

Supporting Information

A Combined Computational-Experimental Study on the Substrate Binding and Reaction Mechanism of Salicylic Acid Decarboxylase

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1. Optimized structures in the pathway of Mg-enzyme

Optimized structures with full model for the transition states (**TS1-A_{Mg}** and **TS2-A_{Mg}**) and intermediates (**Int-A_{Mg}** and **E:P-A_{Mg}**) in the reaction pathway with Mode-A for the Mg-enzyme of SDC. The energies relative to **E:S-A_{Mg}** are given in the parentheses (kcal/mol).

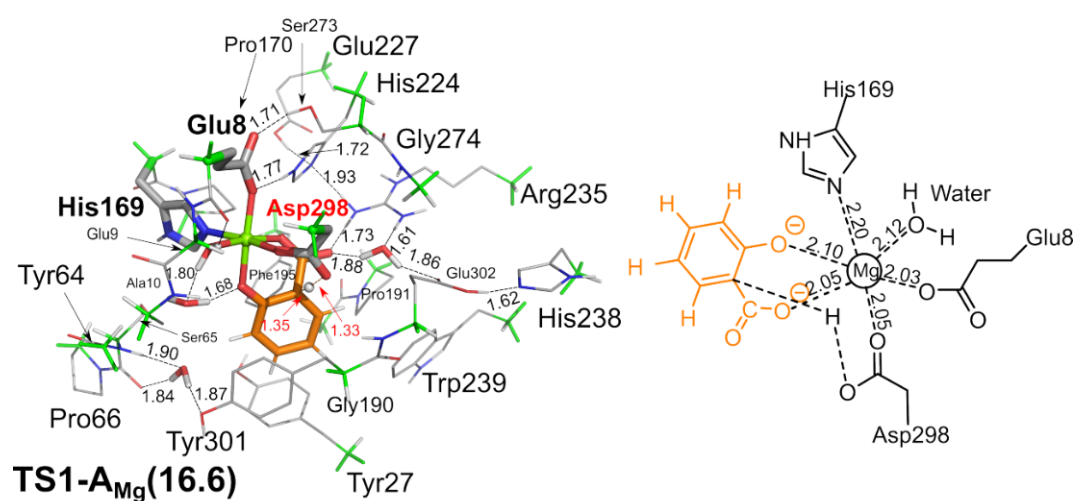


Figure S1. Optimized structure for the transition state of substrate protonation in the pathway with Mode-A for the Mg-enzyme.

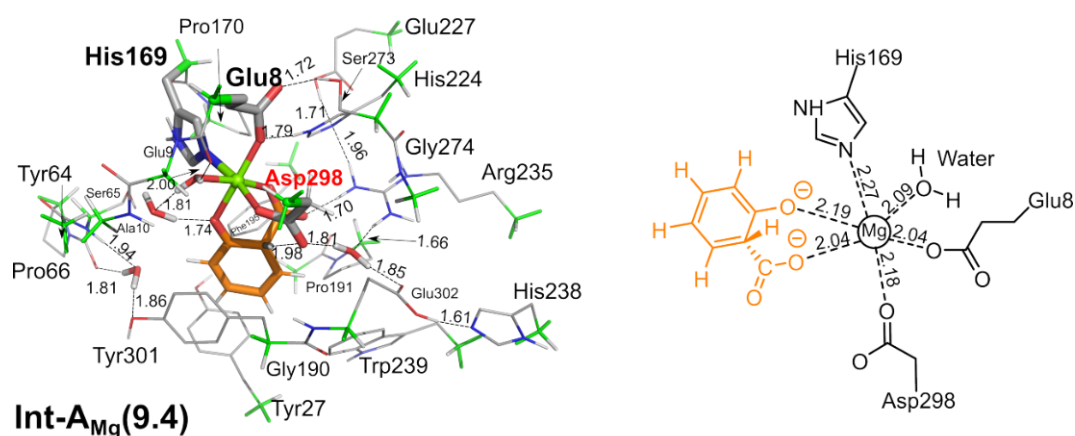
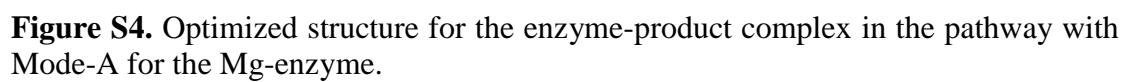
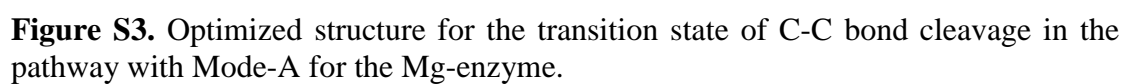


Figure S2. Optimized structure for the intermediate in the pathway with Mode-A for the Mg-enzyme.



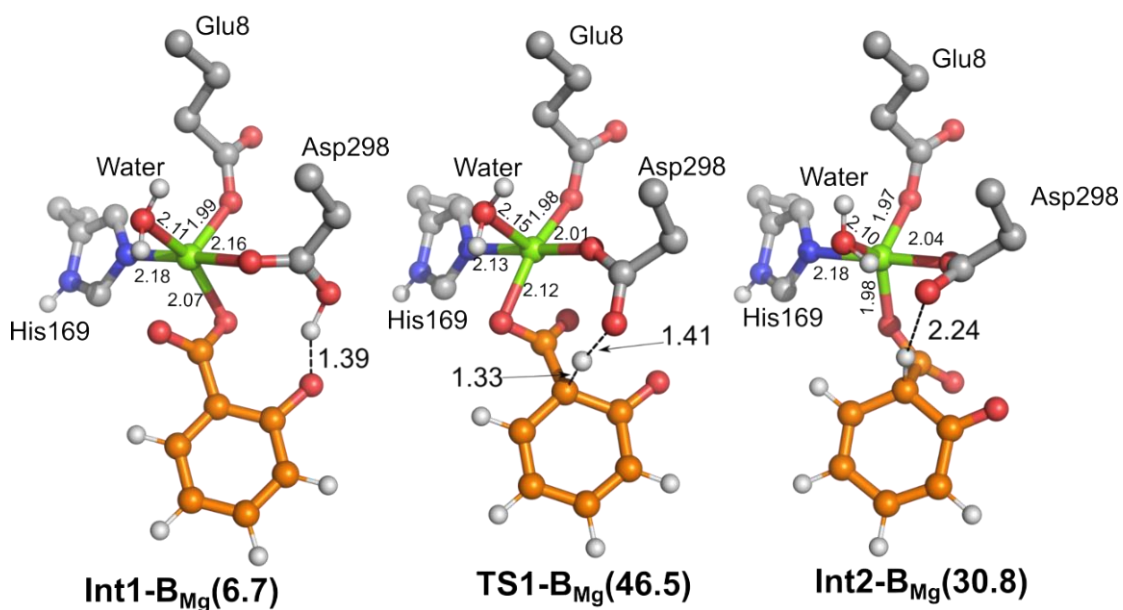


Figure S5. Optimized structures of the transition state (TS1-B_{Mg}) and intermediates (Int1-B_{Mg}, Int1-B_{Mg}) in the pathway with **Mode-B** for the Mg-enzyme. The first intermediate (Int1-B_{Mg}) is resulted by the proton transfer from the hydroxyl group of the substrate to Asp298 and the second intermediate (Int2-B_{Mg}) is formed by the proton transfer from Asp298 to substrate C1. TS1-B_{Mg} is the transition state of the second proton transfer. Only a part of the active site model is shown. The energies relative to E:S-A_{Mg} are given in kcal/mol.

2. Optimized structures in the pathway of Zn-enzyme

Optimized structures for the enzyme-substrate complex (**E:S-A_{Zn}**), transition states (**TS1-A_{Zn}** and **TS2-A_{Zn}**) and intermediates (**Int-A_{Zn}** and **E:P-A_{Zn}**) in the reaction pathway with Mode-A for the Zn-enzyme of SDC. The energies relative to the **E:S-A_{Zn}** are given in the parentheses (kcal/mol).

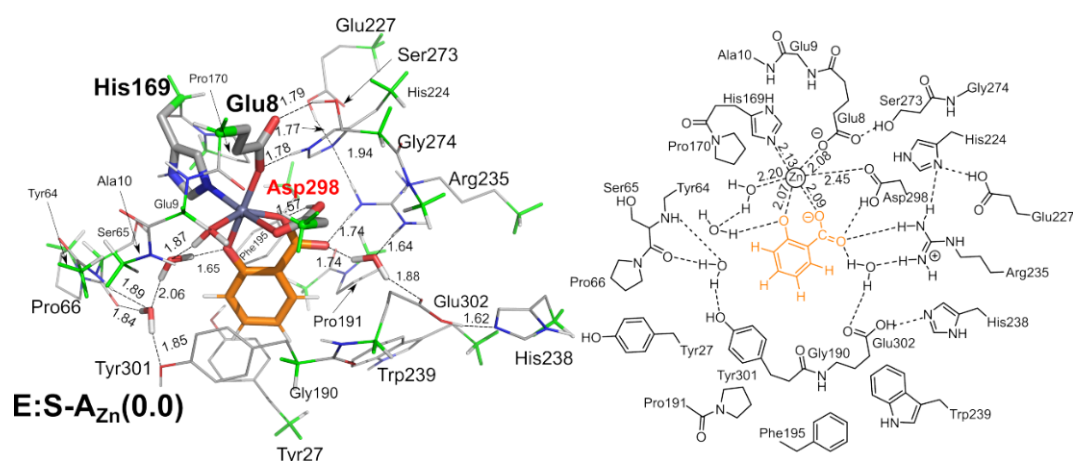


Figure S6. Optimized structure for the enzyme-substrate complex in the pathway with Mode-A for the Zn-enzyme.

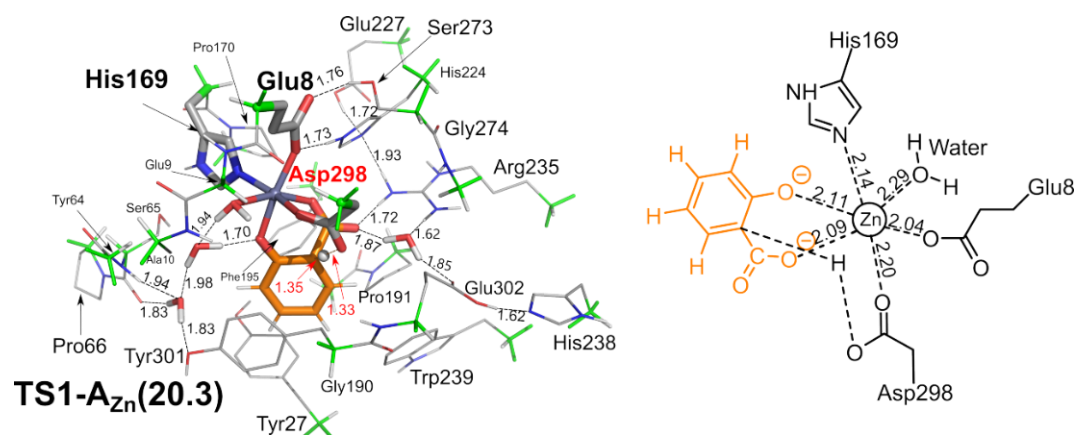


Figure S7. Optimized structure for the transition state of substrate protonation in the pathway with Mode-A for the Zn-enzyme.

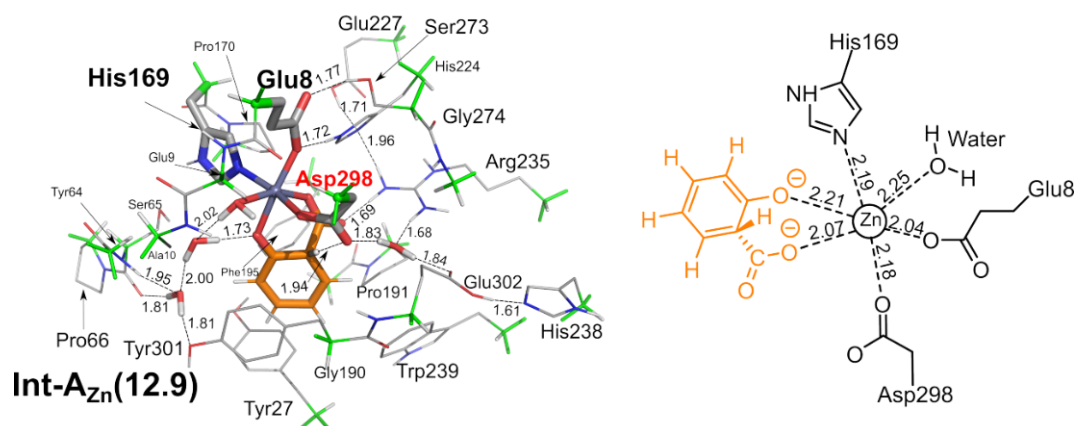


Figure S8. Optimized structure for the intermediate in the pathway with Mode-A for the Zn-enzyme.

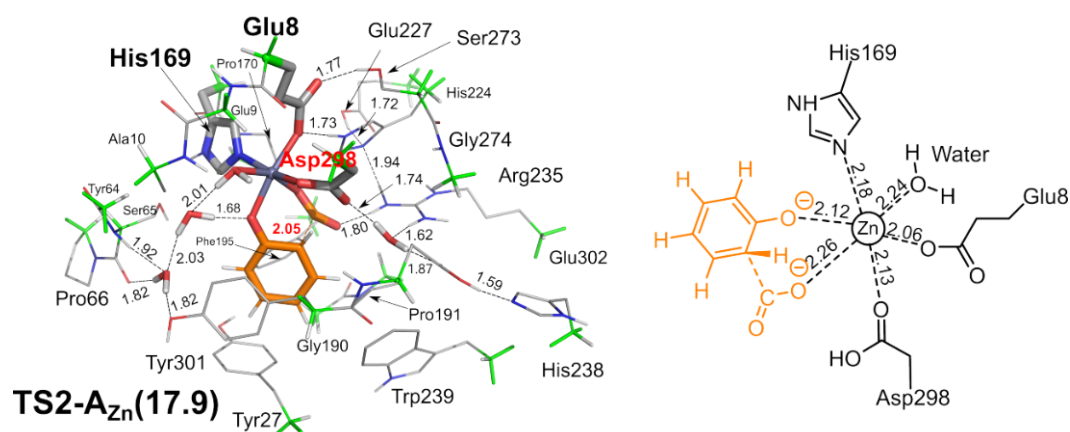


Figure S9. Optimized structure for the transition state of C-C bond cleavage in the pathway with Mode-A for the Zn-enzyme.

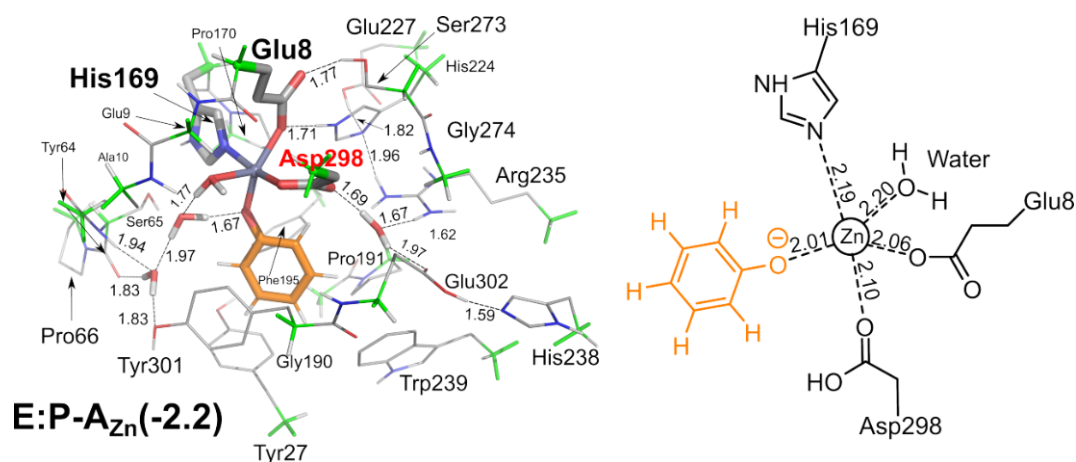


Figure S10. Optimized structure for the enzyme-product complex in the pathway with Mode-A for the Zn-enzyme.

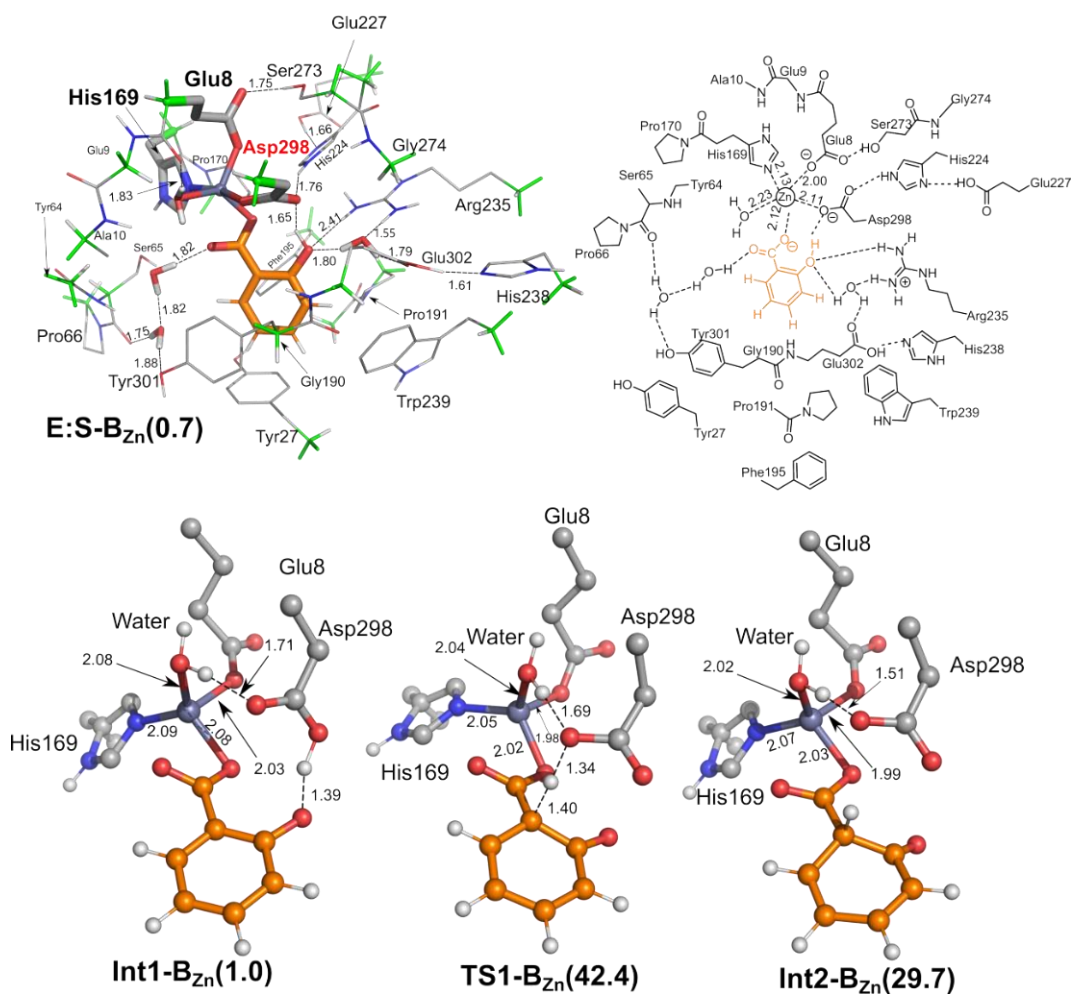


Figure S11. Optimized structures of the enzyme-substrate complex (**E:S-B_{Zn}**), transition state (**TS1-B_{Zn}**) and intermediates (**Int1-B_{Zn}**, **Int2-B_{Zn}**) in the pathway with **Mode-B** for the Zn-enzyme. Only a part of the active site model is shown. The energies relative to **E:S-A_{Zn}** are given in kcal/mol.

3. Optimized structures in the pathway of Mn-enzyme

Optimized structures for the enzyme-substrate complex (**E:S-A_{Mn}**), transition states (**TS1-A_{Mn}** and **TS2-A_{Mn}**) and intermediates (**Int-A_{Mn}** and **E:P-A_{Mn}**) in the reaction pathway with Mode-A for the Zn-enzyme of SDC. The energies relative to the **E:S-A_{Mn}** are given in the parentheses (kcal/mol).

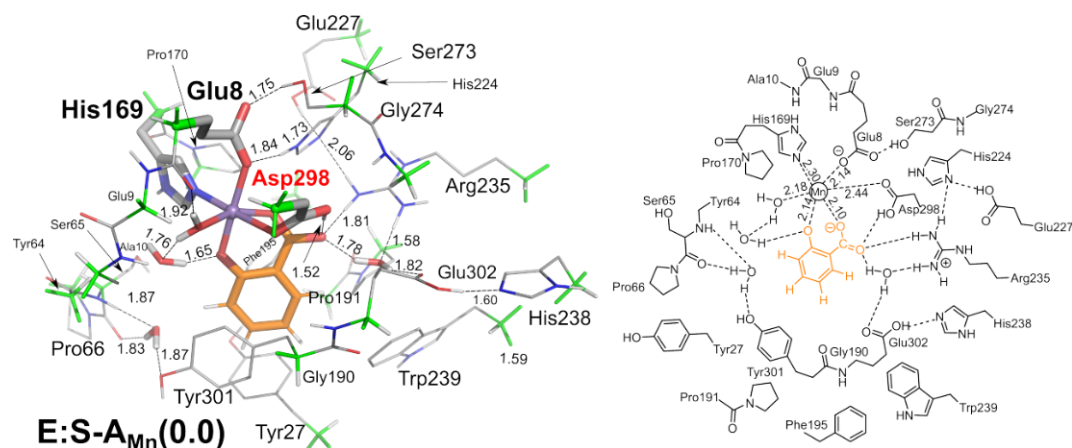


Figure S12. Optimized structure for the enzyme-substrate complex in the pathway with Mode-A for the Mn-enzyme.

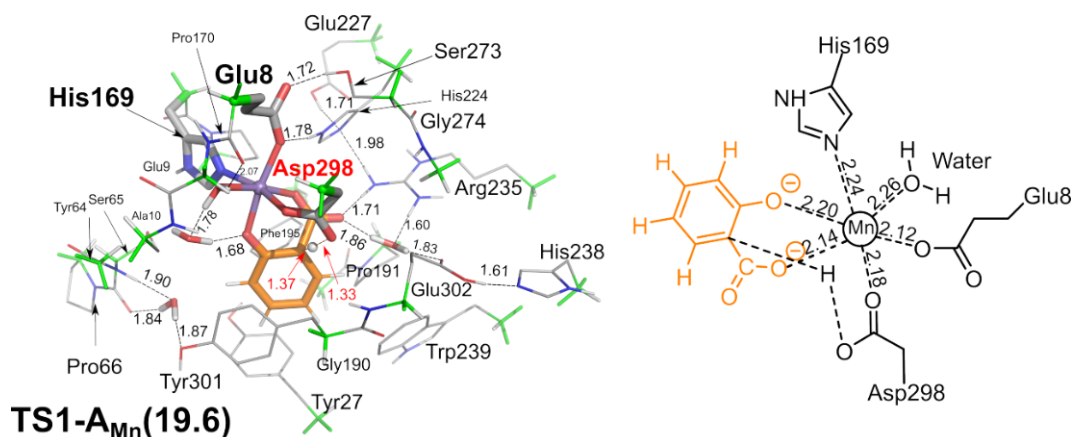


Figure S13. Optimized structure for the transition state of substrate protonation in the pathway with Mode-A for the Mn-enzyme.

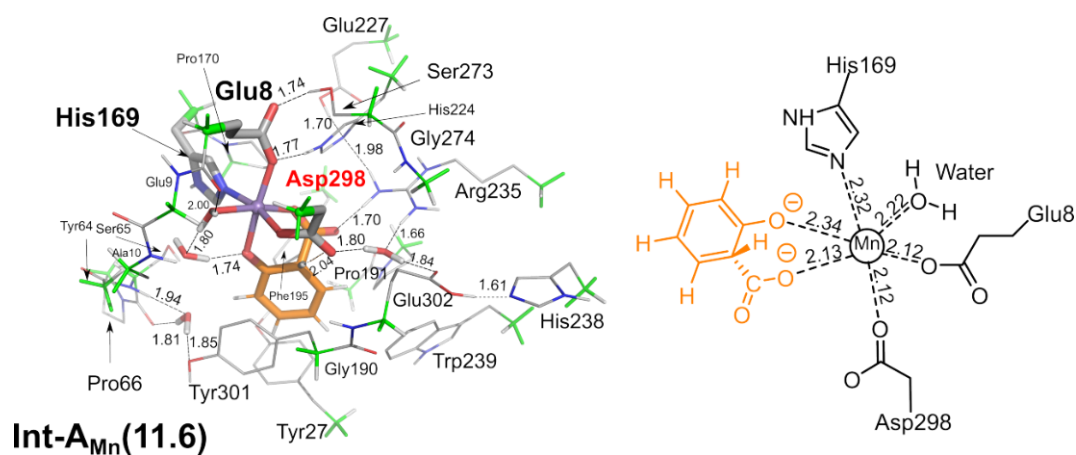


Figure S14. Optimized structure for the intermediate in the pathway with Mode-A for the Mn-enzyme.

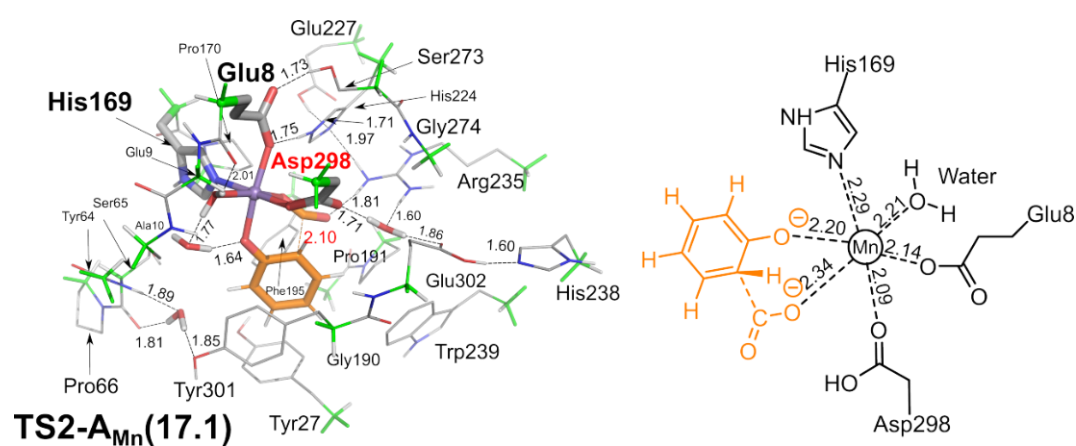


Figure S15. Optimized structure for the transition state of C-C bond cleavage in the pathway with Mode-A for the Mn-enzyme.

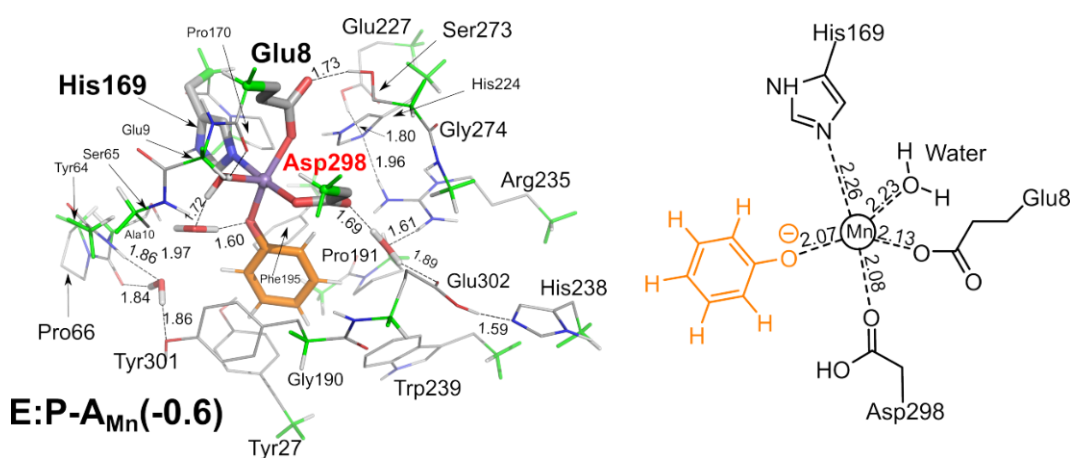


Figure S16. Optimized structure for the enzyme-product complex in the pathway with Mode-A for the Mn-enzyme.

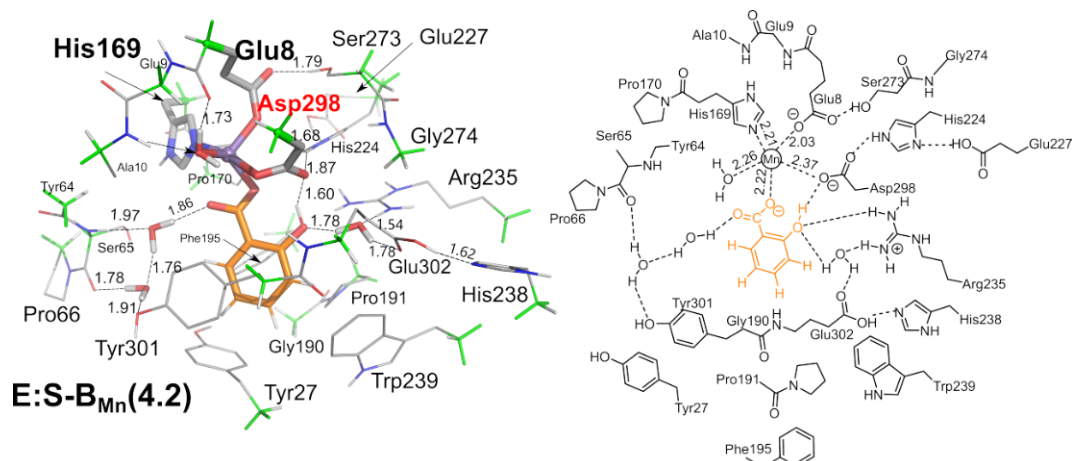


Figure S17. Optimized structure of the enzyme-substrate complex with **Mode-B** for the Mn-enzyme. The energy relative to **E:S-A_{Mn}** is given in kcal/mol.

4. Data collection and refinement statistics of TmSDC crystal

Table S1. Data collection and refinement statistics of TmSDC crystal.

	TmSDC (WT)
<i>Data collection</i>	
Space group	P2 ₁ 2 ₁ 2 ₁
Unit-cell	
<i>a, b, c</i> [Å]	57.91/92.31/128.60
<i>α /β /γ</i> (°)	90/90/90
Resolution (Å)	30.00 - 1.78 (1.84 - 1.78)
Unique reflections	64395 (6204)
Redundancy	5.9 (6.0)
Completeness (%)	96.1 (93.9)
Average I/σ(I)	25.9 (3.2)
CC 1/2	0.99 (0.74)
<i>Refinement</i>	
R_{work} (95% data)	0.165 (0.229)
R_{free} (5% data)	0.194 (0.278)
Rmsd bonds (Å)	0.016
Rmsd angles (°)	1.72
Dihedral angles	
Most favored (%)	96.2
Allowed (%)	3.8
Disallowed (%)	0
Average B-factor/ Number of non-hydrogen atoms	
Protein	17.8 / 5730
ligands	17.6 / 12
solvent	28.5 / 823
<i>PDB ID code</i>	8H41

Values in parentheses are for the outermost resolution shells.

5. Cartesian coordinates

The transition states and intermediates involved in the reaction pathway with **Mode-A** for the Mg-enzyme of SDC.

E:S-A_{Mg} (0.0 kcal/mol)

H	20.66700300	-6.80400000	-16.56500000
H	16.39000500	-5.37400700	-12.30898900
H	24.65800200	-6.75700000	-19.16500100
H	29.36498400	-8.34201700	-18.18000100
H	35.11194200	4.87003000	-6.01592700
H	32.10200100	7.76402000	-10.35100000
H	33.92499400	-0.03000100	-10.21099500
H	31.94999300	-4.27899000	-6.58602100
H	23.18500000	1.49700400	-4.32301200
H	22.41701500	4.62902600	-7.60400500
H	22.25399900	6.38999800	-15.14799900
H	33.53401600	5.46902100	-6.68090600
H	30.78100100	8.84800100	-10.93699500
H	23.93696900	6.31002400	-15.82101900
H	23.80800200	-0.12299700	-3.81399900
H	32.79705500	-3.33893500	-5.29803100
H	32.07502000	0.82301300	-17.96199600
H	30.43495400	-3.27800700	-15.73599000
H	31.70202300	-4.16492500	-14.93605400
H	30.41800400	-9.05997400	-14.20504400
H	20.88601600	-5.04999600	-16.84099500
H	34.15698400	-4.71597100	-10.10796200
H	23.72508500	-8.30802500	-7.05601700
H	21.59202100	-3.72899900	-7.32002500
H	27.89799600	0.15100100	-17.74200100
H	27.15890700	4.34402900	-6.69899600
C	29.55200300	-8.45604300	-13.91494300
C	29.05989800	-7.64379200	-15.10505500
O	28.82223700	-6.43155500	-15.08347500
C	29.77548000	-7.56856400	-12.68631400
C	28.43811300	-7.07634700	-12.10090300
C	28.64527000	-6.00105200	-11.03734800
O	29.42965300	-6.24587300	-10.10347700
O	27.98869100	-4.89811700	-11.14533800
H	28.76676100	-9.19268100	-13.68524900
H	30.33163100	-8.10627300	-11.91459500
H	30.38535000	-6.70728800	-12.97789900
H	27.77846700	-6.70544600	-12.88121000
H	27.93689500	-7.92536200	-11.61601200
N	28.92871800	-8.36821100	-16.23513100
C	28.69001800	-7.77097600	-17.53401000
C	27.23165100	-7.97667600	-17.94717700
O	26.76839400	-9.10571200	-18.05502200
H	29.02824500	-9.37130600	-16.20011000
H	28.99729500	-6.72538900	-17.49103000
N	26.51434800	-6.83388000	-18.11320500
C	25.05599600	-6.84000100	-18.14800000
C	24.50129400	-5.71855200	-17.27817900
H	26.96256900	-5.96261700	-17.86733900
H	24.74041000	-7.81989400	-17.77844500
H	23.41144300	-5.68975500	-17.34107600
H	24.77706200	-5.85250000	-16.23095300
H	24.86773900	-4.73596500	-17.59661500
C	23.25804100	6.03496100	-15.04098300
C	23.21366000	4.49345400	-14.99267500
C	22.29351000	3.92046800	-13.94178700
C	22.59019200	4.04808800	-12.57941500
C	21.14505100	3.19843000	-14.29054100
C	21.79832200	3.45025000	-11.60574800
C	20.33554900	2.59479100	-13.32915600
C	20.67250300	2.71005100	-11.97850700
O	19.88229600	2.08038900	-11.05775300
H	23.64598400	6.44119500	-14.10000200
H	22.89984700	4.12344100	-15.97570700
H	24.22774200	4.10283700	-14.83940900
H	23.47889100	4.59143100	-12.26964500
H	20.89133200	3.08569700	-15.34184200
H	22.06793500	3.52746700	-10.55894800
H	19.46106800	2.01558700	-13.60629300
H	20.30976100	2.15072300	-10.19243300
C	20.86196700	-5.84000000	-16.08300700
C	19.87952500	-5.67147200	-14.93053600
O	19.27131600	-6.63192100	-14.46714700
H	21.87062800	-5.89398500	-15.65559100
N	19.79977100	-4.41391400	-14.40318600
C	19.19502900	-4.19798800	-13.09496900
C	18.17168300	-3.06963600	-13.16159500
O	18.44179900	-1.97440400	-13.68291700
C	20.33311500	-3.89955300	-12.09433500
O	19.90172900	-3.82910800	-10.73647600
H	20.36579400	-3.64303000	-14.77013000
H	18.72438500	-5.14225700	-12.82466000
H	21.03846400	-4.73349900	-12.15847000
H	20.85853400	-2.98759800	-12.40118700
H	19.66826300	-2.91321600	-10.54066000

C	23.90588100	-7.35592000	-7.56599700
C	22.91426000	-6.30367100	-7.09152800
O	21.74503700	-6.60748500	-6.84557900
C	23.64938600	-7.58935000	-9.08439300
C	23.97801400	-6.40079600	-9.92892700
C	25.16078600	-6.04336500	-10.52574600
N	23.13346100	-5.31843500	-10.14520600
C	23.82147900	-4.37018300	-10.83633400
N	25.05599900	-4.78418300	-11.08052100
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C	24.70680800	-4.49575100	-7.24482300
H	21.90285800	-4.31513800	-5.72118100
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H	23.64366600	-2.75698000	-5.31920200
H	24.27258600	-2.65178600	-8.30808300
H	25.39884100	-2.44229400	-6.95876200
H	25.17499300	-4.88130600	-8.15077300
H	25.32910500	-4.77508400	-6.38479200
C	23.17495000	4.07097600	-8.16499400
C	24.47017800	3.93688600	-7.38429300
O	24.49579100	3.84501900	-6.15625400
H	22.78186000	3.06987600	-8.36587300
H	23.32234600	4.57866500	-9.12075200
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C	26.90912800	3.66698800	-7.52200700
C	27.87943200	3.79168800	-8.69954900
C	27.07387200	3.20386700	-9.86098400
C	25.65992100	3.74125400	-9.60698300
H	26.94021000	2.64949800	-7.10470300
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H	27.45312200	3.49304300	-10.84057100
H	27.07667000	2.11222400	-9.80769600
H	25.51525200	4.70732300	-10.10601700
H	24.89310000	3.04798700	-9.95994600
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C	24.29421500	0.47176200	-5.86091800
C	23.61371600	0.54530600	-7.21714700
C	22.22522700	0.60715800	-7.38618600
C	24.40823400	0.48562700	-8.37515700
C	21.64739500	0.55066000	-8.66082600
C	23.84074300	0.44915400	-9.64626600
C	22.45024500	0.46407400	-9.79731500
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C	29.88181900	-2.76942700	-7.07496100
C	30.01622900	-3.58116200	-8.17474600
N	28.59098700	-2.22925400	-7.06537200
C	27.98794100	-2.72662600	-8.15187400
N	28.80924500	-3.53862300	-8.83614700
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H	27.72385700	-2.92566700	-5.69188600
H	30.84549300	-4.16522900	-8.53922800
H	26.99198100	-2.49016100	-8.48945800
H	28.55544000	-4.07117700	-9.68318300
C	33.48001200	-4.18202100	-10.78307400
C	33.31216800	-2.74271800	-10.32643200
O	32.95898200	-2.40736700	-9.20131600
C	32.16445400	-4.97740500	-10.82016400
O	31.99442900	-5.64862300	-9.59235500
H	33.94144100	-4.19983500	-11.77797500
H	31.31875900	-4.30655500	-11.02497600
H	32.21849200	-5.69607200	-11.65517600
H	31.08934800	-6.02286200	-9.62614600
N	33.57143900	-1.80577600	-11.28701200
C	33.30500800	-0.40200700	-11.03299500
H	33.78163900	-2.10348200	-12.22555900
H	33.55059300	0.17171600	-11.92878600
H	32.25256900	-0.24186300	-10.79464600
C	30.70403000	-3.79207500	-14.83692700
C	30.73084700	-2.82207100	-13.64635900
C	29.45725200	-2.77491300	-12.85168500
O	28.36064100	-3.08070700	-13.33856900
O	29.64357800	-2.38057600	-11.61518000
H	30.02139800	-4.62569500	-14.67784700
H	31.53031600	-3.06076900	-12.94094200
H	30.92904000	-1.79196800	-13.96728000
C	27.87500800	1.06299600	-17.13699800
C	29.24852800	1.55941900	-16.73385900
O	29.41572900	2.61297900	-16.12241800

C	27.01367500	0.79945700	-15.88082300
C	25.59912800	0.42043700	-16.23256200
C	24.68007000	1.40265000	-16.61524300
C	25.16671500	-0.90862300	-16.18742400
C	23.36402500	1.07411200	-16.93129700
C	23.85662700	-1.25913100	-16.50278200
C	22.95884100	-0.25890200	-16.86622300
O	21.65060100	-0.63686600	-17.12183100
H	27.40350900	1.84650500	-17.73922400
H	27.47158800	0.00264900	-15.28431500
H	27.02197700	1.69520900	-15.25522500
H	24.98791400	2.44423600	-16.64235200
H	25.84812400	-1.68477400	-15.85088800
H	22.65333200	1.85177500	-17.20277100
H	23.52676100	-2.28525500	-16.38956600
H	21.13118400	0.15264600	-17.32288000
N	30.27400500	0.73636300	-17.07443800
C	31.68296600	1.10898400	-16.98000300
C	32.39305000	0.40193100	-15.82610300
C	31.84663100	0.85274000	-14.47152600
C	32.27016900	2.24044700	-14.02354900
O	33.23136800	2.77020400	-14.75361800
O	31.78808000	2.78736200	-13.03068200
H	30.04996600	-0.09286400	-17.60260100
H	31.73788600	2.19273200	-16.86789100
H	32.24928600	-0.68118800	-15.92835800
H	33.46749000	0.59709600	-15.88478600
H	30.75472900	0.82331000	-14.45852100
H	32.15491200	0.17285300	-13.67113900
C	27.09096200	-0.82387100	-11.37845700
O	27.17813800	-2.07108000	-11.04468300
O	27.91394300	0.02325200	-10.92013600
C	26.00952500	-0.35140300	-12.25842600
C	25.00256900	-1.21496200	-12.78392600
O	25.12262400	-2.52474500	-12.82085100
C	23.81980800	-0.60614700	-13.28260000
C	23.71189100	0.76736400	-13.39995700
C	24.78094200	1.60488900	-13.03586400
C	25.90010800	1.04179400	-12.45681800
H	28.73909100	-2.27591900	-11.16500400
H	23.01061000	-1.24453600	-13.62228800
H	22.80181800	1.19557800	-13.80294300
H	24.71963800	2.67592700	-13.16676400
H	26.71015700	1.66680500	-12.10531300
O	26.35412100	-5.04530600	-13.79802300
H	25.53393600	-4.80943600	-14.29732300
H	27.09206600	-5.19832000	-14.40733900
O	24.08126100	-3.94065700	-14.69292500
H	23.20517900	-4.23461700	-14.41555800
H	24.36313300	-3.27196400	-13.98951300
O	21.02566600	-1.93067900	-14.66969600
H	21.13781800	-1.48944900	-15.52928900
H	20.12690000	-1.70438800	-14.34799200
C	34.22903000	4.62593900	-6.61618500
C	33.56315800	3.35524500	-6.06850600
C	32.24642800	2.98348600	-6.76799700
C	31.91680800	1.49001500	-6.58636000
N	30.54783700	1.11057200	-6.92999800
C	30.09606700	0.92554500	-8.19386600
N	30.78141400	1.41648400	-9.22576600
N	28.93085200	0.30876600	-8.37528100
H	34.58311000	4.44201800	-7.63904200
H	34.27337300	2.52358900	-6.17015500
H	33.37598000	3.46044500	-4.99287000
H	31.41831600	3.58659000	-6.37957600
H	32.32771300	3.23591500	-7.83360600
H	32.62345500	0.87331800	-7.15748000
H	32.05154200	1.22280000	-5.53499900
H	29.97725400	0.70351900	-6.20302000
H	31.61220700	1.95475100	-9.05523800
H	30.54540300	1.17733500	-10.21832700
H	28.66147000	-0.40192700	-7.68574300
H	28.59781000	0.13067100	-9.33928900
C	31.09199500	7.81099700	-10.76999600
C	30.08806800	7.05151000	-9.88402700
C	28.76709700	6.82748600	-10.55762200
C	27.57568000	7.45287000	-10.28671700
C	28.51248300	5.91316500	-11.64897700
C	27.13710400	6.03966500	-11.99105500
C	29.30397200	4.98594500	-12.35143000
N	26.59191300	6.98758800	-11.14553500
C	26.54642400	5.27618200	-13.00283000
C	28.72397900	4.22833000	-13.36256200
C	27.35857900	4.37553900	-13.68376700
H	31.14438100	7.33610500	-11.75614000
H	30.51974900	6.07768400	-9.61440600
H	29.93839300	7.59060800	-8.94131300
H	27.34427300	8.19818400	-9.53901800
H	25.62944300	7.28057100	-11.14031800
H	30.35695500	4.85491500	-12.12238400
H	25.49754000	5.38924500	-13.25505500
H	29.32467900	3.53399600	-13.93725100
H	26.94273200	3.78174900	-14.49061000
O	30.26397200	0.84537300	-11.80534100
H	30.45295400	1.68496800	-12.26478200
H	29.29821800	0.68056500	-11.75142100
N	16.95469900	-3.31930000	-12.63978000
C	16.59799000	-4.44999100	-11.75903700
C	15.33368200	-3.94260400	-11.04534900

C	14.69185500	-3.00252400	-12.07718500
C	15.90139100	-2.29360700	-12.69345200
H	17.41143400	-4.65280700	-11.05923800
H	14.68007200	-4.76106100	-10.73516100
H	15.61374000	-3.37768100	-10.14940200
H	14.16782000	-3.58462400	-12.84324300
H	13.97747300	-2.30204100	-11.63834400
H	15.75145300	-1.96602900	-13.72474700
H	16.20566700	-1.41495700	-12.11104400
C	29.55101400	-2.94402000	-1.16198900
C	28.26525700	-3.75606900	-1.35117200
C	28.03423900	-4.24188400	-2.78309600
C	27.85311000	-3.13489100	-3.80725200
O	28.01218000	-1.94535100	-3.59866100
O	27.53021500	-3.62974200	-5.00913100
H	29.53853200	-2.10752900	-1.86478000
H	28.26224600	-4.62671500	-0.68412300
H	27.41379200	-3.13276000	-1.05339200
H	28.87933700	-4.85028900	-3.13281100
H	27.15879200	-4.89887500	-2.84548900
H	30.46537800	-3.51014700	-1.36794700
H	29.56604500	-2.49724500	-0.16239600
C	34.86196400	8.00000900	-10.31596000
C	35.22942000	6.50223100	-10.33219500
C	35.05396800	5.89246100	-11.68503300
C	34.12531900	5.01956800	-12.19831100
N	35.85691100	6.22554800	-12.76675800
C	35.40107100	5.55603000	-13.86088600
N	34.35446800	4.82047500	-13.54533800
H	35.56703400	8.59423100	-10.90668600
H	36.25518800	6.35170600	-9.97097600
H	34.57769100	5.96184400	-9.63842700
H	36.64042200	6.86057700	-12.74481300
H	33.30775300	4.51565300	-11.70457700
H	35.85672800	5.63115400	-14.83711600
H	33.57877400	3.63500600	-14.32974900
H	34.87101900	8.38159600	-9.28968300
H	33.87106300	8.09547700	-10.77201900
Mg	26.64079100	-3.72966900	-12.17394200

TS1-A_{Mg} (16.6 kcal/mol)

H	20.66699000	-6.80399700	-16.56500100
H	16.39000700	-5.37401200	-12.30898100
H	24.65799900	-6.75700700	-19.16500000
H	29.36499700	-8.34200900	-18.17999400
H	35.11193200	4.87003800	-6.01591600
H	32.10199800	7.76400700	-10.35099500
H	33.92500200	-0.03000800	-10.21099800
H	31.95001000	-4.27900700	-6.58598500
H	23.18501000	1.49700800	-4.32301900
H	22.41702300	4.62903800	-7.60400600
H	22.25399800	6.38997800	-15.14805900
H	33.53402500	5.46902900	-6.68089400
H	30.78102500	8.84801000	-10.93698300
H	23.93695500	6.31002100	-15.82103200
H	23.80798900	-0.12301600	-3.81400600
H	32.79703100	-3.33892000	-5.29801500
H	32.07499800	0.82298500	-17.96199700
H	30.43534600	-3.27780400	-15.73599100
H	31.70208700	-4.16474900	-14.93607700
H	30.41806900	-9.05985200	-14.20510400
H	20.88601600	-5.04999800	-16.84099700
H	34.15696100	-4.71598700	-10.10795100
H	23.72495000	-8.30800900	-7.05603500
H	21.59204800	-3.72899400	-7.32005500
H	27.89798600	0.15101700	-17.74202500
H	27.15884400	4.34404500	-6.69899000
C	29.55193000	-8.45618600	-13.91484700
C	29.02335800	-7.65711500	-15.09585900
O	28.70630000	-6.46373900	-15.05661300
C	29.80103100	-7.57096000	-12.69023200
C	28.48018200	-7.18374100	-12.00062100
C	28.71058000	-6.09057900	-10.96036600
O	29.48127100	-6.34343300	-10.01739300
O	28.10686600	-4.96605900	-11.11956300
H	28.77674500	-9.19687900	-13.66385000
H	30.44587800	-8.08053200	-11.96984300
H	30.32627300	-6.66463700	-13.00864800
H	27.74131900	-6.86184700	-12.73084800
H	28.08821500	-8.06802400	-11.48103500
N	28.94829400	-8.36971000	-16.23869000
C	28.68998400	-7.77099000	-17.53401700
C	27.23027100	-7.97909000	-17.94320100
O	26.76643300	-9.10690000	-18.05646000
H	29.12618400	-9.36199300	-16.21576500
H	28.99351300	-6.72360600	-17.49676600
N	26.51412600	-6.83460100	-18.10838100
C	25.05601700	-6.83998400	-18.14799800
C	24.49925300	-5.70790200	-17.29169200
H	26.96030000	-5.96698700	-17.84591500
H	24.73548300	-7.81599100	-17.77262100
H	23.40910700	-5.68509700	-17.34929000
H	24.77615500	-5.82049200	-16.24254100
H	24.86061700	-4.73031000	-17.63340600
C	23.25808800	6.03494100	-15.04087500
C	23.26875900	4.48880000	-15.03046700
C	22.42494300	3.82340000	-13.97205700
C	22.76987200	3.90718500	-12.61756300

