1.20710	1.71776
	S	-0.00295	0.35074	-2.49247		S	-0.65401	-0.35329	2.45897

	C	-1.66357	-2.11345	-0.77140		C	1.86619	-4.47720	0.20410
	C	-1.70096	-0.97435	0.05620		O	2.01540	-5.52268	-0.43402
	C	-2.94705	-0.58499	0.58687		C	2.38145	-4.37284	1.62192
	C	-4.10336	-1.31029	0.31972		H	3.20433	-3.65480	1.66944
	C	-4.03024	-2.43376	-0.49907		H	1.60774	-4.00476	2.29755
	C	-2.81851	-2.84076	-1.04707		H	2.73289	-5.35451	1.94213
	H	-0.71268	-2.42921	-1.18716		C	1.20485	-3.30824	-0.41115
	H	-2.99545	0.29645	1.22003		N	1.09117	-2.26538	0.35511
	H	-5.05541	-1.00326	0.74404		O	0.53353	-1.19912	-0.17864
	H	-2.77399	-3.72216	-1.68106		O	1.11377	-0.04933	-2.64518
	Cl	-5.49075	-3.35610	-0.83841		H	0.28561	-0.15500	-3.14667
	O	-0.58809	-0.29294	0.34036		H	0.94333	-0.46093	-1.76363
	H	1.65343	4.88852	2.37906		O	1.36617	4.40182	-1.65680
	O	2.35036	4.21910	2.24348		H	1.81184	4.65207	-0.82559
	H	2.55925	4.25521	1.29101		H	0.42772	4.28144	-1.41747
	O	2.16397	1.68850	3.56907		C	0.71501	-3.37464	-1.82792
	H	1.31022	1.27365	3.31712		H	1.30708	-2.72906	-2.48406
	H	2.19942	2.54147	3.09445		H	0.77348	-4.39869	-2.19673
	O	-0.29497	0.49779	2.91433		H	-0.31965	-3.02318	-1.88761
	H	-0.41161	0.24029	1.96019		O	2.53554	2.31048	-3.21275
	H	-1.02384	1.11426	3.10580		H	2.13543	3.02602	-2.68039
						H	2.04736	1.49554	-2.96940
TS1$_{\mathbf{1dbd}}$ $\cdot\cdot 3H_2O$	C	-2.38397	-1.47038	-0.30328	**IN1$_{\mathbf{1dbd}}$**$\cdot\cdot 3H_2O$	O	-0.95204	0.85200	0.02880
	C	-2.19690	-0.16388	0.18289		C	-2.13772	0.18275	0.00794
	C	-3.32479	0.54027	0.64252		C	-2.43352	-0.58151	1.14390
	C	-4.59041	-0.03878	0.63086		C	-3.07445	0.24934	-1.03087
	C	-4.74380	-1.33212	0.14196		C	-3.64461	-1.25589	1.25544
	C	-3.64908	-2.05075	-0.32769		H	-1.70029	-0.64260	1.94351
	H	-1.52557	-2.02636	-0.66409		C	-4.28528	-0.43088	-0.92249
	H	-3.19689	1.55407	1.01328		H	-2.85837	0.81313	-1.92913
	H	-5.45101	0.51495	0.99607		C	-4.56585	-1.17565	0.21691
	H	-3.78038	-3.06163	-0.70408		H	-3.86422	-1.84189	2.14335
	Cl	-6.34133	-2.06969	0.12216		H	-5.00912	-0.37575	-1.73071
	O	-0.97850	0.39946	0.23054		Cl	-6.09689	-2.02742	0.34490
	H	1.73118	4.45109	-1.46868		C	4.12557	-0.57731	-0.00695
	O	1.75723	4.02819	-0.59026		C	3.29140	0.49787	-0.23975
	H	1.49700	3.09723	-0.73603		C	1.91808	0.30781	-0.50746
	O	-0.22119	4.73177	1.34508		C	1.40476	-1.00598	-0.54149
	H	-0.34668	3.83431	1.72373		C	2.24233	-2.08264	-0.31044
	H	0.47314	4.61380	0.66626		C	3.59630	-1.86979	-0.04463

	O	-0.44139	2.09515	2.28145		H	5.17908	-0.42691	0.20100
	H	-0.64447	1.48105	1.52680		H	3.68447	1.50958	-0.21329
	H	-1.09161	1.88900	2.97639		H	0.35942	-1.16975	-0.75627
	C	2.80125	-1.83534	0.18235		H	1.85167	-3.09404	-0.33332
	C	1.74845	-0.99638	-0.14383		O	1.18628	1.41153	-0.69497
	C	2.00653	0.33826	-0.49050		N	4.46092	-2.99895	0.19461
	C	3.32564	0.81750	-0.49992		O	3.97958	-4.13593	0.15209
	C	4.37803	-0.01793	-0.16947		O	5.65510	-2.79156	0.43416
	C	4.10624	-1.34377	0.16595		C	-0.30112	1.32591	-1.27655
	H	2.61647	-2.86805	0.45649		O	-0.42182	0.55408	-2.24848
	H	0.73012	-1.35444	-0.12151		C	-0.63831	2.80443	-1.41083
	H	3.51156	1.85317	-0.76790		H	-0.05993	3.22965	-2.23446
	H	5.39938	0.34568	-0.17504		H	-1.69927	2.89608	-1.65423
	O	1.04019	1.24221	-0.78487		H	-0.43693	3.36319	-0.49534
	N	5.20298	-2.22773	0.50831		H	2.54966	4.40861	-1.07254
	O	6.34996	-1.77501	0.49750		O	2.50484	3.87394	-0.25843
	O	4.94845	-3.39910	0.79746		H	2.02612	3.05283	-0.50149
	C	-0.25157	0.81387	-1.35564		O	0.84394	4.77547	1.86579
	O	-0.25235	-0.16044	-2.10951		H	0.40462	3.92690	2.08392
	C	-1.01102	2.08583	-1.66438		H	1.45731	4.55837	1.13415
	H	-0.59379	2.53013	-2.57353		O	-0.37598	2.26781	2.39665
	H	-2.05366	1.82908	-1.85582		H	-0.53782	1.76874	1.56628
	H	-0.96005	2.80753	-0.84887		H	-1.24538	2.33793	2.83180
TS2$_{\mathbf{dbd}}$ $\cdot\cdot 3H_2O$	O	-0.90406	1.44581	0.64501	**TS1$_{\mathbf{dbe}}$**$\cdot\cdot 3H_2O$	C	-2.57274	-1.53888	-0.03105
	C	-1.99036	0.64905	0.42512		C	-1.41808	-0.83052	0.26025
	C	-2.12193	-0.46475	1.26106		C	-1.49361	0.55107	0.47729
	C	-2.98229	0.91380	-0.52555		C	-2.72333	1.21511	0.39508
	C	-3.23167	-1.29847	1.16559		C	-3.87805	0.51010	0.09737
	H	-1.34406	-0.67286	1.99061		C	-3.79079	-0.86489	-0.10859
	C	-4.08971	0.07572	-0.62764		H	-2.53376	-2.60822	-0.20626
	H	-2.89128	1.76078	-1.19409		H	-0.45899	-1.32707	0.30688
	C	-4.21015	-1.02164	0.21759		H	-2.76339	2.28671	0.56577
	H	-3.32767	-2.15850	1.82212		H	-4.83596	1.01344	0.03123
	H	-4.85886	0.28380	-1.36600		O	-0.39943	1.32930	0.71862
	Cl	-5.61198	-2.07078	0.08427		N	-4.99782	-1.61308	-0.41527
	C	4.29824	0.41412	0.25275		O	-6.06340	-1.00010	-0.49965
	C	3.39528	1.45524	0.31712		O	-4.90896	-2.83103	-0.57901
	C	2.02715	1.25673	0.01455		C	0.70524	0.81286	1.50029
	C	1.59944	-0.03598	-0.36650		O	0.49126	-0.06512	2.32433
	C	2.50624	-1.07747	-0.43311		C	1.70448	1.92443	1.68840

	C	3.85078	-0.85573	-0.12489		H	1.36945	2.55990	2.51477
	H	5.34461	0.57249	0.48925		H	2.66120	1.47672	1.95711
	H	3.72583	2.44721	0.60970		H	1.82261	2.53016	0.79022
	H	0.56258	-0.20727	-0.61500		C	4.32360	-2.24734	0.01625
	H	2.17885	-2.06994	-0.72291		O	4.93930	-3.00679	-0.73465
	O	1.22187	2.30934	0.12562		C	4.75527	-2.08292	1.45589
	N	4.78683	-1.94669	-0.19678		H	5.12000	-1.06661	1.62546
	O	4.37729	-3.06234	-0.53767		H	3.91773	-2.23476	2.13859
	O	5.97177	-1.73350	0.08472		H	5.55232	-2.79658	1.66793
	C	-0.32984	2.27423	-0.47911		C	3.16406	-1.47580	-0.48264
	O	-0.39764	1.78111	-1.61576		N	2.58070	-0.72231	0.39703
	C	-0.72285	3.71816	-0.21626		O	1.54990	-0.00772	-0.03510
	H	-0.17051	4.37147	-0.89506		O	1.77674	1.69765	-2.18340
	H	-1.78992	3.82496	-0.42746		H	1.10789	1.42008	-2.83487
	H	-0.53634	4.01718	0.81622		H	1.70001	1.05712	-1.43243
	H	2.31070	5.38409	0.55084		O	-0.64437	4.16969	0.19321
	O	2.36284	4.64518	1.18458		H	-0.55945	3.22894	0.44162
	H	1.94350	3.87621	0.73877		H	-0.65460	4.66492	1.03351
	O	0.75221	4.73282	3.52152		C	2.72868	-1.60725	-1.91201
	H	0.40516	3.81671	3.49198		H	2.97610	-0.70857	-2.48586
	H	1.34083	4.80075	2.74175		H	3.21921	-2.46279	-2.37632
	O	-0.19703	2.06469	3.31037		H	1.64300	-1.72964	-1.96345
	H	-0.39541	1.84899	2.37378		O	1.65089	4.41689	-1.48735
	H	-1.02576	1.89916	3.79622		H	0.86194	4.44626	-0.91001
						H	1.72543	3.47569	-1.75561
IN1$_{\mathbf{dbe}\cdot\cdot 3H_2O}$	C	2.57273	-1.58917	-0.15539	**TS2**$_{\mathbf{dbe}\cdot\cdot 3H_2O}$	C	2.65049	-1.59326	-0.14504
	C	1.42292	-0.89030	-0.47970		C	1.47733	-0.89258	-0.34846
	C	1.41949	0.51757	-0.43084		C	1.48207	0.52286	-0.37802
	C	2.59661	1.19595	-0.05530		C	2.71592	1.19551	-0.19688
	C	3.74296	0.49755	0.27142		C	3.88633	0.49547	0.01205
	C	3.72597	-0.89764	0.21820		C	3.85324	-0.90303	0.03435
	H	2.58146	-2.67313	-0.18637		H	2.64490	-2.67741	-0.11712
	H	0.52744	-1.41872	-0.77117		H	0.54426	-1.42214	-0.48188
	H	2.58897	2.28106	-0.01994		H	2.72514	2.28110	-0.21779
	H	4.64672	1.02032	0.56400		H	4.82661	1.01677	0.15395
	O	0.34748	1.28381	-0.69261		O	0.38796	1.25186	-0.54249
	N	4.92011	-1.63597	0.55785		N	5.06981	-1.63885	0.24842
	O	5.92899	-1.00803	0.89325		O	6.12406	-1.01313	0.41349
	O	4.89134	-2.86905	0.50158		O	5.02569	-2.87501	0.26091
	C	-0.89626	0.70813	-1.44525		C	-0.99047	0.59979	-1.40951

	O	-0.63645	-0.05503	-2.39485		O	-0.65844	-0.15435	-2.32161
	C	-1.76016	1.94193	-1.65160		C	-1.73589	1.89491	-1.64416
	H	-1.32136	2.55371	-2.44367		H	-1.22296	2.46664	-2.41958
	H	-2.74719	1.60926	-1.97779		H	-2.73679	1.64169	-2.00207
	H	-1.86468	2.54014	-0.74467		H	-1.82305	2.49546	-0.73829
	C	-4.39321	-2.09195	0.05815		C	-4.56066	-1.96749	0.15900
	O	-4.92871	-2.83230	0.87607		O	-5.10327	-2.67639	0.99749
	C	-5.00605	-1.85043	-1.29851		C	-5.20517	-1.69058	-1.17507
	H	-5.25092	-0.79284	-1.42194		H	-5.38140	-0.61930	-1.29736
	H	-4.30024	-2.10536	-2.09176		H	-4.54746	-1.99777	-1.99105
	H	-5.90953	-2.45361	-1.39051		H	-6.14994	-2.23157	-1.23034
	C	-3.11009	-1.40789	0.40745		C	-3.22552	-1.35599	0.46309
	N	-2.63357	-0.65739	-0.52132		N	-2.74437	-0.63423	-0.48286
	O	-1.48393	-0.02332	-0.17824		O	-1.53675	-0.06980	-0.17008
	O	-1.37145	1.62900	2.17552		O	-1.19856	1.52948	2.25532
	H	-0.55510	1.40432	2.65897		H	-0.31593	1.40377	2.65037
	H	-1.35655	1.07315	1.36842		H	-1.17554	1.03144	1.41389
	O	0.69180	4.09036	-0.37905		O	0.67020	4.01452	-0.26639
	H	0.54941	3.14306	-0.58589		H	0.56801	3.04843	-0.43067
	H	0.64697	4.55998	-1.23246		H	0.61406	4.44160	-1.14063
	C	-2.48248	-1.63181	1.74931		C	-2.56322	-1.61627	1.78035
	H	-2.57225	-0.73775	2.37370		H	-2.51253	-0.69981	2.37536
	H	-2.96978	-2.46447	2.25536		H	-3.11791	-2.37294	2.33363
	H	-1.41530	-1.83850	1.63456		H	-1.53488	-1.95238	1.62263
	O	-1.40949	4.38910	1.51734		O	-1.48398	4.27242	1.55933
	H	-0.69075	4.41783	0.85346		H	-0.75116	4.32674	0.91142
	H	-1.44794	3.44860	1.78964		H	-1.45656	3.34276	1.86676

S11 The optimized geometries for the transition states and minima of the reaction in **Table1**, obtained with CAM-B3LYP+IDSCRF/DZVP.

Species	Cartesian coordinates				Species	Cartesian coordinates			
2d$\cdot\cdot 3H_2O1$DMSO	C	1.96153	-0.34535	1.54777	**2e**$\cdot\cdot 3H_2O1$DMSO	C	-4.16152	-0.32354	0.86194
	C	1.34358	0.60664	0.69289		O	-4.97552	0.46575	1.35934
	C	1.95077	0.79900	-0.57787		C	-4.39663	-1.81539	0.98424
	C	3.08793	0.09571	-0.96078		H	-5.37211	-1.97944	1.44442
	C	3.65986	-0.82732	-0.08933		H	-4.35224	-2.30488	0.01001
	C	3.09788	-1.04934	1.16523		H	-3.62055	-2.27277	1.60308
	H	1.52456	-0.51847	2.52848		C	-2.96487	0.16166	0.16501
	H	1.50786	1.51728	-1.26383		C	-2.70449	1.63330	0.02877

	H	3.52958	0.26619	-1.93963		H	-3.57548	2.20064	0.35772
	H	3.54704	-1.77031	1.84388		H	-1.84012	1.94417	0.62509
	Cl	5.10400	-1.71932	-0.57637		H	-2.47332	1.88274	-1.01139
	O	0.27589	1.27174	1.06385		N	-2.17510	-0.76063	-0.32052
	H	-1.03153	0.41442	1.85227		O	-1.09193	-0.34102	-0.94421
	O	-1.86329	-0.00763	2.18725		H	0.07412	-1.58125	-1.26544
	H	-2.49868	0.09119	1.45284		O	0.84751	-2.18368	-1.42618
	O	-1.41767	2.27598	-0.72132		H	1.60849	-1.70065	-1.05179
	H	-0.72579	1.93500	-0.07869		O	0.79594	1.41677	-0.11206
	H	-2.19089	1.68504	-0.59756		H	0.01113	0.86931	-0.37914
	S	-3.91457	-0.60843	-1.16988		H	1.56055	0.80055	-0.13197
	O	-3.48926	0.45729	-0.14365		S	3.65283	-0.83462	1.05004
	C	-5.66422	-0.89754	-0.84261		O	2.84297	-0.49836	-0.21574
	H	-6.19902	0.01133	-1.12120		C	5.26297	-1.37208	0.44174
	H	-6.01421	-1.73296	-1.45282		H	5.74968	-0.50009	0.00314
	H	-5.79933	-1.10515	0.22061		H	5.85941	-1.74623	1.27663
	C	-3.27200	-2.16959	-0.53249		H	5.11908	-2.14573	-0.31493
	H	-3.63086	-2.98816	-1.16015		C	3.03574	-2.43833	1.60099
	H	-2.18382	-2.11628	-0.58192		H	3.64385	-2.78784	2.43813
	H	-3.59484	-2.29875	0.50225		H	2.00561	-2.29322	1.92843
	O	-0.38895	2.29383	-3.25063		H	3.06935	-3.14535	0.76999
	H	-0.77894	2.28859	-2.33999		O	1.05132	3.82122	-1.40108
	H	-0.14643	1.36947	-3.42795		H	0.96064	2.95292	-0.93729
						H	0.93575	3.61853	-2.34448
TS1$_{dad}$ $\cdot\cdot 3H_2O1DMSO$	C	-2.21682	2.70931	0.08459	**TS1$_{dae}$**$\cdot\cdot 3H_2O1DMSO$	C	3.70909	-1.07984	-1.37936
	C	-1.22593	1.76797	-0.14385		C	2.53417	-0.38486	-1.63115
	C	-1.43056	0.77869	-1.10970		C	1.36064	-0.74336	-0.96866
	C	-2.62048	0.72115	-1.83655		C	1.34422	-1.78884	-0.04290
	C	-3.61606	1.66071	-1.61162		C	2.51478	-2.48523	0.21276
	C	-3.39968	2.64637	-0.65251		C	3.68216	-2.12398	-0.45951
	H	-2.08381	3.48454	0.83099		H	4.63163	-0.81975	-1.88602
	H	-0.29649	1.77104	0.41067		H	2.51392	0.43512	-2.34290
	H	-2.75154	-0.06011	-2.57918		H	0.41832	-2.02859	0.46483
	H	-4.54548	1.63417	-2.16921		H	2.53125	-3.29818	0.93004
	O	-0.53858	-0.23605	-1.32460		O	0.26381	0.04743	-1.19704
	N	-4.43872	3.63743	-0.41070		N	4.91119	-2.85950	-0.18995
	O	-5.48192	3.56333	-1.06066		O	4.87262	-3.78589	0.61944
	O	-4.23178	4.50887	0.43413		O	5.93631	-2.52334	-0.78265
	C	0.80167	-0.00460	-1.59805		C	-0.95538	-0.47473	-1.57539
	C	1.46827	-1.32496	-1.84950		C	-1.92607	0.63965	-1.78994

C	2.77949	-1.37082	-2.33253	C	-3.24322	0.35360	-2.16647
C	0.80075	-2.53128	-1.60024	C	-1.54656	1.97591	-1.61449
C	3.41000	-2.59101	-2.56336	C	-4.16198	1.38059	-2.35873
H	3.29695	-0.43991	-2.53611	H	-3.53556	-0.68087	-2.30289
C	1.42892	-3.75061	-1.83836	C	-2.46594	3.00303	-1.81623
H	-0.21465	-2.51697	-1.22137	H	-0.52943	2.21918	-1.33130
C	2.73755	-3.78750	-2.31996	C	-3.77778	2.71099	-2.18594
H	4.43048	-2.60608	-2.93803	H	-5.18287	1.14253	-2.64716
H	0.89312	-4.67711	-1.64688	H	-2.15306	4.03598	-1.68562
H	3.22711	-4.74037	-2.50543	H	-4.49496	3.51322	-2.34160
S	1.26581	1.40412	-2.41741	S	-1.06252	-1.94656	-2.37664
C	2.88234	1.90037	0.55979	C	-4.44358	-2.32802	1.65625
C	2.54856	0.53118	0.53768	O	-4.95808	-2.65460	2.72975
C	3.56557	-0.39946	0.83392	C	-5.17309	-2.58533	0.35622
C	4.85327	0.01599	1.15553	H	-5.47033	-1.63685	-0.09900
C	5.14766	1.37675	1.17064	H	-4.53055	-3.09137	-0.36572
C	4.17138	2.32229	0.87510	H	-6.06127	-3.18376	0.56348
H	2.11135	2.63031	0.33718	C	-3.12430	-1.66741	1.62406
H	3.32484	-1.45852	0.81564	N	-2.67504	-1.38244	0.43806
H	5.62370	-0.71320	1.39121	O	-1.51188	-0.77701	0.37139
H	4.41288	3.38162	0.89561	O	-0.61267	1.34735	1.94729
Cl	6.77650	1.90752	1.57869	H	0.03741	1.86256	1.42301
O	1.30824	0.12834	0.26115	H	-0.89603	0.58128	1.39466
H	-2.85206	-2.85758	-0.45649	O	1.73160	3.92384	-1.68664
O	-3.43365	-3.08288	-1.21684	H	1.65117	3.53937	-0.78670
H	-3.02891	-2.66450	-1.99704	H	1.85471	3.16327	-2.28081
S	-3.38096	-2.07144	2.17017	C	-2.39328	-1.37133	2.90027
O	-2.24198	-2.43073	1.19047	H	-2.39613	-0.29882	3.12056
C	-4.31881	-0.76766	1.34785	H	-2.86400	-1.89645	3.73170
H	-5.21010	-0.54252	1.93810	H	-1.34598	-1.67565	2.81843
H	-3.67461	0.11142	1.30412	S	2.60250	2.88044	1.93109
H	-4.58117	-1.09864	0.34152	O	1.48102	2.86651	0.86958
C	-4.58182	-3.40692	1.99796	C	3.04681	1.14698	2.15809
H	-4.12105	-4.30845	2.40384	H	3.89344	1.07882	2.84506
H	-5.47508	-3.15865	2.57546	H	2.17484	0.65240	2.58817
H	-4.81811	-3.54053	0.94060	H	3.29077	0.70762	1.18921
O	0.33124	-1.75831	1.99253	C	4.07794	3.42193	1.04722
H	0.69433	-1.12768	1.31999	H	3.92500	4.46397	0.76424
H	-0.56232	-2.01684	1.67443	H	4.93956	3.34225	1.71373
O	0.13272	-0.67362	4.50614	H	4.21286	2.80576	0.15659

	H	0.21799	-1.06411	3.60173			
	H	-0.17020	0.23863	4.36199			
2d ··2H$_2$O1DMSO	C	1.28530	-1.43638	0.91048	**2e** ··2H$_2$O1DMSO	O	-2.60525	1.67034	-0.81589
	C	0.94437	-0.06101	1.02871		H	-1.93634	1.22856	-0.24085
	C	1.75082	0.84973	0.29243		H	-3.32940	1.02083	-0.90544
	C	2.81322	0.42140	-0.49512		O	-2.90627	-1.72765	0.78374
	C	3.11036	-0.93673	-0.57934		H	-2.14320	-1.09090	0.87108
	C	2.34741	-1.86628	0.12228		H	-3.44862	-1.34940	0.06452
	H	0.69163	-2.16509	1.45770		C	2.46711	-0.02406	-0.03525
	H	1.52054	1.91070	0.35629		O	3.40936	0.70480	-0.37392
	H	3.41097	1.14480	-1.04432		C	2.68946	-1.51709	0.09803
	H	2.58186	-2.92582	0.05450		H	3.74383	-1.73103	-0.08311
	Cl	4.46033	-1.48125	-1.57954		H	2.40012	-1.87140	1.08902
	O	-0.05373	0.34437	1.77197		H	2.07572	-2.06192	-0.62325
	H	-1.41349	-0.66330	2.09101		C	1.13696	0.53124	0.23349
	O	-2.29065	-1.11511	2.21599		C	0.88307	2.00515	0.11143
	H	-2.92866	-0.52599	1.76798		H	1.81744	2.53317	-0.08022
	O	-1.74037	2.35341	1.03269		H	0.18216	2.22138	-0.70185
	H	-1.05063	1.68499	1.28223		H	0.42512	2.39022	1.02804
	H	-2.53330	1.81904	0.83742		N	0.22045	-0.33266	0.58707
	S	-3.77294	-0.19297	-0.94367		O	-0.97962	0.15135	0.83512
	O	-3.88266	0.49497	0.43284		S	-5.90682	0.04685	0.13083
	C	-4.01668	-1.95282	-0.61953		O	-4.75740	-0.25822	-0.85196
	H	-5.05694	-2.08406	-0.31789		C	-6.30792	-1.53576	0.90284
	H	-3.82811	-2.51335	-1.53800		H	-7.04806	-1.37026	1.68913
	H	-3.34299	-2.26055	0.18303		H	-6.73434	-2.17363	0.12728
	C	-2.00799	-0.24523	-1.32434		H	-5.39313	-1.97624	1.30456
	H	-1.86473	-0.79870	-2.25518		C	-5.12747	0.83328	1.55846
	H	-1.67349	0.78548	-1.44771		H	-4.72198	1.78707	1.21842
	H	-1.46894	-0.71094	-0.49793		H	-5.88414	1.00062	2.32827
						H	-4.32402	0.18838	1.91945
TS1$_{dad}$ ··2H$_2$O1DMSO	C	-2.17224	-2.71068	-0.19060	**IN1$_{dad}$** ··2H$_2$O1DMSO	C	2.28175	-2.47533	-0.92692
	C	-1.20340	-1.73732	-0.00594		C	1.19314	-1.61876	-0.88527
	C	-1.41691	-0.72971	0.93846		C	1.37329	-0.25303	-1.15305
	C	-2.59259	-0.68518	1.68819		C	2.65536	0.23705	-1.45028
	C	-3.56632	-1.65684	1.50707		C	3.74349	-0.61678	-1.49166
	C	-3.34178	-2.66017	0.56850		C	3.54665	-1.97309	-1.23131
	H	-2.03293	-3.50112	-0.91971		H	2.15569	-3.53240	-0.72066
	H	-0.28294	-1.72806	-0.57575		H	0.21075	-2.00106	-0.65197

H	-2.73064	0.11085	2.41365	H	2.77671	1.29828	-1.64215
H	-4.48497	-1.64141	2.08263	H	4.73428	-0.24344	-1.72546
O	-0.54605	0.31355	1.10415	O	0.39675	0.68641	-1.10382
N	-4.35799	-3.68492	0.37305	N	4.67890	-2.87718	-1.27797
O	-5.39055	-3.62114	1.04076	O	5.79232	-2.41355	-1.53483
O	-4.14304	-4.57301	-0.45212	O	4.48639	-4.07515	-1.05865
C	0.79272	0.11745	1.40285	C	-1.02796	0.37243	-1.28407
C	1.44433	1.45687	1.57195	C	-1.65539	1.77433	-1.24373
C	2.73747	1.55175	2.09417	C	-2.07660	2.41634	-2.40832
C	0.77916	2.63414	1.20479	C	-1.76393	2.45268	-0.02474
C	3.35197	2.79195	2.25113	C	-2.60626	3.70507	-2.35879
H	3.25331	0.64381	2.38645	H	-1.99669	1.88564	-3.35090
C	1.39054	3.87356	1.36901	C	-2.30090	3.73734	0.02817
H	-0.21996	2.58071	0.78903	H	-1.43657	1.97684	0.89399
C	2.68109	3.95962	1.89222	C	-2.72482	4.37005	-1.13952
H	4.35851	2.84524	2.65862	H	-2.93109	4.18936	-3.27652
H	0.85689	4.77755	1.08576	H	-2.38598	4.24587	0.98544
H	3.15778	4.92842	2.01972	H	-3.14441	5.37225	-1.09924
S	1.26962	-1.23946	2.29378	C	-3.73272	-0.48798	-0.33380
C	2.89873	-1.89589	-0.64957	C	-2.53403	-0.81055	0.30636
C	2.56347	-0.52619	-0.69829	C	-2.54636	-1.68839	1.39434
C	3.58988	0.38819	-1.01858	C	-3.73964	-2.23963	1.84743
C	4.88277	-0.04248	-1.29562	C	-4.92718	-1.91115	1.20237
C	5.17588	-1.40278	-1.24232	C	-4.92868	-1.04213	0.11833
C	4.19269	-2.33276	-0.92115	H	-3.74302	0.17819	-1.18547
H	2.12306	-2.61465	-0.40701	H	-1.60935	-1.93501	1.88584
H	3.35010	1.44704	-1.05421	H	-3.74074	-2.92033	2.69377
H	5.65871	0.67451	-1.55026	H	-5.86076	-0.79188	-0.38025
H	4.43317	-3.39205	-0.88741	Cl	-6.44013	-2.60339	1.76372
Cl	6.81190	-1.95301	-1.59523	O	-1.30619	-0.29506	-0.00934
O	1.32268	-0.11121	-0.46373	S	-1.36533	-0.62766	-2.71586
H	-2.77869	2.86726	0.21732	O	1.74293	3.35857	-0.45990
O	-3.28383	3.11405	1.02474	H	1.05128	2.76204	-0.79177
H	-2.82679	2.68474	1.76919	H	2.03909	2.93526	0.37540
O	0.29724	1.68852	-2.34832	O	0.16533	0.46882	2.43613
H	0.67162	1.10562	-1.64884	H	0.94028	1.03904	2.24560
H	-0.58831	1.95204	-2.02607	H	-0.18575	0.19789	1.56968
S	-3.48868	2.02316	-2.34682	S	3.84683	1.47009	2.13164
O	-2.29001	2.41004	-1.45536	O	2.43075	2.03406	1.89831
C	-4.35233	0.71960	-1.44581	C	4.27285	1.97594	3.80931

	H	-5.27817	0.47456	-1.97143		H	5.22121	1.51639	4.09609
	H	-3.69506	-0.15073	-1.43289		H	4.37721	3.06162	3.80204
	H	-4.55192	1.06111	-0.42870		H	3.47178	1.67678	4.48788
	C	-4.69478	3.34504	-2.11079		C	3.61548	-0.29195	2.44080
	H	-4.27633	4.24656	-2.56025		H	3.26633	-0.74020	1.51039
	H	-5.62267	3.07669	-2.62077		H	4.57460	-0.73034	2.72560
	H	-4.85905	3.49209	-1.04158		H	2.86944	-0.42944	3.22548
TS2$_{dad}$ $\cdot\cdot 2H_2O1DMSO$	C	2.24211	-2.49617	-0.82091	**TS1$_{dae}$**$\cdot\cdot 2H_2O1DMSO$	C	3.46735	-1.02514	-1.55360
	C	1.22777	-1.57947	-0.62201		C	2.33520	-0.22775	-1.65191
	C	1.42515	-0.20596	-0.91176		C	1.16958	-0.59408	-0.98082
	C	2.68689	0.19741	-1.41758		C	1.11763	-1.74948	-0.19868
	C	3.70489	-0.71555	-1.60863		C	2.24508	-2.54870	-0.09670
	C	3.47917	-2.06484	-1.31216		C	3.40533	-2.17761	-0.77597
	H	2.09297	-3.54504	-0.58870		H	4.38381	-0.76048	-2.06883
	H	0.27241	-1.89994	-0.22617		H	2.34344	0.67925	-2.24915
	H	2.84157	1.24896	-1.63841		H	0.19815	-1.99130	0.32019
	H	4.67047	-0.40010	-1.98852		H	2.23478	-3.44879	0.50777
	O	0.49350	0.70318	-0.70413		O	0.12239	0.29098	-1.03949
	N	4.53537	-3.02075	-1.51343		N	4.59041	-3.01917	-0.66521
	O	5.62881	-2.62163	-1.93176		O	4.52180	-4.03813	0.02159
	O	4.31797	-4.21205	-1.26208		O	5.61017	-2.67534	-1.26268
	C	-1.28327	0.35148	-1.19502		C	-1.13404	-0.08169	-1.46008
	C	-1.64631	1.80755	-1.29484		C	-2.03540	1.10706	-1.45089
	C	-1.64135	2.46634	-2.52876		C	-3.37645	0.96904	-1.82632
	C	-1.99362	2.52744	-0.14690		C	-1.56398	2.37073	-1.07364
	C	-1.98415	3.81187	-2.61477		C	-4.22753	2.06976	-1.82431
	H	-1.37612	1.90894	-3.42090		H	-3.74075	-0.00883	-2.11766
	C	-2.34887	3.87197	-0.23436		C	-2.41517	3.47337	-1.08308
	H	-1.98958	2.03669	0.82025		H	-0.52782	2.49901	-0.78417
	C	-2.34460	4.52025	-1.46736		C	-3.75080	3.32806	-1.45505
	H	-1.97565	4.30971	-3.58120		H	-5.26780	1.94626	-2.11522
	H	-2.62500	4.41524	0.66592		H	-2.03126	4.45018	-0.79955
	H	-2.62038	5.56965	-1.53579		H	-4.41476	4.18901	-1.46047
	C	-3.98673	-0.43687	-0.36721		S	-1.36156	-1.39724	-2.47575
	C	-2.82688	-0.70196	0.36113		C	-4.69481	-2.12891	1.61927
	C	-2.88743	-1.50045	1.50517		O	-5.18555	-2.62969	2.63628
	C	-4.09915	-2.03717	1.92406		C	-5.52825	-1.99621	0.36328
	C	-5.25106	-1.77219	1.18971		H	-5.68533	-0.94158	0.12372
	C	-5.20126	-0.97756	0.05128		H	-5.02034	-2.43961	-0.49482
	H	-3.95673	0.18003	-1.25684		H	-6.49083	-2.48273	0.52697

