

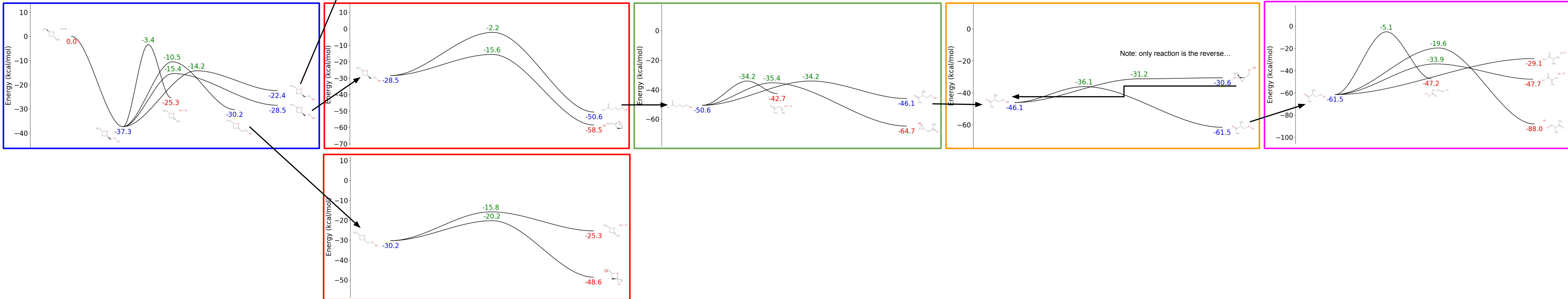
Doner et al., *Faraday Discussions* (2022)