C	21.30873500	3.04823900	-14.31298400	H	30.91452000	-4.03594900	-8.58990400
C	22.04459300	3.22951800	-11.64347400	H	27.00323800	-2.50695200	-8.49703100
C	20.56781400	2.36329500	-13.35131800	H	28.62796900	-3.94638300	-9.76501500
C	20.94082200	2.45117100	-12.00798800	C	33.48008600	-4.18196000	-10.78309800
O	20.20571800	1.76028800	-11.08812900	C	33.35330000	-2.74034900	-10.31916400
H	23.64619900	6.43354800	-14.09701600	O	33.08961400	-2.40302000	-9.16999600
H	22.94010800	4.13680000	-16.01573900	C	32.15868600	-4.96511600	-10.78811100
H	24.30736500	4.14731400	-14.92563600	O	31.99237700	-5.58956400	-9.53906300
H	23.64070000	4.48350900	-12.31693500	H	33.92497200	-4.20954700	-11.78475100
H	21.02448300	2.96341200	-15.35894000	H	31.31544200	-4.29319400	-11.01483100
H	22.34581400	3.27957200	-10.60411100	H	32.19642600	-5.70840900	-11.60159000
H	19.71786500	1.74593000	-13.62224800	H	31.08952700	-5.97671900	-9.55606000
H	20.64943800	1.82754600	-10.23047000	N	33.56014000	-1.80666200	-11.29478900
C	20.86198300	-5.83999800	-16.08300400	C	33.30498800	-0.40202700	-11.03298900
C	19.84579700	-5.63713500	-14.96913400	H	33.63269600	-2.11207700	-12.25222100
O	19.07850600	-6.52932300	-14.62030000	H	33.55866800	0.17158900	-11.92747600
H	21.86511100	-5.86959400	-15.64355800	H	32.25334100	-0.22412600	-10.79992700
N	19.90595800	-4.42377700	-14.33970900	C	30.70344300	-3.79243000	-14.83688600
C	19.19503500	-4.19798000	-13.09496900	C	30.49719300	-2.78521600	-13.69117000
C	18.15572400	-3.08760700	-13.21389900	C	29.03244900	-2.36086400	-13.62249500
O	18.40822400	-2.01128100	-13.78224800	O	28.16775600	-3.26144500	-13.55153700
C	20.24084300	-3.87449400	-12.00202700	O	28.75658500	-1.10529500	-13.64553900
O	19.67873900	-3.68200400	-10.70775300	H	30.02524600	-4.63882000	-14.71711600
H	20.55484200	-3.68841500	-14.62637100	H	30.72487200	-3.24050300	-12.72118800
H	18.70883600	-5.14365300	-12.85696800	H	31.12719300	-1.90108600	-13.80142500
H	20.90966400	-4.73790200	-11.92987400	C	27.87501600	1.06296300	-17.13697700
H	20.83513800	-3.00919600	-12.31756000	C	29.24570900	1.57689200	-16.74868200
H	19.39175100	-2.76238100	-10.64166600	O	29.40658500	2.63493400	-16.14246900
C	23.90608200	-7.35584500	-7.56601800	C	27.04011600	0.78391100	-15.87573600
C	22.91058100	-6.30344900	-7.10218900	C	25.66057800	0.28408100	-16.20849600
O	21.73765600	-6.60471500	-6.87049000	C	24.64898300	1.18008000	-16.56653500
C	23.66534200	-7.59988700	-9.08479200	C	25.35227900	-1.08057600	-16.16087800
C	24.00988400	-6.42011000	-9.93338900	C	23.36279200	0.73404600	-16.86208400
C	25.18037800	-6.09936600	-10.57341600	C	24.07150300	-1.54761800	-16.44981600
N	23.19724900	-5.30658800	-10.10619900	C	23.08281300	-0.63046900	-16.80297100
C	23.89529600	-4.37201400	-10.80833000	O	21.81171400	-1.12340800	-17.04872200
N	25.10023200	-4.83034000	-11.10857800	H	27.38684200	1.83814000	-17.73793800
H	24.94590300	-7.06578900	-7.39954800	H	27.56912100	0.04726700	-15.26750800
H	24.27742500	-8.44420800	-9.41487400	H	26.98343600	1.69811300	-15.28178500
H	22.61640300	-7.88613900	-9.21801300	H	24.86060200	2.24544400	-16.59062900
H	22.28253600	-5.17213500	-9.69621100	H	26.11385000	-1.78703100	-15.84157300
H	26.07335400	-6.69353000	-10.67145600	H	22.57859000	1.44471000	-17.11396800
H	23.51081500	-3.40025300	-11.07765900	H	23.82010800	-2.59774300	-16.34449200
N	23.32713900	-5.00660600	-7.09572600	H	21.24734000	-0.39588300	-17.34271100
C	22.40694600	-3.96407800	-6.62792900	N	30.27026100	0.76398300	-17.10393500
C	23.31551000	-2.76693700	-6.33936700	C	31.68299400	1.10902800	-16.97998700
C	24.51474700	-2.97912900	-7.26995500	C	32.35338800	0.35972900	-15.82628400
C	24.70845300	-4.49882300	-7.24494600	C	31.75945600	0.73862400	-14.46749800
H	21.89816600	-4.32398900	-5.72701100	C	32.11063000	2.12510600	-13.96655100
H	22.81094800	-1.81908400	-6.50876000	O	33.02916100	2.73937100	-14.68434700
H	23.65041000	-2.79475000	-5.29691900	O	31.61814900	2.59918300	-12.94088100
H	24.28074400	-2.63831800	-8.28378000	H	30.04308000	-0.08868400	-17.59145900
H	25.40807500	-2.45183400	-6.93346100	H	31.75761000	2.18867800	-16.84891000
H	25.17521500	-4.87499400	-8.15604200	H	32.22198900	-0.71910200	-15.97831600
H	25.33078800	-4.79076100	-6.38956000	H	33.42820000	0.56334700	-15.83877500
C	23.17494500	4.07094900	-8.16501600	H	30.67135400	0.63197800	-14.46362200
C	24.47154900	3.94032700	-7.38539100	H	32.10529300	0.05096400	-13.68835500
O	24.49572300	3.84711500	-6.15748400	C	27.17119100	-1.06459900	-11.23463700
H	22.78354100	3.06528500	-8.35229600	O	27.09989400	-2.29020700	-10.95703100
H	23.31410100	4.57064800	-9.12578300	O	27.81734800	-0.19257600	-10.59415400
N	25.60430200	3.91098700	-8.13889400	C	26.43262200	-0.55675400	-12.49043700
C	26.90921100	3.66696500	-7.52203100	C	25.26363900	-1.33370700	-12.91651400
C	27.87906100	3.79328600	-8.70150300	O	25.27656700	-2.61666300	-12.95265000
C	27.07244000	3.21286400	-9.86760400	C	24.07437400	-0.62980500	-13.28936400
C	25.66101500	3.75414000	-9.60839400	C	24.05000700	0.73945600	-13.33825400
H	26.93940500	2.64916500	-7.10742300	C	25.20001300	1.51746400	-13.01731800
H	28.09956200	4.84863800	-8.89310300	C	26.32596800	0.89028000	-12.57512200
H	28.82164300	3.27178200	-8.52997800	H	27.51452000	-0.87447600	-13.23270900
H	27.45044200	3.51102000	-10.84541200	H	23.19331000	-1.20790300	-13.55042900
H	27.07247500	2.12023600	-9.82247300	H	23.13525700	1.24034900	-13.63167100
H	25.51940100	4.72382200	-10.10216800	H	25.16282700	2.59740200	-13.08354500
H	24.89233000	3.06427000	-9.96383400	H	27.18383000	1.46961700	-12.25637300
C	23.37401100	0.46299500	-4.62997900	O	26.32040800	-5.34016800	-13.68533900
C	24.36836700	0.47276900	-5.80915600	H	25.46406300	-5.13220500	-14.12277700
C	23.80429900	0.49888600	-7.21754000	H	27.02302900	-5.46624000	-14.34448800
C	22.43646100	0.44725300	-7.50698800	O	23.88932700	-4.31013800	-14.42149500
C	24.70154900	0.48618000	-8.29997600	H	23.18252900	-4.65464400	-13.86138700
C	21.98156500	0.31811700	-8.82448300	H	24.25288400	-3.53625900	-13.91266600
C	24.25389900	0.38956600	-9.61510700	O	21.11272100	-1.88069300	-14.40624500
C	22.88539200	0.28578900	-9.88672200	H	21.27411300	-1.62288000	-15.32977300
H	22.42255400	-0.01492400	-4.87688900	H	20.16169400	-1.71082100	-14.23316000
H	25.03195500	1.33676300	-5.69512900	C	34.22903100	4.62592700	-6.61620900
H	25.01416100	-0.41197100	-5.74814100	C	33.56854900	3.37125400	-6.02230400
H	21.71145900	0.47435000	-6.70117600	C	32.21255600	3.00593300	-6.64240400
H	25.77021200	0.53138100	-8.10570200	C	31.86913800	1.52585800	-6.38986200
H	20.91588100	0.20050600	-9.00872100	N	30.48973300	1.14701900	-6.68816100
H	24.96889200	0.38857300	-10.42743300	C	30.00941300	0.93858700	-7.93729900
H	22.54258900	0.17863000	-10.90949600	N	30.68494400	1.38910500	-8.99180400
C	32.20595800	-3.28008800	-6.21799500	N	28.82189500	0.34648700	-8.07988300
C	30.88106600	-2.53175100	-5.96499500	H	34.57270700	4.42156000	-7.63781300
C	29.88630300	-2.76302500	-7.06586800	H	34.26093900	2.52751100	-6.14510100
C	30.06229300	-3.49344600	-8.21527900	H	33.43875000	3.49628500	-4.94021700
N	28.57397800	-2.28066900	-7.03477100	H	31.41652800	3.63785600	-6.23300100
C	28.00318900	-2.72424500	-8.16173700	H	32.24260900	3.22260100	-7.71792000
N	28.86337700	-3.45130900	-8.88983400	H	32.55724200	0.87822400	-6.94968700
H	32.78876900	-2.80276000	-7.00523000	H	32.02569800	1.30206300	-5.33146900
H	30.43748300	-2.85447200	-5.01432800	H	29.92994000	0.77015700	-5.93711600
H	31.06796300	-1.45476800	-5.84395500	H	31.55230900	1.87445300	-8.84585900
H	27.72491000	-2.95961300	-5.70201300	H	30.44703000	1.11003600	-9.97699700

H	28.58603300	-0.38532600	-7.39807300
H	28.50186800	0.10720200	-9.03370000
C	31.09196500	7.81099400	-10.77002400
C	30.08598800	7.04887100	-9.88787900
C	28.76867000	6.83023800	-10.57049400
C	27.58229200	7.47370300	-10.32118300
C	28.51981900	5.91862800	-11.66550600
C	27.15424700	6.06956300	-12.03583900
C	29.30918000	4.97755300	-12.35157200
N	26.60662900	7.02205200	-11.19684200
C	26.57630900	5.32910500	-13.07182100
C	28.74041200	4.23795500	-13.38209600
C	27.38937500	4.42031900	-13.74176900
H	31.14602500	7.33678500	-11.75643000
H	30.51626500	6.07408500	-9.62018700
H	29.93291100	7.58532200	-8.94422400
H	27.34931900	8.22449000	-9.57945800
H	25.65229600	7.33978900	-11.21793400
H	30.35170800	4.81936300	-12.09404600
H	25.53902200	5.47200200	-13.35464400
H	29.33856800	3.52903400	-13.94050900
H	26.99036900	3.84890600	-14.57320100
O	30.25513200	0.66846100	-11.51228200
H	30.43876900	1.42349500	-12.10503000
H	29.31863000	0.40039300	-11.56153800
N	16.95122700	-3.32633100	-12.65670900
C	16.59798200	-4.44999200	-11.75904500
C	15.33356700	-3.93569400	-11.05287300
C	14.68375900	-3.01953400	-12.10100800
C	15.88661900	-2.31389000	-12.73438600
H	17.41317800	-4.64173900	-11.05974000
H	14.68509800	-4.75148200	-10.72525100
H	15.61333300	-3.35244100	-10.16852700
H	14.16227300	-3.62000200	-12.85449800
H	13.96525100	-2.31570600	-11.67433000
H	15.73292400	-2.01237500	-13.77303100
H	16.18113800	-1.41802000	-12.17331800
C	29.55100800	-2.94399200	-1.16203500
C	28.26335700	-3.75358000	-1.34833600
C	28.02826400	-4.24398100	-2.77774000
C	27.84994200	-3.14419600	-3.81100900
O	28.03343100	-1.95476600	-3.61555300
O	27.50379400	-3.64595600	-5.00114500
H	29.53841000	-2.10850500	-1.86598200
H	28.25865400	-4.62186400	-0.67808100
H	27.41403500	-3.12694800	-1.05084000
H	28.87124900	-4.85668000	-3.12540400
H	27.15128700	-4.89924100	-2.83545300
H	30.46538400	-3.51015100	-1.36790800
H	29.56605100	-2.49726600	-0.16238700
C	34.86196500	8.00000800	-10.31597000
C	35.21485500	6.49740500	-10.32800400
C	34.95452800	5.87293100	-11.66026700
C	33.99933900	4.98930500	-12.10264600
N	35.67278100	6.21026600	-12.79837800
C	35.14412800	5.53378800	-13.85483400
N	34.13054600	4.78943000	-13.46209900
H	35.57009700	8.58822700	-10.90862000
H	36.25684300	6.33964500	-10.02062400
H	34.59547900	5.97425600	-9.59278500
H	36.44888300	6.85359800	-12.83525000
H	33.22728700	4.47930900	-11.54568300
H	35.52589400	5.61016600	-14.86215600
H	33.34367700	3.59984100	-14.23026500
H	34.87102100	8.38159500	-9.28968300
H	33.87105900	8.09548200	-10.77200900
Mg	26.76277300	-3.89142500	-12.19994400

Int-AMg (9.4 kcal/mol)

H	20.66699000	-6.80399800	-16.56500000
H	16.39000600	-5.37401100	-12.30898300
H	24.65800000	-6.75700500	-19.16500000
H	29.36500100	-8.34200500	-18.17999400
H	35.11212100	4.86988000	-6.01613000
H	32.10201300	7.76385100	-10.35105000
H	33.92499700	-0.03001000	-10.21099300
H	31.95004800	-4.27895700	-6.58614700
H	23.18500600	1.49700800	-4.32302200
H	22.41702500	4.62903800	-7.60400300
H	22.25399800	6.38997600	-15.14806100
H	33.53403100	5.46901900	-6.68109200
H	30.78102700	8.84800600	-10.93701100
H	23.93695900	6.31001800	-15.82103000
H	32.80798800	-0.12301500	-3.81400500
H	32.79714900	-3.33873500	-5.29807900
H	32.07465800	0.82262800	-17.96202800
H	30.43538700	-3.27780600	-15.73600400
H	31.70210100	-4.16470700	-14.93609200
H	30.41806600	-9.05985600	-14.20510600
H	20.88601500	-5.04999900	-16.84099800
H	34.15695900	-4.71599500	-10.10795500
H	23.72501000	-8.30800900	-7.05601400
H	21.59204000	-3.72900200	-7.32004900
H	27.89794800	0.15108100	-17.74212300
H	27.15884300	4.34404500	-6.69899000
C	29.55193700	-8.45618800	-13.91485300
C	29.02371700	-7.66163000	-15.09897100
O	28.70756300	-6.46713400	-15.06399300

C	29.81345700	-7.55646500	-12.70277000
C	28.49965400	-7.13183100	-12.01959700
C	28.75953000	-6.01563400	-11.00998300
O	29.46776800	-6.28595100	-10.02456400
O	28.25565900	-4.85464000	-11.24704500
H	28.77649800	-9.19232700	-13.65280000
H	30.44756000	-8.06681000	-11.97327900
H	30.35631400	-6.66564700	-13.03534100
H	27.76586300	-6.81330500	-12.75655500
H	28.09773800	-7.99672800	-11.47657600
N	28.95086700	-8.37322300	-16.24065400
C	28.68997800	-7.77099700	-17.53402000
C	27.22876900	-7.97996500	-17.93660300
O	26.76233100	-9.10807000	-18.03524800
H	29.12939700	-9.36545100	-16.21944300
H	28.99395200	-6.72395100	-17.49527700
N	26.51374600	-6.83625200	-18.10960600
C	25.05601700	-6.83998600	-18.14799800
C	24.49896000	-5.70578200	-17.29450100
H	26.96394400	-5.96455500	-17.86870400
H	24.73516200	-7.81524400	-17.77140300
H	23.40899500	-5.68126500	-17.35487400
H	24.77145700	-5.81838400	-16.24423700
H	24.86389700	-4.72971300	-17.63723700
C	23.25809000	6.03494500	-15.04087400
C	23.25610700	4.48969000	-15.01159300
C	22.38186000	3.86090700	-13.95498200
C	22.69663000	3.97927900	-12.59547200
C	21.25704600	3.09946000	-14.29845000
C	21.93500600	3.34669100	-11.61838800
C	20.47880400	2.46098200	-13.33389000
C	20.82204900	2.58206200	-11.98494700
O	20.05075000	1.93476600	-11.06327300
H	23.64605300	6.43875000	-14.09887800
H	22.93855400	4.12522300	-15.99595400
H	24.28818200	4.13712500	-14.88249700
H	23.57047200	4.54989600	-12.29162800
H	20.99328700	2.99030700	-15.34754400
H	22.21308800	3.42334400	-10.57425200
H	19.62112400	1.85528500	-13.60660200
H	20.48291000	2.00332700	-10.19960800
C	20.86198400	-5.83999400	-16.08300500
C	19.83763900	-5.62969200	-14.97781800
O	19.04149800	-6.50551800	-14.65267500
H	21.86209500	-5.86012100	-15.63665100
N	19.91883300	-4.42664100	-14.33064200
C	19.19503600	-4.19797700	-13.09497000
C	18.15163900	-3.09139100	-13.22220100
O	18.39836700	-2.01779900	-13.79914400
C	20.22461700	-3.87135600	-11.98667000
O	19.63776800	-3.64940300	-10.70877000
H	20.59786300	-3.71126200	-14.59129300
H	18.70509000	-5.14305100	-12.86159000
H	20.88111400	-4.74165400	-11.88646600
H	20.83589300	-3.01921700	-12.30422100
H	19.35796200	-2.72616400	-10.66659200
C	23.90599800	-7.35587100	-7.56603100
C	22.89812900	-6.30450100	-7.12680100
O	21.71848000	-6.60003700	-6.92730000
C	23.75132300	-7.58082400	-9.09954000
C	24.12600500	-6.39462500	-9.93475600
C	25.28540300	-6.09003900	-10.60805600
N	23.32159000	-5.27471400	-10.10407200
C	24.01351500	-4.35405400	-10.83027600
N	25.20674800	-4.82545000	-11.15989500
H	24.93551600	-7.05880500	-7.35050000
H	24.38647500	-8.41770500	-9.40384300
H	22.71371200	-7.87442700	-9.29498300
H	22.42160600	-5.12479600	-9.66805000
H	26.16649900	-6.69910200	-10.72255100
H	23.62993900	-3.38009700	-11.09215300
N	23.32462200	-5.00967500	-7.09663600
C	22.40696900	-3.96405800	-6.62794500
C	23.31436900	-2.76247300	-6.34652700
C	24.53188000	-2.99267400	-7.24964800
C	24.71359600	-4.51279200	-7.20756900
H	21.89935900	-4.31991500	-5.72459300
H	22.81388400	-1.81747800	-6.54560900
H	23.62891700	-2.76731700	-5.29759100
H	24.32304800	-2.65912200	-8.27141300
H	25.42261200	-2.46965000	-6.89906400
H	25.20473700	-4.89880900	-8.10158500
H	25.30900800	-4.80283500	-6.33245000
C	23.17494100	4.07095200	-8.16501500
C	24.47013000	3.93449800	-7.38410200
O	24.49210900	3.83148700	-6.15672600
H	22.78155000	3.06847700	-8.36169600
H	23.32002700	4.57821400	-9.12099800
N	25.60302700	3.91251800	-8.13678900
C	26.90921300	3.66696500	-7.52203100
C	27.87691100	3.80653800	-8.70191100
C	27.07240400	3.23823500	-9.87506500
C	25.66014800	3.77368600	-9.60855700
H	26.94219000	2.64725200	-7.11308000
H	28.09799900	4.86422500	-8.88017500
H	28.81999500	3.28469700	-8.53420500
H	27.45399900	3.54475500	-10.84831200
H	27.06535700	2.14686500	-9.84652500
H	25.51197700	4.74932300	-10.08961600

H	24.89310500	3.08457800	-9.97000500	H	27.12002800	1.50127300	-12.32417500
C	23.37401200	0.46299700	-4.62997000	O	26.43625500	-5.22268500	-13.77388500
C	24.31880100	0.47151300	-5.84295200	H	25.55576000	-5.09692400	-14.18981800
C	23.67496200	0.52293200	-7.21625000	H	27.12183100	-5.43324500	-14.42984900
C	22.29061600	0.53952800	-7.42560000	O	23.85980100	-4.46987100	-14.33287400
C	24.50573000	0.47753400	-8.34813000	H	23.35736100	-4.93820400	-13.65381800
C	21.75295500	0.44601600	-8.71481000	H	24.15010500	-3.63807100	-13.88524900
C	23.97614500	0.41364500	-9.63341800	O	21.10098300	-1.85832600	-14.34103200
C	22.59221100	0.37627400	-9.82713900	H	21.28460000	-1.63857300	-15.27008500
H	22.41501000	-0.01374600	-4.85183600	H	20.13815400	-1.71861400	-14.20469200
H	24.99572600	1.32807400	-5.75373000	C	34.22881200	4.62612600	-6.61576500
H	24.95612200	-0.42049800	-5.82360000	C	33.56754000	3.32874800	-6.13161800
H	21.61515700	0.59763900	-6.57985100	C	32.29939400	2.93665400	-6.91076400
H	25.58494400	0.46560600	-8.22777700	C	31.95743200	1.44213800	-6.72479800
H	20.67310100	0.38978100	-8.83703900	N	30.54958500	1.09848900	-6.91023000
H	24.64959000	0.38989800	-10.47729800	C	29.92843600	0.90455300	-8.09746400
H	22.18474400	0.28863600	-10.82794000	N	30.49289200	1.32370600	-9.22980200
C	32.20577300	-3.28035300	-6.21775400	N	28.72560800	0.33370900	-8.09424700
C	30.87853400	-2.53566800	-5.96394400	H	34.59742300	4.47214100	-7.63973400
C	29.89589200	-2.74423100	-7.08039900	H	34.30374800	2.51786100	-6.21329500
C	30.10323400	-3.40693200	-8.26464500	H	33.31613100	3.40133000	-5.06617500
N	28.56583900	-2.31645300	-7.03087800	H	31.44911200	3.54411700	-6.58125400
C	28.01334300	-2.72675600	-8.17858500	H	32.44692300	3.16405800	-7.97600400
N	28.90487600	-3.37821100	-8.94216600	H	32.57438400	0.81882500	-7.38403800
H	32.78929700	-2.80050600	-7.00292600	H	32.20300700	1.14633800	-5.70136200
H	30.42369000	-2.87904600	-5.02635200	H	30.03660400	0.77910300	-6.10185700
H	31.06513000	-1.46152500	-5.81679100	H	31.28877500	1.93782700	-9.18597300
H	27.74873200	-3.01570400	-5.70201500	H	30.06595300	1.16078100	-10.17314600
H	30.97374300	-3.90999300	-8.64974100	H	28.54959800	-0.39100000	-7.39032700
H	27.00672800	-2.53251000	-8.50729900	H	28.23834700	0.14721000	-8.98663600
H	28.69317600	-3.84804600	-9.83638400	C	31.09195300	7.81107100	-10.76997700
C	33.48008900	-4.18194800	-10.78309600	C	30.08120500	7.04051000	-9.90149800
C	33.36831700	-2.73930600	-10.31694500	C	28.77652500	6.80976200	-10.60472800
O	33.14601200	-2.39774500	-9.16052200	C	27.57906700	7.43678700	-10.36702100
C	32.15729100	-4.96105200	-10.77547300	C	28.55350100	5.90152500	-11.70850800
O	31.98894700	-5.56248900	-9.51558400	C	27.19042300	6.03614600	-12.09405200
H	33.91821100	-4.21228200	-11.78730200	C	29.36347000	4.97553100	-12.39156900
H	31.31695100	-4.29177700	-11.01384500	N	26.62041700	6.97772300	-11.25732700
H	32.19441000	-5.71741000	-11.57694200	C	26.63392000	5.29204100	-13.13907400
H	31.07680500	-5.92690600	-9.52018600	C	28.81668200	4.23501100	-13.43262300
N	33.54452300	-1.80525000	-11.30025500	C	27.46715500	4.39887100	-13.80552400
C	33.30499300	-0.40202700	-11.03299600	H	31.15154800	7.34229000	-11.75894400
H	33.57361100	-2.11125000	-12.26015800	H	30.51652600	6.06966700	-9.62751900
H	33.55507600	0.17604000	-11.92477500	H	29.90876500	7.57486900	-8.96004400
H	32.25616900	-0.20712200	-10.78087800	H	27.32729300	8.18009100	-9.62391500
C	30.70337000	-3.79247300	-14.83686200	H	25.66219100	7.28253000	-11.28779900
C	30.56240000	-2.85370100	-13.62973400	H	30.40473200	4.83071800	-12.12000200
C	29.18957900	-2.18336700	-13.58394100	H	25.59733300	5.42192000	-13.43189800
O	28.17394400	-2.94756700	-13.62453700	H	29.42817400	3.53481600	-13.98793300
O	29.12742000	-0.92537500	-13.53823600	H	27.08764800	3.82904000	-14.64704600
H	30.02282400	-4.63933300	-14.73511300	O	29.65937600	1.15489600	-11.78025000
H	30.66948800	-3.42872100	-12.70442200	H	30.34693700	1.67984300	-12.23662600
H	31.33151900	-2.07590000	-13.63347300	H	29.52387000	0.34630300	-12.31613100
C	27.87495800	1.06284000	-17.13691900	N	16.94949500	-3.32850700	-12.66026300
C	29.24872400	1.61608400	-16.81297600	C	16.59798200	-4.44999400	-11.75904200
O	29.41018300	2.73198400	-16.32241700	C	15.33360900	-3.93482700	-11.05380500
C	27.12121100	0.75955100	-15.82267000	C	14.68130800	-3.02402400	-12.10502700
C	25.73387500	0.24190900	-16.09142600	C	15.88231000	-2.31909200	-12.74280600
C	24.70625000	1.12867300	-16.43041100	H	17.41376900	-4.63880700	-11.06000100
C	25.44130700	-1.12647300	-16.04221400	H	14.68670900	-4.75024700	-10.72217500
C	23.42543000	0.66969600	-16.72583300	H	15.61363900	-3.34764300	-10.17214500
C	24.16388600	-1.60541100	-16.33468200	H	14.15994300	-3.62845400	-12.85542800
C	23.16563300	-0.69980900	-16.68936800	H	13.96217700	-2.31945700	-11.68060900
O	21.90600500	-1.20677400	-16.96450600	H	15.72737200	-2.02340100	-13.78293100
H	27.33263800	1.82445300	-17.70578900	H	16.17509400	-1.41960100	-12.18663600
H	27.69850300	0.03648400	-15.23823300	C	29.55108800	-2.94420200	-1.16180300
H	27.07725600	1.67464500	-15.22720100	C	28.26727700	-3.76305400	-1.33812400
H	24.90626500	2.19632000	-16.45182100	C	28.03628800	-4.27502500	-2.76034600
H	26.21616300	-1.82359000	-15.73377400	C	27.84747200	-3.18755100	-3.80492800
H	22.63122100	1.37250800	-16.96794500	O	27.98993600	-1.99267700	-3.61031900
H	23.92459800	-2.66073800	-16.25608300	O	27.54119000	-3.70610500	-4.99871300
H	21.34830500	-0.48974900	-17.29489100	H	29.53189300	-2.11149500	-1.86880400
N	30.27096800	0.76211000	-17.07194300	H	28.26770100	-4.62154400	-0.65528400
C	31.68351800	1.10951500	-16.97993400	H	27.41444700	-3.13677700	-1.05047400
C	32.38413300	0.35668000	-15.84645500	H	28.88335600	-4.88608000	-3.10036700
C	31.84264900	0.74033200	-14.46942700	H	27.16378100	-4.93731100	-2.80895200
C	32.26524700	2.09925300	-13.95121700	H	30.46537700	-3.51011500	-1.36803900
O	33.15506600	2.71436000	-14.70020100	H	29.56598300	-2.49711300	-0.16245500
O	31.84182500	2.55234600	-12.88354100	C	34.86214800	7.99988800	-10.31617100
H	30.04109400	-0.13942700	-17.46093700	C	35.22577700	6.50064800	-10.32532100
H	31.75441000	2.18953400	-16.85009100	C	35.00860200	5.87385600	-11.66401200
H	32.23490700	-0.72078700	-15.99178700	C	34.09593800	4.95539700	-12.12379100
H	33.46027000	0.54658600	-15.89885700	N	35.73968700	6.23355800	-12.78729300
H	30.75160200	0.67185800	-14.44612500	C	35.25929500	5.53600900	-13.85283700
H	32.17412800	0.01944900	-13.71396500	N	34.26499400	4.75646500	-13.47932000
C	26.87518300	-1.03000800	-11.08997000	H	35.56869300	8.59205500	-10.90718000
O	26.98737400	-2.27556200	-10.95244800	H	36.26093800	6.35209700	-9.99092000
O	27.14942400	-0.14356000	-10.26162100	H	34.59272700	5.97007400	-9.60726500
C	26.33355300	-0.53199400	-12.49504400	H	36.49260100	6.90451000	-12.80959200
C	25.13144000	-1.31587100	-12.90648400	H	33.32982600	4.41794100	-11.58496700
O	25.20088800	-2.57764000	-12.99745500	H	35.65897300	5.62474300	-14.85214500
C	23.91106700	-0.61300800	-13.18103600	H	33.49823400	3.56726000	-14.24614100
C	23.89957900	0.75323700	-13.19989600	H	34.87088400	8.38158600	-9.28967800
C	25.06783800	1.54641400	-12.91564600	H	33.87099200	8.09565600	-10.77183000
C	26.22280900	0.94080300	-12.56386700	Mg	26.87594800	-3.80079300	-12.30284000
H	27.19124000	-0.83259700	-13.13224700				
H	23.02058700	-1.18132500	-13.43179100				
H	22.97572300	1.26288200	-13.44783400				
H	25.00353100	2.62551500	-12.97461600				

TS2-A_{Mg} (15.8 kcal/mol)

H	20.66699100	-6.80399800	-16.56500000
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H	16.39000400	-5.37400900	-12.30898500	N	23.32288900	-5.00614000	-7.10672900
H	24.65800000	-6.75700600	-19.16500000	C	22.40694500	-3.96405500	-6.62793800
H	29.36499900	-8.34200700	-18.17999400	C	23.31287500	-2.76092300	-6.35631200
H	35.11211300	4.86985600	-6.01610800	C	24.50870000	-2.97926500	-7.29030600
H	32.10201300	7.76385400	-10.35104800	C	24.70340400	-4.49915100	-7.25989500
H	33.92499600	-0.03000800	-10.21099700	H	21.90517300	-4.32239300	-5.72294000
H	31.95004300	-4.27895500	-6.58614800	H	22.80414900	-1.81633800	-6.53604500
H	23.18503300	1.49701000	-4.32301200	H	23.65300800	-2.77360900	-5.31537300
H	22.41700800	4.62904500	-7.60403400	H	24.27266100	-2.64255500	-8.30525200
H	22.25399600	6.38997200	-15.14805300	H	25.40098400	-2.44881200	-6.95521000
H	33.53404900	5.46903500	-6.68108300	H	25.16855300	-4.87939500	-8.17066000
H	30.78102900	8.84800600	-10.93701400	H	25.32766800	-4.78787600	-6.40448000
H	23.93695300	6.31000100	-15.82104100	C	23.17501400	4.07090900	-8.16503000
H	23.80795700	-0.12305000	-3.81401300	C	24.46929700	3.93234500	-7.38329700
H	32.79714600	-3.33874400	-5.29807800	O	24.49228500	3.82517700	-6.15626100
H	32.07466400	0.82262900	-17.96202600	H	22.78118400	3.06975800	-8.36604700
H	30.43538200	-3.27781000	-15.73600500	H	23.32246600	4.58127400	-9.11881600
H	31.70211300	-4.16467800	-14.93607800	N	25.60250700	3.91393300	-8.13599000
H	30.41806800	-9.05985800	-14.20509600	C	26.90925100	3.66688600	-7.52199100
H	20.88601500	-5.05000000	-16.84099900	C	27.87537300	3.79697800	-8.70485800
H	34.15695700	-4.71599300	-10.10795100	C	27.06390800	3.22804700	-9.87327900
H	23.72500700	-8.30801600	-7.05602800	C	25.65862300	3.77935300	-9.60815300
H	21.59205100	-3.72899900	-7.32006100	H	26.93925000	2.64857500	-7.10908800
H	27.89794000	0.15107800	-17.74211900	H	28.09988700	4.85260300	-8.89046900
H	27.15884100	4.34406100	-6.69900200	H	28.81734200	3.27230000	-8.53911200
C	29.55192400	-8.45615300	-13.91485100	H	27.44691900	3.51530500	-10.85122800
C	29.03322900	-7.65926800	-15.10182800	H	27.04331700	2.13765400	-9.83119900
O	28.73968600	-6.45928700	-15.07111600	H	25.52565900	4.75816400	-10.08643000
C	29.79766000	-7.55876800	-12.69645500	H	24.88372400	3.10219000	-9.97417100
C	28.47241200	-7.12767800	-12.03983100	C	23.37400900	0.46304100	-4.62999800
C	28.69567500	-6.02574200	-11.00527100	C	24.31257000	0.47105100	-5.84647700
O	29.46404200	-6.26848400	-10.05752400	C	23.66081800	0.53572000	-7.21570500
O	28.08024900	-4.90623200	-11.16483100	C	22.27623700	0.54789100	-7.42004700
H	28.77441900	-9.19390700	-13.66313300	C	24.48790300	0.50969500	-8.35085900
H	30.41512000	-8.07329200	-11.95588700	C	21.73614400	0.47164300	-8.70968800
H	30.35138000	-6.67070900	-13.01768800	C	23.95760500	0.45766900	-9.63680400
H	27.75625000	-6.80074800	-12.79023200	C	22.57226800	0.41931100	-9.82455300
H	28.04816600	-7.99541000	-11.51701900	H	22.41401500	-0.01319600	-4.84885800
N	28.94227300	-8.37504800	-16.23986400	H	24.99640900	1.32196200	-5.75616500
C	28.68998000	-7.77099700	-17.53402000	H	24.94254300	-0.42651400	-5.83498300
C	27.23045600	-7.97773700	-17.94307700	H	21.60282600	0.59240200	-6.57184800
O	26.76665800	-9.10628300	-18.05175200	H	25.56625600	0.50774000	-8.22272800
H	29.09815300	-9.37108100	-16.21615000	H	20.65619000	0.41802200	-8.83142700
H	28.99601100	-6.72484800	-17.49112700	H	24.61722700	0.44476900	-10.49360700
N	26.51386400	-6.83430900	-18.10824400	H	22.16452600	0.34574900	-10.82594900
C	25.05601700	-6.83998500	-18.14799800	C	32.20578900	-3.28034500	-6.21774900
C	24.49575400	-5.71173700	-17.29207000	C	30.88525900	-2.52290600	-5.97811300
H	26.96231300	-5.96321100	-17.86194400	C	29.89664100	-2.74011200	-7.08866400
H	24.73711700	-7.81717200	-17.77445400	C	30.07615600	-3.44121600	-8.25653700
H	23.40638000	-5.68424200	-17.35945500	N	28.57291700	-2.29615800	-7.02940900
H	24.75999900	-5.83292600	-16.24189500	C	27.99458500	-2.74364200	-8.14897900
H	24.86382500	-4.73271000	-17.62229000	N	28.86376300	-3.42760700	-8.91103900
C	23.25807600	6.03493500	-15.04084600	H	32.79587800	-2.80865900	-7.00344500
C	23.25118400	4.49007200	-14.99622500	H	30.42455300	-2.84719400	-5.03667500
C	22.36480300	3.87829400	-13.93918500	H	31.08134300	-1.44928600	-5.84835500
C	22.67021000	4.01106300	-12.57914300	H	27.73933700	-3.00454400	-5.69380800
C	21.23571600	3.12317400	-14.28068000	H	30.93493000	-3.96352000	-8.64435000
C	21.89521700	3.39863300	-11.59994600	H	26.96811200	-2.58765300	-8.43163200
C	20.44497100	2.50325400	-13.31425100	H	28.62585300	-3.93546400	-9.78135100
C	20.78051900	2.63676600	-11.96487400	C	33.48009300	-4.18194300	-10.78309800
O	20.00050700	2.00286000	-11.03934900	C	33.37143600	-2.73871800	-10.31582900
H	23.64539500	6.44518700	-14.10102000	O	33.15197800	-2.39790700	-9.15864500
H	22.93920700	4.11666600	-15.97880500	C	32.15396300	-4.95685400	-10.77955000
H	24.27887000	4.13117400	-14.85348400	O	31.98561300	-5.57178700	-9.52491800
H	23.54697000	4.57766100	-12.27628000	H	33.92000100	-4.21150900	-11.78643500
H	20.97832200	3.00342100	-15.33012100	H	31.31288400	-4.28436900	-11.00771900
H	22.16618300	3.48564500	-10.55483400	H	32.18667000	-5.70602200	-11.58734400
H	19.58460700	1.90089900	-13.58604200	H	31.08041200	-5.95120700	-9.54419100
H	20.43178700	2.07540900	-10.17590700	N	33.55347300	-1.80466200	-11.29912800
C	20.86198600	-5.83999400	-16.08300500	C	33.30499600	-0.40202500	-11.03299900
C	19.84674200	-5.63756200	-14.96768500	H	33.54601100	-2.11252400	-12.25908900
O	19.08372700	-6.53282700	-14.61564100	H	33.55330700	0.17669600	-11.92505500
H	21.86514100	-5.86595000	-15.64364900	C	32.25368300	-0.21609600	-10.78456600
N	19.90240800	-4.42265600	-14.34210600	C	30.70332100	-3.79246800	-14.83683200
C	19.19503900	-4.19797700	-13.09497400	C	30.69985000	-2.83937000	-13.63933300
C	18.15227600	-3.08863400	-13.21345100	C	29.34157200	-2.42167400	-13.07758200
O	18.39776900	-2.01120800	-13.78269100	O	28.32909600	-3.11328500	-13.41833800
C	20.24114800	-3.87510600	-12.00246800	O	29.31948800	-1.44998500	-12.28282100
O	19.67786200	-3.68541200	-10.70754500	H	30.01354300	-4.62240300	-14.68616900
H	20.55266400	-3.68710300	-14.62738100	H	31.21723200	-3.30737200	-12.79378700
H	18.70899700	-5.14375100	-12.85681100	H	31.26600600	-1.92793400	-13.85636000
H	20.91078200	-4.73799600	-11.93261000	C	27.87496000	1.06283700	-17.13692000
H	20.83448200	-3.00887000	-12.31608300	C	29.24617900	1.58702900	-16.76667900
H	19.40038200	-2.76332000	-10.63648200	O	29.40989100	2.65299300	-16.17568400
C	23.90602700	-7.35581500	-7.56603400	C	27.07267500	0.76350400	-15.85369900
C	22.91011600	-6.30616800	-7.09752500	C	25.66333700	0.32353000	-16.14755200
O	21.74364800	-6.60996700	-6.84249900	C	24.68066800	1.27009600	-16.45254500
C	23.69230700	-7.58132300	-9.09360100	C	25.30112800	-1.02824200	-16.13151700
C	24.04916700	-6.40968800	-9.95664900	C	23.37347800	0.88460200	-16.73693400
C	25.19515900	-6.13325400	-10.66256300	C	23.99741800	-1.43494200	-16.40808400
N	23.24793500	-5.28889700	-10.14224300	C	23.04084900	-0.46916000	-16.71479900
C	23.92807500	-4.39737800	-10.91570100	O	21.74884900	-0.90387100	-16.95842500
N	25.11197000	-4.88651700	-11.25050900	H	27.36258000	1.83645900	-17.71778500
H	24.94340600	-7.06479000	-7.38289100	H	27.59059400	-0.01302400	-15.28211700
H	24.30493200	-8.42815300	-9.41643200	H	27.06777300	1.65731800	-15.22683100
H	22.64498400	-7.86517400	-9.24670900	H	24.93473600	2.32619300	-16.45062300
H	22.34984700	-5.12451500	-9.70747500	H	26.03834300	-1.77391500	-15.84830700
H	26.07158700	-6.74912100	-10.77534100	H	22.61376800	1.63274500	-16.95165200
H	23.55021300	-3.42849400	-11.20541000	H	23.70836200	-2.47794200	-16.33106800

H	21.19686600	-0.13826200	-17.16625600
N	30.27052400	0.76321900	-17.10152800
C	31.68350600	1.10951300	-16.97993200
C	32.34735600	0.35626200	-15.82385800
C	31.76404200	0.75093300	-14.46339900
C	32.21888700	2.08754800	-13.91155500
O	33.08124800	2.72392800	-14.67183300
O	31.83407000	2.49930700	-12.81362600
H	30.04461400	-0.08813900	-17.59243100
H	31.75824600	2.18906500	-16.84753200
H	32.19756000	-0.72055000	-15.97061700
H	33.42542800	0.54126300	-15.83758300
H	30.66963100	0.75956900	-14.49145500
H	32.02192200	0.01116700	-13.69865700
C	26.82372500	-1.19040300	-10.79719400
O	26.69043000	-2.38741100	-10.81528000
O	27.10746600	-0.22702000	-10.15014500
C	26.35351000	-0.52317200	-12.75945100
C	25.19331700	-1.32202900	-13.02232500
O	25.28156800	-2.61688400	-13.11541500
C	23.93906700	-0.65125100	-13.15126800
C	23.88115200	0.72521700	-13.10462800
C	25.03714100	1.51642600	-12.87085800
C	26.25275300	0.89551200	-12.71401900
H	27.32929900	-0.96087300	-12.94503300
H	23.04715200	-1.23241900	-13.36511300
H	22.92550200	1.21567100	-13.24991200
H	24.95748000	2.59553100	-12.82696700
H	27.15872400	1.46555300	-12.53027300
O	26.39947000	-5.27875000	-13.87294900
H	25.53452000	-5.08319400	-14.30367300
H	27.09960600	-5.46453400	-14.52072300
O	23.91879200	-4.33922500	-14.49723800
H	23.30708200	-4.74845400	-13.87235000
H	24.27799400	-3.54584600	-14.00298600
O	21.08110700	-1.88094500	-14.38757300
H	21.25729700	-1.56101200	-15.28849800
H	20.12745800	-1.71890800	-14.21962400
C	34.22877200	4.62612400	-6.61580400
C	33.58648800	3.35012800	-6.05870400
C	32.28742000	2.93307800	-6.75991300
C	31.98367100	1.44105600	-6.52324900
N	30.59366800	1.05600100	-6.73762600
C	29.99727900	0.92377700	-7.93992000
N	30.58843800	1.35015400	-9.05024900
N	28.76463900	0.40134400	-7.97273400
H	34.58306000	4.44110100	-7.63843000
H	34.31845900	2.53556200	-6.14362300
H	33.38759400	3.46416300	-4.98586600
H	31.44581400	3.53592700	-6.40113300
H	32.37831200	3.14476300	-7.83364600
H	32.63667600	0.81220500	-7.14210700
H	32.20851200	1.19135900	-5.48321100
H	30.05440900	0.74451300	-5.94344200
H	31.44996700	1.86446900	-8.98329100
H	30.17969400	1.20135900	-10.01616400
H	28.56525700	-0.37506200	-7.32850000
H	28.33971900	0.26105300	-8.88608600
C	31.09195300	7.81107400	-10.76997800
C	30.08362000	7.05196500	-9.88819700
C	28.77315200	6.82379600	-10.58021000
C	27.58168000	7.46458000	-10.34880700
C	28.53996900	5.90155600	-11.66941200
C	27.17737000	6.04130900	-12.05389300
C	29.34095900	4.95728500	-12.33728200
N	26.61745600	7.00077100	-11.23063500
C	26.61133400	5.28216500	-13.08272700
C	28.78467300	4.20201200	-13.36233700
C	27.43498500	4.36939900	-13.73370100
H	31.14514700	7.33621000	-11.75607300
H	30.51512900	6.08052400	-9.61032500
H	29.92222600	7.59499900	-8.94971800
H	27.33782900	8.22118900	-9.61655400
H	25.66077600	7.31048100	-11.26172000
H	30.38138600	4.80854300	-12.06437500
H	25.57384500	5.41080300	-13.37243200
H	29.38834100	3.48575500	-13.90509400
H	27.04374900	3.78173400	-14.55705400
O	29.72441200	1.09478000	-11.54702800
H	30.39866100	1.56910800	-12.07257700
H	29.66806000	0.16766500	-11.87801600
N	16.94820300	-3.32816200	-12.65670300
C	16.59798600	-4.44999200	-11.75904000
C	15.33386500	-3.93730600	-11.05099800
C	14.68108900	-3.02334500	-12.09924400
C	15.88215300	-2.31756700	-12.73607600
H	17.41418800	-4.64122100	-11.06075200
H	14.68719900	-4.75370400	-10.72125900
H	15.61431600	-3.35250500	-10.16786100
H	14.15873900	-3.62554500	-12.85077200
H	13.96267200	-2.31948600	-11.67239400
H	15.72672700	-2.01914700	-13.77536200
H	16.17613400	-1.41962100	-12.17805100
C	29.55108800	-2.94419100	-1.16181100
C	28.26630100	-3.76079300	-1.33850900
C	28.03382200	-4.27029600	-2.76121700
C	27.85789400	-3.18186400	-3.80571100
O	28.02659900	-1.98912900	-3.61898200
O	27.53172500	-3.69630600	-4.99685900

H	29.53334800	-2.11094900	-1.86800100
H	28.26542100	-4.62046100	-0.65731000
H	27.41444600	-3.13393700	-1.04911600
H	28.87683900	-4.88795900	-3.09968300
H	27.15614800	-4.92526500	-2.81245600
H	30.46537500	-3.51011900	-1.36803700
H	29.56598300	-2.49711900	-0.16245200
C	34.86214100	7.99988500	-10.31617100
C	35.22429900	6.50006100	-10.32013600
C	34.99163200	5.86455200	-11.65186900
C	34.07609200	4.93995100	-12.09298800
N	35.70498000	6.22080700	-12.78751900
C	35.21219600	5.51603700	-13.84223800
N	34.22655300	4.73463700	-13.44963800
H	35.56972000	8.59020500	-10.90758200
H	36.26273200	6.35249100	-9.99566200
H	34.59821800	5.97471300	-9.59221300
H	36.45456200	6.89487800	-12.82444400
H	33.31987600	4.40259000	-11.54029000
H	35.59646600	5.60103200	-14.84785800
H	33.44573700	3.56487900	-14.20582000
H	34.87088700	8.38158600	-9.28967800
H	33.87099300	8.09565400	-10.77183300
Mg	26.77755100	-3.88239200	-12.37536800

E:P-A_{Mg}(0.8 kcal/mol)

H	20.66696200	-6.80399600	-16.56499300
H	16.39001100	-5.37402200	-12.30896600
H	24.65800100	-6.75700400	-19.16500000
H	29.36500000	-8.34200500	-18.17999500
H	35.11205800	4.86988300	-6.01603900
H	32.10201300	7.76386000	-10.35104600
H	33.92499700	-0.03000700	-10.21099800
H	31.95004000	-4.27895000	-6.58615800
H	23.18504000	1.49701100	-4.32301100
H	22.41700800	4.62904400	-7.60403400
H	22.25399600	6.38997200	-15.14805200
H	33.53406000	5.46904900	-6.68101800
H	30.78102800	8.84800600	-10.93701400
H	23.93695100	6.31000100	-15.82104200
H	23.80795800	-0.12305200	-3.81401500
H	32.79715300	-3.33874400	-5.29808200
H	32.07469200	0.82265900	-17.96202400
H	30.43537700	-3.27779200	-15.73599300
H	31.70211600	-4.16466600	-14.93609300
H	30.41806500	-9.05986400	-14.20509200
H	20.88600900	-5.05001100	-16.84101100
H	34.15695600	-4.71599800	-10.10795400
H	23.72497700	-8.30802000	-7.05604600
H	21.59205700	-3.72900800	-7.32007100
H	27.89793400	0.15108100	-17.74212300
H	27.15884000	4.34406200	-6.69900200
C	29.55192400	-8.45614000	-13.91485300
C	29.03594000	-7.65705700	-15.10151700
O	28.74874900	-6.45579500	-15.06883300
C	29.79907000	-7.56100300	-12.69444200
C	28.47449200	-7.12813800	-12.03791900
C	28.69684000	-6.04606700	-10.98228200
O	29.46083700	-6.29870500	-10.03600400
O	28.07627600	-4.92394600	-11.12647800
H	28.77364700	-9.19348000	-13.66464700
H	30.41390400	-8.07900200	-11.95405100
H	30.35494300	-6.67347200	-13.01331200
H	27.76590900	-6.78653200	-12.78968700
H	28.03770800	-8.00004500	-11.53314900
N	28.94185200	-8.37322900	-16.23902600
C	28.68997800	-7.77100000	-17.53402200
C	27.22990900	-7.97694800	-17.94105600
O	26.76503900	-9.10557500	-18.04415700
H	29.08781800	-9.37076200	-16.21346500
H	28.99641900	-6.72489300	-17.49195000
N	26.51380200	-6.83353900	-18.10986500
C	25.05601700	-6.83998800	-18.14799700
C	24.49490800	-5.72603000	-17.27061900
H	26.96363000	-5.96041200	-17.87358400
H	24.74208800	-7.82210000	-17.78285000
H	23.40606700	-5.69225500	-17.34868000
H	24.75641100	-5.88125500	-16.22233500
H	24.87124200	-4.74072900	-17.56794100
C	23.25807700	6.03493500	-15.04084500
C	23.25635800	4.49075800	-15.00950700
C	22.39033900	3.85627600	-13.95014800
C	22.71577000	3.97024400	-12.59356800
C	21.27096100	3.08525900	-14.28781500
C	21.96893900	3.32476600	-11.61452400
C	20.50996200	2.42987900	-13.32138600
C	20.86594700	2.54534800	-11.97594600
O	20.11441100	1.87956100	-11.04878400
H	23.64548400	6.44169100	-14.09953400
H	22.93457300	4.12887300	-15.99258400
H	24.28653100	4.13330400	-14.88489100
H	23.58939200	4.54346900	-12.29510700
H	20.99961300	2.98044700	-15.33533400
H	22.25656900	3.39459700	-10.57272200
H	19.65716400	1.81486700	-13.58930200
H	20.55823900	1.95079200	-10.19184700
C	20.86203000	-5.83996500	-16.08300000
C	19.86793600	-5.66151600	-14.94143400