	H	-1.97550	-1.69219	2.06324		C	-3.30553	-1.63918	1.61363
	H	-4.14320	-2.65832	2.81393		N	-2.89156	-1.14679	0.48212
	H	-6.10599	-0.77332	-0.51399		O	-1.66652	-0.68306	0.45413
	Cl	-6.78435	-2.44906	1.70919		O	-0.40088	1.04345	2.31780
	O	-1.58748	-0.18391	0.07719		H	0.12823	1.66564	1.78206
	S	-1.36096	-0.68656	-2.52550		H	-0.83752	0.43357	1.68448
	O	1.74899	3.24343	-0.12892		O	1.88827	4.03506	-1.20056
	H	1.17827	2.50587	-0.42237		H	1.79196	3.58455	-0.33266
	H	2.18402	2.89219	0.67586		H	1.81995	3.32955	-1.86695
	O	0.29413	0.67355	2.36104		C	-2.45943	-1.72711	2.84942
	H	1.16074	1.12892	2.34332		H	-2.20496	-0.73237	3.22879
	H	0.05418	0.55225	1.42512		H	-2.98803	-2.27754	3.62785
	S	4.14952	1.30178	2.14621		H	-1.51233	-2.22914	2.62805
	O	2.78260	2.01222	2.18236		S	2.73341	2.58133	2.28041
	C	4.88184	1.63072	3.76123		O	1.59282	2.80436	1.26524
	H	5.80778	1.06039	3.86223		C	3.06430	0.80853	2.23187
	H	5.10050	2.69841	3.80537		H	3.90274	0.58101	2.89425
	H	4.16712	1.35831	4.54013		H	2.15609	0.31637	2.58312
	C	3.78655	-0.44947	2.37901		H	3.28319	0.50957	1.20509
	H	3.24575	-0.78973	1.49566		C	4.22693	3.15703	1.44887
	H	4.72646	-0.99815	2.47229		H	4.14466	4.23920	1.34096
	H	3.16898	-0.57547	3.27041		H	5.09426	2.91228	2.06602
						H	4.29898	2.68578	0.46710
IN1$_{dae}$ $\cdot\cdot 2H_2O1DMSO$	C	3.42221	-0.97561	-1.33315	**TS2$_{dae}$**$\cdot\cdot 2H_2O1DMSO$	C	-1.72303	-0.49491	-1.05526
	C	2.25164	-0.24880	-1.45537		C	-2.34626	0.78443	-1.52729
	C	1.02583	-0.78855	-1.03465		C	-2.64615	0.98190	-2.87872
	C	0.98328	-2.07808	-0.48471		C	-2.64136	1.80464	-0.61480
	C	2.15458	-2.80763	-0.35995		C	-3.23437	2.16777	-3.30920
	C	3.36334	-2.25600	-0.78295		H	-2.42302	0.19126	-3.58733
	H	4.37040	-0.56362	-1.66017		C	-3.23890	2.98682	-1.04374
	H	2.26119	0.74887	-1.88482		H	-2.40004	1.67809	0.43486
	H	0.04231	-2.49905	-0.16347		C	-3.53813	3.17413	-2.39226
	H	2.13639	-3.80403	0.06733		H	-3.46235	2.30469	-4.36330
	O	-0.03023	0.04694	-1.16387		H	-3.46653	3.76738	-0.32209
	N	4.58282	-3.02743	-0.64911		H	-4.00450	4.09742	-2.72700
	O	4.51376	-4.16219	-0.17156		S	-1.64179	-1.88178	-1.99735
	O	5.64452	-2.51949	-1.01752		C	-3.33695	-1.27858	1.90234
	C	-1.40400	-0.39163	-1.20535		C	-2.25472	-1.21584	2.93356
	C	-2.21260	0.88811	-1.42514		H	-1.51745	-2.00307	2.74608
	C	-3.55747	0.80789	-1.79879		H	-1.72141	-0.26299	2.87982

	C	-1.65320	2.15117	-1.20926		H	-2.67747	-1.35748	3.92734
	C	-4.32332	1.95939	-1.95667		N	-3.18556	-1.03516	0.65169
	H	-3.99049	-0.16949	-1.97659		O	-1.88504	-0.68239	0.35784
	C	-2.41616	3.30706	-1.38045		C	-4.73556	-1.66212	2.29264
	H	-0.61280	2.24363	-0.92198		O	-4.98035	-1.92122	3.46341
	C	-3.75512	3.21761	-1.75177		C	-5.80169	-1.71820	1.22964
	H	-5.36768	1.87505	-2.24764		H	-6.74429	-2.01579	1.68908
	H	-1.95602	4.27942	-1.22234		H	-5.91143	-0.74405	0.74752
	H	-4.35043	4.11781	-1.88413		H	-5.52476	-2.42879	0.44755
	S	-1.72267	-1.72204	-2.33559		C	2.25632	-2.50909	-0.08999
	C	-4.43671	-1.85275	2.09650		C	1.11486	-1.73042	-0.07387
	O	-4.68682	-2.30076	3.20896		C	1.05357	-0.51785	-0.80304
	C	-5.52410	-1.60644	1.08247		C	2.18659	-0.13339	-1.56199
	H	-5.54486	-0.55295	0.79415		C	3.33159	-0.90612	-1.57521
	H	-5.33236	-2.17690	0.17082		C	3.36311	-2.09519	-0.83828
	H	-6.48266	-1.89696	1.51293		H	2.30607	-3.43146	0.47832
	C	-3.01810	-1.53346	1.73081		H	0.25462	-2.03095	0.51141
	N	-2.87058	-1.09171	0.53451		H	2.14265	0.79552	-2.12188
	O	-1.57644	-0.77590	0.24135		H	4.19991	-0.60396	-2.15046
	O	-0.32625	1.18123	2.12557		O	-0.00885	0.26628	-0.77420
	H	0.26981	1.84024	1.71208		N	4.55407	-2.90489	-0.85037
	H	-0.63620	0.60508	1.40542		O	5.52928	-2.51958	-1.50549
	O	1.64457	4.10676	-1.32732		O	4.56420	-3.95959	-0.20535
	H	1.64293	3.70171	-0.43298		O	0.85087	2.98479	-1.32064
	H	1.57386	3.36028	-1.94737		H	0.38928	2.12632	-1.24461
	C	-1.92240	-1.74104	2.73046		H	1.36111	3.05007	-0.48666
	H	-1.50866	-0.78236	3.05661		O	-0.05426	1.35960	1.99260
	H	-2.30781	-2.27652	3.59733		H	0.71118	1.93989	1.79930
	H	-1.10335	-2.30819	2.28090		H	-0.20951	0.87811	1.15832
	S	2.86476	2.88752	2.14300		S	3.62384	2.49463	1.28625
	O	1.63123	2.98548	1.21926		O	2.15167	2.93757	1.18175
	C	3.21120	1.12150	2.27054		C	4.28864	3.42881	2.67815
	H	4.12227	0.97557	2.85525		H	5.30268	3.08527	2.89381
	H	2.35927	0.66877	2.77983		H	4.31066	4.47823	2.38167
	H	3.31453	0.70095	1.26854		H	3.63698	3.29355	3.54347
	C	4.26551	3.36197	1.11116		C	3.58441	0.86654	2.06227
	H	4.15435	4.42135	0.87722		H	3.11635	0.18102	1.35533
	H	5.18928	3.20195	1.67154		H	4.60825	0.54537	2.26663
	H	4.25610	2.77089	0.19375		H	2.99861	0.91733	2.98207
2d ··2H_2O2DMSO	C	-0.29278	0.62640	-1.35559	**2e** ··2H_2O2DMSO	C	3.65832	-5.71092	-3.82858

	C	-0.00051	-0.12428	-0.18378	O	3.89040	-5.27890	-4.96518
	C	0.12999	0.61926	1.02170	C	4.10809	-7.10846	-3.45442
	C	-0.02169	2.00094	1.05246	H	4.42898	-7.62748	-4.35895
	C	-0.30927	2.69449	-0.12077	H	4.94832	-7.05378	-2.75645
	C	-0.44286	2.00862	-1.32538	H	3.31643	-7.66634	-2.95364
	H	-0.40319	0.09247	-2.29601	C	2.97259	-4.88452	-2.82730
	H	0.35368	0.07986	1.93865	C	2.54740	-3.48272	-3.15409
	H	0.08093	2.53953	1.99142	H	2.70859	-3.27973	-4.21316
	H	-0.66983	2.55225	-2.23924	H	1.49074	-3.33592	-2.91080
	Cl	-0.50631	4.44803	-0.08040	H	3.10932	-2.75254	-2.56256
	O	0.13929	-1.42603	-0.21582	N	2.76643	-5.45564	-1.66994
	H	-0.93681	-2.24182	-1.32928	O	2.16185	-4.72990	-0.74794
	O	-1.61358	-2.69166	-1.89684	H	2.97127	-3.17419	-0.27463
	H	-2.45316	-2.23550	-1.68159	O	3.50100	-2.44228	0.11831
	O	1.45844	-2.62256	1.85412	H	4.20702	-2.90885	0.61393
	H	0.92099	-2.19185	1.13975	O	1.37682	-6.50398	1.20424
	H	2.36601	-2.29562	1.69311	H	1.70974	-5.86699	0.52062
	S	4.27046	-1.07716	-0.24310	H	0.48498	-6.75683	0.89015
	O	4.00558	-1.50054	1.20854	S	-1.87531	-5.66162	-0.24228
	C	3.20753	-2.11343	-1.26957	O	-1.22299	-6.99945	0.13552
	H	2.16862	-1.84919	-1.04656	C	-3.47071	-6.10368	-0.96223
	H	3.43233	-1.91578	-2.32061	H	-4.08623	-6.51614	-0.16155
	H	3.39206	-3.16238	-1.02615	H	-3.94745	-5.20978	-1.37025
	C	5.85188	-1.83716	-0.67435	H	-3.31433	-6.85275	-1.74109
	H	6.05796	-1.67828	-1.73507	C	-1.04830	-5.12693	-1.75456
	H	6.62155	-1.35080	-0.07333	H	-1.54226	-4.23072	-2.13790
	H	5.80984	-2.90299	-0.44081	H	-0.01089	-4.90209	-1.49015
	S	-3.91164	-0.91154	0.35985	H	-1.09030	-5.93642	-2.48687
	O	-3.96825	-1.29194	-1.12568	S	4.47663	-5.19067	2.13929
	C	-5.61268	-1.05787	0.94835	O	5.33969	-4.08150	1.51318
	H	-5.87534	-2.11634	0.92150	C	5.45316	-5.81244	3.52611
	H	-5.67880	-0.68811	1.97390	H	5.49734	-5.02149	4.27622
	H	-6.26996	-0.49057	0.28618	H	4.96518	-6.69354	3.94850
	C	-3.78754	0.88777	0.40138	H	6.45881	-6.05526	3.17659
	H	-3.87193	1.23215	1.43445	C	4.64908	-6.61948	1.05496
	H	-2.80655	1.15268	0.00533	H	4.12087	-7.46459	1.49963
	H	-4.57960	1.31406	-0.21830	H	4.17355	-6.36417	0.10635
					H	5.71137	-6.83547	0.91824
TS1$_{dad}$ $\cdot\cdot 2H_2O2DMSO$	C	4.17561	-1.05854	-1.12972	**TS1$_{dae}$**$\cdot\cdot 2H_2O2DMSO$	C	-3.94821	-1.48837	-1.57564
	C	3.04103	-0.46631	-0.59953		C	-2.65877	-1.03702	-1.82394

	C	2.52432	-0.93860	0.60931	C	-2.10281	-0.04975	-1.01230
	C	3.13128	-1.99657	1.28594	C	-2.81644	0.49311	0.05809
	C	4.26630	-2.59578	0.75812	C	-4.10388	0.04597	0.31110
	C	4.77459	-2.11637	-0.44534	C	-4.65390	-0.93833	-0.50962
	H	4.59476	-0.71378	-2.06841	H	-4.40162	-2.25341	-2.19591
	H	2.53701	0.35450	-1.09413	H	-2.07540	-1.44272	-2.64506
	H	2.71569	-2.33318	2.23114	H	-2.34636	1.25373	0.67008
	H	4.75465	-3.41669	1.27086	H	-4.67938	0.44785	1.13760
	O	1.34727	-0.46614	1.13239	O	-0.79201	0.28519	-1.24744
	N	5.96579	-2.73891	-1.00612	N	-6.00785	-1.40857	-0.24119
	O	6.47624	-3.68073	-0.39885	O	-6.62310	-0.91084	0.70117
	O	6.41418	-2.29820	-2.06470	O	-6.47789	-2.28353	-0.96792
	C	1.18051	0.87563	1.45056	C	-0.42241	1.57456	-1.56882
	C	-0.17726	1.05733	2.06246	C	1.04716	1.61874	-1.83054
	C	-0.48264	2.22164	2.77217	C	1.63199	2.76944	-2.36723
	C	-1.16747	0.07555	1.92330	C	1.86747	0.52647	-1.51970
	C	-1.74155	2.39882	3.34255	C	3.00422	2.82484	-2.59656
	H	0.28131	2.98321	2.88329	H	0.99944	3.61744	-2.60355
	C	-2.42288	0.25098	2.49706	C	3.24023	0.58209	-1.74323
	H	-0.96635	-0.82543	1.35577	H	1.43307	-0.36938	-1.09192
	C	-2.71699	1.41265	3.21199	C	3.81351	1.73231	-2.28629
	H	-1.95879	3.31104	3.89275	H	3.44365	3.72648	-3.01623
	H	-3.17859	-0.52186	2.38045	H	3.85615	-0.27016	-1.46771
	H	-3.69851	1.54810	3.65967	H	4.88576	1.77932	-2.46146
	S	2.51973	1.79518	1.92723	S	-1.52505	2.63296	-2.26934
	C	1.64273	3.48682	-0.90330	C	0.68544	5.17975	1.90655
	C	0.52225	2.68719	-0.59878	O	0.76303	5.70725	3.02021
	C	-0.74526	3.30601	-0.58508	C	1.08162	5.95837	0.67183
	C	-0.88962	4.65868	-0.87493	H	1.93323	5.48313	0.17920
	C	0.23871	5.41937	-1.17033	H	0.26915	5.97453	-0.05714
	C	1.50431	4.84302	-1.18789	H	1.34451	6.97515	0.96642
	H	2.62353	3.02380	-0.92399	C	0.22181	3.78625	1.76558
	H	-1.62063	2.70239	-0.36300	N	0.15801	3.33440	0.54745
	H	-1.87386	5.11935	-0.87151	O	-0.23099	2.08750	0.40523
	H	2.37611	5.44609	-1.42723	O	0.86653	-0.10391	1.84176
	Cl	0.05845	7.13278	-1.53874	H	0.64691	-0.92762	1.35417
	O	0.65405	1.38518	-0.34819	H	0.48303	0.64710	1.33469
	S	-0.22559	-3.55376	-0.42491	C	-0.14778	2.98594	2.97970
	O	-1.46736	-2.64903	-0.43706	H	0.55227	2.16093	3.14354
	C	-0.05284	-4.08809	1.28923	H	-0.15100	3.62524	3.86258

	H	0.75139	-4.82342	1.36402		H	-1.13680	2.53550	2.85122
	H	0.19927	-3.20414	1.87592		S	-0.42102	-3.62070	1.57234
	H	-1.00087	-4.50870	1.63126		O	0.39355	-2.62460	0.73211
	C	-0.76948	-5.12496	-1.12657		C	-1.49407	-2.61136	2.61746
	H	-1.00464	-4.94517	-2.17648		H	-2.16572	-3.26368	3.18013
	H	0.03959	-5.85492	-1.05065		H	-0.85107	-2.05671	3.30186
	H	-1.65740	-5.47202	-0.59454		H	-2.05606	-1.91547	1.99144
	O	-1.20756	-0.15486	-1.66774		C	-1.68816	-4.25995	0.45713
	H	-1.28667	-1.02529	-1.21741		H	-1.18088	-4.86141	-0.29855
	H	-0.56203	0.37544	-1.13683		H	-2.38484	-4.88610	1.01909
	O	-3.69424	1.12653	-1.66211		H	-2.20548	-3.42230	-0.01393
	H	-2.80807	0.69824	-1.67570		O	3.64529	-0.28124	2.27325
	H	-4.28184	0.48705	-1.20641		H	2.68362	-0.16280	2.11216
	S	-5.46336	-2.10514	-1.13768		H	3.96758	-0.83623	1.53198
	O	-5.32613	-0.77380	-0.38549		S	4.29579	-3.42004	0.26622
	C	-7.18770	-2.59506	-0.92008		O	4.56251	-1.91181	0.16117
	H	-7.80091	-1.87524	-1.46399		C	5.68050	-4.20077	-0.59008
	H	-7.33872	-3.59450	-1.33365		H	6.57795	-4.00573	-0.00137
	H	-7.43398	-2.57171	0.14343		H	5.51011	-5.27747	-0.65639
	C	-4.70730	-3.34621	-0.07013		H	5.77935	-3.75956	-1.58399
	H	-4.90284	-4.34001	-0.48074		C	3.01081	-3.77123	-0.94892
	H	-3.63175	-3.15109	-0.06198		H	2.89023	-4.85353	-1.04263
	H	-5.12903	-3.25204	0.93321		H	2.08678	-3.32729	-0.57038
						H	3.29969	-3.32960	-1.90533
2d ··H_2O2DMSO	H	0.22543	0.59920	-1.81601	**2e** ··H_2O2DMSO	C	4.92316	0.03864	-0.10258
	O	0.23408	0.75354	-2.79891		O	5.80289	0.61581	-0.76683
	H	0.31692	-0.13150	-3.20993		C	5.26560	-0.40727	1.30545
	C	-0.81407	2.41399	0.20350		H	5.66457	0.45029	1.85435
	C	-0.20268	1.21398	0.67780		H	4.41474	-0.82935	1.83535
	C	-0.06772	1.10982	2.09488		H	6.06520	-1.15214	1.24685
	C	-0.50340	2.10942	2.95669		C	3.59944	-0.21708	-0.65193
	C	-1.09441	3.26130	2.44223		N	2.73165	-0.82046	0.13846
	C	-1.24986	3.41294	1.06598		O	1.54632	-1.05289	-0.34600
	H	-0.93805	2.53775	-0.86992		C	3.26023	0.20351	-2.05126
	H	0.39133	0.21076	2.50016		H	2.39793	0.87872	-2.05780
	H	-0.38397	1.99300	4.03136		H	4.11359	0.70420	-2.50934
	H	-1.71220	4.31299	0.66735		H	2.97640	-0.65749	-2.66554
	Cl	-1.64904	4.53324	3.53830		S	-1.54335	2.18568	-1.83669
	O	0.21073	0.27618	-0.12118		O	-2.05300	0.78334	-2.20095
	S	3.99684	-0.67731	-1.18796		C	-2.07158	3.25033	-3.19704

	O	3.63759	-2.16526	-1.20393		H	-1.84185	4.29107	-2.95841
	C	3.39440	-0.03094	0.38483		H	-1.51448	2.94485	-4.08390
	H	3.77300	0.98511	0.52209		H	-3.14269	3.11557	-3.36118
	H	2.29956	-0.01505	0.33031		C	-2.67558	2.79861	-0.57527
	H	3.74465	-0.68556	1.18671		H	-2.50692	2.19853	0.32389
	C	5.76661	-0.61699	-0.81775		H	-2.45291	3.84976	-0.37535
	H	6.29200	-1.05904	-1.66577		H	-3.69998	2.68248	-0.93698
	H	6.08310	0.42042	-0.68937		O	0.03246	-1.08915	-2.68946
	H	5.96192	-1.19723	0.08672		H	-0.69281	-0.46084	-2.49247
	S	1.75668	-2.13580	-4.75511		H	0.66049	-1.01600	-1.93337
	O	0.46187	-1.80305	-4.00231		S	-2.16076	-0.65797	2.02060
	C	1.22190	-2.96780	-6.26681		O	-1.87497	0.84489	1.93317
	H	0.69156	-2.23169	-6.87264		C	-1.64680	-1.36695	0.44396
	H	2.09428	-3.33423	-6.81223		H	-0.55482	-1.31554	0.39132
	H	0.55321	-3.79009	-6.00396		H	-1.97139	-2.41026	0.40426
	C	2.46075	-3.56410	-3.90996		H	-2.08381	-0.78534	-0.37118
	H	3.29684	-3.95190	-4.49722		C	-3.94763	-0.82666	1.79548
	H	2.81811	-3.21301	-2.93723		H	-4.43016	-0.34818	2.64912
	H	1.68241	-4.32232	-3.79675		H	-4.24182	-0.32827	0.86948
						H	-4.21598	-1.88507	1.76703
TS1 $_{\mathbf{dad}}$ ··$H_2O2DMSO$	C	4.21590	0.24957	-1.00995	**TS1** $_{\mathbf{dae}}$ ··$H_2O2DMSO$	C	1.53687	3.80534	-1.47670
	C	2.91780	0.43231	-0.56213		C	0.88601	2.58478	-1.58818
	C	2.50180	-0.20812	0.60738		C	1.41601	1.45736	-0.96266
	C	3.36999	-1.02955	1.32575		C	2.59232	1.53109	-0.21369
	C	4.67059	-1.21920	0.88001		C	3.24689	2.74695	-0.10079
	C	5.07662	-0.57440	-0.28439		C	2.71281	3.86868	-0.73502
	H	4.56387	0.73204	-1.91649		H	1.14381	4.69430	-1.95669
	H	2.20939	1.06051	-1.08765		H	-0.03385	2.49375	-2.15783
	H	3.02290	-1.50431	2.23861		H	2.96296	0.63697	0.27212
	H	5.36226	-1.85074	1.42589		H	4.15940	2.83456	0.47813
	O	1.20032	-0.14932	1.04148		O	0.66820	0.30958	-1.03478
	N	6.43993	-0.76737	-0.75940		N	3.40156	5.14628	-0.61196
	O	7.18513	-1.50863	-0.11784		O	4.44229	5.19001	0.04435
	O	6.79198	-0.18145	-1.78341		O	2.91471	6.13061	-1.16896
	C	0.61015	1.05818	1.38864		C	1.18761	-0.88633	-1.47544
	C	-0.78610	0.79074	1.86537		C	0.11530	-1.92457	-1.46584
	C	-1.44636	1.71377	2.67909		C	0.38720	-3.21428	-1.93399
	C	-1.46038	-0.37978	1.48939		C	-1.16795	-1.63571	-0.98238
	C	-2.74650	1.47126	3.12002		C	-0.60200	-4.19310	-1.92269
	H	-0.92808	2.62084	2.97027		H	1.38037	-3.43843	-2.30539

	C	-2.75665	-0.62587	1.93137	C	-2.16093	-2.61325	-0.97746
	H	-0.98010	-1.09873	0.83549	H	-1.39581	-0.64245	-0.61221
	C	-3.40501	0.30084	2.75124	C	-1.87935	-3.89647	-1.44666
	H	-3.24364	2.20090	3.75462	H	-0.37511	-5.19169	-2.28820
	H	-3.26821	-1.53742	1.62739	H	-3.15307	-2.36763	-0.60388
	H	-4.41848	0.11040	3.09669	H	-2.65194	-4.66185	-1.44234
	S	1.56505	2.31104	2.00179	S	2.50904	-0.93053	-2.51100
	C	0.39115	3.82113	-0.90104	C	3.57137	-4.24010	1.62063
	C	-0.43029	2.69974	-0.65877	O	4.06937	-4.68642	2.65936
	C	-1.82748	2.90200	-0.64916	C	3.60154	-5.06623	0.35313
	C	-2.37884	4.15618	-0.88775	H	2.58768	-5.26231	-0.00258
	C	-1.53666	5.23852	-1.13018	H	4.11477	-4.52871	-0.44710
	C	-0.15479	5.07998	-1.13824	H	4.11349	-6.00713	0.55919
	H	1.46761	3.68343	-0.90990	C	2.93564	-2.91121	1.60004
	H	-2.47351	2.05078	-0.45404	N	2.44899	-2.53673	0.45189
	H	-3.45700	4.29279	-0.88529	O	1.85983	-1.36634	0.42083
	H	0.49151	5.93219	-1.33102	O	-0.05670	-0.31463	2.24902
	Cl	-2.23215	6.82847	-1.43730	H	-0.77276	0.03130	1.68077
	O	0.09268	1.49618	-0.45532	H	0.62043	-0.68204	1.64039
	S	0.79655	-3.56448	-0.44449	C	2.87653	-2.07610	2.84526
	O	-0.58563	-3.00939	-0.81354	H	1.84522	-1.94685	3.18862
	C	0.74588	-3.80795	1.34275	H	3.45639	-2.54563	3.64004
	H	1.65587	-4.31630	1.66960	H	3.26957	-1.07336	2.65052
	H	0.68892	-2.81873	1.79801	S	-2.05769	2.47179	1.88592
	H	-0.14167	-4.39117	1.59755	O	-2.21269	1.16833	1.08701
	C	0.75853	-5.30140	-0.93516	C	-3.67840	3.26412	1.81605
	H	0.70066	-5.32793	-2.02420	H	-3.68999	4.12983	2.48229
	H	1.67542	-5.79395	-0.60359	H	-3.83790	3.59222	0.78789
	H	-0.12036	-5.78004	-0.49863	H	-4.44226	2.53933	2.10525
	O	-0.71381	-0.54641	-2.19335	C	-2.09307	1.97337	3.62121
	H	-0.66895	-1.39366	-1.70391	H	-1.21003	1.35281	3.78241
	H	-0.47547	0.15188	-1.54174	H	-2.05613	2.86087	4.25694
	S	-4.55257	-3.02146	-0.82235	H	-2.99991	1.39466	3.80918
	O	-4.48379	-3.35823	0.66748	S	-5.72485	-0.18284	-0.05362
	C	-6.16408	-3.62212	-1.38387	O	-5.18626	-1.57778	0.26207
	H	-6.92589	-3.01289	-0.89503	C	-7.06333	-0.43661	-1.24330
	H	-6.24319	-3.50952	-2.46737	H	-7.86237	-0.96790	-0.72396
	H	-6.27770	-4.66837	-1.09195	H	-7.43296	0.52823	-1.59727
	C	-3.53212	-4.25293	-1.66100	H	-6.69230	-1.03985	-2.07469
	H	-3.66400	-4.15864	-2.74159	C	-4.53769	0.57429	-1.18456

	H	-2.49471	-4.03958	-1.39195		H	-4.94866	1.51361	-1.56409
	H	-3.82876	-5.24744	-1.31939		H	-3.63238	0.77076	-0.60573
						H	-4.33474	-0.11779	-2.00499
TS1$_{dbd}$ $\cdot\cdot 2H_2O1DMSO$	C	1.44682	3.10638	-0.39138	**IN1$_{dbd}$**$\cdot\cdot 2H_2O1DMSO$	O	-1.64256	-0.19621	0.56378
	C	0.67274	2.08517	0.13432		C	-2.92042	-0.04248	0.12512
	C	1.28572	1.05638	0.86489		C	-3.21412	-0.62821	-1.11589
	C	2.67601	1.06543	1.05802		C	-3.93596	0.63591	0.81203
	C	3.45130	2.08208	0.52875		C	-4.49025	-0.54698	-1.65909
	C	2.82716	3.09991	-0.19142		H	-2.42753	-1.15820	-1.64509
	H	0.98786	3.90537	-0.96305		C	-5.21701	0.71284	0.26719
	H	-0.39479	2.06274	-0.02526		H	-3.72373	1.12144	1.75553
	H	3.13601	0.26371	1.62796		C	-5.48923	0.12453	-0.96057
	H	4.52564	2.09522	0.67390		H	-4.70454	-1.00711	-2.61960
	O	0.62138	-0.00677	1.37752		H	-5.99932	1.24050	0.80564
	N	3.63058	4.17132	-0.74636		Cl	-7.10657	0.23019	-1.64055
	O	4.85151	4.14142	-0.57543		C	3.45001	1.48272	0.79395
	O	3.06376	5.07240	-1.36864		C	2.51655	0.70362	1.44969
	C	-0.79014	0.09163	1.75045		C	1.14355	0.79250	1.13158
	C	-3.35351	1.20856	0.00252		C	0.73193	1.69921	0.13182
	C	-2.72865	-0.04939	-0.10696		C	1.66646	2.48278	-0.52179
	C	-3.53856	-1.16087	-0.41361		C	3.01956	2.37399	-0.19238
	C	-4.90914	-1.02530	-0.61170		H	4.50386	1.41046	1.03922
	C	-5.49550	0.23096	-0.49211		H	2.82797	0.00543	2.22057
	C	-4.72608	1.34823	-0.18458		H	-0.31565	1.77475	-0.12166
	H	-2.75003	2.07764	0.24023		H	1.35580	3.17693	-1.29500
	H	-3.07024	-2.13715	-0.50465		O	0.31843	-0.02467	1.78794
	H	-5.51710	-1.89252	-0.85501		N	3.98789	3.19386	-0.88027
	H	-5.19327	2.32561	-0.09815		O	3.59071	3.98659	-1.73992
	Cl	-7.22995	0.40902	-0.73962		O	5.18139	3.07435	-0.58562
	O	-1.40836	-0.19657	0.05445		C	-1.22919	0.33088	1.93117
	H	1.99790	-2.96786	1.32472		O	-1.44876	1.54665	2.12905
	O	2.26759	-2.36361	2.05144		C	-1.65524	-0.71333	2.95576
	H	1.68689	-1.58832	1.95685		H	-1.23260	-0.44919	3.92747
	O	-0.29008	-2.26480	-1.44027		H	-2.74405	-0.70652	3.03973
	H	-0.65518	-1.54933	-0.86819		H	-1.32695	-1.71588	2.67591
	H	0.26009	-2.83305	-0.86838		O	1.68130	-2.42443	2.72257
	S	2.91139	-3.82084	-1.19285		H	1.13418	-1.63356	2.56379
	O	1.72911	-3.90737	-0.20233		H	1.99280	-2.67555	1.82708
	C	3.14392	-2.05789	-1.50766		O	-0.29638	-2.38755	-0.76198
	H	3.99764	-1.92473	-2.17602		H	0.61609	-2.59461	-0.47346

	H	2.22749	-1.70403	-1.98277		H	-0.60200	-1.64703	-0.20490
	H	3.30187	-1.53958	-0.56023		S	3.56872	-2.36767	-0.65326
	C	4.38596	-4.10867	-0.19284		O	2.33762	-2.96738	0.05421
	H	4.36150	-5.15089	0.12830		C	4.15987	-3.67994	-1.74018
	H	5.27256	-3.93391	-0.80655		H	4.96719	-3.29446	-2.36665
	H	4.36686	-3.44194	0.67150		H	4.53824	-4.48079	-1.10366
	O	-1.20363	1.16551	2.18749		H	3.32953	-4.04118	-2.34987
	C	-1.16134	-1.24019	2.36233		C	2.90577	-1.26583	-1.91887
	H	-0.75789	-1.28422	3.37866		H	2.42707	-0.43164	-1.40577
	H	-2.24834	-1.30740	2.41737		H	3.72935	-0.89770	-2.53474
	H	-0.77572	-2.07918	1.78381		H	2.17357	-1.80579	-2.52206
TS2$_{dbd}$ $\cdot\cdot 2H_2O1DMSO$	O	-1.68075	-0.22047	0.62845	**TS1$_{dbe}$**$\cdot\cdot 2H_2O1DMSO$	C	1.39801	2.92539	-0.38088
	C	-2.97140	-0.09327	0.20585		C	0.51632	2.00316	0.15923
	C	-3.27336	-0.72329	-1.00954		C	1.01392	0.94425	0.92864
	C	-3.98109	0.59392	0.88904		C	2.38998	0.81085	1.14776
	C	-4.55871	-0.67493	-1.53413		C	3.27410	1.72821	0.60307
	H	-2.48668	-1.26005	-1.53177		C	2.76632	2.78139	-0.15404
	C	-5.27182	0.63729	0.36296		H	1.03321	3.74963	-0.98360
	H	-3.76419	1.11005	1.81546		H	-0.54743	2.07755	-0.02000
	C	-5.55488	0.00666	-0.84093		H	2.75609	-0.01708	1.74755
	H	-4.78258	-1.16838	-2.47567		H	4.34203	1.63631	0.76562
	H	-6.05241	1.17148	0.89728		O	0.22089	-0.03636	1.44792
	Cl	-7.18305	0.07020	-1.49742		N	3.68604	3.75081	-0.72497
	C	3.47462	1.52643	0.70352		O	4.89344	3.59950	-0.53148
	C	2.57216	0.73678	1.38618		O	3.22266	4.68564	-1.38010
	C	1.18923	0.76693	1.07665		C	-1.09041	0.27596	1.94450
	C	0.74885	1.63642	0.04904		O	-1.33188	1.40521	2.34334
	C	1.65250	2.43087	-0.63061		C	-1.69055	-0.97729	2.52252
	C	3.01222	2.37701	-0.30685		H	-1.31002	-1.11168	3.54015
	H	4.53166	1.49578	0.94416		H	-2.77184	-0.84910	2.56258
	H	2.91115	0.07100	2.17413		H	-1.44725	-1.85666	1.92736
	H	-0.30185	1.66912	-0.20362		C	-5.28005	0.91141	-0.70769
	H	1.31605	3.09162	-1.42219		O	-6.00519	1.03246	-1.69950
	O	0.38756	-0.04070	1.74853		C	-5.84850	1.13364	0.67711
	N	3.94692	3.20489	-1.02094		H	-5.84471	0.19754	1.24126
	O	3.52180	3.96127	-1.90208		H	-5.24429	1.84452	1.24290
	O	5.14722	3.13416	-0.73124		H	-6.87242	1.49743	0.58200
	C	-1.26909	0.34654	1.94071		C	-3.86026	0.53793	-0.85315
	O	-1.44694	1.56251	2.10270		N	-3.19280	0.44543	0.25853
	C	-1.59042	-0.66416	3.02711		O	-1.92366	0.09471	0.15248