Supplementary Information

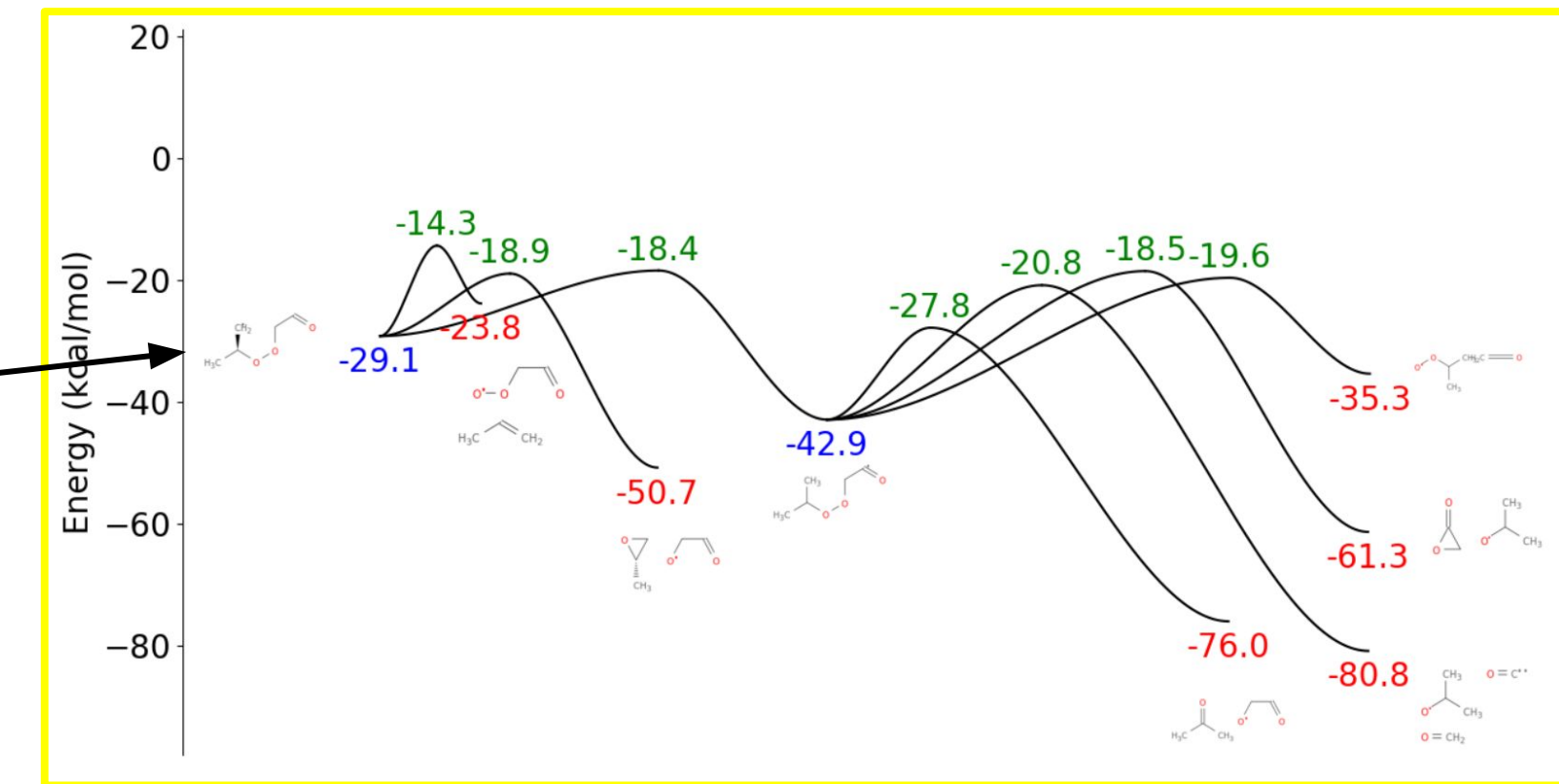
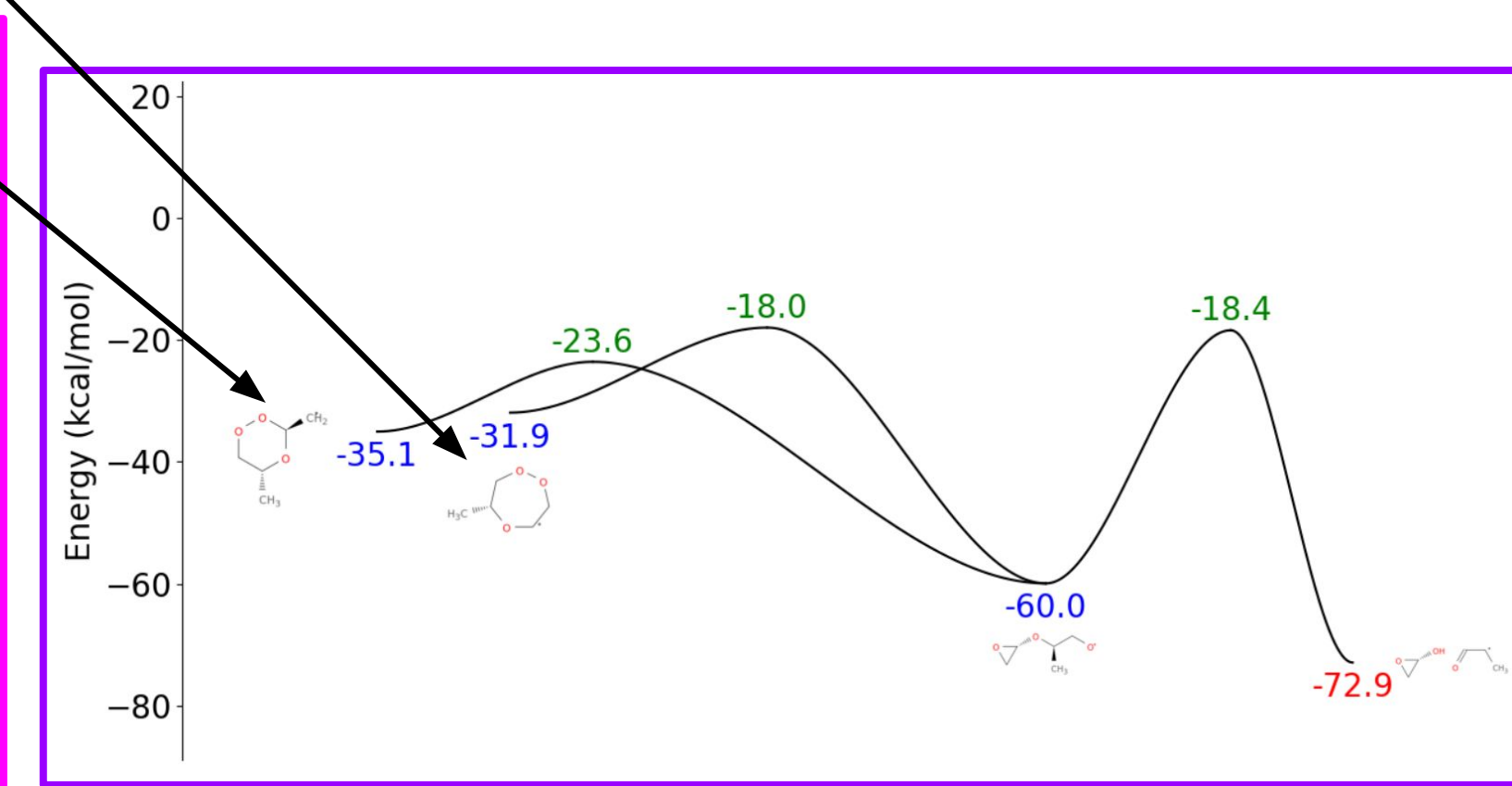
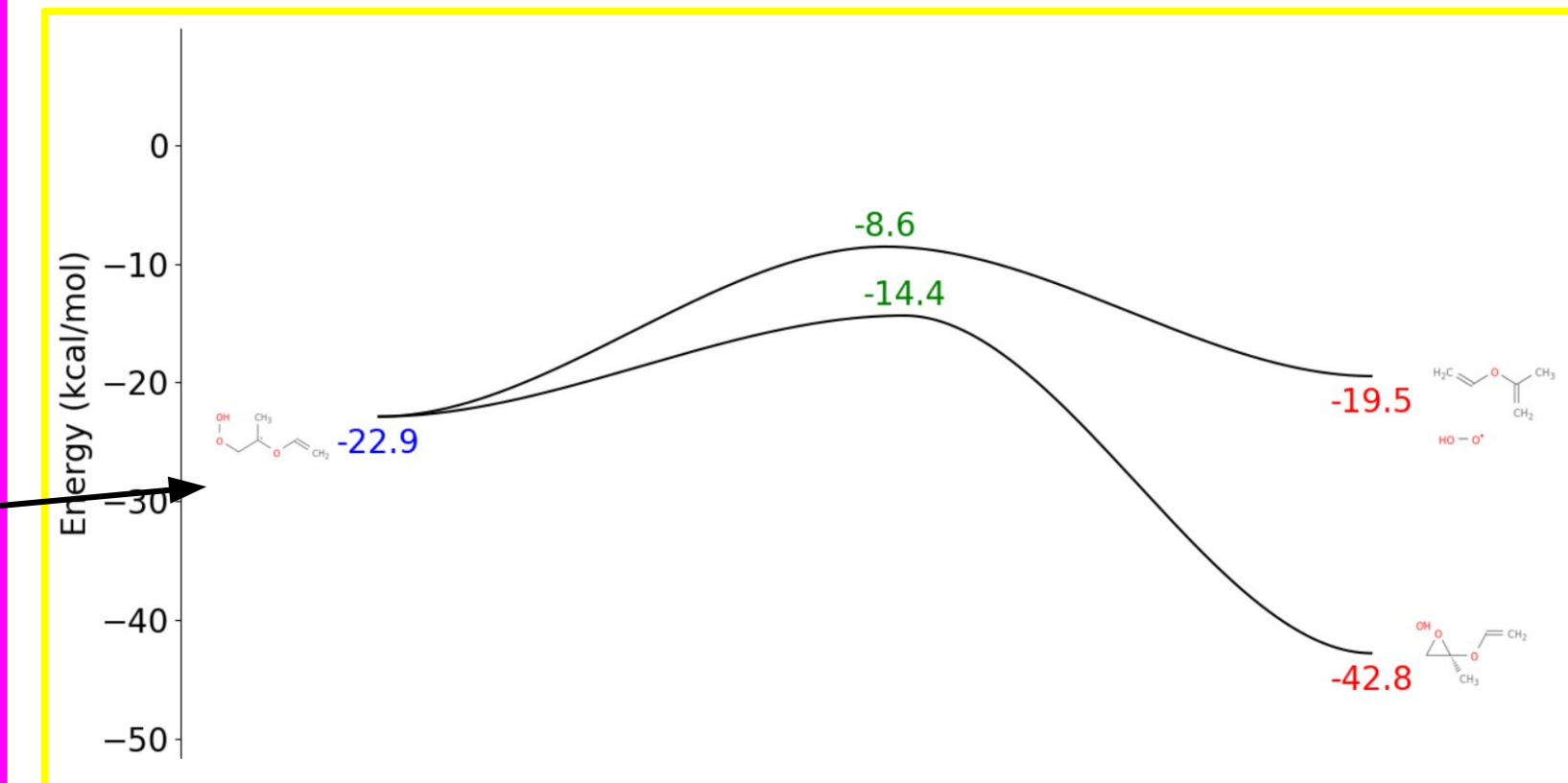
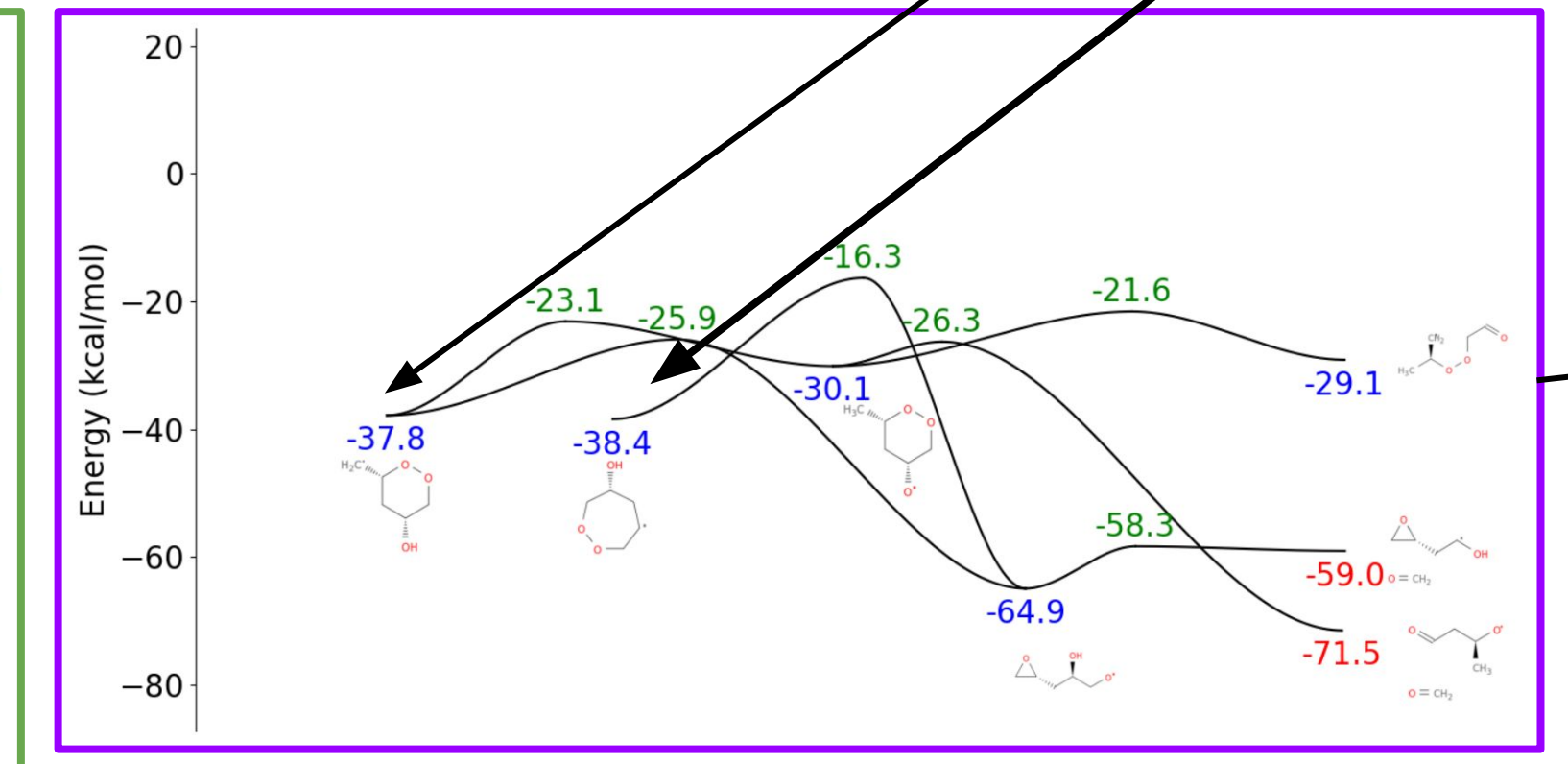
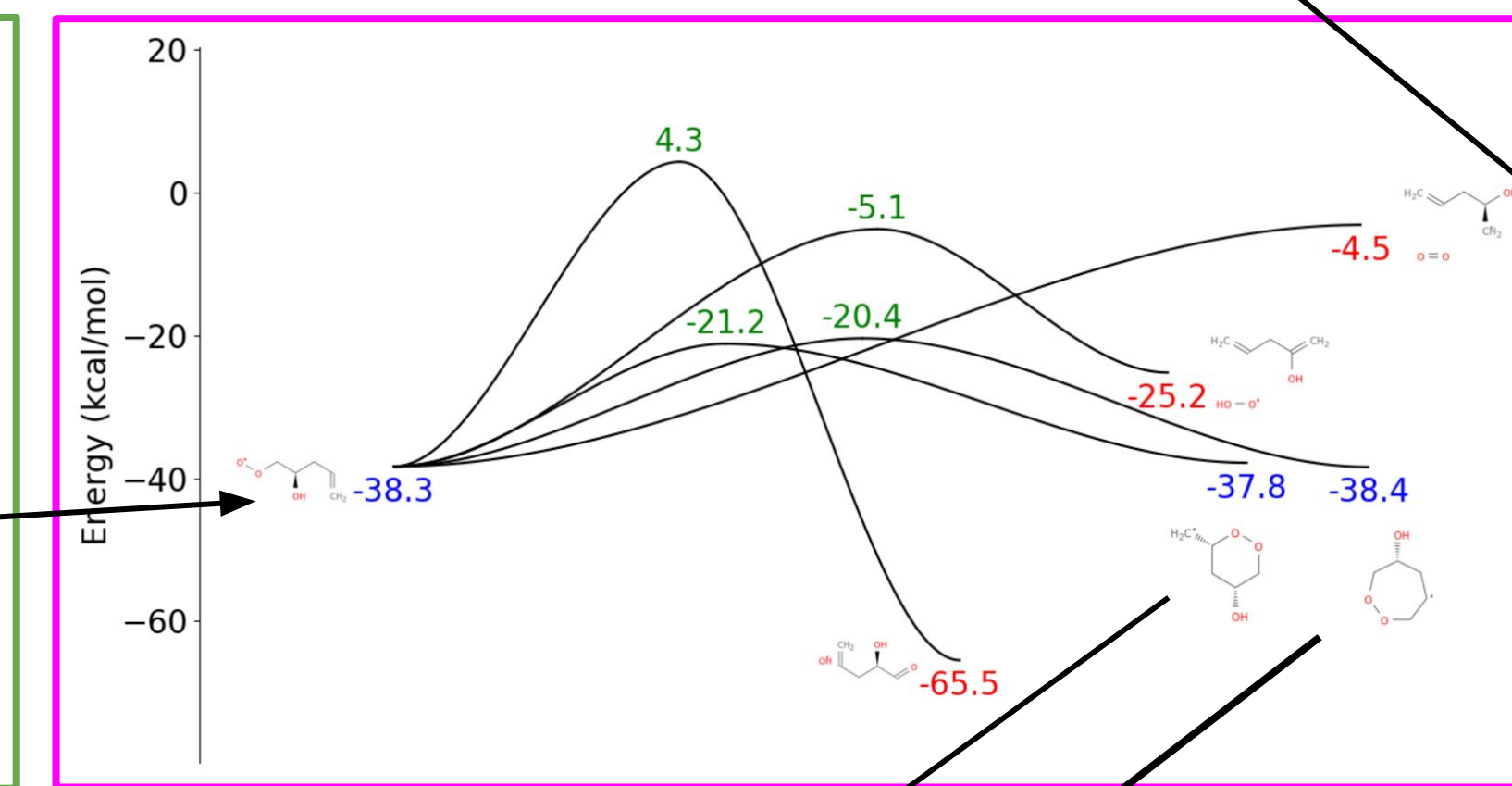
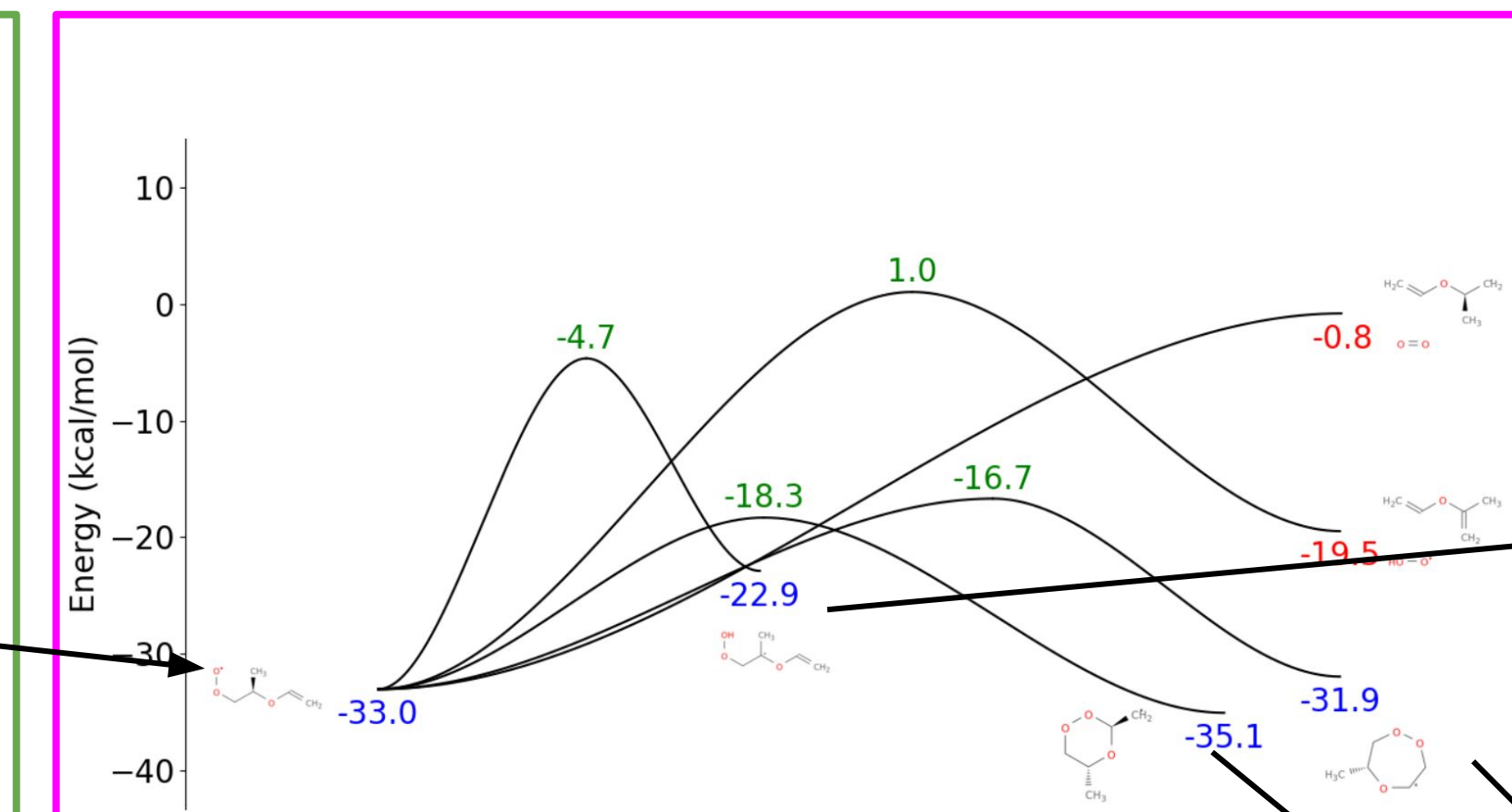
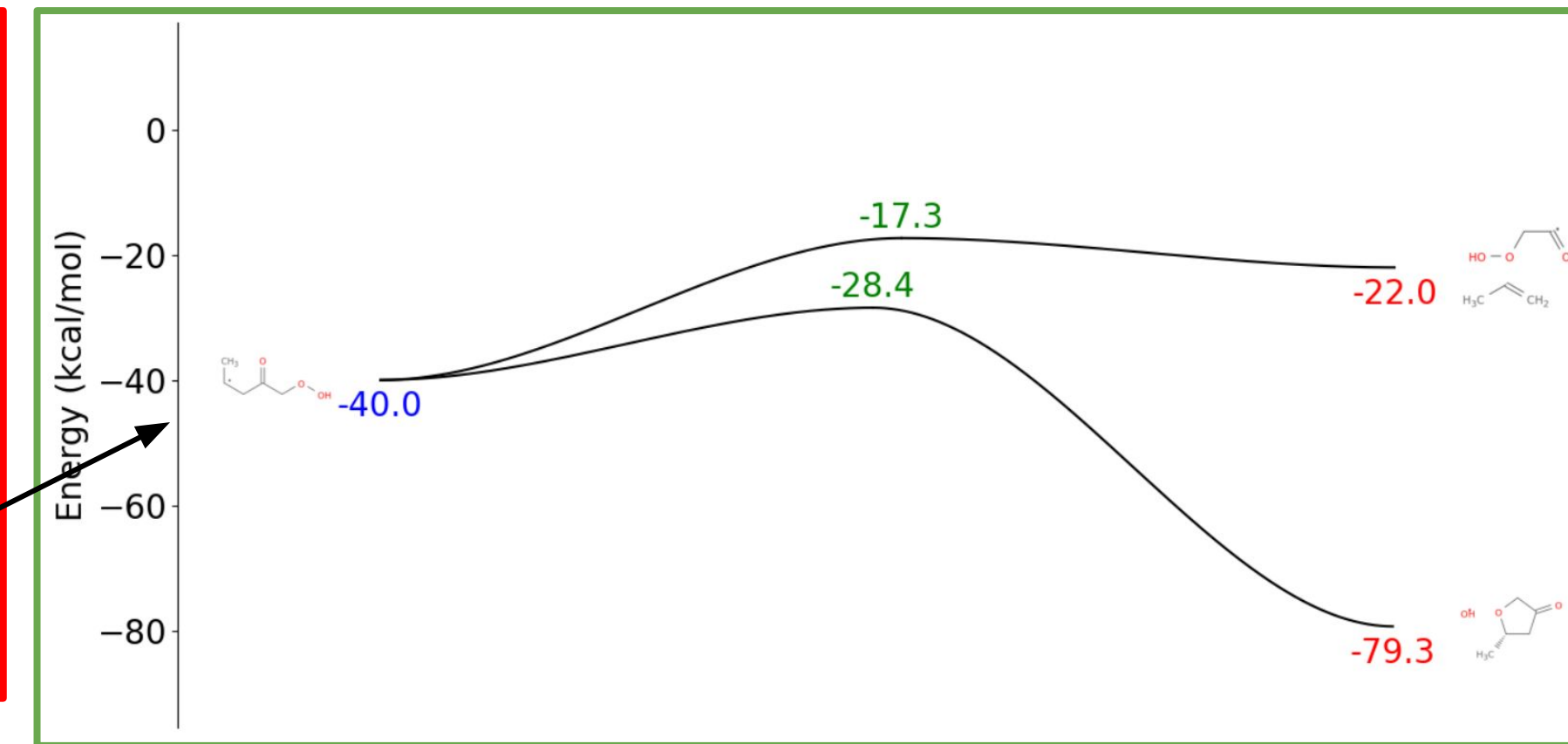
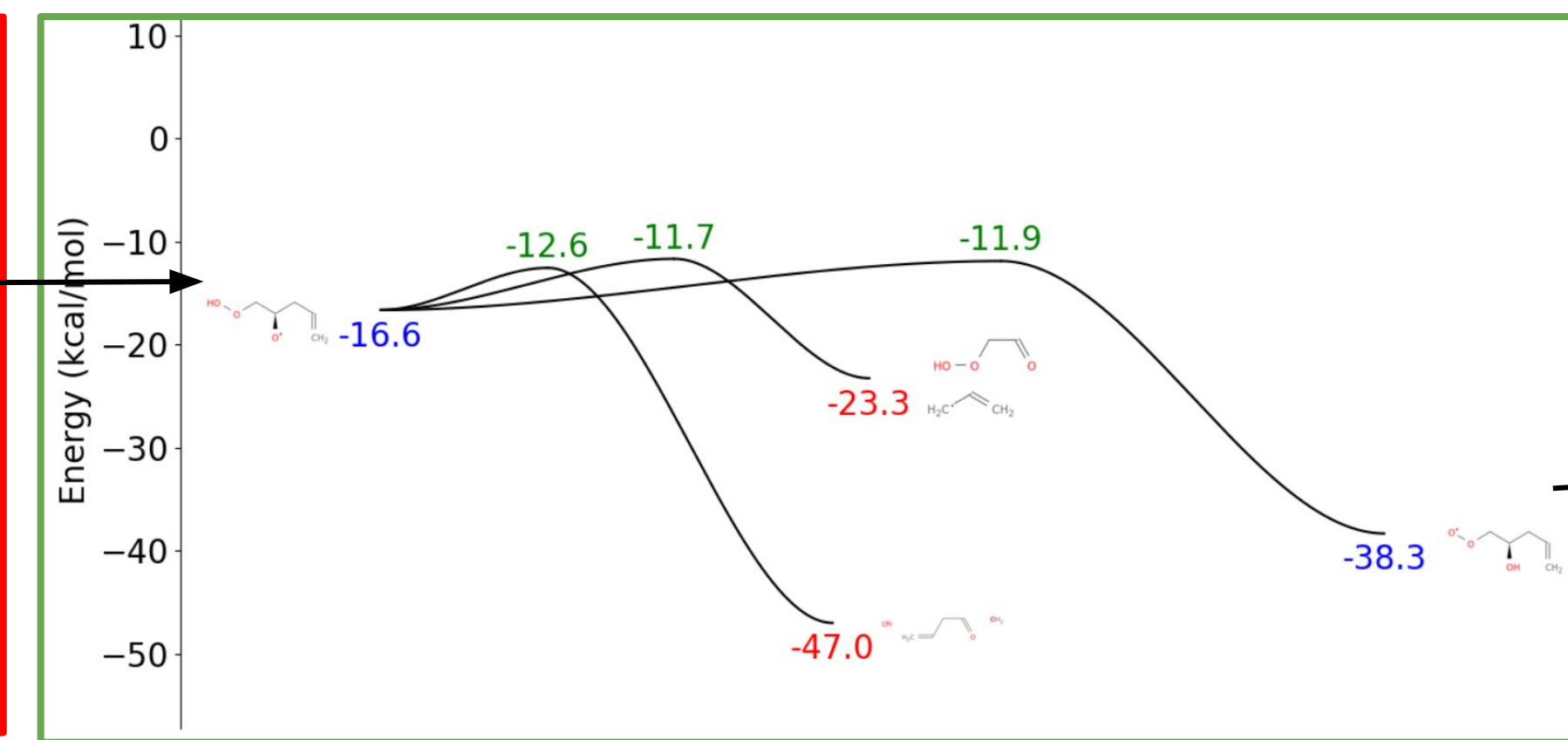