O	19.22846900	-6.61161700	-14.49938500	H	33.54003900	0.18329400	-11.92417200
H	21.86699600	-5.88917400	-15.64657000	H	32.25386000	-0.24347800	-10.77679500
N	19.80880200	-4.40774600	-14.39931700	C	30.70332400	-3.79250400	-14.83681700
C	19.19502400	-4.19800500	-13.09497100	C	30.71107300	-2.83431700	-13.64055200
C	18.18282300	-3.06121000	-13.14520600	C	29.38117300	-2.59524500	-12.92685900
O	18.46795500	-1.95728400	-13.63914200	O	28.36588400	-3.21682600	-13.36675500
C	20.31908600	-3.93132200	-12.06882700	O	29.39680100	-1.83334500	-11.92478100
O	19.84877400	-3.81453300	-10.72701700	H	30.01430900	-4.62149100	-14.68074700
H	20.40507000	-3.64874500	-14.73871500	H	31.38420100	-3.20545000	-12.85988500
H	18.70798600	-5.13966700	-12.84492200	H	31.11420800	-1.85645400	-13.92183800
H	20.98896000	-4.79619100	-12.09546100	C	27.87497500	1.06283400	-17.13691400
H	20.89282000	-3.04918100	-12.37394300	C	29.24829800	1.57447900	-16.75549200
H	19.61561000	-2.89037400	-10.57295900	O	29.41881900	2.63532400	-16.15689200
C	23.90606600	-7.35579000	-7.56602500	C	27.04832100	0.80097700	-15.85956000
C	22.91543800	-6.30797500	-7.08304000	C	25.61676000	0.45451100	-16.16530900
O	21.75808500	-6.61794400	-6.79662300	C	24.70890200	1.45824000	-16.51644900
C	23.66122300	-7.59095500	-9.08626000	C	25.15690200	-0.86355800	-16.10168400
C	24.05026200	-6.43566000	-9.95190700	C	23.37413100	1.16242100	-16.78052900
C	25.23749000	-6.16660300	-10.58551500	C	23.82796200	-1.18042400	-16.36583200
N	23.26715000	-5.31070600	-10.18339600	C	22.94021500	-0.15938700	-16.69167300
C	23.99388000	-4.42520100	-10.91772600	O	21.61324800	-0.50833700	-16.89050600
N	25.19529700	-4.92024200	-11.17719600	H	27.38519700	1.84130800	-17.73124500
H	24.94746100	-7.06868700	-7.40195600	H	27.50758600	-0.00650200	-15.28039000
H	24.24248600	-8.45995200	-9.40868200	H	27.09168800	1.69029200	-15.22750500
H	22.60378800	-7.84271100	-9.22297900	H	25.04251200	2.49113300	-16.56113800
H	22.33838300	-5.14342600	-9.81841000	H	25.83022100	-1.65548600	-15.78850600
H	26.11655000	-6.78705600	-10.63752200	H	22.67302800	1.95449700	-17.03193600
H	23.64717800	-3.45804900	-11.24758500	H	23.48242900	-2.19984700	-16.24796900
N	23.32002400	-5.00628300	-7.11240400	H	21.09227000	0.29770800	-17.00128000
C	22.40693600	-3.96405600	-6.62791900	N	30.27339600	0.75071100	-17.09255500
C	23.31890400	-2.76317500	-6.36255200	C	31.68346200	1.10947300	-16.97993400
C	24.49705400	-2.97801600	-7.32042300	C	32.37152900	0.34757000	-15.84483200
C	24.69629700	-4.49641400	-7.28719700	C	31.77480700	0.68604800	-14.47886700
H	21.90916800	-4.32193900	-5.72080600	C	32.14268900	2.04159700	-13.91075000
H	22.80951000	-1.81638000	-6.52614700	O	33.01416100	2.70920800	-14.63179000
H	23.67731600	-2.78524800	-5.32770800	O	31.68649700	2.43144600	-12.83331700
H	24.23356300	-2.64688600	-8.33039100	H	30.04899400	-0.09211900	-17.59866600
H	25.39659400	-2.44335700	-7.01087400	H	31.75170200	2.18825700	-16.84104200
H	25.15099900	-4.88004400	-8.20131800	H	32.25739700	-0.72938300	-16.02020600
H	25.33289300	-4.77923700	-6.43850900	H	33.44275400	0.56890500	-15.85299100
C	23.17501400	4.07091000	-8.16503000	H	30.68208600	0.62447000	-14.50783500
C	24.47130800	3.93728300	-7.38552400	C	32.09111400	-0.04391300	-13.72628600
O	24.49781500	3.83706300	-6.15814300	C	26.51151100	-0.43293800	-12.41557200
H	22.78418500	3.06675500	-8.35858400	C	25.38057300	-1.22574900	-12.70373400
H	23.31804300	4.57522900	-9.12259400	O	25.43077300	-2.56212500	-12.67587200
N	25.60507100	3.91413200	-8.13913400	C	24.17459900	-0.56864700	-13.03489100
C	26.90925200	3.66688500	-7.52199100	C	24.11575100	0.82075200	-13.09861800
C	27.87944100	3.79304600	-8.70091100	C	25.24565200	1.59902000	-12.82725000
C	27.07071300	3.21752500	-9.86619900	C	26.44089200	0.95903000	-12.48801100
C	25.66368300	3.76844200	-9.61042600	H	27.44455700	-0.92051700	-12.15612400
H	26.93526800	2.64928100	-7.10492200	H	23.29716600	-1.15885500	-13.28496500
H	28.10228100	4.84790200	-8.89220500	H	23.18311000	1.29717700	-13.37678300
H	28.82203600	3.27165700	-8.52712500	H	25.20006100	2.68037400	-12.88346000
H	27.45358800	3.49498500	-10.84704200	H	27.33879400	1.53545800	-12.28892600
H	27.04923300	2.12571200	-9.80812700	O	26.36342600	-5.27864800	-13.94561500
H	25.53374200	4.74316800	-10.09711800	H	25.56181800	-4.91273300	-14.39870000
H	24.89342600	3.08692600	-9.97697000	H	27.08912800	-5.44200200	-14.57169700
C	23.37400300	0.46303800	-4.63000300	O	24.24865600	-3.82155900	-14.60857200
C	24.35491400	0.47309000	-5.81678300	H	23.32129300	-3.96709300	-14.38486100
C	23.76405600	0.51720600	-7.21291500	H	24.60416700	-3.21971600	-13.87629400
C	22.39031800	0.50672900	-7.47471900	O	21.12289500	-1.94531400	-14.49170900
C	24.63906500	0.48151200	-8.31247000	H	21.24921800	-1.44713500	-15.31806400
C	21.90835400	0.40088100	-8.78512600	H	20.21671900	-1.72548600	-14.18618300
C	24.16876200	0.39806600	-9.62040200	C	34.22881400	4.62608000	-6.61595400
C	22.79122200	0.34152200	-9.86259400	C	33.55832900	3.35814400	-6.06335900
H	22.42114700	-0.01498600	-4.87153400	C	32.23558700	2.99293300	-6.75760400
H	25.02698200	1.33088700	-5.70441700	C	31.91088900	1.49619700	-6.59668000
H	24.99294400	-0.41830500	-5.77177700	N	30.55974300	1.10819700	-7.00443300
H	21.68165500	0.55326700	-6.65549400	C	30.16357600	0.99060000	-8.28658800
H	25.71150000	0.49906500	-8.12945500	N	30.88837800	1.47602400	-9.28683600
H	20.83588000	0.32366200	-8.95145400	N	28.97628800	0.42117500	-8.55127500
H	24.86242100	0.35480100	-10.45111000	H	34.58153800	4.43808400	-7.63842400
H	22.43141600	0.24910200	-10.88031500	H	34.26399700	2.52296400	-6.16714600
C	32.20578600	-3.28034500	-6.21773200	H	33.37709900	3.46596000	-4.98719100
C	30.89934200	-2.48367800	-6.01572300	H	31.40907600	3.58836600	-6.35445200
C	29.92356200	-2.67449500	-7.14714500	H	32.30561600	3.26157900	-7.81940500
C	30.07507500	-3.46309900	-8.26217000	H	32.64402700	0.88730400	-7.14232400
N	28.63809600	-2.12069400	-7.15716500	H	32.00149100	1.22079400	-5.54313700
C	28.05473600	-2.59823800	-8.26680600	H	29.95952000	0.67518000	-6.31616200
N	28.88683100	-3.39792300	-8.95300900	H	31.74998800	1.96127600	-9.11468200
H	32.81307000	-2.82724300	-7.00237500	H	30.56730500	1.24298500	-10.25813300
H	30.40933100	-2.78408000	-5.08139800	H	28.67611300	-0.33823900	-7.92781500
H	31.12701000	-1.41539500	-5.88908300	H	28.75294000	0.30182500	-9.53409000
H	27.77286300	-2.82485900	-5.73993300	C	31.09195400	7.81107100	-10.76997800
H	30.90230100	-4.06517100	-8.60158700	C	30.08589000	7.05356400	-9.88361300
H	27.04988700	-2.37038000	-8.59284000	C	28.77407400	6.82571400	-10.57249000
H	28.64699400	-3.93264700	-9.80709600	C	27.58170700	7.46400500	-10.33790300
C	33.48009300	-4.18193700	-10.78309300	C	28.54379400	5.91243500	-11.66959500
C	33.37307600	-2.73638700	-10.32161000	C	27.18284400	6.05650100	-12.05758600
O	33.12965500	-2.39291500	-9.17000200	C	29.34707000	4.97456800	-12.34398300
C	32.14181900	-4.93740600	-10.77906100	N	26.61992900	7.00707100	-11.22581600
O	31.99102200	-5.59310600	-9.54082700	C	26.62171600	5.31171300	-13.09950900
H	33.91997200	-4.21627300	-11.78637000	C	28.79520300	4.23313700	-13.38154600
H	31.30980300	-4.24149900	-10.96734100	C	27.44798300	4.40763100	-13.75834600
H	32.14583600	-5.66121200	-11.60979700	H	31.14313400	7.33458500	-11.75522900
H	31.09302700	-5.98772100	-9.56406600	H	30.51848700	6.08233600	-9.60583100
N	33.57541300	-1.80182100	-11.30149800	H	29.92792200	7.59807700	-8.94539000
C	33.30499500	-0.40202700	-11.03299900	H	27.33619100	8.21523600	-9.60067500
H	33.58943000	-2.10831800	-12.26177500	H	25.66374000	7.31826300	-11.25869300

H	30.38558400	4.82031000	-12.06696400
H	25.58496200	5.44142000	-13.39087800
H	29.40007900	3.52234600	-13.93012700
H	27.05922200	3.82644300	-14.58700400
O	29.77200700	0.76422800	-11.57138100
H	30.26755700	1.29275600	-12.22498500
H	29.76860800	-0.19686500	-11.82393100
N	16.95970700	-3.31531600	-12.63669600
C	16.59798600	-4.44996900	-11.75906300
C	15.33377100	-3.94147100	-11.04549900
C	14.69993800	-2.98808400	-12.06989500
C	15.91539800	-2.28000000	-12.67459300
H	17.41026200	-4.65381500	-11.05832700
H	14.67460300	-4.75907400	-10.74479800
H	15.61382700	-3.38632300	-10.14345000
H	14.17560100	-3.55967100	-12.84364800
H	13.98780900	-2.28821900	-11.62631700
H	15.76864300	-1.93511200	-13.70070400
H	16.22607600	-1.41283200	-12.07827900
C	29.55108500	-2.94420300	-1.16181700
C	28.25978400	-3.73471000	-1.39346100
C	28.05434600	-4.18659100	-2.84250500
C	27.90364700	-3.06183800	-3.85379200
O	28.07842900	-1.87752400	-3.63011700
O	27.58793600	-3.53731000	-5.06720300
H	29.55856200	-2.09931000	-1.85594000
H	28.22970700	-4.62102400	-0.74823800
H	27.40989000	-3.10722200	-1.10014000
H	28.90092600	-4.79672200	-3.18577000
H	27.17493600	-4.83439600	-2.93549400
H	30.46537900	-3.51011600	-1.36802900
H	29.56598400	-2.49711300	-0.16245500
C	34.86212300	7.99988500	-10.31615300
C	35.21670200	6.49794800	-10.31552700
C	34.94281000	5.85662200	-11.63597700
C	33.99793300	4.94868200	-12.04901800
N	35.62982700	6.19760200	-12.79192800
C	35.09421100	5.50063000	-13.83073000
N	34.10550800	4.73882200	-13.40853200
H	35.57172300	8.58599900	-10.90895600
H	36.26210000	6.34567200	-10.01703900
H	34.60590500	5.98256900	-9.56778900
H	36.38933500	6.85886500	-12.85160600
H	33.24755600	4.42948700	-11.47146000
H	35.45155100	5.57553200	-14.84700200
H	33.33525600	3.56141800	-14.15545300
H	34.87090100	8.38159200	-9.28968000
H	33.87099800	8.09564800	-10.77184600
Mg	26.79797600	-3.98448800	-12.39027700

The transition states and intermediates involved in the reaction pathway with **Mode-A** for the Mn-enzyme of SDC.

E:S-A_{Mn} (0.0 kcal/mol)

H	20.66700100	-6.80399900	-16.56500200
H	16.38999700	-5.37400500	-12.30899000
H	24.65788400	-6.75700200	-19.16495600
H	29.36490400	-8.34212700	-18.17998900
H	35.11198300	4.87000600	-6.01597800
H	32.10200100	7.76400800	-10.35100300
H	33.92499300	-0.03000300	-10.21099400
H	31.95001600	-4.27901000	-6.58598400
H	23.18497500	1.49700000	-4.32301400
H	22.41699500	4.62899700	-7.60400300
H	22.25399900	6.39001100	-15.14796100
H	33.53400500	5.46900600	-6.68098300
H	30.78100600	8.84799900	-10.93701800
H	23.93692700	6.31001000	-15.82106000
H	23.80799800	-0.12300700	-3.81400400
H	32.79699400	-3.33901300	-5.29799700
H	32.07500100	0.82299300	-17.96199700
H	30.43503100	-3.27798500	-15.73600100
H	31.70201000	-4.16496500	-14.93603400
H	30.41797600	-9.06002500	-14.20502200
H	20.88600700	-5.04999900	-16.84099900
H	34.15702300	-4.71602400	-10.10804100
H	23.72503500	-8.30800300	-7.05599300
H	21.59199900	-3.72899900	-7.32000000
H	27.89800000	0.15100300	-17.74200400
H	27.15898500	4.34400000	-6.69899600
C	29.55210200	-8.45608100	-13.91504200
C	29.04259600	-7.66205700	-15.10718900
O	28.76832400	-6.45499800	-15.08229300
C	29.81579400	-7.53701100	-12.71517100
C	28.50794200	-6.99684200	-12.09893600
C	28.81176600	-5.88288100	-11.09415000
O	29.41627200	-6.19730700	-10.05579900
O	28.46307400	-4.67880700	-11.40566300
H	28.77162800	-9.18488900	-13.64936300
H	30.37887400	-8.06588000	-11.94185300
H	30.43442700	-6.69632300	-13.04628100

H	27.83999300	-6.63026800	-12.87607000
H	28.01343300	-7.81893900	-11.56774500
N	28.94291300	-8.37692700	-16.24066000
C	28.68992200	-7.77067700	-17.53380400
C	27.22819600	-7.97726700	-17.93397900
O	26.76304000	-9.10718800	-18.02293500
H	29.08045300	-9.37587900	-16.21600200
H	28.99732900	-6.72527900	-17.49008000
N	26.51341200	-6.83514900	-18.10759400
C	25.05622400	-6.84006300	-18.14811200
C	24.49020700	-5.70965200	-17.29554600
H	26.96444700	-5.95860700	-17.88632700
H	24.73742500	-7.81727300	-17.77495800
H	23.40185600	-5.67912800	-17.38020200
H	24.73857600	-5.82877700	-16.24015500
H	24.86609200	-4.73176300	-17.61929300
C	23.25808900	6.03498200	-15.04099300
C	23.21518500	4.49381000	-14.98757800
C	22.29352200	3.92862900	-13.93386400
C	22.59162200	4.06142500	-12.57238900
C	21.14284800	3.20850500	-14.27951100
C	21.79920200	3.46817600	-11.59627700
C	20.33356300	2.60908800	-13.31534600
C	20.67243700	2.72773000	-11.96561700
O	19.88325300	2.10066300	-11.04154700
H	23.64407100	6.44515900	-14.10142300
H	22.90187800	4.11821300	-15.96911000
H	24.22955900	4.10510100	-14.83062600
H	23.48186100	4.60383200	-12.26560800
H	20.88884200	3.09068000	-15.33015800
H	22.06926700	3.54876300	-10.54996500
H	19.45903100	2.02928000	-13.59069900
H	20.31264200	2.17287400	-10.17740000
C	20.86198800	-5.84000100	-16.08300000
C	19.84885400	-5.64590400	-14.96290100
O	19.09668200	-6.54949300	-14.60684900
H	21.86456600	-5.86367400	-15.64099100
N	19.89990100	-4.43199800	-14.34112700
C	19.19499400	-4.19800800	-13.09499700
C	18.14096200	-3.10043600	-13.23534900
O	18.37478100	-2.03692800	-13.83403500
C	20.24003400	-3.83040700	-12.01633100
O	19.67490600	-3.62256400	-10.72545400
H	20.53873100	-3.69063700	-14.64006000
H	18.72300900	-5.14503100	-12.83485900
H	20.92891800	-4.67719200	-11.93117000
H	20.81455100	-2.95989300	-12.35328800
H	19.39403500	-2.70055500	-10.66958200
C	23.90595300	-7.35598500	-7.56603000
C	22.89474500	-6.30561600	-7.13319500
O	21.71836700	-6.60514100	-6.92357200
C	23.76312400	-7.60380700	-9.05276000
C	24.16296400	-6.44036300	-9.94754800
C	25.33892000	-6.15732300	-10.60125600
N	23.36486300	-5.32538600	-10.16816200
C	24.06674500	-4.42886800	-10.91047900
N	25.26914700	-4.91207600	-11.19651200
H	24.93423800	-7.05711200	-7.34660400
H	24.38886100	-8.45562000	-9.37714700
H	22.72388800	-7.88660800	-9.29765800
H	22.45051600	-5.16584300	-9.76605300
H	26.22717200	-6.76471900	-10.66145300
H	23.70513600	-3.46362600	-11.23067900
N	23.31956600	-5.01015500	-7.10897500
C	22.40700500	-3.96400600	-6.62800400
C	23.31765500	-2.75963800	-6.36461100
C	24.52271600	-2.99416900	-7.28446500
C	24.70685100	-4.51325900	-7.23227600
H	21.90802400	-4.31789800	-5.71953600
H	22.81340900	-1.81599900	-6.56311700
H	23.64703200	-2.75740000	-5.32020600
H	24.29655200	-2.66993600	-8.30576500
H	25.41867300	-2.46759800	-6.95157800
H	25.19317400	-4.90582400	-8.12604900
H	25.30863300	-4.79555800	-6.35856800
C	23.17500200	4.07100700	-8.16499800
C	24.46830700	3.93151100	-7.38226000
O	24.49107400	3.82511700	-6.15512800
H	22.78050400	3.07144500	-8.37003500
H	23.32432500	4.58226800	-9.11821500
N	25.60193900	3.91209600	-8.13479400
C	26.90901200	3.66700400	-7.52200200
C	27.87724100	3.80279400	-8.70130200
C	27.06813200	3.24366200	-9.87360400
C	25.65736900	3.77797100	-9.60703000
H	26.94019600	2.64841400	-7.10824500
H	28.10546300	4.85853900	-8.88028900
H	28.81673600	3.27304100	-8.53806600
H	27.45904400	3.54222300	-10.84455400
H	27.06380900	2.15070700	-9.83415500
H	25.51479300	4.75473700	-10.08517700
H	24.88847900	3.09433700	-9.97406800
C	23.37404100	0.46300200	-6.62998900
C	24.29743600	0.47064400	-5.85838900
C	23.62272100	0.55063900	-7.21704900
C	22.23480500	0.60042000	-7.39376200
C	24.42413800	0.51033500	-8.37104800
C	21.66529100	0.55274900	-8.67250100
C	23.86517600	0.48326700	-9.64607600

C	22.47538400	0.48735400	-9.80521200	H	21.22723800	-1.64071900	-15.44436900
H	22.41188600	-0.01273700	-4.84198800	H	20.09526600	-1.72249800	-14.35686200
H	24.98757500	1.31703800	-5.77233200	C	34.22900000	4.62598100	-6.61604600
H	24.92158600	-0.43075100	-5.86101400	C	33.57478700	3.34346600	-6.07743200
H	21.58079900	0.65797000	-6.53140800	C	32.27623100	2.93765200	-6.79751100
H	25.50618800	0.48384000	-8.26191700	C	32.02663200	1.41934600	-6.68902200
H	20.58164000	0.53509700	-8.77089900	N	30.67233600	0.98099700	-7.02705200
H	24.50309500	0.44252700	-10.51788900	C	30.16750800	0.94159300	-8.28044500
H	22.04916200	0.43620600	-10.80077200	N	30.83444700	1.48526200	-9.29808800
C	32.20597300	-3.27997700	-6.21802900	N	28.96651800	0.39057200	-8.47848100
C	30.88839900	-2.52052700	-5.96073000	H	34.58608500	4.44796000	-7.63920100
C	29.93172400	-2.64047900	-7.11301300	H	34.30537300	2.52828700	-6.16808600
C	30.16732500	-3.23805800	-8.32616500	H	33.37035900	3.44430600	-5.00477400
N	28.59844800	-2.22117700	-7.06798800	H	31.41715800	3.47527900	-6.38211300
C	28.06837500	-2.58425100	-8.24211600	H	32.34486500	3.24754400	-7.84793800
N	28.98323400	-3.18635700	-9.02351000	H	32.75870700	0.86957900	-7.29647100
H	32.79495800	-2.80195900	-7.00081100	H	32.18988500	1.10883700	-5.65401800
H	30.39958200	-2.90690100	-5.05841000	H	30.18274600	0.42204500	-6.34237600
H	31.10401700	-1.46469300	-5.73779800	H	31.67513600	1.99842100	-9.09817400
H	27.78243800	-2.93530400	-5.72461100	H	30.34318100	1.69866700	-10.21155000
H	31.04921100	-3.71729200	-8.71277300	H	28.64634900	-0.29359000	-7.79218800
H	27.05925700	-2.39821200	-8.57175800	H	28.65916800	0.20778300	-9.44512900
H	28.80415800	-3.61351300	-9.94170600	C	31.09198400	7.81100500	-10.76996600
C	33.47998600	-4.18197100	-10.78294600	C	30.08316800	7.04355900	-9.89825000
C	33.38954300	-2.73543500	-10.32007500	C	28.75388600	6.85375500	-10.56718700
O	33.18782000	-2.39414200	-9.15953400	C	27.55802600	7.42852900	-10.21623200
C	32.14998400	-4.94780700	-10.76681100	C	28.48754600	6.02259700	-11.72150000
O	31.94988500	-5.49317700	-9.48620600	C	27.09970900	6.14010500	-12.01257300
H	33.91326900	-4.22172400	-11.78921200	C	29.27723400	5.17739800	-12.52007200
H	31.31772200	-4.28533800	-11.04896400	N	26.55953100	7.00872600	-11.08158800
H	32.19875000	-5.73897700	-11.53415500	C	26.49467800	5.43684200	-13.05836600
H	31.02521700	-5.82201900	-9.48356900	C	28.68528800	4.48660100	-13.57017100
N	33.56691800	-1.80273100	-11.30363200	C	27.30715200	4.61429700	-13.83316500
C	33.30500400	-0.40200400	-11.03301200	H	31.14953300	7.34374500	-11.75951600
H	33.55319300	-2.10989800	-12.26329400	H	30.50447900	6.05764400	-9.65636600
H	33.54348200	0.18050500	-11.92576400	H	29.94497100	7.56006300	-8.94108800
C	32.25567100	-0.23437400	-10.77146100	H	27.33260100	8.10673300	-9.40542600
C	30.70396500	-3.79207100	-14.83698100	H	25.59175200	7.27788200	-11.02670300
C	30.90152300	-2.83421800	-13.66072600	H	30.33487600	5.04234100	-12.31708700
C	29.70564900	-2.16408500	-13.04396500	H	25.43478600	5.53526100	-13.26401500
O	28.55013800	-2.32436400	-13.43424300	H	29.27831900	3.83782300	-14.20383900
O	30.07516600	-1.39645600	-12.03508700	H	26.87902700	4.06248000	-14.66430900
H	30.00124800	-4.59641100	-14.62751100	O	29.58197300	2.12628000	-11.52734800
H	31.38893300	-3.36282600	-12.83614100	H	30.24174300	2.25947500	-12.23511100
H	31.60193100	-2.03663200	-13.93881000	H	28.98143200	1.38426300	-11.73850500
C	27.87499900	1.06299600	-17.13699400	N	16.94298400	-3.33289000	-12.66299000
C	29.24572500	1.60019000	-16.78921700	C	16.59800200	-4.44999900	-11.75901300
O	29.41489800	2.68640300	-16.23835200	C	15.33390900	-3.93676600	-11.05199000
C	27.08305500	0.75033100	-15.84165100	C	14.67374200	-3.03676700	-12.10785700
C	25.70067000	0.24096100	-16.15790600	C	15.86921100	-2.33203900	-12.75703700
C	24.71415800	1.12903300	-16.59846600	H	17.41579200	-4.63683600	-11.06151800
C	25.37459000	-1.11621100	-16.05020500	H	14.69203800	-4.75276900	-10.71192600
C	23.43941900	0.68175500	-16.93410600	H	15.61471900	-3.34170500	-10.17585800
C	24.10278400	-1.58285900	-16.38079300	H	14.15144400	-3.64956700	-12.85085400
C	23.14394300	-0.67675900	-16.82897700	H	13.95340700	-2.33172500	-11.68618400
O	21.88351000	-1.16957000	-17.12875700	H	15.71019700	-2.05094500	-13.80063100
H	27.34528300	1.83045600	-17.70936700	H	16.15707400	-1.42326700	-12.21362900
H	27.62486000	0.00356300	-15.25051500	C	29.55096500	-2.94393800	-1.16209300
H	27.02836900	1.65523900	-15.23012600	C	28.26430900	-3.75214500	-1.36188800
H	24.93809700	2.19048000	-16.66276600	C	28.04622300	-4.24199800	-2.79516100
H	26.10818400	-1.81760700	-15.66164600	C	27.87409500	-3.13902400	-3.82726000
H	22.67554300	1.38687300	-17.25557300	O	28.01286600	-1.94754900	-3.61360900
H	23.83702300	-2.62560800	-16.24405600	O	27.58678200	-3.64030700	-5.03449900
H	21.34419900	-0.44659600	-17.47593300	H	29.54260000	-2.10593600	-1.86370400
N	30.26972500	0.76098100	-17.09237800	H	28.25132700	-4.62099400	-0.69249900
C	31.68300200	1.10900900	-16.98000800	H	27.41226100	-3.12468800	-1.07490500
C	32.34248600	0.38056700	-15.80664200	H	28.89315000	-4.85393400	-3.13396100
C	31.77210500	0.85922400	-14.46726700	H	27.17032300	-4.89819300	-2.86212400
C	32.27707500	2.20884000	-13.99237200	H	30.46538600	-3.51016200	-1.36787600
O	33.26484400	2.70379000	-14.70608900	H	29.56609200	-2.49730800	-0.16236900
O	31.82026500	2.75652400	-12.98779600	C	34.86198600	8.00000300	-10.31599400
H	30.04252300	-0.10195700	-17.56207200	C	35.22559200	6.50077500	-10.31822900
H	31.75335600	2.19119300	-16.86210200	C	35.06217600	5.86926500	-11.66264900
H	32.16248100	-0.69668200	-15.91128800	C	34.14874000	4.97379100	-12.16423900
H	33.42424200	0.53740500	-15.83168300	N	35.87490500	6.18274200	-12.74297600
H	30.68013000	0.91722500	-14.50723200	C	35.44016900	5.48090600	-13.82491000
H	31.99392000	0.15415700	-13.65872600	N	34.39751700	4.74204100	-13.50275000
C	27.11899000	-0.83485500	-11.43572400	H	35.57007200	8.58959100	-10.90753600
O	27.08183400	-2.01115900	-10.96664800	H	36.24806800	6.35206300	-9.94678100
O	28.11603500	-0.05739500	-11.14796000	H	34.56762300	5.96985400	-9.62304900
C	26.03543000	-0.31336100	-12.27461200	H	36.65139400	6.82657700	-12.72803400
C	24.99769000	-1.15997900	-12.77889800	H	33.32820100	4.47642200	-11.66885700
O	25.09514200	-2.47334500	-12.82018200	H	35.90620000	5.53660300	-14.79749100
C	23.82434000	-0.52988000	-13.26526500	H	33.63750600	3.55992700	-14.27435800
C	23.74503600	0.84634500	-13.38001800	H	34.87100500	8.38158900	-9.28967900
C	24.83395800	1.66447300	-13.03018200	H	33.87105300	8.09549500	-10.77199200
C	25.95672600	1.08034300	-12.47694600	Mn	26.82895500	-3.61734200	-12.29098600
H	29.28421500	-0.91227400	-11.60333700				
H	22.99714200	-1.15354100	-13.58792900				
H	22.83724600	1.29141700	-13.76872000				
H	24.78991100	2.73739700	-13.15539000				
H	26.78421900	1.69535500	-12.14846100				
O	26.74351900	-4.59547100	-14.23826600				
H	25.79668600	-4.74508600	-14.46994400				
H	27.33613500	-5.28516800	-14.58252100				
O	24.08770000	-4.31774200	-14.38081100				
H	23.63618000	-4.87236600	-13.73222300				
H	24.31378400	-3.48707900	-13.86499100				
O	21.04615200	-1.89536500	-14.52400200				

TS1-A_{Mn} (19.6 kcal/mol)

H	20.66700000	-6.80400000	-16.56500000
H	16.38999500	-5.37400400	-12.30899000
H	24.65788200	-6.75698200	-19.16495400
H	29.36495500	-8.34205800	-18.17999700
H	35.11193700	4.87004700	-6.01592800
H	32.10200200	7.76400700	-10.35100500
H	33.92497300	-0.02996500	-10.21099600
H	31.95001500	-4.27902200	-6.58595000

H	23.18500500	1.49700000	-4.32299500	H	23.65929100	-2.79601100	-5.30361100
H	22.41700000	4.62900600	-7.60400500	H	24.27261800	-2.64024600	-8.29440100
H	22.25402000	6.39005000	-15.14802800	H	25.40815300	-2.45301700	-6.95088800
H	33.53401600	5.46901900	-6.68093100	H	25.17113800	-4.87802800	-8.16689300
H	30.78101200	8.84800200	-10.93701100	H	25.32926900	-4.79128600	-6.40096000
H	23.93691500	6.31003400	-15.82106200	C	23.17500000	4.07099400	-8.16499800
H	23.80798700	-0.12301100	-3.81400100	C	24.47134200	3.93482200	-7.38585500
H	32.79699100	-3.33900700	-5.29799500	O	24.49334600	3.82498900	-6.15890400
H	32.07502700	0.82301700	-17.96199300	H	22.78244100	3.06674400	-8.35657500
H	30.43530200	-3.27793800	-15.73605500	H	23.31605600	4.57484700	-9.12309500
H	31.70204300	-4.16487700	-14.93603800	N	25.60441600	3.91775000	-8.13809800
H	30.41799600	-9.05999500	-14.20502600	C	26.90901300	3.66700900	-7.52200400
H	20.88600300	-5.05000400	-16.84100400	C	27.88027300	3.79859300	-8.70015100
H	34.15687200	-4.71594600	-10.10782800	C	27.07197200	3.24091800	-9.87473900
H	23.72486300	-8.30799000	-7.05602900	C	25.66609400	3.79095400	-9.61090100
H	21.59201300	-3.72896500	-7.32000500	H	26.93617400	2.64855600	-7.10970900
H	27.89799800	0.15100200	-17.74200300	H	28.11186100	4.85404400	-8.87842100
H	27.15898400	4.34399700	-6.69899300	H	28.81747400	3.26615500	-8.53507100
C	29.55202100	-8.45606200	-13.91501800	H	27.46430100	3.53737200	-10.84605700
C	29.04057700	-7.65154800	-15.09906200	H	27.06249400	2.14846300	-9.83959200
O	28.76788700	-6.44741100	-15.06479000	H	25.53526000	4.77250600	-10.08456800
C	29.81980800	-7.57355000	-12.69410700	H	24.89185600	3.11635800	-9.98326500
C	28.51294000	-7.16337300	-11.99015500	C	23.37402700	0.46299100	-4.63002900
C	28.80353900	-6.07538300	-10.96171000	C	24.36895100	0.47111000	-5.80834500
O	29.47853700	-6.38159500	-9.96410200	C	23.80661900	0.50776300	-7.21704000
O	28.37371500	-4.88412100	-11.21267400	C	22.43978300	0.44737400	-7.50924400
H	28.77225800	-9.19102000	-13.66363700	C	24.70553400	0.51679400	-8.29814600
H	30.46278500	-8.09246400	-11.97830400	C	21.98779500	0.33294800	-8.82907000
H	30.35418900	-6.67485800	-13.01933200	C	24.26081100	0.43504200	-9.61519000
H	27.77765400	-6.81955700	-12.71518000	C	22.89344400	0.32395700	-9.89017500
H	28.10974300	-8.03926900	-11.46693200	H	22.42236400	-0.01478600	-4.87672000
N	28.93647800	-8.36929800	-16.23613800	H	25.03785800	1.33026600	-5.69039300
C	28.68988300	-7.77078900	-17.53380900	H	25.00864800	-0.41842400	-5.75040900
C	27.23057700	-7.97761600	-17.94357600	H	21.71336800	0.45841900	-6.70430500
O	26.76628700	-9.10623200	-18.04946800	H	25.77324900	0.57084000	-8.10113900
H	29.06928700	-9.36862000	-16.20706800	H	20.92344200	0.21113100	-9.01767100
H	28.99563500	-6.72443300	-17.49315800	H	24.97620100	0.45327600	-10.42717200
N	26.51391800	-6.83447100	-18.11096300	H	22.55321400	0.23048500	-10.91499900
C	25.05622900	-6.84007300	-18.14810600	C	32.20597100	-3.27997400	-6.21806600
C	24.49836700	-5.71075400	-17.28978900	C	30.88209600	-2.53675400	-5.94718200
H	26.96319200	-5.96213300	-17.87062900	C	29.89976000	-2.72510000	-7.06560500
H	24.73783700	-7.81703400	-17.77373100	C	30.10736900	-3.39704700	-8.24415800
H	23.40868300	-5.68336300	-17.35481100	N	28.57611100	-2.27689500	-7.02932200
H	24.76894700	-5.83306200	-16.24055700	C	28.02793600	-2.68587000	-8.17986000
H	24.86583300	-4.73217000	-17.62177200	N	28.91650500	-3.35630800	-8.93046200
C	23.25807700	6.03489500	-15.04091200	H	32.78523800	-2.79584100	-7.00355200
C	23.26265600	4.48998300	-15.02710800	H	30.43088000	-2.89460300	-5.01331600
C	22.41520800	3.83897500	-13.96345500	H	31.07639200	-1.46738600	-5.78106400
C	22.75865800	3.93954300	-12.60980300	H	27.72904700	-2.95653200	-5.70886600
C	21.30010400	3.05948700	-14.29740300	H	30.97494600	-3.90964400	-8.62388000
C	22.03336800	3.27107600	-11.62951400	H	27.02511700	-2.48279000	-8.51558600
C	20.55992900	2.38304300	-13.32920400	H	28.71807600	-3.82453000	-9.82739300
C	20.93200500	2.48589900	-11.98677700	C	33.48018300	-4.18199700	-10.78331300
O	20.19790400	1.80269600	-11.06020000	C	33.36713100	-2.73970200	-10.31880300
H	23.64639500	6.43364600	-14.09711600	O	33.14107800	-2.39816400	-9.16351800
H	22.93026400	4.13541500	-16.01020100	C	32.15621400	-4.96062100	-10.77474500
H	24.29883500	4.14179700	-14.92094000	O	31.97680800	-5.53637400	-9.50498100
H	23.62948800	4.51945900	-12.31568200	H	33.91736100	-4.21465500	-11.78809100
H	21.01777100	2.96245500	-15.34281200	H	31.31770900	-4.29604100	-11.03682600
H	22.33311400	3.33257600	-10.59056200	H	32.20299200	-5.73303900	-11.56028600
H	19.71120100	1.76140100	-13.59416900	H	31.06901600	-5.91469900	-9.50555000
H	20.64413900	1.87405400	-10.20420600	N	33.54127800	-1.80524600	-11.30219600
C	20.86199300	-5.83999100	-16.08299300	C	33.30503500	-0.40207400	-11.03296700
C	19.84684100	-5.63835600	-14.96756000	H	33.60040900	-2.10966600	-12.26093800
O	19.08753800	-6.53513300	-14.61294500	H	33.54727300	0.17856300	-11.92488200
H	21.86536900	-5.87117200	-15.64385500	H	32.25930000	-0.20871700	-10.76630700
N	19.89854600	-4.42134500	-14.34472500	C	30.70360900	-3.79221800	-14.83681100
C	19.19499200	-4.19801400	-13.09500000	C	30.46830000	-2.80375000	-13.68268100
C	18.16031700	-3.08310300	-13.20488300	C	29.02575400	-2.29996100	-13.69862800
O	18.41862000	-2.00240400	-13.76199500	O	28.10214900	-3.13657800	-13.83791000
C	20.24655300	-3.88486700	-12.00437200	O	28.82160900	-1.03759500	-13.55698000
O	19.68808700	-3.68861200	-10.70888700	H	30.02754700	-4.64216800	-14.73461700
H	20.54776500	-3.68609700	-14.63101800	H	30.60084800	-3.29536500	-12.71204400
H	18.70592200	-5.14275800	-12.85934600	H	31.14772100	-1.94943700	-13.71909400
H	20.90796200	-4.75435500	-11.93452000	C	27.87501200	1.06299800	-17.13699200
H	20.84781100	-3.02463300	-12.32007700	C	29.24634600	1.59157300	-16.77128000
H	19.40899100	-2.76655500	-10.64240000	O	29.40949800	2.67306900	-16.20966000
C	23.90619900	-7.35594100	-7.56600500	C	27.05990300	0.77945900	-15.86370000
C	22.90877100	-6.30442800	-7.10556400	C	25.67673900	0.28372100	-16.18609400
O	21.73783600	-6.60740000	-6.86801800	C	24.67328600	1.18500000	-16.55368900
C	23.67378600	-7.61238200	-9.08366900	C	25.35928100	-1.07827800	-16.12589000
C	24.03801100	-6.44878400	-9.94515700	C	23.38405700	0.74719400	-16.84732400
C	25.20811800	-6.16007100	-10.60231900	C	24.07523800	-1.53655000	-16.41550700
N	23.24600100	-5.32155200	-10.12347300	C	23.09443800	-0.61467100	-16.77789400
C	23.95286300	-4.40896500	-10.84361700	O	21.82009000	-1.10054200	-17.02251100
N	25.14447800	-4.89674400	-11.14971100	H	27.37141700	1.83346200	-17.73070000
H	24.94540100	-7.06527700	-7.39631900	H	27.59524100	0.04008100	-15.26411400
H	24.27839100	-8.46743000	-9.39954900	H	27.01089800	1.69133800	-15.26514900
H	22.62277500	-7.88868700	-9.22194200	H	24.89396000	2.24830400	-16.58692900
H	22.33654000	-5.16673000	-9.70878400	H	26.11282800	-1.78732500	-15.79236000
H	26.08720300	-6.77548400	-10.70513900	H	22.60577300	1.46180900	-17.10638300
H	23.58953600	-3.43217400	-11.12365800	H	23.81621100	-2.58407300	-16.30480300
N	23.32414600	-5.00676500	-7.10407300	H	21.25883200	-0.36933900	-17.31325100
C	22.40696400	-3.96407100	-6.62799300	N	30.27069700	0.76061300	-17.08829500
C	23.31847500	-2.76771600	-6.34408400	C	31.68296000	1.10897700	-16.98000900
C	24.51262500	-2.98046600	-7.28158800	C	32.36866200	0.33964600	-15.84813700
C	24.70560800	-4.50008700	-7.25568300	C	31.82006300	0.71060100	-14.46936600
H	21.90175700	-4.32521500	-5.72578700	C	32.24987100	2.06234800	-13.93649600
H	22.81409800	-1.81924500	-6.51070600	O	33.13730600	2.68445600	-14.68212800

O	31.83503700	2.49850000	-12.86064900
H	30.04310800	-0.10527200	-17.55213600
H	31.75831900	2.18721900	-16.84011400
H	32.21573100	-0.73498900	-16.00962900
H	33.44625300	0.52457400	-15.88533000
H	30.72689700	0.65928500	-14.44619500
H	32.15125800	-0.01661400	-13.71938300
C	27.20848600	-1.01478600	-11.23218200
O	27.11401500	-2.23903300	-10.94342500
O	27.89460700	-0.16854100	-10.60422500
C	26.45712900	-0.49157100	-12.47235800
C	25.26868700	-1.24413500	-12.89698300
O	25.23660000	-2.52699300	-12.93838400
C	24.09445700	-0.51464100	-13.26585000
C	24.09667500	0.85402900	-13.31680000
C	25.26181400	1.60738400	-12.99715400
C	26.37699900	0.95855700	-12.55617200
H	27.56383900	-0.80351900	-13.20799700
H	23.20399600	-1.07884700	-13.52579200
H	23.19213900	1.37112700	-13.61131400
H	25.25050700	2.68817800	-13.06525400
H	27.24646600	1.52635300	-12.24970400
O	26.31902000	-5.45305500	-13.81614800
H	25.47827900	-5.13560600	-14.22168500
H	27.02659000	-5.49552300	-14.48116700
O	23.94394800	-4.25368600	-14.45404600
H	23.23963400	-4.61459000	-13.90113800
H	24.27811900	-3.46849200	-13.94325700
O	21.13084600	-1.89053800	-14.38962700
H	21.29396200	-1.61724900	-15.30858900
H	20.18307500	-1.70866900	-14.21201400
C	34.22903400	4.62591900	-6.61615800
C	33.58244800	3.36590800	-6.01925600
C	32.23794400	2.97163600	-6.64637900
C	31.95149900	1.47185000	-6.43949700
N	30.57799000	1.05732900	-6.71295100
C	30.04927300	0.93570300	-7.95277500
N	30.71145200	1.40944200	-9.00818100
N	28.84361100	0.38039200	-8.08967300
H	34.57313100	4.42222100	-7.63784300
H	34.29087200	2.53430600	-6.13378900
H	33.44471300	3.49378900	-4.93863000
H	31.42000300	3.55978000	-6.21621500
H	32.25951700	3.22505700	-7.71379600
H	32.64758900	0.86853400	-7.03805900
H	32.14227800	1.21806000	-5.39369100
H	30.07086400	0.59365800	-5.97300800
H	31.54459400	1.94833300	-8.85048800
H	30.25963000	1.50207200	-9.95606500
H	28.58663700	-0.33571600	-7.40310700
C	28.52181700	0.14069500	-9.04376000
C	31.09198200	7.81100600	-10.76997100
C	30.07986600	7.04627000	-9.89691600
C	28.77211600	6.82648700	-10.59753900
C	27.57503300	7.45128100	-10.35270100
C	28.55100200	5.93703800	-11.71637600
C	27.19031500	6.08101100	-12.10599900
C	29.36369300	5.02334700	-12.41049500
N	26.61822500	7.00808500	-11.25375400
C	26.63994800	5.35971400	-13.17008700
C	28.82360800	4.30615300	-13.47014600
C	27.47793800	4.48028100	-13.84976500
H	31.14882700	7.33993900	-11.75770400
H	30.50929100	6.07199400	-9.62581400
H	29.91497400	7.58169100	-8.95466700
H	27.32196900	8.18343300	-9.59900200
H	25.66147600	7.31741400	-11.28443300
H	30.39921200	4.86404400	-12.12633300
H	25.60515200	5.49506100	-13.46639600
H	29.43459500	3.60989900	-14.03045100
H	27.10339600	3.92352500	-14.70237300
O	29.62151000	1.72682200	-11.40287200
H	30.31476200	1.82730600	-12.08363300
H	29.11909800	0.89867900	-11.51940500
N	16.95297400	-3.32451500	-12.65435600
C	16.59800600	-4.44999800	-11.75901400
C	15.33365900	-3.93598300	-11.05216900
C	14.68674000	-3.01390700	-12.09686500
C	15.89183400	-2.30800900	-12.72541900
H	17.41271300	-4.64297900	-11.05935500
H	14.68317600	-4.75185200	-10.72873300
H	15.61353200	-3.35705400	-10.16504200
H	14.16493400	-3.60985000	-12.85373000
H	13.96921600	-2.31055600	-11.66774600
H	15.73928200	-1.99912600	-13.76207200
H	16.18906000	-1.41681900	-12.15832300
C	29.55095600	-2.94392500	-1.16211700
C	28.26245400	-3.75115000	-1.35229400
C	28.02958400	-4.24085300	-2.78262800
C	27.85917900	-3.14159900	-3.81809600
O	28.05895700	-1.95407600	-3.62629400
O	27.50232500	-3.64117900	-5.00586600
H	29.54037900	-2.10784300	-1.86535500
H	28.25408300	-4.61985800	-0.68260000
H	27.41355700	-3.12308700	-1.05651800
H	28.87150000	-4.85702600	-3.12705800
H	27.15052700	-4.89302100	-2.84242900
H	30.46538800	-3.51016300	-1.36786100
H	29.56609700	-2.49731900	-0.16236400

C	34.86197400	8.00000400	-10.31598700
C	35.21949600	6.49855300	-10.32041800
C	34.99222800	5.86203700	-11.65328500
C	34.08232700	4.93333100	-12.09855300
N	35.71385300	6.21534000	-12.78469800
C	35.23133700	5.50489900	-13.84047500
N	34.24446000	4.72231700	-13.45330900
H	35.57069500	8.58862000	-10.90771000
H	36.25596900	6.34725200	-9.99125400
H	34.58853800	5.97508400	-9.59534000
H	36.46186000	6.89129900	-12.81828900
H	33.32225400	4.39729700	-11.54976000
H	35.62373400	5.58714600	-14.84321300
H	33.48259100	3.53341700	-14.21871200
H	34.87101600	8.38159200	-9.28968000
H	33.87105400	8.09549400	-10.77199400
Mn	26.81427400	-3.89694900	-12.25763300

Int-A_{Mn} (11.6 kcal/mol)

H	20.66700500	-6.80400200	-16.56499900
H	16.38999600	-5.37400000	-12.30899600
H	24.65787900	-6.75699900	-19.16495400
H	29.36494100	-8.34206200	-18.18000900
H	35.11197400	4.87001500	-6.01596900
H	32.10200300	7.76399200	-10.35100900
H	33.92497200	-0.02996100	-10.21099700
H	31.95001600	-4.27902900	-6.58593200
H	23.18499900	1.49700000	-4.32299900
H	22.41699100	4.62900000	-7.60401100
H	22.25402100	6.39005200	-15.14803500
H	33.53402000	5.46902000	-6.68095000
H	30.78101000	8.84800000	-10.93701700
H	23.93691400	6.31003100	-15.82106400
H	23.80798300	-0.12301200	-3.81400000
H	32.79698100	-3.33902300	-5.29799000
H	32.07484700	0.82280600	-17.96200300
H	30.43534500	-3.27793200	-15.73606400
H	31.70205400	-4.16484000	-14.93606100
H	30.41802600	-9.05994100	-14.20504800
H	20.88601000	-5.04999900	-16.84099900
H	34.15687000	-4.71594100	-10.10782200
H	23.72493900	-8.30799000	-7.05600300
H	21.59201100	-3.72897400	-7.32000500
H	27.89798700	0.15103000	-17.74204600
H	27.15898900	4.34399500	-6.69899300
C	29.55198500	-8.45613500	-13.91499600
C	29.03606600	-7.65678900	-15.10059800
O	28.75001200	-6.45500000	-15.06751300
C	29.82670100	-7.56190000	-12.70297200
C	28.52332000	-7.12631800	-12.00701000
C	28.82458800	-6.02984400	-10.98975100
O	29.46638500	-6.33926400	-9.97256000
O	28.43897100	-4.82886900	-11.27223200
H	28.77314100	-9.18873500	-13.65444900
H	30.46107800	-8.08073600	-11.97940700
H	30.37344900	-6.67405900	-13.03719800
H	27.79525900	-6.78037700	-12.73815300
H	28.10858300	-7.99095700	-11.47441500
N	28.94376200	-8.37197300	-16.23869400
C	28.68990800	-7.77078800	-17.53379400
C	27.22863000	-7.97924100	-17.93500000
O	26.76099000	-9.10780000	-18.02457500
H	29.08970800	-9.36951700	-16.21282500
H	28.99520700	-6.72433300	-17.49371400
N	26.51347200	-6.83661500	-18.11182500
C	25.05622700	-6.84004900	-18.14810800
C	24.49761900	-5.70893700	-17.29229500
H	26.96708600	-5.96076000	-17.89379500
H	24.73725600	-7.81628200	-17.77273600
H	23.40822300	-5.67947400	-17.36055200
H	24.76215700	-5.83189800	-16.24157300
H	24.86911300	-4.73174100	-17.62463900
C	23.25807500	6.03489600	-15.04090100
C	23.24582900	4.49138700	-15.00492000
C	22.36251600	3.88402600	-13.94380700
C	22.67284400	4.02103600	-12.58506000
C	21.23568100	3.12296800	-14.28113100
C	21.90683200	3.40240100	-11.60263800
C	20.45390900	2.49751300	-13.31091000
C	20.79483100	2.63334400	-11.96283000
O	20.02249800	1.99544400	-11.03543100
H	23.64590700	6.44015600	-14.09941500
H	22.92525100	4.12289400	-15.98673800
H	24.27369400	4.12847200	-14.87168800
H	23.54776100	4.59264900	-12.28623900
H	20.97572000	3.00007000	-15.32959600
H	22.18128100	3.49183600	-10.55871000
H	19.59603300	1.88988300	-13.57859000
H	20.45558900	2.06833300	-10.17267400
C	20.86197900	-5.83999600	-16.08300200
C	19.83729200	-5.62999800	-14.97782700
O	19.04428500	-6.50778100	-14.65024200
H	21.86182000	-5.85987900	-15.63605400
N	19.91366900	-4.42450700	-14.33439200
C	19.19499600	-4.19801200	-13.09499900
C	18.15440600	-3.08828700	-13.21589000
O	18.40380500	-2.01166500	-13.78592900

C	20.22943400	-3.88035800	-11.98872300	O	29.13599000	-0.89803200	-13.53751000
O	19.64737100	-3.66205900	-10.70765900	H	30.02518000	-4.64140200	-14.74321000
H	20.59576900	-3.71145200	-14.59291500	H	30.58474100	-3.43525800	-12.70434900
H	18.70281400	-5.14250300	-12.86395600	H	31.32161100	-2.09414000	-13.59425600
H	20.88257000	-4.75390400	-11.89483500	C	27.87496700	1.06293600	-17.13697200
H	20.84336800	-3.02953900	-12.30425400	C	29.24908200	1.61868400	-16.81970500
H	19.37200000	-2.73773600	-10.66028600	O	29.41152500	2.73993400	-16.34160400
C	23.90609400	-7.35597300	-7.56602800	C	27.12586800	0.76546300	-15.81920600
C	22.89917800	-6.30492600	-7.12483000	C	25.73647900	0.25042900	-16.08123200
O	21.72164600	-6.60244700	-6.91678900	C	24.71463500	1.13819700	-16.43523300
C	23.73904000	-7.59596000	-9.09540000	C	25.43743900	-1.11587200	-16.01332300
C	24.11915500	-6.42289600	-9.94374700	C	23.43228600	0.68238300	-16.72817200
C	25.27754800	-6.13859600	-10.62762100	C	24.15815300	-1.59119800	-16.30451000
N	23.32797800	-5.29397600	-10.11384200	C	23.16574600	-0.68524400	-16.67425800
C	24.02500900	-4.38639800	-10.85059500	O	21.90473700	-1.18994300	-16.94725500
N	25.20912200	-4.87687000	-11.18420400	H	27.33090000	1.82307800	-17.70615700
H	24.93743100	-7.05983200	-7.35866200	H	27.70349900	0.04417200	-15.23324100
H	24.36512200	-8.44139500	-9.39474100	H	27.08602200	1.68372300	-15.22829100
H	22.69773300	-7.88296800	-9.28036900	H	24.92098900	2.20429800	-16.47124100
H	22.43082500	-5.13218300	-9.67594600	H	26.20719600	-1.81201500	-15.68929200
H	26.15087400	-6.75914400	-10.74540600	H	22.64250200	1.38584900	-16.98285500
H	23.65485700	-3.40960300	-11.12055000	H	23.91343600	-2.64452200	-16.21725100
N	23.32336800	-5.00921200	-7.10131500	H	21.34811600	-0.47260700	-17.27877400
C	22.40698000	-3.96404900	-6.62800000	N	30.27080000	0.76109400	-17.06915300
C	23.31570500	-2.76191500	-6.35214400	C	31.68323600	1.10926900	-16.97997200
C	24.52756100	-2.99129400	-7.26357000	C	32.38518900	0.35781300	-15.84648600
C	24.71121800	-4.51123600	-7.22081900	C	31.84758800	0.74685600	-14.46951200
H	21.90230500	-4.31993400	-5.72324500	C	32.28172000	2.10245700	-13.95190900
H	22.81357100	-1.81697800	-6.54796900	O	33.17155300	2.71347900	-14.70388200
H	23.63739500	-2.76676600	-5.30539800	O	31.86496600	2.55711200	-12.88209100
H	24.31116000	-2.65903200	-8.28434800	H	30.04052800	-0.14442200	-17.44868100
H	25.41984600	-2.46622500	-6.91963900	H	31.75296000	2.18942600	-16.85082100
H	25.19752200	-4.89837400	-8.11719600	H	32.23301100	-0.71968700	-15.98856700
H	25.31209800	-4.79955600	-6.34888700	H	33.46164600	0.54487600	-15.90189500
C	23.17501600	4.07100000	-8.16499400	H	30.75588300	0.68957300	-14.44707600
C	24.46963300	3.92976700	-7.38413900	H	32.17109300	0.02301700	-13.71348600
O	24.49091500	3.81528400	-6.15775200	C	26.86155700	-0.96752200	-11.10087800
H	22.78069700	3.07011700	-8.36650800	O	26.97913400	-2.21175500	-10.93893700
H	23.32265000	4.58237400	-9.11824900	O	27.14674400	-0.07325200	-10.28411500
N	25.60315000	3.91636100	-8.13606700	C	26.30807700	-0.48574300	-12.50321400
C	26.90900300	3.66701100	-7.52200400	C	25.07089000	-1.23507800	-12.89331700
C	27.87836600	3.81478900	-8.70016300	O	25.09414900	-2.49477300	-12.98963400
C	27.07337300	3.26463200	-9.88124100	C	23.86944100	-0.49482000	-13.15692700
C	25.66299900	3.80136400	-9.60966000	C	23.90096900	0.86905800	-13.18605200
H	26.94160900	2.64634300	-7.11608000	C	25.09636200	1.62852300	-12.91902000
H	28.10486800	4.87349300	-8.86553700	C	26.23832500	0.99190700	-12.58301600
H	28.81889600	3.28675200	-8.53746800	H	27.13605000	-0.81899300	-13.15880500
H	27.45724600	3.58222300	-10.84994700	H	22.96250200	-1.04120200	-13.39819900
H	27.06234200	2.17343400	-9.86719400	H	22.99190700	1.40432800	-13.43040600
H	25.51957800	4.78539900	-10.07518300	H	25.06403200	2.70916300	-12.98112900
H	24.89427300	3.12125500	-9.98402700	H	27.15442700	1.52792600	-12.35936500
C	23.37403600	0.46299500	-4.63001900	O	26.39897100	-5.34795800	-13.86739700
C	24.31749000	0.46920200	-5.84341900	H	25.53448900	-5.10484800	-14.26900700
C	23.67262600	0.53529600	-7.21551500	H	27.08809900	-5.47871300	-14.54072400
C	22.28809200	0.54801500	-7.42384900	O	23.86160400	-4.43698500	-14.35491400
C	24.50294500	0.51193400	-8.34836300	H	23.40196200	-4.93493500	-13.66636600
C	21.74993200	0.47527100	-8.71414100	H	24.11296600	-3.59289300	-13.90821900
C	23.97283900	0.46934800	-9.63430900	O	21.10755000	-1.86067600	-14.32707400
C	22.58877000	0.43018600	-9.82793300	H	21.29224400	-1.63405800	-15.25436800
H	22.41464100	-0.01369500	-4.85058000	H	20.14526300	-1.71735100	-14.19045800
H	25.00219700	1.31902200	-5.75049100	C	34.22898400	4.62595300	-6.61609200
H	24.94639000	-0.42896300	-5.82935900	C	33.56714200	3.32805600	-6.13257900
H	21.61285500	0.58934900	-6.57696900	C	32.29757700	2.93613200	-6.91044800
H	25.58224600	0.50353300	-8.22845600	C	31.95498400	1.44126800	-6.72459100
H	20.67034500	0.41829600	-8.83757000	N	30.54668800	1.09652100	-6.90928400
H	24.64579800	0.46525600	-10.47901300	C	29.92497300	0.90431200	-8.09660000
H	22.18138800	0.36058800	-10.82997700	N	30.48897600	1.32776600	-9.22736600
C	32.20598200	-3.27995300	-6.21809000	N	28.72265100	0.33193800	-8.09627800
C	30.88150300	-2.53150800	-5.95782700	H	34.59789400	4.47265200	-7.64006400
C	29.90672700	-2.71966200	-7.08387000	H	34.30298300	2.51697400	-6.21545500
C	30.14268200	-3.33164600	-8.28905600	H	33.31680400	3.40003100	-5.06684200
N	28.56333200	-2.33739300	-7.02906600	H	31.44791100	3.54392300	-6.57995400
C	28.02999200	-2.72816800	-8.19221500	H	32.44430300	3.16375600	-7.97574500
N	28.94882300	-3.32050700	-8.97299300	H	32.57166100	0.81806000	-7.38416000
H	32.79068200	-2.79940700	-7.00202200	H	32.20091800	1.14537500	-5.70128900
H	30.42002000	-2.88771900	-5.02870200	C	30.03542000	0.77488100	-6.10072200
H	31.07480700	-1.46117400	-5.79159300	H	31.28333500	1.94363600	-9.18014200
H	27.75253400	-3.03203800	-5.70843300	H	30.06421100	1.16942900	-10.17273100
H	31.03048900	-3.79780200	-8.67932600	H	28.54062400	-0.38703400	-7.39023400
H	27.01812100	-2.55990300	-8.51958900	H	28.22878500	0.15798600	-8.98831400
H	28.76479600	-3.78472600	-9.87528900	C	31.09198200	7.81102300	-10.76996100
C	33.48018800	-4.18199700	-10.78332200	C	30.07818300	7.03972900	-9.90579600
C	33.37974300	-2.73862100	-10.31723300	C	28.77766100	6.81105800	-10.61749400
O	33.17911700	-2.39633500	-9.15682500	C	27.57898400	7.43870400	-10.38792300
C	32.15551800	-4.95732400	-10.76429700	C	28.56360300	5.90832300	-11.72745300
O	31.97777300	-5.51930100	-9.48759400	C	27.20446000	6.04673800	-12.12531200
H	33.91210700	-4.21724300	-11.78997500	C	29.37903100	4.98462700	-12.40705600
H	31.31904000	-4.29434500	-11.03141600	N	26.62781600	6.98474900	-11.28905100
H	32.19969200	-5.73751300	-11.54242200	C	26.65747700	5.30954100	-13.18026800
H	31.06371500	-5.87936300	-9.47808100	C	28.84157500	4.25073000	-13.45750700
N	33.54209000	-1.80506900	-11.30286900	C	27.49636500	4.41920100	-13.84363500
C	33.30503800	-0.40208200	-11.03296400	H	31.15311000	7.34357900	-11.75946300
H	33.55415600	-2.11135200	-12.26314800	H	30.51184900	6.06844500	-9.63085600
H	33.55461000	0.17705600	-11.92422500	H	29.90106400	7.57320200	-8.96472900
H	32.25659300	-0.20560900	-10.78000800	H	27.32151300	8.17956700	-9.64433100
C	30.70353800	-3.79225600	-14.83676700	H	25.67100400	7.29292100	-11.32859100
C	30.53652400	-2.85505300	-13.63165800	H	30.41715700	4.83663500	-12.12536400
C	29.18033200	-2.14997800	-13.64530900	H	25.62391400	5.44255500	-13.48259200
O	28.14716700	-2.88766800	-13.79388700	H	29.45694900	3.55205800	-14.01045800