	H	-1.12454	-0.34556	3.96113	O	-1.26555	-2.25669	-1.26783
	H	-2.67377	-0.69051	3.17110	H	-0.71371	-2.81988	-0.69153
	H	-1.24274	-1.66408	2.76544	H	-1.46816	-1.43551	-0.76642
	O	1.72170	-2.40497	2.69389	O	1.56184	-2.58898	2.14862
	H	1.20312	-1.59663	2.51601	H	1.10106	-1.73628	2.07020
	H	2.03524	-2.67714	1.80584	H	1.18911	-3.13863	1.42374
	O	-0.22142	-2.30228	-0.78345	C	-3.26916	0.30996	-2.21306
	H	0.68698	-2.53841	-0.50410	H	-3.02822	-0.74586	-2.37122
	H	-0.51828	-1.59345	-0.18378	H	-3.96930	0.63053	-2.98476
	S	3.65708	-2.38867	-0.63108	H	-2.33102	0.86421	-2.31193
	O	2.39495	-2.97865	0.02802	S	1.81057	-4.02982	-1.17926
	C	4.28916	-3.71130	-1.68202	O	0.71032	-3.98835	-0.09583
	H	5.12237	-3.33292	-2.27819	C	2.16906	-2.30168	-1.56089
	H	4.63922	-4.50762	-1.02395	H	2.97960	-2.25759	-2.29187
	H	3.48352	-4.07595	-2.32205	H	1.25393	-1.88071	-1.98040
	C	3.05206	-1.29474	-1.93159	H	2.44098	-1.77760	-0.64277
	H	2.54929	-0.45864	-1.44534	C	3.33131	-4.42743	-0.29208
	H	3.90234	-0.92888	-2.51149	H	3.24316	-5.45744	0.05618
	H	2.34943	-1.83951	-2.56499	H	4.17676	-4.34283	-0.97856
					H	3.43970	-3.74662	0.55453
IN1$_{\mathbf{dbe}}$ ··2H$_2$O1DMSO	C	1.29617	-0.83246	1.79328	**TS2**$_{\mathbf{dbe}}$ ··2H$_2$O1DMSO	C	1.35825	-0.97550	1.76648
	C	3.59216	-0.83253	-0.94157		C	3.65687	-1.06474	-0.86935
	C	2.81535	-0.43819	-2.16047		C	2.90968	-0.62173	-2.08858
	H	1.86142	-0.97123	-2.18576		H	1.97968	-1.18857	-2.18506
	H	2.58500	0.63129	-2.14499		H	2.63467	0.43383	-2.00723
	H	3.39016	-0.66306	-3.05830		H	3.52344	-0.76844	-2.97637
	N	3.11848	-0.89548	0.25248		N	3.16827	-1.13277	0.31587
	O	1.81692	-0.52804	0.34319		O	1.86284	-0.72665	0.37867
	C	5.03528	-1.20235	-1.05871		C	5.09272	-1.48176	-0.97390
	O	5.58116	-1.18399	-2.15715		O	5.64846	-1.46227	-2.06541
	C	5.79647	-1.58563	0.18602		C	5.82177	-1.91342	0.27295
	H	6.81355	-1.86210	-0.09283		H	6.84043	-2.19606	0.00689
	H	5.81859	-0.74975	0.88934		H	5.83876	-1.10204	1.00435
	H	5.30686	-2.41606	0.69874		H	5.30994	-2.75442	0.74581
	C	-1.89343	-2.69027	-0.51583		C	-2.11066	-2.51807	-0.55165
	C	-0.83587	-2.03711	0.09222		C	-1.01785	-1.89217	0.01385
	C	-1.08175	-0.95004	0.95400		C	-1.18947	-0.78521	0.88433
	C	-2.41204	-0.54482	1.18744		C	-2.51270	-0.35092	1.16072
	C	-3.46755	-1.19427	0.57656		C	-3.60318	-0.97315	0.59091
	C	-3.20252	-2.26971	-0.27404		C	-3.40284	-2.06180	-0.26679

	H	-1.71123	-3.52498	-1.18371	H	-1.97600	-3.35935	-1.22281
	H	0.18023	-2.35454	-0.09111	H	-0.01746	-2.23679	-0.20978
	H	-2.59298	0.29103	1.85660	H	-2.64917	0.49210	1.83160
	H	-4.49023	-0.88117	0.75533	H	-4.61042	-0.63235	0.80429
	O	-0.12314	-0.23479	1.56026	O	-0.18399	-0.13199	1.43143
	N	-4.29979	-2.95636	-0.91374	N	-4.53377	-2.71448	-0.86113
	O	-5.45083	-2.56441	-0.69753	O	-5.66981	-2.29266	-0.60703
	O	-4.05062	-3.91195	-1.65519	O	-4.34204	-3.68074	-1.61112
	O	-1.12872	2.19111	2.88113	O	-0.93499	2.29778	2.76119
	H	-0.70951	1.36967	2.56667	H	-0.63206	1.44438	2.39008
	H	-1.03311	2.81473	2.13119	H	-0.78193	2.94469	2.04302
	O	1.28019	2.17663	-0.61878	O	1.24158	1.99037	-0.66825
	H	0.70307	2.68458	-0.00962	H	0.77807	2.61780	-0.07327
	H	1.35275	1.27552	-0.25017	H	1.21745	1.12186	-0.22704
	S	-1.64355	4.13978	-0.50280	S	-1.36977	4.35049	-0.54377
	O	-0.65290	3.78569	0.62692	O	-0.35342	3.95695	0.54979
	C	-0.61179	4.78246	-1.83686	C	-0.37304	4.66212	-2.01599
	H	-1.23271	4.94650	-2.72044	H	-1.03775	4.83390	-2.86562
	H	-0.19938	5.73304	-1.49607	H	0.21453	5.56061	-1.82247
	H	0.18781	4.06767	-2.04075	H	0.28093	3.80535	-2.18942
	C	-2.09391	2.56488	-1.26344	C	-2.13276	2.80138	-1.07222
	H	-2.66684	2.00098	-0.52630	H	-2.71914	2.42589	-0.23296
	H	-2.71461	2.75884	-2.14125	H	-2.79052	2.99994	-1.92151
	H	-1.18229	2.02689	-1.53019	H	-1.34740	2.09020	-1.33441
	O	1.32373	-2.04481	2.09059	O	1.18253	-2.15119	2.07422
	C	1.93788	0.20499	2.70167	C	1.93338	0.05144	2.71462
	H	1.49294	0.12826	3.69626	H	1.39613	0.00430	3.66266
	H	3.00347	-0.01805	2.77487	H	2.98198	-0.20238	2.88839
	H	1.80918	1.22163	2.32547	H	1.87272	1.06131	2.30918
TS1$_{dbd}$ $\cdot\cdot 2H_2O2DMSO$	C	4.66580	0.45548	-0.41866	**TS1$_{dbe}$**$\cdot\cdot 2H_2O2DMSO$	C	4.75718	0.45949	-0.56618
	C	3.37387	0.54956	0.07032		C	3.54420	0.58198	0.09120
	C	2.71610	-0.60315	0.53180		C	2.94972	-0.55181	0.66544
	C	3.37913	-1.84146	0.49224		C	3.58287	-1.79941	0.57103
	C	4.66778	-1.93929	0.00069		C	4.79237	-1.92587	-0.08986
	C	5.30609	-0.78384	-0.45076		C	5.37270	-0.78948	-0.65163
	H	5.18039	1.33764	-0.78318		H	5.22680	1.32495	-1.02029
	H	2.86018	1.49890	0.08644		H	3.04256	1.53724	0.15343
	H	2.86556	-2.72521	0.85682		H	3.11245	-2.66475	1.02813
	H	5.18049	-2.89405	-0.03025		H	5.28785	-2.88715	-0.16592
	O	1.44606	-0.62704	0.98437		O	1.74275	-0.54429	1.28229

	N	6.65627	-0.87386	-0.96410	N	6.64241	-0.90995	-1.34162
	O	7.20234	-1.97985	-0.99882	O	7.16548	-2.02368	-1.42263
	O	7.21279	0.15795	-1.34855	O	7.15151	0.10527	-1.82156
	C	0.83183	0.57143	1.56673	C	1.29445	0.62093	2.00395
	C	0.72196	3.63309	0.52111	O	2.12688	1.36672	2.51470
	C	-0.06154	2.56654	0.04046	C	-0.02347	0.28006	2.65326
	C	-1.35300	2.85783	-0.43882	H	0.17743	-0.27752	3.57388
	C	-1.84193	4.16104	-0.44320	H	-0.52733	1.21193	2.91127
	C	-1.04810	5.19237	0.04815	H	-0.66351	-0.31649	2.00394
	C	0.23065	4.93585	0.53086	C	-0.65237	4.78666	0.16955
	H	1.71854	3.42906	0.89432	O	-1.01463	5.59254	-0.69057
	H	-1.96981	2.05320	-0.82967	C	-0.70766	5.16003	1.63410
	H	-2.83749	4.37028	-0.82532	H	-1.44398	4.54098	2.15291
	H	0.84652	5.74923	0.90514	H	0.25201	4.98380	2.12261
	Cl	-1.66505	6.84177	0.04915	H	-0.98939	6.21032	1.71873
	O	0.40353	1.30727	0.00252	C	-0.17396	3.44195	-0.21697
	S	-0.28603	-3.74746	0.02324	N	0.19222	2.68222	0.76863
	O	-1.44161	-2.77463	-0.25696	O	0.60308	1.46384	0.44668
	C	-0.06724	-3.72863	1.81333	C	-0.12488	3.04650	-1.66303
	H	0.64197	-4.50854	2.10122	H	-0.97641	2.41424	-1.93634
	H	0.33340	-2.74807	2.07030	H	-0.14686	3.93521	-2.29477
	H	-1.03477	-3.88633	2.29466	H	0.78282	2.47075	-1.86146
	C	-1.00806	-5.39429	-0.13083	O	-0.94641	-0.31488	-1.06849
	H	-1.28240	-5.52974	-1.17786	H	-1.42670	-0.85878	-0.40341
	H	-0.26683	-6.14370	0.15554	H	-0.40462	0.33599	-0.56507
	H	-1.89436	-5.46160	0.50308	S	-1.84184	-3.46895	0.69181
	O	-0.84357	-0.48623	-1.70657	O	-2.32390	-2.00953	0.63756
	H	-1.02768	-1.30216	-1.18739	C	-1.09174	-3.79469	-0.91924
	H	-0.39374	0.13735	-1.08584	H	-0.61468	-4.77706	-0.90161
	O	-3.31061	0.53881	-2.51845	H	-1.89704	-3.79104	-1.65523
	H	-2.42491	0.18709	-2.27221	H	-0.37196	-3.00662	-1.14842
	H	-3.91961	0.20502	-1.82522	C	-0.32905	-3.44389	1.67666
	S	-5.36061	-1.94576	-0.62635	H	-0.61765	-3.21356	2.70329
	O	-4.98861	-0.46068	-0.50917	H	0.13976	-4.43035	1.64153
	C	-7.07792	-2.04506	-0.07796	H	0.34137	-2.67127	1.29539
	H	-7.68538	-1.51921	-0.81586	O	-2.94223	0.59935	-2.80611
	H	-7.38537	-3.09173	-0.02614	H	-2.19824	0.31272	-2.23145
	H	-7.16972	-1.56292	0.89744	H	-3.73445	0.56739	-2.22806
	C	-4.59000	-2.75097	0.79081	S	-5.78559	-0.91688	-0.86231
	H	-4.94335	-3.78322	0.85378	O	-5.15860	0.46567	-1.09194

	H	-3.51101	-2.73590	0.61709		C	-7.56429	-0.61614	-0.78373
	H	-4.85033	-2.19637	1.69522		H	-7.88368	-0.29424	-1.77591
	C	-0.54426	0.14636	2.03493		H	-8.08032	-1.53957	-0.51217
	H	-0.44037	-0.37362	2.99266		H	-7.76108	0.16996	-0.05189
	H	-1.15023	1.03961	2.19499		C	-5.51109	-1.29311	0.87938
	H	-1.03996	-0.50954	1.31919		H	-6.07665	-2.18911	1.14670
	O	1.55112	1.32014	2.23873		H	-4.44040	-1.47942	0.99721
						H	-5.83306	-0.43856	1.47891
TS1$_{dbd}$ $\cdot\cdot$H$_2$O2DMSO	C	4.40836	1.55811	-0.30816	**TS1$_{dbe}$**$\cdot\cdot$H$_2$O2DMSO	C	-4.80797	-0.68333	-0.12189
	C	3.13183	1.25008	0.13077		C	-3.58839	-0.13721	-0.48634
	C	2.83785	-0.05576	0.55652		C	-2.53859	-0.98452	-0.87298
	C	3.84239	-1.03785	0.53172		C	-2.72765	-2.37445	-0.88693
	C	5.11700	-0.73357	0.09053		C	-3.94356	-2.92248	-0.51851
	C	5.39296	0.56950	-0.32501		C	-4.97866	-2.06789	-0.14060
	H	4.64597	2.56102	-0.64514		H	-5.62758	-0.04299	0.18465
	H	2.35398	1.99865	0.13571		H	-3.43157	0.93151	-0.46190
	H	3.60327	-2.04245	0.86718		H	-1.90535	-3.01215	-1.19721
	H	5.89437	-1.48897	0.07066		H	-4.09693	-3.99566	-0.52779
	O	1.62057	-0.47094	0.96162		O	-1.29537	-0.55755	-1.19536
	N	6.72483	0.90002	-0.78503		N	-6.25810	-2.63105	0.24303
	O	7.58038	0.01106	-0.80442		O	-6.38765	-3.85753	0.23769
	O	6.95714	2.05821	-1.14112		O	-7.16936	-1.86338	0.56059
	C	0.64443	0.46501	1.50518		C	-1.08511	0.73863	-1.77905
	C	-0.45658	3.34289	0.29309		O	-1.96322	1.23702	-2.47799
	C	-0.83206	2.03821	-0.08299		C	0.38832	0.87901	-2.06612
	C	-2.17778	1.81596	-0.43847		H	0.60407	0.38543	-3.01929
	C	-3.10438	2.85451	-0.42929		H	0.61990	1.94023	-2.16111
	C	-2.70136	4.13175	-0.05136		H	1.00374	0.43279	-1.28501
	C	-1.38260	4.38261	0.31238		C	-1.24580	5.13487	0.52663
	H	0.57409	3.53224	0.57319		O	-1.40777	5.92901	1.45702
	H	-2.49943	0.81892	-0.72932		C	-1.00073	5.64903	-0.87465
	H	-4.13654	2.66718	-0.71334		H	0.02158	5.41692	-1.18477
	H	-1.07653	5.38416	0.60262		H	-1.66485	5.17001	-1.59545
	Cl	-3.87366	5.44745	-0.03842		H	-1.14520	6.73014	-0.88267
	O	0.05667	1.03841	-0.11928		C	-1.27000	3.67796	0.76682
	S	0.16620	-4.22735	-0.28214		N	-1.10223	2.93738	-0.28701
	O	-1.00191	-3.27200	-0.56192		O	-1.09773	1.63085	-0.08018
	C	0.63743	-3.92975	1.43434		C	-1.49318	3.13942	2.14921
	H	1.39735	-4.65619	1.73264		H	-0.58463	2.67503	2.54520
	H	1.04685	-2.91977	1.48145		H	-1.80014	3.94227	2.81977

	H	-0.24747	-4.00918	2.06940	H	-2.26147	2.36083	2.12788
	C	-0.59305	-5.84953	-0.05831	O	0.75913	0.57117	1.78710
	H	-0.99709	-6.15420	-1.02467	H	1.52998	0.28434	1.25217
	H	0.16496	-6.56563	0.26650	H	0.10111	0.93261	1.15389
	H	-1.39584	-5.76932	0.67732	S	2.72896	-2.19040	0.84097
	O	-0.30287	-0.96992	-2.04939	O	2.89930	-0.70117	0.49774
	H	-0.57661	-1.76825	-1.55234	C	2.46762	-2.25046	2.62849
	H	-0.18264	-0.27111	-1.36662	H	2.21618	-3.27227	2.92164
	S	-4.82141	-2.04244	-0.75422	H	3.40573	-1.95451	3.10045
	O	-4.21020	-0.86356	-1.51036	H	1.66997	-1.55273	2.89188
	C	-6.33584	-1.40440	0.00203	C	1.04953	-2.62018	0.33151
	H	-7.02830	-1.16727	-0.80714	H	1.01383	-2.54747	-0.75596
	H	-6.77535	-2.16504	0.65097	H	0.83357	-3.64525	0.64229
	H	-6.09827	-0.50062	0.56741	H	0.34848	-1.91075	0.77376
	C	-3.85804	-2.22767	0.76237	S	6.69985	-0.95148	-0.75010
	H	-4.34332	-2.96277	1.40963	O	6.89630	-1.90134	0.43161
	H	-2.86621	-2.58185	0.47155	C	8.32738	-0.22863	-1.06957
	H	-3.79185	-1.25714	1.25919	H	8.97551	-1.03121	-1.42492
	C	-0.55352	-0.36440	1.91029	H	8.24492	0.54425	-1.83687
	H	-0.32609	-0.86601	2.85672	H	8.72224	0.18701	-0.13997
	H	-1.40210	0.30234	2.06989	C	5.90670	0.52605	-0.08123
	H	-0.80805	-1.10744	1.15536	H	5.87270	1.29941	-0.85262
	O	1.05401	1.41431	2.17955	H	4.89188	0.23726	0.20524
					H	6.47520	0.86941	0.78632
TS1$_{dbd}$ （DMSO）	O	-1.01490	1.43645	0.96491	**TS1$_{dbe}$** （DMSO）	C	1.97766	0.88915	0.37631
	C	-2.00093	0.62882	0.63967		C	0.94881	-0.03916	0.35494
	C	-2.16752	-0.59760	1.33303		C	1.20623	-1.34019	-0.10196
	C	-2.94725	0.91501	-0.37670		C	2.49200	-1.69434	-0.53560
	C	-3.21546	-1.46671	1.05209		C	3.51882	-0.76727	-0.51741
	H	-1.45099	-0.84784	2.11164		C	3.25131	0.52144	-0.05634
	C	-3.99225	0.04246	-0.66482		H	1.79686	1.90094	0.72185
	H	-2.85087	1.83334	-0.94477		H	-0.04586	0.23344	0.67968
	C	-4.12639	-1.14364	0.05009		H	2.66591	-2.70728	-0.88644
	H	-3.32047	-2.39472	1.60843		H	4.51576	-1.03298	-0.85021
	H	-4.70629	0.28999	-1.44631		O	0.26582	-2.31023	-0.21452
	Cl	-5.45666	-2.24447	-0.31540		N	4.32085	1.50055	-0.02988
	C	4.17669	0.36066	0.28888		O	5.43862	1.16224	-0.42553
	C	3.29801	1.42580	0.36348		O	4.07284	2.63414	0.38673
	C	1.93225	1.24709	0.09092		C	-0.89638	-2.31485	0.60733
	C	1.44889	-0.02306	-0.26116		C	-3.15101	0.79406	-0.58628

	C	2.32856	-1.09034	-0.33895		C	-3.47592	0.62204	-2.04059
	C	3.68272	-0.89465	-0.06705		H	-4.13143	1.42397	-2.37984
	H	5.23213	0.49335	0.49802		H	-2.56185	0.62206	-2.64396
	H	3.65041	2.41628	0.63584		H	-3.96111	-0.34388	-2.21506
	H	0.39724	-0.16461	-0.46070		N	-2.39933	-0.05104	0.07674
	H	1.96975	-2.07825	-0.60547		O	-1.93289	-1.05705	-0.60420
	O	1.16437	2.34839	0.24045		C	-3.66756	1.94014	0.16271
	N	4.59441	-2.01683	-0.15290		O	-4.39502	2.78457	-0.38026
	O	4.14606	-3.11932	-0.47692		C	-3.29453	2.12492	1.61889
	O	5.78685	-1.82877	0.10136		H	-2.54945	2.92451	1.68489
	C	-0.11411	2.46649	-0.39852		H	-4.17908	2.45725	2.16718
	O	-0.29056	1.94516	-1.49678		H	-2.87859	1.22470	2.06619
	C	-0.67605	3.81166	-0.00979		C	-1.73039	-3.50759	0.22465
	H	-0.13847	4.58695	-0.56596		H	-1.26080	-4.40825	0.63358
	H	-1.73010	3.85101	-0.28238		H	-2.72344	-3.39716	0.65886
	H	-0.56673	3.99288	1.05841		H	-1.80984	-3.60590	-0.85719
						O	-0.86770	-1.81515	1.72205

S12 The optimized geometries for the transition states and minima of all the other reactions studied, obtained with CAM-B3LYP+IDSCRF/DZVP.

Species	Cartesian coordinates				Species	Cartesian coordinates			
1bd (MeOH)	C	-0.61968	-1.56735	-0.05984	**1be** (MeOH)	N	-3.20447	0.02563	-0.00001
	C	1.32666	0.37078	0.00717		C	-1.75729	-0.24762	0.00624
	C	-0.98041	-0.21626	-0.00785		C	-1.32113	-1.56301	0.04563
	C	0.71694	-1.94129	-0.07957		C	-0.88501	0.83020	-0.03389
	C	1.70293	-0.96884	-0.04033		C	0.47243	0.56352	-0.03243
	C	0.00030	0.76554	0.01595		H	-1.24910	1.85073	-0.08158
	N	-2.37870	0.21394	0.02340		H	-2.03559	-2.37900	0.07413
	H	0.96424	-2.99779	-0.12845		C	0.04739	-1.81379	0.05181
	H	2.75277	-1.24165	-0.04997		N	1.39445	1.69935	-0.15090
	H	-0.27523	1.81329	0.04795		H	0.42440	-2.83195	0.09585
	N	2.36520	1.40440	0.04651		O	-3.96255	-0.93509	0.04204
	O	-3.22669	-0.59607	0.37703		O	-3.56151	1.19643	-0.04559
	O	-2.61649	1.37467	-0.29622		C	0.93313	-0.75145	0.01998
	O	2.00807	2.57726	0.08835		O	2.49177	1.48121	-0.65082
	O	3.53580	1.03825	0.03474		O	0.99805	2.79059	0.23276
	F	-1.53639	-2.52681	-0.11887		N	2.36600	-1.07790	0.11699
						O	2.84182	-1.75404	-0.78240
						O	2.95465	-0.69223	1.11635

TS1$_{bdb}$ ··2MeOH				
	N	3.66297	-1.18541	-1.08294
	C	2.37171	-1.01275	-0.46375
	C	2.23335	-0.15528	0.64914
	C	1.29606	-1.72984	-0.94986
	C	0.04669	-1.56200	-0.36621
	H	1.41268	-2.42064	-1.77626
	H	3.10100	0.35154	1.06280
	C	1.00322	0.00251	1.22647
	C	-0.15260	-0.61802	0.68093
	N	-1.05463	-2.32030	-0.90130
	H	0.87655	0.61083	2.11639
	O	4.62031	-0.55073	-0.62883
	O	3.76324	-1.95428	-2.04070
	O	-0.80779	-3.27276	-1.64344
	O	-2.20184	-1.97349	-0.60737
	C	-4.91869	0.09697	-1.01472
	H	-5.88706	-0.35974	-0.78181
	H	-5.08991	1.10804	-1.38748
	H	-4.42044	-0.49210	-1.79271
	O	-4.10590	0.21545	0.15463
	H	-3.90233	-0.67562	0.49229
	C	-1.89362	3.39484	0.02561
	C	-1.14089	2.20253	0.61962
	C	-0.77107	1.25728	-1.59972
	C	-1.50423	2.42591	-2.26148
	C	-1.41578	3.68529	-1.39789
	H	-0.08021	2.45621	0.73475
	H	-1.53190	1.94702	1.60843
	H	-2.96722	3.17232	0.02036
	H	-1.74933	4.26785	0.67069
	H	0.30469	1.46850	-1.55634
	H	-0.90303	0.34137	-2.18307
	H	-1.07780	2.60177	-3.25452
	H	-2.55591	2.15194	-2.40996
	H	-0.37562	4.03400	-1.36891
	H	-2.00706	4.49237	-1.84158
	N	-1.22840	1.00625	-0.22833
	H	-2.19915	0.67227	-0.22444
	C	4.86653	2.61652	0.64839
	H	4.34766	3.42840	1.16078

TS1$_{beb}$ ··2MeOH				
	C	-5.13839	-0.16120	-0.33686
	H	-6.17646	-0.17109	0.01274
	H	-5.09336	0.38624	-1.27962
	H	-4.79676	-1.18780	-0.50419
	O	-4.28888	0.52902	0.58465
	H	-4.32691	0.09338	1.45615
	C	-1.77351	3.37388	-0.24576
	C	-1.04434	2.23738	0.47520
	C	-1.17603	0.82551	-1.50426
	C	-1.91051	1.92000	-2.28248
	C	-1.54336	3.30612	-1.75469
	H	0.03918	2.36228	0.35901
	H	-1.26953	2.24755	1.54243
	H	-2.84584	3.30292	-0.02966
	H	-1.42576	4.32929	0.16069
	H	-0.09691	0.90790	-1.68112
	H	-1.49754	-0.15864	-1.85127
	H	-1.66322	1.82477	-3.34475
	H	-2.99165	1.76220	-2.19008
	H	-0.48817	3.51243	-1.97415
	H	-2.12968	4.07579	-2.26614
	N	-1.40100	0.91301	-0.05481
	H	-2.38418	0.70672	0.16360
	C	4.79818	2.72571	0.62521
	H	5.79518	3.12873	0.41194
	H	4.33190	2.41268	-0.31657
	H	4.19206	3.51352	1.07543
	O	4.85525	1.65436	1.56561
	H	5.37087	0.92399	1.17916
	N	3.56292	-1.17911	-1.03125
	C	2.29439	-1.01003	-0.35305
	C	2.18282	-0.08314	0.69670
	C	1.22136	-1.79461	-0.73732
	C	0.00690	-1.62480	-0.09412
	H	1.31611	-2.52788	-1.52981
	H	3.05102	0.48026	1.03054
	C	0.97443	0.07745	1.33094
	N	-1.11469	-2.42728	-0.52306
	H	0.88591	0.74278	2.18427
	O	4.50887	-0.47039	-0.68175

	H	5.85590	2.97302	0.33811		O	3.64172	-2.01829	-1.92833
	H	4.29397	2.33757	-0.24433		C	-0.17866	-0.61846	0.88910
	O	4.96362	1.53406	1.57148		O	-2.24201	-2.05659	-0.18446
	H	5.39462	0.78383	1.12550		O	-0.90117	-3.42006	-1.21648
	F	-1.17572	-0.79082	1.54072		N	-1.15546	-0.89471	2.00467
						O	-1.78717	0.02820	2.49294
						O	-1.16341	-2.04498	2.42058
2c (MeCN)	C	-2.33251	-1.08825	0.40439	**2f** (MeCN)	N	0.00000	-0.29202	-0.08250
	C	-0.84556	-1.22800	0.09917		H	0.00000	-0.97453	0.67643
	C	-0.78501	1.11226	-0.46321		C	1.21666	0.51190	0.01662
	C	-2.27333	1.19924	-0.14534		C	2.46359	-0.36105	-0.02835
	H	-0.27646	-1.10027	1.02729		H	1.22974	1.12873	0.93230
	H	-0.63370	-2.23188	-0.28227		H	1.22711	1.21059	-0.82806
	H	-2.92566	-1.32897	-0.49175		H	3.36831	0.25111	0.02925
	H	-2.63846	-1.75933	1.21166		H	2.48319	-1.06352	0.81206
	H	-0.21200	1.39219	0.42836		H	2.49692	-0.94166	-0.95457
	H	-0.52875	1.82175	-1.25637		C	-1.21666	0.51190	0.01663
	H	-2.53670	2.17777	0.26546		C	-2.46359	-0.36105	-0.02834
	H	-2.86443	1.03536	-1.05998		H	-1.22711	1.21059	-0.82805
	N	-0.36797	-0.23413	-0.86726		H	-1.22974	1.12873	0.93230
	H	-0.76802	-0.44381	-1.78296		H	-3.36831	0.25111	0.02926
	O	-2.64409	0.23444	0.83745		H	-2.49692	-0.94165	-0.95457
						H	-2.48319	-1.06352	0.81206
2b $\cdot\cdot 2H_2O$	O	-3.41003	0.02529	-0.31273	**2f** $\cdot\cdot 2H_2O$	O	0.90400	2.15492	-1.50833
	H	-2.41806	0.07240	-0.20792		H	0.60273	1.41778	-0.90922
	O	0.26600	3.01436	0.36432		O	-1.13707	-2.37069	-1.07932
	H	-0.19921	3.63070	-0.23132		H	-1.78378	-2.16949	-1.78099
	C	1.27196	-0.84348	1.31729		N	0.08482	0.11857	0.27123
	C	-0.24187	-0.70071	1.14388		H	-0.30982	-0.68446	-0.22663
	C	-0.00345	-0.39845	-1.26087		H	-1.62028	-2.93560	-0.44826
	C	1.51840	-0.53089	-1.16783		H	1.27311	2.83151	-0.91567
	C	1.91647	-1.38455	0.03869		C	1.26825	-0.33353	1.00855
	H	-0.69269	-1.69529	1.03057		C	2.29081	-0.96671	0.07441
	H	-0.69280	-0.24694	2.03192		H	0.99405	-1.04859	1.80111
	H	1.69893	0.13889	1.55636		H	1.70988	0.53544	1.51052
	H	1.48696	-1.50043	2.16769		H	3.17054	-1.29863	0.63338
	H	-0.44326	-1.37911	-1.48442		H	1.86555	-1.83738	-0.43476
	H	-0.28511	0.27017	-2.08032		H	2.61499	-0.25206	-0.68751
	H	1.90993	-0.96393	-2.09529		C	-0.95059	0.66739	1.15160
	H	1.95916	0.46963	-1.07114		C	-2.19456	1.05794	0.36459

	H	1.58371	-2.41816	-0.12431		H	-0.53741	1.54919	1.65524
	H	3.00615	-1.41808	0.14255		H	-1.22048	-0.04958	1.94391
	N	-0.62422	0.10223	-0.02628		H	-2.95652	1.47505	1.02933
	H	-0.32217	1.06910	0.12250		H	-1.95337	1.80562	-0.39643
	H	1.21343	3.16043	0.18586		H	-2.62745	0.18745	-0.13866
	H	-3.61084	-0.91839	-0.43156					
TS1$_{bdb}$ $\cdot\cdot 2H_2O$	N	3.52437	-0.35848	-0.94249	**TS1$_{bdf}$**$\cdot\cdot 2H_2O$	N	3.56853	0.38688	0.41174
	C	2.29870	-0.40481	-0.18305		C	2.21369	0.24947	-0.05692
	C	1.99886	0.62716	0.73300		C	1.78333	-0.97074	-0.62726
	C	1.45680	-1.48793	-0.34020		C	1.36623	1.33624	0.01768
	C	0.27122	-1.54244	0.38304		C	0.05578	1.21232	-0.42892
	H	1.70929	-2.29789	-1.01365		H	1.70940	2.28575	0.41036
	H	2.70055	1.44187	0.89579		H	2.47888	-1.79821	-0.74809
	C	0.83091	0.57191	1.44326		C	0.49568	-1.08834	-1.07062
	C	-0.11886	-0.46280	1.22741		C	-0.45257	-0.03500	-0.90654
	N	-0.58110	-2.68638	0.19446		N	-0.79141	2.37085	-0.36249
	H	0.59616	1.32191	2.19219		H	0.16541	-1.99069	-1.57523
	O	4.27837	0.60572	-0.78085		O	4.32270	-0.58618	0.31824
	O	3.77232	-1.27860	-1.72491		O	3.92516	1.46719	0.88986
	O	-0.14869	-3.64540	-0.44933		O	-0.27891	3.46503	-0.10909
	O	-1.71615	-2.65659	0.67810		O	-2.00333	2.22175	-0.54112
	O	-4.08193	-1.24152	-0.25027		O	-4.38733	0.61582	0.39761
	H	-3.75781	-2.15986	-0.21507		H	-4.19650	1.54895	0.18974
	C	-3.26077	2.46748	0.14900		N	-1.74567	-0.77670	0.57663
	C	-2.17406	1.69057	0.89539		H	-2.60579	-0.21689	0.50926
	C	-1.22579	0.88843	-1.20573		O	3.87174	-3.50112	-0.95437
	C	-2.27798	1.64983	-2.01498		H	4.54402	-2.97369	-0.48646
	C	-2.77947	2.87256	-1.24505		H	-4.99613	0.64130	1.15958
	H	-1.31567	2.34786	1.08050		H	3.69533	-4.25909	-0.36763
	H	-2.53843	1.33851	1.86368		C	-2.08629	-2.19092	0.32384
	H	-4.15547	1.83946	0.06549		C	-2.93347	-2.41298	-0.92232
	H	-3.53949	3.34857	0.73663		H	-2.63053	-2.57352	1.19647
	H	-0.32765	1.50718	-1.08795		H	-1.15130	-2.76009	0.27038
	H	-0.93072	-0.02804	-1.72527		H	-3.26636	-3.45435	-0.94460
	H	-1.84669	1.94436	-2.97745		H	-3.81864	-1.77138	-0.90666
	H	-3.11765	0.97878	-2.23136		H	-2.38612	-2.21423	-1.84444
	H	-1.96564	3.60298	-1.15122		C	-1.11499	-0.59948	1.90077
	H	-3.58459	3.36642	-1.79818		C	-1.54034	0.67752	2.61386
	N	-1.69415	0.52603	0.13734		H	-0.02710	-0.62866	1.77265
	H	-2.45728	-0.15782	0.06003		H	-1.37057	-1.45543	2.53461

	O	4.14848	3.06741	1.11094		H	-1.04945	0.72890	3.58929
	H	4.63961	2.65665	0.37752		H	-1.27181	1.58004	2.06226
	F	-0.96667	-0.68585	2.24678		H	-2.62130	0.69227	2.77680
	H	-4.59970	-1.17966	-1.07424		F	-1.44828	-0.00856	-1.81658
	H	3.92059	3.96006	0.79365					
TS1$_{bdf}$ (MeCN)	N	-4.02982	-0.56410	0.51189	**TS1$_{baf}$** (MeCN)	N	4.04163	0.75843	0.74436
	C	-2.77442	-0.15029	-0.05988		C	2.83829	0.23530	0.15765
	C	-2.61432	1.17635	-0.51894		C	2.72028	-1.14921	-0.09960
	C	-1.75349	-1.07075	-0.18967		C	1.81925	1.09829	-0.18802
	C	-0.54018	-0.67019	-0.73462		C	0.65041	0.59263	-0.74369
	H	-1.88604	-2.09962	0.12363		H	1.91294	2.16545	-0.02420
	H	-3.44903	1.86695	-0.46485		H	3.55162	-1.81005	0.12131
	C	-1.42672	1.56939	-1.06673		C	1.58446	-1.64391	-0.67085
	C	-0.30734	0.68582	-1.12240		C	0.44736	-0.81211	-0.95334
	N	0.50546	-1.65150	-0.85718		N	-0.39424	1.53896	-1.03834
	H	-1.30305	2.56695	-1.47774		H	1.52475	-2.69511	-0.93317
	O	-4.93289	0.27213	0.60110		O	4.94444	-0.03474	1.02836
	O	-4.15278	-1.73208	0.89000		O	4.12651	1.97406	0.94309
	O	0.21201	-2.84386	-0.75569		O	-0.09765	2.72578	-1.18643
	O	1.65960	-1.25252	-1.04357		O	-1.55603	1.12079	-1.10191
	N	1.02910	1.43895	0.25780		N	-0.97736	-1.38841	0.39445
	H	1.71990	0.68656	0.30967		H	-1.79094	-0.90241	0.00968
	C	1.67068	2.68536	-0.21644		Cl	-0.46910	-1.32957	-2.38825
	C	2.96878	2.42764	-0.96757		C	-1.18441	-2.85406	0.37741
	H	1.86661	3.33975	0.63857		C	-2.65382	-3.25796	0.33088
	H	0.95424	3.21257	-0.85539		H	-0.69002	-3.27592	1.25533
	H	3.38352	3.37491	-1.32149		H	-0.67797	-3.26601	-0.49955
	H	3.71237	1.96075	-0.31387		H	-2.73510	-4.34778	0.29596
	H	2.81095	1.77925	-1.83096		H	-3.20522	-2.90370	1.20472
	C	0.32603	1.56904	1.54524		H	-3.13676	-2.85878	-0.56625
	C	1.24749	1.67859	2.75673		C	-0.62748	-0.82173	1.70636
	H	-0.31731	0.69182	1.66074		C	-1.68038	-1.01721	2.79380
	H	-0.32828	2.44222	1.47462		H	-0.45403	0.24747	1.56313
	H	0.64844	1.76019	3.66775		H	0.32353	-1.27108	2.00901
	H	1.87937	0.78997	2.84903		H	-1.34926	-0.51679	3.70788
	H	1.89608	2.55679	2.70586		H	-2.63946	-0.58089	2.49977
	F	0.55150	0.92282	-2.13945		H	-1.83642	-2.07208	3.03137
TS1$_{bab}$ $\cdot\cdot 2H_2O$	N	-3.73824	-0.62806	0.66130	**TS1$_{baf}$**$\cdot\cdot 2H_2O$	N	3.78387	0.08695	-0.38261
	C	-2.42464	-0.72765	0.08155		C	2.36638	0.20175	-0.58316
	C	-2.12996	-0.05562	-1.12443		C	1.71995	-0.58262	-1.56738