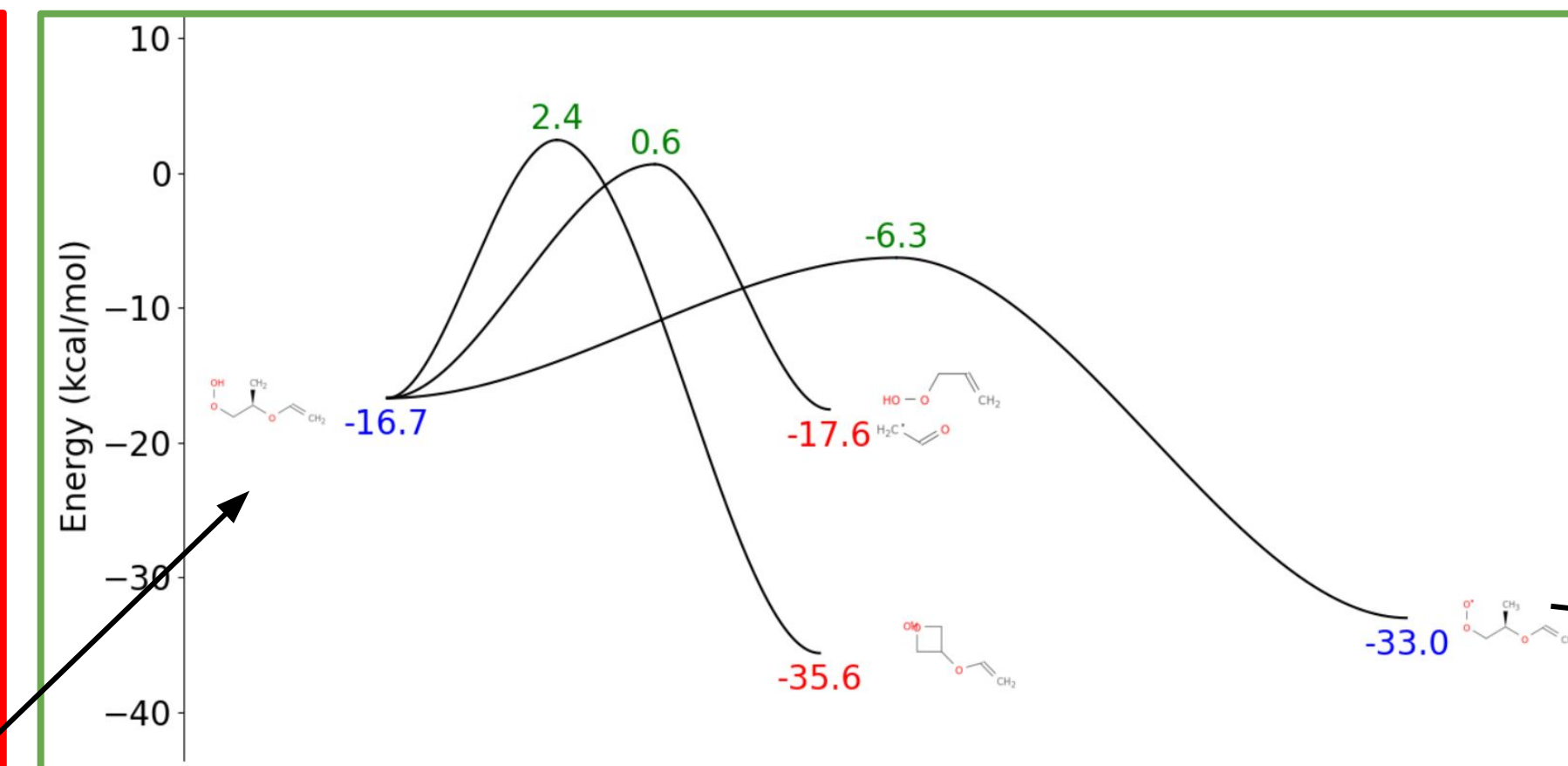
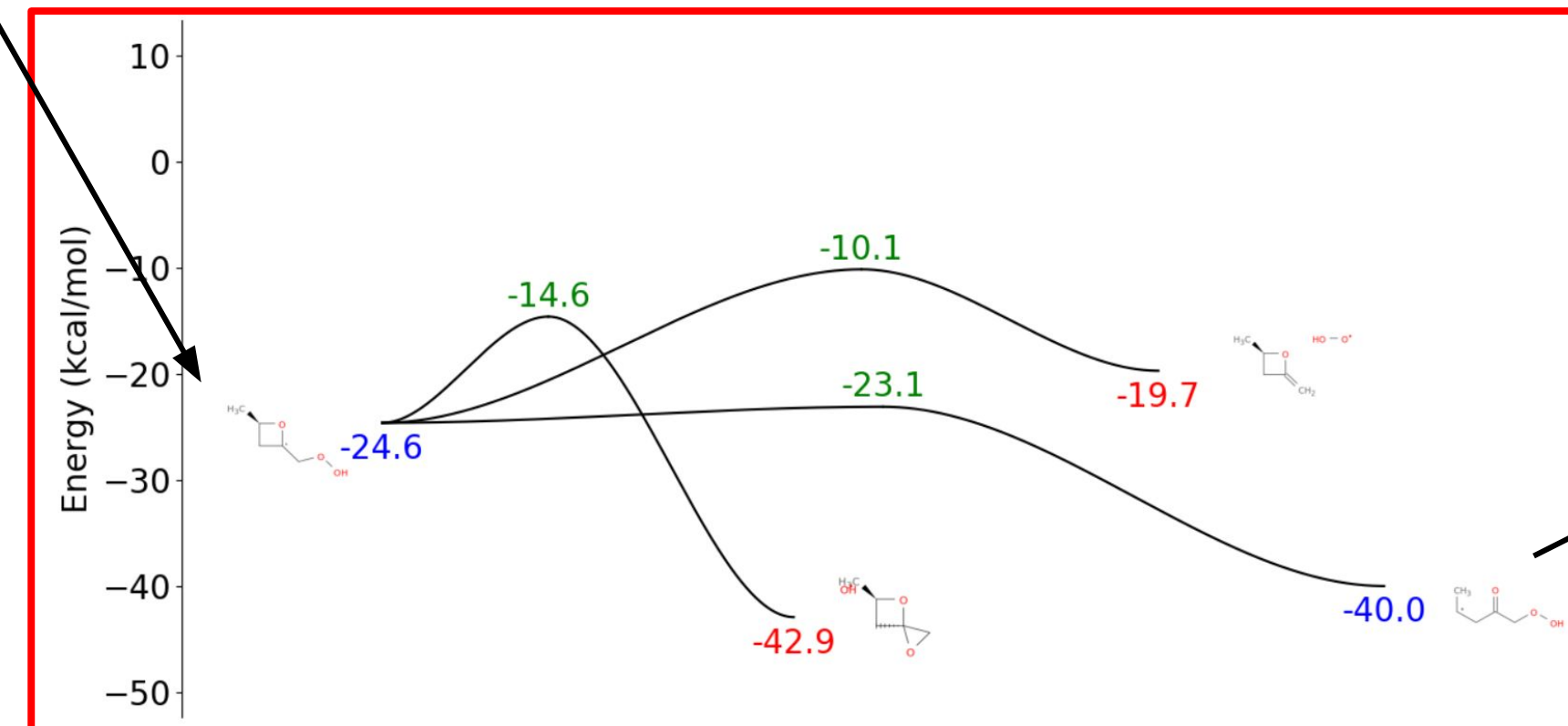
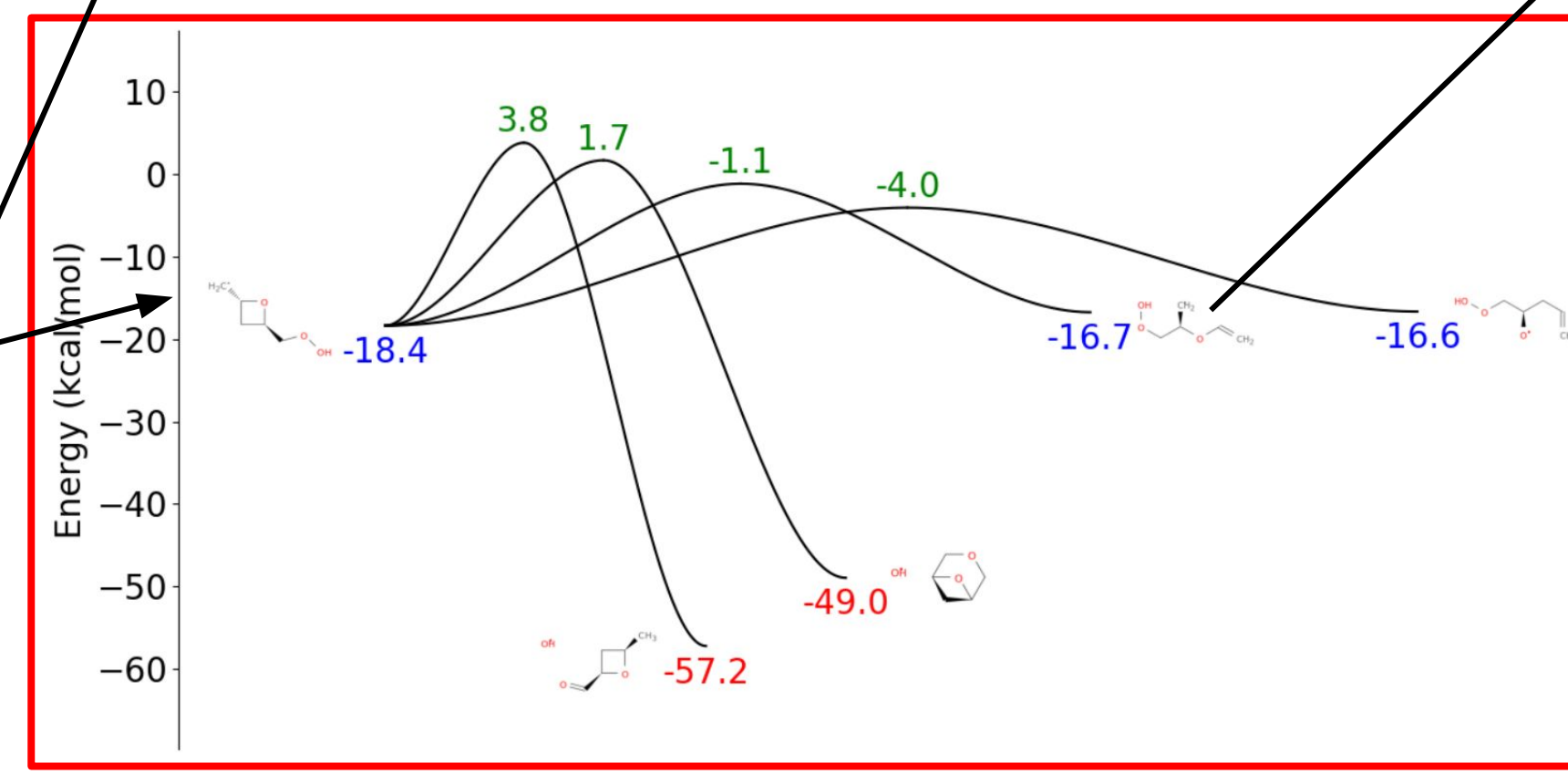
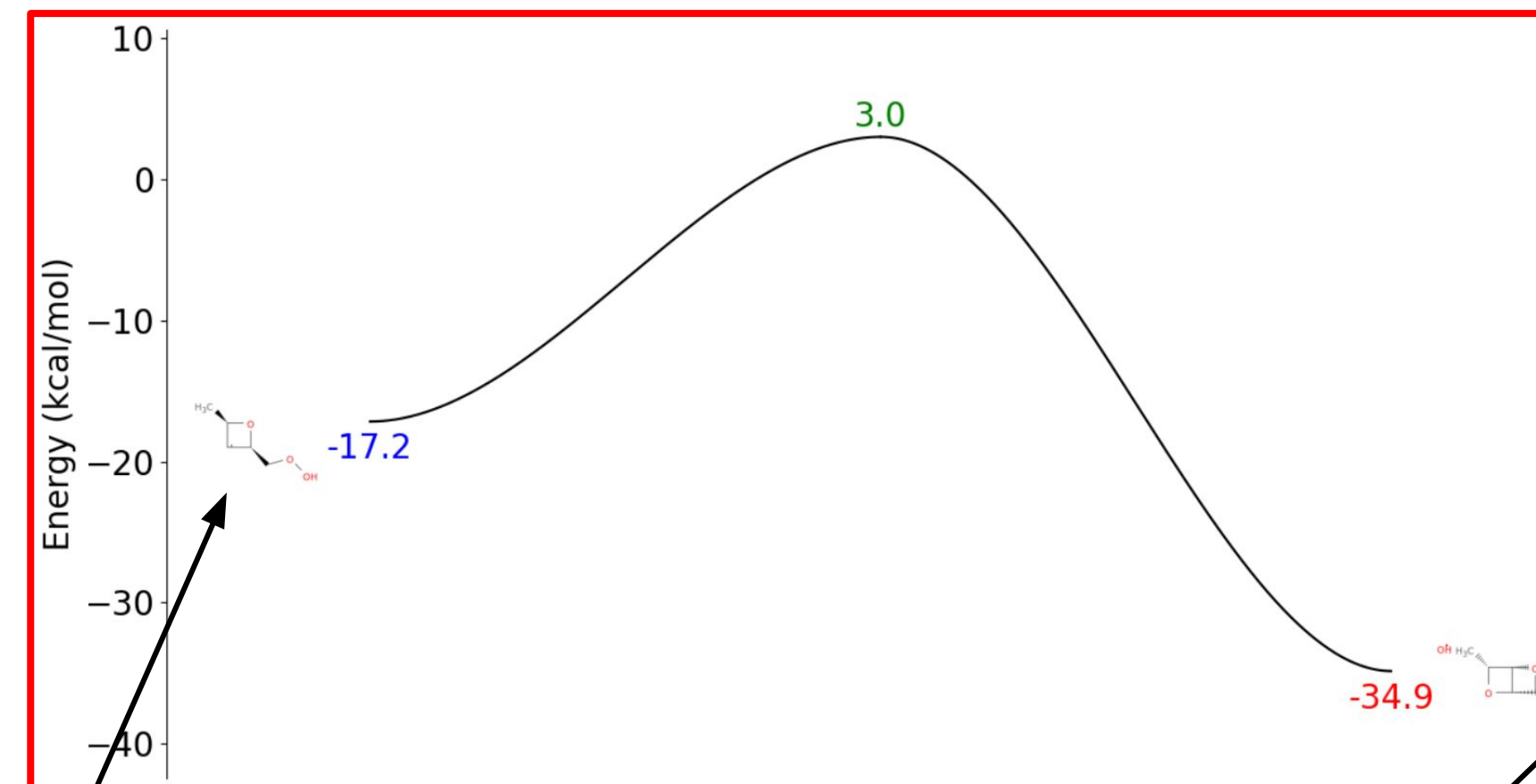
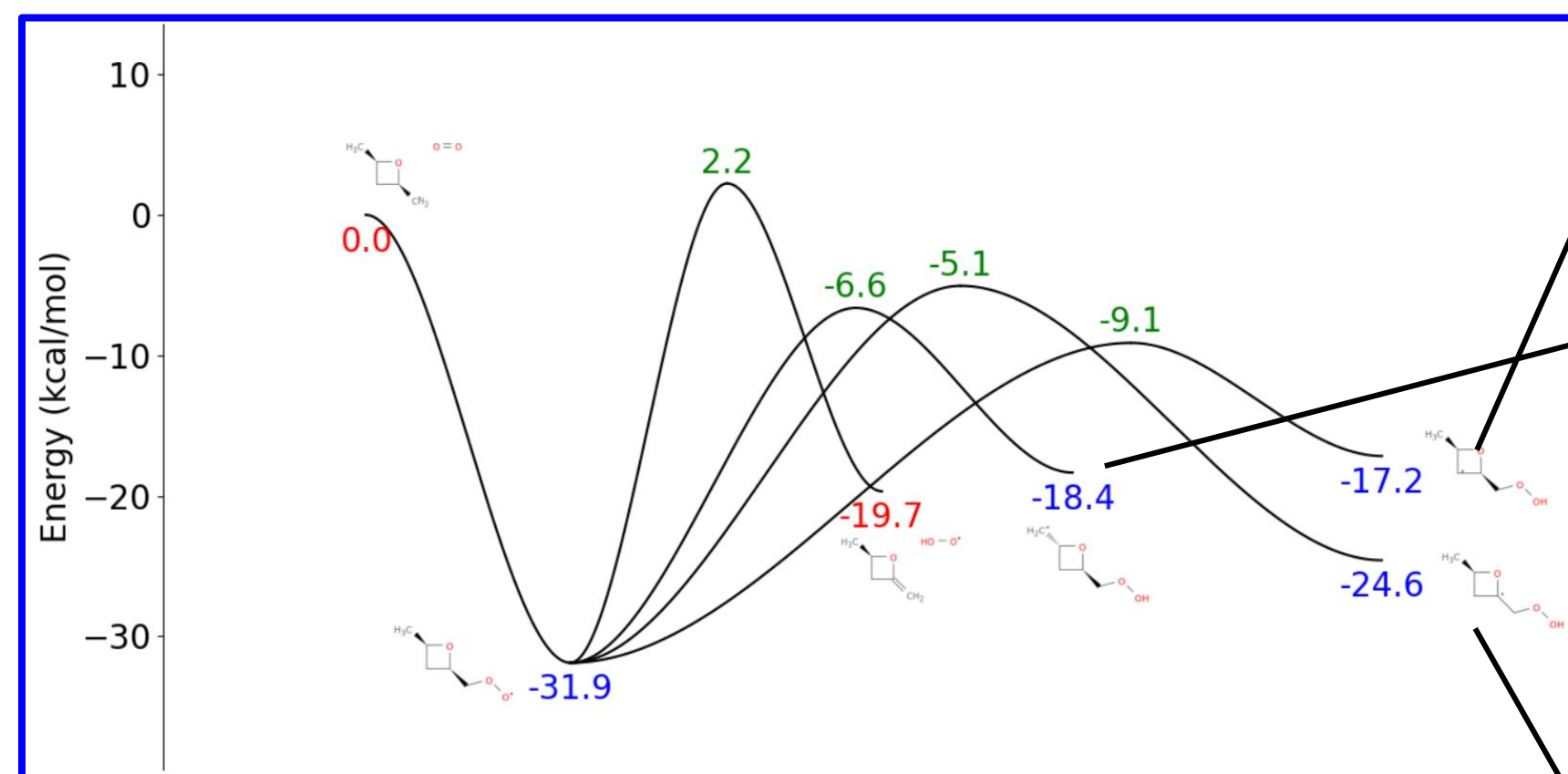
- S1** PES Block Diagrams
- S2** PES Schemes
- S3** PES Examples Before Pruning
- S4** Species Notation
- S5** T1 Diagnostics
- S6** MESS files (located in separate folder)