H	27.12584800	3.85507400	-14.69290600
O	29.67458300	1.17391700	-11.78180800
H	30.36971600	1.69194300	-12.23473900
H	29.53634000	0.36503900	-12.31626100
N	16.95055800	-3.32722000	-12.65813700
C	16.59800500	-4.45000100	-11.75900700
C	15.33357900	-3.93537600	-11.05321800
C	14.68289000	-3.02106000	-12.10236600
C	15.88515900	-2.31566600	-12.73709700
H	17.41344300	-4.63999500	-11.05977400
H	14.68564100	-4.75103000	-10.72419400
H	15.61352200	-3.35078600	-10.16981300
H	14.16152100	-3.62284800	-12.85488600
H	13.96416100	-2.31694900	-11.67650900
H	15.73105000	-2.01573100	-13.77613200
H	16.17920700	-1.41879400	-12.17735500
C	29.55095100	-2.94392100	-1.16213100
C	28.26690900	-3.76223400	-1.33902300
C	28.03788600	-4.27886700	-2.75995600
C	27.85269700	-3.19583900	-3.80991400
O	28.00430600	-2.00082300	-3.62166400
O	27.53996000	-3.71809700	-5.00001900
H	29.53253600	-2.11127200	-1.86922200
H	28.26526800	-4.61866800	-0.65357600
H	27.41401100	-3.13446700	-1.05470800
H	28.88498500	-4.89228400	-3.09580200
H	27.16486400	-4.94048700	-2.80756500
H	30.46539100	-3.51016300	-1.36784900
H	29.56610100	-2.49732400	-0.16236200
C	34.86202700	7.99999200	-10.31605000
C	35.22730200	6.50120000	-10.32514200
C	35.01665700	5.87436500	-11.66488600
C	34.10908600	4.95259700	-12.12799100
N	35.75168100	6.23553900	-12.78517200
C	35.27842700	5.53559600	-13.85230000
N	34.28501000	4.75307100	-13.48261200
H	35.56831300	8.59263700	-10.90687600
H	36.26139100	6.35389900	-9.98683000
H	34.59229500	5.96929800	-9.60979800
H	36.50261100	6.90880200	-12.80462000
H	33.34213600	4.41293300	-11.59261700
H	35.68221800	5.62497200	-14.84989500
H	33.51957100	3.56528600	-14.25038200
H	34.87097000	8.38157800	-9.28967500
H	33.87103800	8.09549500	-10.77195900
Mn	26.91263300	-3.81617800	-12.33785500

TS2-A_{Mn} (17.1 kcal/mol)

H	20.66700200	-6.80400000	-16.56500100
H	16.38999300	-5.37399800	-12.30899800
H	24.65787700	-6.75700100	-19.16495300
H	29.36494000	-8.34206200	-18.18001100
H	35.11196500	4.87002900	-6.01596100
H	32.10200600	7.76397700	-10.35101800
H	33.92493500	-0.02996000	-10.21096900
H	31.95001000	-4.27902800	-6.58593000
H	23.18502600	1.49700000	-4.32298200
H	22.41698300	4.62898700	-7.60400900
H	22.25402100	6.39004400	-15.14806500
H	33.53401500	5.46901600	-6.68094800
H	30.78100200	8.84800000	-10.93700100
H	23.93691700	6.31003800	-15.82105900
H	23.80798500	-0.12299900	-3.81399200
H	32.79696300	-3.33901300	-5.29797800
H	32.07482800	0.82282400	-17.96201600
H	30.43548700	-3.27791400	-15.73609600
H	31.70207400	-4.16477700	-14.93609900
H	30.41801500	-9.05995300	-14.20505600
H	20.88601400	-5.04999800	-16.84099800
H	34.15684400	-4.71595200	-10.10780500
H	23.72491800	-8.30799100	-7.05601200
H	21.59193700	-3.72899300	-7.31992400
H	27.89799500	0.15102000	-17.74203100
H	27.15896500	4.34403000	-6.69901500
C	29.55197700	-8.45612000	-13.91500500
C	29.04109500	-7.65663400	-15.10343200
O	28.76603200	-6.45223200	-15.07409200
C	29.80810500	-7.55823200	-12.69930800
C	28.49078900	-7.10170500	-12.04288400
C	28.75057200	-6.01375900	-11.00268400
O	29.46342300	-6.30127900	-10.02591200
O	28.23387700	-4.84742300	-11.20273200
H	28.77182200	-9.19013000	-13.66169300
H	30.41602100	-8.08046300	-11.95606800
H	30.37573600	-6.67985900	-13.02349000
H	27.78764300	-6.74907600	-12.79436000
H	28.04518200	-7.96297300	-11.52817200
N	28.93879900	-8.37438200	-16.23901700
C	28.68992100	-7.77078600	-17.53381500
C	27.22976200	-7.97721100	-17.93926000
O	26.76397400	-9.10603600	-18.03688000
H	29.07232300	-9.37365700	-16.21229600
H	28.99692900	-6.72505700	-17.49039500
N	26.51332400	-6.83460700	-18.10918900
C	25.05622800	-6.84004500	-18.14810900
C	24.49185900	-5.71601800	-17.29017100
H	26.96583900	-5.95881300	-17.88876300

H	24.73924200	-7.81845900	-17.77644500
H	23.40367200	-5.68094300	-17.37181700
H	24.74146200	-5.85267400	-16.23888100
H	24.87063900	-4.73588900	-17.60469900
C	23.25807900	6.03490600	-15.04089600
C	23.24072100	4.49154400	-14.98758100
C	22.34148700	3.90178600	-13.92894000
C	22.63597100	4.05590900	-12.56871100
C	21.21249500	3.14539300	-14.26791300
C	21.85319400	3.45820800	-11.58671300
C	20.41442000	2.53968800	-13.29838700
C	20.74194200	2.69003600	-11.94879100
O	19.95821800	2.06536200	-11.01995700
H	23.64497100	6.44754400	-14.10191100
H	22.92923600	4.11270100	-15.96821200
H	24.26361400	4.12277400	-14.83623300
H	23.51145100	4.62546200	-12.26767500
H	20.96346400	3.00962900	-15.31739900
H	22.11601700	3.56052100	-10.54091700
H	19.55572400	1.93402600	-13.56800700
H	20.38675500	2.14468600	-10.15579600
C	20.86198200	-5.84000000	-16.08300000
C	19.84636700	-5.63842500	-14.96771100
O	19.08319800	-6.53387000	-14.61634400
H	21.86497100	-5.86507800	-15.64340200
N	19.90225900	-4.42393200	-14.34187000
C	19.19499500	-4.19801100	-13.09500200
C	18.15152300	-3.08942200	-13.21502600
O	18.39615800	-2.01284500	-13.78632000
C	20.24109700	-3.87209600	-12.00335100
O	19.67698300	-3.67598700	-10.70981300
H	20.55341600	-3.68922600	-14.62726200
H	18.70951400	-5.14366700	-12.85521600
H	20.90975600	-4.73552200	-11.92942600
H	20.83576500	-3.00809700	-12.32060300
H	19.40049300	-2.75325900	-10.64327900
C	23.90611200	-7.35598900	-7.56599300
C	22.90842800	-6.30631500	-7.10179400
O	21.74131500	-6.61015300	-6.85005400
C	23.69561900	-7.59306800	-9.09156600
C	24.05615700	-6.42989400	-9.96285700
C	25.19716800	-6.16792900	-10.68286800
N	23.26286600	-5.30305400	-10.14545300
C	23.94119900	-4.42096700	-10.92998300
N	25.11577400	-4.92424500	-11.27478300
H	24.94310700	-7.06426300	-7.38204900
H	24.30759400	-8.44341000	-9.40622800
H	22.64818100	-7.87641700	-9.24485700
H	22.37037600	-5.13010100	-9.70236600
H	26.06690600	-6.79257700	-10.80431900
H	23.57263800	-3.44977700	-11.22340100
N	23.32189200	-5.00654300	-7.10928900
C	22.40708500	-3.96401700	-6.62811700
C	23.31405500	-2.76018100	-6.36053200
C	24.51037100	-2.98102800	-7.29385400
C	24.70314900	-4.50104700	-7.26147900
H	21.90716400	-4.32162600	-5.72188800
H	22.80543500	-1.81597700	-6.54348300
H	23.65397500	-2.76932000	-5.31952800
H	24.27721100	-2.64499700	-8.30967400
H	25.40350800	-2.45198500	-6.95844500
H	25.16863700	-4.88277800	-8.17155100
H	25.32637800	-4.78976100	-6.40533100
C	23.17498000	4.07103400	-8.16494700
C	24.46853300	3.92764000	-7.38309200
O	24.49046600	3.80810300	-6.15711900
H	22.77999300	3.07173300	-8.37116400
H	23.32495600	4.58531800	-9.11610900
N	25.60237200	3.91823300	-8.13477300
C	26.90897800	3.66698800	-7.52189400
C	27.87665100	3.80801100	-8.70291500
C	27.06488700	3.25986800	-9.88054000
C	25.66131300	3.81099400	-9.60889000
H	26.93924300	2.64742600	-7.11302400
H	28.10677400	4.86514000	-8.87288300
H	28.81593800	3.27659800	-8.54343400
H	27.45043500	3.56069100	-10.85324000
H	27.04106800	2.16980800	-9.85547600
H	25.53215100	4.79910000	-10.06914300
H	24.88511500	3.14336400	-9.98915800
C	23.37398900	0.46301200	-4.63002700
C	24.30762700	0.46853200	-5.84956800
C	23.65020700	0.54991400	-7.21532200
C	22.26472800	0.56042800	-7.41407600
C	24.47282600	0.54664000	-8.35406300
C	21.71932100	0.50741700	-8.70268900
C	23.93705700	0.51824600	-9.63840000
C	22.55102600	0.47966500	-9.82156400
H	22.41303100	-0.01300100	-4.84575500
H	25.00048500	1.31174600	-5.75728100
H	24.92790400	-0.43582300	-5.84617800
H	21.59457400	0.58818400	-6.56263100
H	25.55175400	0.54716500	-8.23084900
H	20.63903300	0.45525600	-8.82173900
H	24.59256500	0.52621800	-10.49839400
H	22.13989500	0.42527500	-10.82265900
C	32.20599300	-3.27994400	-6.21813600
C	30.88735000	-2.52101300	-5.97059000
C	29.90515500	-2.71589300	-7.09009600

H	20.88601800	-5.04999900	-16.84099900	C	27.88018900	3.79157200	-8.70004500
H	34.15685400	-4.71596100	-10.10782200	C	27.07056000	3.22163200	-9.86745600
H	23.72474700	-8.30797500	-7.05604300	C	25.66532500	3.77701900	-9.61122800
H	21.59193800	-3.72899700	-7.31992600	H	26.93287900	2.64951400	-7.10402700
H	27.89798800	0.15102300	-17.74203500	H	28.10730600	4.84590800	-8.88925200
C	27.15899900	4.34412500	-6.69910300	H	28.82065500	3.26639100	-8.52603900
C	29.55196900	-8.45610100	-13.91499300	H	27.45600300	3.49961600	-10.84713000
C	29.04179400	-7.65409500	-15.10230800	H	27.04514000	2.12971100	-9.81228700
O	28.76937500	-6.44934800	-15.07054700	H	25.54043000	4.75463200	-10.09337100
C	29.80991700	-7.56195200	-12.69749900	H	24.89250500	3.10097700	-9.98221500
C	28.49404800	-7.10134200	-12.04212600	C	23.37399500	0.46301300	-4.63004400
C	28.76022500	-6.03580900	-10.98199600	C	24.34693400	0.47088700	-5.82233600
O	29.46919100	-6.34084400	-10.00847300	C	23.74433600	0.53011100	-7.21308500
O	28.24841200	-4.86277100	-11.16278900	C	22.36815100	0.53457200	-7.46310900
H	28.77141700	-9.19006100	-13.66287600	C	24.60927300	0.50088200	-8.32066600
H	30.41335600	-8.08905800	-11.95399200	C	21.87361100	0.45440400	-8.77069300
H	30.38215300	-6.68529000	-13.01827000	C	24.12657800	0.44198800	-9.62544000
H	27.79949900	-6.72850600	-12.79209100	C	22.74643500	0.40399000	-9.85662400
H	28.03319900	-7.96516700	-11.54598100	H	22.41972800	-0.01475300	-4.86730700
N	28.93811100	-8.37197200	-16.23790100	H	25.02681500	1.32252900	-5.71039700
C	28.68991800	-7.77078600	-17.53383100	H	24.97771300	-0.42592500	-5.78691700
C	27.22971600	-7.97622300	-17.93974300	H	21.66710800	0.57684400	-6.63718000
O	26.76402600	-9.10505200	-18.03796700	H	25.68341000	0.50659000	-8.14715200
H	29.06777000	-9.37173000	-16.20959000	H	20.79899200	0.39313100	-8.92951000
H	28.99713000	-6.72497900	-17.49168200	H	24.81272300	0.40560200	-10.46263500
N	26.51351000	-6.83330700	-18.11025700	H	22.37713200	0.33278100	-10.87257900
C	25.05625900	-6.84002000	-18.14810000	C	32.20600700	-3.27994800	-6.21815200
C	24.49126900	-5.72835500	-17.27076700	C	30.90237200	-2.48022800	-6.00861400
H	26.96526900	-5.95760800	-17.88778300	C	29.93236900	-2.65249400	-7.14696500
H	24.74352300	-7.82288600	-17.78410400	C	30.10454400	-3.40966000	-8.27992500
H	23.40374500	-5.68724300	-17.36319000	N	28.63660500	-2.12371600	-7.14986500
H	24.73762500	-5.89354000	-16.22062300	C	28.06670700	-2.58815300	-8.27225700
H	24.87721700	-4.74326600	-17.55630900	N	28.91904800	-3.35271700	-8.97502500
C	23.25808300	6.03490100	-15.04089700	H	32.81342400	-2.82581500	-7.00201900
C	23.24256300	4.49230300	-14.99906500	H	30.40763000	-2.79255800	-5.08088500
C	22.35737200	3.88374100	-13.94009600	H	31.13647100	-1.41532200	-5.86399600
C	22.66253500	4.02611400	-12.58145400	H	27.78186000	-2.83574200	-5.73963900
C	21.24115700	3.10828600	-14.27796400	H	30.94390500	-3.99129000	-8.62433200
C	21.90310400	3.39846200	-11.60060400	H	27.05745600	-2.37614500	-8.59568900
C	20.46790100	2.47009300	-13.30955000	H	28.70061200	-3.88393000	-9.84024100
C	20.80769700	2.60857500	-11.96206400	C	33.48018500	-4.18197300	-10.78342300
O	20.04872600	1.95397600	-11.03259800	C	33.37591700	-2.73623700	-10.32162100
H	23.64531300	6.44442100	-14.10070200	O	33.14451900	-2.39259800	-9.16744000
H	22.92379600	4.12468400	-15.98093300	C	32.14733000	-4.94659900	-10.77063400
H	24.26645200	4.12192100	-14.86173200	O	31.98781800	-5.56389400	-9.51433300
H	23.53156700	4.60581400	-12.28211100	H	33.91615400	-4.21803900	-11.78817800
H	20.98457300	2.98256300	-15.32687300	H	31.31040200	-4.26593000	-10.98981700
H	22.17536100	3.49000100	-10.55626400	H	32.16769300	-5.69555400	-11.57870500
H	19.61948400	1.84915400	-13.57759500	H	31.08775100	-5.95596000	-9.52676900
H	20.48402300	2.03807600	-10.17257800	N	33.57199000	-1.80219900	-11.30314000
C	20.86199500	-5.83999100	-16.08300000	C	33.30509100	-0.40208800	-11.03297700
C	19.87006300	-5.66313200	-14.93937400	H	33.56494900	-2.10905200	-12.26354900
O	19.23834000	-6.61574600	-14.49167400	H	33.54153900	0.18289000	-11.92422700
H	21.86765400	-5.89036500	-15.64810500	H	32.25425900	-0.23981200	-10.77540200
N	19.80417600	-4.40770800	-14.40183300	C	30.70337600	-3.79255900	-14.83650000
C	19.19499500	-4.19801400	-13.09500000	C	30.72860200	-2.83179200	-13.64436900
C	18.18303400	-3.06083400	-13.14364100	C	29.38804600	-2.46401900	-13.01338600
O	18.46805500	-1.95660500	-13.63701500	O	28.35015900	-3.02428000	-13.49285500
C	20.32361500	-3.93201300	-12.07373300	O	29.40673800	-1.67188500	-12.03776100
O	19.86060000	-3.82354500	-10.72869600	H	30.01216800	-4.61821400	-14.67449300
H	20.39664900	-3.64703000	-14.74432600	H	31.31431700	-3.26369800	-12.82551900
H	18.70899200	-5.13965300	-12.84292800	H	31.24214400	-1.89918000	-13.90137500
H	20.99611000	-4.79476900	-12.10876900	C	27.87496400	1.06294000	-17.13697400
H	20.89298400	-3.04682000	-12.37803500	C	29.24836500	1.57983700	-16.76424600
H	19.63142400	-2.89987000	-10.56618800	O	29.41945800	2.64705900	-16.17695100
C	23.90636100	-7.35592400	-7.56602600	C	27.05889900	0.79608700	-15.85298100
C	22.91049600	-6.30692700	-7.09572900	C	25.62534400	0.45175900	-16.15162300
O	21.74713300	-6.61374700	-6.83111300	C	24.71896500	1.45674600	-16.50312300
C	23.68574500	-7.59253800	-9.08885700	C	25.16362500	-0.86573900	-16.08706100
C	24.07963100	-6.43039200	-9.94294100	C	23.38457900	1.16251800	-16.77056200
C	25.27805200	-6.13929600	-10.54628200	C	23.83491400	-1.18105700	-16.35566400
N	23.28471800	-5.31618300	-10.18564000	C	22.94959700	-0.15896600	-16.68470100
C	24.01285200	-4.41486600	-10.89770600	O	21.62307500	-0.50656600	-16.89000500
N	25.22716500	-4.89070900	-11.13037200	H	27.37735400	1.83957700	-17.72691400
H	24.94506800	-7.06659900	-7.38851700	H	27.52209700	-0.01468300	-15.28129900
H	24.27825500	-8.45655600	-9.40399700	H	27.10714500	1.68348800	-15.21830500
H	22.63235300	-7.85052700	-9.24332800	H	25.05404200	2.48920400	-16.54725600
H	22.34512200	-5.16593300	-9.84084700	H	25.83630800	-1.65701100	-15.77017200
H	26.16866700	-6.74483200	-10.58241100	H	22.68471100	1.95553700	-17.02275600
H	23.65964000	-3.45366900	-11.23821300	H	23.48758000	-2.20006300	-16.23952100
N	23.32112400	-5.00693900	-7.10887200	H	21.10401900	0.29994400	-17.00617800
C	22.40707300	-3.96402200	-6.62809800	N	30.27284400	0.75235700	-17.09338900
C	23.31728900	-2.76059500	-6.36375800	C	31.68319500	1.10918400	-16.98000300
C	24.50451500	-2.98193100	-7.30902100	C	32.36414700	0.35424900	-15.83598000
C	24.70048800	-4.50022600	-7.26645400	C	31.76970900	0.72197600	-14.47575300
H	21.90861500	-4.31950000	-5.72021100	C	32.16363700	2.07891100	-13.92763900
H	22.80896700	-1.81516200	-6.53970400	O	33.05909200	2.71351000	-14.64892000
H	23.66609100	-2.77362000	-5.32554700	O	31.70569300	2.50108000	-12.86268600
H	24.25149300	-2.65579900	-8.32334500	H	30.04803300	-0.09696400	-17.58837500
H	25.40244200	-2.44777500	-6.99359300	H	31.75126200	2.18872500	-16.84552200
H	25.16680200	-4.88816800	-8.17250200	H	32.23673300	-0.72353000	-15.99610500
H	25.32522400	-4.78039700	-6.40805500	H	33.43782300	0.56276800	-15.84649900
C	23.17498100	4.07099000	-8.16489800	H	30.67625700	0.68044400	-14.50652700
C	24.47114400	3.93519800	-7.38569400	H	32.06790700	-0.00274700	-13.71069900
O	24.49781200	3.83048900	-6.15872900	C	26.43161400	-0.37080300	-12.44452700
H	22.78397900	3.06815400	-8.36332700	C	25.28936900	-1.14798300	-12.72480900
H	23.32075700	4.57861500	-9.12036000	O	25.32046400	-2.48770600	-12.69766500
N	25.60522400	3.91610900	-8.13927100	C	24.08796500	-0.48211800	-13.04801500
C	26.90892700	3.66685700	-7.52182300	C	24.04285300	0.90726900	-13.10648200

C	25.18243300	1.67304500	-12.84003900
C	26.37464700	1.02195800	-12.51293400
H	27.36487800	-0.86728400	-12.20150800
H	23.20546100	-1.06663800	-13.29304500
H	23.11319100	1.39295700	-13.37495300
H	25.14669800	2.75494400	-12.89111300
H	27.27999000	1.58884400	-12.32110200
O	26.33012900	-5.32448200	-14.00056800
H	25.53600200	-4.92010200	-14.43444400
H	27.05787600	-5.45433000	-14.63216900
O	24.21618600	-3.82886100	-14.62599300
H	23.29243200	-3.99521500	-14.40174000
H	24.54547100	-3.19593800	-13.91116300
O	21.11548500	-1.94595700	-14.50066100
H	21.24365500	-1.44711000	-15.32650300
H	20.21017500	-1.72436300	-14.19357800
C	34.22901500	4.62593700	-6.61619400
C	33.55854400	3.35169500	-6.07870900
C	32.24764600	2.98286200	-6.79491600
C	31.93180100	1.48164500	-6.65463800
N	30.57871500	1.09120200	-7.05563100
C	30.16909900	0.98940700	-8.33515400
N	30.87874800	1.49414500	-9.33644300
N	28.98427700	0.41341000	-8.59463700
H	34.58544100	4.44524200	-7.63896600
H	34.27035200	2.52120100	-6.17771400
H	33.36101300	3.45185000	-5.00470900
H	31.41115200	3.56779400	-6.39715400
H	32.33202500	3.26335200	-7.85280700
H	32.66398000	0.88450200	-7.21426300
H	32.03140600	1.19196400	-5.60575100
H	29.99481600	0.63244300	-6.36981100
H	31.72313800	2.00897000	-9.16442200
H	30.52593100	1.31578200	-10.30983500
H	28.68001800	-0.33898500	-7.96704100
H	28.74480200	0.30273400	-9.57394900
C	31.09198700	7.81101700	-10.76997300
C	30.08583000	7.05220000	-9.88505300
C	28.77314900	6.82673200	-10.57319400
C	27.57980400	7.45988100	-10.32980800
C	28.54164500	5.92099200	-11.67637600
C	27.17876900	6.06357400	-12.05810300
C	29.34555400	4.99180000	-12.36195200
N	26.61622700	7.00678400	-11.21768900
C	26.61553100	5.32379500	-13.10241200
C	28.79192300	4.25642500	-13.40291200
C	27.44203900	4.42745300	-13.77146500
H	31.14385600	7.33551400	-11.75568200
H	30.51812300	6.08003800	-9.60983900
H	29.92868900	7.59440800	-8.94535700
H	27.33477500	8.20489700	-9.58614100
H	25.65902300	7.31538500	-11.24473400
H	30.38618200	4.84011700	-12.09163300
H	25.57677300	5.45125600	-13.38759200
H	29.39721000	3.55331000	-13.96099400
H	27.05118000	3.84951500	-14.60150000
O	29.70951800	0.93433800	-11.64003300
H	30.24139500	1.46412500	-12.26495000
H	29.71280400	-0.01848300	-11.91386100
N	16.95978700	-3.31514300	-12.63596300
C	16.59800600	-4.44999500	-11.75901600
C	15.33373500	-3.94182400	-11.04524800
C	14.69993700	-2.98813900	-12.06939000
C	15.91541500	-2.27983900	-12.67380000
H	17.41018700	-4.65433900	-11.05825700
H	14.67461000	-4.75957600	-10.74488200
H	15.61371500	-3.38697700	-10.14300000
H	14.17562500	-3.55948200	-12.84333800
H	13.98779800	-2.28840700	-11.62563300
H	15.76881600	-1.93477300	-13.69987100
H	16.22605800	-1.41283000	-12.07726700
C	29.55095200	-2.94387300	-1.16218400
C	28.26056900	-3.73694500	-1.39090600
C	28.05565700	-4.19408200	-2.83823000
C	27.90146000	-3.07162200	-3.85152700
O	28.06114900	-1.88561000	-3.62583600
O	27.60085900	-3.55059800	-5.06732400
H	29.55693700	-2.09946700	-1.85686500
H	28.23223500	-4.62090200	-0.74237300
H	27.40990500	-3.10953900	-1.09979900
H	28.90304100	-4.80369600	-3.18019800
H	27.17727400	-4.84376400	-2.92879400
H	30.46538500	-3.51017900	-1.36783100
H	29.56610200	-2.49735100	-0.16235000
C	34.86200800	8.00000800	-10.31602900
C	35.21857500	6.49870000	-10.31673200
C	34.96587000	5.86036800	-11.64305300
C	34.02603400	4.95567300	-12.07430200
N	35.67771500	6.19713700	-12.78522900
C	35.16093100	5.50068000	-13.83389200
N	34.16081000	4.74318800	-13.43113400
H	35.57116400	8.58703200	-10.90854400
H	36.25994300	6.34707300	-10.00407400
H	34.59831200	5.97973400	-9.57928500
H	36.44142500	6.85473500	-12.83011500
H	33.26133400	4.44015100	-11.51251600
H	35.53953500	5.57285800	-14.84263500
H	33.39091000	3.56744100	-14.18213000
H	34.87098300	8.38157600	-9.28967400

H	33.87104400	8.09549200	-10.77197300
Mn	26.81028900	-3.89030700	-12.40232100

The transition states and intermediates involved in the reaction pathway with **Mode-A** for the Zn-enzyme of SDC.

E:S-A_{Zn} (0.0 kcal/mol)

H	20.66699700	-6.80400000	-16.56499900
H	16.39000000	-5.37400000	-12.30900100
H	24.65797500	-6.75700000	-19.16499000
H	29.36482300	-8.34219900	-18.18000800
H	35.11201800	4.86999000	-6.01602200
H	32.10199800	7.76399100	-10.35099600
H	33.92502100	-0.03000400	-10.21101500
H	31.94996900	-4.27902700	-6.58590600
H	23.18498600	1.49700100	-4.32301100
H	22.41699300	4.62898300	-7.60399200
H	22.25401000	6.39002300	-15.14801400
H	33.53400000	5.46899900	-6.68101600
H	30.78099800	8.84799900	-10.93700600
H	23.93698200	6.31001500	-15.82101000
H	23.80798500	-0.12302100	-3.81400700
H	32.79691800	-3.33918000	-5.29795900
H	32.07500800	0.82299800	-17.96199700
H	30.43501800	-3.27794000	-15.73597200
H	31.70202200	-4.16493000	-14.93604300
H	30.41826900	-9.05964100	-14.20494400
H	20.88599300	-5.04999900	-16.84099900
H	34.15692800	-4.71601300	-10.10793800
H	23.72497400	-8.30798900	-7.05598800
H	21.59198300	-3.72901300	-7.31998500
H	27.89800600	0.15099700	-17.74199500
H	27.15899000	4.34402600	-6.69901900
C	29.55190000	-8.45625600	-13.91512900
C	29.39154600	-7.66804100	-15.20025100
O	29.92027600	-6.57271600	-15.37960400
C	29.73998400	-7.54812900	-12.70507300
C	28.51062500	-6.65577400	-12.48779600
C	28.59879000	-5.80220100	-11.22681300
O	29.34704800	-6.15038100	-10.29806100
O	27.85239500	-4.75078300	-11.16551200
H	28.71105700	-9.14628400	-13.77575400
H	29.92927100	-8.13391600	-11.80285700
H	30.61624500	-6.91487500	-12.86932900
H	28.34040700	-5.99962500	-13.34420000
H	27.60361300	-7.27173400	-12.39810700
N	28.74362600	-8.31635700	-16.19518900
C	28.69019000	-7.77098900	-17.53409500
C	27.24201500	-7.95902700	-17.98673700
O	26.76879900	-9.08805700	-18.07984800
H	28.29771600	-9.21022500	-16.04694500
H	29.02378600	-6.73420800	-17.48332900
N	26.51607500	-6.82258900	-18.14523500
C	25.05595600	-6.83996200	-18.14803800
C	24.51244700	-5.71008700	-17.27501300
H	26.96991600	-5.94261900	-17.94764600
H	24.75338500	-7.81959200	-17.76964200
H	23.42072600	-5.71867800	-17.27661600
H	24.85510200	-5.80652700	-16.24085900
H	24.83013500	-4.72926300	-17.65059000
C	23.25799700	6.03501700	-15.04100200
C	23.18264600	4.49786600	-14.99338000
C	22.25559100	3.96721900	-13.92752800
C	22.57794600	4.09478000	-12.57126100
C	21.07631300	3.28617600	-14.25462800
C	21.78323800	3.52716900	-11.58250500
C	20.26543900	2.71078500	-13.27716400
C	20.63038600	2.81806500	-11.93295700
O	19.84035800	2.21219100	-10.99685400
H	23.64609400	6.43529300	-14.09785300
H	22.84595200	4.13368800	-15.97129700
H	24.18626200	4.07971400	-14.84991200
H	23.48941700	4.60916400	-12.27928700
H	20.80134900	3.17808100	-15.30121200
H	22.07161500	3.60058000	-10.54092200
H	19.36756400	2.16015000	-13.53698800
H	20.28781600	2.26444200	-10.14025600
C	20.86200900	-5.84000300	-16.08300700
C	19.88805900	-5.68954100	-14.91777000
O	19.38268200	-6.67245300	-14.38565900
H	21.86443200	-5.87899500	-15.63944400
N	19.69028200	-4.41453000	-14.45652500
C	19.19499200	-4.19800000	-13.09498600
C	18.19790000	-3.05322000	-13.11190300
O	18.50003400	-1.94635500	-13.59275500
C	20.40883600	-3.94643300	-12.17376700
O	20.10074200	-4.05595800	-10.78078900
H	20.24210300	-3.65425100	-14.85049700
H	18.73097200	-5.13778900	-12.79935700
H	21.14694700	-4.71886900	-12.39960900
H	20.86456400	-2.97829400	-12.40754200

H	19.86483600	-3.18114000	-10.44878000	O	29.41534600	2.64882900	-16.18321500
C	23.90601600	-7.35601600	-7.56596900	C	27.04288400	0.79406000	-15.86171600
C	22.91197800	-6.30156000	-7.10190500	C	25.62407200	0.41365000	-16.18989500
O	21.73932100	-6.60368200	-6.86903100	C	24.71399300	1.38783300	-16.61315100
C	23.63700700	-7.62194100	-9.07712300	C	25.18145300	-0.90897400	-16.10080200
C	23.91362200	-6.43412800	-9.93701900	C	23.40087200	1.05688900	-16.93520600
C	25.08824100	-6.01581200	-10.50940700	C	23.87510600	-1.26318700	-16.42275700
N	23.01436100	-5.40194700	-10.17380100	C	22.98814900	-0.27160700	-16.83953600
C	23.65682600	-4.42095800	-10.85245100	O	21.68485500	-0.65009200	-17.11762600
N	24.91764200	-4.76721400	-11.06973500	H	27.38558300	1.84172900	-17.73036800
H	24.94807600	-7.06591100	-7.41633400	H	27.51514800	-0.00264600	-15.27614300
H	24.26894800	-8.44884400	-9.41425900	H	27.05973500	1.68906500	-15.23522600
H	22.59561100	-7.94350800	-9.18142700	H	25.02866600	2.42595500	-16.67138600
H	22.04343700	-5.35337000	-9.88556600	H	25.85985900	-1.67420200	-15.73422200
H	26.04532200	-6.51058500	-10.52158100	H	22.69821800	1.82949900	-17.23962800
H	23.20888300	-3.49820600	-11.17987000	H	23.53801300	-2.28547400	-16.30870500
N	23.32818900	-5.00568900	-7.09033800	H	21.18276000	0.13024400	-17.38707500
C	22.40699700	-3.96397300	-6.62798700	N	30.27373900	0.73793800	-17.06769200
C	23.30727000	-2.75309700	-6.36667300	C	31.68298700	1.10899900	-16.97999300
C	24.50301400	-2.97522200	-7.29990100	C	32.39691000	0.40304300	-15.82807300
C	24.70492800	-4.49348000	-7.25262500	C	31.85870700	0.86047500	-14.47303800
H	21.90378400	-4.31305800	-5.71988500	C	32.29389200	2.24569400	-14.02866000
H	22.79310000	-1.81250700	-6.55501600	O	33.25957500	2.76696900	-14.75758500
H	23.64786600	-2.75358000	-5.32572500	O	31.81365300	2.79890000	-13.03773000
H	24.26316100	-2.65279100	-8.31862200	H	30.05003000	-0.11129700	-17.56341900
H	25.39467500	-2.43860200	-6.97363200	H	31.73703000	2.19292600	-16.86953500
H	25.16738500	-4.88016500	-8.16082600	H	32.25004900	-0.67997400	-15.92591500
H	25.33302800	-4.76949000	-6.39561600	H	33.47143300	0.59501200	-15.89337000
C	23.17500300	4.07102800	-8.16500500	H	30.76651900	0.83805500	-14.45658500
C	24.46980200	3.92955500	-7.38550200	H	32.16334500	0.17955100	-13.67221600
O	24.49471000	3.81478000	-6.15941700	C	27.03800000	-0.69886900	-11.37198700
H	22.77982200	3.07263800	-8.37178100	O	27.89653900	0.13050200	-10.95207900
H	23.32449500	4.58461200	-9.11694600	O	27.11473500	-1.94303900	-11.01905500
N	25.60464100	3.91709300	-8.13792400	C	25.94595200	-0.20947000	-12.22938400
C	26.90901600	3.66696200	-7.52197900	C	24.84794900	-1.01988800	-12.64833700
C	27.88308800	3.80196800	-8.69657900	O	24.81825800	-2.32694100	-12.53586100
C	27.07440400	3.25011300	-9.87311900	C	23.71837900	-0.35472400	-13.19689000
C	25.66781600	3.80028100	-9.61075900	C	23.71483300	1.00841600	-13.40766000
H	26.93623900	2.64815700	-7.10913500	C	24.84422600	1.78546100	-13.09627000
H	28.11616100	4.85784700	-8.86970300	C	25.93213500	1.17439700	-12.50945800
H	28.81974000	3.26795800	-8.52902400	H	28.64541100	-2.21758000	-11.23325400
H	27.46066300	3.55641100	-10.84471200	H	22.85871200	-0.95056100	-13.48385000
H	27.06333000	2.15782900	-9.84594200	H	22.83615500	1.47462300	-13.83330000
H	25.54130900	4.78510800	-10.07784000	H	24.86068300	2.85001700	-13.28093500
H	24.89329600	3.13148700	-9.99164300	H	26.79495200	1.75778100	-12.21696400
C	23.37403200	0.46302100	-4.62998300	Zn	26.38529200	-3.59079800	-12.07154700
C	24.28805400	0.46784600	-5.86308600	O	26.09003800	-4.46172300	-14.07064500
C	23.60290200	0.57626200	-7.21417100	H	25.18988700	-4.22018500	-14.38458200
C	22.21300400	0.60402100	-7.38133800	H	26.74403200	-3.95044000	-14.56912300
C	24.39791800	0.59188100	-8.37286500	O	23.38942500	-3.76330800	-14.21011700
C	21.63546200	0.58744700	-8.65733700	H	22.62093600	-3.26425700	-14.52948400
C	23.83029800	0.60118600	-9.64381500	H	23.79673200	-3.15859000	-13.53070800
C	22.44005400	0.57827400	-9.79560200	O	21.04910500	-1.95398900	-14.72514600
H	22.41042600	-0.01258600	-4.83581400	H	21.10352500	-1.45789000	-15.56121300
H	24.99394800	1.30061600	-5.77432200	H	20.17949100	-1.74776200	-14.31418100
H	24.89539400	-0.44467900	-5.88098700	C	34.22899800	4.62602600	-6.61595300
H	21.56334000	0.62136500	-6.51410100	C	33.56569700	3.35529000	-6.06513700
H	25.48096900	0.58537700	-8.27255400	C	32.24713300	2.98131100	-6.75975100
H	20.55166700	0.55474200	-8.75075900	C	31.92890900	1.48401700	-6.59016900
H	24.46380800	0.61030300	-10.51894300	N	30.56422700	1.09834400	-6.94138900
H	22.00999700	0.55038000	-10.79031600	C	30.11055100	0.94230200	-8.20746900
C	32.20612400	-3.27977400	-6.21810500	N	30.80076000	1.44117400	-9.23252500
C	30.88917400	-2.51133300	-5.98639200	N	28.93468800	0.34779300	-8.39795700
C	29.88287200	-2.74436700	-7.07900100	H	34.58235100	4.44092100	-7.63882200
C	30.00064200	-3.55347300	-8.18318800	H	34.27685100	2.52464900	-6.16872600
N	28.60007600	-2.18533800	-7.06090200	H	33.38271300	3.46094200	-4.98887100
C	27.98454800	-2.66975800	-8.14597800	H	31.41719100	3.57451200	-6.36019200
N	28.79024100	-3.49045600	-8.83831400	H	32.31808800	3.24444400	-7.82320100
H	32.79725300	-2.81259200	-7.00573700	H	32.64224300	0.87665900	-7.16333100
H	30.43807300	-2.80891300	-5.03078700	H	32.06241100	1.20909400	-5.54069300
H	31.09125300	-1.43550800	-5.88615700	H	29.99172400	0.68245600	-6.22092200
H	27.73546100	-2.90212100	-5.68670200	H	31.65712400	1.93550600	-9.05546300
H	30.82009200	-4.14755800	-8.55531300	H	30.56545000	1.20712700	-10.22696100
H	26.99154700	-2.41522800	-8.47955000	H	28.65534100	-0.36366900	-7.71379700
H	28.51365700	-4.01254600	-9.68316600	H	28.59940900	0.18867700	-9.36336700
C	33.47999200	-4.18203900	-10.78310500	C	31.09200000	7.81100600	-10.77000100
C	33.31849100	-2.74237600	-10.32276500	C	30.08241800	7.05011400	-9.89159800
O	32.98128700	-2.40644500	-9.19277100	C	28.76971700	6.82871000	-10.58223000
C	32.15867700	-4.96441900	-10.85358500	C	27.57479000	7.45479500	-10.32952600
O	31.92763200	-5.62461400	-9.62873200	C	28.53483800	5.92561100	-11.68694800
H	33.95051000	-4.19514200	-11.77382100	C	27.16738300	6.05964200	-12.05680100
H	31.33013000	-4.28393300	-11.09445000	C	29.33959600	5.00484200	-12.38239500
H	32.23247700	-5.69048900	-11.67938200	N	26.60709600	6.99979000	-11.21239000
H	31.02430800	-5.99264100	-9.70537400	C	26.59846900	5.31271700	-13.09311700
N	33.56997600	-1.80615200	-11.28635700	C	28.78118500	4.26358800	-13.41728900
C	33.30496800	-0.40201500	-11.03296800	C	27.42481700	4.42113000	-13.76939800
H	33.74594600	-2.10686600	-12.23119500	H	31.14711600	7.33848600	-11.75714900
H	33.55316900	0.17080100	-11.92867700	H	30.51143900	6.07594600	-9.61930800
H	32.25264200	-0.23804300	-10.79604200	H	29.92310100	7.58820100	-8.94996400
C	30.70393000	-3.79212800	-14.83683700	H	27.33042400	8.19507800	-9.58096900
C	30.70076800	-2.81373500	-13.65520900	H	25.64651800	7.29863700	-11.22658700
C	29.38751000	-2.70070200	-12.92626700	H	30.38636800	4.86719700	-12.13024800
O	28.28945900	-2.91100900	-13.46101300	H	25.55616400	5.43365100	-13.36855200
O	29.54992700	-2.34956400	-11.67231600	H	29.39248800	3.57479000	-13.98727400
H	30.04340700	-4.63809500	-14.68328300	H	27.03014100	3.84394200	-14.59860000
H	31.44905800	-3.07743600	-12.90474000	O	30.28480900	0.87237300	-11.80977700
C	30.95833900	-1.79510600	-13.97250600	H	30.49108600	1.70744300	-12.27115300
C	27.87500700	1.06301300	-17.13701200	H	29.31655500	0.72333300	-11.76683800
C	29.25012000	1.57407200	-16.75703300	N	16.96962600	-3.30594700	-12.61957900

C	16.59799800	-4.45000600	-11.75900200
C	15.33145300	-3.94419800	-11.04659700
C	14.70658800	-2.97898500	-12.06548400
C	15.92765000	-2.26755800	-12.65479400
H	17.40472100	-4.66658300	-11.05477000
H	14.66816100	-4.76270700	-10.75804100
H	15.60755700	-3.39859100	-10.13761800
H	14.18584000	-3.54125200	-12.84835900
H	13.99344000	-2.28202700	-11.61922800
H	15.78918800	-1.91314200	-13.67881100
H	16.23668500	-1.40756000	-12.04776400
C	29.55091300	-2.94380900	-1.16226500
C	28.26556800	-3.75654300	-1.35150800
C	28.03395700	-4.23803200	-2.78471900
C	27.84827700	-3.12584300	-3.80235900
O	27.98162700	-1.93566100	-3.58118900
O	27.55111900	-3.61621500	-5.01312800
H	29.53838900	-2.10671000	-1.86445400
H	28.26441100	-4.62890900	-0.68676500
H	27.41391500	-3.13469300	-1.05153600
H	28.87911600	-4.84391200	-3.13819400
H	27.15904300	-4.89581800	-2.84850200
H	30.46540100	-3.51018200	-1.36775500
H	29.56614300	-2.49740400	-0.16232600
C	34.86200500	8.00000500	-10.31599600
C	35.23123800	6.50274000	-10.33180400
C	35.06490500	5.89242900	-11.68559600
C	34.14179300	5.01651000	-12.20353600
N	35.87492900	6.22476700	-12.76230200
C	35.42857900	5.55183900	-13.85816200
N	34.38118600	4.81478500	-13.54848400
H	35.56676300	8.59483100	-10.90650700
H	36.25521200	6.35355500	-9.96496500
H	34.57659800	5.96103100	-9.64179600
H	36.65745800	6.86086300	-12.73606900
H	33.32166000	4.51193500	-11.71484700
H	35.89119400	5.62562400	-14.83120800
H	33.61159900	3.63146000	-14.33409400
H	34.87099300	8.38159000	-9.28967900
H	33.87104900	8.09550700	-10.77198100

TS1-A_{Zn} (20.3 kcal/mol)

H	20.66694100	-6.80396900	-16.56503700
H	16.39007100	-5.37410900	-12.30884600
H	24.65797500	-6.75700600	-19.16499000
H	29.36481800	-8.34221100	-18.18000300
H	35.11200200	4.86999900	-6.01600200
H	32.10199600	7.76394600	-10.35099700
H	33.92503000	-0.03001800	-10.21101600
H	31.94995600	-4.27902300	-6.58590800
H	23.18498400	1.49699800	-4.32300300
H	22.41697500	4.62897000	-7.60400100
H	22.25400600	6.39000200	-15.14804600
H	33.53399900	5.46899900	-6.68100300
H	30.78100300	8.84800500	-10.93698000
H	23.93698400	6.30999100	-15.82101700
H	23.80798700	-0.12302400	-3.81401100
H	32.79689700	-3.33916200	-5.29794400
H	32.07502400	0.82298300	-17.96198600
H	30.43502000	-3.27794800	-15.73597800
H	31.70209400	-4.16471500	-14.93613300
H	30.41824100	-9.05969400	-14.20491400
H	20.88589800	-5.05002200	-16.84102600
H	34.15692600	-4.71598100	-10.10791100
H	23.72484400	-8.30795600	-7.05597300
H	21.59197300	-3.72901200	-7.31997300
H	27.89806000	0.15092600	-17.74188700
H	27.15897700	4.34402600	-6.69901600
C	29.55197400	-8.45617500	-13.91521300
C	29.40960500	-7.67115100	-15.20336600
O	29.98416100	-6.60258800	-15.39830300
C	29.77928400	-7.57121100	-12.70073600
C	28.57885800	-6.65734800	-12.45494000
C	28.69818600	-5.85675400	-11.16585300
O	29.41943500	-6.26819600	-10.24323400
O	28.00347600	-4.77140000	-11.09198600
H	28.70581500	-9.13842400	-13.77340700
H	29.96916500	-8.17481300	-11.81034300
H	30.66795900	-6.95657200	-12.87098500
H	28.44021300	-5.95959400	-13.28320200
H	27.65231200	-7.24659400	-12.39331800
N	28.73087000	-8.30426900	-16.18974100
C	28.69018700	-7.77097000	-17.53408300
C	27.24281800	-7.95694800	-17.99015700
O	26.76802600	-9.08503900	-18.08694600
H	28.26202600	-9.18461400	-16.03197700
H	29.02543400	-6.73419000	-17.48908700
N	26.51603700	-6.81996800	-18.14549000
C	25.05595100	-6.83995100	-18.14804200
C	24.50975500	-5.71840500	-17.26764000
H	26.97026800	-5.93947100	-17.95119600
H	24.75690200	-7.82223400	-17.77367500
H	23.41803100	-5.72516700	-17.27305400
H	24.84935200	-5.83210300	-16.23460700
H	24.83068100	-4.73329600	-17.62901500
C	23.25800300	6.03506800	-15.04095800
C	23.24560100	4.49282700	-15.01650500

C	22.38049200	3.87360600	-13.94858600
C	22.71720300	3.99455100	-12.59483600
C	21.25832400	3.10170800	-14.27591400
C	21.98195700	3.34729400	-11.60826400
C	20.50850900	2.44579200	-13.30085900
C	20.87702500	2.56387700	-11.95854800
O	20.13653700	1.89723300	-11.02591300
H	23.64527100	6.43619500	-14.09784800
H	22.91162500	4.13300800	-15.99702900
H	24.27503600	4.12860800	-14.90123800
H	23.59243400	4.57029800	-12.30573400
H	20.98015900	2.99127200	-15.32110800
H	22.27668600	3.42256200	-10.56904400
H	19.65387700	1.82946600	-13.55944400
H	20.58181700	1.97258800	-10.16976900
C	20.86217900	-5.84001400	-16.08296300
C	19.87978700	-5.68125900	-14.92714100
O	19.34476700	-6.65605100	-14.41071700
H	21.86270500	-5.87695800	-15.63578000
N	19.70271400	-4.40565400	-14.45244800
C	19.19495300	-4.19788200	-13.09501000
C	18.20019400	-3.05134100	-13.10833400
O	18.50589000	-1.94251500	-13.58381900
C	20.39557300	-3.96639800	-12.14867300
O	20.07348800	-4.13957800	-10.76546600
H	20.27405700	-3.65140700	-14.82433700
H	18.72338000	-5.13913600	-12.81581500
H	21.14818700	-4.71753600	-12.39721400
H	20.84002900	-2.98299100	-12.33367700
H	19.81301900	-3.28527200	-10.40019100
C	23.90620400	-7.35609400	-7.56598900
C	22.91152700	-6.30102900	-7.10321700
O	21.73940300	-6.60256200	-6.86769000
C	23.65527700	-7.60320100	-9.08309000
C	23.96422200	-6.41462300	-9.93456500
C	25.15538700	-6.01035000	-10.48334300
N	23.07692200	-5.38162300	-10.21080000
C	23.74354000	-4.41625700	-10.89219600
N	25.00632500	-4.77130700	-11.07152200
H	24.94681800	-7.06609400	-7.40466300
H	24.27875500	-8.43732600	-9.41831000
H	22.61078500	-7.90731200	-9.20742500
H	22.09962700	-5.32457700	-9.94517900
H	26.10952600	-6.51144400	-10.46434100
H	23.29493000	-3.50680700	-11.25487000
N	23.32772700	-5.00420900	-7.09689600
C	22.40697800	-3.96394100	-6.62799700
C	23.31061800	-2.76185300	-6.34299700
C	24.51429500	-2.97631300	-7.26707500
C	24.70932400	-4.49550500	-7.23487800
H	21.89948700	-4.32330900	-5.72597200
H	22.80355400	-1.81633100	-6.52058600
H	23.64125700	-2.78069800	-5.29898000
H	24.28625400	-2.64102900	-8.28427800
H	25.40483800	-2.44743600	-6.92613600
H	25.18311600	-4.87326500	-8.14071800
H	25.32448400	-4.78333000	-6.37253100
C	23.17502800	4.07105000	-8.16498500
C	24.47076100	3.93205500	-7.38554900
O	24.49316500	3.81532200	-6.15970800
H	22.78262700	3.06811000	-8.36151600
H	23.31890200	4.57981300	-9.11999200
N	25.60478200	3.92054300	-8.13753800
C	26.90902500	3.66695600	-7.52199000
C	27.88229300	3.80761900	-8.69813000
C	27.07306700	3.26453100	-9.87961100
C	25.66729800	3.81334200	-9.61079200
H	26.93725400	2.64740300	-7.11345500
H	28.11546100	4.86459700	-8.86494000
H	28.81853100	3.27168200	-8.53706700
H	27.45759900	3.58277800	-10.84851600
H	27.06248400	2.17173800	-9.86153300
H	25.53961400	4.80118700	-10.07234500
H	24.89261200	3.14534600	-9.99345700
C	23.37403200	0.46302800	-4.62998800
C	24.36223100	0.46748700	-5.81270300
C	23.79008300	0.52759300	-7.21663600
C	22.42059000	0.47777900	-7.49912600
C	24.68029000	0.55443400	-8.30461500
C	21.95696400	0.39500600	-8.81728300
C	24.22391000	0.50362500	-9.61921000
C	22.85406900	0.40564600	-9.88535100
H	22.42127500	-0.01488200	-4.87275100
H	25.04430800	1.31563600	-5.69113400
H	24.98896600	-0.43166600	-5.76710400
H	21.70096100	0.47591700	-6.68814100
H	25.74981600	0.59947200	-8.11580500
H	20.89036000	0.28494100	-9.00056900
H	24.93329600	0.53520400	-10.43599500
H	22.50518800	0.33618400	-10.90902100
C	32.20615700	-3.27979600	-6.21812100
C	30.88857300	-2.52478500	-5.94883900
C	29.88476900	-2.71977400	-7.04708500
C	30.03957400	-3.43486200	-8.20939700
N	28.57954400	-2.22086200	-6.99339200
C	27.99050500	-2.64216700	-8.11928800
N	28.83294200	-3.36821400	-8.86833600
H	32.78720600	-2.80058400	-7.00542800
H	30.44466600	-2.86444200	-5.00382200