	C	-1.47629	-1.51968	0.69790		C	1.65579	1.12849	0.15262
	C	-0.20229	-1.61505	0.15163		C	0.28126	1.23533	-0.01854
	H	-1.70948	-2.06459	1.60468		H	2.15430	1.77234	0.86725
	H	-2.89725	0.51593	-1.64110		H	2.29394	-1.24541	-2.20985
	C	-0.87981	-0.16645	-1.66664		C	0.37296	-0.46298	-1.74563
	C	0.17617	-0.87600	-1.01261		C	-0.44672	0.37054	-0.90626
	N	0.74789	-2.43252	0.86420		N	-0.39828	2.21863	0.78339
	H	-0.66490	0.29118	-2.62658		H	-0.11067	-0.99953	-2.55491
	O	-4.58284	0.06870	0.08834		O	4.41282	-0.72853	-1.06803
	O	-3.97431	-1.23789	1.70795		O	4.32620	0.80000	0.46681
	O	0.32326	-3.28620	1.64755		O	0.25641	3.14751	1.26503
	O	1.95012	-2.22630	0.68069		O	-1.60937	2.07720	0.98111
	O	4.22017	-0.34245	-0.08437		O	-4.03733	0.30321	1.03849
	H	4.11419	-1.29418	0.09854		H	-4.89536	0.10217	0.61965
	C	2.39064	2.92850	-0.77078		N	-1.48009	-0.95587	0.27729
	C	1.52562	1.76634	-1.26459		H	-2.39133	-0.50250	0.43816
	C	0.94620	1.14765	1.02096		O	3.60085	-2.50790	-3.45661
	C	1.78750	2.29557	1.58466		H	4.29739	-2.16681	-2.86860
	C	1.89022	3.44319	0.57931		H	-3.88057	1.24917	0.86289
	H	0.50794	2.12280	-1.46247		H	3.59501	-3.47089	-3.30844
	H	1.92324	1.35234	-2.19495		C	-1.66341	-2.25355	-0.40096
	H	3.42859	2.58823	-0.67890		C	-2.75672	-2.25661	-1.46054
	H	2.37806	3.72559	-1.52140		H	-1.89841	-3.01169	0.35253
	H	-0.09176	1.47536	0.88549		H	-0.69877	-2.53983	-0.83486
	H	0.94106	0.30253	1.71421		H	-2.88911	-3.27660	-1.83101
	H	1.34104	2.63683	2.52432		H	-3.71109	-1.92381	-1.04282
	H	2.78963	1.92004	1.82330		H	-2.51931	-1.61767	-2.31188
	H	0.90280	3.90434	0.45044		C	-0.78356	-1.10684	1.56821
	H	2.55625	4.22352	0.96053		C	-1.66770	-1.65910	2.68483
	N	1.43833	0.68070	-0.27993		H	-0.41188	-0.12813	1.87384
	H	2.36363	0.24511	-0.17149		H	0.08968	-1.74591	1.40459
	O	-4.48831	1.67739	-2.57624		H	-1.09698	-1.68692	3.61732
	H	-5.02668	1.46564	-1.79294		H	-2.54152	-1.01997	2.83263
	Cl	1.38809	-1.53033	-2.11855		H	-2.01396	-2.67495	2.47878
	H	4.79205	-0.00720	0.63151		Cl	-1.85122	1.05204	-1.75696
	H	-4.40889	2.64875	-2.57218					
TS1$_{bac}$ (MeCN)	N	-3.92882	0.31772	-1.06724	**TS1$_{bbb}$** (MeCN)	N	-4.10022	0.52585	-1.18036
	C	-2.76821	0.02712	-0.27154		C	-2.90796	0.18840	-0.44845
	C	-2.58724	-1.26477	0.27121		C	-2.71824	-1.12733	0.02437
	C	-1.85578	1.02802	-0.00735		C	-1.97345	1.16888	-0.18353

	C	-0.72741	0.74630	0.75201		C	-0.81770	0.84123	0.51448
	H	-2.00266	2.03107	-0.39055		H	-2.12430	2.18815	-0.51911
	H	-3.34341	-2.02600	0.11147		H	-3.48643	-1.87526	-0.14044
	C	-1.49058	-1.53876	1.03529		C	-1.59154	-1.44305	0.73086
	C	-0.45078	-0.57013	1.25498		C	-0.54204	-0.49303	0.94608
	N	0.20946	1.82057	0.95354		N	0.14206	1.89960	0.71240
	H	-1.39195	-2.50745	1.51408		H	-1.48211	-2.43613	1.15315
	O	-4.73536	-0.59361	-1.27692		O	-4.92672	-0.36642	-1.39116
	O	-4.07477	1.46088	-1.51051		O	-4.24930	1.68791	-1.56860
	O	-0.18180	2.98268	0.83218		O	-0.24454	3.06892	0.65960
	O	1.38227	1.52675	1.21255		O	1.32134	1.58536	0.89870
	Cl	0.32839	-0.72483	2.84820		C	2.30289	-3.11660	-1.11349
	C	2.52240	-3.16180	-0.48149		C	1.17980	-2.61460	-0.20436
	C	1.37768	-2.67719	0.40160		C	0.79489	-0.68433	-1.65055
	C	0.94661	-0.93355	-1.22839		C	1.90216	-1.13562	-2.60466
	C	2.10050	-1.48351	-2.06012		C	2.08748	-2.65224	-2.55390
	H	0.46197	-3.21412	0.13807		H	0.22737	-3.06188	-0.50942
	H	1.60348	-2.85647	1.45485		H	1.36389	-2.88955	0.83660
	H	3.46686	-2.69147	-0.17159		H	3.26365	-2.74262	-0.73962
	H	2.62854	-4.24503	-0.39447		H	2.34085	-4.20900	-1.05559
	H	0.00478	-1.39193	-1.54588		H	-0.17254	-1.08482	-1.97521
	H	0.87386	0.14850	-1.35962		H	0.72032	0.40534	-1.63794
	H	1.89537	-1.34294	-3.12322		H	1.65144	-0.80466	-3.61737
	H	3.03123	-0.95378	-1.81035		H	2.83830	-0.63612	-2.32756
	N	1.13108	-1.23915	0.19905		H	1.19718	-3.14316	-2.96614
	H	1.90077	-0.68270	0.58590		H	2.93305	-2.95165	-3.18039
	O	2.26465	-2.87808	-1.84898		N	1.01897	-1.15367	-0.27533
						H	1.83337	-0.68298	0.12875
						Br	0.40136	-0.76740	2.62453
TS1$_{bbb}$ $\cdot\cdot 2H_2O$	N	-3.89935	-0.87124	0.62081	**TS1$_{bbf}$**$\cdot\cdot 2H_2O$	N	3.77953	0.07251	-0.38861
	C	-2.53658	-0.87236	0.15568		C	2.36135	0.19108	-0.58465
	C	-2.21915	-0.33518	-1.10975		C	1.70961	-0.58836	-1.56863
	C	-1.55815	-1.43893	0.94778		C	1.65524	1.11515	0.15870
	C	-0.23915	-1.44042	0.51039		C	0.28014	1.22552	-0.00908
	H	-1.80279	-1.87736	1.90772		H	2.15715	1.75347	0.87594
	H	-2.99964	0.06472	-1.75267		H	2.27942	-1.25076	-2.21506
	C	-0.92111	-0.35873	-1.54326		C	0.36152	-0.46408	-1.74282
	C	0.14702	-0.83559	-0.72300		C	-0.45069	0.37004	-0.89944
	N	0.73506	-2.01354	1.40727		N	-0.39270	2.20662	0.80239
	H	-0.68447	-0.00831	-2.54215		H	-0.12148	-1.00011	-2.55258

	O	-4.76898	-0.38842	-0.11132		O	4.40542	-0.74044	-1.07998
	O	-4.14920	-1.35023	1.73035		O	4.32527	0.77979	0.46296
	O	0.34925	-2.79972	2.27645		O	0.26598	3.13236	1.28445
	O	1.91309	-1.67133	1.28316		O	-1.60276	2.06561	1.00606
	O	4.02239	0.39380	0.52487		O	-4.06274	0.29474	1.04940
	H	4.01603	-0.51791	0.87017		H	-4.90427	0.12353	0.58615
	C	1.89930	3.22393	-0.90496		N	-1.49818	-0.96093	0.28164
	C	1.23278	1.89841	-1.28152		H	-2.41481	-0.51657	0.43570
	C	0.49830	1.54509	1.01474		O	3.61714	-2.49151	-3.45625
	C	1.13305	2.86515	1.46039		H	4.28492	-2.16153	-2.83009
	C	1.20353	3.85819	0.29978		H	-3.88061	1.24209	0.90791
	H	0.20569	2.08548	-1.61645		H	3.62149	-3.45934	-3.34428
	H	1.76908	1.41137	-2.10000		C	-1.65871	-2.26605	-0.38827
	H	2.95477	3.04060	-0.67268		C	-2.76110	-2.30323	-1.43720
	H	1.87134	3.89471	-1.76997		H	-1.86824	-3.02486	0.37185
	H	-0.55200	1.70787	0.74334		H	-0.69175	-2.53290	-0.82938
	H	0.52324	0.81679	1.82944		H	-2.87271	-3.32921	-1.79795
	H	0.55279	3.27629	2.29289		H	-3.71941	-1.98945	-1.01369
	H	2.14210	2.66564	1.84006		H	-2.54614	-1.66639	-2.29593
	H	0.18745	4.16055	0.01620		C	-0.80579	-1.09760	1.57675
	H	1.72914	4.76701	0.60905		C	-1.68634	-1.66096	2.69078
	N	1.17332	0.96428	-0.15090		H	-0.45080	-0.11351	1.88320
	H	2.12579	0.67323	0.10430		H	0.07770	-1.72383	1.41865
	O	-4.60774	1.05195	-2.92759		H	-1.11888	-1.67756	3.62552
	H	-5.18675	0.87506	-2.16465		H	-2.57042	-1.03494	2.83347
	Br	1.62524	-1.56605	-1.73754		H	-2.01618	-2.68253	2.48623
	H	4.43519	0.92979	1.22789		Br	-1.96113	1.14803	-1.85603
	H	-4.54607	2.02338	-2.97578					
TS1$_{bbf}$ (MeCN)	N	4.22008	0.84478	0.58085	**TS1$_{bbc}$** (MeCN)	N	-4.05464	0.45477	-1.06841
	C	2.95362	0.28107	0.19699		C	-2.83766	0.06431	-0.40931
	C	2.72096	-1.10372	0.34719		C	-2.56347	-1.30192	-0.18154
	C	1.98473	1.09624	-0.34965		C	-1.96042	1.03446	0.03016
	C	0.75625	0.55374	-0.70874		C	-0.77911	0.65731	0.65699
	H	2.16304	2.15538	-0.49413		H	-2.17500	2.08690	-0.11434
	H	3.50952	-1.74370	0.72832		H	-3.28764	-2.05306	-0.47848
	C	1.52479	-1.64145	-0.03365		C	-1.41360	-1.67258	0.45551
	C	0.44490	-0.82959	-0.51480		C	-0.41707	-0.71587	0.84463
	N	-0.22939	1.46852	-1.22719		N	0.11793	1.71593	1.04428
	H	1.37895	-2.71516	0.01966		H	-1.24484	-2.71725	0.69420
	O	5.07487	0.08949	1.05298		O	-4.82838	-0.43356	-1.43769

	O	4.40263	2.05579	0.42626		
	O	0.14670	2.53689	-1.71248		
	O	-1.41999	1.15048	-1.13551		
	N	-0.97388	-0.89772	0.98082		
	H	-1.76978	-0.47881	0.49429		
	C	-1.27589	-2.28653	1.38993		
	C	-2.76884	-2.57309	1.51036		
	H	-0.76248	-2.48070	2.33436		
	H	-0.84562	-2.96748	0.65036		
	H	-2.92151	-3.61846	1.79242		
	H	-3.24814	-1.94400	2.26376		
	H	-3.27266	-2.40896	0.55300		
	C	-0.52133	-0.01138	2.06401		
	C	-1.52234	0.18506	3.19963		
	H	-0.29214	0.95878	1.61682		
	H	0.41623	-0.42487	2.44908		
	H	-1.11137	0.89686	3.92082		
	H	-2.46846	0.58987	2.82865		
	H	-1.72793	-0.74594	3.73310		
	Br	-0.64526	-1.73184	-1.85929		
1e (MeCN)	S	-3.80210	0.80365	-0.10643	**TS1$_{eb}$** (MeCN)	S	1.29269	-0.77467	-0.77435
	O	-2.34950	0.81790	-0.15419		O	1.64232	-0.83961	-2.17835
	O	-4.52282	2.06503	-0.06126		O	0.81333	-1.87604	0.03892
	O	-4.25261	-0.07994	1.21602		O	-0.85308	-0.44244	-1.61902
	C	-3.90631	0.43193	2.46911		C	-2.00627	-0.43402	-1.04403
	C	-2.69687	0.04779	3.03926		C	-2.26380	-1.06720	0.21552
	C	-4.80896	1.26067	3.12771		C	-3.11247	0.22915	-1.67169
	C	-2.37851	0.50624	4.31086		C	-3.51253	-1.03028	0.79216
	H	-2.02301	-0.60498	2.49332		H	-1.45492	-1.59927	0.70273
	C	-4.49330	1.72081	4.39937		C	-4.35794	0.26249	-1.09393
	H	-5.74469	1.53216	2.64923		H	-2.93440	0.71114	-2.62904
	C	-3.28261	1.33587	4.96660		C	-4.56923	-0.36491	0.14799
	H	-1.44647	0.22602	4.78847		H	-3.69409	-1.51759	1.74417
	H	-5.17282	2.36614	4.94445		H	-5.18274	0.77058	-1.58198
	C	-4.46689	-0.26265	-1.34527		C	0.95249	0.84341	-0.14740
	C	-3.65898	-1.27233	-1.86346		C	1.18990	1.93899	-0.97421
	C	-5.77767	-0.05905	-1.77085		C	0.47644	0.96864	1.15444
	C	-4.19087	-2.10710	-2.84150		C	0.94904	3.20954	-0.46327
	H	-2.63722	-1.39708	-1.51713		H	1.53678	1.80118	-1.99395
	C	-6.29288	-0.90339	-2.74959		C	0.24145	2.25043	1.64556
						O	-4.27755	1.65668	-1.24036
						O	-0.33274	2.85201	1.20074
						O	1.31575	1.44026	1.17499
						Br	0.51234	-1.22101	2.48536
						C	2.56083	-2.68778	-1.59698
						C	1.44859	-2.47757	-0.57491
						C	0.89641	-0.40231	-1.69843
						C	2.02267	-0.68572	-2.68699
						H	0.53482	-2.96540	-0.92636
						H	1.72946	-2.90521	0.38990
						H	3.50778	-2.27679	-1.21797
						H	2.69627	-3.75430	-1.78788
						H	-0.04746	-0.80136	-2.08319
						H	0.79018	0.67509	-1.55356
						H	1.76382	-0.29230	-3.67204
						H	2.95066	-0.20169	-2.34960
						N	1.15632	-1.04537	-0.40176
						H	1.92657	-0.57278	0.08217
						O	2.23134	-2.08201	-2.83850

	H	-6.37726	0.74467	-1.35368		H	0.28359	0.09392	1.76801
	C	-5.50226	-1.92295	-3.28017		C	0.47852	3.36405	0.84177
	H	-3.57897	-2.89971	-3.26257		H	1.12362	4.07999	-1.08928
	H	-7.31155	-0.76227	-3.09935		H	-0.13196	2.37389	2.65814
	H	-5.91064	-2.57766	-4.04558		H	0.29120	4.36066	1.23245
	N	-2.94840	1.81998	6.30870		N	-5.85568	-0.32962	0.74945
	O	-3.75427	2.55197	6.87779		O	-6.78231	0.25808	0.16483
	O	-1.87818	1.47100	6.80055		O	-6.02819	-0.88655	1.84770
						C	5.53475	-0.20169	-0.39226
						C	4.08660	0.11951	-0.75087
						C	3.30594	-0.90472	1.36582
						C	4.74298	-1.24211	1.75258
						C	5.73308	-0.26374	1.12173
						H	3.80310	1.10566	-0.37586
						H	3.91967	0.08676	-1.82816
						H	5.81770	-1.15690	-0.85032
						H	6.17092	0.56640	-0.84118
						H	3.02694	0.08373	1.73772
						H	2.59918	-1.64213	1.74816
						H	4.81139	-1.22201	2.84397
						H	4.97154	-2.26741	1.43818
						H	5.58744	0.73416	1.55214
						H	6.75815	-0.56464	1.35407
						N	3.16110	-0.87099	-0.12122
						H	3.40207	-1.80877	-0.48603
1dc (MeCN)	C	-2.66919	-1.73924	0.09767	**1fa** (H_2O)	C	-2.79209	-0.24900	1.22077
	C	-1.28727	-1.75032	-0.01079		C	-1.41458	-0.42314	1.22012
	C	-0.57981	-0.56806	-0.20298		C	-0.74186	-0.49689	0.00547
	C	-1.28263	0.64245	-0.28234		C	-1.40736	-0.40381	-1.21196
	C	-2.66225	0.67618	-0.15053		C	-2.78469	-0.22948	-1.21802
	C	-3.33463	-0.52066	0.02972		C	-3.45358	-0.15408	0.00010
	H	-3.22415	-2.65988	0.24239		H	-3.34688	-0.18881	2.15025
	H	-0.72966	-2.67986	0.05542		H	-0.86207	-0.50631	2.15151
	H	-3.19633	1.61800	-0.20260		H	-0.84961	-0.47231	-2.14142
	O	0.77862	-0.68276	-0.33754		H	-3.33392	-0.15446	-2.14973
	N	-4.79524	-0.49286	0.15157		O	0.62655	-0.74187	0.00883
	O	-5.35707	0.59603	0.08937		N	-4.90534	0.02766	-0.00285
	O	-5.37590	-1.56181	0.30925		O	-5.47850	0.10878	-1.08710
	C	3.02535	-0.23719	0.25719		O	-5.48512	0.09099	1.07904
	C	3.96267	0.36795	1.10190		C	2.89184	-0.06374	-0.00158

	C	3.45012	-1.01416	-0.82642		C	3.85549	0.95013	-0.00903
	C	5.32085	0.19579	0.86350		C	3.28469	-1.40647	0.00598
	H	3.61703	0.96886	1.93773		C	5.20667	0.62274	-0.00871
	C	4.81097	-1.18207	-1.06034		H	3.53542	1.98775	-0.01493
	H	2.72193	-1.48247	-1.48013		C	4.63833	-1.72906	0.00606
	C	5.74488	-0.57897	-0.21738		H	2.53604	-2.19168	0.01168
	H	6.05026	0.66482	1.51802		C	5.59838	-0.71685	-0.00123
	H	5.14470	-1.78411	-1.90093		H	5.95564	1.40995	-0.01436
	C	1.59485	-0.02066	0.55163		H	4.94573	-2.77124	0.01180
	O	1.14134	0.63944	1.45800		H	6.65498	-0.97257	-0.00107
	N	-0.61255	1.92016	-0.53575		C	1.46398	0.33548	-0.00237
	O	-1.14841	2.93468	-0.10505		O	1.05242	1.47566	-0.01134
	O	0.42741	1.90720	-1.18559					
	H	6.80748	-0.71297	-0.40353					
$TS1_{dcb}$ (MeCN)	C	-3.03602	-2.80038	0.65649	**$TS1_{dcc}$** (MeCN)	C	3.53167	-1.11522	-0.04978
	C	-2.44314	-1.39867	0.73567		C	2.17883	-1.30874	0.19195
	C	-2.88078	-1.06478	-1.68266		C	1.19570	-0.29126	-0.06015
	C	-3.48766	-2.45722	-1.78137		C	1.71179	0.94771	-0.56126
	C	-4.08314	-2.90925	-0.44958		C	3.04873	1.14754	-0.78090
	H	-3.21163	-0.66105	0.97350		C	3.96394	0.10932	-0.52475
	H	-1.64454	-1.34252	1.47109		H	4.23716	-1.91329	0.14601
	H	-2.23169	-3.52688	0.48925		H	1.00774	1.74517	-0.76462
	H	-3.47036	-3.03142	1.63331		H	3.41086	2.10098	-1.15045
	H	-3.63943	-0.31588	-1.43924		O	-0.05567	-0.48723	0.13382
	H	-2.37936	-0.77331	-2.60447		N	5.37125	0.31907	-0.75400
	H	-4.24884	-2.43398	-2.56647		O	5.73681	1.41723	-1.18303
	H	-2.71652	-3.16473	-2.10899		O	6.15639	-0.60303	-0.51531
	H	-4.94753	-2.28217	-0.20097		C	-1.44422	0.54565	-0.82887
	H	-4.44610	-3.93757	-0.52842		C	-1.70991	1.68550	0.11020
	N	-1.85136	-1.00217	-0.58601		C	-2.28581	2.82074	-0.47176
	H	-1.09805	-1.67140	-0.80808		C	-1.41516	1.68282	1.47661
	C	3.80843	-0.35344	1.03250		C	-2.58300	3.93456	0.30910
	C	2.48493	-0.76912	1.04644		H	-2.49567	2.82891	-1.53756
	C	1.41026	0.05536	0.57090		C	-1.70528	2.80204	2.25063
	C	1.79477	1.34982	0.09700		H	-0.93172	0.82398	1.92716
	C	3.09856	1.77165	0.10266		C	-2.29403	3.92643	1.67206
	C	4.11078	0.91492	0.57152		H	-3.03401	4.81005	-0.15020
	H	4.58861	-1.01304	1.39224		H	-1.46319	2.79819	3.30997
	H	1.01873	2.00869	-0.27141		O	-1.09266	0.69209	-1.98027
	H	3.35844	2.76359	-0.25122		N	1.79548	-2.60912	0.70487

	O	0.19351	-0.35537	0.55931		O	0.74743	-2.72320	1.33868
	N	5.48253	1.35894	0.57889		O	2.55622	-3.56131	0.49375
	O	5.73277	2.49213	0.15896		H	-2.51920	4.79749	2.28203
	O	6.35248	0.59252	1.00191		C	-3.61274	-2.37012	0.70144
	C	-1.10005	0.37516	-0.67676		C	-2.75121	-1.11792	0.75623
	C	-1.72425	1.49450	0.11186		C	-3.57584	-0.58230	-1.49443
	C	-2.36583	2.48075	-0.64574		C	-4.40522	-1.85441	-1.43168
	C	-1.68994	1.60897	1.50430		H	-3.31228	-0.28767	1.18548
	C	-2.98347	3.55903	-0.01716		H	-1.84024	-1.29425	1.32457
	H	-2.37381	2.40265	-1.72916		H	-3.02931	-3.22158	0.32189
	C	-2.29995	2.69331	2.12805		H	-3.95448	-2.61025	1.70958
	H	-1.16413	0.87001	2.09747		H	-4.14101	0.27030	-1.11143
	C	-2.95231	3.66672	1.37169		H	-3.24500	-0.37616	-2.51226
	H	-3.48239	4.31768	-0.61426		H	-5.32897	-1.70647	-1.99362
	H	-2.25938	2.78119	3.21047		H	-3.85355	-2.69070	-1.88530
	O	-0.56161	0.54782	-1.75455		N	-2.35385	-0.72362	-0.63304
	N	2.23387	-2.10245	1.55929		H	-1.75579	-1.47216	-1.01969
	O	1.13311	-2.36555	2.03976		O	-4.76735	-2.17386	-0.09903
	O	3.15591	-2.92465	1.50528					
	H	-3.42791	4.51107	1.86407					
TS1$_{\mathbf{fad}}$ $\cdot\cdot 3H_2O$	C	3.13359	-2.12463	-0.47964	**TS1$_{\mathbf{fae}}$**$\cdot\cdot 3H_2O$	C	-3.92910	-0.97529	-0.17001
	C	2.02356	-1.29607	-0.49901		C	-2.62915	-1.44802	-0.20160
	C	2.18879	0.08810	-0.34253		C	-1.56593	-0.58028	-0.49229
	C	3.47350	0.62521	-0.16447		C	-1.81468	0.77537	-0.75092
	C	4.58202	-0.20223	-0.14268		C	-3.11716	1.24813	-0.72134
	C	4.40297	-1.57559	-0.30393		C	-4.16324	0.37348	-0.43374
	H	3.01976	-3.19677	-0.59504		H	-4.75621	-1.63953	0.05392
	H	1.03348	-1.70752	-0.62195		H	-2.41973	-2.49359	-0.00121
	H	3.58779	1.69732	-0.04259		H	-0.99577	1.44477	-0.96675
	H	5.57693	0.20611	-0.00529		H	-3.32497	2.29428	-0.91663
	O	1.16804	0.98336	-0.30981		O	-0.32693	-1.14195	-0.45671
	N	5.55927	-2.44946	-0.28485		N	-5.52357	0.87666	-0.40554
	O	6.67392	-1.94833	-0.12003		O	-5.71611	2.06930	-0.65092
	O	5.38567	-3.66118	-0.43389		O	-6.43561	0.09188	-0.13705
	C	-0.13259	0.66389	-0.88705		C	0.79845	-0.51016	-1.10136
	C	-1.00795	1.88368	-0.70423		C	2.01617	-1.36275	-0.85524
	C	-1.81658	2.27186	-1.77104		C	2.94434	-1.48974	-1.88771
	C	-1.02996	2.62755	0.47891		C	2.23883	-2.02648	0.35452
	C	-2.63713	3.39491	-1.66475		C	4.08615	-2.27228	-1.71835
	H	-1.79424	1.68543	-2.68451		H	2.76164	-0.97046	-2.82360

	C	-1.84500	3.75084	0.58502		C	3.37702	-2.80949	0.52379
	H	-0.42283	2.31865	1.32304		H	1.53015	-1.92417	1.16926
	C	-2.65129	4.13903	-0.48700		C	4.30481	-2.93493	-0.51218
	H	-3.26347	3.68903	-2.50329		H	4.80384	-2.36550	-2.52957
	H	-1.85650	4.32355	1.50913		H	3.54375	-3.32131	1.46833
	H	-3.28848	5.01579	-0.40143		H	5.19376	-3.54618	-0.37743
	C	-2.15043	-1.90647	-0.46534		C	2.94514	3.73375	0.26183
	C	-1.86958	-0.88869	0.46481		O	3.19123	4.70936	0.97364
	C	-2.89623	-0.48966	1.34028		C	3.58126	3.60753	-1.10393
	C	-4.15173	-1.08879	1.29982		H	4.18815	4.49383	-1.29220
	C	-4.40000	-2.09002	0.36633		H	4.20681	2.71327	-1.15343
	C	-3.40817	-2.50090	-0.51846		H	2.81976	3.50204	-1.87919
	H	-1.36975	-2.22510	-1.14746		C	2.02661	2.67331	0.73457
	H	-2.69604	0.30157	2.05774		N	1.84160	1.69110	-0.09088
	H	-4.93243	-0.77501	1.98740		O	1.02838	0.72900	0.31271
	H	-3.61197	-3.28743	-1.24006		O	-0.15000	-0.18159	2.69186
	Cl	-5.98651	-2.85006	0.30828		H	-1.02505	0.24428	2.73636
	O	-0.65605	-0.32324	0.54118		H	0.28633	0.19644	1.89304
	H	1.72472	4.45198	0.26067		O	-0.56269	-3.97515	0.35641
	O	2.17501	3.61114	0.46712		H	0.02466	-4.71891	0.12222
	H	1.65362	2.91684	0.02193		H	-0.23096	-3.20918	-0.14757
	O	1.87438	2.71864	3.18474		C	1.37292	2.78686	2.07885
	H	1.39051	1.87080	3.08110		H	1.66715	1.96122	2.73329
	H	2.00389	3.06450	2.27946		H	1.64904	3.72951	2.55081
	O	0.45992	0.29162	2.94102		H	0.28392	2.73924	1.98065
	H	0.03917	0.07202	2.06830		O	-0.25159	-2.97737	3.03485
	H	-0.24460	0.19735	3.60687		H	-0.37854	-3.36615	2.14672
	O	-0.16777	-0.00923	-1.91827		H	-0.23023	-2.00602	2.89924
						O	0.62636	0.10934	-2.14640
TS1$_{fad}$ $\cdot\cdot 2H_2O1DMSO$	C	-1.50375	-2.87268	1.00284	**TS1$_{fae}$**$\cdot\cdot 2H_2O1DMSO$	C	2.59381	-2.77533	-0.83070
	C	-0.68021	-1.75850	0.98853		C	2.00957	-1.53483	-1.01149
	C	-1.22143	-0.49350	1.26256		C	0.61948	-1.37954	-0.88187
	C	-2.58932	-0.36236	1.54889		C	-0.18573	-2.48694	-0.57085
	C	-3.41204	-1.47480	1.56289		C	0.40030	-3.72938	-0.39235
	C	-2.86010	-2.72611	1.29005		C	1.78182	-3.86807	-0.52337
	H	-1.10030	-3.85604	0.78836		H	3.66588	-2.90432	-0.92889
	H	0.37035	-1.85989	0.76182		H	2.61342	-0.66395	-1.25338
	H	-2.99006	0.62637	1.74985		H	-1.25389	-2.36676	-0.46840
	H	-4.46937	-1.38145	1.78479		H	-0.20804	-4.59289	-0.14738
	O	-0.51457	0.66452	1.23807		O	0.16399	-0.11566	-1.03834

N	-3.71446	-3.89716	1.30487	N	2.38539	-5.17061	-0.33563
O	-4.91391	-3.74804	1.54944	O	1.65448	-6.12926	-0.07288
O	-3.21075	-4.99833	1.07211	O	3.60991	-5.27528	-0.44497
C	0.91273	0.66188	1.47590	C	-1.21447	0.14283	-1.37407
C	1.36127	2.10573	1.46552	C	-1.37518	1.63786	-1.52718
C	2.25056	2.52206	2.45436	C	-2.43629	2.10127	-2.30515
C	0.90479	3.02787	0.52067	C	-0.51327	2.55986	-0.92659
C	2.68699	3.84627	2.50039	C	-2.64386	3.46872	-2.47927
H	2.59758	1.79874	3.18638	H	-3.09403	1.37644	-2.77478
C	1.33799	4.34961	0.56556	C	-0.71774	3.92660	-1.10465
H	0.22472	2.70667	-0.26109	H	0.32238	2.21831	-0.32590
C	2.23141	4.76363	1.55602	C	-1.78390	4.38697	-1.87857
H	3.38131	4.16070	3.27564	H	-3.47492	3.81745	-3.08749
H	0.98129	5.06017	-0.17596	H	-0.04112	4.63794	-0.63659
H	2.56959	5.79637	1.58893	H	-1.94059	5.45429	-2.01445
O	1.38333	-0.16233	2.26060	O	-1.81243	-0.65013	-2.10757
C	3.65671	-0.23853	0.16517	C	-5.05828	-0.80660	1.53716
C	2.44347	-0.47571	-0.51417	O	-5.64690	-1.01801	2.59915
C	2.44416	-1.45939	-1.52594	C	-5.81222	-0.84705	0.22736
C	3.59928	-2.15887	-1.85961	H	-5.75404	0.11888	-0.27936
C	4.77972	-1.89899	-1.17088	H	-5.37364	-1.58374	-0.44893
C	4.81130	-0.94432	-0.15968	H	-6.85415	-1.09797	0.42900
H	3.69044	0.50750	0.95037	C	-3.60749	-0.51217	1.53024
H	1.51678	-1.66076	-2.05618	N	-3.08938	-0.30142	0.36105
H	3.57753	-2.90609	-2.64841	O	-1.79257	-0.03686	0.34587
H	5.73763	-0.74480	0.37260	O	0.23567	0.74974	2.31826
Cl	6.24535	-2.78562	-1.58261	H	0.96504	1.16601	1.81535
O	1.32070	0.19266	-0.25895	H	-0.43825	0.48607	1.66197
H	-2.70124	2.81144	0.26850	O	3.54664	1.51400	-1.47002
O	-2.58456	3.01128	1.22316	H	3.00949	1.87411	-2.19818
H	-1.74816	2.57603	1.45697	H	3.01154	1.64512	-0.65443
O	-0.44900	0.84043	-2.31447	C	-2.83586	-0.48515	2.81484
H	0.16089	0.56591	-1.59084	H	-2.42119	0.50934	3.00460
H	-1.10803	1.43312	-1.89910	H	-3.48101	-0.76639	3.64690
S	-3.84731	1.84770	-2.34603	H	-1.98491	-1.17106	2.76528
O	-2.67820	2.36405	-1.48190	S	3.37933	2.85143	1.82975
C	-3.26658	2.01271	-4.04687	O	2.40578	1.99272	0.99485
H	-3.99593	1.55722	-4.72033	C	4.98416	2.04229	1.66089
H	-3.18681	3.07981	-4.25827	H	5.74995	2.66511	2.12857
H	-2.29090	1.53081	-4.13540	H	4.91863	1.08689	2.18317