S1 PES Block Diagrams

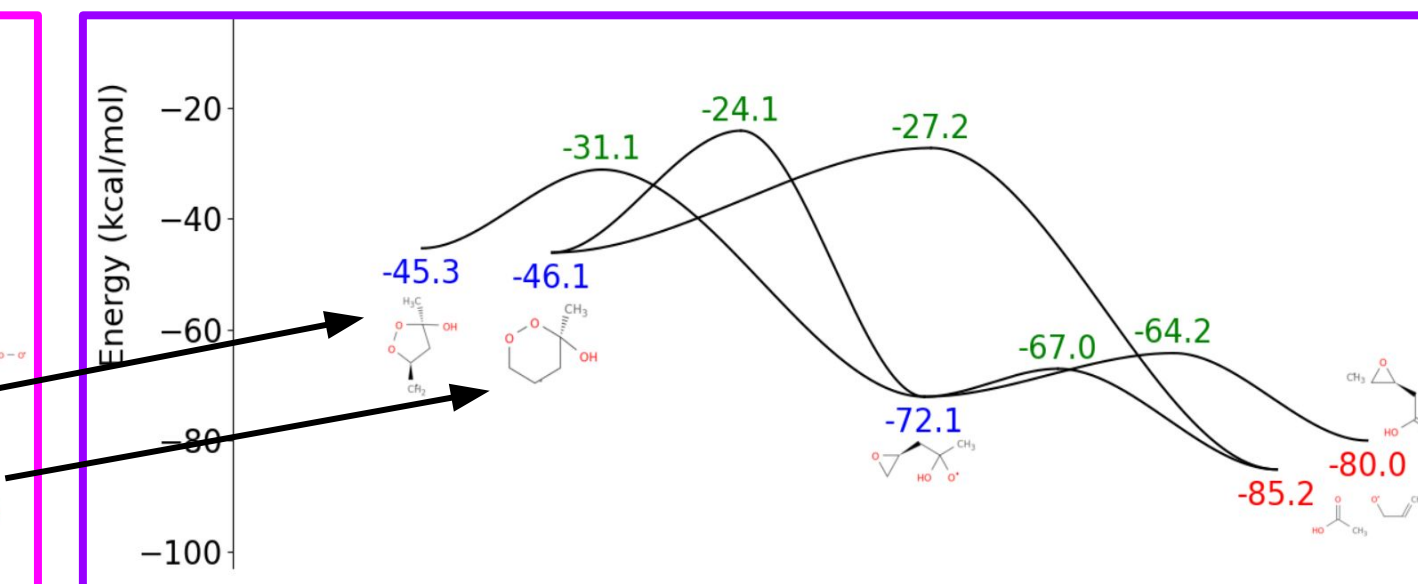
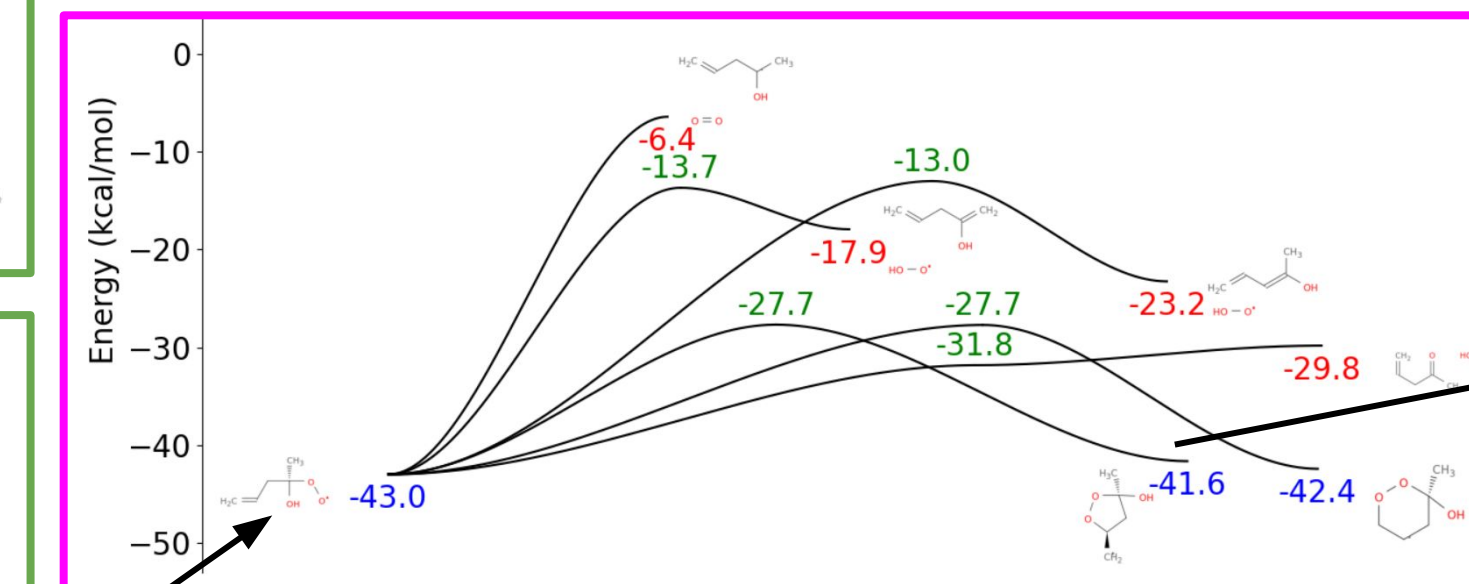
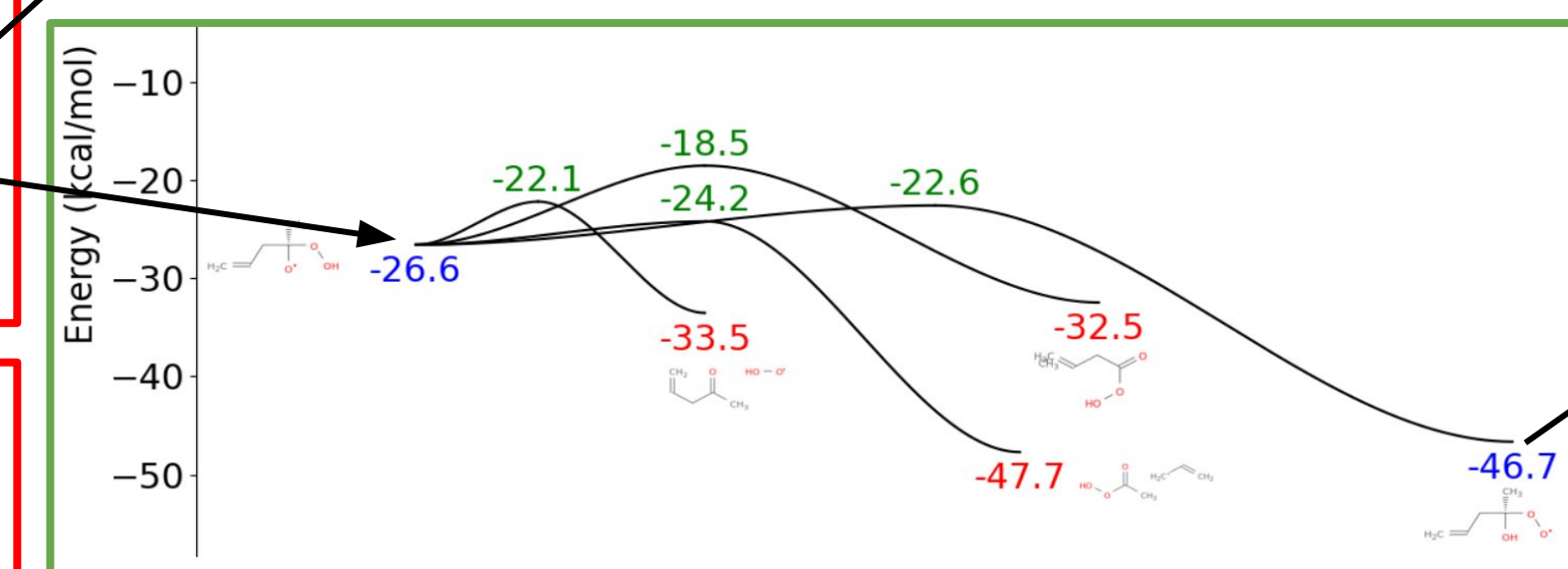
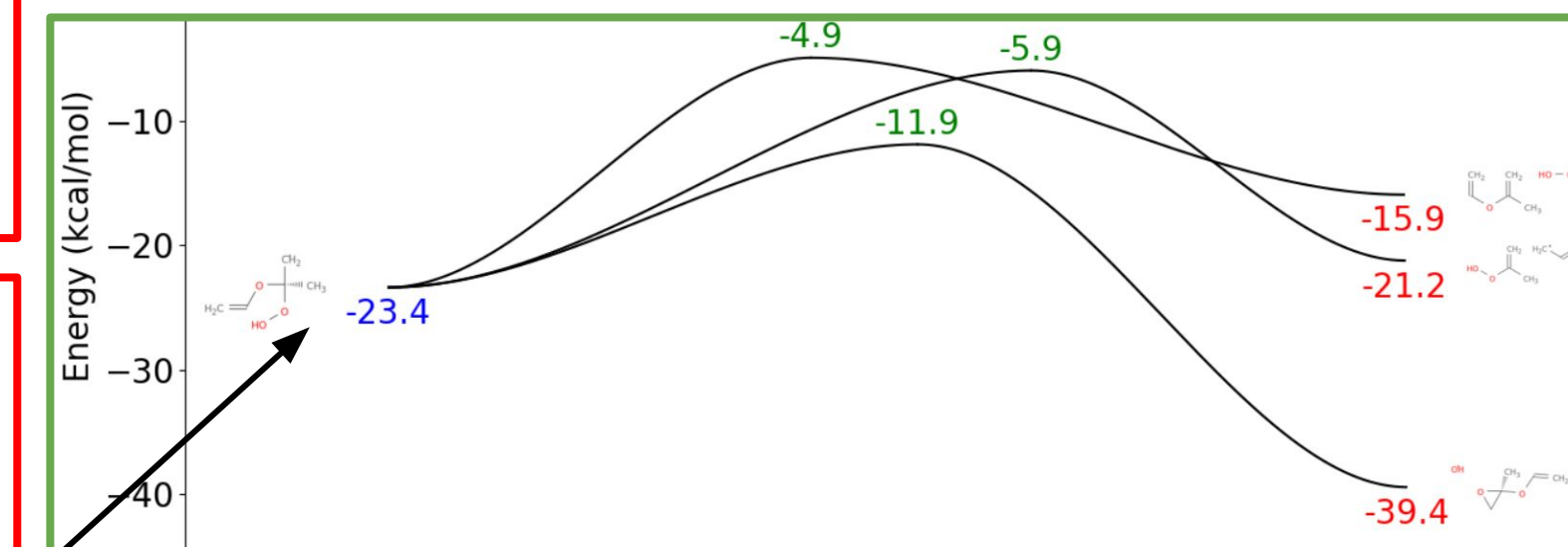
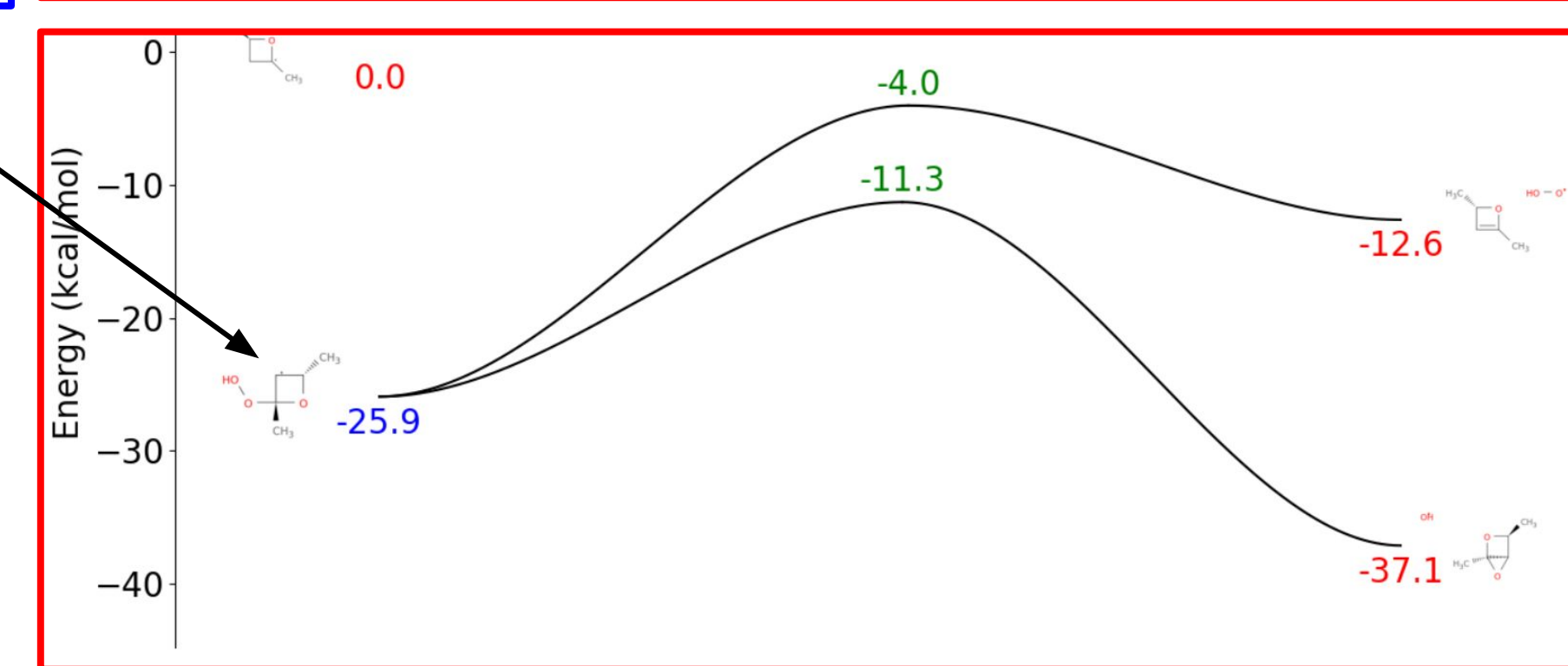
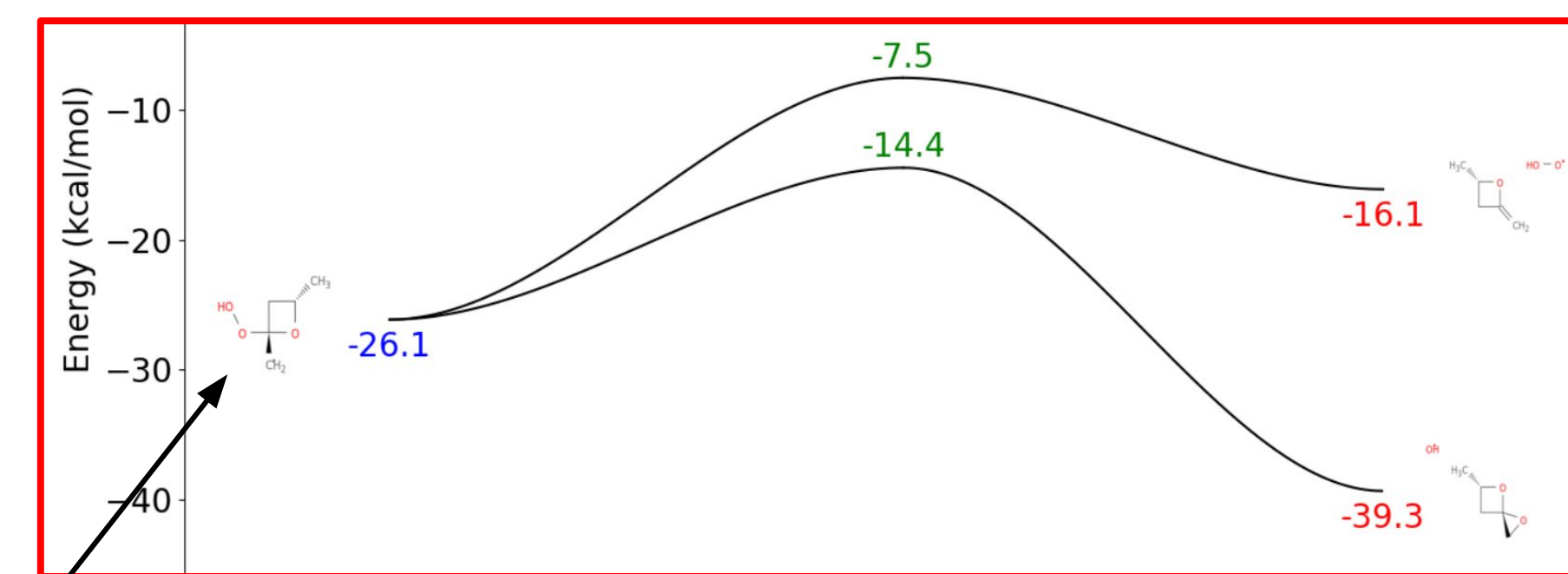
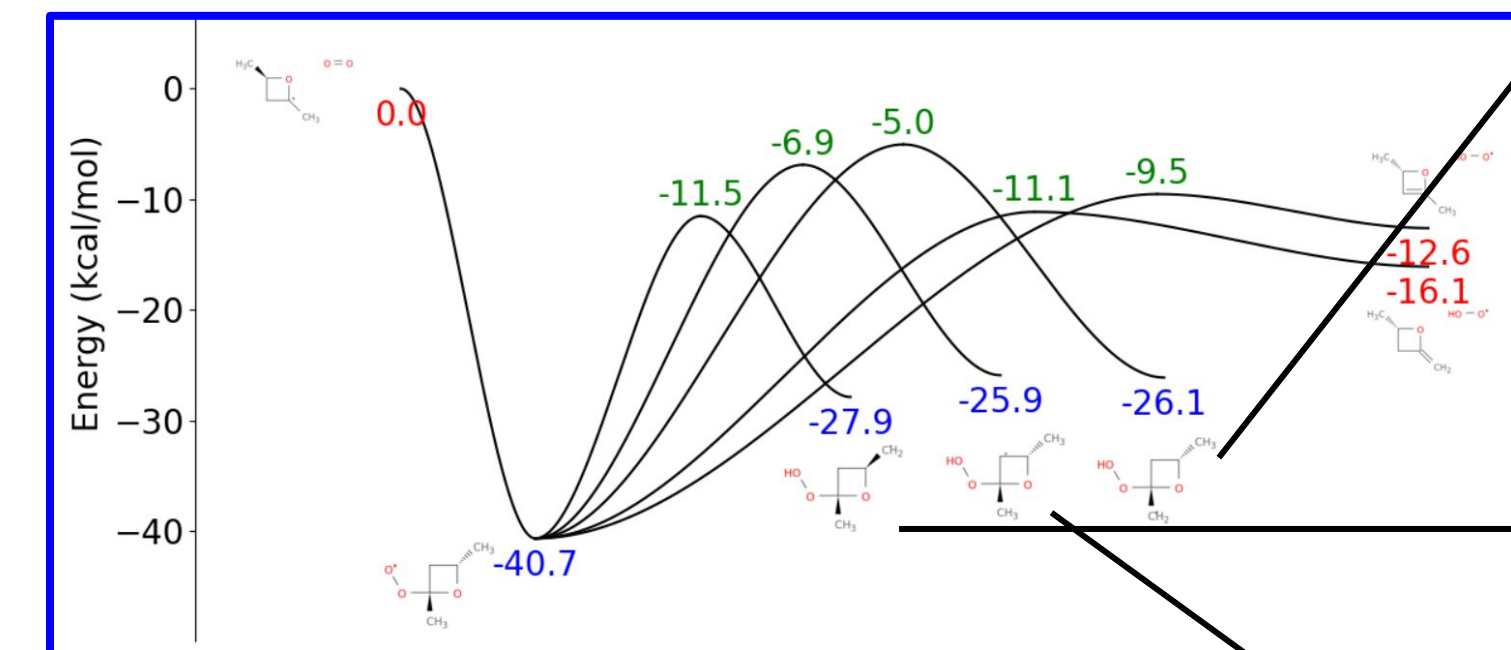
anti-ROO1