H	31.08844100	-1.45312400	-5.80424200
H	27.73599100	-2.94786700	-5.67627300
H	30.88121600	-3.98177900	-8.60298800
H	26.99025600	-2.40657200	-8.44123600
H	28.57003700	-3.85119000	-9.74366500
C	33.48000200	-4.18207600	-10.78313500
C	33.34757000	-2.74074700	-10.31854100
O	33.07786700	-2.40296900	-9.17069700
C	32.16055600	-4.96424000	-10.81756700
O	31.92480100	-5.54494700	-9.55764700
H	33.93319500	-4.20514300	-11.78121100
H	31.33508500	-4.29657200	-11.10985600
H	32.23487700	-5.73582200	-11.60029500
H	31.02834200	-5.93703500	-9.61642600
N	33.55799800	-1.80720300	-11.29337300
C	33.30495800	-0.40199500	-11.03296500
H	33.64055400	-2.11268300	-12.25001500
H	33.56013700	0.17048100	-11.92771200
H	32.25341100	-0.22252300	-10.80116700
C	30.70382300	-3.79243700	-14.83666400
C	30.40818300	-2.82508900	-13.67505900
C	28.93498800	-2.40148000	-13.66662400
O	28.04272500	-3.28886300	-13.69274400
O	28.68280300	-1.14209200	-13.62028200
H	30.05978300	-4.66286400	-14.75918400
H	30.57422900	-3.31490300	-12.70878100
H	31.02633800	-1.92545700	-13.69805600
C	27.87495400	1.06310500	-17.13710400
C	29.24695500	1.58305300	-16.76066300
O	29.40626700	2.65276000	-16.17439900
C	27.04880100	0.80015100	-15.86891500
C	25.64887600	0.35751700	-16.19185400
C	24.68549500	1.29234800	-16.58273500
C	25.27368600	-0.98744600	-16.11004600
C	23.38227300	0.90218800	-16.88003200
C	23.97542500	-1.39959900	-16.40363900
C	23.03616800	-0.44522300	-16.79089500
O	21.74439700	-0.87926600	-17.04695600
H	27.38537100	1.83636400	-17.73941600
H	27.55744400	0.04093600	-15.27111600
H	27.03186500	1.71248000	-15.26978400
H	24.95029800	2.34459400	-16.63463700
H	25.99848700	-1.71992900	-15.76491100
H	22.63691900	1.64271500	-17.16189800
H	23.68012300	-2.43447800	-16.27145100
H	21.22096100	-0.13128200	-17.36400800
N	30.27020900	0.76441900	-17.10186500
C	31.68299000	1.10903600	-16.98000100
C	32.35210800	0.35628300	-15.82762900
C	31.76549000	0.74139300	-14.46740500
C	32.13463200	2.12468800	-13.96848400
O	33.06123100	2.72617200	-14.68589400
O	31.64590100	2.60936900	-12.94552200
H	30.04382100	-0.09945600	-17.56990700
H	31.75770900	2.18856600	-16.84853300
H	32.21281500	-0.72165100	-15.97759100
H	33.42813500	0.55234800	-15.84364000
H	30.67585500	0.65016100	-14.46219400
H	32.10278800	0.04788300	-13.68968000
C	27.13835500	-0.90625700	-11.21270700
O	27.81128000	-0.03722800	-10.59755500
O	27.04031200	-2.12011800	-10.89445700
C	26.40778300	-0.40899500	-12.47686900
C	25.18624000	-1.12811000	-12.85176700
O	25.11259500	-2.40717100	-12.84614800
C	24.03402000	-0.37280100	-13.23739100
C	24.08101800	0.99123700	-13.32473500
C	25.27249500	1.71508500	-13.03228700
C	26.37401600	1.03997000	-12.60020100
H	27.45541700	-0.83069700	-13.21936000
H	23.12460400	-0.91192300	-13.48165900
H	23.19271700	1.52919900	-13.62704300
H	25.29163300	2.79401400	-13.11878100
H	27.26622000	1.58308700	-12.31468900
Zn	26.56869700	-3.74701600	-12.12065900
O	25.93358300	-4.96806000	-13.94995100
H	25.01282700	-4.72961600	-14.17388000
H	26.50882400	-4.46300800	-14.54390900
O	23.28740300	-3.85318800	-14.15298900
H	22.49951200	-3.33608800	-14.38820600
H	23.84152700	-3.21844300	-13.63993800
O	21.11605500	-1.92643300	-14.54823300
H	21.18206600	-1.50452500	-15.42386300
H	20.21323100	-1.74475300	-14.19993400
C	34.22902200	4.62602000	-6.61599000
C	33.57567300	3.37153700	-6.01516200
C	32.21982400	2.99707100	-6.62788100
C	31.89324900	1.51270700	-6.38062700
N	30.51866500	1.12448600	-6.68168200
C	30.02809400	0.95048900	-7.93058700
N	30.71053100	1.39847500	-8.98313900
N	28.82190100	0.39795300	-8.07382500
H	34.57146000	4.41944600	-7.63749800
H	34.27215800	2.53103700	-6.13763600
H	33.45052200	3.49990100	-4.93293100
H	31.42027100	3.61807500	-6.20877100
H	32.23742900	3.21904900	-7.70214600
H	32.58819000	0.87363000	-6.94228200
H	32.05176500	1.28493600	-5.32341700

H	29.95432800	0.75045000	-5.93284100
H	31.61167500	1.81753000	-8.83540000
H	30.46775600	1.12732100	-9.96839600
H	28.57173600	-0.32875200	-7.39238200
H	28.49259700	0.17797500	-9.02950200
C	31.09198900	7.81102200	-10.77004300
C	30.08035300	7.04893900	-9.89425100
C	28.77013700	6.83677100	-10.59243300
C	27.58162000	7.48154100	-10.35790600
C	28.53954200	5.94088900	-11.70382700
C	27.18270500	6.10281000	-12.10059000
C	29.34061300	5.00733300	-12.38613000
N	26.62126000	7.04433500	-11.25824300
C	26.62659000	5.38423600	-13.16362900
C	28.79319900	4.28877300	-13.44251200
C	27.45272600	4.48573800	-13.83212000
H	31.14814300	7.33869100	-11.75719300
H	30.50625400	6.07271500	-9.62519100
H	29.92021200	7.58420000	-8.95117300
H	27.33711100	8.22496100	-9.61250300
H	25.67078700	7.37161400	-11.29843100
H	30.37570700	4.83948700	-12.10586400
H	25.59643200	5.53644000	-13.46775700
H	29.39975600	3.58501500	-13.99823200
H	27.07432900	3.93277200	-14.68537800
O	30.27788600	0.69774800	-11.51696900
H	30.47840600	1.45739900	-12.09931900
H	29.33223700	0.46344200	-11.55849300
N	16.97135800	-3.30424000	-12.61829700
C	16.59789100	-4.44996800	-11.75913200
C	15.33174800	-3.94377600	-11.04645000
C	14.70861500	-2.97555200	-12.06347700
C	15.93078500	-2.26403800	-12.65017900
H	17.40462000	-4.66860600	-11.05551100
H	14.66730900	-4.76209300	-10.76019500
H	15.60777400	-3.40060900	-10.13597600
H	14.18785100	-3.53532200	-12.84807800
H	13.99597200	-2.27887400	-11.61605500
H	15.79316800	-1.90611100	-13.67306500
H	16.24116000	-1.40668000	-12.04011600
C	29.55092000	-2.94380800	-1.16231800
C	28.26618100	-3.76171800	-1.33511800
C	28.02307900	-4.25577800	-2.76106300
C	27.82685400	-3.15241800	-3.78668600
O	27.95239700	-1.95922800	-3.57133500
O	27.53253900	-3.65339600	-4.99113200
H	29.53133400	-2.11007500	-1.86806000
H	28.27353500	-4.62764900	-0.66193500
H	27.41582700	-3.13903500	-1.03296800
H	28.86600100	-4.86328300	-3.11689500
H	27.14874300	-4.91560400	-2.81183000
H	30.46540900	-3.51018300	-1.36771600
H	29.56613300	-2.49740900	-0.16232300
C	34.86198400	7.99999100	-10.31600900
C	35.21575600	6.49759700	-10.32656900
C	34.96624100	5.87081600	-11.65993300
C	34.01798300	4.98228400	-12.10741500
N	35.69401000	6.20557000	-12.79279500
C	35.17762500	5.52284100	-13.85120900
N	34.16273800	4.77683500	-13.46477600
H	35.57016800	8.58823300	-10.90858000
H	36.25577600	6.34095700	-10.01196200
H	34.59205700	5.97409900	-9.59524200
H	36.46899400	6.85051100	-12.82510200
H	33.24232100	4.47197000	-11.55580500
H	35.56862400	5.59616500	-14.85520700
H	33.38212700	3.58624000	-14.23357500
H	34.87100800	8.38158600	-9.28967800
H	33.87104900	8.09552800	-10.77197600

Int-A_{Zn} (12.9 kcal/mol)

H	20.66696600	-6.80398100	-16.56502200
H	16.39006300	-5.37409300	-12.30886900
H	24.65797500	-6.75700600	-19.16499000
H	29.36482200	-8.34221000	-18.18000000
H	35.11213100	4.86994400	-6.01617000
H	32.10199700	7.76390900	-10.35100500
H	33.92503000	-0.03001400	-10.21101800
H	31.94997100	-4.27902300	-6.58591900
H	23.18498300	1.49699500	-4.32299600
H	22.41696300	4.62894500	-7.60399400
H	22.25400800	6.39000700	-15.14805300
H	33.53406900	5.46905100	-6.68107300
H	30.78101700	8.84801000	-10.93697700
H	23.93698600	6.30998200	-15.82101800
H	23.80798400	-0.12303100	-3.81401500
H	32.79693100	-3.33914500	-5.29796400
H	32.07472200	0.82269300	-17.96202300
H	30.43512300	-3.27793100	-15.73600000
H	31.70212600	-4.16462500	-14.93615200
H	30.41824100	-9.05967800	-14.20494600
H	20.88588700	-5.05002200	-16.84102700
H	34.15693300	-4.71599400	-10.10792800
H	23.72483800	-8.30794500	-7.05595300
H	21.59196600	-3.72900200	-7.31996100
H	27.89806400	0.15093000	-17.74189300
H	27.15900700	4.34393000	-6.69894600

C	29.55199100	-8.45621800	-13.91518400	H	27.46132500	3.65826400	-10.85086400
C	29.41164200	-7.67478600	-15.20594600	H	27.06111100	2.22722700	-9.90071200
O	29.99339400	-6.61078500	-15.40341000	H	25.52673300	4.84822800	-10.04679700
C	29.78346400	-7.56290400	-12.70797800	H	24.89717800	3.18374300	-10.00539000
C	28.58274700	-6.64714100	-12.46525900	C	23.37403400	0.46304400	-4.62999100
C	28.74198200	-5.80112100	-11.20886100	C	24.30890600	0.46629800	-5.84803000
O	29.40627500	-6.23629800	-10.25515900	C	23.65349200	0.55612900	-7.21352100
O	28.14997200	-4.65366200	-11.20210600	C	22.26751400	0.56746800	-7.41287000
H	28.70562600	-9.13715700	-13.76911900	C	24.47643700	0.56256000	-8.35161500
H	29.97698500	-8.15711600	-11.81219900	C	21.72096600	0.52511500	-8.70114500
H	30.66995500	-6.94821100	-12.88919800	C	23.93796300	0.55006100	-9.63430200
H	28.41648300	-5.98542100	-13.31741600	C	22.55312200	0.51114200	-9.82063300
H	27.66588900	-7.24395100	-12.35308300	H	22.41321500	-0.01348600	-4.84559500
N	28.72741200	-8.30493800	-16.19002100	H	25.00636100	1.30526300	-5.75334500
C	28.69017300	-7.77096900	-17.53408500	H	24.92425400	-0.44110100	-5.84706300
C	27.24340600	-7.95563000	-17.99309200	H	21.59763500	0.58694900	-6.56103700
O	26.76927700	-9.08355600	-18.09554300	H	25.55625900	0.55635200	-8.23926500
H	28.25566700	-9.18370300	-16.03218000	H	20.64070000	0.47057800	-8.82003700
H	29.02625500	-6.73456700	-17.48804900	H	24.60515100	0.56981200	-10.48300400
N	26.51618100	-6.81840700	-18.14481400	H	22.13976400	0.46547600	-10.82155900
C	25.05595700	-6.83995000	-18.14804500	C	32.20610200	-3.27981700	-6.21808100
C	24.50862100	-5.71793200	-17.26915500	C	30.88632900	-2.52859000	-5.94651800
H	26.96868300	-5.93928600	-17.94028100	C	29.89427200	-2.70307900	-7.05869500
H	24.75705800	-7.82224700	-17.77350200	C	30.08537400	-3.34202300	-8.25893200
H	23.41700800	-5.72856300	-17.27049600	N	28.56761300	-2.26967400	-6.98436900
H	24.85297400	-5.82669300	-16.23735100	C	28.00001600	-2.65545700	-8.13300400
H	24.82543300	-4.73310100	-17.63483700	N	28.87888700	-3.29449700	-8.92036000
C	23.25800100	6.03506300	-15.04093600	H	32.78797100	-2.79800600	-7.00313100
C	23.22758100	4.49520700	-14.99284100	H	30.43241800	-2.88762400	-5.01401200
C	22.32753700	3.92177300	-13.92753300	H	31.08544100	-1.45982800	-5.77745200
C	22.62944300	4.08654800	-12.56987100	H	27.75855000	-3.01202100	-5.67452700
C	21.98575000	3.16059600	-14.25671500	H	30.94854500	-3.84258900	-8.66486600
C	21.85742300	3.48744000	-11.58055600	H	26.99078300	-2.44985400	-8.44682600
C	20.41140900	2.55352000	-13.27908800	H	28.64197900	-3.75227700	-9.81690800
C	20.74765400	2.71100500	-11.93203300	C	33.48000100	-4.18206100	-10.78311400
O	19.97316100	2.08719000	-10.99785300	C	33.36364000	-2.73986600	-10.31598700
H	23.64500800	6.44331300	-14.10040200	O	33.13832400	-2.39716800	-9.16036100
H	22.90453100	4.12115900	-15.97152500	C	32.15771100	-4.95893400	-10.80739800
H	24.24767400	4.11570700	-14.84976300	O	31.91499700	-5.51256800	-9.53701400
H	23.50484500	4.66064800	-12.27752600	H	33.92704000	-4.20789300	-11.78363600
H	20.94352100	3.01988500	-15.30414100	H	31.33809300	-4.29358600	-11.11614400
H	22.12575800	3.59637900	-10.53704900	H	32.23302500	-5.74505600	-11.57552400
H	19.55169700	1.94493900	-13.53896600	H	31.00861700	-5.88267400	-9.58405900
H	20.40781300	2.16343100	-10.13608000	N	33.53986500	-1.80590100	-11.29929400
C	20.86216200	-5.84000100	-16.08296900	C	33.30495600	-0.40200600	-11.03296400
C	19.88121700	-5.68208200	-14.92616000	H	33.58446200	-2.11185400	-12.25859900
O	19.35115200	-6.65749400	-14.40618800	H	33.55728700	0.17444000	-11.92521300
H	21.86278100	-5.87744300	-15.63593200	H	32.25598500	-0.20409400	-10.78334000
N	19.69960600	-4.40600500	-14.45339300	C	30.70364900	-3.79252900	-14.83661900
C	19.19492500	-4.19790400	-13.09504800	C	30.46726900	-2.88266600	-13.62256700
C	18.20053800	-3.05110300	-13.10572600	C	29.07597800	-2.24116200	-13.62961200
O	18.50686500	-1.94053700	-13.57810800	O	28.05953200	-3.01123600	-13.75234600
C	20.39582500	-3.96865200	-12.14770500	O	28.99286800	-0.98949300	-13.52286700
O	20.06639700	-4.11974900	-10.76489000	H	30.05663000	-4.66200900	-14.77345700
H	20.26522800	-3.64996900	-14.82889400	H	30.52802400	-3.47459100	-12.70344100
H	18.72232400	-5.13850800	-12.81564500	H	31.20801400	-2.08090600	-13.55100100
H	21.13978800	-4.73241400	-12.38525100	C	27.87484500	1.06309500	-17.13709800
H	20.85222700	-2.99316700	-12.34435400	C	29.24996600	1.61615700	-16.81821200
H	19.81343500	-3.25752800	-10.41302400	O	29.41054200	2.73411700	-16.33126400
C	23.90620500	-7.35615700	-7.56598700	C	27.12091400	0.78821000	-15.81896800
C	22.89745200	-6.30163200	-7.13252000	C	25.69955100	0.37396800	-16.07900900
O	21.71746200	-6.59695300	-6.93333400	C	24.74642600	1.33244000	-16.43946400
C	23.74896400	-7.58668100	-9.09856700	C	25.30025900	-0.96438200	-16.00545100
C	24.08540900	-6.39254200	-9.93983800	C	23.43506100	0.97002600	-16.73263700
C	25.26981600	-6.00116600	-10.51817500	C	23.99228700	-1.34871500	-16.29898800
N	23.19958200	-5.35972200	-10.22152700	C	23.06920700	-0.37377700	-16.67233000
C	23.85834800	-4.41056900	-10.93224100	O	21.77353100	-0.78232400	-16.94895900
N	25.11734900	-4.77175600	-11.13230600	H	27.33961900	1.82517100	-17.71227000
H	24.93564300	-7.05773200	-7.35163000	H	27.65425700	0.02135300	-15.24927000
H	24.40104800	-8.41043900	-9.40332300	H	27.14546200	1.69793100	-15.21391000
H	22.71792900	-7.90364400	-9.28958400	H	25.03123900	2.37966700	-16.48348100
H	22.22840200	-5.29615900	-9.93711300	H	26.01886000	-1.71212800	-15.68019800
H	26.21971700	-6.51095600	-10.50540000	H	22.70068900	1.72734500	-16.99757500
H	23.40463000	-3.50303400	-11.29320700	H	23.68220900	-2.38166600	-16.18946900
N	23.32438000	-5.00761500	-7.09799700	H	21.26268500	-0.01924300	-17.25001700
C	22.40698200	-3.96393500	-6.62801500	N	30.27094100	0.76299900	-17.07654900
C	23.31061700	-2.75872800	-6.35042900	C	31.68350000	1.10941000	-16.97997700
C	24.52781400	-2.98867300	-7.25374100	C	32.37638300	0.34459900	-15.84934600
C	24.71171500	-4.50861000	-7.20924000	C	31.82772500	0.71538000	-14.47136300
H	21.90069300	-4.31908600	-5.72345200	C	32.25415100	2.06842600	-13.93794500
H	22.80695800	-1.81543000	-6.55189000	O	33.14565700	2.68845800	-14.67945200
H	23.62609900	-2.75855900	-5.30172900	O	31.82963000	2.51181300	-12.86663200
H	24.31949400	-2.65828300	-8.27681400	H	30.04250500	-0.14030300	-17.46261500
H	25.41700400	-2.46426400	-6.90167900	H	31.75654300	2.18836800	-16.84493200
H	25.20172900	-4.89419200	-8.10321800	H	32.22709300	-0.73103000	-16.00627400
H	25.30802600	-4.79590400	-6.33339700	H	33.45292600	0.53356100	-15.89241700
C	23.17503800	4.07110500	-8.16499100	H	30.73540000	0.65696100	-14.45677500
C	24.46837600	3.92306400	-7.38346000	H	32.15144500	-0.01529100	-13.72180600
O	24.48770000	3.79092700	-6.15894100	C	26.82905700	-0.85624500	-11.04691100
H	22.77923700	3.07291500	-8.37423000	O	27.11945100	0.03371200	-10.22889800
H	23.32662400	4.58902400	-9.11392600	O	26.92999000	-2.10043300	-10.88352400
N	25.60290200	3.92227400	-8.13375600	C	26.29056700	-0.36680100	-12.45194700
C	26.90900100	3.66702700	-7.52208300	C	25.03643400	-1.08799300	-12.82102300
C	27.88039200	3.83587400	-8.69659200	O	25.01917400	-2.35100500	-12.86631500
C	27.07547200	3.31771700	-9.89097400	C	23.85973500	-0.32568700	-13.12203300
C	25.66649800	3.85051900	-9.60914600	C	23.92414000	1.03553300	-13.17573000
H	26.94435800	2.64408800	-7.12434300	C	25.13288700	1.76914600	-12.90432500
H	28.11250400	4.89713200	-8.83661500	C	26.25722000	1.10910400	-12.55087700
H	28.81805900	3.29937900	-8.54562700	H	27.12018400	-0.72696900	-13.09972100

H	22.94519400	-0.85567600	-13.36834400
H	23.03276300	1.58678200	-13.44275300
H	25.12889200	2.84931400	-12.98064700
H	27.18585800	1.62475900	-12.33153800
Zn	26.67258200	-3.66784000	-12.20925100
O	26.08377200	-4.77494600	-14.07586100
H	25.17184800	-4.54682300	-14.33623100
H	26.69272300	-4.23674600	-14.60884800
O	23.27043000	-3.89066200	-14.21489500
H	22.48250700	-3.37480600	-14.45386100
H	23.77765700	-3.26446300	-13.65332700
O	21.11015000	-1.92222500	-14.51859300
H	21.18650700	-1.46995300	-15.37839700
H	20.20096700	-1.75350600	-14.17712300
C	34.22877800	4.62602500	-6.61572900
C	33.57240900	3.32640500	-6.13324400
C	32.31085600	2.92683900	-6.91808600
C	31.97293100	1.43137900	-6.73002800
N	30.56315300	1.09083600	-6.89577800
C	29.91643900	0.91595500	-8.07090200
N	30.46957300	1.32090900	-9.21431800
N	28.69783200	0.38026700	-8.04411600
H	34.59828100	4.47357400	-7.63971400
H	34.31365900	2.51972600	-6.21082000
H	33.31552500	3.39828000	-5.06903700
H	31.45648700	3.53163700	-6.59425200
H	32.46201900	3.15204400	-7.98324800
H	32.57919900	0.80794600	-7.39896700
H	32.23307300	1.13241600	-5.71115600
H	30.05200500	0.79630300	-6.07708200
H	31.29536800	1.89505400	-9.19033600
H	30.04175700	1.13730700	-10.15052900
H	28.52228400	-0.34302300	-7.33890200
H	28.18931800	0.21607800	-8.92983300
C	31.09197500	7.81101300	-10.77005800
C	30.07295300	7.04051000	-9.91154400
C	28.77738000	6.82068700	-10.63501900
C	27.58109800	7.45797100	-10.42073000
C	28.57208500	5.92489600	-11.75187000
C	27.22058800	6.07741400	-12.17037100
C	29.38970100	4.99577200	-12.42104400
N	26.63938300	7.01597900	-11.33811000
C	26.68478300	5.35118500	-13.23865500
C	28.86274400	4.27125300	-13.48321000
C	27.52649200	4.45604300	-13.89227200
H	31.15484000	7.34500400	-11.76015000
H	30.50107700	6.06683700	-9.63687300
H	29.89175500	7.57229900	-8.97037400
H	27.31918500	8.19889300	-9.67876600
H	25.68693300	7.33519900	-11.39239300
H	30.42103000	4.83566100	-12.12172000
H	25.65812400	5.49653000	-13.55870400
H	29.47991000	3.56796200	-14.02812400
H	27.16643100	3.90024800	-14.75145700
O	29.66457400	1.09221300	-11.78277000
H	30.35268100	1.61812700	-12.23743100
H	29.52138300	0.28500200	-12.31704600
N	16.97148000	-3.30409100	-12.61794700
C	16.59791000	-4.44997600	-11.75908100
C	15.33174600	-3.94387800	-11.04629800
C	14.70896400	-2.97470600	-12.06261300
C	15.93142600	-2.26316600	-12.64858200
H	17.40476600	-4.66809300	-11.05555000
H	14.66706400	-4.76224200	-10.76081100
H	15.60783000	-3.40158600	-10.13534800
H	14.18806700	-3.53359300	-12.84774900
H	13.99660700	-2.27804300	-11.61473300
H	15.79409000	-1.90396900	-13.67105300
H	16.24243500	-1.40686000	-12.03739600
C	29.55091600	-2.94385200	-1.16225600
C	28.27021500	-3.77156800	-1.32255400
C	28.02959700	-4.28985400	-2.73990400
C	27.82303000	-3.20091800	-3.77898800
O	27.90963200	-2.00364900	-3.56788600
O	27.56646800	-3.71893300	-4.98446000
H	29.52402000	-2.11339500	-1.87151800
H	28.28376500	-4.62631200	-0.63522500
H	27.41649000	-3.14894900	-1.03028600
H	28.87568100	-4.89734100	-3.08763200
H	27.15904300	-4.95577500	-2.77918900
H	30.46540800	-3.51017200	-1.36774700
H	29.56613800	-2.49737600	-0.16233700
C	34.86214500	7.99995900	-10.31615700
C	35.22365100	6.49986900	-10.32123200
C	34.99853900	5.86498900	-11.65487100
C	34.08815500	4.93782200	-12.10175500
N	35.71995700	6.22034300	-12.78568400
C	35.23684200	5.51218300	-13.84277200
N	34.24952000	4.72963500	-13.45684500
H	35.56962000	8.59041600	-10.90756800
H	36.26040200	6.35148600	-9.99174600
H	34.59405900	5.97366500	-9.59697100
H	36.46926700	6.89494700	-12.81792300
H	33.32900800	4.40033500	-11.55320300
H	35.62934300	5.59563500	-14.84536100
H	33.48865200	3.53943000	-14.21874400
H	34.87087600	8.38153600	-9.28965800
H	33.87101000	8.09563500	-10.77187000

TS2-A_{Zn} (17.9 kcal/mol)

H	20.66694600	-6.80396900	-16.56503800
H	16.39005300	-5.37409400	-12.30886400
H	24.65797500	-6.75700700	-19.16499000
H	29.36482200	-8.34220900	-18.18000000
H	35.11211600	4.86996200	-6.01615500
H	32.10199200	7.76390000	-10.35099400
H	33.92503500	-0.03001500	-10.21102200
H	31.94997700	-4.27903600	-6.58588700
H	23.18497800	1.49699400	-4.32299500
H	22.41694900	4.62894600	-7.60401400
H	22.25403100	6.39002200	-15.14821700
H	33.53409000	5.46907000	-6.68104200
H	30.78105100	8.84802500	-10.93694500
H	23.93693000	6.30998400	-15.82106600
H	23.80795700	-0.12305500	-3.81401700
H	32.79691200	-3.33919800	-5.29795600
H	32.07471100	0.82269700	-17.96202900
H	30.43519800	-3.27793000	-15.73602200
H	31.70214900	-4.16455100	-14.93619500
H	30.41823100	-9.05968700	-14.20495600
H	20.88587800	-5.05002000	-16.84102600
H	34.15693200	-4.71599400	-10.10792700
H	23.72482700	-8.30796000	-7.05598500
H	21.59199600	-3.72898600	-7.31999100
H	27.89804300	0.15092400	-17.74188500
H	27.15900800	4.34385500	-6.69888500
C	29.55201000	-8.45621600	-13.91517500
C	29.40908000	-7.67387800	-15.20548000
O	29.98438600	-6.60593700	-15.40049200
C	29.77444400	-7.55681000	-12.70506800
C	28.58763000	-6.61381900	-12.48581000
C	28.69620800	-5.79246300	-11.20487600
O	29.41528400	-6.18848000	-10.27398700
O	27.99346200	-4.70874600	-11.14417200
H	28.70589500	-9.13776800	-13.77022700
H	29.94108800	-8.15231600	-11.80452500
H	30.67582800	-6.95965800	-12.86965200
H	28.47822600	-5.92630300	-13.32694700
H	27.64839100	-7.18380700	-12.43411400
N	28.72868400	-8.30653200	-16.19079300
C	28.69017100	-7.77096700	-17.53408600
C	27.24398600	-7.95397800	-17.99514300
O	26.77168600	-9.08190600	-18.10585000
H	28.25871800	-9.18631700	-16.03352600
H	29.02708200	-6.73488500	-17.48665000
N	26.51598500	-6.81644600	-18.14092300
C	25.05595800	-6.83995000	-18.14804600
C	24.50032200	-5.72318100	-17.26961300
H	26.96663600	-5.93854700	-17.92751000
H	24.75795200	-7.82371000	-17.77636900
H	23.40895800	-5.73001400	-17.28674100
H	24.82847400	-5.84307900	-16.23493500
H	24.82496200	-4.73623400	-17.62261000
C	23.25804200	6.03503500	-15.04069500
C	23.22860700	4.49460500	-14.97881300
C	22.31858800	3.92858100	-13.91699400
C	22.60558600	4.10593400	-12.55791400
C	21.18981700	3.16917900	-14.24978200
C	21.81861100	3.52284600	-11.57075300
C	20.38823000	2.57698500	-13.27473700
C	20.71059100	2.74660700	-11.92594900
O	19.92491200	2.13327600	-10.99236200
H	23.64440600	6.45029000	-14.10266000
H	22.91442700	4.11213700	-15.95687500
H	24.24621100	4.11448000	-14.82171500
H	23.47992500	4.67972200	-12.26180600
H	20.94582000	3.01769600	-15.29830900
H	22.07556600	3.64215700	-10.52541200
H	19.52971700	1.96818500	-13.53808100
H	20.35469500	2.21382600	-10.12882400
C	20.86219900	-5.84002300	-16.08295300
C	19.88511700	-5.68553600	-14.92168500
O	19.37397400	-6.66527300	-14.38998000
H	21.86358500	-5.87569000	-15.63746500
N	19.68662600	-4.40876600	-14.45901600
C	19.19492600	-4.19789700	-13.09503800
C	18.20155800	-3.04985000	-13.10172800
O	18.50717700	-1.93799000	-13.56984500
C	20.40953900	-3.96514800	-12.16791500
O	20.10234700	-4.10332200	-10.77760600
H	20.24415800	-3.64916900	-14.84312700
H	18.72571300	-5.13755100	-12.80715600
H	21.14583600	-4.73454300	-12.41044700
H	20.86664600	-2.99333200	-12.38085600
H	19.86466200	-3.23572400	-10.42832600
C	23.90622000	-7.35610000	-7.56595900
C	22.90903900	-6.30374600	-7.10318700
O	21.74254400	-6.60794500	-6.84719500
C	23.69170600	-7.58928200	-9.09296200
C	24.01843500	-6.41548500	-9.96673500
C	25.19072900	-6.06831600	-10.59459200
N	23.14375800	-5.37412300	-10.25784100
C	23.79833300	-4.46498300	-11.02402300
N	25.04248500	-4.85943900	-11.24703300
H	24.94332500	-7.06349400	-7.38340800

H	24.31707400	-8.42811900	-9.41272300	H	27.11694200	1.67292100	-15.21325900
H	22.64937500	-7.89147500	-9.24222000	H	25.02596900	2.43120300	-16.49173000
H	22.17873600	-5.28288600	-9.95968800	H	25.92213600	-1.69817400	-15.77225100
H	26.13031700	-6.59645900	-10.59389300	H	22.68113800	1.83799400	-17.00938200
H	23.35842700	-3.55896300	-11.40593200	H	23.58010700	-2.30588600	-16.27816300
N	23.32203000	-5.00439500	-7.10916900	H	21.18464600	0.13638200	-17.21234200
C	22.40694700	-3.96398400	-6.62797200	N	30.27096700	0.76149700	-17.09741000
C	23.31005700	-2.75818000	-6.35975600	C	31.68350500	1.10941100	-16.97996200
C	24.50467200	-2.97496800	-7.29550000	C	32.35542600	0.34412400	-15.83648900
C	24.70048900	-4.49501000	-7.26832300	C	31.77622400	0.70924300	-14.46726100
H	21.90655800	-4.32234300	-5.72208000	C	32.20741300	2.04789300	-13.90068200
H	22.79802400	-1.81495700	-6.53983100	O	33.05965400	2.70546700	-14.65361500
H	23.65173700	-2.76757200	-5.31923200	O	31.81391700	2.44051500	-12.79898400
H	24.27171800	-2.63684900	-8.31055400	H	30.04606000	-0.09749500	-17.57556500
H	25.39665300	-2.44627300	-6.95733800	H	31.75809600	2.18791100	-16.84162800
H	25.15995800	-4.87182800	-8.18275200	H	32.21473200	-0.73147500	-15.99997700
H	25.32965400	-4.78466100	-6.41644700	H	33.43183300	0.53826000	-15.85169300
C	23.17506600	4.07109800	-8.16496500	H	30.68144500	0.69280100	-14.48469900
C	24.46812700	3.92456500	-7.38308600	H	32.06150000	-0.03551100	-13.71683400
O	24.48940200	3.79581900	-6.15819200	C	26.69782300	-1.01386700	-10.73940600
H	22.77959700	3.07335200	-8.37579100	O	27.09037400	-0.06304800	-10.11955400
H	23.32741400	4.58928400	-9.11358400	O	26.48164900	-2.20183900	-10.67403900
N	25.60254500	3.92233500	-8.13408400	C	26.26522500	-0.39739700	-12.64873600
C	26.90898900	3.66712400	-7.52217300	C	25.06964200	-1.13929900	-12.93533300
C	27.87836600	3.81904500	-8.70084500	O	25.08763400	-2.43167700	-13.01150300
C	27.06672100	3.28884300	-9.88624100	C	23.85351500	-0.41030200	-13.10897300
C	25.66384100	3.83821000	-9.60908500	C	23.86516600	0.96463500	-13.09480200
H	26.94009800	2.64627900	-7.11793700	C	25.05622200	1.70466800	-12.85694500
H	28.11233100	4.87753200	-8.85696900	C	26.23340400	1.03087500	-12.65519200
H	28.81561000	3.28226100	-8.54741900	H	27.22205600	-0.87594500	-12.85086700
H	27.45340000	3.60424500	-10.85386300	H	22.94058800	-0.95336000	-13.33191300
H	27.04113800	2.19894300	-9.87581700	H	22.93929000	1.49666600	-13.26880000
H	25.53711000	4.83373200	-10.05458500	H	25.03045700	2.78727900	-12.84443600
H	24.88733100	3.17798800	-10.00124800	H	27.16329900	1.55914500	-12.46807100
C	23.37408100	0.46306700	-4.63000000	Zn	26.58556200	-3.75640800	-12.31641100
C	24.29958900	0.46699900	-5.85370100	O	26.09811300	-4.84718400	-14.20893000
C	23.63129300	0.56528600	-7.21266100	H	25.20004200	-4.56870900	-14.47391100
C	22.24441200	0.57725000	-7.40213500	H	26.73290900	-4.32968700	-14.72905900
C	24.44618500	0.57983200	-8.35624600	O	23.31153200	-3.89481700	-14.32143800
C	21.69045000	0.54410600	-8.68786500	H	22.52041000	-3.37480300	-14.53597600
C	23.90208500	0.57000300	-9.63682600	H	23.85067700	-3.27227000	-13.77292700
C	22.51526400	0.53356400	-9.81214200	O	21.08450600	-1.94289500	-14.59432600
H	22.41198600	-0.01288500	-4.84147800	H	21.15599500	-1.44989400	-15.43150300
H	25.00154700	1.30255400	-5.76158700	H	20.19339700	-1.75506400	-14.22026900
H	24.91017700	-0.44369800	-5.86132500	C	34.22876000	4.62597900	-6.61578000
H	21.57981400	0.59231100	-6.54609500	C	33.58842700	3.34683700	-6.06459400
H	25.52557200	0.57978300	-8.24047400	C	32.29541300	2.92489800	-6.77378600
H	20.60934200	0.49576400	-8.80139800	C	31.98535100	1.43548600	-6.52501600
H	24.55307000	0.58980300	-10.49945900	N	30.58944000	1.06095900	-6.71371100
H	22.09751700	0.49356600	-10.81116100	C	29.96663600	0.92724400	-7.90212600
C	32.20612100	-3.27974800	-6.21812200	N	30.54624700	1.32697300	-9.02919300
C	30.88959500	-2.52089400	-5.96219500	N	28.72236900	0.43354100	-7.90114400
C	29.89318800	-2.70755100	-7.07000000	H	34.58465700	4.44410300	-7.63856300
C	30.05874900	-3.37889900	-8.25743400	H	34.32435000	2.53549300	-6.14616600
N	28.57258500	-2.25928900	-6.98620800	H	33.38216900	3.45823500	-4.99280600
C	27.98153400	-2.67370500	-8.11155500	H	31.45226700	3.53288000	-6.42733100
N	28.83968600	-3.34112000	-8.89940000	H	32.39474900	3.12491200	-7.84913800
H	32.79353700	-2.80483800	-7.00359700	H	32.62205100	0.79770200	-7.15146400
H	30.43075600	-2.86306500	-5.02585200	H	32.22586400	1.18803500	-5.48792500
H	31.09185900	-1.45111000	-5.81040100	H	30.05145200	0.78945900	-5.90431600
H	27.75036100	-3.01128000	-5.67146000	H	31.42436600	1.81536000	-8.98607800
H	30.91134700	-3.89645300	-8.66556900	H	30.14168200	1.13930200	-9.98612200
H	26.95663400	-2.49922400	-8.38870200	H	28.53099700	-0.33811900	-7.24875600
H	28.57670100	-3.82815400	-9.77539200	H	28.26911800	0.29642500	-8.80347200
C	33.48000500	-4.18206400	-10.78311400	C	31.09193800	7.81099900	-10.77011500
C	33.36081800	-2.73989500	-10.31612400	C	30.07775200	7.05160100	-9.89573700
O	33.12709800	-2.39806000	-9.16194500	C	28.77325900	6.83230900	-10.60186900
C	32.15786000	-4.96076400	-10.80288900	C	27.58313900	7.48051200	-10.38543800
O	31.93112000	-5.53484000	-9.53760800	C	28.55118300	5.91988900	-11.70129600
H	33.92660500	-4.20801800	-11.78364900	C	27.19623500	6.07272500	-12.10756100
H	31.32821000	-4.29640500	-11.08652300	C	29.35635800	4.97363100	-12.36108100
H	32.22371000	-5.73535400	-11.58298700	N	26.62983900	7.02996300	-11.28632700
H	31.02896100	-5.91269100	-9.58968300	C	26.64301500	5.32637500	-13.15260100
N	33.54613000	-1.80557900	-11.29790700	C	28.81253500	4.23028600	-13.40140700
C	33.30494800	-0.40200500	-11.03296000	C	27.47160600	4.41275500	-13.79652300
H	33.57802700	-2.11232900	-12.25753000	H	31.14769600	7.33833100	-11.75716700
H	33.55632600	0.17485500	-11.92520800	H	30.50376400	6.07773000	-9.61836200
H	32.25442800	-0.20943500	-10.78618900	H	29.91065900	7.59202700	-8.95682600
C	30.70351800	-3.79260500	-14.83654100	H	27.33320200	8.23480800	-9.65287200
C	30.58814500	-2.86374800	-13.63284100	H	25.67669500	7.34861100	-11.33182500
C	29.17936500	-2.47380900	-13.17925300	H	30.38990100	4.81332000	-12.06926900
O	28.18356900	-3.17043000	-13.58930400	H	25.61185200	5.46571300	-13.45989800
O	29.08665200	-1.51068500	-12.38270400	H	29.41956900	3.51193700	-13.93778400
H	30.04895200	-4.65082000	-14.73015100	H	27.09240900	3.83621100	-14.63324900
H	31.03486500	-3.33733800	-12.75120600	O	29.73023600	0.98391900	-11.54172900
H	31.14736700	-1.93346300	-13.77423300	H	30.40113200	1.45528800	-12.07340400
C	27.87487300	1.06309800	-17.13711200	N	29.63142500	0.06808100	-11.88833500
C	29.24803100	1.59095100	-16.77597500	N	16.97105400	-3.30444000	-12.61691400
O	29.41052200	2.66629100	-16.20193900	C	16.59792100	-4.44997700	-11.75909300
C	27.07995700	0.78229100	-15.84411600	C	15.33147700	-3.94479500	-11.04580700
C	25.65234400	0.40395800	-16.12901100	C	14.70893500	-2.97464500	-12.06134900
C	24.72019000	1.38927200	-16.46898500	C	15.93176000	-2.26306100	-12.64653300
C	25.22451000	-0.92635400	-16.08415200	H	17.40431200	-4.66836800	-11.05496500
C	23.40010800	1.06023100	-16.76256700	H	14.66674100	-4.76342100	-10.76103900
C	23.90838300	-1.27753500	-16.37550600	H	15.60749200	-3.40318300	-10.13441700
C	23.00315900	-0.27528000	-16.71751900	H	14.18801300	-3.53283700	-12.84699400
O	21.69486200	-0.65041600	-16.97914700	H	13.99661800	-2.27821300	-11.61296700
H	27.36235800	1.83562100	-17.71907300	H	15.79450800	-1.90269500	-13.66862600
H	27.57381500	-0.01726900	-15.28234400	H	16.24297700	-1.40732800	-12.03459300

C	29.55089600	-2.94380800	-1.16231600
C	28.26928700	-3.76923700	-1.32409300
C	28.02968100	-4.28724000	-2.74162400
C	27.83599700	-3.19933100	-3.78316000
O	27.95006000	-2.00257100	-3.58201200
O	27.55845500	-3.71721700	-4.98463900
H	29.52569000	-2.11291400	-1.87087800
H	28.28014900	-4.62420800	-0.63712700
H	27.41613900	-3.14545200	-1.03245000
H	28.87316300	-4.90069300	-3.08558100
H	27.15499300	-4.94726100	-2.78380900
H	30.46541200	-3.51017900	-1.36770900
H	29.56615500	-2.49740900	-0.16232200
C	34.86213900	7.99963000	-10.31615500
C	35.22176800	6.49924200	-10.31794900
C	34.97286900	5.85868100	-11.64428300
C	34.05511800	4.92873800	-12.06953800
N	35.66788900	6.21487100	-12.79115300
C	35.16303200	5.50518100	-13.83668600
N	34.18663500	4.72052500	-13.42763100
H	35.57043800	8.58895900	-10.90791400
H	36.26331300	6.35088000	-10.00408900
H	34.60259500	5.97799400	-9.58126800
H	36.41388000	6.89212200	-12.84078700
H	33.31005600	4.38977600	-11.50337900
H	35.53216800	5.58891300	-14.84805500
H	33.41311700	3.54750200	-14.17973900
H	34.87088100	8.38153500	-9.28965800
H	33.87101000	8.09564200	-10.77186900

E:P-A_{Zn} (-2.2 kcal/mol)

H	20.66694600	-6.80396900	-16.56503800
H	16.39005300	-5.37409400	-12.30886400
H	24.65797500	-6.75700700	-19.16499000
H	29.36482200	-8.34220900	-18.18000000
H	35.11211600	4.86996200	-6.01615500
H	32.10199200	7.76390000	-10.35099400
H	33.92503500	-0.03001500	-10.21102200
H	31.94997700	-4.27903600	-6.58588700
H	23.18497800	1.49699400	-4.32299500
H	22.41694900	4.62894600	-7.60401400
H	22.25403100	6.39002200	-15.14821700
H	33.53409000	5.46907000	-6.68104200
H	30.78105100	8.84802500	-10.93694500
H	23.93693000	6.30998400	-15.82106600
H	23.80795700	-0.12305500	-3.81401700
H	32.79691200	-3.33919800	-5.29795600
H	32.07471100	0.82269700	-17.96202900
H	30.43519800	-3.27793000	-15.73602200
H	31.70214900	-4.16455100	-14.93619500
H	30.41823100	-9.05968700	-14.20495600
H	20.88587800	-5.05002000	-16.84102600
H	34.15693200	-4.71599400	-10.10792700
H	23.72482700	-8.30796000	-7.05598500
H	21.59199600	-3.72898600	-7.31999100
H	27.89804300	0.15092400	-17.74188500
H	27.15900800	4.34385500	-6.69888500
C	29.55201000	-8.45621600	-13.91517500
C	29.41137500	-7.67353700	-15.20543200
O	29.98953400	-6.60717900	-15.39970000
C	29.77165000	-7.55696100	-12.70272700
C	28.58095100	-6.61890700	-12.47494600
C	28.67681200	-5.81412600	-11.18047200
O	29.40968600	-6.20245300	-10.25768500
O	27.94321900	-4.75092900	-11.09697600
H	28.70595600	-9.13815200	-13.77160400
H	29.94343300	-8.15458700	-11.80445000
H	30.66981500	-6.95530500	-12.86827400
H	28.47342000	-5.91976700	-13.30781100
H	27.64349100	-7.19305600	-12.43430200
N	28.73063100	-8.30579100	-16.19047000
C	28.69017100	-7.77096700	-17.53408600
C	27.24272700	-7.95639000	-17.99026700
O	26.76876800	-9.08486700	-18.08846800
H	28.25748000	-9.18382100	-16.03261600
H	29.02588400	-6.73439700	-17.48810200
N	26.51589900	-6.81959600	-18.14349800
C	25.05595800	-6.83995000	-18.14804600
C	24.50559700	-5.71411400	-17.27623500
H	26.96945500	-5.93955400	-17.94570900
H	24.75558000	-7.82090700	-17.77142900
H	23.41371700	-5.72303000	-17.28953900
H	24.84196400	-5.81822600	-16.24132900
H	24.82642500	-4.73164100	-17.64530400
C	23.25804200	6.03503500	-15.04069500
C	23.23404500	4.49376300	-14.99535800
C	22.33980200	3.90362400	-13.93411300
C	22.62693300	4.08255300	-12.57581000
C	21.23873100	3.10533200	-14.26780800
C	21.86393100	3.46723900	-11.59015900
C	20.46456600	2.47639800	-13.29411300
C	20.78583400	2.65122800	-11.94626100
O	20.02641600	2.00539700	-11.01153600
H	23.64453500	6.44470300	-14.10036900
H	22.91372600	4.12287000	-15.97593300
H	24.25456200	4.11554700	-14.85281000
H	23.48629700	4.67863300	-12.28047500

H	20.99836400	2.95002900	-15.31662300
H	22.12011800	3.58839200	-10.54480800
H	19.62949500	1.83565900	-13.55743900
H	20.45647800	2.10274900	-10.15022800
C	20.86219900	-5.84002300	-16.08295300
C	19.86778000	-5.66999800	-14.93828600
O	19.28111500	-6.63429100	-14.45783900
H	21.86153000	-5.87768300	-15.63315400
N	19.73926400	-4.40029400	-14.43731300
C	19.19492600	-4.19789700	-13.09503800
C	18.20344200	-3.04865200	-13.10591000
O	18.51280800	-1.93530000	-13.56652700
C	20.37377600	-3.97761300	-12.12054600
O	19.98837400	-4.01626000	-10.74456600
H	20.34271600	-3.65671600	-14.78474200
H	18.70906800	-5.13752400	-12.83551200
H	21.07830300	-4.79735800	-12.27924000
H	20.89553500	-3.04639500	-12.36311500
H	19.75976000	-3.11974700	-10.46961400
C	23.90622000	-7.35610000	-7.56595900
C	22.90956200	-6.30635600	-7.09912100
O	21.74535200	-6.61301200	-6.83589200
C	23.67426800	-7.61341900	-9.08492700
C	24.01035000	-6.44870100	-9.95866700
C	25.18424100	-6.11536300	-10.58755400
N	23.16702900	-5.36863400	-10.19206300
C	23.84246300	-4.44633400	-10.92270100
N	25.06962600	-4.87386300	-11.18100200
H	24.94528600	-7.06405800	-7.39640500
H	24.29034200	-8.46131400	-9.39853400
H	22.62775400	-7.90793900	-9.21981700
H	22.21571500	-5.25940700	-9.86154000
H	26.10519400	-6.67436000	-10.62035400
H	23.43604100	-3.50674200	-11.25496900
N	23.32032500	-5.00715200	-7.10692800
C	22.40694700	-3.96398400	-6.62797200
C	23.31760000	-2.76026500	-6.37031800
C	24.49201800	-2.97683200	-7.33230000
C	24.69327600	-4.49535600	-7.29744000
H	21.90916000	-4.31689900	-5.71880300
H	22.80547300	-1.81478800	-6.53591100
H	23.67987400	-2.77697600	-5.33672400
H	24.22607500	-2.64811200	-8.34249800
H	25.39244000	-2.44211500	-7.02596500
H	25.13788400	-4.87937800	-8.21617800
H	25.33956000	-4.77554000	-6.45506600
C	23.17506600	4.07109800	-8.16496500
C	24.47096800	3.92997300	-7.38665000
O	24.49724600	3.80837500	-6.16134500
H	22.78308100	3.07018400	-8.36889200
H	23.32309200	4.58325700	-9.11754000
N	25.60625000	3.92370000	-8.13902400
C	26.90898900	3.66712400	-7.52217300
C	27.88354400	3.80612200	-8.69689900
C	27.07369600	3.26451800	-9.87693400
C	25.67189100	3.82392200	-9.61341800
H	26.93210600	2.64793400	-7.11017200
H	28.11702100	4.86253200	-8.86622600
H	28.82049200	3.27241900	-8.53137500
H	27.46281000	3.56202800	-10.84954300
H	27.04131400	2.17184400	-9.84460400
H	25.55789400	4.81538300	-10.07037200
H	24.89574800	3.16477700	-10.00633500
C	23.37408100	0.46306700	-4.63000000
C	24.34460000	0.46649100	-5.82188200
C	23.74004100	0.55387300	-7.20943900
C	22.36397000	0.53907800	-7.45969600
C	24.60521400	0.57529600	-8.31639600
C	21.87054300	0.49102200	-8.76923900
C	24.12328500	0.55085100	-9.62181000
C	22.74449400	0.49294700	-9.85516000
H	22.41916400	-0.01468900	-4.86487100
H	25.04043100	1.30378800	-5.70207400
H	24.95816700	-0.44268100	-5.79784000
H	21.66225000	0.54352700	-6.63335900
H	25.67896200	0.59739000	-8.14258400
H	20.79732300	0.41630100	-8.93144100
H	24.81063900	0.55454000	-10.45801400
H	22.37678200	0.44509200	-10.87276400
C	32.20612100	-3.27974800	-6.21812200
C	30.90660100	-2.47507700	-6.00768800
C	29.92118000	-2.63664700	-7.13491500
C	30.03310700	-3.43594600	-8.24806500
N	28.65555100	-2.03926500	-7.13210100
C	28.04370200	-2.50238300	-8.23251200
N	28.83883800	-3.33330000	-8.92487100
H	32.81371900	-2.82739400	-7.00286000
H	30.41589800	-2.78410000	-5.07608200
H	31.14562900	-1.41119000	-5.86576900
H	27.78213200	-2.78088400	-5.72040900
H	30.83780600	-4.06280800	-8.59899300
H	27.04482600	-2.24022400	-8.55128100
H	28.55945300	-3.85838600	-9.77542800
C	33.48000500	-4.18206400	-10.78311400
C	33.35820900	-2.73770100	-10.32283400
O	33.08742100	-2.39261700	-9.17761800
C	32.14361200	-4.93966700	-10.80429600
O	31.94214100	-5.57633700	-9.56263900
H	33.92775200	-4.21197700	-11.78304500

H	31.31906200	-4.24655500	-11.02923900
H	32.17333600	-5.67608900	-11.62200400
H	31.04938400	-5.97387900	-9.62661800
N	33.57103900	-1.80264700	-11.29958100
C	33.30494800	-0.40200500	-11.03296000
H	33.63610000	-2.10707300	-12.25820300
H	33.54128400	0.18135700	-11.92499600
H	32.25379000	-0.24225300	-10.78014700
C	30.70351800	-3.79260500	-14.83654100
C	30.59031900	-2.86267400	-13.63061600
C	29.19441400	-2.66845300	-13.03128400
O	28.20907100	-3.28254200	-13.56610100
O	29.11204500	-1.94439400	-12.00743000
H	30.05091700	-4.65185400	-14.72921000
H	31.19852200	-3.23207800	-12.79834100
H	30.98497400	-1.86469700	-13.84621200
C	27.87487300	1.06309800	-17.13711200
C	29.24863100	1.59011400	-16.77888700
O	29.41626700	2.66789100	-16.21084800
C	27.07718900	0.79401600	-15.84104300
C	25.64761100	0.42209700	-16.12334800
C	24.73079500	1.40501300	-16.50831300
C	25.20160200	-0.89865200	-16.02501900
C	23.40602400	1.08463900	-16.78941900
C	23.88285200	-1.24186900	-16.31098700
C	22.99004400	-0.24168000	-16.68832200
O	21.67615200	-0.61171100	-16.93065200
H	27.36498100	1.83520800	-17.72206700
H	27.56080300	-0.00278100	-15.26657400
H	27.11468700	1.68778900	-15.21487800
H	25.05125700	2.44094400	-16.57129600
H	25.88823700	-1.66699900	-15.68141600
H	22.69871400	1.86182800	-17.06920600
H	23.54030700	-2.26240100	-16.19066400
H	21.16430400	0.17827100	-17.14873100
N	30.27206800	0.75691100	-17.09423200
C	31.68350500	1.10941100	-16.97996200
C	32.36704800	0.33080300	-15.85246000
C	31.75172600	0.62649500	-14.48499300
C	32.07574800	1.98042300	-13.88646700
O	32.94707800	2.67604300	-14.58141100
O	31.58837000	2.34343700	-12.81431300
H	30.04753000	-0.10007000	-17.57622400
H	31.75579000	2.18659200	-16.83326700
H	32.26983700	-0.74333300	-16.05347200
H	33.43521900	0.56607700	-15.84370800
H	30.66144300	0.53395900	-14.52470200
H	32.08426300	-0.11020800	-13.74589600
C	26.43235200	-0.27032100	-12.37032700
C	25.25740800	-1.01631300	-12.59510300
O	25.21857400	-2.34276500	-12.45507300
C	24.08850100	-0.31923300	-12.97078600
C	24.09880800	1.06369400	-13.10485900
C	25.26490300	1.79941500	-12.87218100
C	26.43083500	1.11715400	-12.51393800
H	27.33743600	-0.79685800	-12.09164100
H	23.17688500	-0.87242100	-13.17492700
H	23.18808900	1.56677600	-13.39957300
H	25.26995300	2.87853200	-12.96947200
H	27.35591600	1.65971600	-12.34653000
Zn	26.59476800	-3.79905000	-12.33217200
O	25.92549100	-4.73382700	-14.20777300
H	25.00949900	-4.39591500	-14.36478600
H	26.52472700	-4.25685700	-14.79978500
O	23.46687300	-3.61829600	-13.97957100
H	22.70542700	-3.07858500	-14.25059800
H	24.01546400	-3.03334900	-13.38644900
O	21.13067300	-1.92265300	-14.53135300
H	21.19000900	-1.42601700	-15.36727300
H	20.23835500	-1.74464200	-14.15759100
C	34.22876600	4.62597900	-6.61578000
C	33.56166800	3.35877700	-6.05793800
C	32.23996400	2.98670900	-6.74968300
C	31.92622000	1.48771000	-6.59146700
N	30.58500000	1.09243600	-7.02178300
C	30.19799900	1.00623400	-8.30724100
N	30.94249600	1.49813600	-9.29582800
N	29.00001100	0.47747000	-8.59502000
H	34.58052700	4.43584800	-7.63815100
H	34.27032600	2.52567500	-6.15881300
H	33.38181300	3.47040400	-4.98197600
H	31.41018400	3.57411300	-6.34156300
H	32.30105700	3.25724000	-7.81095500
H	32.67372600	0.88316200	-7.12308300
H	32.00127400	1.21239900	-5.53677000
H	29.97644600	0.64753100	-6.34807200
H	31.85982400	1.86358600	-9.11496500
H	30.65669500	1.21447100	-10.25346900
H	28.66495100	-0.26422500	-7.97044400
H	28.79311600	0.37121300	-9.58452000
C	31.09193800	7.81099900	-10.77011500
C	30.08034400	7.05057900	-9.89252600
C	28.77548200	6.83076200	-10.59736000
C	27.58308600	7.47417300	-10.37798100
C	28.56084200	5.93369300	-11.71067000
C	27.20959100	6.09384700	-12.12555000
C	29.37189900	4.99995300	-12.38106500
N	26.63583900	7.03534200	-11.29083500
C	26.66809000	5.37404400	-13.19497400

C	28.83898800	4.28224800	-13.44483200
C	27.50367800	4.47700500	-13.85213000
H	31.14656900	7.33745800	-11.75664100
H	30.50909600	6.07730900	-9.61632800
H	29.91504500	7.59098000	-8.95326100
H	27.32838800	8.21882500	-9.63721300
H	25.68404200	7.35738800	-11.34145900
H	30.40124700	4.83017200	-12.08027400
H	25.63946600	5.51794700	-13.50819200
H	29.45005500	3.57435600	-13.99014000
H	27.13346900	3.91630100	-14.70325600
O	29.75681200	0.58718100	-11.50821900
H	30.16148600	1.12834200	-12.20971600
H	29.67590000	-0.36133500	-11.79144100
N	16.97174500	-3.30446100	-12.62061000
C	16.59792100	-4.44997700	-11.75909300
C	15.33237800	-3.94258800	-11.04600800
C	14.71218700	-2.96852700	-12.05917800
C	15.93684200	-2.25887800	-12.64246400
H	17.40553800	-4.66510500	-11.05566100
H	14.66533600	-4.76002900	-10.76295800
H	15.60947300	-3.40359200	-10.13336900
H	14.19002900	-3.52356900	-12.84628600
H	14.00152300	-2.27139300	-11.60911900
H	15.79908100	-1.89204100	-13.66220400
H	16.25193200	-1.40741100	-12.02634500
C	29.55089600	-2.94380800	-1.16231600
C	28.26043200	-3.73705500	-1.38987600
C	28.04947300	-4.18045100	-2.84032700
C	27.88729400	-3.04527000	-3.83771700
O	28.01959700	-1.86028400	-3.59166500
O	27.61100900	-3.51061600	-5.06511900
H	29.55641400	-2.09852400	-1.85599000
H	28.23710100	-4.62646300	-0.74876000
H	27.41049300	-3.11323600	-1.08948100
H	28.89562300	-4.78504300	-3.19356100
H	27.17108900	-4.82992100	-2.93381800
H	30.46541200	-3.51017900	-1.36770900
H	29.56615500	-2.49740900	-0.16232200
C	34.86213900	7.99996300	-10.31615500
C	35.21171600	6.49636200	-10.30928300
C	34.90062900	5.84342300	-11.61535300
C	33.94072700	4.93575100	-11.99300500
N	35.55415200	6.17270800	-12.79360800
C	34.98555700	5.46962100	-13.81048100
N	34.00700400	4.71490600	-13.35318800
H	35.57333600	8.58273500	-10.91006200
H	36.26349500	6.34245000	-10.03530800
H	34.61757500	5.99093100	-9.54166700
H	36.31362000	6.83095700	-12.88099600
H	33.20619200	4.42604700	-11.38719000
H	35.31301200	5.53448200	-14.83745000
H	33.24323100	3.52905400	-14.09131800
H	34.87088100	8.38153500	-9.28965800
H	33.87101000	8.09564200	-10.77186900

The transition states and intermediates involved in the reaction pathway with **Mode-B** for the Mg-enzyme of SDC.