	C	-3.77776	0.04731	-2.22608		H	5.19490	1.88463	0.60136
	H	-4.04714	-0.21782	-1.20317		C	3.71353	4.30449	0.81326
	H	-4.50189	-0.38320	-2.92168		H	2.78451	4.87247	0.74874
	H	-2.76067	-0.28220	-2.44829		H	4.48250	4.91054	1.29747
						H	4.03336	3.97996	-0.17869
1fb (H_2O)	C	1.12850	1.16444	-0.16506	**1fc** (H_2O)	C	1.11922	1.21602	-0.21624
	C	-0.24474	1.19087	-0.36434		C	-0.25748	1.18779	-0.38519
	C	-0.93140	-0.01420	-0.46624		C	-0.95235	-0.02688	-0.44425
	C	-0.27873	-1.23584	-0.37829		C	-0.24931	-1.22040	-0.32798
	C	1.09810	-1.25074	-0.17793		C	1.12422	-1.21278	-0.13948
	C	1.81364	-0.05326	-0.06845		C	1.78476	0.00968	-0.08384
	H	1.68854	2.09062	-0.08292		H	1.65202	2.15925	-0.18285
	H	-0.78563	2.12985	-0.44482		H	-0.79763	-2.15572	-0.39387
	H	-0.84352	-2.15951	-0.46888		H	1.67860	-2.13992	-0.04044
	H	1.60224	-2.20963	-0.11025		O	-2.29790	-0.07971	-0.71480
	O	-2.30167	0.00641	-0.73355		N	3.23846	0.02967	0.11288
	C	-3.15824	0.01114	0.32538		O	3.81561	-1.04759	0.21498
	C	-4.58284	0.03648	-0.14303		O	3.79659	1.12073	0.16435
	H	-4.75407	0.92571	-0.75412		C	-3.16563	-0.05256	0.35493
	H	-4.78082	-0.83696	-0.76862		C	-4.58096	0.00535	-0.12265
	H	-5.25144	0.03962	0.71584		H	-4.75087	0.97493	-0.59793
	O	-2.78231	-0.00352	1.47547		H	-4.76024	-0.76942	-0.87062
	C	3.29364	-0.02854	0.14591		H	-5.25733	-0.11565	0.72149
	O	3.88935	1.03877	0.23505		O	-2.77492	-0.07428	1.49466
	C	4.04203	-1.33485	0.25118		N	-0.94092	2.47765	-0.51574
	H	3.66377	-1.93365	1.08477		O	-2.12752	2.54328	-0.21297
	H	3.91876	-1.92820	-0.65944		O	-0.27590	3.42933	-0.91093
	H	5.10066	-1.12821	0.40660					
TS1$_{fbd}$ $\cdot\cdot 3H_2O$	C	-2.34566	-1.46130	-0.31572	**TS1$_{fbe}$**$\cdot\cdot 3H_2O$	C	2.57166	-1.55255	0.06826
	C	-2.21535	-0.14051	0.14317		C	1.40248	-0.85391	-0.18766
	C	-3.36980	0.53894	0.56444		C	1.46899	0.51940	-0.45201
	C	-4.61638	-0.08066	0.54167		C	2.70355	1.17287	-0.45089
	C	-4.71725	-1.38856	0.07960		C	3.86701	0.46214	-0.18392
	C	-3.59109	-2.08232	-0.35185		C	3.81971	-0.91280	0.07503
	H	-1.46128	-1.99347	-0.64691		H	2.53143	-2.61752	0.27647
	H	-3.28058	1.56443	0.91354		H	0.43969	-1.34713	-0.17711
	H	-5.50141	0.45275	0.87726		H	2.74227	2.23857	-0.65746
	H	-3.68279	-3.10512	-0.70698		H	4.81245	0.99604	-0.18699
	Cl	-6.28879	-2.17784	0.04545		O	0.35977	1.29596	-0.65979
	O	-1.01180	0.46632	0.21453		C	-0.75480	0.77571	-1.43707

	H	1.67850	4.45720	-1.37719		O	-0.53100	-0.08702	-2.28433
	O	1.72911	4.04688	-0.49425		C	-1.72489	1.91344	-1.65257
	H	1.48504	3.10700	-0.62433		H	-1.35586	2.53816	-2.47224
	O	-0.22584	4.78987	1.44168		H	-2.68651	1.48946	-1.94239
	H	-0.40091	3.89372	1.80188		H	-1.85021	2.52597	-0.75935
	H	0.46176	4.64709	0.76000		C	-4.41249	-2.17802	-0.01178
	O	-0.58043	2.14611	2.33020		O	-5.03564	-2.92725	0.74150
	H	-0.73287	1.54748	1.55497		C	-4.85746	-1.98875	-1.44373
	H	-1.28750	1.94230	2.96810		H	-5.17526	-0.95595	-1.60698
	C	2.82161	-1.74919	0.34438		H	-4.03709	-2.17893	-2.13788
	C	1.75715	-0.91215	0.05059		H	-5.68927	-2.66440	-1.64614
	C	2.00802	0.38065	-0.43052		C	-3.22323	-1.44216	0.47841
	C	3.32867	0.81072	-0.60228		N	-2.63676	-0.69612	-0.40244
	C	4.38611	-0.03527	-0.29672		O	-1.57723	-0.01499	0.02573
	C	4.15042	-1.33218	0.17736		O	-1.73646	1.66853	2.22158
	H	2.63437	-2.75108	0.71924		H	-1.03399	1.39091	2.83684
	H	0.73527	-1.23483	0.19412		H	-1.67585	1.04979	1.45347
	H	3.51403	1.81372	-0.97599		O	0.63055	4.11785	-0.17436
	H	5.39895	0.32909	-0.43988		H	0.53960	3.16923	-0.39572
	O	1.02723	1.28686	-0.69983		H	0.61483	4.59025	-1.02734
	C	-0.26565	0.83757	-1.28138		C	-2.76997	-1.60275	1.89903
	O	-0.23243	-0.14165	-2.04228		H	-2.97664	-0.70109	2.48396
	C	-0.99028	2.11555	-1.66463		H	-3.28263	-2.44529	2.36301
	H	-0.52797	2.52506	-2.56780		H	-1.68865	-1.76341	1.93186
	H	-2.02922	1.87095	-1.89185		O	-1.61952	4.39943	1.55296
	H	-0.96207	2.86231	-0.86997		H	-0.84611	4.42104	0.95406
	C	5.25280	-2.27064	0.50905		H	-1.69875	3.45700	1.81442
	O	5.01646	-3.40488	0.92034		C	5.04164	-1.71138	0.35981
	C	6.68357	-1.81450	0.33414		O	4.97021	-2.92010	0.56819
	H	6.87940	-1.53478	-0.70495		C	6.38333	-1.01625	0.39152
	H	6.89193	-0.93696	0.95277		H	6.60115	-0.54610	-0.57177
	H	7.35383	-2.62469	0.62106		H	6.39671	-0.22792	1.14950
						H	7.15883	-1.74777	0.61813
TS1$_{fcd}$ $\cdot\cdot 3H_2O$	C	-2.38326	-1.25137	-0.38069	**TS1$_{fce}$**$\cdot\cdot 3H_2O$	C	0.90914	0.57495	1.80455
	C	-2.13527	0.01850	0.17398		O	0.94086	-0.35475	2.58172
	C	-3.23702	0.76831	0.62868		C	1.70968	1.83807	1.91591
	C	-4.53323	0.26888	0.54483		H	1.30009	2.42974	2.74171
	C	-4.74572	-0.98880	-0.01132		H	2.73947	1.57261	2.15298
	C	-3.67908	-1.75096	-0.47712		H	1.67489	2.42568	1.00042
	H	-1.54493	-1.84131	-0.73616		C	4.82835	-2.01708	-0.39700

	H	-3.05997	1.75355	1.05237		O	5.57481	-2.43876	-1.28762
	H	-5.37262	0.85678	0.90624		C	5.11350	-2.36074	1.04972
	H	-3.85662	-2.73353	-0.90602		H	5.30295	-1.45449	1.62959
	Cl	-6.38334	-1.62495	-0.12197		H	4.25632	-2.85570	1.51023
	O	-0.89146	0.50462	0.28576		H	5.98716	-3.01264	1.08941
	H	0.82049	5.11291	-0.61567		C	3.66396	-1.17925	-0.72122
	O	0.93786	4.63009	0.22315		N	2.93710	-0.80320	0.29412
	H	1.43983	3.82806	-0.00989		O	1.89025	-0.05810	0.02355
	O	-1.12243	4.30523	2.16142		O	0.94381	1.81027	-1.74239
	H	-0.92094	3.38413	2.43555		H	0.03874	1.83355	-1.38676
	H	-0.46421	4.49017	1.46220		H	1.39943	1.10499	-1.21828
	O	-0.36398	1.65777	2.66767		O	-0.94603	5.25803	-0.21576
	H	-0.54049	1.24022	1.78163		H	-1.48443	4.44537	-0.23864
	H	-0.84705	1.11588	3.31664		H	-0.99673	5.57616	0.70477
	C	-0.05452	0.92178	-1.31376		C	3.35980	-0.80912	-2.14257
	O	0.01204	-0.07486	-2.02219		H	3.44214	0.27239	-2.29480
	C	-0.82840	2.16528	-1.66988		H	4.05140	-1.31153	-2.81889
	H	-0.36823	2.61512	-2.55511		H	2.33261	-1.08457	-2.40112
	H	-1.85152	1.88059	-1.91715		O	1.66494	4.47541	-1.11644
	H	-0.83070	2.88633	-0.85409		H	0.80148	4.79708	-0.78674
	C	4.51567	-0.03527	-0.11078		H	1.50565	3.53879	-1.36218
	C	3.50019	0.84770	-0.45534		C	-3.38687	-0.57221	-0.16090
	C	2.13438	0.50723	-0.33088		C	-2.38047	0.31306	0.18436
	C	1.83149	-0.77766	0.15945		C	-1.12680	-0.11229	0.67085
	C	2.82972	-1.65671	0.52118		C	-0.88980	-1.49374	0.73961
	C	4.16775	-1.27664	0.38436		C	-1.87405	-2.39096	0.36708
	H	5.55403	0.25172	-0.22531		C	-3.11486	-1.92612	-0.06796
	H	0.78868	-1.04135	0.26636		H	-4.34754	-0.21175	-0.51183
	H	2.58431	-2.63654	0.91657		H	0.06939	-1.84712	1.08665
	O	1.19483	1.39070	-0.66798		H	-1.68520	-3.45817	0.41339
	N	5.22337	-2.20232	0.76867		O	-0.25594	0.84252	1.02250
	O	4.89538	-3.31019	1.18978		N	-4.15063	-2.87929	-0.44486
	O	6.39189	-1.83567	0.65430		O	-3.89381	-4.07754	-0.35306
	N	3.92613	2.13745	-0.98582		O	-5.23023	-2.43914	-0.83495
	O	3.22473	3.12861	-0.79540		N	-2.66708	1.73420	0.01270
	O	4.99433	2.17501	-1.59356		O	-1.78680	2.44754	-0.47485
						O	-3.77670	2.14111	0.32929
1ga (MeCN)	C	-3.58620	-1.67843	-0.31271	**1gb** (MeCN)	C	-3.38985	-1.76252	0.13064
	C	-2.20228	-1.62199	-0.38181		C	-2.00781	-1.75284	0.02556
	C	-1.54283	-0.40318	-0.28453		C	-1.31838	-0.56271	-0.18611

	C	-2.28565	0.77346	-0.13142	C	-2.04197	0.63384	-0.28896
	C	-3.67138	0.73919	-0.08036	C	-3.42203	0.64799	-0.15960
	C	-4.29658	-0.49315	-0.16064	C	-4.07538	-0.55635	0.04042
	H	-4.10967	-2.62613	-0.38015	H	-3.92997	-2.68944	0.29057
	H	-1.61350	-2.52438	-0.51896	H	-1.43530	-2.67173	0.11028
	H	-4.24231	1.65427	0.02649	H	-3.97121	1.57997	-0.22924
	O	-0.17662	-0.38250	-0.44693	O	0.04064	-0.65644	-0.31366
	N	-5.76195	-0.54081	-0.09017	N	-5.53604	-0.55039	0.15955
	O	-6.36511	0.51907	0.03950	O	-6.11570	0.52811	0.07970
	O	-6.30099	-1.63957	-0.16533	O	-6.09993	-1.62602	0.33290
	C	2.04467	-0.37544	0.36659	C	2.27049	-0.14208	0.26844
	C	2.94548	-0.51072	1.42580	C	3.20246	0.50672	1.08236
	C	2.50227	-0.14371	-0.93287	C	2.72343	-0.94738	-0.78950
	C	4.31033	-0.41733	1.19301	C	4.56601	0.36647	0.85948
	H	2.57101	-0.68907	2.42887	H	2.85132	1.13007	1.89941
	C	3.86617	-0.04779	-1.17806	C	4.07712	-1.09345	-1.02058
	H	1.79891	-0.03706	-1.75138	H	2.01142	-1.45744	-1.42973
	C	4.74242	-0.18724	-0.10843	C	5.00831	-0.43796	-0.19852
	H	5.02764	-0.51975	1.99939	H	5.26463	0.88292	1.50753
	H	4.24567	0.13205	-2.17750	H	4.44442	-1.71173	-1.83459
	C	0.59512	-0.48282	0.67872	C	0.84510	0.05326	0.55619
	O	0.12373	-0.65279	1.77587	O	0.37053	0.73180	1.44025
	N	-1.64425	2.08786	-0.03393	N	-1.39241	1.91661	-0.56723
	O	-2.31084	3.06433	-0.35837	O	-1.93227	2.92914	-0.13659
	O	-0.49024	2.14321	0.37686	O	-0.36544	1.90908	-1.23753
	N	6.18712	-0.08754	-0.36392	O	6.30896	-0.64404	-0.50636
	O	6.95090	-0.21568	0.58813	C	7.30763	-0.00510	0.28687
	O	6.55612	0.11843	-1.51619	H	8.26335	-0.30876	-0.13832
					H	7.21466	1.08399	0.23419
					H	7.25170	-0.33319	1.32936
$TS1_{gab}$ (MeCN)	C	-3.46382	-2.39474	0.78164	**$TS1_{gac}$** (MeCN)	C	3.25905	-1.47137	-0.50408
	C	-2.73260	-1.05829	0.80887		C	1.94627	-1.36785	-0.06776
	C	-3.43558	-0.61904	-1.53406		C	1.29709	-0.11408	0.14121
	C	-4.18409	-1.94350	-1.57323		C	2.04992	1.03829	-0.21518
	C	-4.64736	-2.37315	-0.18286		C	3.33840	0.94998	-0.68544
	H	-3.39105	-0.25685	1.15002		C	3.94201	-0.31021	-0.82015
	H	-1.84675	-1.10196	1.43673		H	3.72807	-2.44168	-0.61829
	H	-2.75944	-3.18745	0.50262		H	1.57855	2.00641	-0.08030
	H	-3.79211	-2.61051	1.80223		H	3.89779	1.84271	-0.94397
	H	-4.07813	0.19329	-1.18297		O	0.11290	-0.02221	0.65502

	H	-3.02695	-0.35410	-2.50834		N	5.30425	-0.40580	-1.30173
	H	-5.03244	-1.82380	-2.25299		O	5.89532	0.63691	-1.58709
	H	-3.53442	-2.71151	-2.00953		O	5.81523	-1.52238	-1.40544
	H	-5.40878	-1.67491	0.18417		C	-1.21786	0.76158	-0.50220
	H	-5.11483	-3.36017	-0.23061		C	-1.72970	1.89401	0.35319
	N	-2.27154	-0.68988	-0.57457		C	-2.42213	2.89705	-0.33282
	H	-1.62529	-1.42959	-0.89458		C	-1.53619	1.99759	1.73227
	C	3.53024	-1.24131	-0.13460		C	-2.94023	3.98979	0.35107
	C	2.18703	-1.37234	0.18935		H	-2.54948	2.82666	-1.40892
	C	1.25097	-0.28839	0.05826		C	-2.04222	3.08871	2.42665
	C	1.80682	0.94257	-0.42195		H	-0.96568	1.24296	2.25888
	C	3.13528	1.07964	-0.72421		C	-2.74120	4.06293	1.72358
	C	4.00229	-0.02001	-0.57941		H	-3.48156	4.77200	-0.16918
	H	4.19886	-2.08641	-0.02652		H	-1.89356	3.18679	3.49614
	H	1.13793	1.78779	-0.53499		O	-0.74258	0.94702	-1.60488
	H	3.52823	2.02897	-1.07217		N	1.24771	-2.61529	0.18617
	O	0.00653	-0.41193	0.33112		O	0.02911	-2.67713	-0.01515
	N	5.40165	0.12228	-0.89264		O	1.90360	-3.58272	0.56283
	O	5.80288	1.21841	-1.29445		C	-3.34104	-2.26000	0.84111
	O	6.14524	-0.85269	-0.74972		C	-2.64419	-0.91031	0.93315
	C	-1.40896	0.58869	-0.73975		C	-3.04894	-0.65434	-1.47617
	C	-1.72826	1.73486	0.18369		C	-3.73422	-2.01098	-1.44618
	C	-2.34834	2.83152	-0.42496		H	-3.36518	-0.12628	1.16796
	C	-1.42687	1.77028	1.54698		H	-1.85355	-0.93097	1.68087
	C	-2.68951	3.95161	0.32252		H	-2.60800	-3.05978	0.66840
	H	-2.56014	2.81108	-1.48984		H	-3.85432	-2.45905	1.78335
	C	-1.75408	2.88844	2.30272		H	-3.76944	0.14744	-1.29789
	H	-0.90862	0.94113	2.01211		H	-2.54169	-0.48643	-2.42598
	C	-2.38600	3.95672	1.67753		H	-4.53523	-2.02308	-2.18722
	H	-3.17419	4.80589	-0.13668		H	-3.01730	-2.80589	-1.69742
	H	-1.51798	2.93476	3.35992		N	-2.02001	-0.58082	-0.38644
	O	-0.97670	0.75334	-1.85799		H	-1.28234	-1.28527	-0.55270
	N	1.76188	-2.67640	0.65670		O	-4.32401	-2.26552	-0.18223
	O	0.74738	-2.76950	1.34584		N	-3.28064	5.21479	2.45634
	O	2.45312	-3.65537	0.34877		O	-3.08974	5.27014	3.66806
	N	-2.73675	5.13799	2.47647		O	-3.89734	6.06610	1.82175
	O	-2.45567	5.13120	3.67151					
	O	-3.29448	6.07334	1.90965					
TS1$_{gbb}$ (MeCN)	C	-3.53113	-2.45410	0.73867	**TS1$_{gbc}$** (MeCN)	C	3.53606	-1.07892	-0.01510
	C	-2.69085	-1.18286	0.76186		C	2.18082	-1.28661	0.19885

	C	-3.57466	-0.54252	-1.46224		C	1.18926	-0.29420	-0.10881
	C	-4.43464	-1.79824	-1.50169		C	1.69636	0.93779	-0.63331
	C	-4.79662	-2.27953	-0.09808		C	3.03567	1.15267	-0.82500
	H	-3.24384	-0.35665	1.21221		C	3.96043	0.13833	-0.51527
	H	-1.75589	-1.33059	1.29658		H	4.24872	-1.85928	0.22200
	H	-2.92843	-3.28169	0.34541		H	0.98554	1.71594	-0.88132
	H	-3.77636	-2.70814	1.77386		H	3.39172	2.10034	-1.21472
	H	-4.11037	0.29321	-1.00382		O	-0.06344	-0.51206	0.06098
	H	-3.24261	-0.24647	-2.45635		N	5.36986	0.36478	-0.71621
	H	-5.33185	-1.56996	-2.08417		O	5.72844	1.45608	-1.16761
	H	-3.89782	-2.58628	-2.04337		O	6.16294	-0.53714	-0.43177
	H	-5.45725	-1.54835	0.38277		C	-1.43885	0.52938	-0.84427
	H	-5.34859	-3.22177	-0.15293		C	-1.67080	1.66242	0.10499
	N	-2.33711	-0.76087	-0.63451		C	-2.20505	2.83313	-0.45534
	H	-1.78812	-1.52044	-1.06555		C	-1.38207	1.64323	1.46896
	C	3.57563	-1.04138	-0.00152		C	-2.46344	3.94135	0.33193
	C	2.22332	-1.26609	0.21100		H	-2.41516	2.86906	-1.52043
	C	1.21945	-0.28694	-0.09370		C	-1.62845	2.75512	2.26948
	C	1.70903	0.95273	-0.61357		H	-0.92799	0.76687	1.91675
	C	3.04626	1.18583	-0.80307		C	-2.17806	3.90956	1.70331
	C	3.98401	0.18348	-0.49697		H	-2.88138	4.84763	-0.09720
	H	4.29806	-1.81349	0.23325		H	-1.37820	2.70693	3.32315
	H	0.98947	1.72256	-0.86043		O	-1.12755	0.68184	-2.00912
	H	3.38960	2.13990	-1.18857		N	1.80406	-2.57667	0.74316
	O	-0.03121	-0.52792	0.07754		O	0.74681	-2.68494	1.36242
	N	5.39085	0.42974	-0.69591		O	2.58022	-3.52434	0.57366
	O	5.73498	1.52724	-1.14304		C	-3.61384	-2.38742	0.69691
	O	6.19534	-0.46258	-0.41383		C	-2.72249	-1.15613	0.75111
	C	-1.38046	0.47818	-0.82379		C	-3.62543	-0.53552	-1.44424
	C	-1.63226	1.62233	0.11370		C	-4.48102	-1.79033	-1.38539
	C	-2.17968	2.77966	-0.46040		H	-3.24787	-0.32715	1.22558
	C	-1.34940	1.62306	1.47860		H	-1.79377	-1.36783	1.27736
	C	-2.45532	3.89390	0.31319		H	-3.06615	-3.23988	0.26928
	H	-2.38527	2.80117	-1.52671		H	-3.91957	-2.64983	1.71107
	C	-1.61277	2.74098	2.26628		H	-4.15417	0.31703	-1.01225
	H	-0.88927	0.75643	1.93901		H	-3.33319	-0.30498	-2.46865
	C	-2.17461	3.88172	1.68559		H	-5.42352	-1.60531	-1.90355
	H	-2.88302	4.78985	-0.12798		H	-3.96784	-2.62411	-1.88640
	H	-1.36648	2.70741	3.32149		N	-2.37275	-0.72930	-0.64100
	O	-1.05610	0.63764	-1.98842		H	-1.81041	-1.47881	-1.07544

	N	1.86285	-2.56260	0.75311		O	-4.79569	-2.14339	-0.04898
	O	0.82185	-2.67770	1.39717		O	-2.45938	5.04311	2.39400
	O	2.63763	-3.50581	0.55646		C	-2.18615	5.06847	3.79229
	O	-2.47305	5.02029	2.36299		H	-1.11864	4.92712	3.98899
	C	-2.20400	5.06401	3.76122		H	-2.48981	6.05612	4.13748
	H	-1.13543	4.93746	3.96265		H	-2.76428	4.30449	4.32179
	H	-2.52028	6.05160	4.09529					
	H	-2.77421	4.29895	4.29787					
1gc (MeCN)	C	-2.66653	-1.74187	0.09344	**1gd** (MeCN)	C	-2.66974	-1.74477	0.08118
	C	-1.28428	-1.75352	-0.01270		C	-1.28788	-1.75463	-0.02739
	C	-0.57678	-0.57115	-0.20134		C	-0.57995	-0.57027	-0.20616
	C	-1.27809	0.64016	-0.28000		C	-1.28340	0.64072	-0.27197
	C	-2.65797	0.67407	-0.15072		C	-2.66287	0.67338	-0.13905
	C	-3.33099	-0.52286	0.02652		C	-3.33535	-0.52544	0.02764
	H	-3.22219	-2.66247	0.23583		H	-3.22466	-2.66699	0.21556
	H	-0.72717	-2.68343	0.05292		H	-0.73031	-2.68486	0.02870
	H	-3.19167	1.61615	-0.20199		H	-3.19686	1.61582	-0.18006
	O	0.78298	-0.68603	-0.33381		O	0.77784	-0.68293	-0.34073
	N	-4.79194	-0.49439	0.14739		N	-4.79564	-0.49898	0.15103
	O	-5.35254	0.59531	0.09030		O	-5.35742	0.59079	0.10458
	O	-5.37340	-1.56369	0.29899		O	-5.37662	-1.56989	0.29421
	C	3.02698	-0.24066	0.26067		C	3.02177	-0.23421	0.25631
	C	3.96511	0.36302	1.10363		C	3.96438	0.36979	1.09627
	C	3.45456	-1.01203	-0.82435		C	3.45408	-1.00492	-0.82803
	C	5.32338	0.20014	0.86920		C	5.31973	0.20184	0.85264
	H	3.62472	0.96165	1.94308		H	3.62429	0.97127	1.93411
	C	4.81229	-1.17984	-1.06651		C	4.81417	-1.16566	-1.06271
	H	2.73115	-1.48243	-1.48173		H	2.73084	-1.47420	-1.48676
	C	5.73242	-0.57162	-0.21633		C	5.76649	-0.56941	-0.22835
	H	6.05762	0.66625	1.51926		H	6.04483	0.67839	1.50836
	H	5.15351	-1.77674	-1.90687		H	5.14204	-1.76285	-1.91027
	C	1.59601	-0.02810	0.55777		C	1.59470	-0.02131	0.55134
	O	1.14676	0.62713	1.46905		O	1.13727	0.63489	1.45952
	N	-0.60649	1.91814	-0.52882		N	-0.61324	1.92067	-0.51254
	O	-1.14655	2.93260	-0.10374		O	-1.14098	2.92933	-0.05859
	O	0.43966	1.90517	-1.16884		O	0.41821	1.91561	-1.17594
	Cl	7.43654	-0.78065	-0.51757		C	7.23938	-0.77154	-0.46924
						H	7.81203	0.12031	-0.20337
						H	7.61662	-1.59713	0.14350
						H	7.44405	-1.01571	-1.51398

1ge (MeCN)				
	C	-2.64977	-1.70741	0.53849
	C	-1.26558	-1.70540	0.47391
	C	-0.57644	-0.61085	-0.04236
	C	-1.30742	0.49674	-0.49594
	C	-2.69066	0.52597	-0.41319
	C	-3.34162	-0.58486	0.09653
	H	-3.18779	-2.56130	0.93576
	H	-0.68950	-2.55474	0.82886
	H	-3.24404	1.39295	-0.75547
	O	0.78358	-0.71334	-0.09714
	N	-4.80437	-0.56832	0.16993
	O	-5.38991	0.43584	-0.22374
	O	-5.36595	-1.56118	0.62211
	C	2.98291	-0.00128	0.37719
	C	3.89349	0.87233	0.99224
	C	3.48965	-1.07121	-0.37716
	C	5.25519	0.69274	0.86504
	H	3.51481	1.70506	1.57807
	C	4.84973	-1.26378	-0.51482
	H	2.80777	-1.76165	-0.86304
	C	5.77826	-0.38614	0.10388
	H	5.91973	1.39237	1.35699
	H	5.19640	-2.10188	-1.10677
	C	1.55753	0.24305	0.54730
	O	1.03530	1.14346	1.17247
	N	-0.66000	1.65765	-1.10941
	O	-1.20555	2.74716	-0.97446
	O	0.37004	1.47162	-1.74830
	N	7.12270	-0.57240	-0.02768
	C	7.63526	-1.68295	-0.81542
	H	8.72383	-1.66165	-0.79948
	H	7.31189	-2.64867	-0.41065
	H	7.31270	-1.62006	-1.86095
	C	8.05590	0.34142	0.61319
	H	9.07471	0.02653	0.39282
	H	7.93390	1.36706	0.24671
	H	7.93355	0.34595	1.70223

$TS1_{gcb}$ (MeCN)				
	C	-3.00608	-2.82968	0.63597
	C	-2.43805	-1.41800	0.71890
	C	-2.90227	-1.07948	-1.69482
	C	-3.48207	-2.48312	-1.79672
	C	-4.05875	-2.95373	-0.46313
	H	-3.21900	-0.69601	0.96459
	H	-1.63498	-1.35298	1.44846
	H	-2.18939	-3.54021	0.46042
	H	-3.42892	-3.07251	1.61491
	H	-3.67261	-0.34703	-1.43823
	H	-2.41538	-0.77306	-2.61962
	H	-4.24940	-2.46960	-2.57599
	H	-2.69962	-3.17303	-2.13469
	H	-4.93377	-2.34546	-0.20531
	H	-4.40132	-3.98873	-0.54474
	N	-1.86186	-1.00432	-0.60609
	H	-1.09891	-1.66007	-0.83718
	C	3.79740	-0.35872	1.07109
	C	2.47141	-0.76588	1.08792
	C	1.40435	0.04989	0.57793
	C	1.80127	1.33015	0.07312
	C	3.10725	1.74386	0.07615
	C	4.11139	0.89382	0.57539
	H	4.57083	-1.01191	1.45625
	H	1.03174	1.98283	-0.31984
	H	3.37609	2.72389	-0.30333
	O	0.18744	-0.35318	0.56244
	N	5.48532	1.32858	0.57839
	O	5.74609	2.44772	0.12763
	O	6.34806	0.56895	1.02835
	C	-1.14129	0.38003	-0.69958
	C	-1.75788	1.49075	0.10432
	C	-2.38980	2.49326	-0.63825
	C	-1.72335	1.58957	1.49719
	C	-2.99974	3.57047	-0.00380
	H	-2.40150	2.43444	-1.72270
	C	-2.32132	2.66710	2.14039
	H	-1.20316	0.84338	2.08565
	C	-2.96018	3.64511	1.38391
	H	-3.49323	4.34438	-0.58412

				H	-2.28378	2.74825	3.22263
				O	-0.59919	0.56506	-1.77052
				N	2.20693	-2.07918	1.64242
				O	1.09960	-2.31892	2.12063
				O	3.12396	-2.90886	1.62649
				Cl	-3.71529	4.99615	2.19230
TS1$_{gcc}$ (MeCN)	C	3.41721	-0.69510	0.42786	**TS1$_{gdb}$** (MeCN)	C	-3.16638	-2.92653	0.90408
	C	2.06554	-1.00582	0.44214		C	-2.50126	-1.56223	0.76463
	C	1.11088	-0.34936	-0.40232		C	-3.28644	-1.40573	-1.58060
	C	1.63381	0.69914	-1.22214		C	-3.96786	-2.76175	-1.46118
	C	2.96366	1.03273	-1.21580		C	-4.37394	-3.06444	-0.02032
	C	3.85967	0.32820	-0.39128		H	-3.18882	-0.76127	1.04186
	H	4.10786	-1.23287	1.06628		H	-1.59905	-1.49304	1.36711
	H	0.94449	1.21974	-1.87643		H	-2.43282	-3.71269	0.68810
	H	3.33551	1.83098	-1.84933		H	-3.45718	-3.04725	1.95151
	O	-0.12228	-0.70834	-0.43625		H	-3.96063	-0.59374	-1.29503
	N	5.26033	0.67263	-0.39303		H	-2.92014	-1.22272	-2.58983
	O	5.63560	1.59210	-1.12535		H	-4.83814	-2.75702	-2.12372
	O	6.02831	0.03702	0.33428		H	-3.29093	-3.53996	-1.83366
	C	-1.58696	0.45294	-1.06289		H	-5.15984	-2.36771	0.29460
	C	-1.60857	1.49855	0.01484		H	-4.79268	-4.07198	0.05005
	C	-2.09142	2.75108	-0.37784		N	-2.09777	-1.31659	-0.66075
	C	-1.17830	1.31316	1.33218		H	-1.42233	-2.04858	-0.92953
	C	-2.16716	3.80141	0.53044		C	3.74745	-0.69634	0.30488
	H	-2.40930	2.90572	-1.40448		C	2.42329	-1.06922	0.48431
	C	-1.24260	2.35913	2.24490		C	1.32590	-0.29088	-0.01642
	H	-0.76315	0.36396	1.64920		C	1.68953	0.91348	-0.69883
	C	-1.74191	3.59286	1.83750		C	2.99589	1.29570	-0.85728
	H	-2.54764	4.77053	0.22184		C	4.03029	0.48606	-0.35423
	H	-0.89845	2.21665	3.26495		H	4.54426	-1.31986	0.69147
	O	-1.43692	0.71742	-2.23738		H	0.89661	1.53380	-1.09632
	N	1.64938	-2.04706	1.36322		H	3.24099	2.22027	-1.36898
	O	0.50743	-2.02056	1.82314		O	0.10725	-0.66880	0.12960
	O	2.47566	-2.90971	1.67366		N	5.40457	0.88910	-0.51995
	C	-3.63291	-2.53400	0.49962		O	5.63688	1.94718	-1.11130
	C	-2.71952	-1.31877	0.54764		O	6.29468	0.16392	-0.06708
	C	-3.85137	-0.52154	-1.47972		C	-1.30136	-0.00114	-0.99542
	C	-4.71918	-1.76793	-1.41774		C	-1.76380	1.22574	-0.26107
	H	-3.18002	-0.52402	1.13504		C	-2.42927	2.18293	-1.03211
	H	-1.74248	-1.57483	0.95299		C	-1.56886	1.47130	1.10138

	H	-3.15246	-3.35532	-0.05187		C	-2.90676	3.35319	-0.44825
	H	-3.82627	-2.87207	1.51896		H	-2.57065	2.00985	-2.09520
	H	-4.30973	0.30109	-0.92619		C	-2.04019	2.64652	1.67304
	H	-3.67289	-0.21603	-2.51045		H	-1.02532	0.75882	1.71105
	H	-5.71029	-1.53184	-1.80879		C	-2.71979	3.60551	0.91251
	H	-4.28302	-2.56523	-2.03711		H	-3.42820	4.08122	-1.06552
	N	-2.51827	-0.79225	-0.84176		H	-1.87154	2.82438	2.73303
	H	-2.02861	-1.51752	-1.39147		O	-0.91098	0.02653	-2.14901
	O	-4.88680	-2.22089	-0.08527		N	2.19460	-2.30807	1.20329
	Cl	-1.82519	4.90426	2.98617		O	1.13294	-2.46995	1.80209
						O	3.09685	-3.15357	1.19769
						C	-3.20533	4.88491	1.54439
						H	-2.37433	5.58218	1.69313
						H	-3.94839	5.38316	0.91780
						H	-3.65228	4.69848	2.52448
TS1$_{gdc}$ (MeCN)	C	3.75540	-0.63591	0.34259	**TS1$_{geb}$** (MeCN)	C	-2.03186	3.92637	-1.07731
	C	2.43496	-1.03292	0.49943		C	-1.67275	2.47074	-0.80150
	C	1.33357	-0.28349	-0.03923		C	-2.51183	2.68698	1.51609
	C	1.69091	0.91753	-0.73368		C	-2.89295	4.13933	1.26318
	C	2.99217	1.32215	-0.87024		C	-3.19971	4.39358	-0.21135
	C	4.03062	0.54050	-0.32998		H	-2.51045	1.81147	-1.03564
	H	4.55541	-1.23677	0.75728		H	-0.79694	2.15913	-1.36568
	H	0.89400	1.51464	-1.15905		H	-1.15333	4.55850	-0.89962
	H	3.23164	2.24204	-1.39295		H	-2.27171	4.01374	-2.14093
	O	0.12039	-0.67760	0.08197		H	-3.33681	2.01093	1.27594
	N	5.39982	0.96690	-0.47218		H	-2.20987	2.52073	2.54921
	O	5.62523	2.02049	-1.07461		H	-3.75709	4.37327	1.89170
	O	6.29382	0.26594	0.01070		H	-2.07517	4.79044	1.59494
	C	-1.34345	-0.00555	-1.04692		H	-4.10876	3.85083	-0.49670
	C	-1.80218	1.20644	-0.29435		H	-3.39592	5.45620	-0.37883
	C	-2.47143	2.17326	-1.05096		N	-1.35608	2.27105	0.65074
	C	-1.59776	1.43446	1.06996		H	-0.54681	2.86542	0.88490
	C	-2.94662	3.33477	-0.44924		C	4.05248	-0.06377	-0.42760
	H	-2.61495	2.01538	-2.11614		C	2.87610	0.65571	-0.57730
	C	-2.06750	2.60152	1.65875		C	1.67230	0.32373	0.12708
	H	-1.04220	0.71925	1.66534		C	1.75289	-0.82087	0.97966
	C	-2.75595	3.56730	0.91475		C	2.90750	-1.54862	1.11039
	H	-3.46617	4.07334	-1.05538		C	4.06259	-1.16762	0.40536
	H	-1.88636	2.76958	2.71815		H	4.94247	0.23026	-0.97046
	O	-0.97305	0.02014	-2.20258		H	0.87082	-1.10696	1.53683