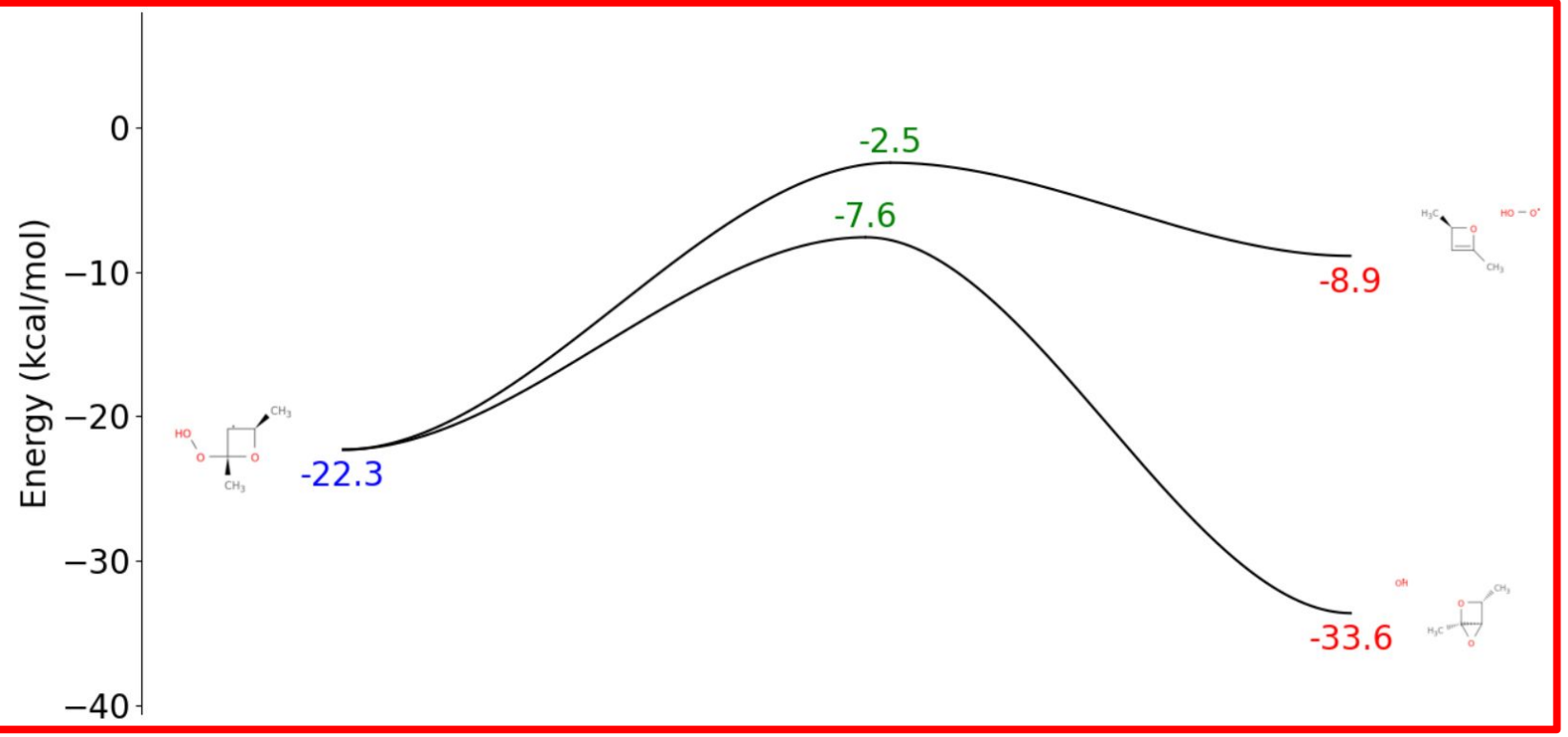
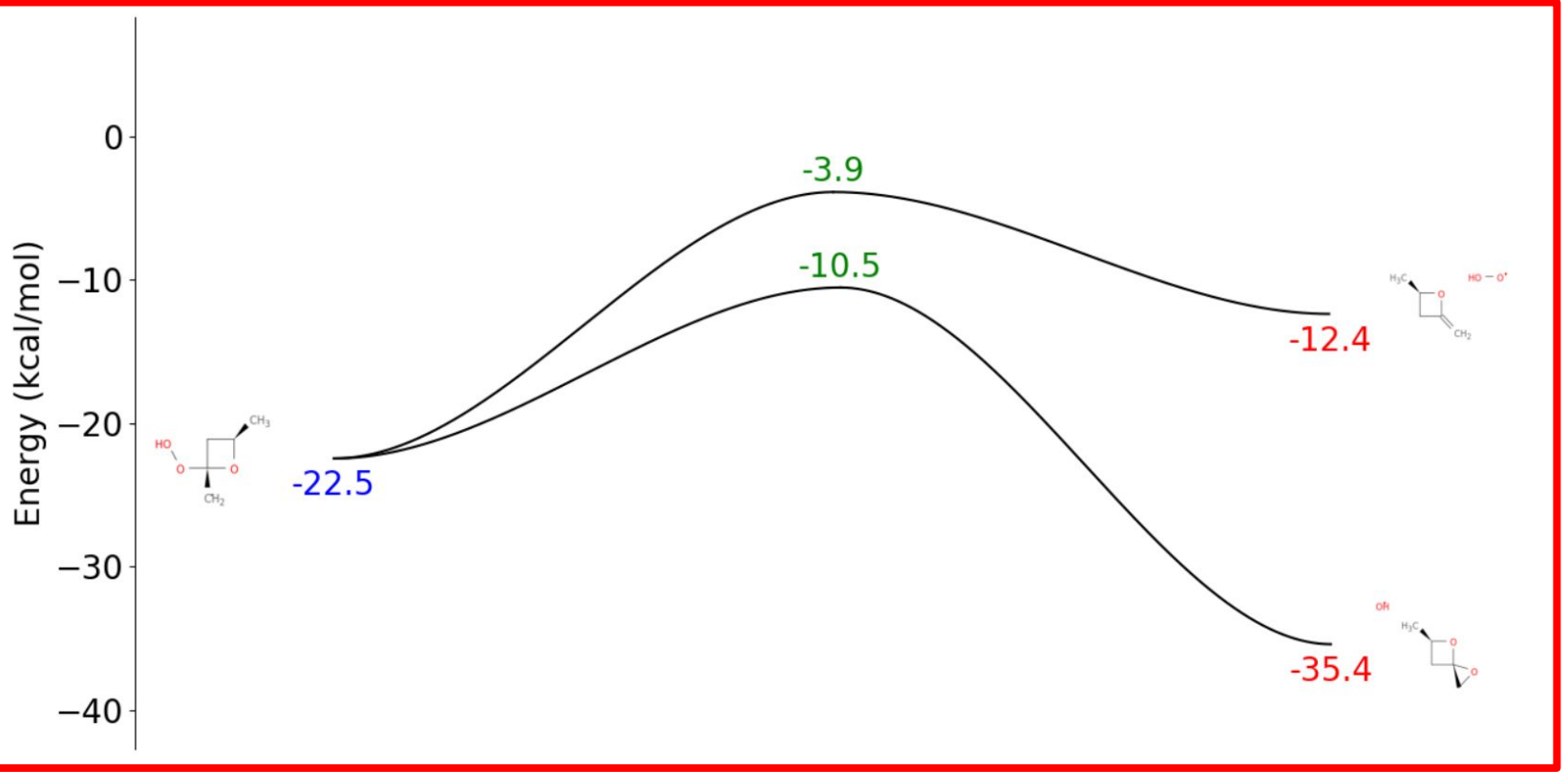
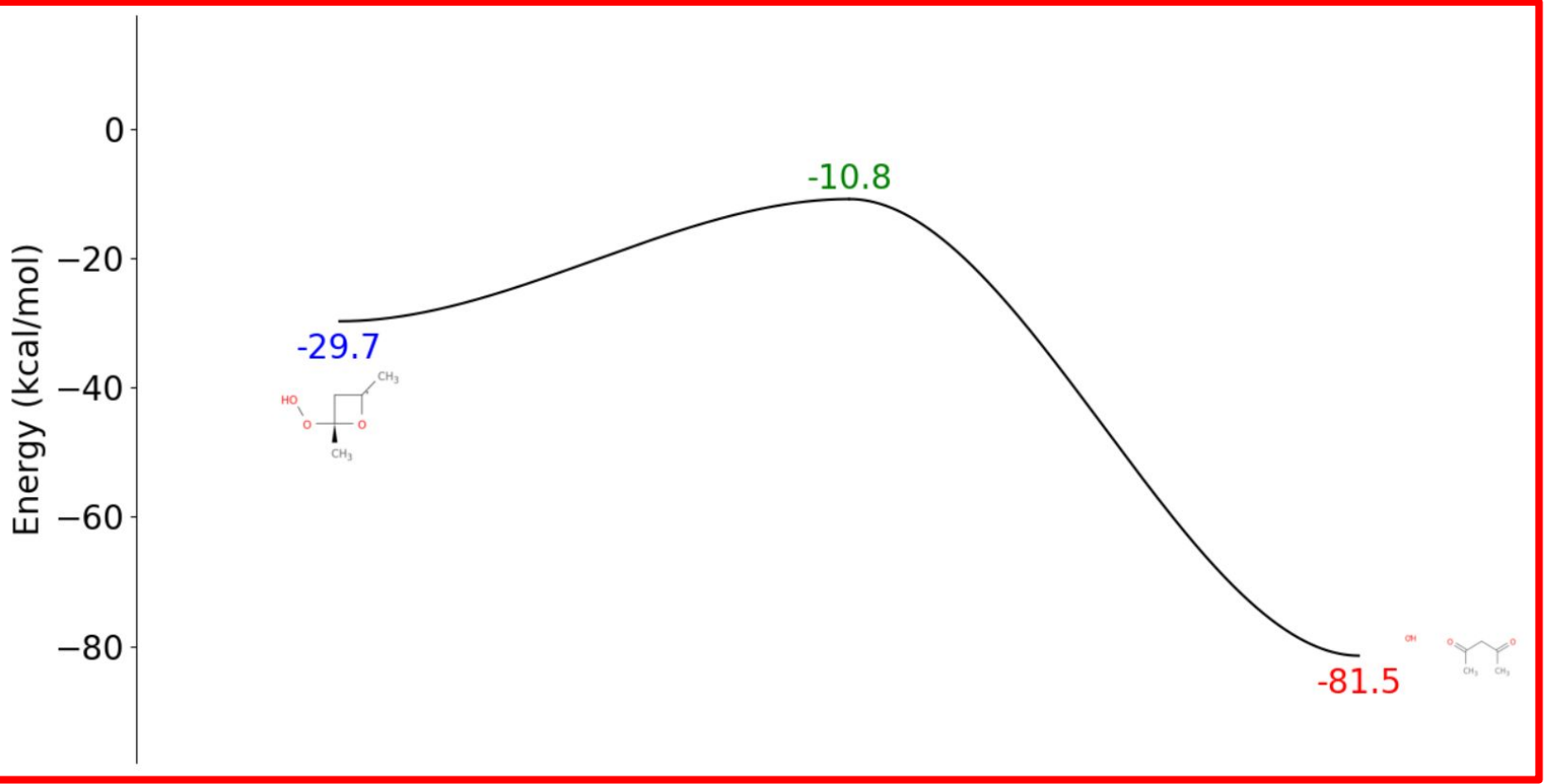
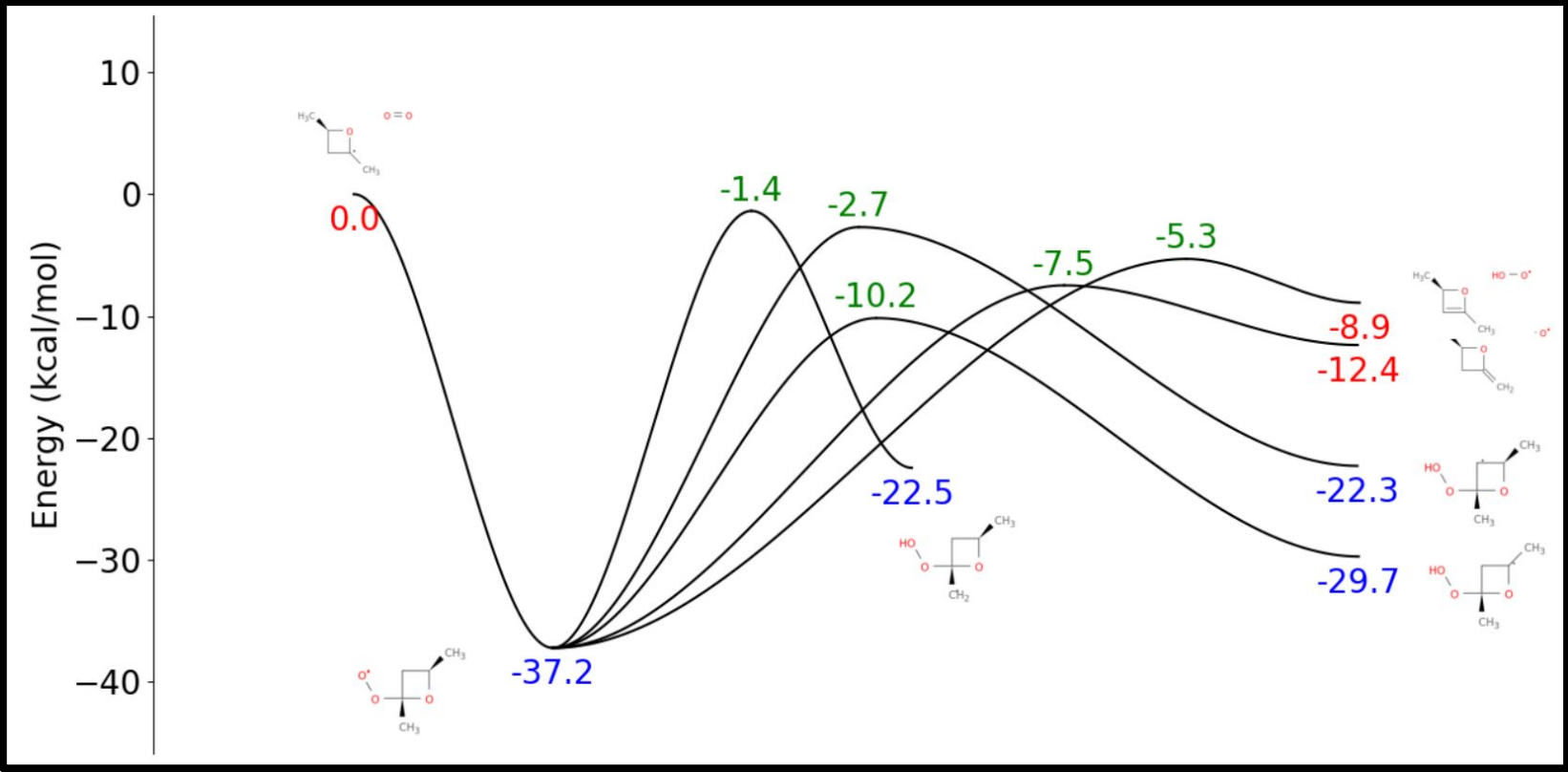
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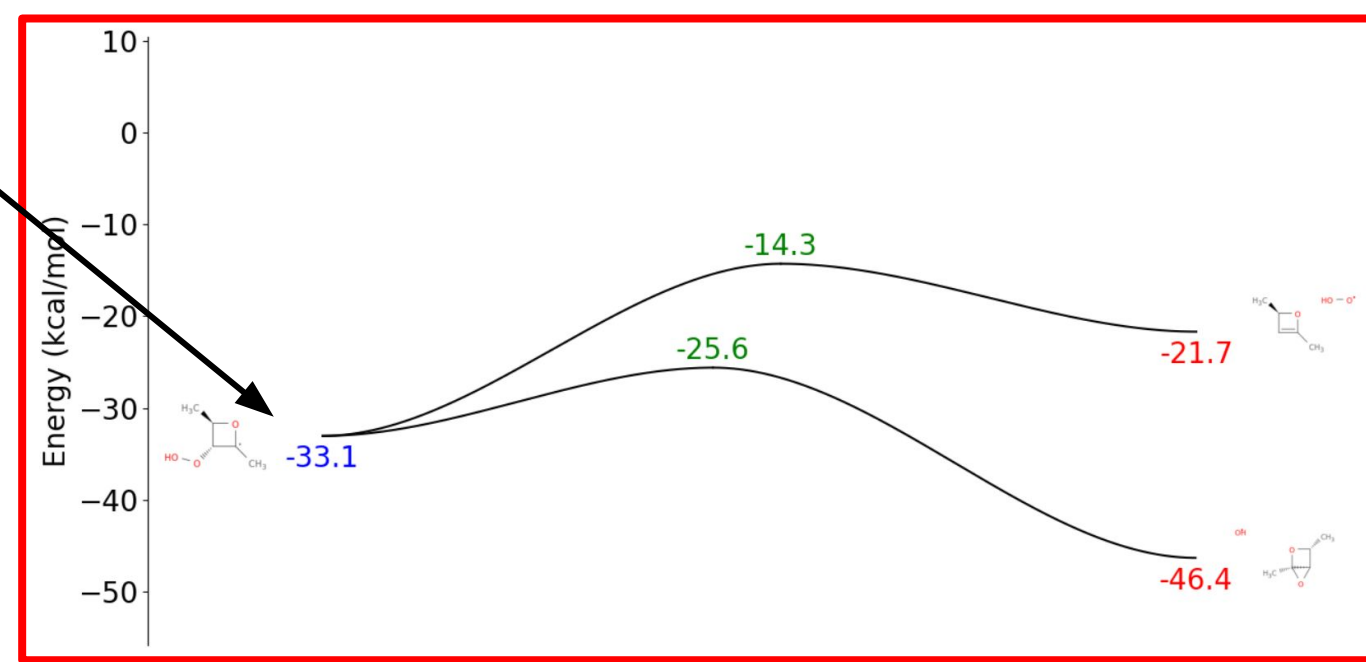
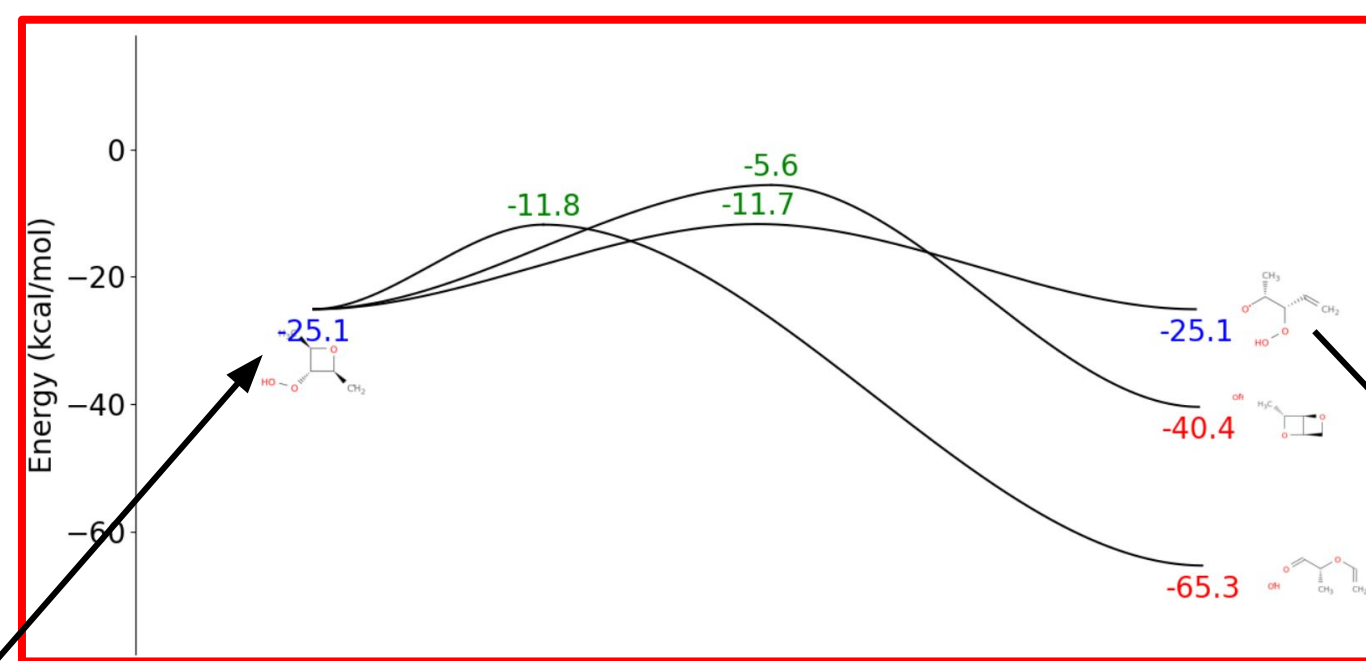
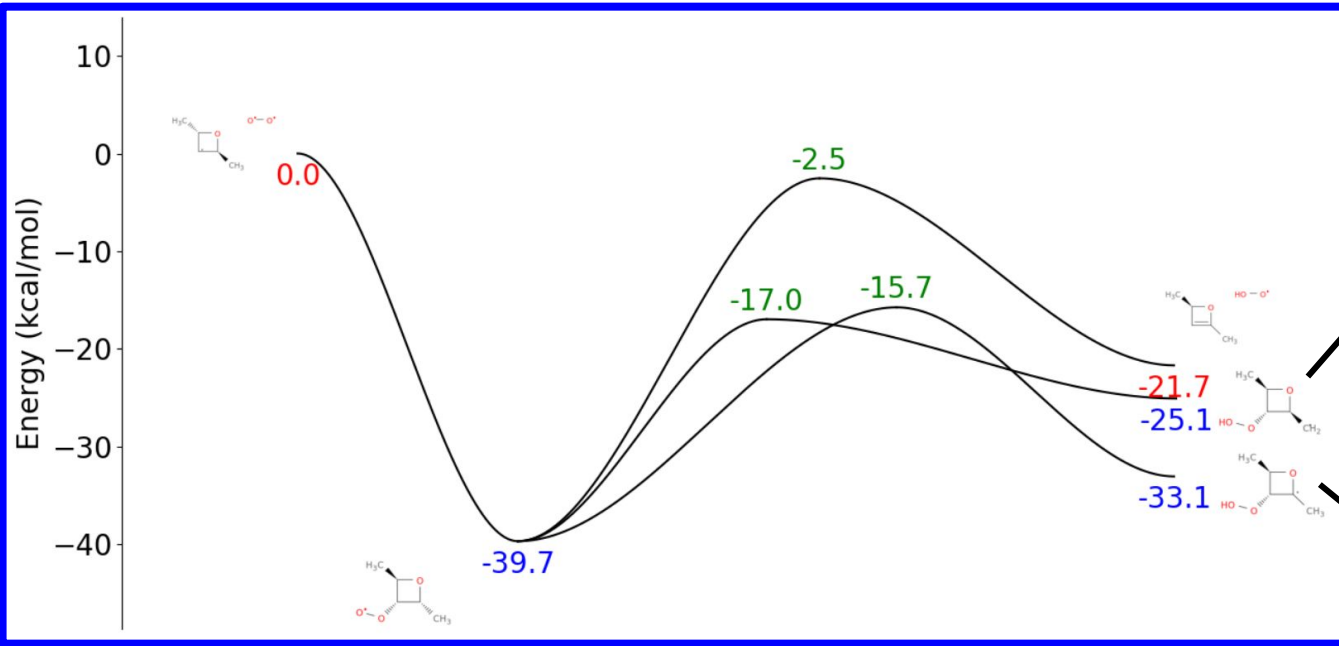
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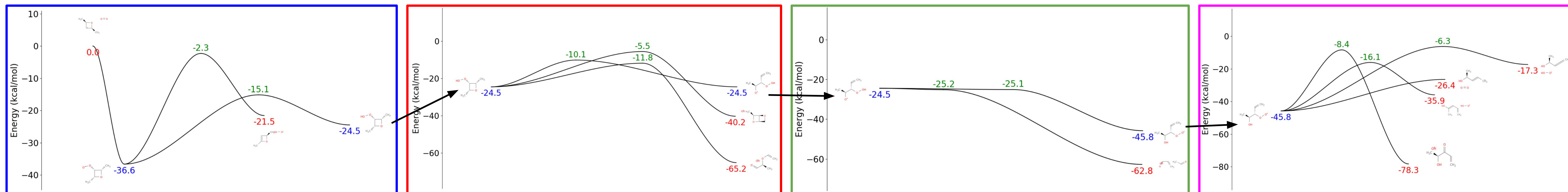
syn-ROO2