E:S-B_{Mg} (1.9 kcal/mol)

H	20.66706600	-6.80406200	-16.56490500
H	16.38995900	-5.37400500	-12.30897300
H	24.65804700	-6.75722800	-19.16503700
H	29.36460500	-8.34236600	-18.18009000
H	35.11198500	4.87001000	-6.01598300
H	32.10200100	7.76399400	-10.35100200
H	33.92510700	-0.02999300	-10.21108400
H	31.95000500	-4.27896200	-6.58610400
H	23.18522500	1.49712900	-4.32329800
H	22.41700900	4.62901700	-7.60400600
H	22.25386600	6.38954500	-15.14827300
H	33.53399800	5.46899800	-6.68099800
H	30.78100300	8.84800000	-10.93700000
H	23.93862300	6.30925300	-15.81983900
H	23.80780000	-0.12316500	-3.81401100
H	32.79714400	-3.33879100	-5.29807800
H	32.07507100	0.82308700	-17.96199500
H	30.43491900	-3.27775200	-15.73583400
H	31.70201300	-4.16491400	-14.93618300
H	30.41799700	-9.06001500	-14.20497600
H	20.88596600	-5.05007400	-16.84107900
H	34.15715900	-4.71603300	-10.10818600
H	23.72468000	-8.30785100	-7.05583600
H	21.59201500	-3.72880000	-7.31994900
H	27.89809000	0.15097800	-17.74196200
H	27.15896100	4.34410100	-6.69907100
C	29.55218400	-8.45631100	-13.91551100
C	29.05964600	-7.65433300	-15.10210200
O	28.81402400	-6.44065900	-15.07833100
C	29.82534200	-7.58685900	-12.68609900
C	28.53258000	-7.23256600	-11.93330800

C	28.80807500	-6.12163000	-10.91072900	C	24.33239900	0.45492900	-5.82812400
O	29.56833600	-6.40440100	-9.96921500	C	23.71962100	0.59054100	-7.20792100
O	28.27343900	-4.97883600	-11.13254900	C	22.34497300	0.52709000	-7.46198400
H	28.76973700	-9.19137500	-13.67347500	C	24.58035400	0.71285400	-8.30997200
H	30.50266600	-8.09854800	-11.99816400	C	21.85119900	0.53007800	-8.77200200
H	30.32649700	-6.66783200	-13.00656500	C	24.09447000	0.74690500	-9.61241100
H	27.75404500	-6.92894800	-12.63569900	C	22.72177700	0.63669600	-9.85560100
H	28.17936100	-8.12599800	-11.40416400	H	22.41578100	-0.01294800	-4.85578200
N	28.94418200	-8.36766600	-16.23583800	H	25.05859000	1.26443800	-5.70080000
C	28.69016600	-7.77022900	-17.53345200	H	24.91144800	-0.47697900	-5.82649200
C	27.22762700	-7.98306000	-17.92846700	H	21.64431600	0.45363600	-6.63801800
O	26.75974400	-9.11276300	-17.99582900	H	25.65225600	0.77129500	-8.13744500
H	29.05736600	-9.36966800	-16.20490900	H	20.78275700	0.41819000	-8.94066300
H	28.99547200	-6.72398100	-17.49517700	H	24.78149900	0.84048000	-10.44051100
N	26.51527400	-6.84243800	-18.12628500	H	22.34956000	0.62666000	-10.87299500
C	25.05614300	-6.83990900	-18.14801200	C	32.20580900	-3.28026700	-6.21781300
C	24.51911000	-5.71023200	-17.27003700	C	30.90819500	-2.47208800	-6.00148100
H	26.97241200	-5.96600600	-17.91899300	C	30.02537400	-2.43813200	-7.22365800
H	24.73908800	-7.81603500	-17.77114800	C	30.40413600	-2.42591700	-8.54705400
H	23.42724100	-5.70223100	-17.28118000	N	28.63226900	-2.49027100	-7.16464800
H	24.85331200	-5.82937300	-16.23421500	C	28.20575500	-2.54632200	-8.42922600
H	24.85477100	-4.73026500	-17.63166000	N	29.24790600	-2.49816500	-9.28571600
C	23.25606600	6.03698800	-15.04213200	H	32.82867800	-2.82885400	-6.99372800
C	23.17259800	4.49849900	-15.03156600	H	30.33025500	-2.89303800	-5.17559400
C	22.26005900	3.91688500	-13.97759700	H	31.16334900	-1.44922400	-5.68044800
C	22.42571700	4.22990400	-12.62336700	H	27.91761400	-3.20801800	-5.84099400
C	21.28348900	2.96682600	-14.30794300	H	31.38395600	-2.42280000	-8.98708600
C	21.66844900	3.60395500	-11.63764200	H	27.18278600	-2.61735700	-8.76656200
C	20.52549500	2.31708900	-13.33665200	H	29.18428200	-2.50019800	-10.30839100
O	20.72506100	2.63422000	-11.99061300	C	33.47990000	-4.18206100	-10.78263200
O	19.98242200	1.96973200	-11.05534600	C	33.54897200	-2.73111500	-10.32972700
H	23.64623100	6.42508500	-14.09520400	O	33.62602100	-2.38617700	-9.15236900
H	22.82534000	4.16830200	-16.01703700	C	32.08684900	-4.81577400	-10.66083600
H	24.17704600	4.07036400	-14.92065100	O	31.77510900	-5.02390600	-9.31247300
H	23.18017000	4.95232000	-12.32351700	H	33.84318900	-4.28025900	-11.81182000
H	21.14745800	2.69307000	-15.35054200	H	31.33613600	-4.17267800	-11.14870000
H	21.82524200	3.84548100	-10.59152500	H	32.10031900	-5.76119900	-11.22860100
H	19.83137400	1.52624300	-13.59555700	H	30.88080100	-5.43605900	-9.31866300
H	20.35017600	2.15878100	-10.18083100	N	33.53386100	-1.80127000	-11.33080900
C	20.86193200	-5.83974700	-16.08300800	C	33.30483900	-0.40190500	-11.03293900
C	19.76940700	-5.54633600	-15.05610800	H	33.27376800	-2.11475700	-12.25446500
O	18.77269700	-6.24838000	-14.92673300	H	33.55324000	0.18929500	-11.91873400
H	21.84197500	-5.85673000	-15.59658500	H	32.25377500	-0.21037000	-10.79230500
N	19.99290700	-4.42909600	-14.28926500	C	30.70430000	-3.79269300	-14.83716500
C	19.19490800	-4.19819100	-13.09497300	C	30.68818900	-2.83239700	-13.64917300
C	18.14399800	-3.10489700	-13.25372600	C	29.33714500	-2.59248800	-12.98824000
O	18.38174100	-2.04040100	-13.84800600	O	28.31627600	-3.17104900	-13.45727700
C	20.16180700	-3.85098100	-11.93769500	O	29.35866300	-1.82087800	-11.98328000
O	19.50451500	-3.63906900	-10.69409300	H	30.02210400	-4.62682300	-14.68471900
H	20.91644500	-4.00167600	-14.32659300	H	31.33063200	-3.20629200	-12.84576100
H	18.69448100	-5.14212600	-12.87382100	H	31.09632900	-1.84863800	-13.91260000
H	20.83468200	-4.70345100	-11.80882900	C	27.87487500	1.06305200	-17.13700000
H	20.77758100	-2.99049000	-12.21554200	C	29.25242500	1.59113000	-16.79376000
H	19.21357300	-2.71892100	-10.66557100	O	29.42119400	2.70452200	-16.29833700
C	23.90649100	-7.35674400	-7.56585800	C	27.06163300	0.81322100	-15.84924400
C	22.89712700	-6.30717100	-7.13070300	C	25.61560900	0.50196400	-16.13702800
O	21.73073800	-6.61670600	-6.87956800	C	24.76835400	1.50085300	-16.62759900
C	23.70085900	-7.69077600	-9.06782100	C	25.07949300	-0.76928200	-15.90974100
C	24.10262300	-6.59931800	-9.99496600	C	23.42108100	1.24811200	-16.87202400
C	25.31034000	-6.32522000	-10.58209600	C	23.73452100	-1.04222200	-16.14958200
N	23.28059600	-5.54654500	-10.36651100	C	22.90745600	-0.02382800	-16.61994100
C	23.99701000	-4.69591900	-11.14874500	O	21.56773800	-0.31827300	-16.78944500
N	25.23452500	-5.14573700	-11.29448900	H	27.37731200	1.83555900	-17.73147000
H	24.94209400	-7.05859500	-7.38898100	H	27.51365900	-0.00757500	-15.28177500
H	24.29232200	-8.57816900	-9.31250100	H	27.13382800	1.70390800	-15.21919500
H	22.64802200	-7.95755300	-9.21269600	H	25.15851400	2.50035100	-16.80051400
H	22.33259400	-5.39995200	-10.04893900	H	25.70277400	-1.54496300	-15.47526700
H	26.22468900	-6.89211800	-10.51890800	H	22.77137300	2.03876800	-17.23928600
H	23.58309300	-3.82172600	-11.62514700	H	23.31154700	-2.01346500	-15.91836900
N	23.30999200	-5.00970500	-7.13069100	H	21.11029800	0.46643500	-17.11880700
C	22.40692000	-3.96388400	-6.62809400	N	30.27478700	0.73322100	-17.04438700
C	23.33164600	-2.76569100	-6.38784400	C	31.68296500	1.10887100	-16.98008700
C	24.48398500	-2.98401200	-7.37880000	C	32.40995600	0.42808600	-15.82142700
C	24.68229100	-4.50273800	-7.34287100	C	31.90038300	0.94394300	-14.47645500
H	21.92095900	-4.31799800	-5.71353800	C	32.38774600	2.32653400	-14.08201100
H	22.81884100	-1.81793700	-6.53829300	O	33.39678000	2.77641400	-14.79512700
H	23.71738200	-2.78791900	-5.36284900	O	31.90228100	2.94694800	-13.13165700
H	24.19313000	-2.66035600	-8.38393900	H	30.04995900	-0.15193900	-17.47250600
H	25.39532500	-2.44907600	-7.10164700	H	31.72778000	2.19508100	-16.88519000
H	25.11043600	-4.89046400	-8.26820700	H	32.24446600	-0.65482400	-15.87798800
H	25.34156800	-4.78300200	-6.51051300	H	33.48574400	0.60087800	-15.91057600
C	23.17498400	4.07100100	-8.16499700	H	30.80807800	0.95736500	-14.45370500
C	24.47296300	3.92422100	-7.39293800	H	32.18855700	0.27883000	-13.65624700
O	24.50098200	3.77036900	-6.17193100	C	25.84007700	-1.93740900	-12.23620100
H	22.78042000	3.07137300	-8.36747500	O	25.37382500	-2.77262100	-13.08859600
H	23.31823700	4.57711400	-9.12204800	O	26.56324700	-2.32504300	-11.27241600
N	25.61311300	3.93954400	-8.14142700	C	25.60130200	-0.49225000	-12.43933100
C	26.90904800	3.66685200	-7.52193500	C	26.61609000	0.45459100	-12.20533300
C	27.90234300	3.86426700	-8.66903900	O	27.83817300	0.16542900	-11.67340500
C	27.11374400	3.40749900	-9.89201300	C	26.38091700	1.79426400	-12.52983500
C	25.70041700	3.93499200	-9.61548300	C	25.12757600	2.20460000	-12.96507000
H	26.93664200	2.64208900	-7.12862700	C	24.09630700	1.27938100	-13.14148000
H	28.14610800	4.92712700	-8.76939400	C	24.35736000	-0.06213700	-12.91571100
H	28.83351600	3.31604600	-8.52132100	H	28.15856400	-0.79168000	-11.76616300
H	27.52052000	3.79103700	-10.82486600	H	27.19241000	2.50232100	-12.43872600
H	27.09485300	2.31581100	-9.94366400	H	24.96734100	3.25509200	-13.16793100
H	25.58317400	4.95161600	-10.01248500	H	23.11905600	1.58680000	-13.47801600
H	24.93450700	3.29696700	-10.05992000	H	23.58248200	-0.79817100	-13.08063400
C	23.37403400	0.46301100	-4.62955100	O	26.58199300	-5.23580000	-14.06462700

H	26.30583400	-4.48788400	-14.61273100
H	27.41896200	-5.57005700	-14.45630400
O	22.64526500	-3.14860900	-13.86284900
H	22.17375700	-2.28504500	-13.90804100
H	23.59389700	-2.96928300	-13.71446600
O	20.94377900	-1.02239100	-14.07154500
H	21.03263100	-0.76874800	-15.00547500
H	20.04109000	-1.40916800	-14.00536300
C	34.22900400	4.62597000	-6.61602700
C	33.55359800	3.34810900	-6.08051100
C	32.22719300	2.98651700	-6.77899500
C	31.89342200	1.48586100	-6.62803600
N	30.52508300	1.10155300	-6.99943500
C	30.08329400	1.01409400	-8.27121500
N	30.79444000	1.52142600	-9.26685700
N	28.86368900	0.49128800	-8.51141600
H	34.58505100	4.44662700	-7.63910200
H	34.25941400	2.51455300	-6.19421600
H	33.37097400	3.44198700	-5.00331900
H	31.40252400	3.58132200	-6.37111200
H	32.30011900	3.26458100	-7.83807100
H	32.61007200	0.87672100	-7.19522500
H	32.00785100	1.20026900	-5.57981500
H	29.97620400	0.61492500	-6.30438800
H	31.67905700	1.95103500	-9.05892100
H	30.52679600	1.41287700	-10.28943600
H	28.53259800	-0.24189900	-7.88891300
H	28.58876300	0.36202900	-9.48216000
C	31.09199800	7.81099800	-10.76999800
C	30.06388000	7.03714500	-9.92546600
C	28.77665100	6.83315900	-10.66926100
C	27.56722400	7.44077500	-10.44194200
C	28.60333000	5.99882200	-11.83741000
C	27.25823400	6.15643800	-12.27394800
C	29.45009200	5.12687400	-12.54565600
N	26.64757100	7.03512700	-11.39850400
C	26.75655600	5.49229800	-13.39839000
C	28.95746100	4.46560500	-13.66421200
C	27.62642700	4.65510300	-14.08994300
H	31.16036400	7.35153100	-11.76259700
H	30.48563600	6.05885500	-9.65630000
H	29.87445600	7.56052100	-8.98128800
H	27.28186600	8.13876900	-9.66770400
H	25.69621800	7.35634100	-11.46234300
H	30.47929400	4.96863200	-12.23987500
H	25.73274200	5.63630500	-13.72747100
H	29.59762100	3.80898200	-14.23985100
H	27.29144200	4.13578900	-14.98151400
O	30.29770000	1.24435800	-11.80745000
H	30.61658000	2.00297500	-12.33853100
H	29.37500700	1.00549500	-12.02278900
N	16.94826000	-3.33522500	-12.67244900
C	16.59812800	-4.44991300	-11.75908000
C	15.33369600	-3.92883700	-11.05934600
C	14.67928900	-3.03016600	-12.11948900
C	15.87850000	-2.33020400	-12.76614800
H	17.41360600	-4.63282800	-11.05969100
H	14.68803900	-4.74146100	-10.71820600
H	15.61389300	-3.33197400	-10.18405700
H	14.15868800	-3.64373200	-12.86298500
H	13.95910000	-2.32226100	-11.70219000
H	15.72186600	-2.04732100	-13.80952900
H	16.16856100	-1.42277200	-12.22115400
C	29.55102500	-2.94411200	-1.16185000
C	28.26591500	-3.74920500	-1.38353500
C	28.10402300	-4.30949600	-2.79997800
C	27.98216300	-3.27529100	-3.91089800
O	28.15526700	-2.07439300	-3.77078200
O	27.70598000	-3.85211000	-5.08115200
H	29.55147800	-2.10800700	-1.86680000
H	28.21552000	-4.58734700	-0.67740300
H	27.40798800	-3.10349900	-1.16066600
H	28.96066700	-4.94385900	-3.06594800
H	27.22904200	-4.96669500	-2.86519200
H	30.46536900	-3.51013000	-1.36804000
H	29.56603700	-2.49717300	-0.16242800
C	34.86196300	8.00000400	-10.31596400
C	35.24317900	6.50637800	-10.33478500
C	35.12906600	5.90218600	-11.69701700
C	34.22266900	5.03324200	-12.25387600
N	35.99152700	6.22190000	-12.73629500
C	35.59081100	5.54776000	-13.84884200
N	34.52266700	4.82199400	-13.58557200
H	35.56394300	8.59959600	-10.90517900
H	36.25640300	6.36355100	-9.93690100
H	34.57266800	5.95299500	-9.66955000
H	36.77988300	6.84851600	-12.67602300
H	33.37489800	4.53996400	-11.80291700
H	36.09970400	5.61224800	-14.79915900
H	33.76909600	3.64286900	-14.38670700
H	34.87102400	8.38159400	-9.28968200
H	33.87106100	8.09550900	-10.77200700
Mg	26.90430300	-4.13401400	-12.26061100

Int1-B_{Mg} (6.7 kcal/mol)

H	20.66706200	-6.80406200	-16.56490400
H	16.38996600	-5.37400800	-12.30897200

H	24.65804800	-6.75722700	-19.16503700
H	29.36459900	-8.34237300	-18.18009000
H	35.11195600	4.87004000	-6.01595300
H	32.10200600	7.76395000	-10.35101800
H	33.92491300	-0.02994200	-10.21096100
H	31.95014400	-4.27900300	-6.58609000
H	23.18523100	1.49712700	-4.32328700
H	22.41700000	4.62901800	-7.60401900
H	22.25386600	6.38956200	-15.14822000
H	33.53402200	5.46902100	-6.68095900
H	30.78099900	8.84799600	-10.93701400
H	23.93865300	6.30924700	-15.81981500
H	23.80780400	-0.12316000	-3.81401000
H	32.79738200	-3.33851800	-5.29821400
H	32.07503400	0.82300500	-17.96198600
H	30.43521800	-3.27768800	-15.73588700
H	31.70201100	-4.16498600	-14.93594000
H	30.41801800	-9.06002600	-14.20488900
H	20.88596700	-5.05007200	-16.84107700
H	34.15710200	-4.71617000	-10.10823600
H	23.72471400	-8.30785000	-7.05582100
H	21.59202500	-3.72878600	-7.31995700
H	27.89805000	0.15102600	-17.74203500
H	27.15901300	4.34413300	-6.69911300
C	29.55211000	-8.45625300	-13.91559300
C	29.06989800	-7.65212700	-15.10519900
O	28.83718100	-6.43467400	-15.08035000
C	29.81821800	-7.57957600	-12.69138200
C	28.50900900	-7.18458600	-11.98581100
C	28.77246100	-6.06322800	-10.98300900
O	29.46012800	-6.32191000	-9.98529000
O	28.29688800	-4.89736400	-11.26492800
H	28.76744800	-9.18926600	-13.67575400
H	30.46320600	-8.09898500	-11.97843500
H	30.35012600	-6.67788600	-13.01090100
H	27.75798600	-6.88226200	-12.71647100
H	28.12515200	-8.05769500	-11.44579900
N	28.95482200	-8.36417300	-16.23639100
C	28.69020800	-7.77022800	-17.53345000
C	27.22277400	-7.98846800	-17.90520500
O	26.74943100	-9.11786800	-17.91941000
H	29.04434400	-9.36871700	-16.20237800
H	28.99388800	-6.72346400	-17.50020100
N	26.51464900	-6.85265600	-18.13490700
C	25.05612900	-6.83990600	-18.14799800
C	24.52829100	-5.70473600	-17.27154900
H	26.98332000	-5.96903300	-17.99636500
H	24.73700700	-7.81354100	-17.76745400
H	23.43645400	-5.68955000	-17.28038800
H	24.86278600	-5.82439500	-16.23598100
H	24.86890500	-4.72747000	-17.63588000
C	23.25601500	6.03700700	-15.04223200
C	23.13975000	4.50019600	-15.03581900
C	22.20644200	3.94114300	-13.98584900
C	22.35794500	4.26849700	-12.63318600
C	21.22354200	2.99722900	-14.31456700
C	21.59205900	3.65480500	-11.64672300
C	20.45314800	2.36199300	-13.34298300
C	20.64967400	2.68353600	-11.99740800
O	19.90616400	2.02225900	-11.06025200
H	23.65111200	6.41632500	-14.09347400
H	22.78632100	4.18256200	-16.02330100
H	24.13053700	4.04293300	-14.92182900
H	23.11115800	4.99199100	-12.33298700
H	21.09094900	2.71672300	-15.35597700
H	21.74389700	3.90531100	-10.60158900
H	19.75329000	1.57559000	-13.60059300
H	20.27710000	2.21033200	-10.18683800
C	20.86193800	-5.83974600	-16.08300400
C	19.77121600	-5.54807000	-15.05393100
O	18.77775400	-6.25417400	-14.92139600
H	21.84248600	-5.85679500	-15.59725300
N	19.99314100	-4.42986400	-14.28892500
C	19.19490700	-4.19819500	-13.09498400
C	18.14199300	-3.10690000	-13.25755900
O	18.37670000	-2.04630900	-13.85931400
C	20.16070000	-3.85055700	-11.93674600
O	19.50343000	-3.65213000	-10.69082200
H	20.91347500	-3.99674500	-14.33063600
H	18.69569200	-5.14269200	-12.87344200
H	20.83973100	-4.69939700	-11.81506200
H	20.76974500	-2.98380200	-12.20863800
H	19.21787200	-2.73080800	-10.64955300
C	23.90645500	-7.35673100	-7.56588200
C	22.89628100	-6.30801200	-7.13016000
O	21.73234000	-6.62013300	-6.87290300
C	23.71473200	-7.68274500	-9.07191900
C	24.12142200	-6.59113200	-9.99975500
C	25.32331400	-6.32924900	-10.60536200
N	23.30201800	-5.53690400	-10.37314200
C	24.01169800	-4.69790400	-11.17208300
N	25.24649300	-5.15564600	-11.33004600
H	24.94073800	-7.05743500	-7.38081300
H	24.30743000	-8.56977400	-9.31515300
H	22.66327900	-7.94929400	-9.22730700
H	22.35674100	-5.38286800	-10.05024100
H	26.23194100	-6.90588000	-10.54764100
H	23.59651600	-3.82553900	-11.65152100
N	23.30803000	-5.01013700	-7.13424800

C	22.40691300	-3.96390100	-6.62808100	N	30.27395000	0.73888000	-16.99609600
C	23.33089600	-2.76368100	-6.39564000	C	31.68299500	1.10898900	-16.98007800
C	24.47415600	-2.98182200	-7.39635800	C	32.43804200	0.42231800	-15.83543900
C	24.67685600	-4.49939600	-7.35659000	C	31.95585400	0.83534200	-14.43354000
H	21.92349300	-4.31735200	-5.71214400	C	32.55488000	2.11233500	-13.87959500
H	22.81562300	-1.81677600	-6.54369700	O	32.84205600	3.01137900	-14.81511600
H	23.72492600	-2.78297300	-5.37369800	O	32.75223900	2.29669800	-12.68358900
H	24.17268800	-2.66310900	-8.39986100	H	30.04048900	-0.20642900	-17.26081600
H	25.38775600	-2.44506100	-7.13346100	H	31.72773700	2.19274400	-16.87628500
H	25.10266800	-4.88970500	-8.28171300	H	32.31589300	-0.66475500	-15.93846100
H	25.34165300	-4.77411800	-6.52639500	H	33.50853200	0.62679700	-15.94673700
C	23.17500000	4.07098900	-8.16497000	H	30.86856800	0.96932600	-14.40909300
C	24.47453000	3.92832500	-7.39520000	H	32.15821500	0.05450100	-13.69770100
O	24.50275800	3.77467200	-6.17421300	C	25.84983700	-1.88506600	-12.24394100
H	22.78133100	3.07070300	-8.36422800	O	25.36981700	-2.73840600	-13.08658200
H	23.31449200	4.57328200	-9.12487200	O	26.61667600	-2.28857600	-11.31810600
N	25.61526000	3.94639700	-8.14353100	C	25.56154300	-0.45375700	-12.43073300
C	26.90897700	3.66682000	-7.52190300	C	26.57385600	0.52202900	-12.23744700
C	27.91024700	3.84836100	-8.66422400	O	27.80204000	0.24300200	-11.81060600
C	27.11912900	3.42128100	-9.89754800	C	26.24658000	1.85744000	-12.55745000
C	25.70244600	3.94099100	-9.61655700	C	24.96694700	2.21561800	-12.94775600
H	26.92360800	2.64469600	-7.12077900	C	23.96194000	1.25379000	-13.09070600
H	28.18576800	4.90419200	-8.75279400	C	24.28505500	-0.07304600	-12.86502100
H	28.82349500	3.27124000	-8.51391500	H	28.51970900	-0.92308100	-12.04658500
H	27.53099200	3.82338200	-10.82171900	H	27.01888500	2.61066200	-12.48783700
H	27.10082900	2.33228500	-9.97721800	H	24.75630600	3.25939600	-13.13918700
H	25.57438300	4.95617600	-10.01289400	H	22.96288200	1.52289800	-13.39381500
H	24.94157200	3.29705300	-10.06123300	H	23.53071400	-0.83714200	-12.99435600
C	23.37402500	0.46301000	-4.62956000	O	26.62715600	-5.15836400	-14.14730900
C	24.32518700	0.45609900	-5.83257100	H	26.33821600	-4.45082000	-14.73991500
C	23.69828800	0.59676400	-7.20534200	H	27.45177300	-5.53254300	-14.52993900
C	22.31969700	0.55242600	-7.44250300	O	22.65305700	-3.15363700	-13.82629200
C	24.54720200	0.71229400	-8.31746800	H	22.16687300	-2.29730600	-13.87060200
C	21.80958200	0.57004600	-8.74637400	H	23.59970800	-2.94839800	-13.69458800
C	24.04564400	0.76031900	-9.61344600	O	20.94625900	-1.03169100	-14.02014900
C	22.66805200	0.67085700	-9.83967900	H	21.06516200	-0.75745000	-14.94511000
H	22.41447700	-0.01255800	-4.85220400	H	20.03863400	-1.40970900	-13.98654600
H	25.05267400	1.26479700	-5.70873700	C	34.22901500	4.62592800	-6.61609500
H	24.90625800	-0.47446700	-5.83692100	C	33.55062100	3.29024700	-6.27181500
H	21.62815600	0.48657400	-6.61028900	C	32.35150100	2.95255100	-7.19519500
H	25.62190900	0.75705600	-8.15759800	C	32.16129300	1.42840500	-7.36775400
H	20.73706600	0.47707100	-8.90191500	N	30.83071900	0.99758500	-7.80628700
H	24.72349100	0.84754600	-10.44959400	C	30.30111200	1.13454700	-9.04351300
H	22.28480500	0.67264400	-10.85287100	N	30.89985500	1.86356900	-9.98696600
C	32.20530300	-3.28051900	-6.21769600	N	29.10749900	0.57762500	-9.27261300
C	30.92124100	-2.44913600	-6.03660800	H	34.62379700	4.53235600	-7.64018000
C	29.97695900	-2.56382600	-7.20506500	H	34.30452300	2.49633700	-6.35714500
C	30.08196200	-3.39868400	-8.29113300	H	33.21365100	3.27536000	-5.22877100
N	28.75948400	-1.87826300	-7.27235800	H	31.42864700	3.38261800	-6.79164200
C	28.16217700	-2.32134800	-8.38754500	H	32.50287300	3.42206500	-8.17538800
N	28.93065400	-3.22816200	-9.02599500	H	32.92978600	1.01974200	-8.03782900
H	32.82628200	-2.84087900	-7.00011600	H	32.31403100	0.93907700	-6.40251200
H	30.38816100	-2.76593900	-5.13144000	H	30.36086900	0.31457900	-7.22398400
H	31.18220800	-1.39457400	-5.85822900	H	31.85874400	2.14365200	-9.86591800
H	27.86142200	-2.61639300	-5.73793500	H	30.50855900	1.89645000	-10.95865800
H	30.85991200	-4.08050500	-8.59139200	H	28.76796500	-0.09833100	-8.59390000
H	27.20711200	-1.99891200	-8.77883600	H	28.67936400	0.54536100	-10.20611400
H	28.68626900	-3.75619400	-9.87405500	C	31.09200000	7.81102500	-10.76997600
C	33.48011900	-4.18184600	-10.78257900	C	30.05703300	6.97550000	-9.99942900
C	33.34791600	-2.73781700	-10.32580400	C	28.83458900	6.70320000	-10.82964000
O	33.04682500	-2.40208000	-9.18492300	C	27.56054400	7.16782400	-10.62054400
C	32.15435200	-4.96084600	-10.76474800	C	28.79211400	5.93377200	-12.05504200
O	32.01780700	-5.61048000	-9.52227500	C	27.45212300	5.97829300	-12.53617600
H	33.91663600	-4.21879700	-11.78734100	C	29.75099600	5.21657800	-12.79554100
H	31.30699600	-4.28314800	-10.94978100	N	26.72414900	6.73405400	-11.63896600
H	32.16554400	-5.69037100	-11.59179700	C	27.05657800	5.33741000	-13.71584200
H	31.11626300	-5.99490800	-9.52236700	C	29.36761300	4.59434800	-13.98122300
N	33.57356200	-1.80342700	-11.29434000	C	28.03078700	4.65263300	-14.43353000
C	33.30513300	-0.40198000	-11.03309900	H	31.19794300	7.38642100	-11.77569300
H	33.70949500	-2.10286500	-12.24640500	H	30.51697700	6.01977400	-9.71251300
H	33.52250300	0.19458700	-11.91642800	H	29.77238700	7.47169900	-9.06481200
H	32.25450800	-0.25009400	-10.77234500	H	27.17546300	7.77989500	-9.81743700
C	30.70391400	-3.79274000	-14.83755600	H	25.74449500	6.94940300	-11.71834100
C	30.70526700	-2.86748200	-13.62559600	H	30.78095400	5.14921300	-12.45707500
C	29.34524800	-2.43971900	-13.12441600	H	26.02871700	5.38297000	-14.06320000
O	28.30350600	-2.99863400	-13.51590100	H	30.09345000	4.06318800	-14.58791900
O	29.41428700	-1.47753600	-12.26479900	H	27.78971500	4.15394700	-15.36518200
H	30.02548200	-4.63270200	-14.69832300	O	29.73859400	1.87653200	-12.43938700
H	31.18656600	-3.35983000	-12.77331400	H	29.42709300	2.74705700	-12.72704400
H	31.29007500	-1.95999900	-13.80420500	H	28.94036200	1.28987800	-12.32425400
C	27.87493200	1.06298000	-17.13693600	N	16.94772900	-3.33586800	-12.67274400
C	29.25761500	1.63839800	-16.90779200	C	16.59812200	-4.44990700	-11.75907500
O	29.43124700	2.82590500	-16.64026800	C	15.33348200	-3.92889300	-11.05973900
C	27.13342800	0.80910900	-15.80701000	C	14.67791800	-3.03279600	-12.12137500
C	25.67685100	0.50426800	-16.04924300	C	15.87615600	-2.33301300	-12.77019100
C	24.82428600	1.51016100	-16.51629600	H	17.41360200	-4.63277600	-11.05972300
C	25.14354200	-0.77001300	-15.83788900	H	14.68867000	-4.74148100	-10.71687700
C	23.47756900	1.25904700	-16.76086800	H	15.61349900	-3.33015600	-10.18567500
C	23.79792600	-1.04174600	-16.07826200	H	14.15734300	-3.64829300	-12.86330300
C	22.96838900	-0.01840900	-16.53142000	H	13.95737800	-2.32465900	-11.70511200
O	21.62831100	-0.31205000	-16.70882500	H	15.71921400	-2.05408400	-13.81458500
H	27.32311600	1.81255000	-17.71084500	H	16.16473900	-1.42325400	-12.22842100
H	27.60709200	-0.01195200	-15.25860100	C	29.55106300	-2.94493100	-11.16092400
H	27.22985700	1.69907700	-15.17788400	C	28.26165700	-3.72883300	-1.42598500
H	25.21309000	2.51219200	-16.67637400	C	28.07520200	-4.12587800	-2.89545200
H	25.77068700	-1.55048200	-15.41864800	C	27.88536000	-2.95550700	-3.84955300
H	22.82486800	2.05451900	-17.11118400	O	27.87776200	-1.78198000	-3.53366700
H	23.37583000	-2.01673200	-15.86231400	O	27.74505000	-3.38053400	-5.11795000
H	21.17315600	0.47803500	-17.02839400	H	29.56915100	-2.09187600	-1.84734900

H	28.22832700	-4.63799300	-0.81372200
H	27.40800100	-3.11258100	-1.12224600
H	28.93604200	-4.69937300	-3.26271100
H	27.21086300	-4.79020300	-3.01790700
H	30.46537100	-3.50996700	-1.36848000
C	29.56599900	-2.49659100	-0.16268800
C	34.86194500	7.99996200	-10.31594800
C	35.27687200	6.51984100	-10.40198400
C	35.02526200	5.97698900	-11.77245200
C	34.18792300	4.99482300	-12.23968100
N	35.58409500	6.53434000	-12.91509800
C	35.07472400	5.88542200	-13.99914400
N	34.22891400	4.94988100	-13.61990500
H	35.54572000	8.63139400	-10.89566400
H	36.32830500	6.39526900	-10.11138900
H	34.68835700	5.92412900	-9.69731200
H	36.24309400	7.29747600	-12.93824200
H	33.57111200	4.29436900	-11.69822400
H	35.34684200	6.12567400	-15.01638900
H	33.33000400	3.79591700	-14.38902200
H	34.87103700	8.38161700	-9.28969100
H	33.87106300	8.09554800	-10.77200700
Mg	26.84611800	-4.07371400	-12.34556100

TS1-B_{Mg} (46.5 kcal/mol)

H	20.66705300	-6.80405600	-16.56491100
H	16.38990300	-5.37396500	-12.30902200
H	24.65803900	-6.75726900	-19.16503700
H	29.36458200	-8.34239600	-18.18008800
H	35.11183800	4.87010900	-6.01580900
H	32.10201200	7.76393100	-10.35102700
H	33.92491500	-0.02993300	-10.21096800
H	31.95010600	-4.27903600	-6.58597300
H	23.18524400	1.49712300	-4.32326500
H	22.41704300	4.62909000	-7.60403300
H	22.25386900	6.38956300	-15.14824500
H	33.53414100	5.46913800	-6.68069500
H	30.78099900	8.84799500	-10.93702300
H	23.93863600	6.30931600	-15.81980600
H	23.80779600	-0.12317700	-3.81401700
H	32.79729200	-3.33858200	-5.29816100
H	32.07501300	0.82297300	-17.96198500
H	30.43545400	-3.27780300	-15.73602200
H	31.70195500	-4.16529500	-14.93533400
H	30.41807900	-9.05983300	-14.20511000
H	20.88599200	-5.05006500	-16.84106900
H	34.15717400	-4.71610700	-10.10826000
H	23.72447000	-8.30782700	-7.05586600
H	21.59203500	-3.72878600	-7.31996900
H	27.89807500	0.15101700	-17.74202000
H	27.15893700	4.34428400	-6.69921400
C	29.55202300	-8.45656100	-13.91530600
C	29.06060600	-7.64870100	-15.09850300
O	28.79451100	-6.43937700	-15.06565400
C	29.79183300	-7.61066000	-12.66295900
C	28.48112700	-7.36886600	-11.90062300
C	28.66409200	-6.34631100	-10.78046800
O	29.53855300	-6.55561700	-9.92736900
O	27.88439200	-5.32207300	-10.79265100
H	28.77104600	-9.20138300	-13.69745500
H	30.50402600	-8.10153200	-11.99571500
H	30.22842700	-6.65053400	-12.95418700
H	27.69390600	-7.05138300	-12.58680500
H	28.15749500	-8.31472700	-11.44680100
N	28.96474800	-8.35840200	-16.23569100
C	28.69023500	-7.77016300	-17.53343900
C	27.22285300	-7.98872500	-17.90588100
O	26.74966100	-9.11788600	-17.93185000
H	29.08422200	-9.35967500	-16.20364500
H	28.99141400	-6.72215100	-17.50628400
N	26.51473400	-6.85094300	-18.13127400
C	25.05614900	-6.83985900	-18.14800600
C	24.52497700	-5.70897400	-17.26740200
H	26.97997000	-5.96938800	-17.96898300
H	24.73707300	-7.81464300	-17.76984600
H	23.43314000	-5.69241200	-17.28214300
H	24.85340500	-5.83874100	-16.23099300
H	24.86947100	-4.72923000	-17.62127300
C	23.25610900	6.03675600	-15.04210900
C	23.27134900	4.49073900	-15.06296600
C	22.44683900	3.77826500	-14.01949000
C	22.60351600	4.04353600	-12.65451000
C	21.56828100	2.74912300	-14.38623500
C	21.90565500	3.31589700	-11.69385100
C	20.87375700	1.99781600	-13.44237000
C	21.03801900	2.29178800	-12.08686200
O	20.33268900	1.55188900	-11.17951400
H	23.64880200	6.42479600	-14.09516500
H	22.93839800	4.16046800	-16.05410200
H	24.31511600	4.15264000	-14.98411500
H	23.29143100	4.81981000	-12.32844700
H	21.45539000	2.50400600	-15.43859300
H	22.04299200	3.52938200	-10.63900800
H	20.25923000	1.15448800	-13.73522800
H	20.65981900	1.76347900	-10.29435100
C	20.86191000	-5.83974700	-16.08299600
C	19.76458300	-5.54406700	-15.06217400

O	18.75440400	-6.22897200	-14.94790600
H	21.84043400	-5.85414400	-15.59384900
N	19.99912800	-4.43765500	-14.28402100
C	19.19499800	-4.19828300	-13.09491700
C	18.13292900	-3.12124200	-13.28168500
O	18.35953600	-2.07778000	-13.91531900
C	20.16528900	-3.80977700	-11.95517700
O	19.52770500	-3.62717400	-10.69676400
H	20.93221000	-4.03248100	-14.30708800
H	18.71009900	-5.14454900	-12.84977200
H	20.87612600	-4.63156400	-11.84034600
H	20.73583000	-2.92185900	-12.24790800
H	19.17476900	-2.72880100	-10.66903400
C	23.90676800	-7.35667600	-7.56586300
C	22.93580100	-6.30899800	-7.05154200
O	21.80673100	-6.63630600	-6.67921900
C	23.48808400	-7.72815800	-9.01913800
C	23.82817200	-6.68477000	-10.01134500
C	25.00072300	-6.49678700	-10.68734000
N	23.06587000	-5.56107700	-10.29234000
C	23.79135100	-4.74602100	-11.10411600
N	24.97029900	-5.29343000	-11.35387000
H	24.96062500	-7.08084700	-7.51521700
H	24.00299300	-8.64950500	-9.30755600
H	22.41532100	-7.94793600	-9.00724800
H	22.16056700	-5.34651100	-9.89775400
H	25.87122600	-7.13178600	-10.70331600
H	23.42966500	-3.81962200	-11.51943200
N	23.30777900	-5.00436000	-7.14522100
C	22.40686800	-3.96390700	-6.62804900
C	23.33806400	-2.77343800	-6.39263900
C	24.43359300	-2.95667700	-7.45154400
C	24.65117700	-4.47438500	-7.46259500
H	21.92753900	-4.32731100	-5.71497300
H	22.81994200	-1.82176800	-6.47899500
H	23.77709000	-2.83565300	-5.39066900
H	24.08372400	-2.61197200	-8.43021900
H	25.35308500	-2.41775800	-7.21828300
H	25.00943400	-4.83965600	-8.42692800
H	25.37799600	-4.76273600	-6.69195300
C	23.17495300	4.07090500	-8.16495300
C	24.47233500	3.92610700	-7.39009600
O	24.49573900	3.78307500	-6.16808900
H	22.78281000	3.06668700	-8.35884700
H	23.31474100	4.57187700	-9.12518300
N	25.61162800	3.93269200	-8.13879700
C	26.90907900	3.66666400	-7.52183800
C	27.90487300	3.88022500	-8.66107800
C	27.12399700	3.42743200	-9.88780900
C	25.69189300	3.90287000	-9.61139600
H	26.94438800	2.64174800	-7.13064200
H	28.14691500	4.94414200	-8.74836300
H	28.83520800	3.32936000	-8.51632500
H	27.51824900	3.84163500	-10.81295800
H	27.14370900	2.33790100	-9.95367600
H	25.52694500	4.90488200	-10.02797700
H	24.95148400	3.22230400	-10.03922700
C	23.37401600	0.46303700	-4.62957400
C	24.39995700	0.46194100	-5.78353900
C	23.89335400	0.51646400	-7.21208600
C	22.54393300	0.41307200	-7.56439300
C	24.83517700	0.57239000	-8.25415400
C	22.15325000	0.30734700	-8.90403100
C	24.45036200	0.49991400	-9.59058200
C	23.10097500	0.35248800	-9.92703300
H	22.42641600	-0.01442300	-4.89168100
H	25.08337700	1.30443600	-5.63591900
H	25.01952900	-0.44128100	-5.71044200
H	21.78456800	0.38126200	-6.79064200
H	25.89102500	0.65011100	-8.00643200
H	21.10510500	0.14492600	-9.14107300
H	25.19981100	0.53812600	-10.37089100
H	22.80411400	0.26881700	-10.96631700
C	32.20544700	-3.28041900	-6.21784800
C	30.91038400	-2.47047900	-6.03147700
C	29.93900800	-2.65862900	-7.16585000
C	29.98293000	-3.60155900	-8.16465800
N	28.74369300	-1.93890600	-7.27059300
C	28.10056100	-2.46711000	-8.32262500
N	28.81509600	-3.46230200	-8.88143100
H	32.81696500	-2.83579800	-7.00434200
H	30.41100700	-2.76091100	-5.09779800
H	31.15213600	-1.40495400	-5.90430500
H	27.81823300	-2.68177000	-5.73676100
H	30.73390200	-4.32463800	-8.43985700
H	27.16052100	-2.13117900	-8.73566000
H	28.50083400	-4.08737000	-9.63899400
C	33.48002600	-4.18195000	-10.78252500
C	33.32963300	-2.74040600	-10.32513100
O	33.00331100	-2.40657300	-9.19009600
C	32.15447700	-4.96594600	-10.77158600
O	32.03808700	-5.65094500	-9.54522100
H	33.91961500	-4.21284300	-11.78603200
H	31.30392600	-4.28450500	-10.93308100
H	32.15883500	-5.67300900	-11.61716000
H	31.16871100	-6.10320300	-9.56944000
N	33.56179700	-1.80495000	-11.29090000
C	33.30513600	-0.40196800	-11.03308700
H	33.73065600	-2.10364400	-12.23789300

H	33.52486900	0.19393000	-11.91571000
H	32.25750700	-0.23732200	-10.76643300
C	30.70353000	-3.79203900	-14.83814000
C	30.44293300	-2.75395500	-13.72038200
C	28.92639600	-2.59619400	-13.54192400
O	28.35681200	-3.56661000	-12.99141500
O	28.34665000	-1.54963400	-14.00072900
H	30.04359100	-4.65093400	-14.71274100
H	30.83791500	-3.08883400	-12.75701500
H	30.89224000	-1.78889700	-13.96578100
C	27.87492600	1.06298600	-17.13694800
C	29.25286700	1.59907500	-16.80753000
O	29.41875200	2.75295200	-16.41378400
C	27.00668700	0.80666700	-15.90057800
C	25.64322200	0.29468600	-16.29412100
C	24.67293900	1.17032100	-16.78985000
C	25.30208500	-1.05530100	-16.14634100
C	23.39031300	0.72474000	-17.10402000
C	24.02121200	-1.51837400	-16.44238600
C	23.06608300	-0.61928700	-16.91750500
O	21.79475000	-1.10610500	-17.16038100
H	27.39667000	1.82831500	-17.75862700
H	27.51458600	0.08562000	-15.25988700
H	26.91346700	1.73373200	-15.33053500
H	24.90959900	2.22528200	-16.90088900
H	26.03131700	-1.74055300	-15.72417600
H	22.64085500	1.42243300	-17.47155000
H	23.72992900	-2.54409600	-16.24407100
H	21.25898100	-0.39989000	-17.54579900
N	30.27644000	0.72631800	-16.99653500
C	31.68301900	1.10903500	-16.98007200
C	32.46605300	0.41286600	-15.86172800
C	32.03153900	0.81774500	-14.44543600
C	32.64905200	2.09506100	-13.91146800
O	32.86319200	3.01623000	-14.84731300
O	32.92323300	2.26365900	-12.72977300
H	30.04526800	-0.20438600	-17.30953500
H	31.72439400	2.19200300	-16.86808900
H	32.33422200	-0.67216700	-15.96834800
H	33.53387400	0.61273500	-16.00552800
H	30.94395600	0.93639700	-14.39181700
H	32.26527100	0.03369200	-13.72309900
C	26.00112100	-2.10470500	-12.17120200
O	25.44749300	-2.94006100	-12.98263400
O	26.50985000	-2.48479300	-11.09101200
C	26.13488000	-0.70472600	-12.70400000
C	27.03683000	0.30437300	-12.12824300
O	28.09434200	-0.00714700	-11.50526200
C	26.74190800	1.67304100	-12.47339400
C	25.53624600	2.04237600	-13.00290500
C	24.55364700	1.07929600	-13.36289000
C	24.87000000	-0.23838200	-13.25776000
H	27.09384300	-1.12877400	-13.51542500
H	27.47714400	2.42262600	-12.22997300
H	25.33159500	3.09683100	-13.15581600
H	23.59216400	1.38916800	-13.74588500
H	24.15125200	-0.99002600	-13.54911400
O	26.51542800	-5.40788100	-13.96664200
H	26.15410700	-4.65811900	-14.46118200
H	27.36623400	-5.65041500	-14.39285700
O	22.74664500	-3.27419700	-13.91268900
H	22.29366300	-2.40805000	-14.00181400
H	23.67873800	-3.11555300	-13.67386800
O	20.96517700	-1.24494000	-14.40719600
H	21.08192200	-1.28120800	-15.37113000
H	20.04883700	-1.56675600	-14.24884700
C	34.22894800	4.62570000	-6.61657100
C	33.56672400	3.32082000	-6.15420500
C	32.31497400	2.93756700	-6.96966200
C	32.11729000	1.41012100	-7.01960500
N	30.79039000	0.96978500	-7.44653200
C	30.29419300	1.06790500	-8.69845500
N	30.93617100	1.76337800	-9.64099300
N	29.09901200	0.52170400	-8.94040900
H	34.60137700	4.48189700	-7.64101300
H	34.31077200	2.51717100	-6.23683700
H	33.30165900	3.37635200	-5.09180200
H	31.41889000	3.40011400	-6.54207800
H	32.40768800	3.34189000	-7.98460900
H	32.89002800	0.94407200	-7.64737200
H	32.25387600	0.99931200	-6.01605700
H	30.30571800	0.31144000	-6.84969300
H	31.89199400	2.03355000	-9.48239500
H	30.59716900	1.77649800	-10.63089500
H	28.78735200	-0.18981200	-8.27427500
H	28.76685100	0.40061400	-9.90450600
C	31.09199900	7.81104000	-10.76996000
C	30.06445300	7.00351300	-9.95830500
C	28.83124300	6.72203700	-10.76567400
C	27.57337700	7.24276800	-10.59669200
C	28.77637000	5.89420000	-11.95017800
C	27.44812800	5.96815400	-12.45633500
C	29.72060500	5.10532700	-12.63418300
N	26.73364100	6.78637000	-11.60378000
C	27.05281700	5.29632500	-13.61854300
C	29.33497600	4.44343100	-13.79649100
C	28.01186600	4.54012400	-14.28217100
H	31.18043600	7.36780900	-11.76851700
H	30.52049600	6.05223600	-9.65196300