	N	2.21414	-2.26354	1.23302		H	2.93882	-2.41832	1.75799
	O	1.13088	-2.45163	1.78486		O	0.60783	1.03607	-0.00110
	O	3.14299	-3.07832	1.28827		N	5.27681	-1.93368	0.54562
	C	-3.15475	-2.96043	0.84358		O	5.26564	-2.91569	1.29259
	C	-2.46162	-1.61057	0.73916		O	6.27756	-1.57934	-0.08331
	C	-3.29679	-1.48008	-1.56537		C	-0.85501	0.84189	1.13283
	C	-3.95808	-2.83036	-1.34265		C	-1.60602	-0.31022	0.54208
	H	-3.13493	-0.81228	1.05162		C	-2.41086	-1.04896	1.41679
	H	-1.54927	-1.59148	1.33195		C	-1.55123	-0.71848	-0.79461
	H	-2.45919	-3.77108	0.58183		C	-3.15453	-2.13398	0.98017
	H	-3.48551	-3.11085	1.87256		H	-2.44947	-0.76821	2.46557
	H	-3.97422	-0.66583	-1.29900		C	-2.28073	-1.80638	-1.24551
	H	-2.97350	-1.36490	-2.59990		H	-0.90360	-0.20264	-1.49496
	H	-4.88005	-2.87681	-1.92475		C	-3.11986	-2.53995	-0.37366
	H	-3.29386	-3.63930	-1.68022		H	-3.75966	-2.66855	1.70253
	N	-2.08541	-1.34930	-0.68737		H	-2.18505	-2.09131	-2.28635
	H	-1.38824	-2.05680	-0.97101		O	-0.48761	0.86686	2.29986
	O	-4.30684	-3.02066	0.01791		N	2.92230	1.78529	-1.48782
	C	-3.28541	4.81395	1.57533		O	1.88901	2.15353	-2.04321
	H	-3.48884	5.59870	0.84335		O	4.01776	2.32295	-1.68368
	H	-4.22078	4.60208	2.10373		N	-3.86562	-3.60296	-0.82323
	H	-2.57762	5.20464	2.31092		C	-3.68735	-4.08655	-2.18184
						H	-2.66545	-4.44333	-2.36803
						H	-4.37278	-4.91444	-2.36021
						H	-3.91738	-3.30608	-2.91430
						C	-4.58124	-4.43447	0.12959
						H	-5.32238	-3.85243	0.68706
						H	-5.11649	-5.21641	-0.40804
						H	-3.90800	-4.91595	0.85142

TS1$_{gec}$ (MeCN)				
	C	-4.04376	-0.06354	0.43803
	C	-2.86834	0.66011	0.57973
	C	-1.67504	0.34465	-0.15165
	C	-1.76650	-0.78756	-1.02119
	C	-2.91962	-1.51784	-1.14460
	C	-4.06406	-1.15316	-0.41282
	H	-4.92546	0.21691	1.00108
	H	-0.89233	-1.05996	-1.59799
	H	-2.95914	-2.37643	-1.80643
	O	-0.61065	1.05568	-0.03562
	N	-5.27737	-1.92159	-0.54502
	O	-5.27521	-2.89103	-1.30849
	O	-6.26879	-1.58215	0.10667
	C	0.88913	0.84767	-1.17078
	C	1.61692	-0.30713	-0.56753
	C	2.42221	-1.05920	-1.43159
	C	1.54237	-0.70866	0.77100
	C	3.14890	-2.14960	-0.98220
	H	2.47627	-0.78283	-2.48088
	C	2.25474	-1.80170	1.23412
	H	0.89117	-0.18410	1.46147
	C	3.09463	-2.54912	0.37357
	H	3.75680	-2.69363	-1.69506
	H	2.14530	-2.08106	2.27508
	O	0.54160	0.89084	-2.33925
	N	-2.90463	1.77397	1.50885
	O	-1.85912	2.16047	2.02890
	O	-4.00351	2.28259	1.75712
	C	2.09272	3.91442	1.03967
	C	1.67329	2.47344	0.79186
	C	2.53067	2.72320	-1.48988
	C	2.91974	4.14766	-1.13029
	H	2.48665	1.79330	1.04510
	H	0.77974	2.22053	1.35989
	H	1.25569	4.59883	0.83799
	H	2.38321	4.02664	2.08563
	H	3.35032	2.03155	-1.28353
	H	2.24263	2.64585	-2.53820
	H	3.81986	4.42440	-1.68195
	H	2.11497	4.84365	-1.40898

2ga (MeCN)				
	C	5.54988	0.69319	-0.46255
	C	4.05027	0.95670	-0.29754
	C	3.60587	-1.40050	0.06951
	C	5.09067	-1.78139	-0.06954
	C	5.96193	-0.56971	0.30094
	H	3.84084	1.21100	0.74992
	H	3.73862	1.81619	-0.89989
	H	5.78421	0.58749	-1.52863
	H	6.12127	1.55623	-0.10161
	H	3.37965	-1.23775	1.13124
	H	2.96931	-2.22688	-0.26576
	H	5.29076	-2.57963	0.65664
	H	5.85863	-0.37765	1.37692
	H	7.01962	-0.79660	0.12496
	N	3.20489	-0.18823	-0.65048
	H	3.26863	-0.35168	-1.65487
	C	5.41606	-2.33575	-1.45992
	H	6.47172	-2.61677	-1.53210
	H	4.81853	-3.22831	-1.67378
	H	5.21829	-1.61037	-2.25544

2gb (MeCN)				
	C	5.53597	0.64385	-0.43398
	C	4.04185	0.94951	-0.30090
	C	3.59686	-1.39533	0.08851
	C	5.09099	-1.70085	-0.04480
	H	3.82168	1.23473	0.73622
	H	3.76575	1.79991	-0.93384
	H	5.78144	0.49269	-1.49340
	H	6.13439	1.49165	-0.08305
	H	3.35130	-1.24396	1.14787
	H	2.99844	-2.24316	-0.26233
	H	5.36738	-2.55142	0.58780
	N	3.18509	-0.19174	-0.64343
	H	3.26953	-0.37400	-1.64466
	H	5.31079	-1.98592	-1.08206
	N	5.94764	-0.55970	0.29786
	H	5.86328	-0.37747	1.29905

	N	1.36474	2.28138	-0.65927				
	H	0.54769	2.86576	-0.89658				
	O	3.21609	4.27393	0.25072				
	N	3.82031	-3.61797	0.83459				
	C	4.56769	-4.44243	-0.09981				
	H	5.08140	-5.23095	0.44884				
	H	3.91754	-4.91589	-0.84700				
	H	5.32855	-3.85768	-0.62777				
	C	3.65138	-4.07349	2.20411				
	H	4.32228	-4.91172	2.38846				
	H	3.90425	-3.28472	2.92045				
	H	2.62560	-4.40773	2.40746				
1h (MeCN)	S	-1.44391	-0.63395	0.84082	**2gc** (MeCN)	C	-1.14730	-0.99799	0.14001
	O	-0.97925	0.42632	1.71916		C	-1.25490	0.52505	0.03137
	O	-1.34055	-2.01643	1.26600		C	1.20972	0.66006	0.00004
	O	-0.56795	-0.48204	-0.57683		C	1.26462	-0.86618	0.10599
	C	0.80336	-0.42744	-0.45889		H	-1.37742	0.81329	-1.02104
	C	1.47847	0.77071	-0.19005		H	-2.12155	0.89554	0.58533
	C	1.52914	-1.60112	-0.62768		H	-1.17761	-1.28514	1.19744
	C	2.85860	0.80072	-0.07855		H	-2.00638	-1.46215	-0.35276
	C	2.91448	-1.58575	-0.54324		H	1.27227	0.96629	-1.05267
	H	0.99058	-2.52256	-0.82765		H	2.03085	1.12932	0.54296
	C	3.55344	-0.38330	-0.26835		H	2.15472	-1.23694	-0.41016
	H	3.37652	1.72807	0.13949		N	-0.04621	1.14935	0.55917
	H	3.49157	-2.49368	-0.68200		H	1.35513	-1.14750	1.16140
	C	-3.03866	-0.28717	0.18069		N	0.08319	-1.53370	-0.44153
	C	-3.42502	1.04414	0.03440		H	0.06201	-1.40974	-1.45483
	C	-3.86433	-1.35425	-0.16550		C	-0.08419	2.12506	1.48548
	C	-4.68935	1.30767	-0.48084		O	0.89592	2.70438	1.96144
	H	-2.75712	1.85207	0.31821		H	-1.11143	2.37454	1.80185
	C	-5.12613	-1.06955	-0.67898					
	H	-3.53239	-2.37926	-0.02993					
	C	-5.53393	0.25475	-0.83597					
	H	-5.01599	2.33637	-0.60304					
	H	-5.79052	-1.88368	-0.95391					
	H	-6.52126	0.46937	-1.23648					
	N	5.01828	-0.35741	-0.17116					
	O	5.61981	-1.41273	-0.33726					
	O	5.55782	0.71699	0.07079					
	N	0.76741	2.04358	-0.03026					

	O	1.24077	2.85205	0.76002				
	O	-0.23266	2.23533	-0.71084				
TS2$_{hc}$ (MeCN)	S	1.00259	0.11692	0.33218	**TS2$_{h2ga}$** (MeCN)	S	1.12752	0.19646	-0.82237
	O	1.36502	0.59695	1.65053		O	1.39889	1.27487	-1.75448
	O	0.83665	0.91187	-0.87212		O	0.87445	-1.19750	-1.15274
	O	-1.00522	0.36631	0.94979		O	-0.82116	0.75759	-0.87556
	C	-2.10206	0.52104	0.29035		C	-1.90612	0.11834	-0.55657
	C	-2.17258	0.59535	-1.13574		C	-1.95202	-1.24605	-0.15164
	C	-3.35654	0.67471	0.97118		C	-3.17268	0.77665	-0.64584
	C	-3.35688	0.79217	-1.79997		C	-3.13782	-1.87820	0.13906
	H	-1.25266	0.51656	-1.69897		H	-1.02699	-1.80320	-0.10025
	C	-4.54971	0.90365	0.30552		C	-4.37277	0.13708	-0.38655
	C	-4.55151	0.94559	-1.07789		C	-4.35021	-1.18547	0.02271
	H	-3.37677	0.83888	-2.88356		H	-3.14177	-2.91759	0.44952
	H	-5.46851	1.03102	0.86519		H	-5.30951	0.67238	-0.48736
	C	0.56895	-1.59851	0.21774		C	1.07595	0.63641	0.89804
	C	0.58491	-2.35950	1.38319		C	1.22661	1.97760	1.23757
	C	0.23154	-2.12372	-1.02559		C	0.88341	-0.36487	1.84386
	C	0.25552	-3.70769	1.28773		C	1.18702	2.32072	2.58531
	H	0.83375	-1.90870	2.33941		H	1.35866	2.73422	0.46982
	C	-0.09669	-3.47537	-1.09730		C	0.84461	0.00095	3.18759
	H	0.21796	-1.50216	-1.91625		H	0.76587	-1.40348	1.54953
	C	-0.08300	-4.26251	0.05296		C	0.99664	1.33643	3.55587
	H	0.25874	-4.32329	2.18274		H	1.30066	3.36144	2.87533
	H	-0.36462	-3.90911	-2.05650		H	0.69455	-0.76377	3.94440
	H	-0.34113	-5.31610	-0.01181		H	0.96464	1.61357	4.60613
	N	-5.79472	1.15560	-1.77627		N	-5.59515	-1.85338	0.32356
	O	-6.82939	1.29164	-1.11745		O	-6.64741	-1.22127	0.20633
	O	-5.77436	1.19148	-3.00975		O	-5.55328	-3.03128	0.68578
	N	-3.43603	0.61678	2.42126		C	5.54293	0.64754	-0.61023
	O	-4.32077	1.27918	2.97414		C	4.06643	0.96974	-0.39423
	O	-2.64973	-0.09655	3.03801		C	3.59340	-1.38338	0.13929
	C	5.22546	-1.10073	0.51589		C	5.06523	-1.78300	-0.03443
	C	3.74016	-1.08682	0.85651		C	5.96626	-0.56554	0.22036
	C	3.28222	-0.71754	-1.51460		H	3.88658	1.24945	0.64764
	C	4.78652	-0.74346	-1.75755		H	3.73378	1.78779	-1.03523
	H	3.33653	-2.10043	0.81158		H	5.72619	0.47453	-1.67648
	H	3.57056	-0.67235	1.85199		H	6.13270	1.52605	-0.33168
	H	5.65242	-0.09429	0.63516		H	3.40782	-1.11100	1.18162
	H	5.75070	-1.78199	1.18773		H	2.92585	-2.20540	-0.12709

	H	2.87076	-1.72278	-1.62469		H	5.26457	-2.52519	0.74675
	H	2.78309	-0.04168	-2.21139		H	5.91600	-0.30091	1.28354
	H	4.99287	-1.16313	-2.74382		H	7.00879	-0.82288	0.00924
	H	5.19597	0.27652	-1.71929		N	3.21448	-0.20975	-0.68580
	N	3.00188	-0.26015	-0.13096		H	3.33005	-0.44975	-1.67845
	H	3.32862	0.71499	-0.04243		N	-3.26475	2.17567	-1.04092
	O	5.44299	-1.56778	-0.80675		O	-4.25405	2.51925	-1.69411
						O	-2.38406	2.95500	-0.69126
						C	5.33588	-2.45569	-1.38357
						H	6.37703	-2.78544	-1.44200
						H	4.69901	-3.33546	-1.51736
						H	5.16221	-1.78959	-2.23511
TS2$_{h2gb}$ (MeCN)	S	1.30941	0.21013	-0.88874	**TS2$_{h2gc}$** (MeCN)	S	0.90343	0.43932	-0.95070
	O	1.60555	1.44320	-1.59385		O	1.05233	1.75731	-1.52970
	O	0.96324	-1.07256	-1.48127		O	0.58770	-0.79092	-1.65171
	O	-0.61515	0.86875	-0.73793		O	-1.17611	0.97959	-0.68966
	C	-1.72473	0.23293	-0.51673		C	-2.23859	0.28063	-0.50696
	C	-1.83451	-1.18242	-0.39586		C	-2.26069	-1.15084	-0.55430
	C	-2.95679	0.95466	-0.42368		C	-3.51603	0.90039	-0.27929
	C	-3.04421	-1.80382	-0.19654		C	-3.41317	-1.87279	-0.38312
	H	-0.93965	-1.78140	-0.49211		H	-1.33178	-1.66710	-0.75709
	C	-4.18214	0.33260	-0.25529		C	-4.68739	0.17360	-0.13542
	C	-4.22049	-1.04520	-0.12473		C	-4.63368	-1.20887	-0.16942
	H	-3.09604	-2.88338	-0.10390		H	-3.39304	-2.95675	-0.42023
	H	-5.09098	0.92091	-0.21053		H	-5.62886	0.68672	0.01860
	C	1.33675	0.29154	0.88530		C	0.90031	0.35954	0.81825
	C	1.57266	1.52620	1.48254		C	1.05792	1.54529	1.53043
	C	1.12342	-0.87246	1.61612		C	0.74645	-0.87957	1.43279
	C	1.59986	1.58725	2.87226		C	1.07026	1.47592	2.91954
	H	1.71837	2.41721	0.87898		H	1.15203	2.49686	1.01532
	C	1.15243	-0.78837	3.00642		C	0.76022	-0.92475	2.82446
	H	0.93819	-1.82210	1.12290		H	0.61409	-1.78654	0.84999
	C	1.39052	0.43479	3.63056		C	0.92277	0.24643	3.56274
	H	1.78046	2.54001	3.36190		H	1.18943	2.38695	3.49902
	H	0.98744	-1.68411	3.59845		H	0.64122	-1.87969	3.32829
	H	1.41106	0.49193	4.71554		H	0.93131	0.20207	4.64848
	N	-5.49105	-1.70059	0.07898		N	-5.84466	-1.96722	0.00967
	O	-6.51048	-1.00873	0.13288		O	-6.90529	-1.36061	0.18676
	O	-5.50358	-2.92866	0.19045		O	-5.77421	-3.19953	-0.02137
	N	-2.98519	2.40723	-0.52345		N	-3.64999	2.34486	-0.20837

	O	-3.97473	2.92319	-1.05117	O	-4.73167	2.83892	-0.54714
	O	-2.05266	3.05710	-0.06138	O	-2.70807	3.01869	0.20099
	C	4.29939	0.73407	-0.45209	C	3.80399	1.13597	-0.48686
	C	5.74606	0.35280	-0.78308	C	5.26958	0.90596	-0.84771
	C	5.17725	-1.98745	-0.71883	C	4.85173	-1.50948	-1.02103
	C	3.72153	-1.64465	-0.38419	C	3.38730	-1.27969	-0.65846
	H	5.88323	0.36962	-1.87115	H	5.41520	1.05558	-1.92504
	H	6.41775	1.10554	-0.36192	H	5.88931	1.63504	-0.32110
	H	4.16856	0.82301	0.62974	H	3.67103	1.10177	0.59656
	H	4.01930	1.67956	-0.92088	H	3.46113	2.10075	-0.86395
	H	5.27642	-2.12080	-1.80298	H	4.97043	-1.54869	-2.11126
	H	5.43450	-2.94181	-0.25172	H	5.19352	-2.45715	-0.60475
	H	3.03160	-2.38025	-0.80296	H	2.74732	-2.01286	-1.15177
	N	6.12795	-0.96676	-0.29162	N	5.67348	-0.44008	-0.47908
	H	6.18828	-0.95350	0.72726	H	3.25307	-1.35064	0.42276
	H	3.58354	-1.60501	0.69936	N	2.94988	0.07585	-1.08034
	N	3.36510	-0.31334	-0.93150	H	3.02141	0.13622	-2.10907
	H	3.44088	-0.36162	-1.95801	C	6.74782	-0.69258	0.30568
					O	7.13296	-1.81172	0.63323
					H	7.26213	0.22524	0.63690
2d ··4H_2O-A	C	0.42680	-1.19137	0.10444	**2d** ··4H_2O-B	C	0.75135	-1.19659	0.18592
	C	-0.30071	0.02577	0.05854		C	0.01028	0.00870	0.29122
	C	0.46224	1.22191	0.06592		C	0.73255	1.21547	0.10419
	C	1.85175	1.20260	0.11608		C	2.09609	1.21741	-0.16871
	C	2.52679	-0.01412	0.15928		C	2.78509	0.01141	-0.26414
	C	1.81650	-1.21120	0.15323		C	2.11495	-1.19587	-0.08732
	H	-0.12443	-2.12861	0.10344		H	0.23110	-2.14128	0.32629
	H	-0.06225	2.17359	0.02913		H	0.19635	2.15870	0.17773
	H	2.40937	2.13582	0.12018		H	2.62254	2.15845	-0.30706
	H	2.34646	-2.15978	0.18784		H	2.65607	-2.13583	-0.16161
	Cl	4.29014	-0.03891	0.22199		Cl	4.51554	0.01326	-0.61016
	O	-1.61563	0.04588	0.01104		O	-1.27761	0.00720	0.55437
	O	-5.66327	-1.26308	-0.00056		H	-2.24985	-1.28938	0.35681
	H	-4.72854	-1.59404	-0.06058		O	-2.98775	-1.96455	0.23672
	O	-5.68970	1.54022	-0.36594		H	-2.76923	-2.46072	-0.57192
	H	-5.70499	0.56825	-0.23380		O	-4.96939	-0.04816	-0.11153
	O	-3.03032	2.26429	0.19042		H	-3.08340	2.48420	0.91605
	H	-2.44700	1.44663	0.12224		H	-4.35908	-0.81731	-0.00981
	H	-4.76709	1.81580	-0.17025		H	-4.37791	0.73882	-0.03884
	H	-5.98994	-1.54990	0.87053		O	-3.02710	1.92181	0.12335

	H	-2.92070	2.59192	1.10027		H	-2.27736	1.27175	0.29568
	O	-3.08794	-2.10259	-0.15282		O	-7.14331	-0.04080	1.55931
	H	-2.46780	-1.30394	-0.09350		H	-6.77798	-0.09315	2.45833
	H	-2.87833	-2.54697	-0.99353		H	-6.35748	-0.04363	0.95959
2d ··4H_2O-C	C	-0.85208	4.93718	0.65286	**2d** ··4H_2O-D	C	0.75160	0.97218	-0.27318
	C	-1.79810	5.99443	0.70654		C	0.19885	-0.24529	0.20554
	C	-1.30482	7.26498	1.10411		C	1.12496	-1.25856	0.57034
	C	0.03370	7.46398	1.42348		C	2.49862	-1.06977	0.46289
	C	0.92783	6.39870	1.35678		C	2.99664	0.14027	-0.01246
	C	0.48687	5.13552	0.97199		C	2.12483	1.16191	-0.38047
	H	-1.19344	3.94898	0.35329		H	0.07244	1.77087	-0.56252
	H	-2.00167	8.09826	1.15622		H	0.73979	-2.20433	0.94463
	H	0.38129	8.44922	1.72418		H	3.18195	-1.86512	0.75047
	H	1.18753	4.30582	0.92098		H	2.51697	2.10579	-0.75106
	Cl	2.62739	6.65109	1.76115		Cl	4.74026	0.38056	-0.14889
	O	-3.06147	5.81044	0.40275		O	-1.09711	-0.42121	0.30934
	H	-3.74589	4.39564	0.01061		O	-3.06646	0.92628	-0.90463
	O	-4.34113	3.61305	-0.21812		H	-2.26992	0.51714	-0.46329
	H	-4.09101	3.33624	-1.11737		H	-3.35957	1.65780	-0.32213
	O	-6.65736	5.10567	-0.03100		O	-2.36391	-2.72898	0.43349
	H	-5.55433	7.19980	1.48565		H	-1.79830	-1.89620	0.41811
	H	-5.91398	4.46237	-0.13801		O	-4.58075	-1.43662	-0.78233
	H	-6.21913	5.98248	-0.10824		H	-4.15119	-0.55600	-0.87165
	O	-5.17249	7.42864	0.61475		H	-1.91948	-3.36259	-0.15662
	H	-4.31210	6.92190	0.56435		H	-3.88844	-1.99152	-0.36301
	O	-6.72723	5.99229	2.59764		O	-3.93339	3.04780	0.77127
	H	-6.24456	5.41084	3.21194		H	-4.35222	2.74372	1.59881
	H	-6.82387	5.47802	1.76122		H	-3.21456	3.64364	1.05512
2e ··4H_2O-A	C	2.73114	-0.32099	-0.09851	**2e** ··4H_2O-B	O	-2.28367	1.65718	-0.49766
	O	3.81659	0.27026	-0.09820		H	-1.51444	1.08057	-0.23708
	C	2.68643	-1.81200	-0.35842		H	-2.34490	2.34844	0.18554
	H	3.70787	-2.17969	-0.46519		O	-2.30612	-2.22514	0.13344
	H	2.18223	-2.33677	0.45517		H	-1.56272	-1.53995	0.17282
	H	2.12178	-2.02520	-1.26909		O	-4.24074	-0.33267	-0.46286
	C	1.47493	0.40598	0.14503		H	-3.63954	0.44797	-0.48926
	C	1.48876	1.88370	0.40165		H	-2.09057	-2.81580	-0.60970
	H	2.51586	2.24381	0.46071		H	-3.64409	-1.09292	-0.25773
	H	0.96796	2.42979	-0.39116		C	2.98546	-0.03914	0.13061
	H	0.97031	2.11381	1.33816		O	3.88580	0.80756	0.09550
	N	0.39296	-0.32070	0.13113		C	3.33775	-1.51178	0.14855

	O	-0.75222	0.30644	0.34643		H	4.42383	-1.61186	0.16826
	O	-5.06341	-0.24588	0.25295		H	2.90072	-2.00780	1.01731
	H	-4.18885	-0.71864	0.26340		H	2.93749	-2.01330	-0.73555
	O	-4.58236	2.44008	-0.45580		C	1.57094	0.36219	0.15114
	H	-4.77895	1.51298	-0.20109		C	1.18849	1.81235	0.13473
	O	-1.80875	2.75336	-0.04146		H	2.08136	2.43661	0.16837
	H	-1.30610	1.90598	0.10126		H	0.61712	2.06038	-0.76566
	H	-3.61899	2.55365	-0.30842		H	0.54924	2.05120	0.99107
	H	-5.44021	-0.36627	1.14247		N	0.70644	-0.61374	0.19050
	H	-1.58554	3.32475	0.71422		O	-0.56983	-0.27283	0.21042
	O	-2.65300	-1.47053	0.29116		O	-5.86501	-0.65411	-2.64730
	H	-1.89362	-0.79482	0.30613		H	-6.76517	-0.59236	-2.28630
	H	-2.48988	-2.04707	-0.47597		H	-5.26521	-0.53929	-1.87016
2e ··4H_2O-C	O	-1.70683	2.41012	-1.20458	**2e** ··4H_2O-D	O	-2.41051	0.83588	-0.84469
	H	-1.16891	1.64619	-0.87732		H	-1.54757	0.42237	-0.59230
	H	-2.20001	2.72823	-0.42066		H	-2.50190	1.64291	-0.29543
	O	-2.91680	-1.36673	-0.60177		O	-1.74632	-2.89656	0.43783
	H	-2.01945	-0.90897	-0.48162		H	-1.12925	-2.11757	0.25655
	O	-4.14377	0.96171	-1.40632		O	-4.04572	-1.36482	-0.18421
	H	-3.31400	1.42120	-1.66197		H	-3.56662	-0.54248	-0.42969
	H	-2.79181	-2.03349	-1.29990		H	-1.53246	-3.56940	-0.23178
	H	-3.83703	0.06005	-1.13753		H	-3.32996	-1.99395	0.05187
	C	2.52370	-0.70904	0.93199		C	3.11984	0.10651	0.02075
	O	3.60329	-0.15472	1.17122		O	3.87063	1.07615	-0.14391
	C	2.36152	-2.18846	1.21337		C	3.70581	-1.24278	0.38241
	H	3.28869	-2.56596	1.64680		H	4.79002	-1.14560	0.45424
	H	1.52998	-2.36704	1.89794		H	3.30129	-1.60012	1.33172
	H	2.13545	-2.73304	0.29386		H	3.45006	-1.99105	-0.37089
	C	1.39284	0.04473	0.37363		C	1.66540	0.24131	-0.12897
	C	1.52152	1.50823	0.07262		C	1.05128	1.56299	-0.48329
	H	2.52413	1.85624	0.32130		H	1.82729	2.32041	-0.59443
	H	1.32408	1.70829	-0.98546		H	0.48146	1.49401	-1.41542
	H	0.78919	2.08975	0.64206		H	0.34730	1.88391	0.29221
	N	0.30144	-0.64144	0.16908		N	0.97043	-0.84626	0.07141
	O	-0.72474	0.01779	-0.33488		O	-0.33743	-0.74172	-0.05693
	O	-3.83025	2.73800	0.69851		O	-2.73149	3.16382	0.73522
	H	-3.73587	2.30564	1.56620		H	-3.58747	3.17152	1.20462
	H	-4.15717	2.03909	0.08322		H	-2.05943	3.28202	1.43343
TS1$_{dad}$ ··4H_2O-A	C	2.96920	-2.31905	0.17943	**TS1$_{dad}$** ··4H_2O-B	C	2.88029	-2.35053	0.27949
	C	1.87804	-1.47526	0.05033		C	1.79446	-1.52077	0.05244

	C	2.07273	-0.17153	-0.41245	C	1.95615	-0.38327	-0.74348
	C	3.34919	0.29357	-0.73431	C	3.19773	-0.07115	-1.30110
	C	4.44369	-0.54886	-0.60469	C	4.28815	-0.89747	-1.07539
	C	4.23921	-1.84904	-0.15266	C	4.11406	-2.03257	-0.28814
	H	2.84369	-3.33354	0.54072	H	2.78042	-3.23597	0.89716
	H	0.87926	-1.79429	0.31427	H	0.82522	-1.72363	0.48727
	H	3.47663	1.31280	-1.08421	H	3.29356	0.82074	-1.91312
	H	5.44195	-0.20683	-0.85303	H	5.25815	-0.67206	-1.50364
	O	1.05536	0.74878	-0.49693	O	0.96156	0.53204	-0.94914
	N	5.38266	-2.73936	-0.01815	N	5.25159	-2.90678	-0.04702
	O	6.49939	-2.30780	-0.30725	O	6.33776	-2.60766	-0.54523
	O	5.18745	-3.88861	0.37885	O	5.08333	-3.91130	0.64555
	C	-0.19587	0.44455	-1.03752	C	-0.32996	0.17466	-1.31583
	C	-1.05735	1.66858	-0.92958	C	-1.13097	1.43307	-1.49481
	C	-2.15886	1.83820	-1.77108	C	-2.39449	1.38612	-2.09012
	C	-0.78555	2.65432	0.03049	C	-0.64098	2.66959	-1.05358
	C	-2.96525	2.97024	-1.66827	C	-3.15133	2.54529	-2.24600
	H	-2.37371	1.07689	-2.51295	H	-2.77473	0.43259	-2.43947
	C	-1.58631	3.78705	0.12825	C	-1.39491	3.82852	-1.21606
	H	0.04559	2.52927	0.71527	H	0.33338	2.72655	-0.58322
	C	-2.68147	3.95141	-0.72134	C	-2.65512	3.77305	-1.81208
	H	-3.81782	3.08450	-2.33298	H	-4.13238	2.48767	-2.71092
	H	-1.35713	4.54282	0.87531	H	-0.99603	4.78081	-0.87455
	H	-3.30785	4.83657	-0.64321	H	-3.24296	4.67892	-1.93804
	S	-0.32170	-0.65400	-2.30889	S	-0.58470	-1.19103	-2.29002
	C	-2.24212	-2.26684	0.09240	C	-2.30934	-2.11022	0.53067
	C	-2.07313	-0.94163	0.54105	C	-2.11095	-0.72063	0.64156
	C	-3.22602	-0.22361	0.92068	C	-3.22538	0.08355	0.95116
	C	-4.48743	-0.80754	0.87592	C	-4.48191	-0.47529	1.15990
	C	-4.61673	-2.12170	0.43461	C	-4.64295	-1.85325	1.04622
	C	-3.50279	-2.85565	0.04128	C	-3.56580	-2.67525	0.73253
	H	-1.36590	-2.83431	-0.20391	H	-1.46091	-2.74328	0.29395
	H	-3.11583	0.80401	1.25593	H	-3.09128	1.15867	1.03107
	H	-5.36532	-0.24447	1.18091	H	-5.33061	0.15639	1.40748
	H	-3.61656	-3.88138	-0.29895	H	-3.70416	-3.74990	0.65081
	Cl	-6.21172	-2.86579	0.38016	Cl	-6.23085	-2.56538	1.31109
	O	-0.86261	-0.38866	0.60877	O	-0.89924	-0.18280	0.47209
	H	2.35244	4.07151	0.48845	H	2.16335	4.85523	-0.48364
	O	2.33595	4.33476	1.43693	O	2.72460	4.07432	-0.31848
	H	3.13930	4.86715	1.57931	H	2.78008	3.60875	-1.17413

	O	2.31122	2.06924	3.15555		O	2.42578	2.62403	2.07841
	H	1.44017	1.62884	3.05498		H	1.50156	2.27896	2.12448
	H	2.29630	2.84468	2.55729		H	2.50195	3.11127	1.23126
	O	-0.19352	0.79899	2.94154		O	-0.15865	1.68831	2.26870
	H	-0.44995	0.39163	2.07011		H	-0.43831	1.02334	1.58109
	H	-0.92648	1.39366	3.17890		H	-0.80293	2.41562	2.20630
	O	2.29190	3.42706	-1.19338		O	3.37689	3.91112	4.30726
	H	1.64804	2.69580	-1.18331		H	4.03758	3.29788	4.66996
	H	1.96076	4.05937	-1.86014		H	3.02079	3.46147	3.50332
TS1$_{dae}$ $\cdot\cdot 4H_2O$-A	C	4.08769	0.57010	-0.54946	**TS1$_{dae}$**$\cdot\cdot 4H_2O$-B	C	4.17234	0.07569	-0.99122
	C	2.80156	1.06886	-0.69977		C	2.88814	0.50333	-1.29571
	C	1.70436	0.23344	-0.48574		C	1.78666	-0.16001	-0.75471
	C	1.87765	-1.10211	-0.11390		C	1.95323	-1.25320	0.09947
	C	3.16113	-1.60320	0.03474		C	3.23373	-1.68502	0.40521
	C	4.25107	-0.76315	-0.18711		C	4.32804	-1.01763	-0.14429
	H	4.95267	1.20257	-0.71382		H	5.04060	0.57673	-1.40382
	H	2.64000	2.10509	-0.97902		H	2.72573	1.35075	-1.95513
	H	1.01000	-1.72363	0.06011		H	1.07912	-1.73802	0.51469
	H	3.32142	-2.63539	0.32516		H	3.39028	-2.52808	1.06872
	O	0.46483	0.82538	-0.57586		O	0.55925	0.38375	-1.03040
	N	5.59868	-1.29422	-0.03167		N	5.67227	-1.47377	0.18102
	O	5.72881	-2.47720	0.28297		O	5.79661	-2.44319	0.92970
	O	6.55146	-0.53803	-0.22133		O	6.62933	-0.87091	-0.30552
	C	-0.60442	0.23218	-1.24715		C	-0.51594	-0.37164	-1.45352
	C	-1.79595	1.13004	-1.11661		C	-1.69222	0.52283	-1.67320
	C	-2.79764	1.13406	-2.09045		C	-2.87564	0.00355	-2.20779
	C	-1.92544	1.98428	-0.01242		C	-1.64149	1.88091	-1.33537
	C	-3.90188	1.97523	-1.96922		C	-3.98177	0.82428	-2.40806
	H	-2.70080	0.47489	-2.94643		H	-2.91627	-1.04823	-2.46559
	C	-3.02683	2.82454	0.10798		C	-2.74730	2.70188	-1.54053
	H	-1.17726	1.97632	0.77159		H	-0.73761	2.29820	-0.90831
	C	-4.02078	2.82535	-0.87137		C	-3.92242	2.17820	-2.07829
	H	-4.67084	1.96688	-2.73760		H	-4.89457	0.40511	-2.82409
	H	-3.10941	3.47225	0.97681		H	-2.69016	3.75488	-1.27630
	H	-4.88256	3.48155	-0.77748		H	-4.78558	2.81980	-2.23771
	S	-0.34753	-0.79160	-2.54240		S	-0.28425	-1.80471	-2.30268
	C	-3.18129	-3.78391	0.58310		C	-3.72883	-2.84758	1.64256
	O	-3.56440	-4.62448	1.40181		O	-4.15203	-3.34603	2.68850
	C	-3.67217	-3.84529	-0.84611		C	-4.48337	-3.04224	0.34664
	H	-4.47251	-3.11113	-0.98204		H	-4.82286	-2.08043	-0.04480