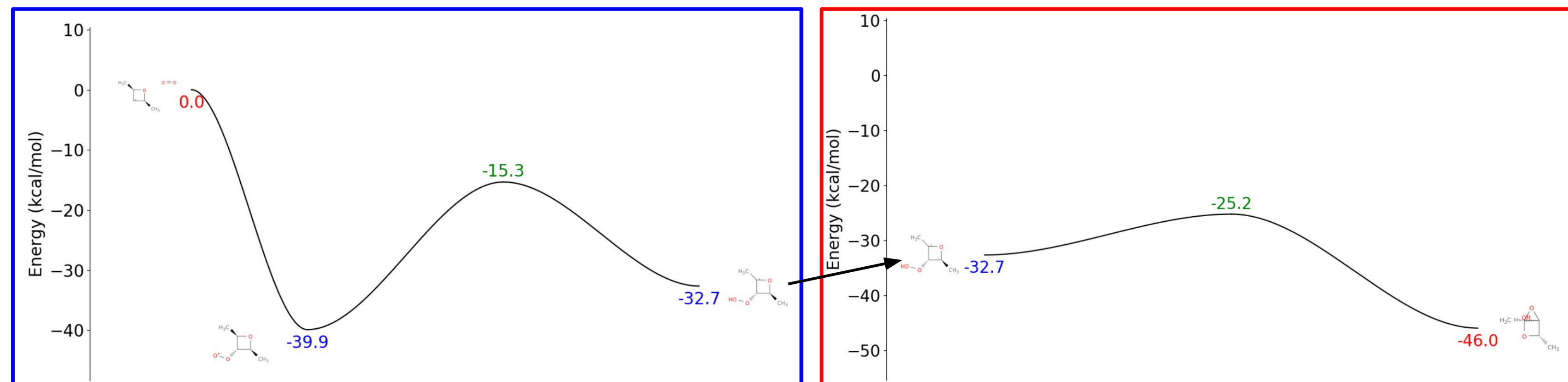
anti-R003



syn-syn-ROO3

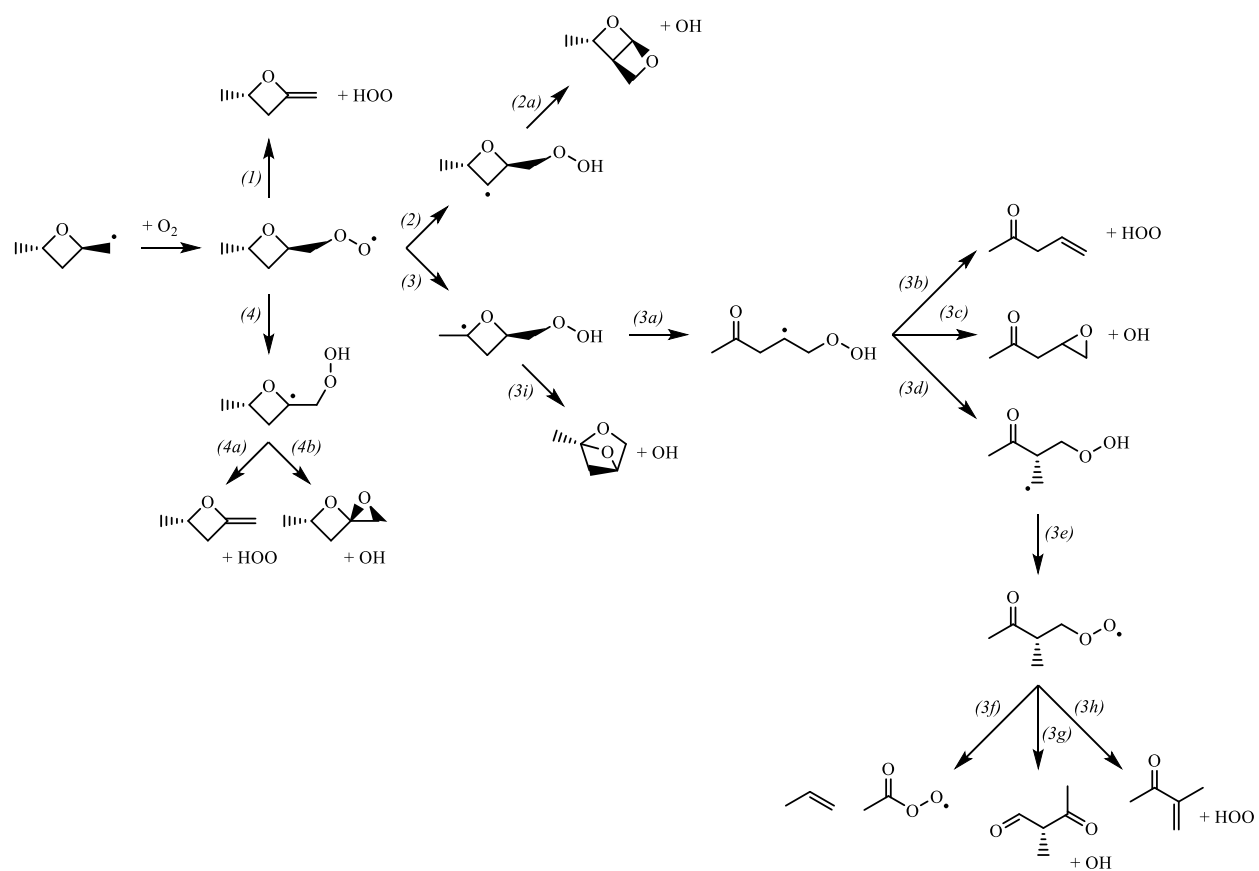


syn-anti-ROO3

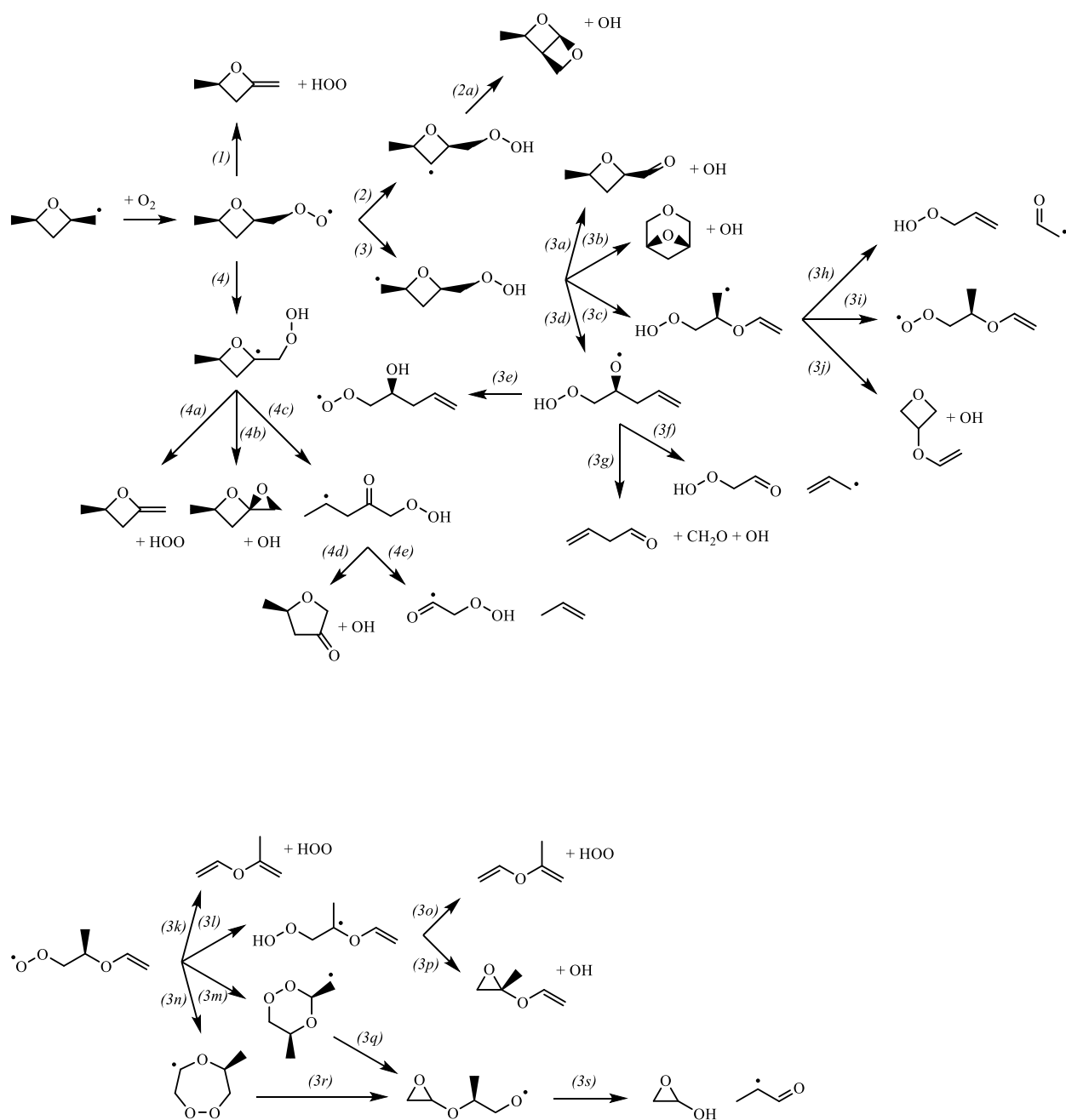


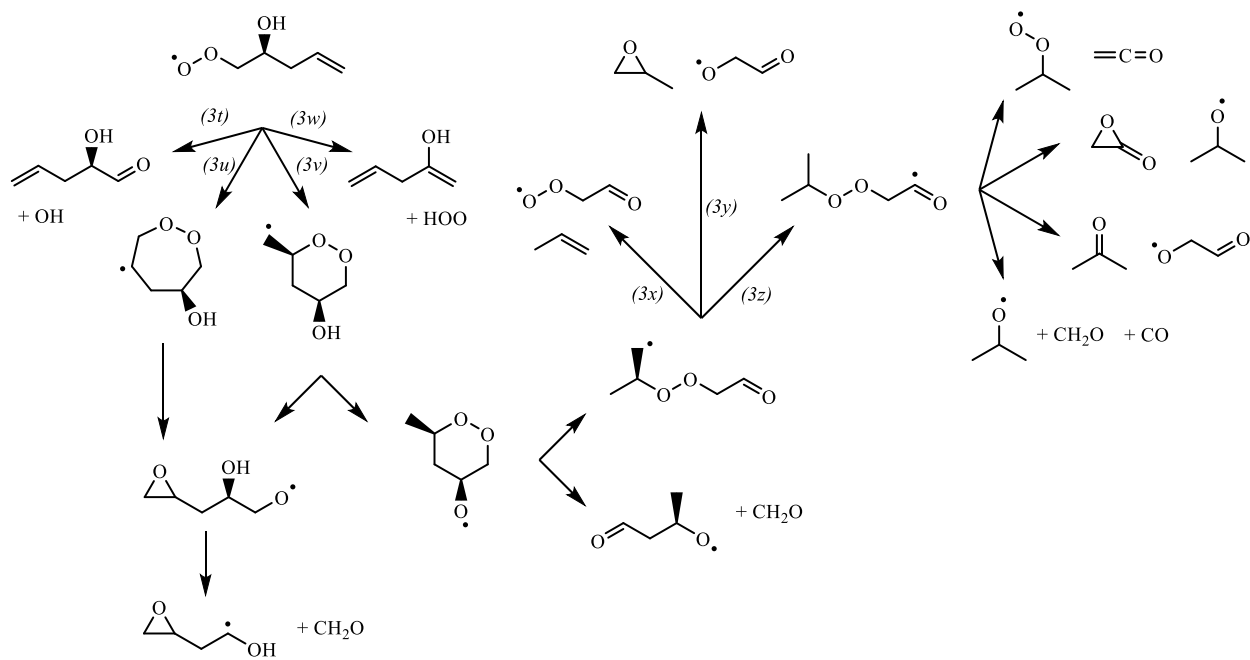
S2 PES Schemes

anti-ROO-1

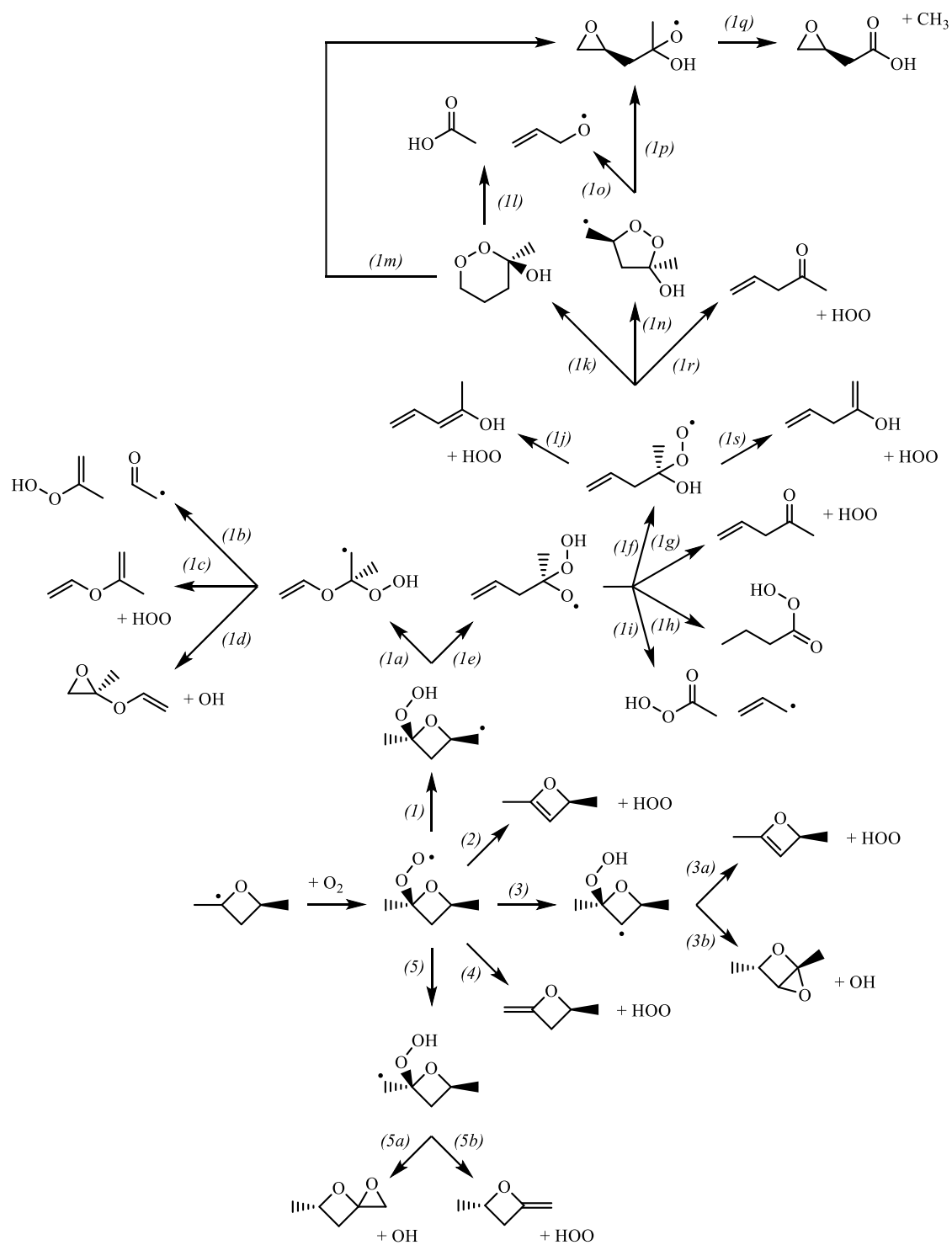


syn-ROO-1

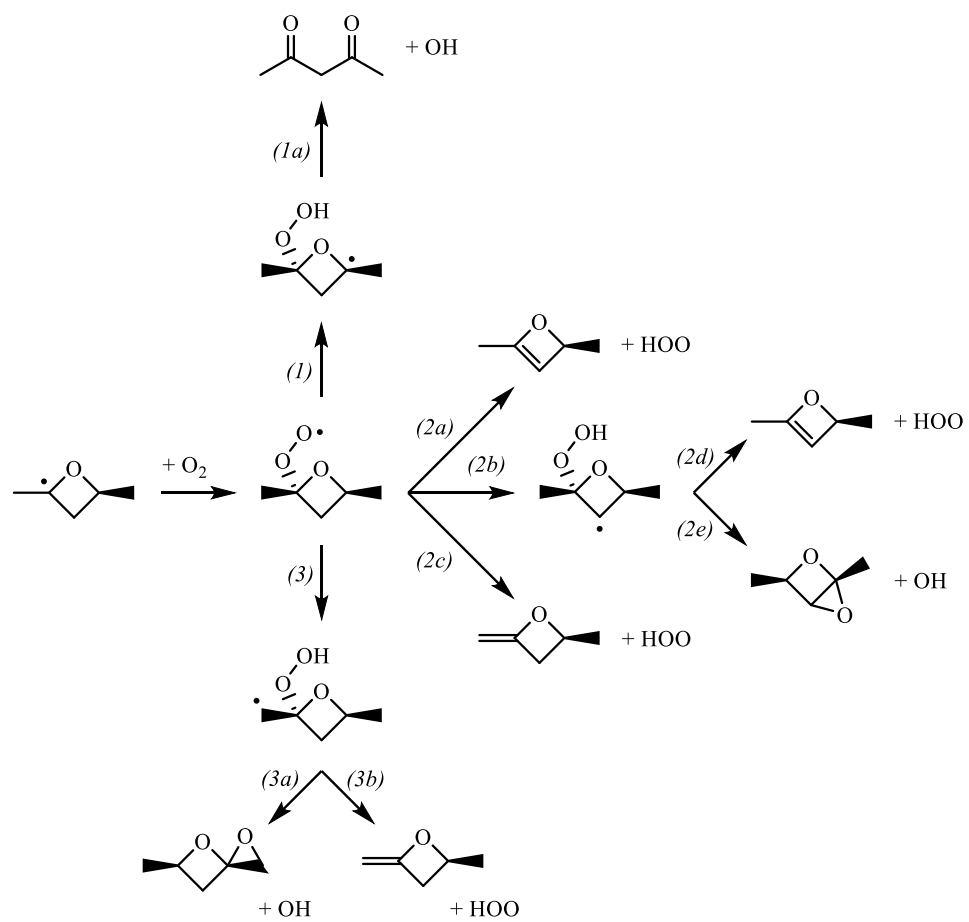




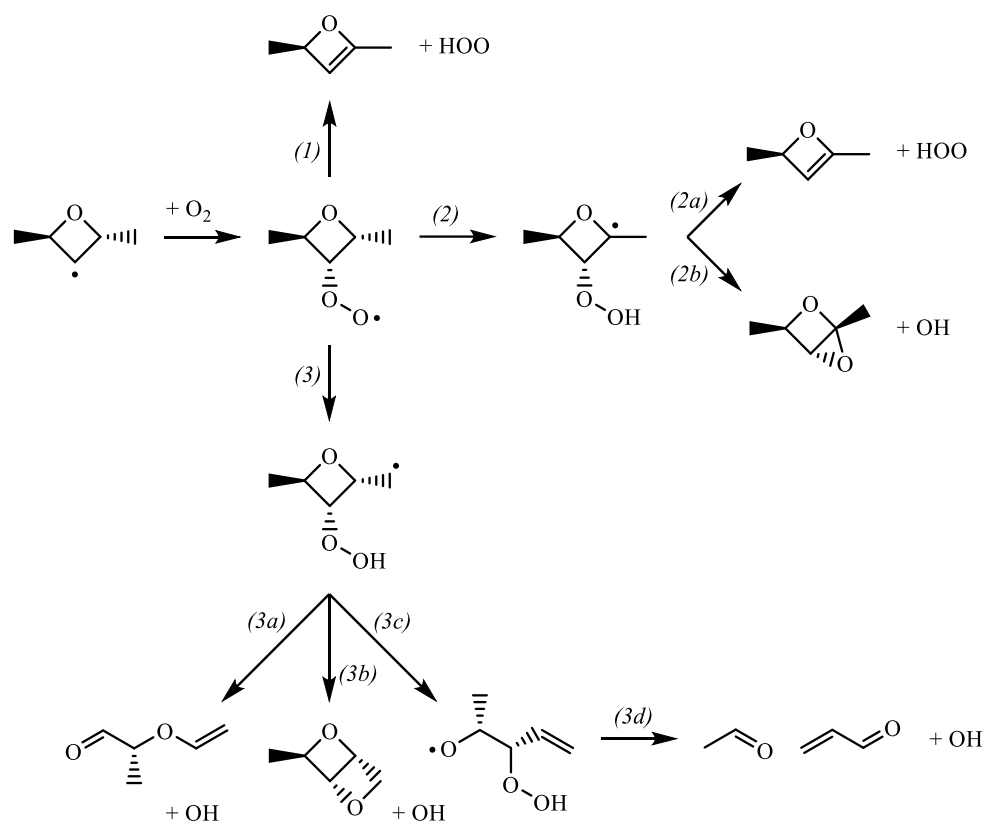
anti-ROO-2



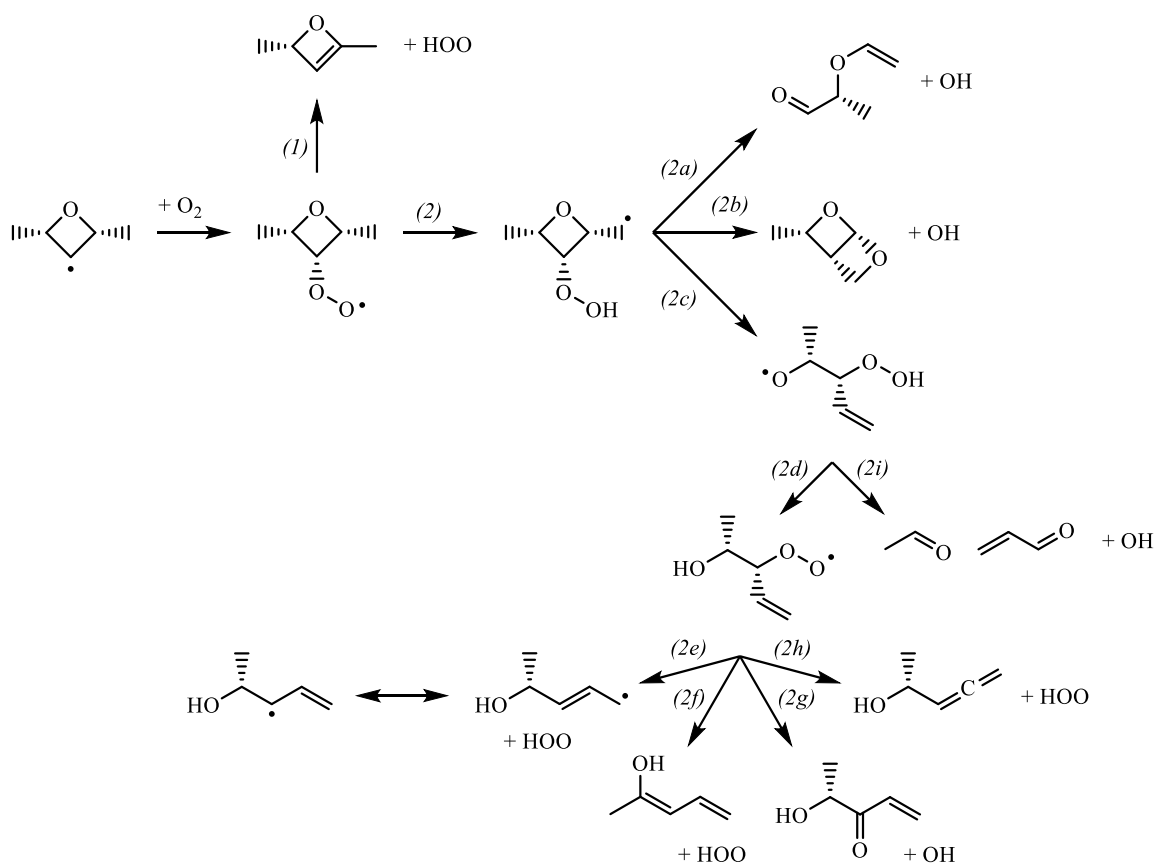
syn-ROO-2



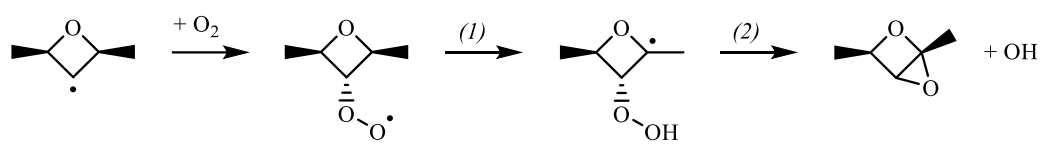
anti-ROO-3



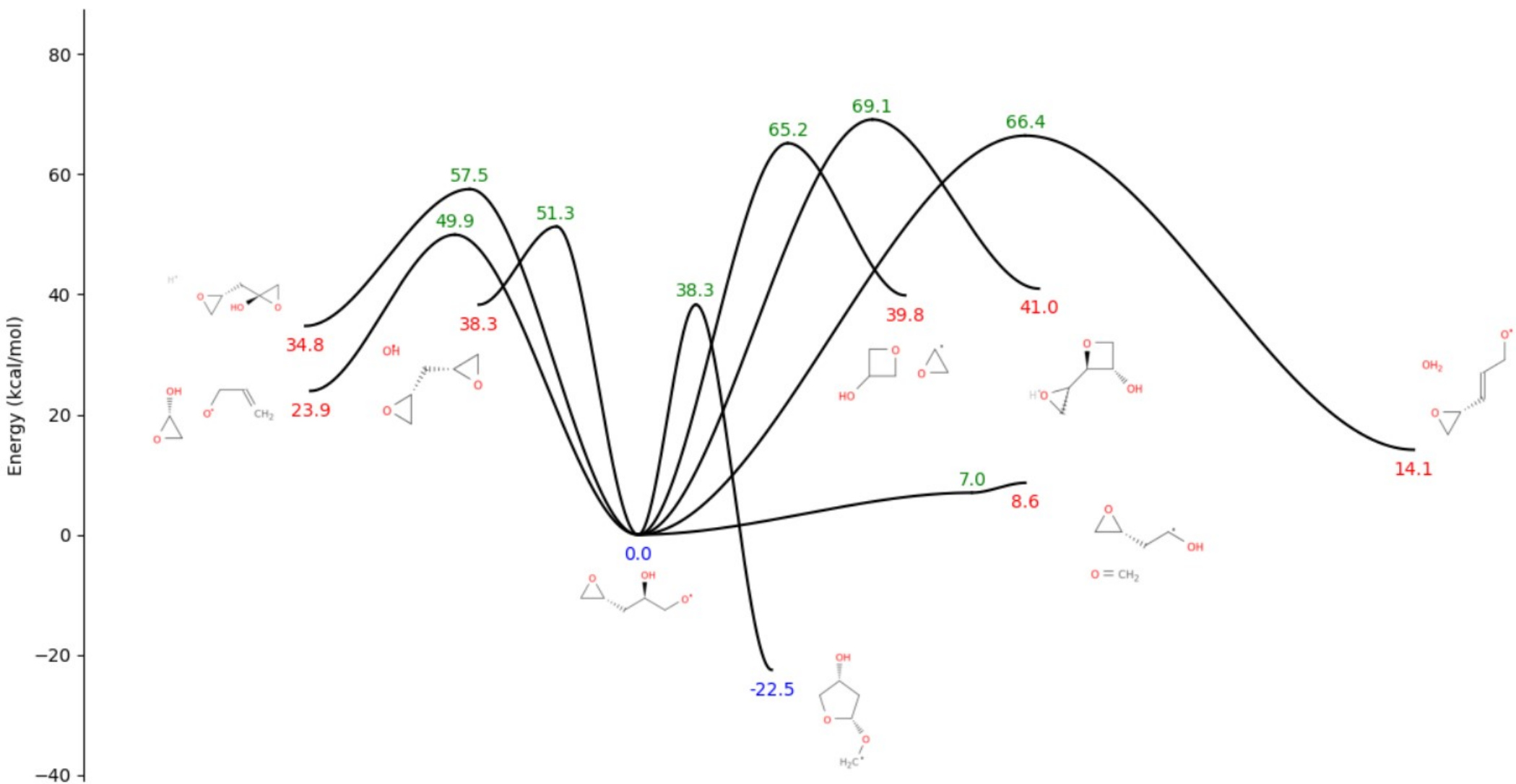
syn-syn-ROO-3

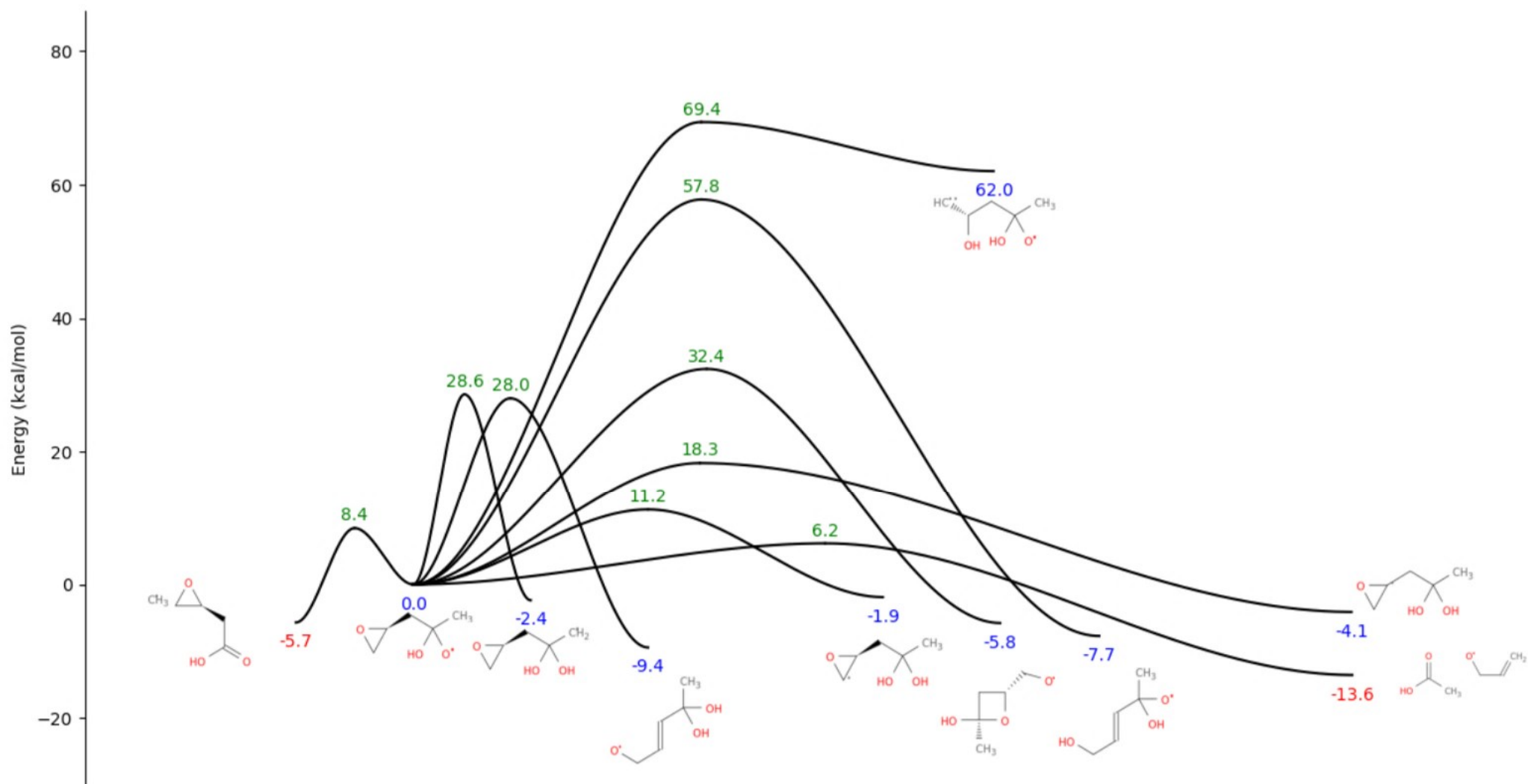


syn-anti-ROO-3



S3 PES Examples Before Pruning





S4 Species Notation

anti-ROO2

w_1	[H][C]([H])([H])[C]1([H])[O][C]([O])[C]([H])([H])([H])[C]1([H])[H]	
w_2	[H][O][O][C]1([O])[C]([H])([C]([H])([H])([H])[C]1([H])([H])[C]([H])([H]	
w_3	[H][O][O][C]1([O])[C]([H])([C]1[H])[C]([H])([H])([H])[C]([H])([H])([H]	
w_4	[H][O][O][C]1([O])[C]([H])([C]([H])([H])[C]1([H])([H])[C]([H])([H])([H]	
w_5	[H][O][O][C]([O])[C]([H])=[C]([H])([H])([C]([H])([H])[C]([H])([H])([H]	
w_6	[H][O][O][C]([O])([C]([H])([H])([H])[C]([H])([H])[C]([H])=[C]([H])([H]	
w_7	[H][O][C]([O][O])([C]([H])([H])([H])[C]([H])([H])[C]([H])=[C]([H])([H]	
w_8	[H][O][C]1([O][O][C]([H])([C]([H])([H])[C]1([H])([H])[C]([H])([H])([H]	
w_9	[H][O][C]1([O][O][C]([H])([H])[C]([H])[C]1([H])([H])[C]([H])([H])([H]	
w_10	[H][O][C]([O])([C]([H])([H])([H])[C]([H])([H])[C]1([H])([O])[C]1([H])([H]	
pr_1	[H][C]([H])=[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])([H]	[H][O][O]
pr_2	[H][C]1=[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_3	[H][C]([H])([H])[C]1([H])[O][C]2([O][C]2([H])([H])[C]1([H])([H]	[H][O]
pr_4	[H][C]([H])([H])[C]1([H])[O][C]2([O][C]12[H])[C]([H])([H])([H]	[H][O]
pr_5	[H][O][O][C]([C]([C]([H])([H])[C]([H])([H])([H]	[H][C]([H])=[C]([H])([O]
pr_6	[H][C]([H])=[C]([H])[O][C]([C]([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_7	[H][C]([H])=[C]([H])[O][C]1([O][C]1([H])([H])[C]([H])([H])([H]	[H][O]
pr_8	[H][C]([H])([H]	[H][O][O][C]([C]([O])([H])([H])[C]([H])=[C]([H])([H]
pr_9	[H][O][O][C]([O])([O])([C]([H])([H])([H]	[H][C]([H])[C]([H])=[C]([H])([H]
pr_10	[H][C]([H])=[C]([H])[C]([H])([H])[C]([C]([O])([H])([H])([H]	[H][O][O]
pr_11	[H][O][C]([C]([C]([H])([H])[C]([H])([H])[C]([H])=[C]([H])([H]	[H][O][O]
pr_12	[H][O][C]([C]([C]([H])([H])[C]([H])=[C]([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_14	[H][O][C]([C]([O])([C]([H])([H])([H]	[H][C]([H])=[C]([H])[C]([H])([H])([O]
pr_15	[H][C]([H])([H]	[H][O][C]([C]([O])([H])([H])[C]1([H])([O])[C]1([H])([H]
r_o2	[H][C]([H])([H])[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])([H]	[O][O]
rnew_o2	[H][O][C]([C]([H])([H])([H])[C]([H])([H])[C]([H])=[C]([H])([H]	[O][O]

anti-ROO3

w_1	[H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])([H])[C]1([H])[O][O]	
w_2	[H][O][O][C]1([H])[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	
w_3	[H][O][O][C]1([H])[C]([H])([O][C]1([H])[C]([H])([H])([H])[C]([H])([H]	
w_4	[H][O][O][C]([H])([C]([H])=[C]([H])([H])[C]([H])([O])[C]([H])([H])([H]	
pr_1	[H][C]1=[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_2	[H][C]([H])([H])[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])[O]	[H][O]
pr_3	[H][C]([H])([H])[C]1([H])[O][C]2([H])[C]([H])([H])[O][C]12[H]	[H][O]
pr_4	[H][C]([C]([O])([C]([H])([O][C]([H])=[C]([H])([H])[C]([H])([H])([H]	[H][O]
t_1	C=CC=O	CC=O
pr_6	[H][O][O][C]([H])([C]([H])=[O])([C]([H])=[C]([H])([H]	[H][C]([H])([H]
r_o2		[O][O]

syn-anti-ROO3

w_1	[H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])([H])[C]1([H])[O][O]	
w_2	[H][O][O][C]1([H])[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	
pr_1	[H][C]1=[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_2	[H][C]([H])([H])[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])[O]	[H][O]
r_o2	[H][C]1[C]([H])([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[O][O]

syn-roo2

w_1	[H][C]([H])([H])[C]1([H])[O][C]([O][O])([C]([H])([H])([H])[C]1([H])([H]	
w_2	[H][O][O][C]1([O])[C]([H])([C]([H])([H])([H])[C]1([H])([H])[C]([H])([H]	
w_3	[H][O][O][C]1([O])[C]([H])([C]1[H])[C]([H])([H])([H])[C]([H])([H])([H]	
w_4	[H][O][O][C]1([O])[C]([C]([H])([H])([H])[C]1([H])([H])[C]([H])([H])([H]	
w_5	[H][C]([H])[C]([H])([O][C]([O][O])[C]([H])([H])([H])[C]([H])([H])([H]	
pr_1	[H][C]([H])=[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])([H]	[H][O][O]
pr_2	[H][C]1=[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_3	[H][C]([H])([H])[C]1([H])[O][C]2([O][C]2([H])([H])[C]1([H])([H]	[H][O]
pr_4	[H][C]([H])([H])[C]1([H])[O][C]2([O][C]12[H])[C]([H])([H])([H]	[H][O]
pr_5	[H][C]([H])([H])[C]([C]([C]([O])([C]([H])([H])[C]([C]([O])([C]([H])([H])([H]	[H][O]
r_o2	[H][C]([H])([H])[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])([H]	[O][O]

syn-syn-ROO3