H	29.80044400	7.52971500	-9.03416200
H	27.20143100	7.91007800	-9.83236300
H	25.77094100	7.05372200	-11.72321000
H	30.74295300	5.02401500	-12.27563600
H	26.03854600	5.37991800	-13.99776100
H	30.05263300	3.87433300	-14.37836000
H	27.77483400	4.02015500	-15.20260200
O	30.03436600	1.66300400	-12.17946200
H	29.66179500	2.47127700	-12.56050900
H	29.29399500	1.01292200	-12.07032900
N	16.94672600	-3.33793300	-12.67604900
C	16.59821100	-4.44989700	-11.75908700
C	15.33238200	-3.92772800	-11.06369900
C	14.67174000	-3.04731600	-12.13544100
C	15.86527000	-2.34768000	-12.79386500
H	17.41342100	-4.63226300	-11.05903300
H	14.69191900	-4.73969100	-10.71143300
H	15.61010500	-3.31789900	-10.19653100
H	14.15423500	-3.67455100	-12.86957300
H	13.94717900	-2.33877300	-11.72702700
H	15.70821000	-2.08916200	-13.84347800
H	16.14375300	-1.42563000	-12.26801900
C	29.55100600	-2.94479800	-1.16124300
C	28.26261700	-3.73320700	-1.41765300
C	28.07357000	-4.14741600	-2.88165500
C	27.88154400	-2.99103000	-3.85082800
O	27.90696200	-1.81093800	-3.55916900
O	27.69886600	-3.43506800	-5.10677600
H	29.56543200	-2.09400400	-1.85013500
H	28.23192400	-4.63583800	-0.79571500
H	27.40819000	-3.11572400	-1.11813200
H	28.93530100	-4.72313200	-3.24384400
H	27.21111300	-4.81539800	-2.99526300
H	30.46541100	-3.50998700	-1.36824800
H	29.56603500	-2.49671100	-0.16263500
C	34.86193100	7.99994700	-10.31596000
C	35.28449300	6.52314400	-10.41585000
C	35.03716500	5.99355900	-11.79311600
C	34.22653700	4.99334200	-12.26910300
N	35.57229300	6.58276700	-12.93144200
C	35.07472400	5.93350700	-14.02108000
N	34.25945400	4.96806700	-13.65040600
H	35.54203500	8.63793200	-10.89332400
H	36.33640600	6.40188500	-10.12539700
H	34.69886300	5.91623300	-9.71830000
H	36.20907100	7.36460000	-12.94848500
H	33.63819500	4.26451300	-11.73343000
H	35.33280400	6.19647600	-15.03642500
H	33.35848500	3.79858700	-14.43052300
H	34.87105100	8.38162600	-9.28969500
H	33.87105700	8.09554900	-10.77199500
Mg	26.73820800	-4.37138500	-12.10234700

Int2-B_{Mg} (30.8 kcal/mol)

H	20.66707300	-6.80405000	-16.56493100
H	16.38993600	-5.37395800	-12.30904700
H	24.65803900	-6.75726400	-19.16503400
H	29.36458900	-8.34239100	-18.18008400
H	35.11186000	4.87008700	-6.01583300
H	32.10200600	7.76398400	-10.35100600
H	33.92491100	-0.02993500	-10.21096400
H	31.95010800	-4.27903300	-6.58598200
H	23.18525300	1.49712100	-4.32325300
H	22.41704800	4.62908900	-7.60402500
H	22.25385400	6.38957300	-15.14806600
H	33.53413400	5.46913000	-6.68072300
H	30.78100200	8.84800000	-10.93699800
H	23.93872700	6.30932900	-15.81972100
H	32.80778900	-0.12318900	-3.81402200
H	32.79729800	-3.33856400	-5.29816400
H	32.07501500	0.82295900	-17.96198000
H	30.43544200	-3.27780300	-15.73601800
H	31.70195400	-4.16530000	-14.93533100
H	30.41807500	-9.05982700	-14.20513300
H	20.88599900	-5.05004200	-16.84104400
H	34.15717800	-4.71610500	-10.10826300
H	23.72441900	-8.30780900	-7.05585100
H	21.59202500	-3.72878600	-7.31995700
H	27.89809500	0.15103400	-17.74204500
H	27.15895500	4.34420000	-6.69915000
C	29.55202300	-8.45656600	-13.91526700
C	29.00323300	-7.65510700	-15.08102800
O	28.59133000	-6.49033000	-15.01128900
C	29.79803200	-7.60184600	-12.66891400
C	28.48064000	-7.28162900	-11.95094400
C	28.67875100	-6.32013400	-10.78028600
O	29.55093200	-6.57894100	-9.94107000
O	27.89505700	-5.29876900	-10.73736800
H	28.78077700	-9.20500000	-13.67234500
H	30.46177900	-8.11877700	-11.97186300
H	30.29661900	-6.67029500	-12.95601500
H	27.75359800	-6.87531700	-12.65592800
H	28.06277800	-8.21501700	-11.54954400
N	29.01254200	-8.34000200	-16.23985400
C	28.69022600	-7.77016700	-17.53345100
C	27.21707500	-7.99827100	-17.88104000
O	26.73711200	-9.12418200	-17.88088100

H	29.25932400	-9.31738400	-16.22005200	H	20.62038100	0.60821300	-8.79727600
H	28.97914300	-6.71720200	-17.53280700	H	24.57529000	0.63624200	-10.47195900
N	26.51434900	-6.86053200	-18.13133100	H	22.10774800	0.62194500	-10.80075000
C	25.05615100	-6.83986800	-18.14800700	C	32.20543600	-3.28044200	-6.21784100
C	24.53730700	-5.67918700	-17.29712000	C	30.93816800	-2.44351000	-6.01090300
H	26.98093800	-5.98056500	-17.96285200	C	29.96222000	-2.61780800	-7.13454400
H	24.72501000	-7.80430900	-17.75450300	C	29.99991800	-3.56206500	-8.13114200
H	23.44472900	-5.66873000	-17.29233300	N	28.76144600	-1.90943800	-7.21279700
H	24.89233900	-5.75257900	-16.26391700	C	28.09458900	-2.45670800	-8.23775900
H	24.87292000	-4.71635400	-17.70182900	N	28.81088300	-3.44411600	-8.81310400
C	23.25602800	6.03672100	-15.04241000	H	32.82195700	-2.84106900	-7.00374200
C	23.22114700	4.49939800	-14.96284800	H	30.43922400	-2.72561300	-5.07411000
C	22.30509000	3.92846400	-13.90199300	H	31.20726500	-1.38409800	-5.87962500
C	22.29701600	4.42155100	-12.59096300	H	27.84616500	-2.64252400	-5.70406900
C	21.49723900	2.81706900	-14.17928400	H	30.75443100	-4.27454900	-8.42300300
C	21.51698300	3.83116200	-11.59902600	H	27.14201400	-2.12688700	-8.61954300
C	20.71898800	2.20478800	-13.20108100	H	28.50267800	-4.07510700	-9.56324200
C	20.72521000	2.71880500	-11.90172100	C	33.48001600	-4.18195400	-10.78252000
O	19.94565100	2.10073100	-10.96514100	C	33.34384900	-2.73854500	-10.32588600
H	23.64912300	6.46423900	-14.11213100	O	33.03435700	-2.40255000	-9.18699800
H	22.91514000	4.10281100	-15.93837100	C	32.14764600	-4.95434000	-10.75388100
H	24.24248200	4.12268100	-14.80262700	O	32.03836800	-5.62851400	-9.51992100
H	22.91820100	5.27312600	-12.32792800	H	33.91129700	-4.22001300	-11.78926100
H	21.49953600	2.39832400	-15.18108200	H	31.29995100	-4.26935400	-10.91235900
H	21.52521800	4.22848500	-10.58835100	H	32.14085200	-5.66971400	-11.59267300
H	20.14809700	1.31023100	-13.42349300	H	31.16966300	-6.08066500	-9.53567400
C	20.23886800	2.37711200	-10.08582400	N	33.56994400	-1.80346300	-11.29402200
C	20.86188100	-5.83981400	-16.08301200	C	33.30514300	-0.40196300	-11.03309300
C	19.76843900	-5.54863800	-15.05543200	H	33.71343200	-2.10310300	-12.24499600
O	18.78041500	-6.25995800	-14.91776600	H	33.51948100	0.19831500	-11.91424800
H	21.84181200	-5.86228600	-15.59588500	H	32.25806800	-0.24773000	-10.75973700
N	19.98145700	-4.42034200	-14.30013200	C	30.70354700	-3.79203600	-14.83814800
C	19.19502700	-4.19823100	-13.09493600	C	30.49195000	-2.80698900	-13.67261800
C	18.14213300	-3.10735900	-13.25297300	C	28.98930000	-2.72293300	-13.44312000
O	18.37604600	-2.04722600	-13.85971600	O	28.54982900	-3.08617500	-12.31361600
C	20.17156800	-3.85908000	-11.94338000	O	28.24998000	-2.43000400	-14.43607000
O	19.54972500	-3.80332900	-10.66464100	H	30.04716100	-4.66061400	-14.73837100
O	20.90633600	-3.99208400	-14.33174500	H	30.97217000	-3.13271200	-12.74890500
H	18.70176700	-5.14538200	-12.87105200	H	30.88404300	-1.81832400	-13.93438600
H	20.91784900	-4.65627800	-11.90620900	C	27.87489300	1.06297700	-17.13692200
H	20.69814300	-2.92526300	-12.16398000	C	29.25688900	1.66583800	-16.97016700
H	19.22987200	-2.90388900	-10.52200500	O	29.42972000	2.87459700	-16.82375200
C	23.90683700	-7.35671400	-7.56587900	C	27.20879600	0.73143800	-15.78674200
C	22.92028400	-6.30934200	-7.07743600	C	25.81487400	0.20275600	-16.01891200
O	21.77496000	-6.63091300	-6.75317400	C	24.76688800	1.08060500	-16.31636500
C	23.58001000	-7.68659600	-9.05414200	C	25.55128700	-1.17236700	-16.02553600
C	23.92171300	-6.60751300	-10.02000800	C	25.49098200	0.60929700	-16.61447100
C	25.06887000	-6.40387900	-10.73768600	C	24.27956400	-1.66061800	-16.33414300
N	23.14259800	-5.48556400	-10.27355300	C	23.25285900	-0.76471700	-16.63091000
C	23.83673900	-4.65761500	-11.09729400	O	21.99816600	-1.28251600	-16.91363200
N	25.01399800	-5.18905000	-11.39539300	H	27.26915200	1.79850700	-17.67291100
H	24.95456900	-7.07114900	-7.45627700	H	27.80860400	-0.00790200	-15.24812900
H	24.13878100	-8.58141100	-9.34437800	H	27.17890100	1.64018900	-15.17960600
H	22.51575800	-7.94171500	-9.10721100	H	24.94797400	2.15174800	-16.30732200
H	22.24765700	-5.27904300	-9.85075500	H	26.35486600	-1.86102900	-15.78413800
H	25.94189900	-7.03237400	-10.78496200	H	22.68562000	1.30489900	-16.83578900
H	23.45939100	-3.71710100	-11.46517100	H	24.08202300	-2.72754700	-16.38382700
N	23.30991300	-5.00710000	-7.13470900	H	21.49331600	-0.61750700	-17.40141400
C	22.40686600	-3.96389300	-6.62805600	N	30.26920500	0.75697800	-16.98076900
C	23.32715700	-2.75817200	-6.41345800	C	31.68302400	1.10904300	-16.98007800
C	24.45033900	-2.96733200	-7.43873300	C	32.42795400	0.42246500	-15.83124200
C	24.66579400	-4.48402300	-7.41084700	C	31.94686400	0.86111300	-14.43356700
H	21.92805600	-4.31523500	-5.70970300	C	32.59570200	2.12118500	-13.90097100
H	22.80245900	-1.81397700	-6.54873000	O	32.65541400	3.10455500	-14.79642000
H	23.74219400	-2.77681400	-5.39975700	O	33.03378400	2.22472100	-12.76281100
H	24.13681700	-2.64471000	-8.43643200	H	30.02522300	-0.21556900	-17.10071200
H	25.36443800	-2.42637700	-7.19064300	H	31.73775100	2.19327700	-16.88106000
H	25.05793400	-4.86680000	-8.35455700	H	32.29028600	-0.66364300	-15.92000400
H	25.36333700	-4.75903600	-6.60872800	H	33.50252500	0.60669400	-15.94250300
C	23.17494700	4.07089100	-8.16495100	H	30.86504100	1.03331500	-14.43882800
C	24.47729600	3.95099400	-7.39585300	H	32.12633200	0.07824100	-13.69519300
O	24.51095700	3.84789300	-6.17021100	C	26.35572900	-1.31967800	-11.05680300
H	22.78759500	3.06621900	-8.35401500	O	26.03990800	-2.55265000	-10.96449000
H	23.30916200	4.56233700	-9.13168600	O	26.73647600	-0.56909600	-10.15698500
N	25.61514200	3.94170600	-8.15056100	C	26.16098800	-0.71988100	-12.50783000
C	26.90906300	3.66677200	-7.52189000	C	26.83358900	0.61870300	-12.58443200
C	27.89994400	3.76025200	-8.68418700	O	28.06864000	0.66097600	-12.43500700
C	27.08860000	3.23485600	-9.87370100	C	26.01265400	1.78734700	-12.80382000
C	25.68306600	3.80226200	-9.61921900	C	24.67526700	1.64936000	-13.02383300
H	26.90184700	2.65365700	-7.09504200	C	24.00703200	0.37043900	-13.06874700
H	28.17888700	4.80409700	-8.86067700	C	24.71045500	-0.75569400	-12.83354500
H	28.81146000	3.19006500	-8.49862600	H	26.72446500	-1.39608100	-13.16636800
H	27.49908500	3.54812200	-10.83526000	H	26.49249900	2.76003400	-12.81017400
H	27.05112400	2.14179000	-9.85868000	H	24.06886600	2.53346800	-13.16904800
H	25.56230800	4.77951200	-10.10307500	H	22.94728200	0.33572000	-13.29435800
H	24.90357000	3.13383400	-9.99000700	H	24.22508500	-1.72407900	-12.83246000
C	23.37401900	0.46305700	-4.62957400	O	26.71434900	-4.50404600	-13.95215900
C	24.30483400	0.46135900	-5.84623800	H	27.20346900	-3.70229200	-14.30748100
C	23.64104900	0.58999900	-7.20277400	H	27.22158600	-5.26733000	-14.28808300
C	22.25390100	0.62967000	-7.39327700	O	22.59027300	-3.13820000	-13.75995700
C	24.45766700	0.60282200	-8.34236200	H	22.07199200	-2.29991600	-13.87195700
C	21.70104000	0.63406700	-8.67897800	H	23.34496100	-3.04968800	-14.35553200
C	23.91251900	0.63490600	-9.62113200	O	20.89995200	-1.10316800	-14.26563100
C	22.52803800	0.63525000	-9.80220000	H	21.06746600	-1.15869300	-15.22129800
H	22.41258600	-0.01302500	-8.44424100	H	19.98561300	-1.45833500	-14.13822000
H	25.02526300	1.27950400	-5.74030200	C	34.22892800	4.62572900	-6.61651600
H	24.89794200	-0.46068800	-5.86196200	C	33.55613400	3.30231600	-6.20909300
H	21.58866000	0.63975000	-6.53756100	C	32.33447900	2.92266600	-7.08324800
H	25.53628400	0.54915900	-8.23545500	C	32.16632800	1.39077800	-7.20366400

N	30.8666500	0.92213400	-7.69744100	H	32.10198800	7.76408400	-10.35096200
C	30.40371100	1.07066700	-8.95849800	H	33.92494300	-0.02994800	-10.21098000
N	31.04142800	1.84121300	-9.84113900	H	31.94951700	-4.27861900	-6.58669800
N	29.24837100	0.48520300	-9.28137800	H	23.18505000	1.49693200	-4.32274300
H	34.61231900	4.50502800	-7.64102100	H	22.41699200	4.62900700	-7.60401800
H	34.30970300	2.50679000	-6.28217600	H	22.25410300	6.39038000	-15.14770600
H	33.24995000	3.32989600	-5.15690700	H	33.53401100	5.46901200	-6.68094900
H	31.41620300	3.35087100	-6.66737200	H	30.78104100	8.84801300	-10.93699800
H	32.45212700	3.36942200	-8.07752600	H	23.93794400	6.31003000	-15.82016800
H	32.97558400	0.96785900	-7.81570300	H	23.80807100	-0.12266300	-3.81379600
H	32.27341700	0.94439800	-6.21191400	H	32.79670700	-3.33983100	-5.29786500
H	30.40999600	0.18913800	-7.16567200	H	32.07487100	0.82265900	-17.96195200
H	31.99061700	2.11662300	-9.65680500	H	30.43510100	-3.27790900	-15.73597800
H	30.66151500	2.01375700	-10.80227200	H	31.70222600	-4.16434100	-14.93620000
H	28.81296900	-0.16620400	-8.63301300	H	30.41802300	-9.05988300	-14.20517500
H	28.89007000	0.47287100	-10.23019200	H	20.88592700	-5.04998000	-16.84098200
C	31.09200500	7.81099400	-10.76999700	H	34.15698700	-4.71598600	-10.10797700
C	30.05565500	6.95927600	-10.02477400	H	23.72515600	-8.30785200	-7.05566700
C	28.84392100	6.68067700	-10.86962900	H	21.59184700	-3.72889700	-7.31978500
C	27.54508500	7.03557400	-10.60378700	H	27.89763000	0.15105900	-17.74210300
C	28.82353900	5.98186800	-12.13749500	H	27.15901100	4.34388500	-6.69890900
C	27.46914200	5.94232000	-12.57605000	C	29.55203600	-8.45629400	-13.91500600
C	29.80909900	5.38626500	-12.95106000	C	29.06555300	-7.64752600	-15.10154100
N	26.71441500	6.59811900	-11.62414200	O	28.84968400	-6.42992800	-15.07967100
C	27.08501800	5.32175700	-13.77056400	C	29.83721400	-7.60116500	-12.67868400
C	29.43259100	4.77139900	-14.14357000	C	28.55853700	-7.24674300	-11.90617900
C	28.08047400	4.73484100	-14.54540600	C	28.87374900	-6.24210700	-10.79073500
H	31.21150100	7.40167800	-11.78010000	O	29.70835100	-6.59323800	-9.93977100
H	30.52205700	6.00445000	-9.74411800	O	28.28369100	-5.10078400	-10.81858200
H	29.75352600	7.43884800	-9.08704500	H	28.76754200	-9.19052600	-13.67768200
H	27.13832000	7.56454300	-9.75377400	H	30.51532100	-8.12511900	-12.00099200
H	25.71812600	6.73322200	-11.66063200	H	30.34157100	-6.68116700	-12.99166900
H	30.85545900	5.39932200	-12.65886300	H	27.79595800	-6.86344500	-12.58565100
H	26.04487300	5.30641900	-14.08300300	H	28.16090000	-8.16019600	-11.44586300
H	30.17479200	4.29476900	-14.77523600	N	28.92268400	-8.36706500	-16.23148800
H	27.84270900	4.24111300	-15.48120400	C	28.68983300	-7.77110800	-17.53382800
O	30.02217400	2.33584900	-12.27129900	C	27.23260500	-7.97752000	-17.95243100
H	29.82175500	3.25475700	-12.49993800	O	26.77255700	-9.10715400	-18.06564100
H	29.19381000	1.81841600	-12.42679300	H	29.01512100	-9.37100600	-16.19534500
N	16.95039400	-3.33205700	-12.66669100	H	28.99770400	-6.72573700	-17.49007500
C	16.59815800	-4.44991200	-11.75904000	N	26.51591500	-6.83479700	-18.12042600
C	15.33290300	-3.93041500	-11.05973400	C	25.05604000	-6.83991900	-18.14808200
C	14.67782600	-3.03379400	-12.12123400	C	24.51113900	-5.71527400	-17.26771700
C	15.87582200	-2.33149700	-12.76785000	H	26.96248100	-5.96660000	-17.86097500
H	17.41286900	-4.63982800	-11.06057200	H	24.74081600	-7.81833300	-17.77480400
H	14.68858700	-4.74407100	-10.71893700	H	23.41974500	-5.70892800	-17.28441700
H	15.61081600	-3.33263700	-10.18431800	H	24.83548200	-5.83465300	-16.22935900
H	14.15875600	-3.64890800	-12.86441200	H	24.84610100	-4.73268100	-17.62264400
H	13.95621200	-2.32686200	-11.70510300	C	23.25674600	6.03497800	-15.04229300
H	15.72144000	-2.05440200	-13.81303300	C	23.17430100	4.49613500	-15.02950800
H	16.16185400	-1.42116600	-12.22620300	C	22.25950700	3.92335400	-13.97318700
C	29.55101300	-2.94481000	-1.16122900	C	22.46714400	4.19440500	-12.61533300
C	28.26445900	-3.74135000	-1.40268000	C	21.22601100	3.03769100	-14.30667000
C	28.06167800	-4.15040500	-2.86523400	C	21.70260200	3.58113300	-11.62850700
C	27.85885200	-2.98307800	-3.81940700	C	20.45248300	2.40807000	-13.33318900
O	27.83554100	-1.80991400	-3.50126200	C	20.70060700	2.67285700	-11.98376700
O	27.72582400	-3.40830900	-5.08648900	O	19.94624900	2.02218200	-11.04922400
H	29.55798500	-2.09597100	-1.85220400	H	23.64657200	6.42211900	-14.09482600
H	28.24788300	-4.64491600	-0.78145100	H	22.82855600	4.16113600	-16.01415300
H	27.41022200	-3.12911300	-1.09252900	H	24.17859200	4.06963600	-14.91305200
H	28.91915900	-4.72379500	-3.23995400	H	23.26283600	4.87105900	-12.31523400
H	27.19672900	-4.81648000	-2.97383400	H	21.04709600	2.80747400	-15.35364000
H	30.46541000	-3.50998600	-1.36825800	H	21.89684000	3.78360900	-10.58087500
H	29.56602800	-2.49670100	-0.16263900	H	19.67992700	1.69311700	-13.59568400
C	34.86193200	7.99993800	-10.31595900	H	20.33219600	2.18323900	-10.17683300
C	35.28073500	6.52308900	-10.43134500	C	20.86191400	-5.83991500	-16.08290600
C	34.98430700	6.00978000	-11.80529900	H	19.86281500	-5.65677200	-14.94782500
C	34.14534300	5.02579100	-12.26523800	O	19.26955000	-6.61290500	-14.46010900
N	35.47324600	6.61850100	-12.95423500	H	21.85678500	-5.85654900	-15.62403400
C	34.92231400	5.99658100	-14.03382800	N	19.71894400	-4.37954800	-14.45271100
N	34.11638200	5.02968500	-13.64689900	C	19.19480600	-4.19824000	-13.09530400
H	35.54018500	8.64041700	-10.89283100	C	18.19027000	-3.05385700	-13.10498000
H	36.34089600	6.39746500	-10.17562300	O	18.47755700	-1.93859400	-13.57523800
H	34.71528100	5.91262200	-9.72052500	C	20.38705900	-3.98058400	-12.13250700
H	36.11539100	7.39558600	-12.98347000	O	20.09356200	-4.33425300	-10.77541800
H	33.58127000	4.28710500	-11.71751700	H	20.34292400	-3.65090200	-14.78339600
H	35.13741600	6.27823700	-15.05412900	H	18.72362800	-5.14675700	-12.84162300
H	33.18697000	3.87383700	-14.40007300	H	21.18804700	-4.63854300	-12.47503800
H	34.87105000	8.38162800	-9.28969600	H	20.75705000	-2.95281700	-12.20512300
H	33.87106000	8.09554600	-10.77200000	H	19.88016100	-3.53216100	-10.28422200
Mg	26.83760000	-4.10573800	-11.89216900	C	23.90574100	-7.35677100	-7.56610400
				C	22.92482700	-6.30727900	-7.06889300
				O	21.78531900	-6.62677000	-6.72493400
				C	23.57380500	-7.67495500	-9.05219600
				C	23.99572800	-6.61132100	-10.00185700
				C	25.24397000	-6.35086100	-10.50400100
				N	23.19514400	-5.58190200	-10.47403200
				C	23.96451400	-4.75870700	-11.23306300
				N	25.21228500	-5.20234900	-11.26190800
				H	24.95502600	-7.07586500	-7.45820000
				H	24.08361000	-8.60227000	-9.33178300
				H	22.49847800	-7.86761400	-9.12433700
				H	22.20708500	-5.44084100	-10.28607500
				H	26.15901500	-6.89825000	-10.34441300
				H	23.58881400	-3.91375000	-11.78481800
				N	23.31133500	-5.00335500	-7.13653800
				C	22.40719100	-3.96386600	-6.62833100
				C	23.32722300	-2.76112900	-6.39509900
				C	24.46120900	-2.96563000	-7.41002600

The transition states and intermediates involved in the reaction pathway with **Mode-B** for the Zn-enzyme of SDC.

E:S-B_{Zn} (0.7 kcal/mol)

H	20.66712700	-6.80403900	-16.56497400
H	16.38996900	-5.37394900	-12.30907600
H	24.65797200	-6.75707800	-19.16499700
H	29.36510800	-8.34186900	-18.18000400
H	35.11194200	4.87001700	-6.01592200

C	24.67240700	-4.48330300	-7.38711400	C	31.87605800	0.91793300	-14.47441500
H	21.92513800	-4.32064100	-5.71343700	C	32.34728600	2.30074300	-14.06257100
H	22.80626900	-1.81476700	-6.52688200	O	33.34146600	2.77578300	-14.77975400
H	23.73250900	-2.79061800	-5.37780900	O	31.86254700	2.89819600	-13.09705300
H	24.14824800	-2.63798200	-8.40714000	H	30.04972700	-0.13823800	-17.50314300
H	25.37339700	-2.42459000	-7.14797400	H	31.73194700	2.19502200	-16.88050800
H	25.07724000	-4.86308500	-8.32586500	H	32.23930800	-0.66321500	-15.88997200
H	25.35647500	-4.76218600	-6.57459100	H	33.47663700	0.59697500	-15.89698900
C	23.17500300	4.07098200	-8.16494800	H	30.78338200	0.92265100	-14.46081200
C	24.47280200	3.92442100	-7.39236800	H	32.16370200	0.24682200	-13.65896000
O	24.50061800	3.77603900	-6.17072600	C	25.80862600	-2.00337900	-12.32084300
H	22.78042100	3.07167100	-8.36871300	O	25.37431500	-2.82097700	-13.19136000
H	23.31985000	4.57960900	-9.12049100	O	26.50352300	-2.37389000	-11.32373000
N	25.61214700	3.93611500	-8.14180300	C	25.55856500	-0.55369900	-12.50581300
C	26.90900700	3.66713400	-7.52215500	C	26.56035700	0.39626800	-12.23267200
C	27.89984500	3.85605400	-8.67266400	O	27.77928400	0.10174900	-11.69343400
C	27.11003100	3.38239300	-9.88912600	C	26.32305500	1.74064900	-12.53170500
C	25.69641100	3.91152100	-9.61623500	C	25.07495600	2.14905100	-12.98230900
H	26.93675600	2.64303300	-7.12651500	C	24.05398000	1.22037100	-13.19970600
H	28.13963100	4.91851500	-8.78559200	C	24.31962700	-0.12577600	-13.00020100
H	28.83301900	3.31237500	-8.52065700	H	28.06078400	-0.86113100	-11.74976200
H	27.51473600	3.75501000	-10.82746300	H	27.12725800	2.45251300	-12.41180800
H	27.09221800	2.28986000	-9.92752900	H	24.91247000	3.20187000	-13.16820400
H	25.57688700	4.92249200	-10.02660800	H	23.08339200	1.53368900	-13.55336800
H	24.93070400	3.26579400	-10.05003900	H	23.56045900	-0.86763900	-13.21878500
C	23.37391600	0.46277700	-4.63050100	Zn	26.95661000	-4.30163900	-12.07949900
C	24.32797600	0.45663200	-5.83337600	O	26.53875000	-5.34825100	-13.99965500
C	23.70923900	0.58734600	-7.21192500	H	26.18024800	-4.53262600	-14.38221500
C	22.33190400	0.54840100	-7.45673900	H	27.39289000	-5.52467100	-14.44483400
C	24.56493800	0.68062600	-8.32145800	O	22.95040900	-3.71143100	-14.24910700
C	21.82939400	0.54869500	-8.76374000	H	22.33663300	-2.95387200	-14.20504700
C	24.07164900	0.70820100	-9.62179600	H	23.80641800	-3.35787300	-13.94232400
C	22.69505300	0.62531000	-9.85396100	O	21.07245900	-1.64513800	-14.33315100
H	22.41519800	-0.01350800	-4.85460200	H	21.10986900	-1.24257500	-15.21739900
H	25.05092100	1.26983500	-5.71038100	H	20.12875900	-1.63112100	-14.05135200
H	24.91126100	-0.47244000	-5.83281100	C	34.22904800	4.62597100	-6.61615300
H	21.63576800	0.49807000	-6.62721200	C	33.55530800	3.34758600	-6.08078200
H	25.63897900	0.71910800	-8.15632000	C	32.23251100	2.98063700	-6.78253300
H	20.75730700	0.45876700	-8.92381500	C	31.89619700	1.48238200	-6.61587400
H	24.75400100	0.77497300	-10.45697200	N	30.52480300	1.09905500	-6.97607400
H	22.31811700	0.61511000	-10.86979600	C	30.07418100	1.00110000	-8.24315900
C	32.20724500	-3.27932200	-6.21713300	N	30.77843000	1.49360400	-9.25091800
C	30.90840300	-2.47564700	-5.98924600	N	28.84820500	0.48381700	-8.46780900
C	30.02067500	-2.43731600	-7.20674100	H	34.58552300	4.44699700	-7.63916000
C	30.39687600	-2.42661400	-8.53070100	H	34.26374400	2.51571300	-6.19044500
N	28.62749600	-2.48441600	-7.14478800	H	33.36860400	3.44304300	-5.00437600
C	28.19922900	-2.53927800	-8.40912300	H	31.40677100	3.58115700	-6.38523200
N	29.23941000	-2.49306600	-9.26681200	H	32.31128800	3.24591100	-7.84454200
H	32.82692700	-2.82423400	-6.99308600	H	32.60768900	0.86561700	-7.18121100
H	30.33625100	-2.90444900	-5.16313400	H	32.01526100	1.20595400	-5.56572300
H	31.16172800	-1.45403300	-5.66246800	H	29.97642300	0.62459000	-6.27228100
H	27.91104400	-3.20818600	-5.83184000	H	31.67013600	1.91585000	-9.05817300
H	31.37588100	-2.42848300	-8.97300300	H	30.50202300	1.36492000	-10.26832100
H	27.17500100	-2.61157000	-8.74295800	H	28.52589200	-0.25026000	-7.84079200
H	29.17642100	-2.49582400	-10.29185900	H	28.57497700	0.33951300	-9.43594700
C	33.47997700	-4.18194900	-10.78301800	C	31.09196500	7.81092100	-10.77002100
C	33.54698100	-2.73058800	-10.33194400	C	30.06782900	7.04192200	-9.91609800
O	33.60939000	-2.38369800	-9.15416000	C	28.77366800	6.83795800	-10.64722100
C	32.08612800	-4.81318600	-10.65134900	C	27.56890700	7.45246500	-10.41389500
O	31.78991200	-5.02756500	-9.30014300	C	28.58572400	5.99252400	-11.80500000
H	33.83939600	-4.28207500	-11.81328100	C	27.23666000	6.15013500	-12.22900000
H	31.33346600	-4.16406000	-11.12995000	C	29.42219000	5.10995700	-12.51234800
H	32.09059800	-5.75610700	-11.22158000	N	26.63793900	7.04001100	-11.35649900
H	30.93332600	-5.51440100	-9.29806900	C	26.72073600	5.47441600	-13.33993500
N	33.54246300	-1.80000000	-11.33271200	C	28.91580300	4.43804300	-13.61836500
C	33.30508200	-0.40214900	-11.03312000	C	27.58080100	4.62719500	-14.03156400
H	33.29968300	-2.11257500	-12.26127500	H	31.15653500	7.34772900	-11.76102700
H	33.54874300	0.19186500	-11.91824900	H	30.48940500	6.06351000	-9.64713700
H	32.25335500	-0.21789400	-10.79022800	H	29.88774100	7.56889500	-8.97207500
C	30.70355500	-3.79291200	-14.83671600	H	27.29388300	8.15912700	-9.64379700
C	30.68020800	-2.83303800	-13.64824600	H	25.68810000	7.36653200	-11.41574400
C	29.34377700	-2.70757500	-12.93066700	H	30.45394700	4.95106300	-12.21547200
O	28.37943200	-3.40822900	-13.34981500	H	25.69401200	5.61793000	-13.65984200
O	29.32233600	-1.91328600	-11.94530600	H	29.54808600	3.77380600	-14.19401900
H	30.02359100	-4.62793800	-14.68447500	H	27.23399600	4.10047800	-14.91422500
H	31.38235500	-3.15879000	-12.87336000	O	30.26305600	1.16735700	-11.78590400
H	30.99974600	-1.82049700	-13.92178500	H	30.57892400	1.92677600	-12.31780000
C	27.87559500	1.06282800	-17.13696600	H	29.34660100	0.91672100	-12.01288700
C	29.25141500	1.58654800	-16.78227400	N	16.96163200	-3.31002900	-12.61938300
O	29.41878200	2.68768200	-16.25932500	C	16.59819100	-4.44990800	-11.75881600
C	27.05442600	0.81195900	-15.85437700	C	15.33542600	-3.94825900	-11.03675000
C	25.62271700	0.45132700	-16.15369600	C	14.70292400	-2.98279600	-12.05072400
C	24.73341300	1.42744100	-16.61392200	C	15.91987900	-2.27142300	-12.64883800
C	25.14316700	-0.84922400	-15.96907800	H	17.40982800	-4.67060900	-11.06125400
C	23.39971200	1.12132100	-16.87358100	H	14.67559500	-4.76835000	-10.74488600
C	23.81388300	-1.17745600	-16.22547500	H	15.61629000	-3.40311200	-10.12885300
C	22.94615700	-0.18203200	-16.67129500	H	14.17645100	-3.54498400	-12.82978600
O	21.62241000	-0.53186400	-16.87583300	H	13.99310700	-2.28573000	-11.59929200
H	27.38074200	1.83632000	-17.73299600	H	15.77456100	-1.91799600	-13.67220300
H	27.52386900	0.01311100	-15.26989400	H	16.23381400	-1.41093300	-12.04504700
H	27.09516900	1.71303200	-15.23692100	C	29.55086100	-2.94355300	-1.16237800
H	25.07879000	2.44874900	-16.75053900	C	28.26604200	-3.75061600	-1.37865200
H	25.79725000	-1.60961300	-15.55372000	C	28.09995700	-4.31248100	-2.79354400
H	22.71494300	1.89388900	-17.21605000	C	27.97311700	-3.27813700	-3.90344300
H	23.44252100	-2.17692000	-16.02407400	O	28.14083800	-2.07640800	-3.76205400
H	21.13017100	0.25079400	-17.15599400	O	27.69905900	-3.85473400	-5.07379500
N	30.27420900	0.73671300	-17.05441700	H	29.54941100	-2.10806100	-1.86785300
C	31.68294000	1.10953600	-16.97982200	H	28.21954000	-4.58766200	-0.67097000
C	32.40058000	0.41950000	-15.82052000	H	27.40813100	-3.10564200	-1.15357900

H	28.95629000	-4.94602700	-3.06229200
H	27.22538900	-4.97055200	-2.85568200
H	30.46534700	-3.51022800	-1.36786600
H	29.56614100	-2.49758300	-0.16224600
C	34.86201600	7.99992900	-10.31604800
C	35.23899200	6.50501800	-10.33374200
C	35.10414000	5.89795400	-11.69267200
C	34.18901500	5.02841400	-12.23436700
N	35.94811900	6.21923100	-12.74644300
C	35.52884600	5.54568600	-13.85241100
N	34.46610900	4.81884400	-13.57108200
H	35.56487100	8.59781400	-10.90581500
H	36.25671600	6.36009500	-9.94838600
H	34.57506100	5.95603200	-9.65838300
H	36.73669900	6.84668900	-12.69929100
H	33.35028500	4.53324000	-11.76862100
H	36.02103700	5.61115400	-14.81140900
H	33.70816500	3.64163800	-14.36498600
H	34.87098200	8.38160300	-9.28968400
H	33.87104000	8.09550800	-10.77195900

Int1-B_{Zn} (1.0 kcal/mol)

H	20.66679000	-6.80396300	-16.56498800
H	16.38980100	-5.37393300	-12.30903600
H	24.65840100	-6.75695400	-19.16515500
H	29.36474700	-8.34255400	-18.17977300
H	35.11184600	4.87009700	-6.01581500
H	32.10198600	7.76409600	-10.35095700
H	33.92497800	-0.02981600	-10.21106700
H	31.95006600	-4.27904600	-6.58592000
H	23.18515900	1.49703000	-4.32300200
H	22.41702400	4.62906400	-7.60403000
H	22.25398000	6.38984100	-15.14833700
H	33.53406300	5.46906600	-6.68081600
H	30.78106800	8.84802700	-10.93695600
H	23.93722900	6.31011500	-15.82076100
H	23.80797600	-0.12296500	-3.81396100
H	32.79715300	-3.33908200	-5.29810200
H	32.07508000	0.82311700	-17.96200200
H	30.43499800	-3.27805100	-15.73602700
H	31.70211100	-4.16463700	-14.93622900
H	30.41810000	-9.06000500	-14.20469600
H	20.88583700	-5.05018800	-16.84120000
H	34.15684600	-4.71631800	-10.10809500
H	23.72500000	-8.30797800	-7.05596000
H	21.59208200	-3.72897200	-7.32008700
H	27.89805300	0.15098800	-17.74198000
H	27.15897800	4.34412300	-6.69909500
C	29.55198900	-8.45619000	-13.91564500
C	29.09083800	-7.65226200	-15.11264800
O	28.92031100	-6.42617800	-15.10285500
C	29.80946700	-7.58339200	-12.69050400
C	28.49252900	-7.14049000	-12.03057900
C	28.77521900	-6.05983600	-10.99000300
O	29.46142000	-6.36602300	-10.00707300
O	28.32409500	-4.87058000	-11.22867200
H	28.76535500	-9.19003800	-13.68515000
H	30.41023000	-8.11932600	-11.95201200
H	30.38169400	-6.70154500	-12.99530300
H	27.79265400	-6.78337900	-12.78857700
H	28.04254900	-8.00648100	-11.53141000
N	28.92620300	-8.37083100	-16.23365200
C	28.69015700	-7.77016700	-17.53405800
C	27.22734200	-7.97972700	-17.92937700
O	26.76216600	-9.11188900	-17.99066000
H	28.97078600	-9.37833400	-16.19524600
H	29.00003400	-6.72607600	-17.48984900
N	26.51456100	-6.84115900	-18.12256300
C	25.05567100	-6.84019200	-18.14771900
C	24.51390100	-5.69839200	-17.28780000
H	26.96901200	-5.96183700	-17.92017800
H	24.73613500	-7.81381700	-17.76685000
H	23.42195000	-5.69740600	-17.30269600
H	24.84726600	-5.78777100	-16.24919000
H	24.84611200	-4.72356400	-17.66350700
C	23.25777000	6.03522600	-15.04097500
C	23.15200600	4.49815800	-15.03658900
C	22.23513200	3.92870400	-13.97838500
C	22.38411900	4.27038000	-12.62916100
C	21.27331100	2.95980000	-14.29669800
C	21.62989600	3.65136600	-11.63664500
C	20.51798200	2.31707800	-13.31858700
C	20.70634600	2.65900400	-11.97720200
O	19.97140800	1.99671200	-11.03256900
H	23.65126600	6.41801000	-14.09354800
H	22.79168600	4.17927800	-16.02123900
H	24.14783200	4.04998500	-14.93340400
H	23.12442100	5.00993400	-12.33678600
H	21.14772300	2.66483400	-15.33475800
H	21.77514200	3.91640900	-10.59425600
H	19.83910300	1.51010300	-13.56782200
H	20.33971800	2.20044100	-10.16174200
C	20.86233400	-5.83970300	-16.08269700
C	19.77896700	-5.55097200	-15.04707900
O	18.79364500	-6.26628200	-14.90160800
H	21.84583200	-5.85770500	-15.60268300
N	19.99595000	-4.42817900	-14.28703500

C	19.19503200	-4.19823800	-13.09501000
C	18.13740700	-3.11140700	-13.26522200
O	18.36345000	-2.05854800	-13.88250900
C	20.15601300	-3.85199800	-11.93287700
O	19.50137200	-3.68888000	-10.67987700
H	20.90533600	-3.97388300	-14.34048200
H	18.69816600	-5.14468800	-12.87654300
H	20.84832800	-4.69256600	-11.82999300
H	20.75086800	-2.97121600	-12.18880100
H	19.20222400	-2.77298100	-10.61857500
C	23.90599400	-7.35604100	-7.56600000
C	22.90284600	-6.30721700	-7.11716300
O	21.74558600	-6.62416300	-6.83769600
C	23.65818500	-7.70745500	-9.05879200
C	24.05345000	-6.64559800	-10.02177500
C	25.24404000	-6.42723600	-10.66108100
N	23.24494600	-5.58498000	-10.40310800
C	23.94193400	-4.77781100	-11.23927700
N	25.16404200	-5.27162200	-11.41316600
H	24.94658600	-7.06202200	-7.41358900
H	24.22606300	-8.60978100	-9.30438600
H	22.59749400	-7.95716800	-9.17135600
H	22.30727000	-5.40872900	-10.06764200
H	26.14506000	-7.01649500	-10.61243100
H	23.53972500	-3.90217600	-11.72793900
N	23.30704000	-5.00787200	-7.14216300
C	22.40695900	-3.96403900	-6.62788900
C	23.33244200	-2.76739400	-6.39007300
C	24.46580800	-2.97431100	-7.40393500
C	24.67105100	-4.49281600	-7.38288300
H	21.92510900	-4.32399500	-5.71406600
H	22.81791300	-1.81819200	-6.52302700
H	23.73635800	-2.79954700	-5.37244600
H	24.15215800	-2.64204800	-8.39954800
H	25.37981500	-2.43869800	-7.14156500
H	25.08123500	-4.87490400	-8.31965400
H	25.35126200	-4.77450400	-6.56805600
C	23.17496900	4.07093500	-8.16496700
C	24.47414800	3.92177700	-7.39490700
O	24.50012200	3.75858700	-6.17443900
H	22.78009000	3.07144200	-8.36727900
H	23.31725600	4.57479800	-9.12329800
N	25.61448100	3.94277700	-8.14194600
C	26.90901600	3.66683200	-7.52195100
C	27.90873700	3.87454900	-8.66101200
C	27.12606900	3.45063900	-9.89876100
C	25.70739200	3.96229500	-9.61600900
H	26.93471600	2.64181300	-7.12934200
H	28.16540400	4.93641500	-8.73742800
H	28.83232300	3.31360900	-8.51543600
H	27.53649500	3.86364000	-10.81720700
H	27.11642400	2.36233100	-9.98805500
H	25.58061700	4.98418000	-9.99557300
H	24.94902900	3.32493300	-10.07391500
C	23.37384700	0.46292100	-4.62991700
C	24.33983800	0.45504100	-5.82249900
C	23.73654800	0.58849400	-7.20621900
C	22.36405700	0.51931100	-7.47002000
C	24.60489300	0.72253200	-8.30121000
C	21.87924300	0.53321400	-8.78352400
C	24.12802500	0.76839100	-9.60667800
C	22.75666900	0.65597600	-9.85960600
H	22.41597400	-0.01243600	-4.85946700
H	25.06279600	1.26644100	-5.69109100
H	24.92397600	-0.47404200	-5.81376100
H	21.65787100	0.43877700	-6.65120700
H	25.67515800	0.78808000	-8.12038700
H	20.81220700	0.42330200	-8.96197200
H	24.81964700	0.87412900	-10.42987800
H	22.39225800	0.66061800	-10.87968900
C	32.20561100	-3.27982800	-6.21765600
C	30.91249700	-2.46355800	-6.01754700
C	29.96200900	-2.57681700	-7.18016000
C	30.11055500	-3.34183200	-8.31126400
N	28.70617200	-1.96199700	-7.20888900
C	28.13176500	-2.37718500	-8.34655900
N	28.94894800	-3.19800400	-9.03539200
H	32.81970500	-2.83107000	-6.99968400
C	30.39091100	-2.79474400	-5.11102800
H	31.16384200	-1.40811200	-5.83384600
H	27.83262000	-2.69337400	-5.74241500
H	30.92185200	-3.97016900	-8.63855900
H	27.15961500	-2.08433200	-8.71706500
H	28.72290600	-3.69752100	-9.90580200
C	33.48034500	-4.18142800	-10.78334400
C	33.37052200	-2.73713600	-10.31979000
O	33.13097300	-2.39994200	-9.16549100
C	32.15093500	-4.95142000	-10.76001500
O	31.99833200	-5.56636000	-9.50183500
H	33.91189100	-4.22021700	-11.78980000
H	31.31072000	-4.27305200	-10.97256300
H	32.16720300	-5.70225600	-11.56735000
H	31.09782100	-5.95215500	-9.50018100
N	33.56284800	-1.80439900	-11.29850800
C	33.30507100	-0.40245600	-11.03285700
H	33.60686000	-2.10894200	-12.25801700
H	33.55695200	0.17410700	-11.92523600
H	32.25334800	-0.22418200	-10.79026700
C	30.70377800	-3.79238000	-14.83669500

C	30.72765300	-2.84696700	-13.64109600
C	29.46500000	-2.05334900	-13.38437700
O	28.48136500	-2.09506500	-14.14463500
O	29.55896900	-1.33215800	-12.31544400
H	30.03351600	-4.63465100	-14.68865400
H	30.95561300	-3.38708300	-12.71847100
H	31.52899900	-2.10387400	-13.74929700
C	27.87488600	1.06301600	-17.13696800
C	29.25495000	1.62743000	-16.86787800
O	29.42995100	2.79782100	-16.53201000
C	27.11927000	0.80074300	-15.81579600
C	25.66679400	0.48614600	-16.06759600
C	24.80896100	1.48483600	-16.53988200
C	25.13988000	-0.78961900	-15.84290400
C	23.46099700	1.22851400	-16.77384000
C	23.79257100	-1.06514300	-16.07142300
C	22.95732300	-0.04764400	-16.52756200
O	21.61491900	-0.34586500	-16.69362000
H	27.33781100	1.82124600	-17.71409100
H	27.59322500	-0.01846200	-15.26677500
H	27.20029300	1.69325300	-15.18834600
H	25.19401400	2.48678400	-16.70983300
H	25.77495700	-1.56670000	-15.42988900
H	22.80393000	2.01859900	-17.12895500
H	23.37487000	-2.04077600	-15.84993300
H	21.15891900	0.43935800	-17.02376000
N	30.27516100	0.73635800	-16.99958300
C	31.68290800	1.10883700	-16.98002900
C	32.43810500	0.45014600	-15.82590700
C	31.99899100	1.03160100	-14.48183000
C	32.55797600	2.40966700	-14.16675600
O	33.71051900	2.66687900	-14.76549700
O	32.02177800	3.19040400	-13.38437300
H	30.04298600	-0.20217600	-17.28776100
H	31.72081800	2.19736300	-16.90115300
H	32.24072700	-0.62976700	-15.83811300
H	33.51378700	0.58691900	-15.96414200
H	30.91246500	1.07759300	-14.40216100
H	32.30923200	0.38606300	-13.65302700
C	25.98798900	-1.79866800	-12.25635000
O	25.30534500	-2.64688800	-12.93930900
O	26.90501700	-2.23595700	-11.48072500
C	25.72483200	-0.36428700	-12.42379200
C	26.72372400	0.62944000	-12.22479600
O	27.94220300	0.39232300	-11.75978200
C	26.38136100	1.95688200	-12.56932000
C	25.09974300	2.30187000	-12.95824700
C	24.10085800	1.32871300	-13.08450500
C	24.43928500	0.00967900	-12.85373000
H	28.71145200	-0.71283100	-12.11307300
H	27.15551700	2.70969200	-12.51696400
H	24.88326500	3.34219300	-13.16341300
H	23.09782000	1.58535900	-13.38525800
H	23.69535500	-0.76524600	-12.97738800
Zn	26.72097200	-4.16515800	-12.24959400
O	27.26429100	-4.45380400	-14.23298000
H	27.72853000	-3.60161600	-14.43742700
H	27.86455900	-5.18101100	-14.49515700
O	22.64658100	-3.09992200	-13.73338800
H	22.14214800	-2.25453100	-13.79820500
H	23.59125600	-2.86373600	-13.64533800
O	20.91629900	-1.01677100	-14.00651900
H	21.05827100	-0.75702200	-14.93303600
H	20.01188800	-1.40247700	-13.99199200
C	34.22908200	4.62582600	-6.61641100
C	33.54321600	3.32957400	-6.14838800
C	32.25260400	2.99567400	-6.92899000
C	31.97050600	1.47787900	-6.96717800
N	30.62904500	1.09568400	-7.42092300
C	30.21946900	1.13110800	-8.71288500
N	30.91541600	1.79653800	-9.62795000
N	29.06672400	0.53575500	-9.03545300
H	34.59810400	4.47607900	-7.64086200
H	34.25806800	2.50359800	-6.26129900
H	33.31071200	3.38244500	-5.07835700
H	31.39125600	3.50901200	-6.48826600
H	32.34815100	3.39540900	-7.94663200
H	32.72847100	0.96715300	-7.57707700
H	32.06709000	1.07582500	-5.95555300
H	30.09925500	0.47512000	-6.82173900
H	31.74978600	2.28179000	-9.35049600
H	30.61803500	1.79582100	-10.64933700
H	28.71666200	-0.17887100	-8.40266200
H	28.71238300	0.51641400	-9.99965200
C	31.09193500	7.81089100	-10.77008800
C	30.05441300	7.00606700	-9.96898600
C	28.78892700	6.79560600	-10.75051500
C	27.55420200	7.34227200	-10.50524700
C	28.65733200	6.01421000	-11.96175700
C	27.30919500	6.13864700	-12.40072900
C	29.54237300	5.21911400	-12.71310200
N	26.65877600	6.95000300	-11.48974500
C	26.83837800	5.50985100	-13.55878500
C	29.08110700	4.59660400	-13.86755400
C	27.74270400	4.74347800	-14.28640800
H	31.17941700	7.37099900	-11.77068600
H	30.48553800	6.02912800	-9.70916400
H	29.82932900	7.50455700	-9.01912600
H	27.23531600	7.98714500	-9.69866500