	H	-2.88647	-3.59581	-1.55868	H	-3.83771	-3.47947	-0.41747
	H	-4.07429	-4.84114	-1.03769	H	-5.34041	-3.69089	0.53243
	C	-2.26564	-2.70036	0.99236	C	-2.48865	-2.04437	1.64021
	N	-1.90578	-1.88069	0.04911	N	-2.12914	-1.58004	0.48212
	O	-1.10009	-0.90198	0.38526	O	-1.03942	-0.84154	0.45422
	O	-0.24159	0.42570	2.69730	O	-0.30636	1.22277	2.15391
	H	0.70913	0.22127	2.74640	H	0.51430	0.89844	2.56575
	H	-0.58997	-0.09632	1.93636	H	-0.60565	0.49857	1.55050
	O	0.59769	4.79766	1.80444	O	1.01379	4.51883	-0.77453
	H	0.20545	5.68695	1.74139	H	0.45855	4.75500	-1.54157
	H	0.69791	4.48376	0.87641	H	1.64769	3.85692	-1.10969
	C	-1.80369	-2.60142	2.41577	C	-1.73124	-1.81863	2.91522
	H	-2.15004	-1.67378	2.88158	H	-1.78085	-0.77098	3.22763
	H	-2.18027	-3.44725	2.99071	H	-2.14166	-2.44194	3.70967
	H	-0.71058	-2.58866	2.46737	H	-0.67256	-2.05718	2.77396
	O	-0.98107	3.06756	3.40098	O	-0.34692	3.93483	1.62253
	H	-0.42900	3.65520	2.84326	H	0.12950	4.10616	0.78274
	H	-0.73809	2.15303	3.14888	H	-0.33966	2.95926	1.76223
	O	0.88292	3.80344	-0.78290	O	0.30823	5.54297	3.75487
	H	0.42267	4.31432	-1.47638	H	1.23411	5.33066	3.95915
	H	0.48814	2.91278	-0.80964	H	0.07212	4.96274	2.99219
2d··2H_2O2DMSO-A	H	-0.22814	0.32179	-1.06798	**2d**··2H_2O2DMSO-B	C	2.76932	-0.48388	0.80002
	O	-0.37516	0.06099	-2.01294		C	1.73633	0.47171	0.57235
	H	-1.17146	-0.50796	-1.98313		C	2.16932	1.76816	0.16561
	O	0.36153	-1.63777	2.16503		C	3.51462	2.07593	-0.00360
	H	0.17041	-0.79559	1.67890		C	4.48625	1.10553	0.22975
	H	1.23388	-1.91876	1.82075		C	4.11411	-0.17489	0.63264
	S	2.88183	-1.82125	-0.52132		H	2.48095	-1.48488	1.11334
	O	2.87688	-2.24286	0.95663		H	1.41745	2.53335	-0.01416
	C	4.55871	-2.16453	-1.09764		H	3.80914	3.07539	-0.31519
	H	4.68872	-3.24771	-1.09750		H	4.87437	-0.93072	0.81525
	H	4.68203	-1.77894	-2.11203		Cl	6.19614	1.49988	0.01582
	H	5.27282	-1.69987	-0.41467		O	0.47816	0.17273	0.73479
	C	2.97650	-0.02045	-0.51345		O	-1.38542	1.66090	-0.43523
	H	3.09520	0.33652	-1.53898		H	-0.66474	1.11978	0.01130
	H	2.03064	0.34297	-0.10169		H	-2.23909	1.36006	-0.05390
	H	3.82154	0.28472	0.10808		S	-4.48581	-0.42167	-0.04128
	S	-2.41123	-2.39928	-0.29982		O	-3.82613	0.78897	0.63073
	O	-2.65004	-1.61537	-1.60110		C	-6.19708	0.07097	-0.33747
	C	-3.84196	-3.49067	-0.14393		H	-6.18057	0.85434	-1.09640

	H	-3.77747	-4.23121	-0.94244		H	-6.76636	-0.78558	-0.70490
	H	-3.81374	-3.99179	0.82613		H	-6.62429	0.45530	0.59095
	H	-4.75468	-2.90085	-0.25081		C	-4.79450	-1.59965	1.29144
	C	-2.81458	-1.25675	1.03454		H	-5.37533	-2.44160	0.90866
	H	-2.74164	-1.78121	1.98930		H	-3.82339	-1.95200	1.64178
	H	-2.06514	-0.46224	0.99867		H	-5.32564	-1.09371	2.10022
	H	-3.82076	-0.86335	0.87196		O	-0.75840	4.33974	-0.17219
	C	-0.15178	2.96389	0.30628		H	-1.00904	3.39638	-0.31792
	C	-0.14951	1.81427	1.14254		H	-0.59185	4.39052	0.79232
	C	-0.24253	2.05311	2.54070		S	-1.34367	3.16926	3.21482
	C	-0.33092	3.33931	3.06159		O	-0.37616	4.20763	2.62694
	C	-0.32935	4.43628	2.20384		C	-1.63354	3.71227	4.91262
	C	-0.23988	4.25025	0.82672		H	-2.18022	4.65507	4.86377
	H	-0.08417	2.82015	-0.76939		H	-2.23289	2.96581	5.43828
	H	-0.24226	1.19760	3.21187		H	-0.67253	3.86013	5.40953
	H	-0.40053	3.48858	4.13633		C	-0.34644	1.71237	3.57943
	H	-0.23939	5.10918	0.16004		H	-0.95022	1.00529	4.15414
	Cl	-0.44122	6.07004	2.86512		H	-0.05215	1.25789	2.62711
	O	-0.06584	0.60265	0.65162		H	0.53099	2.02341	4.15109
2d ··2H_2O2DMSO-C	C	-0.09431	0.26505	-1.21930	**2d** ··2H_2O2DMSO-D	C	-2.63091	-1.84017	-1.20457
	C	-0.00319	-0.47682	-0.00802		C	-1.77115	-1.17217	-0.28665
	C	0.09060	0.28930	1.18786		C	-2.41713	-0.42096	0.73725
	C	0.09103	1.67971	1.17403		C	-3.80224	-0.35361	0.83851
	C	0.00173	2.36250	-0.03701		C	-4.60056	-1.02814	-0.08201
	C	-0.08995	1.65543	-1.23387		C	-4.01568	-1.77065	-1.10502
	H	-0.16825	-0.28332	-2.15504		H	-2.17577	-2.42224	-2.00281
	H	0.16268	-0.24008	2.13461		H	-1.79968	0.11305	1.45613
	H	0.16289	2.23382	2.10679		H	-4.26232	0.22828	1.63368
	H	-0.15991	2.19064	-2.17775		H	-4.64127	-2.29517	-1.82335
	Cl	0.00476	4.12654	-0.05503		Cl	-6.36088	-0.94031	0.04685
	O	-0.00551	-1.78359	0.00530		O	-0.47152	-1.24013	-0.38697
	H	-1.08286	-2.52053	-1.15519		O	1.02002	-0.81923	1.77954
	O	-1.76700	-2.91546	-1.75416		H	0.41520	-0.95167	0.98832
	H	-2.56834	-2.37530	-1.59514		H	1.92709	-0.86574	1.40776
	O	1.75250	-2.88490	1.78766		S	3.40165	-2.23043	-0.57902
	H	1.06970	-2.50001	1.18070		O	3.48678	-1.08463	0.44178
	H	2.55539	-2.35016	1.61859		C	5.00558	-2.23577	-1.40707
	S	3.97959	-0.80338	-0.30720		H	5.75082	-2.54359	-0.67233
	O	4.00019	-1.25755	1.15843		H	4.98652	-2.94903	-2.23391
	C	5.71354	-0.75239	-0.81011		H	5.22428	-1.22800	-1.76593

	H	6.07846	-1.78040	-0.82148		C	2.40785	-1.59462	-1.94358
	H	5.79187	-0.32290	-1.81123		H	2.42202	-2.31743	-2.76333
	H	6.27861	-0.16097	-0.08675		H	1.38616	-1.46980	-1.57069
	C	3.68134	0.97546	-0.26471		H	2.82854	-0.63916	-2.26581
	H	3.78289	1.38334	-1.27277		O	0.25524	1.56063	2.97016
	H	2.66028	1.12311	0.08867		H	0.55068	0.69556	2.59992
	H	4.39556	1.44018	0.41869		H	0.19946	2.14661	2.18621
	S	-3.98608	-0.78464	0.29961		S	1.19762	2.60937	-0.44530
	O	-4.00918	-1.26932	-1.15617		O	0.16233	3.07258	0.59055
	C	-5.71949	-0.71756	0.80244		C	1.58390	4.08684	-1.40952
	H	-6.08769	-1.74392	0.83564		H	2.09001	4.78635	-0.74269
	H	-5.79573	-0.26690	1.79438		H	2.24603	3.82165	-2.23655
	H	-6.28321	-0.13965	0.06720		H	0.65493	4.52544	-1.77963
	C	-3.68221	0.99196	0.21968		C	0.26670	1.71650	-1.70513
	H	-3.78165	1.42115	1.21907		H	0.91486	1.53564	-2.56643
	H	-2.66095	1.12891	-0.13739		H	-0.04795	0.76253	-1.26950
	H	-4.39547	1.44458	-0.47277		H	-0.59619	2.32137	-1.99390

S13 The energy, enthalpy, free energy (au) and entropy (cal·mol^{-1}·K^{-1}) for the studied reactions in **Table 1**, **Fig.1** and **Fig.4**, obtained with CAM-B3LYP+IDSCRF/DZVP.

species	E	H	G(gas)	G(sol)	G_{qRRHO}(l)	S(gas)	S(sol)	S_{qRRHO}(l)
MeOH 313.15K								
1a	-2810.14187	-2809.94840	-2809.99857	-2809.98742	-2809.98602	100.5	78.2	75.4
2a	-265.42555	-265.31856	-265.35613	-265.34460	-265.34421	75.3	52.2	51.4
TS_{aa}	-3075.53829	-3075.23689	-3075.30773	-3075.29679	-3075.29021	142.0	120.0	106.95
	18.28	18.87	29.47	22.11	25.09	-33.9	-10.3	-19.8
P_{aa}	-3075.60385	-3075.29896	-3075.36872	-3075.35793	-3075.35320	139.8	118.2	108.7
	-22.86	-20.08	-8.80	-16.26	-14.41	-36.0	-12.2	-18.1
MeOH 273.15K								
1ba	-1100.63122	-1100.52439	-1100.56845	-1100.55691	-1100.55578	101.2	74.7	72.1
2b	-251.78621	-251.61957	-251.65089	-251.64053	-251.64053	72.0	48.1	48.1
$TS1_{bab}$	-1352.40652	-1352.13176	-1352.18732	-1352.17646	-1352.17434	127.6	102.7	97.8
	6.85	7.66	20.09	13.17	13.79	-45.5	-20.2	-22.4
$IN1_{bab}$	-1352.44935	-1352.17145	-1352.22807	-1352.21700	-1352.21479	130.1	104.6	99.6
	-20.03	-17.25	-5.48	-12.27	-11.6	-43.1	-18.2	-20.7
$TS2_{bab}$	-1604.23719	-1603.79389	-1603.86553	-1603.85511	-1603.85025	164.6	140.6	129.5
	-21.05	-19.05	2.91	-10.79	-8.42	-80.6	-30.3	-38.8
P_{bab}	-1604.25726	-1603.80887	-1603.88331	-1603.87299	-1603.86726	171.0	147.3	134.1
	-33.65	-28.45	-8.21	-21.97	-19.09	-74.1	-23.7	-34.3

MeOH 273.15K								
1ba	-1100.63122	-1100.52439	-1100.56845	-1100.55691	-1100.55578	101.2	74.7	72.1
2b ··MeOH	-367.49212	-367.26734	-367.31083	-367.30118	-367.29909	99.9	77.7	72.9
TS1$_{bab}$ ··MeOH	-1468.10400	-1467.77163	-1467.83840	-1467.82807	-1467.82416	153.4	129.7	120.7
	12.14	12.61	25.65	18.84	19.27	-47.8	-22.8	-24.4
MeOH 273.15K								
1ba	-1100.63122	-1100.52439	-1100.56845	-1100.55691	-1100.55578	101.2	74.7	72.1
2b ··2MeOH	-483.18996	-482.90768	-482.96445	-482.95516	-482.95052	130.4	109.1	98.4
TS1$_{bab}$ ··2MeOH	-1583.80412	-1583.41399	-1583.49108	-1583.48122	-1583.47586	177.1	154.4	142.1
	10.71	11.35	26.24	19.36	19.10	-54.5	-29.3	-28.4
MeOH 273.15K								
1bb	-3214.25377	-3214.14734	-3214.19272	-3214.18125	-3214.17996	104.2	77.9	74.9
2b ··2MeOH	-483.18996	-482.90768	-482.96445	-482.95516	-482.95052	130.4	109.1	98.4
TS$_{bbb}$ ··2MeOH	-3697.42600	-3697.03624	-3697.11464	-3697.10480	-3697.09921	180.1	157.5	144.7
	11.13	11.78	26.69	19.84	19.62	-54.6	-29.5	-28.7
MeOH 273.15K								
1bc	-1420.52205	-1420.30816	-1420.36657	-1420.35528	-1420.35215	134.2	108.2	101.0
2b ··2MeOH	-483.18996	-482.90768	-482.96445	-482.95516	-482.95052	130.4	109.1	98.4
TS$_{bcb}$ ··2MeOH	-1903.69817	-1903.20074	-1903.29104	-1903.28121	-1903.27388	207.4	184.9	168.0
	8.68	9.48	25.09	18.34	18.07	-57.1	-32.4	-31.4
MeOH 273.15K								
1bd	-740.31207	-740.20407	-740.24720	-740.23542	-740.23427	99.1	72.0	69.4
2b ··2MeOH	-483.18996	-482.90768	-482.96445	-482.95516	-482.95052	130.4	109.1	98.4
TS$_{bdb}$ ··2MeOH	-1223.49116	-1223.09999	-1223.17774	-1223.16802	-1223.16185	178.6	156.3	142.1
	6.82	7.38	21.28	14.16	14.40	-50.9	-24.8	-25.7
MeOH 273.15K								
1be	-845.53202	-845.41199	-845.45996	-845.44768	-845.44569	110.2	82.0	77.4
2b ··2MeOH	-483.18996	-482.90768	-482.96445	-482.95516	-482.95052	130.4	109.1	98.4
TS$_{beb}$ ··2MeOH	-1328.71112	-1328.30774	-1328.38803	-1328.37807	-1328.37201	184.5	161.6	147.7
	6.81	7.49	22.83	15.54	15.19	-56.2	-29.5	-28.2
MeOH 293.15K								
1ca	-1216.92221	-1216.85301	-1216.89432	-1216.88236	-1216.88202	88.4	62.8	62.1
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{cab}$ ··2MeOH	-1700.08705	-1699.73339	-1699.81637	-1699.80594	-1699.79831	177.6	155.3	139.0
	15.76	16.15	29.25	21.99	23.21	-44.7	-19.9	-24.1
MeOH 293.15K								
1cb	-3330.54585	-3330.47699	-3330.51960	-3330.50753	-3330.50711	91.2	65.4	64.5
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{cab}$ ··2MeOH	-3813.70926	-3813.35590	-3813.43935	-3813.42874	-3813.42137	178.6	155.9	140.1

	16.66	17.07	30.70	23.48	24.49	-46.5	-21.9	-25.3
MeOH 293.15K								
1cc	-1267.97949	-1267.80591	-1267.86580	-1267.85366	-1267.85022	128.2	102.2	94.9
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{ccb}$ ··2MeOH	-1751.14804	-1750.69004	-1750.79005	-1750.77951	-1750.76905	214.1	191.5	169.1
	13.43	13.80	27.87	20.57	21.62	-48.0	-23.1	-26.7
MeOH 293.15K								
1cd	-1216.91997	-1216.85080	-1216.89264	-1216.88059	-1216.87979	89.6	63.8	62.1
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{cdb}$ ··2MeOH	-1700.08693	-1699.73308	-1699.81541	-1699.80478	-1699.79747	176.2	153.5	137.8
	14.43	14.96	28.80	21.61	22.34	-47.2	-22.7	-25.2
MeOH 293.15K								
1ce	-3330.54357	-3330.47477	-3330.51786	-3330.50562	-3330.50480	92.3	66.0	64.3
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{ceb}$ ··2MeOH	-3813.70925	-3813.35571	-3813.43755	-3813.42694	-3813.42043	175.2	152.5	138.5
	15.24	15.80	30.74	23.41	23.63	-51.0	-26.0	-26.7
MeOH 293.15K								
1cf	-1536.81515	-1536.63809	-1536.69546	-1536.68325	-1536.68077	122.8	96.7	91.4
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{cfb}$ ··2MeOH	-2019.98412	-2019.52228	-2019.61559	-2019.60483	-2019.59776	199.7	176.7	161.6
	13.17	13.76	30.46	23.25	22.77	-56.9	-32.4	-30.7
MeOH 293.15K								
1cg	-1267.97855	-1267.80494	-1267.86404	-1267.85183	-1267.84863	126.5	100.4	93.5
2b ··2MeOH	-483.18996	-482.90612	-482.96867	-482.95863	-482.95328	133.9	112.4	101.0
TS$_{cgb}$ ··2MeOH	-1751.14960	-1750.69117	-1750.78870	-1750.77813	-1750.76886	208.8	186.2	166.3
	11.87	12.48	27.62	20.29	20.74	-51.6	-26.6	-28.2
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d	-766.43561	-766.34566	-766.38408	-766.37134	-766.37126	80.9	54.1	53.9
TS1$_{dad}$	-1945.42021	-1945.11647	-1945.19449	-1945.18235	-1945.17655	164.2	138.7	126.5
	3.57	4.15	17.97	10.02	11.05	-46.4	-19.7	-23.1
IN1$_{dad}$	-1945.43368	-1945.12807	-1945.20578	-1945.19386	-1945.18810	163.5	138.5	126.3
	-4.88	-3.12	10.89	2.79	3.80	-47.0	-19.9	-23.2
TS2$_{dad}$	-1945.42842	-1945.12457	-1945.20265	-1945.19071	-1945.18482	164.3	139.2	126.8
	-1.58	-0.93	12.85	4.77	5.86	-46.2	-19.1	-22.8
P$_{dad}$	-1945.42842	-1945.12457	-1945.20265	-1945.19071	-1945.18482	164.3	139.2	126.8
4-NO$_2$-PhO$^-$	-511.37144	-511.26766	-511.30914	-511.29568	-511.29527	87.3	59.0	58.1
	-13.97	-13.83	-13.4	-13.22	-13.52	-1.4	-2.0	-1.1
H_2O 298.15K								

1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d ··H_2O	-842.86858	-842.75134	-842.79825	-842.78582	-842.78432	98.7	72.6	69.4
TS1$_{dad}$ ··H_2O	-2021.84956	-2021.51839	-2021.60535	-2021.59319	-2021.58546	183.0	157.4	141.2
	5.84	6.51	20.05	12.30	13.65	-45.4	-19.4	-24.0
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d ··$2H_2O$	-919.30017	-919.15549	-919.21171	-919.19936	-919.19606	118.3	92.3	85.4
TS1$_{dad}$ ··$2H_2O$	-2098.27536	-2097.91665	-2098.01010	-2097.99824	-2097.98988	196.7	171.7	154.1
	9.48	10.21	25.51	17.63	18.25	-51.3	-24.9	-27.0
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d ··$4H_2O$-A	-1072.16638	-1071.96624	-1072.03459	-1072.02209	-1072.01651	143.8	117.5	105.8
TS1$_{dad}$ ··$4H_2O$-A	-2251.13177	-2250.71745	-2250.82302	-2250.81118	-2250.80217	222.2	197.3	178.3
	15.62	16.45	31.76	23.77	23.37	-51.3	-24.6	-23.2
2d ··$4H_2O$-B	-1072.16518	-1071.96495	-1072.03430	-1072.02198	-1072.01593	146.0	120.0	107.3
TS1$_{dad}$ ··$4H_2O$-B	-2251.13208	-2250.71845	-2250.82874	-2250.81670	-2250.80584	232.1	206.8	184.0
	14.68	15.02	27.99	20.24	20.70	-43.5	-17.5	-19.0
2d ··$4H_2O$-C	-1072.16416	-1071.96305	-1072.02962	-1072.01709	-1072.01222	140.1	113.7	103.5
2d ··$4H_2O$-D	-1072.16110	-1071.96076	-1072.03308	-1072.02083	-1072.01376	152.2	126.4	111.5
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d ··$3H_2O$	-995.73538	-995.56254	-995.62214	-995.60943	-995.60584	125.4	98.7	91.1
TS1$_{dad}$ ··$3H_2O$	-2174.70494	-2174.31887	-2174.41915	-2174.40693	-2174.39869	211.1	185.3	168.0
	13.01	13.24	26.38	18.49	18.86	-44.1	-17.6	-18.8
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e	-361.20364	-361.09628	-361.13758	-361.12673	-361.12606	86.9	64.1	62.7
TS1$_{dae}$	-1540.19251	-1539.87141	-1539.95358	-1539.94239	-1539.93557	172.9	149.4	135.0
	0.89	1.44	14.46	7.10	8.4	-43.7	-19.0	-23.3
IN1$_{dae}$	-1540.20903	-1539.88619	-1539.96640	-1539.95541	-1539.94966	168.8	145.7	133.6
	-9.48	-7.83	6.42	-1.07	-0.44	-47.8	-22.7	-24.8
TS2$_{dae}$	-1540.19636	-1539.87554	-1539.95740	-1539.94639	-1539.93973	172.3	149.1	135.1
	-1.52	-1.15	12.07	4.59	5.79	-44.3	-19.2	-23.3
P$_{dae}$	-1540.19636	-1539.87554	-1539.95740	-1539.94639	-1539.93973	172.3	149.1	135.1
4-NO_2-PhO$^-$	-511.37144	-511.26766	-511.30914	-511.29568	-511.29527	87.3	59.0	58.1
	-12.91	-13.03	12.68	11.96	12.48	-1.1	-3.4	-1.9
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e ··H_2O	-437.63419	-437.49939	-437.54930	-437.53816	-437.53606	105.1	81.6	77.2

TS1$_{dae}$ $\cdots H_2O$	-1616.62089	-1616.27232	-1616.36147	-1616.35040	-1616.34272	187.6	164.3	148.2
	2.25	2.82	16.87	9.24	10.19	-47.1	-21.5	-24.7
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e $\cdots 2H_2O$	-514.06546	-513.90275	-513.95937	-513.94842	-513.94544	119.2	96.1	89.8
TS1$_{dae}$ $\cdots 2H_2O$	-1693.04599	-1692.66990	-1692.76781	-1692.75667	-1692.74719	206.1	182.6	162.7
	6.12	6.45	19.21	11.75	13.27	-42.8	-17.8	-22.9
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e $\cdots 4H_2O$-A	-666.93202	-666.71445	-666.78519	-666.77404	-666.76839	148.9	125.4	113.5
TS1$_{dae}$ $\cdots 4H_2O$-A	-1845.90155	-1845.46979	-1845.57836	-1845.56716	-1845.55802	228.5	204.9	185.7
	13.03	13.86	28.79	21.24	21.54	-50.1	-24.8	-23.6
2e $\cdots 4H_2O$-B	-666.93104	-666.71332	-666.78666	-666.77553	-666.76861	154.4	130.9	116.4
TS1$_{dae}$ $\cdots 4H_2O$-B	-1845.90150	-1845.47061	-1845.58522	-1845.57398	-1845.56218	241.2	217.6	192.7
	12.44	12.64	25.41	17.90	18.41	-42.8	-17.6	-19.3
2e $\cdots 4H_2O$-C	-666.93034	-666.71181	-666.77993	-666.76877	-666.76416	143.4	119.9	110.2
2e $\cdots 4H_2O$-D	-666.92738	-666.70957	-666.78257	-666.77128	-666.76487	153.6	129.9	116.4
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e $\cdots 3H_2O$	-590.50131	-590.31097	-590.37325	-590.36212	-590.35828	131.1	107.7	99.6
TS1$_{dae}$ $\cdots 3H_2O$	-1769.47475	-1769.07138	-1769.17726	-1769.16629	-1769.1564	222.8	199.8	178.9
	10.57	10.68	21.99	14.31	15.55	-37.9	-12.2	-16.4
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2d $\cdots 3H_2O$	-995.73538	-995.56254	-995.62214	-995.60943	-995.60584	125.4	98.7	91.1
TS1$_{dbd}$ $\cdots 3H_2O$	-1660.15672	-1659.82434	-1659.91437	-1659.90262	-1659.89576	189.5	164.7	150.5
	10.10	10.84	25.07	17.34	17.55	-47.7	-21.8	-22.5
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2e $\cdots 3H_2O$	-590.50131	-590.31097	-590.37325	-590.36212	-590.35828	131.1	107.7	99.6
TS1$_{dbe}$ $\cdots 3H_2O$	-1254.92856	-1254.57877	-1254.67154	-1254.66053	-1254.65255	195.2	172.1	155.3
	6.39	7.07	21.27	14.07	14.87	-47.6	-23.5	-26.2
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d $\cdots 3H_2O$1DMSO	-1548.85292	-1548.59000	-1548.66977	-1548.65886	-1548.65157	167.9	144.9	129.6
TS1$_{dad}$ $\cdots 3H_2O$1DMSO	-2727.82688	-2727.35090	-2727.47082	-2727.45958	-2727.44688	252.4	228.7	202.0
	10.25	10.37	23.85	16.47	17.32	-45.2	-20.4	-23.3
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7

2d ··2H$_2$O1DMSO	-1472.42354	-1472.18788	-1472.25856	-1472.24747	-1472.24219	148.8	125.4	114.3
TS1$_{dad}$ ··2H$_2$O1DMSO	-2651.39696	-2650.94841	-2651.05973	-2651.04854	-2651.03766	234.3	210.7	187.8
	10.59	10.60	23.77	16.25	17.22	-44.2	-19.0	-22.2
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2d ··2H$_2$O1DMSO	-1472.42260	-1472.18692	-1472.25757	-1472.24644	-1472.24119	148.7	125.3	114.2
TS1$_{dad}$ ··2H$_2$O1DMSO	-2651.39593	-2650.94734	-2651.05862	-2651.04732	-2651.03641	234.2	210.4	187.5
	10.53	10.55	23.71	16.27	17.27	-44.1	-19.2	-22.5
H$_2$O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2d ··2H$_2$O2DMSO	-2025.53882	-2025.21402	-2025.30401	-2025.29352	-2025.28476	189.4	167.3	148.9
TS1$_{dad}$ ··2H$_2$O2DMSO	-3204.51931	-3203.98052	-3204.10836	-3204.09774	-3204.08557	269.1	246.7	221.1
	6.15	6.86	21.77	14.28	13.86	-50.0	-24.9	-23.5
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2d ··2H$_2$O2DMSO	-2025.53763	-2025.21281	-2025.30261	-2025.29212	-2025.28346	189.0	166.9	148.7
TS1$_{dad}$ ··2H$_2$O2DMSO	-3204.51795	-3203.97911	-3204.10621	-3204.09557	-3204.08376	267.5	245.1	220.3
	6.14	6.86	22.11	14.66	14.08	-51.2	-26.1	-24.2
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2d ··H$_2$O2DMSO	-1949.10074	-1948.80433	-1948.89073	-1948.88046	-1948.87144	181.9	160.2	141.2
TS1$_{dad}$ ··H$_2$O2DMSO	-3128.08227	-3127.57172	-3127.69480	-3127.68412	-3127.67251	259.0	236.6	212.1
	5.38	6.18	21.82	14.53	13.60	-52.5	-28.0	24.9
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2d	-766.43475	-766.34480	-766.38323	-766.37030	-766.37022	80.9	53.7	53.5
TS1$_{dad}$	-1945.41944	-1945.11569	-1945.19374	-1945.18179	-1945.17598	164.3	139.1	126.9
	3.40	3.98	17.78	9.61	10.66	-46.3	-18.9	-22.4
H$_2$O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e ··3H$_2$O1DMSO	-1143.61843	-1143.33815	-1143.42278	-1143.41258	-1143.40395	178.1	156.6	138.5
TS1$_{dae}$ ··3H$_2$O1DMSO	-2322.59657	-2322.10320	-2322.22744	-2322.21670	-2322.20305	261.5	238.9	210.2
	7.62	7.77	21.58	14.34	14.82	-46.3	-22.1	-24.0
H$_2$O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e ··2H$_2$O1DMSO	-1067.18962	-1066.93664	-1067.01150	-1067.00122	-1066.99494	157.6	135.9	122.7
TS1$_{dae}$ ··2H$_2$O1DMSO	-2246.16724	-2245.70139	-2245.81686	-2245.80609	-2245.79448	243.0	220.3	195.9
	7.95	7.96	21.14	13.87	14.66	-44.2	-19.8	-22.5
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8

2e ··2H_2O1DMSO	-1067.18861	-1066.93561	-1067.00991	-1066.99945	-1066.99346	156.4	134.4	121.8
TS1$_{dae}$ ··2H_2O1DMSO	-2246.16618	-2245.70028	-2245.81494	-2245.80418	-2245.79295	241.3	218.7	195.1
	7.87	7.89	21.22	13.86	14.59	-44.7	-20.0	-22.5
H_2O 298.15K								
1da	-1178.99029	-1178.77743	-1178.83905	-1178.82697	-1178.82290	129.7	104.3	95.7
2e ··2H_2O2DMSO	-1620.30535	-1619.96310	-1620.05652	-1620.04662	-1620.03732	196.6	175.8	156.2
TS1$_{dae}$ ··2H_2O2DMSO	-2799.28950	-2798.73343	-2798.86467	-2798.85452	-2798.84123	276.2	254.9	226.9
	3.85	4.46	19.39	11.97	12.72	-50.1	-25.2	-25.0
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2e ··2H_2O2DMSO	-1620.30420	-1619.96194	-1620.05553	-1620.04555	-1620.03617	197.0	176.0	156.2
TS1$_{dae}$ ··2H_2O2DMSO	-2799.28812	-2798.73201	-2798.86301	-2798.85279	-2798.83962	275.7	254.2	226.5
	3.88	4.50	19.68	12.28	12.11	-50.9	-26.1	-25.5
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2e ··H_2O2DMSO	-1543.86809	-1543.55401	-1543.64114	-1543.63123	-1543.62309	183.4	162.5	145.4
TS1$_{dae}$ ··H_2O2DMSO	-2722.85272	-2722.32490	-2722.45148	-2722.44138	-2722.42795	266.4	245.2	216.9
	3.44	3.98	17.88	10.45	11.22	-46.6	-21.7	-24.3
DMSO 298.15K								
1da	-1178.99011	-1178.77724	-1178.83884	-1178.82681	-1178.82274	129.6	104.3	95.8
2e	-361.20277	-361.09542	-361.13668	-361.12587	-361.12522	86.8	64.1	62.7
TS1$_{dae}$	-1540.19170	-1539.87058	-1539.95258	-1539.94150	-1539.93478	172.6	149.3	135.1
	0.74	1.31	14.40	7.02	8.27	-43.9	-19.1	-23.4
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2d ··2H_2O1DMSO	-1472.42354	-1472.18788	-1472.25856	-1472.24747	-1472.24219	148.8	125.4	114.3
TS1$_{dbd}$ ··2H_2O1DMSO	-2136.84790	-2136.45311	-2136.55387	-2136.54290	-2136.53524	212.1	189.0	172.8
	8.21	8.68	23.14	15.94	15.74	-48.5	-24.3	-23.4
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2d ··2H_2O1DMSO	-1472.42260	-1472.18692	-1472.25757	-1472.24644	-1472.24119	148.7	125.3	114.2
TS1$_{dbd}$ ··2H_2O1DMSO	-2136.84699	-2136.45217	-2136.55263	-2136.54185	-2136.53387	211.4	188.8	172.0
	8.07	8.55	23.17	15.76	15.68	-49.0	-24.2	-23.9
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2d ··2H_2O2DMSO	-2025.53882	-2025.21402	-2025.30401	-2025.29352	-2025.28476	189.4	167.3	148.9
TS1$_{dbd}$ ··2H_2O2DMSO	-2689.96916	-2689.48473	-2689.60283	-2689.59252	-2689.58268	248.6	226.9	206.2
	4.46	5.25	20.93	13.70	12.58	-52.6	-28.3	-24.6
DMSO 298.15K								