w_1	[H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])([H])[C]1([H])[O][O]	
w_2	[H][O][O][C]1([H])[C]([H])([O][C]1([H])[C]([H])([H])([H])[C]([H])([H]	
w_3	[H][O][O][C]([H])([C]([H])=[C]([H])([H])[C]([H])([O])[C]([H])([H])([H]	
w_4	[H][O][C]([H])([C]([H])([H])([H])[C]([H])([O][O])[C]([H])=[C]([H])([H]	
pr_2	[H][C]1=[C]([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[H][O][O]
pr_3	[H][C]([H])([H])[C]1([H])[O][C]2([H])[C]([H])([H])[O][C]12[H]	[H][O]
pr_4	[H][C]([C]([O])([C]([H])([O][C]([H])=[C]([H])([H])[C]([H])([H])([H]	[H][O]
pr_5	C=CC=O	CC=O
pr_6	[H][O][C]([C]([C]([H])([C]([H])=[C]([H])([H])[C]([H])([H])([H]	[H][O][O]
r_o2	[H][C]1[C]([H])([O][C]1([H])[C]([H])([H])([H])[C]([H])([H])([H]	[O][O]

ROO1

w_1 [H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])[O][O])[C]1([H])[H]
w_2 [H][O][O][C]([H])([H])[C]1[O][C]([H])([C]([H])([H])([H])[C]1([H])[H]
w_3 [H][O][O][C]([H])([H])[C]1([H])[O][C]([H])([C]1[H])[C]([H])([H])[H]
w_4 [H][O][O][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])[C]1([H])[H]
w_5 [H][O][O][C]([H])([H])[C]1([H])[O][C]([H])([H])[C]([H])([H])[H]
w_6 [H][O][O][C]([H])([H])[C]([H])([O][C]([H])=C([H])[H])[C]([H])[H]
w_7 [H][O][O][C]([H])([H])[C]([H])([O][C]([H])([H])[C]([H])=C([H])[H]
w_8 [H][C]([H])=C([H])[O][C]([H])([C]([H])([H])[H])[C]([H])([H])[O][O]
w_9 [H][O][C]([H])([C]([H])([H])[O][O])[C]([H])([H])[C]([H])=C([H])[H]
w_10 [H][O][O][C]([H])([H])[C]([O][C]([H])=C([H])[H])[C]([H])([H])[H]
w_11 [H][C]([H])[C]1([H])[O][O][C]([H])([H])[C]([H])([O]1)[C]([H])([H])[H]
w_12 [H][C]1[O][C]([H])([C]([H])([H])([H])[C]([H])([H])[O][O][C]1([H])[H]
w_13 [H][O][C]1([H])[C]([H])([H])[O][O][C]([H])([C]([H])([H])[C]1([H])[H]
w_14 [H][O][C]1([H])[C]([H])([H])[O][O][C]([H])([H])[C]([H])[C]1([H])[H]
w_15 [H][C]([H])([H])[C]([H])([O][C]1([H])[O][C]1([H])[H])[C]([H])([H])[O]
w_16 [H][C]([H])([H])[C]1([H])[O][O][C]([H])([H])[C]([H])([O])[C]1([H])[H]
w_17 [H][O][C]([H])([C]([H])([H])[O][C]([H])([H])[C]1([H])[O][C]1([H])[H]
w_18 [H][C]([H])[C]([H])([O][O][C]([H])([H])[C]([H])=O)[C]([H])([H])[H]
w_19 [H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])[O][O])[C]1([H])[H]
w_20 [H][O][O][C]([H])([H])[C]1([H])[O][C]([H])([C]1[H])[C]([H])([H])[H]
w_21 [H][O][O][C]([H])([H])[C]1([H])[O][C]([C]([H])([H])([H])[C]1([H])[H]
w_22 [H][O][O][C]([H])([H])[C]([H])[C]([H])([H])[C]([H])([H])[C]([H])([H])[H]
w_23 [H][O][O][C]([H])([H])[C]([H])([C]([H])([H])[C]([H])([H])[C]([H])([H])[H]
w_24 [H][C]([H])([H])[C]([H])([C]([H])([C]([H])([H])([H])[C]([H])([H])[O][O]
w_25 [H][O][O][C]([H])([H])[C]1([H])[C]([H])([H])[C]1([O])[C]([H])([H])[H]
pr_1 [H][C]([H])=C[1][O][C]([H])([C]([H])([H])[H])[C]1([H])[H] [H][O][O]
pr_2 [H][C]([H])([H])[C]1([H])[O][C]2([O][C]2([H])[H])[C]1([H])[H] [H][O]
pr_3 [H][C]([H])([H])[C]1([H])[O][C]2([H])[C]([H])([H])[O][C]12[H] [H][O]
pr_4 [H][C]([H])([H])[C]1([H])[O][C]([H])([C]([H])([H])[H])[C]1([H])[H] [H][O]
pr_5 [H][C]1([H])[O][C]([H])([H])[C]2([H])[O][C]1([H])[C]2([H])[H] [H][O]
pr_6 [H][C]1([H])[O][C]([H])([C]([H])([H])[H])[C]([H])([H])[C]1=[O] [H][O]
pr_7 [H][O][O][C]([H])([H])[C]=[O] [H][C]([H])=C([H])[C]([H])([H])[H]
pr_8 [H][O][O][C]([H])([H])[C]([H])=C([H])[H] [H][C]([H])=C([H])[O]
pr_9 [H][C]([H])=C([H])[O][C]1([H])[C]([H])([H])[O][C]1([H])[H] [H][O]
t_1 C=CCC=O [H][O]
pr_12 [H][O][O][C]([H])([H])[C]([H])=O [H][C]([H])[C]([H])=C([H])[H]
pr_13 [H][O][O][C]([H])([H])[C]([H])=O)[C]([H])([H])[C]([H])=C([H])[H] [H]
pr_14 [H][C]([H])=C([H])[O][C]([H])([H])[C]([H])([H])[H] [H][O][O]
pr_15 [H][O][C]([H])([C]([H])=O)[C]([H])([H])[C]([H])=C([H])[H] [H][O]
pr_16 [H][O][C]([H])([C]([H])([H])[C]([H])([H])[C]([H])=C([H])[H] [H][O][O]
pr_17 [H][C]([H])=C([H])[O][C]1([O][C]1([H])[H])[C]([H])([H])[H] [H][O]
pr_18 [H][C]([O])=C([H])[C]([H])([H])[H] [H][O][C]1([H])[O][C]1([H])[H]
pr_19 [H][C]([H])([H])[C]([H])([C]([H])([O])[C]([H])([H])[H] [H][C]([H])=O
pr_20 [H][C]1([H])[O][O][C]([H])([C]([H])([H])[H])[C]([H])([H])[C]1=[O] [H]
pr_21 [H][O][C]([H])[C]([H])([H])[C]1([H])[O][C]1([H])[H] [H][C]([H])=O
pr_22 [H][C]([H])=O)[C]([H])([H])[O][O] [H][C]([H])=C([H])[C]([H])([H])[H]
pr_23 [H][C]([H])([H])[C]([H])([H])[O] [H][C]([H])([H])[C]1([H])[O][C]1([H])[H]
pr_24 [H][C]([H])([H])[C]1([H])[O][C]2([H])[C]([H])([H])[O][C]12[H] [H][O]
pr_25 [H][C]([H])([H])[C]12[O][C]([H])([H])[C]([H])([O]1)[C]2([H])[H] [H][O]
pr_26 [H][C]([H])=C([H])[C]([H])([H])[C]([H])([H])[C]([H])([H])[H] [H][O][O]
pr_27 [H][C]([H])=C([C]([H])([H])[H])[C]([H])([H])[H] [H][O][O]
rs_o2 [H][C]([H])[C]1([H])[O][C]([H])([C]([H])([H])[H])[C]1([H])[H] [O][O]
ra_o2 [H][C]([H])[C]1([H])[O][C]([H])([C]([H])([H])[H])[C]1([H])[H] [O][O]
rnew1 [H][C]([H])[C]([H])([O][C]([H])=C([H])[H])[C]([H])([H])[H] [O][O]
rnew2 [H][O][C]([H])([C]([H])[C]([H])([H])[C]([H])=C([H])[H] [O][O]
rnew3 [H][C]([H])[C]([H])([C]([H])([H])[H])[C]([H])([H])[H] [O][O]