H	25.69360300	7.22902100	-11.54200700
H	30.57726500	5.09094700	-12.41331100
H	25.80875100	5.62338800	-13.88168600
H	29.75146000	4.00057400	-14.47527300
H	27.43290900	4.24572900	-15.19902400
O	30.14809100	1.68491400	-12.11066100
H	30.32705700	2.46973100	-12.65034600
H	29.20130000	1.38710400	-12.15385800
N	16.94664500	-3.33691600	-12.67217200
C	16.59832500	-4.44995800	-11.75911100
C	15.33324000	-3.92965300	-11.06019400
C	14.67441700	-3.04016200	-12.12543100
C	15.86998400	-2.34022700	-12.77943000
H	17.41370200	-4.63410500	-11.06009600
H	14.69093800	-4.74242200	-10.71304400
H	15.61259400	-3.32620700	-10.18909300
H	14.15441800	-3.66069300	-12.86354700
H	13.95251400	-2.33187300	-11.71184700
H	15.71258600	-2.07140600	-13.82638100
H	16.15404400	-1.42436500	-12.24582500
C	29.55093400	-2.94390800	-1.16184000
C	28.26040300	-3.72993800	-1.41439100
C	28.06639900	-4.14842100	-2.87623900
C	27.89077600	-2.99445000	-3.85202200
O	27.95002700	-1.81374000	-3.56688200
O	27.68631900	-3.44077600	-5.10273200
H	29.56552600	-2.09349500	-1.85055400
H	28.22776700	-4.63020600	-0.78898500
H	27.40859400	-3.10865400	-1.11500100
H	28.92192400	-4.73586600	-3.23483800
H	27.19639200	-4.80702600	-2.98682300
H	30.46534500	-3.51015300	-1.36808700
H	29.56612900	-2.49731000	-0.16236800
C	34.86194100	7.99995600	-10.31596100
C	35.25446700	6.50953400	-10.32028700
C	35.25398700	5.89967700	-11.68467600
C	34.38942700	5.04074100	-12.31805200
N	36.22951300	6.17612800	-12.63263700
C	35.93028000	5.48507400	-13.76769400
N	34.82265500	4.79022500	-13.60585400
H	35.56448400	8.59937100	-10.90473700
H	36.23766100	6.37595100	-9.84977400
H	34.54432900	5.94847500	-9.70414900
H	37.02316300	6.78483100	-12.50128400
H	33.48230100	4.58302600	-11.95316000
H	36.53896900	5.51677300	-14.65932200
H	34.09095700	3.54489200	-14.41657300
H	34.87104400	8.38161900	-9.28969100
H	33.87106200	8.09551200	-10.77200300

TS1-B_{Zn} (42.4 kcal/mol)

H	20.66678000	-6.80395300	-16.56500300
H	16.38976100	-5.37393200	-12.30902300
H	24.65834500	-6.75695400	-19.16513300
H	29.36481200	-8.34246200	-18.17978700
H	35.11181100	4.87013700	-6.01577800
H	32.10198100	7.76411300	-10.35094300
H	33.92492900	-0.02997800	-10.21095700
H	31.94998600	-4.27910700	-6.58569900
H	23.18515500	1.49703000	-4.32300100
H	22.41702100	4.62906900	-7.60403900
H	22.25403700	6.38991000	-15.14863400
H	33.53405200	5.46906100	-6.68075300
H	30.78103100	8.84802300	-10.93691400
H	23.93719000	6.31009800	-15.82080100
H	23.80795000	-0.12309000	-3.81403900
H	32.79687200	-3.33914200	-5.29792600
H	32.07534300	0.82337600	-17.96197300
H	30.43505500	-3.27789800	-15.73595700
H	31.70219000	-4.16431700	-14.93662900
H	30.41808600	-9.06004200	-14.20466100
H	20.88585300	-5.05017500	-16.84118500
H	34.15668300	-4.71567600	-10.10742400
H	23.72492900	-8.30801200	-7.05605000
H	21.59206100	-3.72900200	-7.32007200
H	27.89815800	0.15099200	-17.74198300
H	27.15893400	4.34407200	-6.69904000
C	29.55200400	-8.45607600	-13.91560300
C	29.07629500	-7.64914700	-15.10270100
O	28.85884900	-6.42971200	-15.08918100
C	29.83355000	-7.62703800	-12.66433600
C	28.56707000	-7.36587100	-11.84449000
C	28.87249800	-6.44887600	-10.65233600
O	29.82889800	-6.76583600	-9.92966700
O	28.12998100	-5.41320700	-10.48714800
H	28.76781000	-9.19509500	-13.69247400
H	30.55263900	-8.13784700	-12.02079000
H	30.28947600	-6.67474800	-12.95483800
H	27.77696400	-6.95328300	-12.47910600
H	28.19458700	-8.32155900	-11.45302700
N	28.94024500	-8.36373600	-16.23222600
C	28.68995800	-7.77026100	-17.53409100
C	27.22727100	-7.98109500	-17.92987100
O	26.76346400	-9.11237000	-18.00679400
H	29.02620500	-9.36840600	-16.19600300
H	28.99644200	-6.72449500	-17.49818300
N	26.51431300	-6.84019600	-18.11654000

C	25.05582400	-6.84020300	-18.14775100	C	32.20612300	-3.27973600	-6.21831600
C	24.50441800	-5.70197800	-17.28849800	C	30.91473400	-2.46760200	-5.99911500
H	26.96568000	-5.96514400	-17.89031600	C	30.01021500	-2.41182000	-7.20437600
H	24.73489400	-7.81452800	-17.76932100	C	30.32908100	-2.25247200	-8.53639000
H	23.41337600	-5.68964600	-17.33233300	N	28.62811000	-2.54358500	-7.09561100
H	24.80245400	-5.80487300	-16.24085100	C	28.14545000	-2.48834000	-8.33385900
H	24.85395300	-4.72571900	-17.64531400	N	29.14021800	-2.31187200	-9.22860400
C	23.25773300	6.03513400	-15.04056200	H	32.82723300	-2.83088300	-6.99656900
C	23.31467400	4.49299900	-14.98933000	H	30.33832800	-2.88488100	-5.17001800
C	22.49214300	3.79285100	-13.92959700	H	31.17899400	-1.44639700	-5.68126900
C	22.31459000	4.31786700	-12.64603400	H	27.95684200	-3.30336100	-5.81709700
C	21.94179200	2.52955700	-14.19675700	H	31.28801900	-2.14754100	-9.01220200
C	21.59435200	3.62271000	-11.67453800	H	27.11377500	-2.57279200	-8.63366500
C	21.23597600	1.81066900	-13.23689000	H	28.94146700	-2.09969900	-10.20506600
C	21.04534100	2.37248200	-11.97144100	C	33.48012300	-4.18222200	-10.78403300
O	20.30692500	1.66532800	-11.06094500	C	33.52315000	-2.73194000	-10.33031400
H	23.65005600	6.46720300	-14.11168200	O	33.54321200	-2.38388600	-9.15242000
H	23.01665500	4.10196000	-15.96960600	C	32.08708400	-4.81643400	-10.66514600
H	24.36733300	4.19526700	-14.87084500	O	31.74265700	-4.95555800	-9.31690000
H	22.73737200	5.28509500	-12.39054600	H	33.84500800	-4.28024600	-11.81286700
H	22.09943100	2.08153400	-15.17311800	H	31.35954300	-4.19133700	-11.21256700
H	21.45552500	4.05325000	-10.68606300	H	32.11472800	-5.78888800	-11.18203800
H	20.85839100	0.81550500	-13.45020700	H	30.93878300	-5.52048100	-9.30049500
H	20.40917600	2.08120500	-10.19477500	N	33.53497500	-1.80017200	-11.32867100
C	20.86231300	-5.83972700	-16.08268900	C	33.30512700	-0.40207000	-11.03299900
C	19.85649500	-5.65417400	-14.95417500	H	33.39213000	-2.10883600	-12.27805400
O	19.22357400	-6.60036600	-14.49770300	H	33.54937800	0.19191800	-11.91672300
H	21.85861200	-5.86304100	-15.62639000	H	32.25766800	-0.20296600	-10.78386600
N	19.75564900	-4.38564000	-14.43555400	C	30.70379600	-3.79293700	-14.83604700
C	19.19509300	-4.19824400	-13.09497900	C	30.51224500	-2.85140600	-13.62019800
C	18.17133300	-3.07030700	-13.14557600	C	29.48674700	-1.71835100	-13.78230400
O	18.43947400	-1.97458700	-13.66832300	O	28.24559100	-2.06003100	-14.04760500
C	20.36636900	-3.93209200	-12.11494900	O	29.83713700	-0.54725700	-13.63791000
O	20.10415600	-4.38155000	-10.77846700	H	30.05087300	-4.66071300	-14.77074100
H	20.40329600	-3.66826800	-14.74774000	H	30.20633100	-3.43541600	-12.74493100
H	18.73903400	-5.15289500	-12.83599400	H	31.44841500	-2.35336000	-13.35945900
H	21.21856600	-4.50190900	-12.48938800	C	27.87482200	1.06301400	-17.13686800
H	20.65046700	-2.87470000	-12.13269600	C	29.25590300	1.59293100	-16.79913000
H	19.88239900	-3.62016400	-10.22982400	O	29.42937000	2.74711200	-16.41110400
C	23.90612600	-7.35589700	-7.56598100	C	27.00472100	0.82699200	-15.89699900
C	22.95326300	-6.30570800	-7.02328500	C	25.62004400	0.36518500	-16.27765600
O	21.84393100	-6.63776900	-6.60003900	C	24.70499600	1.25690500	-16.84499900
C	23.40697100	-7.74571400	-8.99374700	C	25.20536400	-0.95477700	-16.05860800
C	23.81289800	-6.77850000	-10.03537800	C	23.40578900	0.85745000	-17.15932300
C	25.05685600	-6.62314200	-10.57697400	C	23.90818200	-1.37084600	-16.35120800
N	23.06622300	-5.71403400	-10.51716800	C	23.00805900	-0.45219300	-16.89068400
C	23.86143400	-4.95909500	-11.31301200	O	21.71035000	-0.88261400	-17.11447800
N	25.07805700	-5.49259500	-11.36155300	H	27.40633100	1.83217300	-17.76065400
H	24.96383900	-7.09304600	-7.56255500	H	27.48678400	0.09247600	-15.24934900
H	23.82932600	-8.72155300	-9.25315700	H	26.95321200	1.75647900	-15.32631300
H	22.32110500	-7.86994200	-8.94428400	H	24.99838600	2.28871600	-17.02002400
H	22.09014100	-5.50673600	-10.31888300	H	25.89371500	-1.65797300	-15.59873100
H	25.94334600	-7.21359300	-10.40840400	H	22.70179300	1.56747100	-17.58909200
H	23.54038800	-4.08830000	-11.85970100	H	23.57800500	-2.37325800	-16.09978600
N	23.30666600	-4.99932700	-7.15406800	H	21.20390100	-0.15812600	-17.50510500
C	22.40698200	-3.96402700	-6.62790000	N	30.28049300	0.71468200	-16.97556700
C	23.33538900	-2.77121700	-6.39347500	C	31.68252400	1.10849200	-16.98007600
C	24.42274200	-2.94473200	-7.46298200	C	32.49648700	0.47388600	-15.85553600
C	24.64310800	-4.46332900	-7.48937200	C	32.11495000	1.05869000	-14.50248200
H	21.93121100	-4.33207900	-5.71534500	C	32.75789900	2.36353500	-14.10268000
H	22.81587300	-1.81910400	-6.47127300	O	33.66486200	2.85127900	-14.91746000
H	23.78289900	-2.83817300	-5.39588100	O	32.44669300	2.90522500	-13.03436600
H	24.06037100	-2.58908500	-8.43361500	H	30.05220000	-0.21553900	-17.29116600
H	25.33982200	-2.40165000	-7.22766900	H	31.70565600	2.19744000	-16.90478700
H	24.98310600	-4.82296100	-8.46303300	H	32.30912100	-0.60664100	-15.84296500
H	25.38396600	-4.75716100	-6.73455500	H	33.56262100	0.61922000	-16.05404000
C	23.17497500	4.07090800	-8.16498400	H	31.03342200	1.19878900	-14.45351300
C	24.46734600	3.91388200	-7.38439300	H	32.32623500	0.35489800	-13.69364100
O	24.48406600	3.73607000	-6.16586100	C	26.29915200	-2.09230800	-12.02624900
H	22.78058100	3.06936600	-8.36652500	O	25.40490700	-2.78910400	-12.58028300
H	23.31558000	4.57034700	-9.12512100	O	27.12277000	-2.62199600	-11.9633200
N	25.60697900	3.94039500	-8.12795200	C	26.51728800	-0.69667400	-12.49688900
C	26.90909600	3.66690900	-7.52204400	C	27.50837400	0.19233800	-11.85973100
C	27.89642800	3.92991400	-8.66415800	O	28.39868800	-0.19930600	-11.05627900
C	27.10688000	3.52476100	-9.90012100	C	27.43911900	1.57709800	-12.27753800
C	25.68842600	4.00936100	-9.59931200	C	26.31157200	2.09148400	-12.85063700
H	26.95902100	2.63640500	-7.15262600	C	25.19996500	1.26591100	-13.19860400
H	28.13250300	4.99852300	-8.70802300	C	25.32160000	-0.07902000	-13.05900900
H	28.83155200	3.37972200	-8.55164100	H	27.38872100	-1.21324900	-13.46250400
H	27.50019600	3.94268400	-10.82393300	H	28.28408200	2.20317100	-12.02885000
H	27.10468300	2.43851900	-9.98708500	H	26.26486100	3.15781500	-13.04575100
H	25.54352500	5.04075500	-9.94820600	H	24.29587200	1.70386400	-13.60103400
H	24.93607000	3.37320000	-10.07179800	H	24.51565600	-0.74264600	-13.34300300
C	23.37387600	0.46306800	-4.62985500	Zn	26.85414200	-4.54718800	-11.72761400
C	24.42068400	0.45184000	-5.76670200	O	27.53300800	-4.59239400	-13.65105700
C	23.95651100	0.53407000	-7.20808800	H	27.81687300	-3.68691400	-13.94158300
C	22.62032100	0.42964900	-7.60747100	H	28.06452900	-5.28117700	-14.10002400
C	24.93006400	0.63287500	-8.21624000	O	23.09175400	-3.49867400	-14.04441100
C	22.27334500	0.38351500	-8.96226000	H	22.47397700	-2.74410000	-14.06015800
C	24.59081700	0.61496200	-9.56671100	H	23.94005500	-3.14773300	-13.71612100
C	23.25329400	0.48133700	-9.95046300	O	21.02479400	-1.62256000	-14.44169400
H	22.42914600	-0.01427600	-4.90255900	H	21.08275800	-1.35508800	-15.37488900
H	25.11671600	1.27914000	-5.59447500	H	20.06962800	-1.64316200	-14.19946200
H	25.01811000	-0.46598900	-5.68598400	C	34.22913500	4.62577400	-6.61650700
H	21.83740700	0.36688400	-6.85865300	C	33.55711900	3.36079000	-6.05001100
H	25.97522800	0.71806700	-7.93185700	C	32.20742200	3.00856200	-6.70049500
H	21.23494300	0.25683800	-9.25070800	C	31.85477400	1.52000900	-6.50141500
H	25.36226700	0.69795900	-10.32303400	N	30.48944400	1.14777000	-6.88328900
H	22.98865400	0.45626500	-11.00158000	C	30.06492400	1.04407400	-8.16254100

N	30.83623500	1.46424600	-9.15640500
N	28.82625300	0.59645900	-8.42403900
H	34.57781800	4.43404500	-7.63920800
H	34.25007600	2.51802000	-6.17593600
H	33.41064800	3.46849200	-4.96838600
H	31.40493800	3.62598400	-6.28193800
H	32.24798200	3.25886800	-7.76738100
H	32.57454700	0.88377200	-7.03521900
H	31.95119500	1.26903200	-5.44239000
H	29.92544100	0.67824000	-6.18947600
H	31.75126000	1.82018200	-8.94288700
H	30.57067600	1.43267700	-10.17735000
H	28.42552400	-0.05543900	-7.75853800
H	28.62361100	0.37067700	-9.41462600
C	31.09198400	7.81089200	-10.77014300
C	30.04758500	7.01897300	-9.96264400
C	28.80395500	6.80842100	-10.77595200
C	27.58327500	7.41814200	-10.63115100
C	28.72211700	6.00413100	-11.97472900
C	27.42309400	6.19258100	-12.52270300
C	29.61884300	5.13941800	-12.62847400
N	26.74361600	7.04549100	-11.67218600
C	27.02556500	5.58777200	-13.72018700
C	29.22187900	4.52290200	-13.80745200
C	27.94517900	4.75921800	-14.35674800
H	31.17517300	7.36437400	-11.76767300
H	30.47144100	6.04547200	-9.68136700
H	29.80900100	7.53546800	-9.02590500
H	27.24066200	8.10171900	-9.86725700
H	25.80281800	7.37523900	-11.80668600
H	30.60799100	4.94699300	-12.22430400
H	26.03915200	5.76384700	-14.13897300
H	29.89179000	3.85556800	-14.33483600
H	27.69659700	4.27032700	-15.29224100
O	30.49151800	1.56358000	-11.74148800
H	31.17370900	2.05073200	-12.25248200
N	30.18089300	0.79681100	-12.25307600
N	16.95398100	-3.31717400	-12.63003300
C	16.59837600	-4.44994300	-11.75916800
C	15.33634400	-3.94670000	-11.03814500
C	14.69165500	-3.00333200	-12.06545500
C	15.89933100	-2.29241600	-12.68373800
H	17.41271500	-4.66657500	-11.06356700
H	14.68425000	-4.76676200	-10.72931700
H	15.61825500	-3.38444300	-10.14105300
H	14.16493100	-3.58321300	-12.83123700
H	13.97887500	-2.30412000	-11.62221700
H	15.74802200	-1.96661800	-13.71528900
H	16.20465000	-1.41352800	-12.10275500
C	29.55095300	-2.94390300	-1.16221100
C	28.27147600	-3.76582400	-1.35715600
C	28.10789000	-4.36200000	-2.75708600
C	27.96882200	-3.35009000	-3.88608500
O	28.08320600	-2.14050800	-3.75376400
O	27.74668200	-3.95168800	-5.05283700
H	29.53774400	-2.11382100	-1.87353900
H	28.23461700	-4.58548100	-0.62870200
H	27.40908500	-3.12232300	-1.14586800
H	28.96799400	-4.99501700	-3.01373200
H	27.23746200	-5.02738200	-2.80281800
H	30.46540300	-3.51016500	-1.36779600
H	29.56609300	-2.49734300	-0.16235200
C	34.86174200	7.99992000	-10.31581100
C	35.30195200	6.52621400	-10.34978300
C	35.29472500	5.95089700	-11.72832300
C	34.47842900	5.02820100	-12.33034500
N	36.17529800	6.34641300	-12.72652000
C	35.86851400	5.65999300	-13.86223500
N	34.84592800	4.85511000	-13.65146000
H	35.54906600	8.62515500	-10.89772000
H	36.29690500	6.42063900	-9.89709000
H	34.62211200	5.92519300	-9.73742300
H	36.91362400	7.02669800	-12.62824600
H	33.65208600	4.46805300	-11.92262700
H	36.40850200	5.77662800	-14.79024300
H	34.09845400	3.68296700	-14.49595100
H	34.87119600	8.38167400	-9.28971400
H	33.87110600	8.09550700	-10.77210100

Int2-B_{Zn} (29.7 kcal/mol)

H	20.66677600	-6.80395200	-16.56500400
H	16.38975100	-5.37392700	-12.30902800
H	24.65831500	-6.75658100	-19.16509100
H	29.36446700	-8.34323800	-18.17945600
H	35.11183500	4.87009300	-6.01579700
H	32.10197500	7.76416100	-10.35092100
H	33.92491900	-0.02997500	-10.21095100
H	31.94997700	-4.27910200	-6.58570600
H	23.18515800	1.49703000	-4.32300000
H	22.41701500	4.62905900	-7.60404000
H	22.25403700	6.38990600	-15.14864600
H	33.53409100	5.46909900	-6.68068900
H	30.78102700	8.84802400	-10.93690400
H	23.93718900	6.31010000	-15.82080100
H	23.80794500	-0.12309300	-3.81403800
H	32.79680700	-3.33921600	-5.29789000
H	32.07539700	0.82339900	-17.96195800

H	30.43501900	-3.27791300	-15.73595500
H	31.70219900	-4.16429100	-14.93663900
H	30.41816900	-9.05998700	-14.20452500
H	20.88585800	-5.05017100	-16.84118100
H	34.15667700	-4.71567200	-10.10741500
H	23.72494500	-8.30801800	-7.05605600
H	21.59204400	-3.72901500	-7.32005700
H	27.89817300	0.15100500	-17.74200000
H	27.15894300	4.34404800	-6.69902300
C	29.55185300	-8.45602900	-13.91564500
C	29.08510200	-7.65821700	-15.11124300
O	28.90912900	-6.43439400	-15.10490600
C	29.84038000	-7.60049900	-12.68547800
C	28.56162600	-7.25415500	-11.91083700
C	28.89351500	-6.22220500	-10.82787700
O	29.65707400	-6.58318900	-9.92065600
O	28.41585400	-5.03537000	-10.96848000
H	28.76819900	-9.19116300	-13.67900700
H	30.52080300	-8.12130500	-12.00790900
H	30.33956800	-6.67839600	-12.99961000
H	27.79653600	-6.88562900	-12.60112800
H	28.17754300	-8.16563000	-11.43765000
N	28.91990000	-8.37673500	-16.23415100
C	28.69030700	-7.77010100	-17.53431200
C	27.22995700	-7.97574200	-17.94146900
O	26.76661500	-9.10705000	-18.02944800
H	28.97987900	-9.38339700	-16.19982500
H	29.00188000	-6.72695000	-17.48499700
N	26.51463800	-6.83530600	-18.11777300
C	25.05563300	-6.84057800	-18.14778400
C	24.50824900	-5.70145500	-17.28700100
H	26.96363900	-5.96020400	-17.88582800
H	24.73758400	-7.81553100	-17.76898400
H	23.41625100	-5.70344900	-17.30555300
H	24.83904200	-5.79239000	-16.24755800
H	24.83935200	-4.72494700	-17.65970800
C	23.25773500	6.03513100	-15.04054900
C	23.26779400	4.49493700	-14.97900800
C	22.40362900	3.86240400	-13.91135400
C	22.37226500	4.34795700	-12.59949100
C	21.67597800	2.69574200	-14.18904500
C	21.63129700	3.70500800	-11.60914600
C	20.94908900	2.02404300	-13.21040000
C	20.91693400	2.54278900	-11.91362200
O	20.17296000	1.87879500	-10.97550600
H	23.64977800	6.46275700	-14.10971700
H	22.95682400	4.10350700	-15.95472500
H	24.30571500	4.15468700	-14.84926300
H	22.93683000	5.23761700	-12.33526700
H	21.71730300	2.27341600	-15.18840400
H	21.60915000	4.10291100	-10.59862700
H	20.45522300	1.08452800	-13.43485500
H	20.39661000	2.22894500	-10.10287700
C	20.86230600	-5.83972700	-16.08268300
C	19.77541400	-5.54232300	-15.05373200
O	18.76564700	-6.22740500	-14.93342700
H	21.84517100	-5.85769800	-15.60180600
N	20.01470300	-4.44029000	-14.27074200
C	19.19511300	-4.19826500	-13.09497900
C	18.12152300	-3.13302500	-13.30069300
O	18.32912900	-2.10163500	-13.96019200
C	20.13621900	-3.80140700	-11.93168600
O	19.46067100	-3.58843800	-10.69887500
H	20.93467500	-4.00643500	-14.30569200
H	18.70979600	-5.14610000	-12.85658100
H	20.83072300	-4.63277000	-11.78048400
H	20.73274300	-2.93023200	-12.21695700
H	19.12292200	-2.68389100	-10.69804800
C	23.90608500	-7.35590100	-7.56594900
C	22.90318700	-6.30567800	-7.12236400
O	21.74306800	-6.62010300	-6.85115900
C	23.63849000	-7.73783100	-9.04779000
C	24.06405300	-6.70361000	-10.02097900
C	25.27444700	-6.51115700	-10.62753100
N	23.29246200	-5.61929100	-10.40772800
C	24.03041700	-4.82016600	-11.21555200
N	25.24256300	-5.34421700	-11.36422700
H	24.94869100	-7.06426600	-7.42781700
H	24.18258600	-8.65924800	-9.27514500
H	22.57110200	-7.96210400	-9.14854100
H	22.35355600	-5.42251000	-10.08903800
H	26.16089100	-7.12104200	-10.56183500
H	23.66691000	-3.92228800	-11.68954900
N	23.30860900	-5.00660100	-7.14296200
C	22.40702600	-3.96402300	-6.62793500
C	23.33484200	-2.77212500	-6.37664100
C	24.47733500	-2.97610300	-7.38142000
C	24.67673300	-4.49612100	-7.37012300
H	21.92273600	-4.32842700	-5.71698400
H	22.82525200	-1.82034700	-6.50737000
H	23.72976200	-2.81280400	-5.35586500
H	24.17314700	-2.63415900	-8.37685100
H	25.38902400	-2.44314600	-7.10333200
H	25.09028300	-4.87322000	-8.30790300
H	25.35077100	-4.78770900	-6.55387200
C	23.17497100	4.07091100	-8.16498700
C	24.46748900	3.90885300	-7.38614400
O	24.48612300	3.72252500	-6.16897100
H	22.77794600	3.07249000	-8.37313700

H	23.32089000	4.57652100	-9.12082600	O	27.14956400	-2.44103900	-11.55869400
N	25.60814100	3.94084000	-8.12947800	C	26.23152200	-0.47828000	-12.59889800
C	26.90908600	3.66694500	-7.52205300	C	27.13096100	0.45165000	-11.81681200
C	27.90094600	3.94467400	-8.65620400	O	27.74017900	0.14262200	-10.79603500
C	27.11929700	3.55934200	-9.90268900	C	27.15929200	1.80365300	-12.38908200
C	25.69497500	4.02852300	-9.59930600	C	26.00946000	2.29561000	-12.91181500
H	26.96242100	2.63469900	-7.15845700	C	24.82156400	1.47653900	-13.08449400
H	28.13895100	5.01348600	-8.68260200	C	24.91006500	0.14371100	-12.94420400
H	28.83604400	3.39275900	-8.54879600	H	26.80011700	-0.53968600	-13.55011200
H	27.51392800	4.00431200	-10.81255300	H	28.04753500	2.40131200	-12.24013400
H	27.13201800	2.47544100	-10.01220600	H	25.96994500	3.34057700	-13.19990500
H	25.54349600	5.06304200	-9.93608300	H	23.89002600	1.94266000	-13.37075900
H	24.94778500	3.39408700	-10.08226000	H	24.07596600	-0.51866600	-13.13624200
C	23.37388000	0.46306900	-4.62985500	Zn	26.92098100	-4.38033700	-12.10134800
C	24.38106000	0.45107100	-5.79372800	O	27.30663800	-4.53566000	-14.08107600
C	23.84553500	0.55686100	-7.20721200	H	27.74362400	-3.65400800	-14.37205000
C	22.48832600	0.47212900	-7.53698100	H	27.87825500	-5.26103000	-14.40180700
C	24.76610900	0.66894100	-8.26090700	O	22.67615200	-3.11024500	-13.72735200
C	22.06769200	0.45813300	-8.87132800	H	22.16688800	-2.27707700	-13.84584100
C	24.35110200	0.68362800	-9.58852000	H	23.60930900	-2.86344600	-13.59416300
C	22.99549000	0.56826000	-9.90674700	O	20.87381000	-1.13413100	-14.26888500
H	22.42264400	-0.01373700	-4.88075200	H	21.04926400	-1.09869000	-15.22503400
H	25.09090900	1.27081600	-5.64357800	H	19.96537800	-1.50664500	-14.18904600
H	24.97087900	-0.47374100	-5.74773300	C	34.22905300	4.62580900	-6.61655300
H	21.74481900	0.40117300	-6.75048900	C	33.56290800	3.35246600	-6.06829500
H	25.82613500	0.74090500	-8.03292200	C	32.23405500	2.98559700	-6.75012900
H	21.01333600	0.34362400	-9.10384800	C	31.87135500	1.50347300	-6.52128400
H	25.08179600	0.78005100	-10.37816900	N	30.47994700	1.15184500	-6.80887400
H	22.67637100	0.56489600	-10.94242900	C	29.95933600	1.01305000	-8.04556700
C	32.20625200	-3.27968100	-6.21835600	N	30.63695000	1.40945200	-9.11347200
C	30.90970500	-2.46094300	-6.03481800	N	28.70645200	0.54280600	-8.17684200
C	30.01224400	-2.42896100	-7.25188600	H	34.58295100	4.44292800	-7.63946800
C	30.34021700	-2.31644600	-8.58611400	H	34.26879100	2.51874800	-6.18134800
N	28.62439600	-2.53284600	-7.14908400	H	33.38819700	3.45404300	-4.99008100
C	28.14928600	-2.50834000	-8.39185000	H	31.42250500	3.61751300	-6.37220800
N	29.15184300	-2.36685400	-9.28396900	H	32.31135500	3.20429900	-7.82312200
H	32.83642000	-2.84036300	-6.99550200	H	32.53796700	0.85153100	-7.10082400
H	30.32242700	-2.85813700	-5.20367700	H	32.03375600	1.25373200	-5.46989400
H	31.16721500	-1.43220300	-5.73942800	H	29.90439200	0.83202100	-6.04396700
H	27.93844700	-3.27329000	-5.83607200	H	31.53153500	1.85036600	-8.98398400
H	31.30345500	-2.25087300	-9.05868000	H	30.34200400	1.23359600	-10.11547800
H	27.11576700	-2.58053000	-8.69126100	H	28.41199700	-0.17404100	-7.52102300
H	28.98726200	-2.32290100	-10.28405200	H	28.36779100	0.41159000	-9.13443800
C	33.48013200	-4.18222400	-10.78403400	C	31.09199100	7.81087800	-10.77016300
C	33.52693200	-2.73286600	-10.32692300	C	30.04388300	7.00316500	-9.98419600
O	33.57098400	-2.38781500	-9.14799600	C	28.81542200	6.78600300	-10.81977900
C	32.08794900	-4.81573000	-10.67893700	C	27.59135000	7.39276400	-10.69184500
O	31.72823700	-4.94627500	-9.33270200	C	28.75333900	5.98505400	-12.02319000
H	33.85019700	-4.27663300	-11.81121200	C	27.46200700	6.17464400	-12.58983500
H	31.36604500	-4.19796200	-11.23929000	C	29.65873500	5.12180300	-12.66849700
H	32.12457200	-5.79195200	-11.19029100	N	26.76759600	7.02127900	-11.74554900
H	30.87879800	-5.44113050	-9.32805900	C	27.08161200	5.57556600	-13.79573400
N	33.51988800	-1.80293100	-11.32537500	C	29.27704500	4.50983500	-13.85582500
C	33.30513200	-0.40208000	-11.03300500	C	28.00803400	4.74765600	-14.42272800
H	33.33252600	-2.11562700	-12.26632500	H	31.18505000	7.37264500	-11.77101500
H	33.56040100	0.18745600	-11.91665300	H	30.47397500	6.03238700	-9.70303700
H	32.25711800	-0.18786100	-10.79616300	H	29.78384600	7.50979200	-9.04780700
C	30.70382300	-3.79296800	-14.83601700	H	27.23672300	8.07413200	-9.93146000
C	30.47581500	-2.81277000	-13.66588800	H	25.83280500	7.35971400	-11.89969400
C	29.29963100	-1.83942300	-13.90451100	H	30.64272400	4.92684700	-12.25266500
O	28.30189300	-2.26276800	-14.57786100	H	26.10199900	5.75705600	-14.22893600
O	29.37673400	-0.67546000	-13.44140500	H	29.95463400	3.84643800	-14.37939700
H	30.04647700	-4.65539200	-14.75799400	H	27.77500900	4.26409500	-15.36493700
H	30.25640800	-3.35926400	-12.73981800	O	30.26696200	1.16479400	-11.68339300
H	31.36079900	-2.20076100	-13.46240600	H	30.93567300	1.69748500	-12.16073400
C	27.87479300	1.06301800	-17.13686000	H	29.99537300	0.40965100	-12.25357000
C	29.25535300	1.63092000	-16.87354900	N	16.94166600	-3.34429800	-12.68287700
O	29.43168700	2.81232300	-16.57595200	C	16.59839500	-4.44993100	-11.75917300
C	27.10359100	0.78077600	-15.83961900	C	15.33248100	-3.92699500	-11.06527700
C	25.69697000	0.32615200	-16.13963400	C	14.66410600	-3.06227000	-12.14497900
C	24.75821400	1.23558400	-16.63764700	C	15.85174800	-2.36505500	-12.81705500
C	25.29783000	-1.00184900	-15.94071200	H	17.41472600	-4.62730700	-11.06005000
C	23.45487700	0.84077000	-16.93031100	H	14.69729900	-4.73810800	-10.70163100
C	23.99199900	-1.41028700	-16.21298600	H	15.61069700	-3.30618100	-10.20605700
C	23.07656100	-0.48372700	-16.71106000	H	14.14639900	-3.70067600	-12.86927900
O	21.78501900	-0.92162500	-16.95425700	H	13.93793700	-2.35189300	-11.74262600
H	27.34086800	1.81871400	-17.72174600	H	15.69155400	-2.12616000	-13.87079200
H	27.64303100	0.02226000	-15.26793200	H	16.12405900	-1.43186100	-12.30807600
H	27.09075800	1.69245500	-15.23752500	C	29.55096600	-2.94384800	-1.16230100
H	25.04386900	2.27355900	-16.78725100	C	28.26825400	-3.75574100	-1.37411400
H	26.01130300	-1.71386400	-15.53624100	C	28.10963000	-4.33742800	-2.78174000
H	22.73578400	1.55914800	-17.31875200	C	27.98237600	-3.31944800	-3.90631100
H	23.66285800	-2.42255800	-16.00601600	O	28.13406600	-2.11406100	-3.77908600
H	21.28777800	-0.20628200	-17.37293600	O	27.72632000	-3.91428300	-5.07222200
N	30.27438600	0.73905600	-16.99097400	H	29.54712100	-2.11001600	-1.86977900
C	31.68244400	1.10844000	-16.98009400	H	28.22085200	-4.58360200	-0.65577900
C	32.45335100	0.39479000	-15.86897200	H	27.40797300	-3.10991700	-1.16106700
C	32.00913300	0.84024200	-14.47955700	H	28.96906200	-4.97159700	-3.03859500
C	32.54860500	2.17128700	-14.00271000	H	27.23746100	-4.99943700	-2.83776600
O	33.38399200	2.77010500	-14.82079100	H	30.46540400	-3.51018000	-1.36774800
O	32.24055300	2.62878200	-12.89559500	H	29.56608400	-2.49738200	-0.16233500
H	30.03835500	-0.21696900	-17.21204900	C	34.86170800	7.99988900	-10.31565100
H	31.73279200	2.19224400	-16.87166300	C	35.25691100	6.51066100	-10.34404700
H	32.28781100	-0.68630600	-15.96142200	C	35.12698300	5.91060400	-11.70686700
H	33.52482400	0.56965200	-16.00368400	C	34.28127400	4.96063600	-12.22459200
H	30.91681300	0.86319800	-14.41668300	N	35.89634800	6.32140600	-12.78700200
H	32.30562100	0.10722100	-13.72266700	C	35.50100800	5.62096900	-13.88528800
C	26.18597400	-1.93672500	-12.22989000	N	34.52602400	4.79103000	-13.57359300
O	25.28162100	-2.65183900	-12.73175300	H	35.55937500	8.60826700	-10.90188000

H	36.27766600	6.37916100	-9.96112100
H	34.60256700	5.94639700	-9.67204100
H	36.61948900	7.02425700	-12.76271200
H	33.51525800	4.37720200	-11.73689500
H	35.94438000	5.74611600	-14.86204200
H	33.77767100	3.61001000	-14.37718100
H	34.87118800	8.38172000	-9.28973100
H	33.87116600	8.09546100	-10.77224200

The enzyme-substrate complex with
Mode-B for the Mn-enzyme of SDC.

E:S-B_{Mn} (4.2 kcal/mol)

H	20.66706400	-6.80406200	-16.56490400
H	16.38996100	-5.37400500	-12.30897400
H	24.65804400	-6.75725100	-19.16503800
H	29.36460100	-8.34237500	-18.18008600
H	35.11199200	4.87000600	-6.01599100
H	32.10199900	7.76401000	-10.35099500
H	33.92510800	-0.02999900	-10.21108200
H	31.95000600	-4.27896400	-6.58609900
H	23.18522000	1.49712900	-4.32330000
H	22.41701400	4.62902500	-7.60400800
H	22.25386800	6.38955300	-15.14826800
H	33.53399900	5.46899900	-6.68100000
H	30.78100300	8.84800100	-10.93699200
H	23.93862500	6.30926700	-15.81983300
H	23.80779800	-0.12317000	-3.81401300
H	32.79715300	-3.33877400	-5.29808300
H	32.07507900	0.82309800	-17.96199500
H	30.43482300	-3.27774000	-15.73579800
H	31.70201100	-4.16491900	-14.93618100
H	30.41799100	-9.06001500	-14.20499400
H	20.88596700	-5.05007300	-16.84107800
H	34.15716400	-4.71604900	-10.10820400
H	23.72467700	-8.30785000	-7.05583500
H	21.59201500	-3.72881300	-7.31995300
H	27.89809600	0.15097700	-17.74196100
H	27.15896200	4.34410800	-6.69907700
C	29.55217800	-8.45638400	-13.91548900
C	29.09673800	-7.66329600	-15.11722600
O	28.96487400	-6.43216800	-15.11454000
C	29.83765200	-7.57552300	-12.69963200
C	28.54643300	-7.14608800	-11.98376200
C	28.86162500	-6.01684400	-10.99596400
O	29.48248200	-6.31247100	-9.96525100
O	28.51939200	-4.82640600	-11.35418100
H	28.76631600	-9.18627400	-13.67165500
H	30.47521700	-8.10495600	-11.98708400
H	30.38509400	-6.68687400	-13.02845000
H	27.80339600	-6.82050500	-12.71699600
H	28.14201700	-8.00761500	-11.44073100
N	28.89354700	-8.38296000	-16.23238800
C	28.69016100	-7.77024200	-17.53347500
C	27.23525000	-7.96867400	-17.96392300
O	26.77933500	-9.09929700	-18.08995500
H	28.92030100	-9.39125700	-16.19593900
H	29.00698900	-6.72935300	-17.47344700
N	26.51615000	-6.82730000	-18.11559300
C	25.05618500	-6.83989200	-18.14800600
C	24.50752700	-5.69586500	-17.29449500
H	26.95441300	-5.95973000	-17.83892100
H	24.73919700	-7.81389200	-17.76542300
H	23.41579400	-5.71903000	-17.28716600
H	24.86783300	-5.75249600	-16.26285000
H	24.81020800	-4.72234600	-17.69821700
C	23.25605400	6.03699200	-15.04215700
C	23.15129300	4.50087100	-15.03361500
C	22.23204600	3.93955300	-13.97412900
C	22.38939600	4.27851900	-12.62525900
C	21.26370000	2.97648000	-14.29122000
C	21.63407500	3.66303900	-11.63122300
C	20.50971800	2.33560500	-13.31124900
C	20.70274400	2.67696900	-11.97013100
O	19.96493000	2.01944500	-11.02559700
H	23.64784900	6.42083900	-14.09429500
H	22.79212500	4.17788000	-16.01722800
H	24.14704300	4.05285100	-14.92801200
H	23.13680900	5.01176200	-12.33490700
H	21.13491500	2.68166700	-15.32897100
H	21.78312300	3.92624300	-10.58902100
H	19.82717200	1.53149800	-13.55916000
H	20.33253600	2.22078900	-10.15387300
C	20.86193400	-5.83974700	-16.08300600
C	19.77371100	-5.54626800	-15.05229800
O	18.77644900	-6.24804200	-14.92152900
H	21.84416100	-5.85736100	-15.60078500
N	20.00031600	-4.43215000	-14.28251600
C	19.19491000	-4.19819200	-13.09497200
C	18.13915600	-3.10990300	-13.26382800
O	18.36810500	-2.05122400	-13.87133400
C	20.14903100	-3.84554700	-11.92778900
O	19.47646800	-3.60974100	-10.69632300

H	20.91924000	-3.99339200	-14.32332000
H	18.69377100	-5.14223200	-12.87548500
H	20.80956600	-4.70440200	-11.77661800
H	20.77966300	-2.99706500	-12.20673400
H	19.18451700	-2.68941300	-10.69119800
C	23.90650100	-7.35674100	-7.56585700
C	22.89249500	-6.30873500	-7.13883700
O	21.72716000	-6.61956200	-6.88724000
C	23.72655900	-7.70023000	-9.06977400
C	24.14836000	-6.63359800	-10.01951900
C	25.33835900	-6.42525600	-10.66755600
N	23.34946300	-5.56430500	-10.39712500
C	24.05584700	-4.76726200	-11.23795500
N	25.27118000	-5.26866100	-11.42150400
H	24.93924100	-7.05594600	-7.37539500
H	24.31446800	-8.59554500	-9.29290400
H	22.67460900	-7.96255300	-9.23026800
H	22.41691300	-5.37768500	-10.05488200
H	26.23298200	-7.02486800	-10.62381200
H	23.66163800	-3.88465100	-11.71582800
N	23.30573300	-5.01076900	-7.14047000
C	22.40691500	-3.96387200	-6.62809500
C	23.33556800	-2.76800300	-6.39106700
C	24.48384000	-2.98783400	-7.38681700
C	24.67918000	-4.50683500	-7.35140300
H	21.92437800	-4.32013500	-5.71278800
H	22.82461000	-1.81901500	-6.53973900
H	23.72507500	-2.79119300	-5.36757500
H	24.18859100	-2.66332200	-8.39053300
H	25.39752100	-2.45452000	-7.11430100
H	25.10774900	-4.89623200	-8.27646500
H	25.33812800	-4.78839000	-6.51913100
C	23.17498000	4.07098600	-8.16499200
C	24.47284700	3.92121100	-7.39357400
O	24.50045400	3.75591500	-6.17394200
H	22.77940500	3.07227300	-8.36836700
H	23.31807200	4.57693600	-9.12195100
N	25.61388100	3.94376600	-8.14063200
C	26.90904500	3.66685800	-7.52192200
C	27.90528800	3.87907300	-8.66416900
C	27.11911100	3.44698300	-9.89651700
C	25.70596300	3.97090500	-9.61382900
H	26.93791900	2.64064500	-7.13344500
H	28.15298300	4.94271600	-8.74548600
H	28.83454200	3.32597200	-8.52358700
H	27.52858200	3.84742100	-10.82084500
H	27.09905700	2.35682300	-9.96860800
H	25.59171000	4.99607000	-9.98946300
H	24.94064300	3.34431000	-10.07489400
C	23.37404300	0.46301600	-4.62954400
C	24.33143700	0.45229300	-5.82781100
C	23.71837800	0.59926000	-7.20583600
C	22.34481500	0.52397600	-7.46297800
C	24.57908400	0.75004200	-8.30383200
C	21.85234500	0.54572600	-8.77333800
C	24.09410300	0.80518600	-9.60547100
C	22.72308900	0.68389300	-9.85321000
H	22.41518900	-0.01239800	-4.85472800
H	25.06344000	1.25597100	-5.69794500
H	24.90366800	-0.48396800	-5.82985100
H	21.64377400	0.42920200	-6.64146000
H	25.64984200	0.81925600	-8.12892400
H	20.78539600	0.42844400	-8.94666800
H	24.78099800	0.92560700	-10.42970600
H	22.35196800	0.69194400	-10.87094000
C	32.20579200	-3.28028800	-6.21781100
C	30.91016100	-2.46535700	-6.01822000
C	30.03941500	-2.43056500	-7.25026100
C	30.42954100	-2.40600800	-8.57050900
N	28.64630200	-2.48850900	-7.20379000
C	28.23008300	-2.53356200	-8.47225700
N	29.27989800	-2.47569300	-9.32049200
H	32.83468800	-2.83463400	-6.99267300
H	30.32124200	-2.87933600	-5.19700600
H	31.16695400	-1.44231900	-5.69973000
H	27.93126900	-3.20145400	-5.86077200
H	31.41319600	-2.39216500	-9.00149600
H	27.21001500	-2.59714200	-8.82021100
H	29.22522600	-2.47436100	-10.34198200
C	33.47987500	-4.18205600	-10.78262200
C	33.55551600	-2.73159200	-10.32882300
O	33.65463100	-2.38972700	-9.15218500
C	32.08797700	-4.81591700	-10.65557500
O	31.78601000	-5.03205100	-9.30454300
H	33.84031900	-4.28179600	-11.81246500
H	31.33025600	-4.17431300	-11.13153900
H	32.09968800	-5.75946000	-11.22785500
H	30.87483100	-5.39791400	-9.30061600
N	33.52291400	-1.80283500	-11.32933200
C	33.30483600	-0.40189600	-11.03294100
H	33.24146100	-2.11727500	-12.24649400
H	33.55832500	0.18625700	-11.91941900
H	32.25468600	-0.20144900	-10.79449000
C	30.70439100	-3.79264100	-14.83721100
C	30.70570400	-2.82695100	-13.65162900
C	29.35654100	-2.38434900	-13.09687300
O	28.28585400	-2.70925000	-13.69744100
O	29.40584200	-1.69904000	-12.03636400
H	30.03036300	-4.63073800	-14.67933500

H	31.23321900	-3.26917600	-12.80235700	H	30.64240800	2.07593300	-12.35934100
H	31.25703400	-1.90830100	-13.89390700	H	29.38404400	1.09990500	-12.03559100
C	27.87487400	1.06305800	-17.13699500	C	16.94627600	-3.33780700	-12.67539200
C	29.25331600	1.60551000	-16.82242400	C	16.59812700	-4.44991200	-11.75907900
O	29.42504500	2.73987100	-16.37788800	C	15.33346600	-3.92837000	-11.06049000
C	27.09447100	0.79298200	-15.83100800	C	14.67574800	-3.03716200	-12.12488100
C	25.64171500	0.49111400	-16.09551500	C	15.87241200	-2.33801700	-12.77742700
C	24.79970400	1.49501500	-16.58525000	H	17.41389600	-4.63058400	-11.05975400
C	25.09752000	-0.77477100	-15.85583400	H	14.69011600	-4.74061500	-10.71403100
C	23.44970300	1.25229800	-16.82294800	H	15.61364900	-3.32606600	-10.18889300
C	23.74884900	-1.03694800	-16.09046000	H	14.15555600	-3.65627500	-12.86406600
C	22.92863600	-0.01515800	-16.56505900	H	13.95437200	-2.32853800	-11.71081400
O	21.58593400	-0.30005000	-16.73593300	H	15.71451100	-2.06436800	-13.82307300
H	27.35486700	1.83090400	-17.71687700	H	16.15894700	-1.42485600	-12.24019400
H	27.55579300	-0.03953600	-15.28826400	C	29.55103300	-2.94412200	-1.16182700
H	27.18123800	1.67495800	-15.18995500	C	28.26543000	-3.74471600	-1.39629500
H	25.19733800	2.49029000	-16.76568600	C	28.11381200	-4.30123400	-2.81628700
H	25.71583400	-1.55503900	-15.42237900	C	27.99812200	-3.26643900	-3.92780000
H	22.80463800	2.04610600	-17.19161800	O	28.17337800	-2.06621300	-3.78787000
H	23.31969300	-2.00508100	-15.85873200	O	27.72445700	-3.84349500	-5.09977500
H	21.13948000	0.48259100	-17.08461400	H	29.55706700	-2.10583100	-1.86462200
N	30.27478000	0.73381400	-17.03203600	H	28.20657700	-4.58535400	-0.69383400
C	31.68295600	1.10885800	-16.98009100	H	27.40725700	-3.09762300	-1.17861000
C	32.41634000	0.43392200	-15.82198400	H	28.97290500	-4.93440300	-3.07729900
C	31.91915800	0.96498000	-14.47843600	H	27.24009200	-4.95936600	-2.88831100
C	32.42865400	2.34261800	-14.09437500	H	30.46536600	-3.51013100	-1.36804800
O	33.45303100	2.76718000	-14.80127200	H	29.56603400	-2.49716200	-0.16243300
O	31.94551800	2.98283200	-13.15604300	C	34.86196500	8.00001300	-10.31595800
H	30.04827200	-0.16779100	-17.42371000	C	35.24799100	6.50784000	-10.33413800
H	31.72579900	2.19562400	-16.88934200	C	35.15418600	5.90390700	-11.69805900
H	32.24475800	-0.64864500	-15.86838400	C	34.25830900	5.03179300	-12.26651700
H	33.49231200	0.59978000	-15.92083500	N	36.03246200	6.22210700	-12.72457300
H	30.82719600	0.99362600	-14.45259800	C	35.65052400	5.54367900	-13.84122200
H	32.19927500	0.30140200	-13.65409600	N	34.57972600	4.81658900	-13.59268900
C	25.80208800	-1.82131800	-12.17026100	H	35.56311100	8.60115900	-10.90469100
O	25.24044400	-2.64356700	-12.97163500	H	36.25685300	6.36833600	-9.92405200
O	26.58316800	-2.22226000	-11.25403600	H	34.57174500	5.95078400	-9.67778000
C	25.60126700	-0.37563500	-12.39512900	H	36.81866900	6.85033400	-12.65393900
C	26.63438500	0.55740700	-12.19219800	H	33.40382100	4.53901000	-11.82808000
O	27.85638100	0.25823600	-11.66382500	H	36.17421600	5.60645800	-14.78358900
C	26.41683500	1.89422400	-12.53971400	H	33.83186200	3.63312900	-14.39804800
C	25.16549700	2.31598700	-12.96944200	H	34.87102300	8.38159200	-9.28968100
C	24.12080800	1.40234800	-13.12638300	H	33.87106300	8.09550400	-10.77201300
C	24.36241600	0.06257300	-12.87870700	Mn	26.90704100	-4.11742600	-12.37174000
H	28.18578400	-0.69372700	-11.79007600				
H	27.23972100	2.59157300	-12.47017200				
H	25.01926500	3.36583800	-13.18657800				
H	23.14732500	1.71675700	-13.46432200				
H	23.57874300	-0.66770400	-13.02951800				
O	26.92908500	-4.78139800	-14.53216500				
H	27.46047100	-3.97448900	-14.70390400				
H	27.56449100	-5.50139900	-14.72607600				
O	22.58960900	-3.08295400	-13.81910800				
H	22.10886900	-2.22377300	-13.86318200				
H	23.53681600	-2.88464600	-13.68566200				
O	20.89647200	-0.95800800	-14.03299300				
H	21.01282400	-0.71202200	-14.96637200				
H	20.00387500	-1.37075900	-13.99512800				
C	34.22900400	4.62598400	-6.61600900				
C	33.55228200	3.34860300	-6.08101700				
C	32.22257000	2.99382200	-6.77680700				
C	31.88955800	1.49154400	-6.64231800				
N	30.52347000	1.11026400	-7.02426600				
C	30.08840600	1.03621700	-8.29972100				
N	30.80674300	1.55293500	-9.28524100				
N	28.87114300	0.51541600	-8.55262000				
H	34.58482400	4.44674800	-7.63917600				
H	34.25526700	2.51329500	-6.19928200				
H	33.37355700	3.44019800	-5.00301900				
H	31.39945500	3.58349800	-6.35853100				
H	32.29016900	3.28463400	-7.83273700				
H	32.60938800	0.88915700	-7.21272400				
H	31.99989800	1.19531400	-5.59659700				
H	29.96944400	0.61994100	-6.33605900				
H	31.68573300	1.98780100	-9.06505800				
H	30.54282700	1.46395200	-10.31183000				
H	28.53250400	-0.22010900	-7.93803000				
H	28.59168600	0.40650600	-9.52543300				
C	31.09199900	7.81098500	-10.77001100				
C	30.05742800	7.02778700	-9.94236100				
C	28.78224100	6.82401700	-10.70773100				
C	27.56740000	7.42600400	-10.49461100				
C	28.63167400	6.00415300	-11.88961900				
C	27.29480800	6.16610300	-12.34942700				
C	29.49270900	5.14330600	-12.59446500				
N	26.66605800	7.03091600	-11.47291300				
C	26.81638900	5.52025200	-13.49466800				
C	29.02186300	4.49793700	-13.73158600				
C	27.69957500	4.69299700	-14.18120000				
H	31.16721900	7.35807000	-11.76535400				
H	30.48009400	6.04979100	-9.67361200				
H	29.85182200	7.54422600	-8.99776000				
H	27.26682600	8.11416000	-9.71730900				
H	25.71617200	7.35316900	-11.55161600				
H	30.51622900	4.98217900	-12.27176900				
H	25.79953100	5.67053600	-13.84248600				
H	29.67263300	3.84898900	-14.30409000				
H	27.38408900	4.18423600	-15.08577600				
O	30.31188300	1.32408800	-11.82601500				