1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2d ··2H_2O2DMSO	-2025.53763	-2025.21281	-2025.30261	-2025.29212	-2025.28346	189.0	166.9	148.7
TS1$_{dbd}$ ··2H_2O2DMSO	-2689.96784	-2689.48336	-2689.60179	-2689.59141	-2689.58145	249.3	227.4	206.5
	4.42	5.22	20.58	13.32	12.35	-51.5	-27.2	-23.9
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2d ··H_2O2DMSO	-1949.10074	-1948.80433	-1948.89073	-1948.88046	-1948.87144	181.9	160.2	141.2
TS1$_{dbd}$ ··H_2O2DMSO	-2613.53122	-2613.07515	-2613.18721	-2613.17980	-2613.16973	235.9	220.3	199.1
	4.25	5.05	22.28	13.29	12.13	-57.8	-27.6	-23.8
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2d	-766.43475	-766.34480	-766.38323	-766.37030	-766.37022	80.9	53.7	53.5
TS1$_{dbd}$	-1430.86883	-1430.61953	-1430.68885	-1430.67735	-1430.67291	145.9	121.7	112.3
	1.99	2.60	16.54	8.45	9.40	-46.8	-19.6	-22.8
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2e ··2H_2O1DMSO	-1067.18962	-1066.93664	-1067.01150	-1067.00122	-1066.99494	157.6	135.9	122.7
TS1$_{dbe}$ ··2H_2O1DMSO	-1731.61981	-1731.20773	-1731.31280	-1731.30243	-1731.29275	221.1	199.3	179.0
	4.55	5.01	19.38	12.31	12.66	-48.2	-24.5	-25.6
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2e ··2H_2O1DMSO	-1067.18861	-1066.93561	-1067.00991	-1066.99945	-1066.99346	156.4	134.4	121.8
TS1$_{dbe}$ ··2H_2O1DMSO	-1731.61888	-1731.20677	-1731.31175	-1731.30143	-1731.29180	220.9	199.2	179.0
	4.38	4.84	18.91	11.63	12.13	-47.2	-22.8	-24.4
H_2O 298.15K								
1db	-664.43744	-664.27907	-664.33218	-664.32083	-664.31797	111.8	87.9	81.9
2e ··2H_2O2DMSO	-1620.30535	-1619.96310	-1620.05652	-1620.04662	-1620.03732	196.6	175.8	156.2
TS1$_{dbe}$ ··2H_2O2DMSO	-2284.74135	-2284.23963	-2284.36170	-2284.35173	-2284.34059	256.9	235.9	212.5
	0.90	1.59	16.94	9.86	9.22	-51.5	-27.7	-25.4
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2e ··2H_2O2DMSO	-1620.30420	-1619.96194	-1620.05553	-1620.04555	-1620.03617	197.0	176.0	156.2
TS1$_{dbe}$ ··2H_2O2DMSO	-2284.74005	-2284.23828	-2284.35946	-2284.34941	-2284.33917	255.0	233.9	212.4
	0.88	1.59	17.60	10.45	9.20	-53.7	-29.7	-25.5
DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2e ··H_2O2DMSO	-1543.86809	-1543.55401	-1543.64114	-1543.63123	-1543.62309	183.4	162.5	145.4
TS1$_{dbe}$ ··H_2O2DMSO	-2208.30399	-2207.83075	-2207.94913	-2207.93920	-2207.92654	249.1	228.3	201.6
	0.85	1.34	15.05	7.88	8.93	-46.0	-21.9	-25.4

DMSO 298.15K								
1db	-664.43725	-664.27887	-664.33198	-664.32052	-664.31767	111.8	87.7	81.7
2e	-361.20277	-361.09542	-361.13668	-361.12587	-361.12522	86.8	64.1	62.7
TS1$_{dbe}$	-1025.64242	-1025.37569	-1025.44765	-1025.43694	-1025.43228	151.5	128.9	119.1
	-1.51	-0.88	13.18	5.93	6.66	-47.2	-22.8	-25.3

S14 The energy, enthalpy, free energy (au) and entropy (cal·mol^{-1}·K^{-1}) for the reactions in **Fig.1**, obtained with different models.

species	E	H	G(gas)	G(sol)	G_{qRRHO}(l)	S(gas)	S(sol)	S_{qRRHO}(l)
MeOH 313.15K CAM-B3LYP+IDSCRF/TZVP								
1a	-2810.69342	-2810.50090	-2810.55115	-2810.53985	-2810.53841	100.7	78.0	75.2
2a	-265.48638	-265.37965	-265.41721	-265.40562	-265.40518	75.3	52.0	51.2
TS$_{aa}$	-3076.15068	-3075.85049	-3075.92139	-3075.91042	-3075.90380	142.1	120.1	107.0
	18.27	18.86	29.47	21.99	24.96	-33.9	-10.0	-19.4
P$_{aa}$	-3076.21660	-3075.91290	-3075.98299	-3075.97195	-3075.96698	140.5	118.3	108.4
	-23.09	-20.30	-9.18	-16.62	-14.68	-35.5	-11.8	-17.9
MeOH 313.15K CAM-B3LYP+IDSCRF/6-311++G(d,p)								
1a	-2810.64389	-2810.45181	-2810.50204	-2810.49073	-2810.48931	100.7	78.0	75.1
2a	-265.47123	-265.36468	-265.40235	-265.39072	-265.39023	75.5	52.2	51.2
TS$_{aa}$	-3076.08605	-3075.78654	-3075.85744	-3075.84642	-3075.8399	142.1	120.0	106.7
	18.24	18.79	29.46	21.98	24.90	-34.1	-10.2	-19.6
P$_{aa}$	-3076.15209	-3075.84906	-3075.91906	-3075.90788	-3075.90302	140.3	117.9	108.1
	-23.20	-20.44	-9.21	-16.59	-14.73	-35.9	-12.3	-18.2
MeOH 313.15K B3LYP+IDSCRF/DZVP								
1a	-2810.19948	-2810.00783	-2810.05822	-2810.04690	-2810.04549	101.0	78.3	75.5
2a	-265.56510	-265.45933	-265.49700	-265.48561	-265.48523	75.5	52.6	51.9
TS$_{aa}$	-3075.73756	-3075.43926	-3075.51096	-3075.50010	-3075.49329	143.7	121.9	108.3
	16.96	17.51	27.77	20.34	23.49	-32.8	-9.0	-19.1
P$_{aa}$	-3075.79594	-3075.49407	-3075.56456	-3075.55369	-3075.54872	141.2	119.5	109.5
	-19.68	-16.89	-5.86	-13.29	-11.30	-35.2	-11.5	-17.8
MeOH 313.15K M062x+IDSCRF/DZVP								
1a	-2810.06682	-2809.87337	-2809.92351	-2809.91226	-2809.91086	100.5	77.9	75.1
2a	-265.44255	-265.33546	-265.37291	-265.36128	-265.36098	75.0	51.7	51.1
TS$_{aa}$	-3075.48346	-3075.18204	-3075.25286	-3075.24185	-3075.23521	141.9	119.9	106.4
	16.26	16.81	27.33	19.89	22.99	-33.6	-9.8	-19.8
P$_{aa}$	-3075.54778	-3075.24306	-3075.31277	-3075.30187	-3075.29714	139.7	117.8	108.4
	-24.10	-21.48	-10.26	-17.78	-15.88	-35.8	-11.8	-17.9
MeOH 313.15K ωB97x+IDSCRF/DZVP								
1a	-2810.11824	-2809.92418	-2809.97424	-2809.96312	-2809.96174	100.3	78.0	75.3

2a	-265.48457	-265.37710	-265.41458	-265.40298	-265.40263	75.1	51.9	51.2
TS_{aa}	-3075.57234	-3075.26995	-3075.34107	-3075.33012	-3075.32338	142.5	120.6	107.1
	19.12	19.66	29.96	22.58	25.72	-32.9	-9.3	-19.4
P_{aa}	-3075.64058	-3075.33474	-3075.40464	-3075.39363	-3075.38877	140.1	118.0	108.3
	-23.70	-21.00	-9.93	-17.28	-15.31	-35.4	-11.9	18.2
MeOH 313.15K ωB97xD +IDSCRF/DZVP								
1a	-2810.14836	-2809.95474	-2810.00486	-2809.99362	-2809.99221	100.4	77.9	75.1
2a	-265.46959	-265.36244	-265.39997	-265.38843	-265.38806	75.2	52.1	51.3
TS_{aa}	-3075.59114	-3075.28946	-3075.35995	-3075.34906	-3075.34264	141.3	119.4	106.5
	16.82	17.39	28.16	20.70	23.61	-34.4	-10.5	-19.9
P_{aa}	-3075.65854	-3075.35330	-3075.42356	-3075.41275	-3075.40767	140.8	119.1	108.9
	-25.47	-22.67	-11.75	-19.26	-17.19	-34.8	-10.8	-17.5
MeOH 313.15K CAM-B3LYP/DZVP								
1a	-2810.13914	-2809.94622	-2809.9930	–	–	98.5	–	–
2a	-265.41657	-265.31001	-265.34529	–	–	74.2	–	–
TS_{aa}	-3075.51251	-3075.21175	-3075.27714	–	–	137.6	–	–
	27.10	27.91	38.37	–	–	-35.1	–	–
MeOH 313.15K M062x/DZVP								
1a	-2810.06494	-2809.87187	-2809.91844	–	–	98.0	–	–
2a	-265.433315	-265.327832	-265.361285	–	–	70.4	–	–
TS_{aa}	-3075.45889	-3075.15820	-3075.22307	–	–	136.5	–	–
	24.70	26.04	35.55	–	–	-31.9	–	–
MeOH 313.15K B2PLYP+IDSCRF/DZVP								
1a	-2809.07812	–	–	–	–	–	–	–
2a	-264.980550	–	–	–	–	–	–	–
TS_{aa}	-3074.02844	–	–	–	–	–	–	–
	18.97	–	–	–	–	–	–	–
MeOH 273.15K CAM-B3LYP+IDSCRF/TZVP								
1ba	-251.84825	-251.68241	-251.71372	-251.70334	-251.70334	72.0	48.1	48.1
2b	-1100.82169	-1100.71540	-1100.75962	-1100.74804	-1100.74685	101.6	75.0	72.2
$TS1_{bab}$	-1352.65620	-1352.38252	-1352.43808	-1352.42734	-1352.42519	127.6	103.0	98.0
	8.62	9.59	22.13	15.09	15.69	-45.9	-20.1	-22.3
$IN1_{bab}$	-1352.70211	-1352.42566	-1352.48256	-1352.47190	-1352.46955	130.7	106.2	100.8
	-20.19	-17.48	-5.79	-12.88	-12.15	-42.8	-16.8	-19.5
$TS2_{bab}$	-1604.55079	-1604.10932	-1604.18107	-1604.17065	-1604.16573	164.8	140.9	129.6
	-20.46	-18.26	3.76	-10.00	-7.66	-80.8	-30.3	-38.8
P_{bab}	-1604.56962	-1604.12323	-1604.19762	-1604.18732	-1604.18164	170.9	147.2	134.2
	-32.27	-27.00	-6.63	-20.46	-17.65	-74.7	-24.0	-34.2
MeOH 273.15K CAM-B3LYP+IDSCRF/6-311++G(d,p)								

1ba	-251.83287	-251.66744	-251.69879	-251.68859	-251.68859	72.0	48.6	48.6
2b	-1100.78662	-1100.68021	-1100.72437	-1100.71306	-1100.71188	101.5	75.5	72.8
TS1$_{bab}$	-1352.60757	-1352.33439	-1352.39000	-1352.37879	-1352.37663	127.8	102.0	97.0
	7.48	8.32	20.81	14.34	14.96	-45.7	-22.0	24.3
IN1$_{bab}$	-1352.65304	-1352.37672	-1352.43365	-1352.42305	-1352.42070	130.8	106.4	101.0
	-21.05	-18.24	-6.58	-13.43	-12.69	-42.7	-17.6	-20.3
TS2$_{bab}$	-1604.48896	-1604.04812	-1604.12044	-1604.10978	-1604.10453	166.1	141.6	129.6
	-22.97	-20.73	0.95	-12.26	-9.71	-79.4	-31.1	-40.4
P $_{bab}$	-1604.5088	-1604.06316	-1604.13833	-1604.12783	-1604.12174	172.7	148.6	134.6
	-35.42	-30.16	-10.28	-23.59	-20.51	-72.8	-24.1	-35.4
MeOH 273.15K B3LYP+IDSCRF/DZVP								
1ba	-251.93390	-251.76900	-251.80041	-251.79014	-251.79014	72.2	48.6	48.6
2b	-1100.89782	-1100.79279	-1100.83711	-1100.82576	-1100.82460	101.8	75.7	73.1
TS1$_{bab}$	-1352.82025	-1352.54890	-1352.60470	-1352.59388	-1352.59176	128.2	103.3	98.5
	7.20	8.09	20.59	13.82	14.42	-45.8	-21.0	-23.2
IN1$_{bab}$	-1352.85706	-1352.58290	-1352.64008	-1352.62930	-1352.62699	131.3	106.6	101.3
	-15.90	-13.25	-1.61	-8.41	-7.69	-42.6	-17.7	-20.3
TS2$_{bab}$	-1604.79021	-1604.35222	-1604.42475	-1604.41415	-1604.40903	166.6	142.3	130.5
	-15.43	-13.45	8.27	-5.09	-2.61	-79.5	-30.6	-39.6
P $_{bab}$	-1604.81965	-1604.37651	-1604.45383	-1604.44376	-1604.43672	177.6	154.5	138.3
	-33.9	-28.69	-9.98	-23.67	-19.98	-68.5	-18.4	-31.8
MeOH 273.15K M062x+IDSCRF/DZVP								
1ba	-251.80077	-251.63419	-251.66547	-251.65513	-251.65513	71.9	48.1	48.1
2b	-1100.59573	-1100.48877	-1100.53275	-1100.52109	-1100.51999	101.0	74.2	71.7
TS1$_{bab}$	-1352.39895	-1352.12445	-1352.17979	-1352.16876	-1352.16674	127.1	101.8	97.2
	-1.54	-0.93	11.57	4.68	5.26	-45.7	-20.6	-22.7
IN1$_{bab}$	-1352.43862	-1352.16089	-1352.21732	-1352.20670	-1352.20447	129.7	105.2	100.1
	-26.43	-23.80	-11.99	-19.13	18.42	-43.2	-17.1	-19.7
TS2$_{bab}$	-1604.24642	-1603.80298	-1603.87333	-1603.86276	-1603.85824	161.6	137.3	127
	-30.84	-28.76	-6.05	-19.71	-17.56	-83.2	-33.1	-40.9
P $_{bab}$	-1604.26772	-1603.81993	-1603.8928	-1603.88241	-1603.87743	167.4	143.5	132.1
	-44.21	-39.39	-18.27	-32.04	-29.61	-77.4	-26.9	-35.8
MeOH 273.15K ωB97x+IDSCRF/DZVP								
1ba	-251.86009	-251.69280	-251.72406	-251.71379	-251.71379	71.8	48.2	48.2
2b	-1100.69937	-1100.59191	-1100.63597	-1100.62426	-1100.62311	101.2	74.3	71.7
TS1$_{bab}$	-1352.55156	-1352.27558	-1352.33080	-1352.32004	-1352.31801	126.9	102.1	97.5
	4.96	5.73	18.34	11.30	11.85	-46.2	-20.4	-22.4
IN1$_{bab}$	-1352.59708	-1352.31770	-1352.37427	-1352.36361	-1352.36133	129.9	105.5	100.2
	-23.61	-20.70	-8.94	-16.04	-15.33	-43.1	-17.1	-19.7

TS2$_{bab}$	-1604.46072	-1604.01589	-1604.08773	-1604.07714	-1604.07213	165	140.7	129.2
	-25.83	-24.08	-2.28	-15.87	-13.45	-79.8	-30.0	-38.9
P $_{bab}$	-1604.48438	-1604.03421	-1604.10643	-1604.09619	-1604.09157	165.9	142.4	131.8
	-40.68	-35.58	-14.02	-27.83	-25.64	-78.9	-28.3	-36.3
MeOH 273.15K ωB97xD+IDSCRF/DZVP								
1ba	-251.85343	-251.68654	-251.71778	-251.70738	-251.70738	71.8	47.9	47.9
2b	-1100.64924	-1100.54237	-1100.58667	-1100.57532	-1100.57410	101.8	75.7	72.9
TS1$_{bab}$	-1352.50184	-1352.22664	-1352.28218	-1352.27145	-1352.26928	127.6	102.9	98.0
	0.52	1.42	13.97	7.06	7.66	-46.0	-20.7	-22.8
IN1$_{bab}$	-1352.54410	-1352.26582	-1352.32273	-1352.31190	-1352.30950	130.7	105.9	100.3
	-26.00	-23.16	-11.47	-18.32	-17.58	-42.8	-17.7	-20.4
TS2$_{bab}$	-1604.40508	-1603.96091	-1604.03288	-1604.02081	-1604.01561	165.3	137.6	125.6
	-30.74	-28.53	-6.68	-19.28	-16.78	-80.1	-33.9	-43.1
P $_{bab}$	-1604.4305	-1603.98122	-1604.05386	-1604.04365	-1604.03876	166.9	143.4	132.2
	-46.69	-41.27	-19.845	-33.62	-31.31	-78.5	-28.1	-36.5
MeOH 273.15K CAM-B3LYP/DZVP								
1ba	-1100.61941	-1100.51063	-1100.56030	–	–	104.6	–	–
2b	-251.782564	-251.614787	-251.64991	–	–	73.9	–	–
TS1$_{bab}$	-1352.38796	8.79416213	-1352.17223	–	–	131.6	–	–
	8.79	9.85	23.83	–	–	-46.9	–	–
MeOH 273.15K M062x/DZVP								
1ba	-1100.58395	-1100.47483	-1100.52421	–	–	103.9	–	–
2b	-251.796982	-251.629412	-251.664526	–	–	73.9	–	–
TS1$_{bab}$	-1352.38108	-1352.10288	-1352.16482	–	–	130.3	–	–
	-0.09	0.85	15.00	–	–	-47.5	–	–
MeOH 273.15K B2PLYP+IDSCRF/DZVP								
1ba	-1099.44561	–	–	–	–	–	–	–
2b	-251.33028	–	–	–	–	–	–	–
TS1$_{bab}$	-1350.75506	–	–	–	–	–	–	–
	13.07	–	–	–	–	–	–	–
H_2O 298.15K CAM-B3LYP+IDSCRF/TZVP								
1da	-1179.21659	-1179.00432	-1179.06690	-1179.05508	-1179.05049	131.7	106.9	97.2
2d	-766.56622	-766.47669	-766.51518	-766.50239	-766.50230	81.0	54.1	53.9
TS1$_{dad}$	-1945.77440	-1945.47157	-1945.54978	-1945.53794	-1945.53200	164.6	139.7	127.2
	5.28	5.92	20.27	12.26	13.05	-48.1	-21.3	-23.9
IN1$_{dad}$	-1945.78679	-1945.48225	-1945.56048	-1945.54864	-1945.54264	164.7	139.7	127.1
	-2.50	-0.78	13.55	5.54	6.37	-48.1	-21.2	-24.0
TS2$_{dad}$	-1945.78170	-1945.47893	-1945.55742	-1945.54551	-1945.53944	165.2	140.1	127.4
	0.70	1.31	15.47	7.51	8.38	-47.6	-20.8	-23.7

P_{dad}	-1434.32247	-1434.12358	-1434.18191	-1434.17011	-1434.16659	122.8	97.9	90.5
4-NO_2-PhO^-	-511.48103	-511.37803	-511.41988	-511.40637	-511.40583	88.1	59.6	58.5
	-12.98	-12.93	-12.37	-11.93	-12.32	-1.8	-3.5	-2.1
H_2O 298.15K CAM-B3LYP+IDSCRF/6-311++G(d,p)								
1da	-1179.16994	-1178.95783	-1179.02046	-1179.00873	-1179.00410	131.8	107.1	97.4
2d	-766.55308	-766.46350	-766.50189	-766.48897	-766.48888	80.8	53.6	53.4
$TS1_{dad}$	-1945.71347	-1945.41071	-1945.48881	-1945.47681	-1945.47090	164.4	139.1	126.7
	5.99	6.66	21.05	13.11	13.86	-48.3	-21.6	-24.1
$IN1_{dad}$	-1945.72624	-1945.42159	-1945.49954	-1945.48744	-1945.48150	164.1	138.6	126.1
	-2.02	-0.16	14.31	6.44	7.20	-48.6	-22.1	-24.7
$TS2_{dad}$	-1945.72106	-1945.41822	-1945.49662	-1945.48454	-1945.47843	165.0	139.6	126.7
	1.23	1.95	16.15	8.26	9.13	-47.6	-21.2	-24.1
P_{dad}	-1434.2912	-1434.09246	-1434.1506	-1434.13893	-1434.13549	122.4	97.8	90.6
4-NO_2-PhO^-	-511.45221	-511.34911	-511.39078	-511.37717	-511.37666	87.7	59.1	58
	-12.79	-12.70	-11.94	-11.55	-12.10	-2.5	-3.8	-2.2
H_2O 298.15K B3LYP+IDSCRF/DZVP								
1da	-1179.37909	-1179.16898	-1179.23100	-1179.21921	-1179.21511	130.5	105.7	97.1
2d	-766.59465	-766.50585	-766.54449	-766.53209	-766.53200	81.3	55.2	55.0
$TS1_{dad}$	-1945.96443	-1945.66461	-1945.74284	-1945.73094	-1945.72526	164.6	139.6	127.6
	5.84	6.41	20.49	12.78	13.71	-47.2	-21.3	-24.5
$IN1_{dad}$	-1945.97380	-1945.67237	-1945.75075	-1945.73866	-1945.73299	164.9	139.5	127.6
	-0.04	1.54	15.52	7.93	8.86	-46.9	-21.4	-24.5
$TS2_{dad}$	-1945.97123	-1945.67126	-1945.75068	-1945.73878	-1945.73242	167.1	142.1	128.7
	1.58	2.24	15.57	7.86	9.22	-44.7	-18.8	-23.4
P_{dad}	-1434.39882	-1434.20198	-1434.26020	-1434.24856	-1434.24529	122.5	98.0	91.2
4-NO_2-PhO^-	-511.59947	-511.49705	-511.53868	-511.52545	-511.52504	87.6	59.8	58.9
	-15.40	-15.19	-14.68	-14.25	-14.57	-1.7	-3.1	-2.0
H_2O 298.15K M062x+IDSCRF/DZVP								
1da	-1179.00884	-1178.79616	-1178.85804	-1178.84613	-1178.84194	130.2	105.2	96.3
2d	-766.43291	-766.34307	-766.38154	-766.36911	-766.36903	81.0	54.8	54.6
$TS1_{dad}$	-1945.44800	-1945.14462	-1945.22273	-1945.21092	-1945.20515	164.4	139.5	127.4
	-3.92	-3.38	10.57	2.71	3.65	-46.8	-20.4	-23.6
$IN1_{dad}$	-1945.46357	-1945.15816	-1945.23520	-1945.22307	-1945.21766	162.1	136.6	125.2
	-13.69	-11.88	2.75	-4.91	-4.20	-49.1	-23.4	-25.7
$TS2_{dad}$	-1945.45379	-1945.15023	-1945.22832	-1945.21681	-1945.21096	164.4	140.1	127.8
	-7.56	-6.90	7.07	-0.99	0.01	-46.8	-19.8	-23.1
P_{dad}	-1434.08677	-1433.88787	-1433.94627	-1433.93453	-1433.93104	122.9	98.2	90.9
4-NO_2-PhO^-	-511.37692	-511.27318	-511.31469	-511.30134	-511.30094	87.4	59.3	58.4
	-13.77	-13.697	-13.42	-12.94	-13.18	-0.9	-2.5	-1.6

H_2O 298.15K ωB97x+IDSCRF/DZVP								
1da	-1179.12523	-1178.91154	-1178.97344	-1178.96161	-1178.95735	130.3	105.4	96.4
2d	-766.48012	-766.38984	-766.42821	-766.41537	-766.41529	80.7	53.7	53.6
$TS1_{dad}$	-1945.60534	-1945.30050	-1945.37808	-1945.36609	-1945.36044	163.3	138.0	126.2
	0.01	0.55	14.79	6.83	7.66	-47.7	-21.1	-23.8
$IN1_{dad}$	-1945.62093	-1945.31411	-1945.39135	-1945.37964	-1945.37403	162.6	137.9	126.1
	-9.78	-7.99	6.46	-1.67	-0.87	-48.4	-21.2	-23.9
$TS2_{dad}$	-1945.61250	-1945.30765	-1945.38647	-1945.37462	-1945.36829	165.9	141.0	127.6
	-4.49	-3.93	9.53	1.48	2.73	-45.1	-18.1	-22.3
P_{dad}	-1434.18018	-1433.98028	-1434.03876	-1434.02713	-1434.02353	123.1	98.6	91
4-NO_2-PhO^-	-511.44527	-511.34115	-511.38266	-511.36875	-511.36831	87.4	58.1	57.2
	-12.61	-12.58	-12.40	-11.86	-12.06	-0.5	-2.4	-1.8
H_2O 298.15K ωB97xD+IDSCRF/DZVP								
1da	-1179.07288	-1178.85991	-1178.92184	-1178.90994	-1178.90572	130.4	105.3	96.4
2d	-766.46009	-766.37013	-766.40856	-766.39600	-766.39591	80.9	54.4	54.3
$TS1_{dad}$	-1945.53566	-1945.23156	-1945.30901	-1945.29729	-1945.29176	163.0	138.3	126.7
	-1.69	-0.95	13.42	5.43	6.19	-48.2	-21.4	-24.0
$IN1_{dad}$	-1945.54886	-1945.24292	-1945.31980	-1945.30798	-1945.30263	161.8	136.9	125.7
	-9.97	-8.08	6.65	-1.28	-0.63	-49.4	-22.8	-25.0
$TS2_{dad}$	-1945.54194	-1945.23798	-1945.31643	-1945.30461	-1945.29851	165.1	140.2	127.4
	-5.63	-4.98	8.77	0.83	1.96	-46.1	-19.5	-23.3
P_{dad}	-1434.14514	-1433.9457	-1434.00364	-1433.99214	-1433.98884	121.9	97.7	90.8
4-NO_2-PhO^-	-511.40899	-511.3052	-511.34677	-511.33326	-511.3328	87.5	59.1	58.1
	-13.28	-13.09	-12.56	-12.21	-12.54	-1.9	-2.9	-1.8
H_2O 298.15K B2PLYP+IDSCRF/DZVP								
1da	-1177.55797	–	–	–	–	–	–	–
2d	-765.724709	–	–	–	–	–	–	–
$TS1_{dad}$	-1943.26990	–	–	–	–	–	–	–
	8.02	–	–	–	–	–	–	–
H_2O 298.15K CAM-B3LYP+IDSCRF/TZVP								
1da	-1179.21659	-1179.00432	-1179.06690	-1179.05508	-1179.05049	131.7	106.9	97.2
2e	-361.28378	-361.17702	-361.21828	-361.20733	-361.20664	86.9	63.8	62.4
$TS1_{dae}$	-1540.49655	-1540.17669	-1540.25868	-1540.24755	-1540.24078	172.6	149.1	134.9
	2.40	2.92	16.63	9.32	10.26	-46.0	-21.5	-24.7
$IN1_{dae}$	-1540.51193	-1540.19031	-1540.27040	-1540.25929	-1540.25357	168.6	145.2	133.2
	-7.25	-5.63	9.27	1.96	2.23	-50.0	-25.5	-26.4
$TS2_{dae}$	-1540.49877	-1540.17916	-1540.26080	-1540.24978	-1540.24319	171.8	148.6	134.8
	1.00	1.37	15.30	7.93	8.75	-46.8	-22.0	-24.8
P_{dae}	-1029.03772	-1028.8222	-1028.88281	-1028.87224	-1028.86884	127.6	105.3	98.1

4-NO_2-PhO^-	-511.48103	-511.37803	-511.41988	-511.40637	-511.40583	88.1	59.6	58.5
	-11.53	-11.85	-10.99	-10.16	-11.00	-2.9	-5.8	-3.0
H_2O 298.15K CAM-B3LYP+IDSCRF/6-311++G(d,p)								
1da	-1179.16994	-1178.95783	-1179.02046	-1179.00873	-1179.00410	131.8	107.1	97.4
2e	-361.26572	-361.15917	-361.20095	-361.18985	-361.18888	87.9	64.6	62.5
$TS1_{dae}$	-1540.43090	-1540.11133	-1540.19382	-1540.18277	-1540.17571	173.6	150.4	135.5
	2.99	3.56	17.31	9.92	10.84	-46.1	-21.3	-24.4
$IN1_{dae}$	-1540.44632	-1540.12491	-1540.20531	-1540.19425	-1540.18836	169.2	145.9	133.5
	-6.69	-4.96	10.10	2.72	2.90	-50.5	-25.8	-26.4
$TS2_{dae}$	-1540.43451	-1540.11616	-1540.19501	-1540.18392	-1540.17827	166.0	142.6	130.7
	0.72	0.53	16.57	9.20	9.23	-53.8	-29.1	-29.2
P_{dae}	-1029.00162	-1028.78639	-1028.84714	-1028.83657	-1028.83309	127.9	105.6	98.3
4-NO_2-PhO^-	-511.45221	-511.34911	-511.39078	-511.37717	-511.37666	87.7	59.1	58
	-11.40	-11.61	-10.36	-9.51	-10.56	-4.1	-7.0	-3.6
H_2O 298.15K B3LYP+IDSCRF/DZVP								
1da	-1179.37909	-1179.16898	-1179.23100	-1179.21921	-1179.21511	130.5	105.7	97.1
2e	-361.37028	-361.26415	-361.30545	-361.29448	-361.29390	86.9	63.8	62.6
$TS1_{dae}$	-1540.74549	-1540.42841	-1540.51076	-1540.49979	-1540.49307	173.3	150.2	136.1
	2.43	2.96	16.12	8.72	10.00	-44.1	-19.3	-23.6
$IN1_{dae}$	-1540.75323	-1540.43480	-1540.51579	-1540.50470	-1540.49885	170.5	147.1	134.8
	-2.42	-1.05	12.96	5.64	6.38	-47.0	-22.4	-24.9
$TS2_{dae}$	-1540.74599	-1540.42926	-1540.51176	-1540.50065	-1540.49385	173.6	150.3	135.9
	2.12	2.43	15.49	8.18	9.51	-43.8	-19.3	-23.7
P_{dae}	-1029.17192	-1028.95829	-1029.01907	-1029.00865	-1029.00535	127.9	106.0	99.0
4-NO_2-PhO^-	-511.59947	-511.49705	-511.53868	-511.52545	-511.52504	87.6	59.8	58.9
	-13.82	-13.94	-13.37	-12.81	-13.42	-1.9	-3.8	-1.7
H_2O 298.15K M062x+IDSCRF/DZVP								
1da	-1179.00884	-1178.79616	-1178.85804	-1178.84613	-1178.84194	130.2	105.2	96.3
2d	-361.20192	-361.09455	-361.13691	-361.12605	-361.12488	89.2	66.3	63.8
$TS1_{dae}$	-1540.21670	-1539.89576	-1539.97732	-1539.96634	-1539.96010	171.7	148.6	135.4
	-3.73	-3.17	11.06	3.66	4.22	-47.7	-22.9	-24.7
$IN1_{dae}$	-1540.23767	-1539.91465	-1539.99591	-1539.98490	-1539.97855	171.0	147.9	134.5
	-16.89	-15.02	-0.60	-7.98	-7.36	-48.4	-23.6	-25.7
$TS2_{dae}$	-1540.22554	-1539.90459	-1539.98533	-1539.97406	-1539.96800	169.9	146.2	133.5
	-9.27	-8.71	6.04	-1.18	-0.74	-49.4	-25.2	-26.7
P_{dae}	-1028.85473	-1028.63846	-1028.69913	-1028.68854	-1028.68515	127.7	105.4	98.3
4-NO_2-PhO^-	-511.37692	-511.27318	-511.31469	-511.30134	-511.30094	87.4	59.3	58.4
	-13.11	-13.13	-11.84	-11.11	-12.04	-4.3	-6.8	-3.4
H_2O 298.15K ωB97x+IDSCRF/DZVP								

1da	-1179.12523	-1178.91154	-1178.97344	-1178.96161	-1178.95735	130.3	105.4	96.4
2e	-361.25951	-361.15181	-361.19391	-361.18302	-361.18190	88.6	65.7	63.3
TS1$_{dae}$	-1540.38804	-1540.06592	-1540.14841	-1540.13730	-1540.13035	173.6	150.2	135.6
	-2.07	-1.61	11.89	4.60	5.58	-45.2	-20.8	-24.1
IN1$_{dae}$	-1540.40722	-1540.08303	-1540.16329	-1540.15223	-1540.14635	168.9	145.6	133.3
	-14.11	-12.35	2.55	-4.77	-4.46	-49.9	-25.4	-26.5
TS2$_{dae}$	-1540.39256	-1540.07052	-1540.15131	-1540.14018	-1540.13402	170.0	146.6	133.6
	-4.91	-4.50	10.07	2.79	3.28	-48.8	-24.4	-26.1
P$_{dae}$	-1028.95818	-1028.74108	-1028.80202	-1028.79135	-1028.78777	128.3	105.8	98.3
4-NO$_2$-PhO$^-$	-511.44527	-511.34115	-511.38266	-511.36875	-511.36831	87.4	58.1	57.2
	-11.74	-11.85	-10.87	-9.71	-10.54	-3.2	-7.2	-4.2
H_2O 298.15K ωB97xD+IDSCRF/DZVP								
1da	-1179.07288	-1178.85991	-1178.92184	-1178.90994	-1178.90572	130.4	105.3	96.4
2e	-361.23685	-361.12957	-361.17287	-361.16187	-361.16020	91.1	68.0	64.4
TS1$_{dae}$	-1540.31436	-1539.99330	-1540.07514	-1540.06400	-1540.05755	172.2	148.8	135.2
	-2.91	-2.40	12.28	4.90	5.25	-49.2	-24.5	-25.6
IN1$_{dae}$	-1540.33106	-1540.00790	-1540.08848	-1540.07750	-1540.07154	169.6	146.5	133.9
	-13.38	-11.56	3.91	-3.57	-3.53	-51.9	-26.8	-26.9
TS2$_{dae}$	-1540.31909	-1539.99814	-1540.07909	-1540.06801	-1540.06184	170.4	147.0	134.1
	-5.87	-5.43	9.80	2.38	2.56	-51.1	-26.2	-26.8
P$_{dae}$	-1028.91978	-1028.70342	-1028.76441	-1028.75383	-1028.75024	128.4	106.1	98.5
4-NO$_2$-PhO$^-$	-511.40899	-511.3052	-511.34677	-511.33326	-511.3328	87.5	59.1	58.1
	-11.95	-12.01	-10.33	-9.59	-10.74	-5.6	-8.1	-4.2
H_2O 298.15K B2PLYP+IDSCRF/DZVP								
1da	-1177.55797	–	–	–	–	–	–	–
2e	-360.624629	–	–	–	–	–	–	–
TS1$_{dae}$	-1538.17435	–	–	–	–	–	–	–
	5.18	–	–	–	–	–	–	–