S5 T1 Diagnostics

anti-ROO1

MESS file name	Filename	T1 Diagnostic
rxn_55 w_24 pr_27	1173013994994301920512_beta_delta_17_14_10_1_12.out	0.02459912
rxn_54 w_24 w_23	1173013994994301920512_intra_H_migration_17_4.out	0.02361543
w_24	1173013994994301920512.out	0.02462728
rxn_53 w_22 pr_26	1173053884192912421402_r12_insertion_R_1_10_14.out	0.02936419
rxn_52 w_22 w_23	1173053884192912421402_r12_insertion_R_1_2_3.out	0.01499945
rxn_47 w_19 pr_1	1173295116796376003302_HO2_Elimination_from_PeroxyRadical_12_17.out	0.0250386
rxn_45 w_19 w_2	1173295116796376003302_intra_H_migration_17_12.out	0.02220961
rxn_46 w_19 w_21	1173295116796376003302_intra_H_migration_17_13.out	0.0183091
w_19	1173295116796376003302.out	0.02392361
rxn_56 w_25 w_23	1173295257356674602682_intra_R_migration_11_2.out	0.01395221
w_25	1173295257356674602682.out	0.02527521
w_2	1173334856415776143602.out	0.0157914
rxn_50 w_21 pr_25	1173334856565945863262_Cyclic_Ether_Formation_3_14.out	0.06087459
rxn_51 w_21 w_22	1173334856565945863262_Intra_R_Add_ExoTetCyclic_F_3_1_12.out	0.04933962
rxn_48 w_20 w_19	1173335006286015853312_intra_H_migration_2_4.out	0.02153859
rxn_49 w_20 pr_24	1173335006286015853312_r12_insertion_R_1_10_14.out	0.02212386
fr_1	3304901700000000000002.out	0.03612816

syn-ROO1

MESS file name	Filename	T1 Diagnostic
fr_19	10000000000000000002.out	0
fr_22	1002603503632461390421.out	0.0130349
fr_8	1002844405685474742511.out	0.01268728
fr_6	1002844515855304501641.out	0.01252068
fr_13	1002884375184413302101.out	0.01199625
fr_24	1002884375244242811101.out	0.01215954
fr_7	1003125527628350066821.out	0.0110283
fr_3	1003125527687848164041.out	0.01159454
fr_5	1003125528188889085181.out	0.01113159
fr_20	1162923714042892271041.out	0.01330065
fr_28	1163164726165736114171.out	0.01334134
rxn_11 w_5 pr_6	1173053884193062571252_Cyclic_Ether_Formation_3_14.out	0.02166728
w_5	1173053884193062571252.out	0.01444193
rxn_12 w_5 pr_7	1173053884193062571252_R_Addition_MultipleBond_3_2_1.out	0.01980673
rxn_24 w_8 pr_14	1173053964353482550992_HO2_Elimination_from_PeroxyRadical_12_17.out	0.02490802
rxn_22 w_8 w_6	1173053964353482550992_intra_H_migration_17_4.out	0.02178358
w_8	1173053964353482550992.out	0.02462213
rxn_23 w_8 w_12	1173053964353482550992_r12_insertion_R_10_14_17.out	0.02943193
rxn_43 w_18 pr_23	1173054004062572231862_Cyclic_Ether_Formation_2_17.out	0.02248258
w_18	1173054004062572231862.out	0.01371358
rxn_44 w_18 pr_22	1173054004062572231862_r12_insertion_R_2_3_17.out	0.01872289
w_9	1173054104573422330912.out	0.02492851
rxn_25 w_9 pr_16	1173054104573422330912_r12_insertion_R_12_1_10.out	0.02523657
rxn_26 w_9 pr_15	1173054104573422330912_r13_insertion_ROR_15_10_14_17.out	0.01681602
rxn_18 w_7 t_1	1173054144423212331042_intra_R_migration_11_10.out	0.01920274
rxn_19 w_7 w_4	1173054144423212331042_intra_R_migration_11_3.out	0.03103585
w_7	1173054144423212331042.out	0.01826471
rxn_20 w_7 pr_12	1173054144423212331042_r13_insertion_ROR_2_1_10_14.out	0.01797954
rxn_21 w_7 pr_13	1173054144423212331042_R_Addition_MultipleBond_11_1_12.out	0.01579437
rxn_27 w_10 w_8	1173093704083332811182_intra_H_migration_1_12.out	0.02272232
w_10	1173093704083332811182.out	0.01575056
rxn_28 w_10 pr_14	1173093704083332811182_r12_insertion_R_1_10_14.out	0.02823903
rxn_29 w_10 pr_17	1173093704083332811182_r12_insertion_R_14_10_1.out	0.02527138
rxn_13 w_6 pr_9	1173093964163312551122_Intra_R_Add_ExoTetCyclic_F_2_14_17.out	0.02216869
rxn_14 w_6 w_4	1173093964163312551122_Intra_R_Add_ExoTetCyclic_F_2_3_13.out	0.01888544
w_6	1173093964163312551122.out	0.0128487
rxn_16 w_6 pr_8	1173093964163312551122_R_Addition_MultipleBond_2_1_11.out	0.03554904
rxn_3 w_1 pr_1	1173295116796376003302_HO2_Elimination_from_PeroxyRadical_12_17.out	0.02504523
rxn_1 w_1 w_2	1173295116796376003302_intra_H_migration_17_12.out	0.02185541
rxn_2 w_1 w_4	1173295116796376003302_intra_H_migration_17_7.out	0.02120171
w_1	1173295116796376003302.out	0.02396528
rxn_41 w_16 pr_20	1173295156546226474582_h2_elim_5_12.out	0.01616514
w_16	1173295156546226474582.out	0.01736703
rxn_39 w_16 pr_19	1173295156546226474582_r12_insertion_R_11_1_10.out	0.01874241
rxn_40 w_16 w_18	1173295156546226474582_R_Addition_MultipleBond_11_1_2.out	0.01777452
w_15	1173295315514344533202.out	0.01597795
rxn_38 w_15 pr_18	1173295315514344533202_r13_insertion_ROR_15_10_1_11.out	0.01845664
w_17	1173295415994844132602.out	0.01579625
rxn_42 w_17 pr_21	1173295415994844132602_R_Addition_MultipleBond_14_10_1.out	0.01740733
rxn_4 w_2 pr_2	1173334856415776143602_Intra_R_Add_ExoTetCyclic_F_1_14_17.out	0.0259728
w_2	1173334856415776143602.out	0.01579135
rxn_6 w_2 pr_1	1173334856415776143602_r12_insertion_R_17_14_10.out	0.0283444
rxn_5 w_2 w_5	1173334856415776143602_r12_insertion_R_2_3_11.out	0.01589386
rxn_32 w_12 w_15	1173334865705255465842_Cyclic_Ether_Formation_3_17.out	0.06595837
w_12	1173334865705255465842.out	0.01537175
rxn_36 w_14 w_17	1173335005885495585602_Cyclic_Ether_Formation_3_17.out	0.03050471
w_14	1173335005885495585602.out	0.01289123
rxn_37 w_14 w_9	1173335005885495585602_R_Addition_MultipleBond_3_6_17.out	0.01833615
rxn_48 w_20 w_19	1173335006286015853312_intra_H_migration_2_4.out	0.02156562

rxn_8 w_3 pr_3	1173335006286015853312_Intra_R_Add_ExoTetCyclic_F_2_14_17.out	0.02207003
w_3	1173335006286015853312.out	0.01284694
w_11	1173335015985986894622.out	0.01258443
rxn_30 w_11 w_15	1173335015985986894622_r12_insertion_R_3_17_14.out	0.02013723
rxn_31 w_11 w_8	1173335015985986894622_R_Addition_MultipleBond_6_3_17.out	0.0183451
rxn_33 w_13 w_16	1173335116506266514542_intra_H_migration_6_7.out	0.019454
w_13	1173335116506266514542.out	0.01220966
rxn_34 w_13 w_17	1173335116506266514542_r12_insertion_R_17_3_6.out	0.01944551
rxn_35 w_13 w_9	1173335116506266514542_R_Addition_MultipleBond_6_3_17.out	0.01814863
rxn_9 w_4 pr_4	1173335116606245723142_intra_H_migration_6_15.out	0.01371671
w_4	1173335116606245723142.out	0.01252903
rxn_10 w_4 pr_5	1173335116606245723142_r12_insertion_R_10_14_17.out	0.02133964
fr_4	17017000000000000002.out	0.00745827
t_1	30054036000000000001.out	0.01471681
fr_1	33049017000000000002.out	0.03612776
fr_17	411131060600080000002.out	0.0115383
fr_9	421261230750120000001.out	0.01117466
fr_11	430910860380000000002.out	0.02288009
fr_25	571411531050570000002.out	0.02026246
fr_31	581822822681320120001.out	0.01056084
fr_32	591191480870000000002.out	0.02806926
fr_26	601642622200720040001.out	0.01145621
t_1	701782141760940380001.out	0.0135229
fr_12	741902131801040490041.out	0.012109
fr_30	751511761490490000002.out	0.03023637
fr_10	751551631410490170002.out	0.01843356
fr_18	761681931620660190001.out	0.0137265
fr_21	842322632731771270201.out	0.01280225
fr_23	842322772951711050121.out	0.01210046
fr_2	842563785064103440441.out	0.01217796
rs_o2	852694215404703600442.out	0.01196262
fr_27	872193043041600570002.out	0.01921486
fr_29	872513863953021940722.out	0.01451204
	992714273963142831922.out	0.01776007

anti-ROO2

MESS file name	Filename	T1 Diagnostic
rxn_21 w_7 pr_10	1173054105433651990502_HO2_Elimination_from_PeroxyRadical_11_15.out	0.02306557
rxn_22 w_7 pr_12	1173054105433651990502_HO2_Elimination_from_PeroxyRadical_16_15.out	0.02527429
rxn_19 w_7 w_9	1173054105433651990502_intra_R_migration_15_8.out	0.0193616
w_7	1173054105433651990502.out	0.02412833
rxn_20 w_7 pr_11	1173054105433651990502_r13_insertion_ROR_3_1_2_14.out	0.02597048
rxn_18 w_6 pr_10	1173054145133682070612_HO2_Elimination_from_PeroxyRadical_3_15.out	0.05684123
rxn_15 w_6 pr_9	1173054145133682070612_intra_R_migration_10_6.out	0.03567069
w_6	1173054145133682070612.out	0.01923085
rxn_17 w_6 pr_8	1173054145133682070612_r12_insertion_R_14_2_1.out	0.01909416
rxn_16 w_6 w_7	1173054145133682070612_r12_insertion_R_6_2_10.out	0.0587516
rxn_12 w_5 pr_7	1173093964873782290692_Cyclic_Ether_Formation_6_14.out	0.01979339
rxn_13 w_5 pr_5	1173093964873782290692_Intra_RH_Add_Exocyclic_F_8_11.out	0.03018972
rxn_14 w_5 pr_6	1173093964873782290692_r12_insertion_R_6_2_14.out	0.01701781
rxn_2 w_1 pr_2	1173295117657316901962_HO2_Elimination_from_PeroxyRadical_17_15.out	0.0268919
w_1	1173295117657316901962.out	0.02330584
rxn_1 w_1 pr_1	1173295117657316901962_r12_insertion_R_3_1_2.out	0.02603205
w_10	1173295416594694282302.out	0.01885271
rxn_28 w_10 pr_14	1173295416594694282302_r13_insertion_ROR_2_6_7_15.out	0.01646898
rxn_29 w_10 pr_15	1173295416594694282302_R_Addition_MultipleBond_14_2_1.out	0.01795394
rxn_27 w_9 pr_14	1173335006745986544402_r12_insertion_R_10_2_6.out	0.10450883
rxn_6 w_3 w_1	1173335006997196792272_intra_H_migration_6_17.out	0.02325287
rxn_7 w_3 pr_4	1173335006997196792272_Intra_R_Add_ExoTetCyclic_F_6_14_15.out	0.01603807
rxn_8 w_3 pr_2	1173335006997196792272_r12_insertion_R_6_2_14.out	0.0179384
rxn_3 w_2 w_1	1173335117317276642402_intra_H_migration_1_3.out	0.02116752
rxn_4 w_2 pr_3	1173335117317276642402_r12_insertion_R_14_2_1.out	0.01740494
rxn_5 w_2 pr_1	1173335117317276642402_R_Addition_MultipleBond_1_2_14.out	0.01713684
rxn_24 w_8 w_10	1173335117366906284062_Intra_R_Add_ExoTetCyclic_F_8_15_14.out	0.02495874
rxn_25 w_8 w_7	1173335117366906284062_R_Addition_MultipleBond_8_7_15.out	0.02026798
rxn_11 w_4 w_6	1173335117467446362062_HO2_Elimination_from_PeroxyRadical_16_15.out	0.03159435
rxn_9 w_4 w_1	1173335117467446362062_intra_H_migration_8_11.out	0.02004194
rxn_10 w_4 w_5	1173335117467446362062_r13_insertion_ROR_7_6_2_10.out	0.01918204
fr_1	3304901700000000000002.out	0.03612795
fr_13	4111310606000800000002.out	0.00022618
fr_7	4309108603800000000002.out	0.02288092
fr_20	5714116810504200000002.out	0.02079591

syn-ROO2

MESS file name	Filename	T1 Diagnostic
fr_7	1002563284042141800181.out	0.01420073
fr_4	1003125527687848164041.out	0.0115648
fr_6	1003125528249208123901.out	0.01183092
rxn_4 w_1 pr_1	1173295117657316901962_HO2_Elimination_from_PeroxyRadical_3_17.out	0.0260806
rxn_5 w_1 pr_2	1173295117657316901962_HO2_Elimination_from_PeroxyRadical_9_17.out	0.02679088
rxn_1 w_1 w_2	1173295117657316901962_intra_H_migration_17_3.out	0.02120344
rxn_2 w_1 w_5	1173295117657316901962.out	0.02343036
rxn_3 w_1 w_4	1173295117657316901962_r12_insertion_R_16_7_6.out	0.02241723
rxn_11 w_4 pr_5	1173334857426846762522_Intra_R_Add_ExoTetCyclic_F_7_17_16.out	0.06089403
w_4	1173334857426846762522.out	0.01465265
rxn_9 w_3 pr_4	1173335006997196792272_Cyclic_Ether_Formation_6_15.out	0.01585593
rxn_8 w_3 w_1	1173335006997196792272_intra_H_migration_6_9.out	0.02345627
w_3	1173335006997196792272.out	0.01277059
rxn_10 w_3 pr_2	1173335006997196792272_r12_insertion_R_1_2_15.out	0.01722421
w_5	1173335015744814652002.out	0.01304722
rxn_6 w_2 pr_3	1173335117317276642402_Cyclic_Ether_Formation_1_15.out	0.01701217
w_2	1173335117317276642402.out	0.01305188
rxn_7 w_2 pr_1	1173335117317276642402_r12_insertion_R_17_15_2.out	0.01704359
fr_5	17017000000000000002.out	0.00745824
fr_1	33049017000000000002.out	0.03612781
fr_3	842563674744023760481.out	0.01243657
fr_2	842563785064103440441.out	0.01217773
o2	o2.out	0.00787012

anti-ROO3

MESS file name

Filename

T1 Diagnostic

fr_6	1002603363412521610501.out	0.01357079
fr_5	1003125528188889085181.out	0.01109325
fr_3	1003125528249208123901.out	0.01183071
fr_9	1022423043222461060041.out	0.01363506
rxn_9 w_4 t_1	1173054144834072410222_intra_R_migration_14_17.out	0.01819746
w_4	1173054144834072410222.out	0.03296173
rxn_10 w_4 pr_6	1173054144834072410222_r12_insertion_R_7_10_11.out	0.01697166
rxn_2 w_1 pr_1	1173295117357746382402_HO2_Elimination_from_PeroxyRadical_16_17.out	0.02607788
rxn_1 w_1 w_3	1173295117357746382402_intra_H_migration_17_3.out	0.02164129
w_1	1173295117357746382402.out	0.02399322
rxn_3 w_2 w_1	1173334856977256692612_intra_H_migration_2_15.out	0.02614664
w_2	1173334856977256692612.out	0.01568477
rxn_4 w_2 pr_1	1173334856977256692612_r12_insertion_R_2_6_9.out	0.02877979
rxn_5 w_2 pr_2	1173334856977256692612_r12_insertion_R_6_9_17.out	0.05558475
w_3	1173335117167576252452.out	0.01317067
rxn_8 w_3 w_4	1173335117167576252452_r12_insertion_R_1_2_14.out	0.03017885
rxn_6 w_3 pr_3	1173335117167576252452_r12_insertion_R_17_9_6.out	0.02224458
rxn_7 w_3 pr_4	1173335117167576252452_R_Addition_MultipleBond_1_2_6.out	0.01903879
fr_10	150390060000000000002.out	0.00658023
fr_4	170170000000000000002.out	0.00745823
fr_1	330490170000000000002.out	0.0361281
t_1	441041030570000000001.out	0.01386666
t_1	561281360900380000001.out	0.01469341
fr_2	842563674744023760481.out	0.01243622

syn-syn-ROO3

MESS file name	Filename	T1 Diagnostic
fr_6	1002603363412521610501.out	0.01357079
fr_5	1003125528188889085181.out	0.01113196
rxn_8 w_4 pr_6	1173054104984172260162_HO2_Elimination_from_PeroxyRadical_12_13.out	0.02887203
w_4	1173054104984172260162.out	0.02348412
rxn_7 w_4 w_3	1173054104984172260162_r12_insertion_R_5_2_3.out	0.10404046
rxn_5 w_3 w_2	1173054144834072410222_intra_R_migration_10_1.out	0.03030012
w_3	1173054144834072410222.out	0.02054561
rxn_6 w_3 pr_5	1173054144834072410222_r12_insertion_R_2_3_12.out	0.0164226
rxn_1 w_1 w_2	1173295117357746382402_intra_H_migration_13_7.out	0.0215416
w_1	1173295117357746382402.out	0.02417688
w_2	1173335117167576252452.out	0.01313701
rxn_3 w_2 pr_3	1173335117167576252452_r12_insertion_R_1_2_5.out	0.02222474
rxn_4 w_2 pr_4	1173335117167576252452_R_Addition_MultipleBond_11_1_2.out	0.01917017
fr_1	17017000000000000002.out	0.00745824
fr_2	33049017000000000002.out	0.03612773
pr_5	441041030570000000001.out	0.01386677
pr_5	561281360900380000001.out	0.0146934
fr_9	842322662801781200161.out	0.01254318
rnew_o2	852453093031931240162.out	0.01679256

syn-anti-ROO3

MESS file name

Filename

T1 Diagnostic

fr_3	1003125528249208123901.out	0.01183072
rxn_1 w_1 pr_1	1173295117357746382402_HO2_Elimination_from_PeroxyRadical_14_17.out	0.02587893
w_1	1173295117357746382402.out	0.02405744
rxn_3 w_2 w_1	1173334856977256692612_intra_H_migration_7_14.out	0.0261714
rxn_2 w_2 pr_2	1173334856977256692612_intra_H_migration_7_16.out	0.05560292
w_2	1173334856977256692612.out	0.01568477
rxn_4 w_2 pr_1	1173334856977256692612_r12_insertion_R_7_6_15.out	0.02877979
fr_4	17017000000000000002.out	0.00745824
fr_1	330490170000000000002.out	0.03612794
fr_2	842563674744023760481.out	0.01243779