

脯氨酸硫酯自然化学连接反应中的轨道相互作用

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Orbital Interactions in Native Chemical Ligation Reaction of Proline Thioesters

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Path-Ala 和 Path-Pro 路径中重要中间体结构

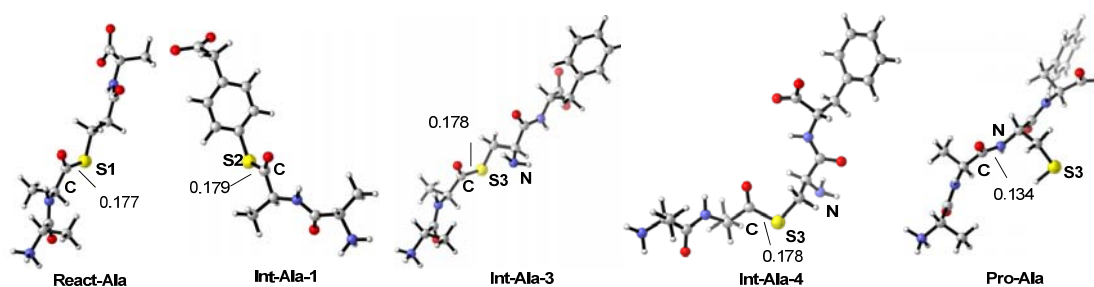


Fig.S1 Path-Ala 中重要的中间体结构

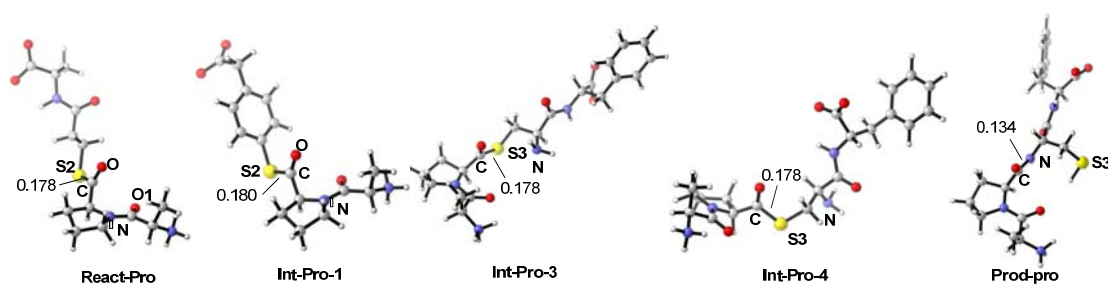


Fig.S2 Path-Pro 中重要的中间体结构

采用 M06 进行构型优化的计算结果

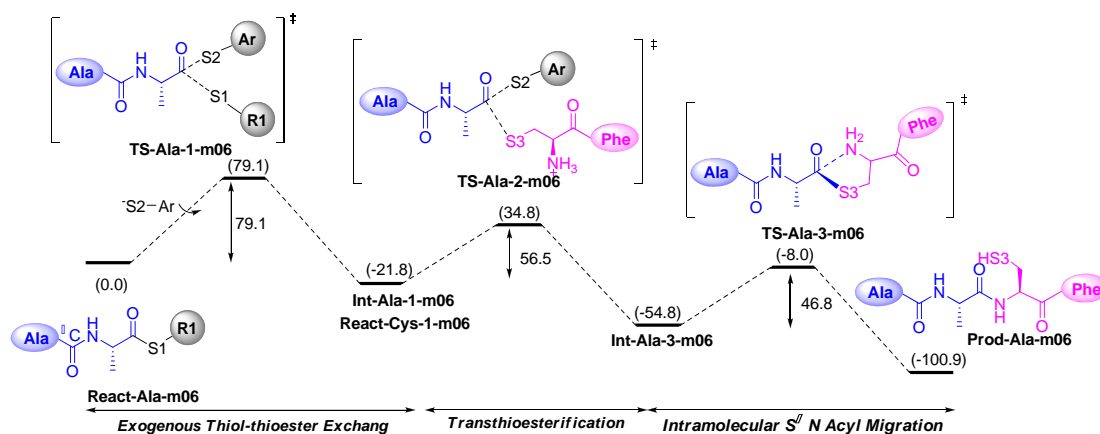


Fig.S3 Calculation result of Path-Ala

(Values in parentheses are Gibbs free energy in $\text{kJ}\cdot\text{mol}^{-1}$).

采用 M06/6-311++G(d,p)/M06/6-31+G(d)对 Path-Ala 进行计算。如 Figure S3 所示, 该路径的三个主要步骤的能垒分别为 79.1, 56.5 和 46.8 kJ/mol , 由此可知第一步是决速步骤。根据这一结论, 进一步考察 Path-Pro 路径的决速步骤, 可知其能垒为 97.6 kJ/mol 。总结得到如下结论: (1) 两种路径的第一步是决速步; (2) Path-Pro 的能垒高于 Path-Ala, 前者仍非优势路径。这与采用 B3LYP 方法得到的结论一样。

采用 M06-2X 进行单点能量计算的计算结果

Table S1 Calculation results of M06 and M06-2X method

Path	Method	Step 1	Step 2	Step 3
Path-Ala	M06	66.6	55.7	55.7
	M06-2X	74.5	60.7	52.8
Path-Pro	M06	76.6	64.5	66.6
	M06-2X	82.1	69.1	62.4

Values in parentheses are Gibbs free energy in $\text{kJ}\cdot\text{mol}^{-1}$.

我们采用 M06-2X 重新计算 Path-Ala 和 Path-Pro 中三个步骤的能垒。结果发现 (Table S1): 两条路径中的第一步硫醇-硫酯交换仍然是决速步; 并且 Path-Ala 仍比 Path-Pro 优势。这与采用 M06 计算能量得到的计算结果是一致的, 我们的结论并不依赖于方法的改变而变化。

React-Ala 和 React-Cys 直接交换的过程

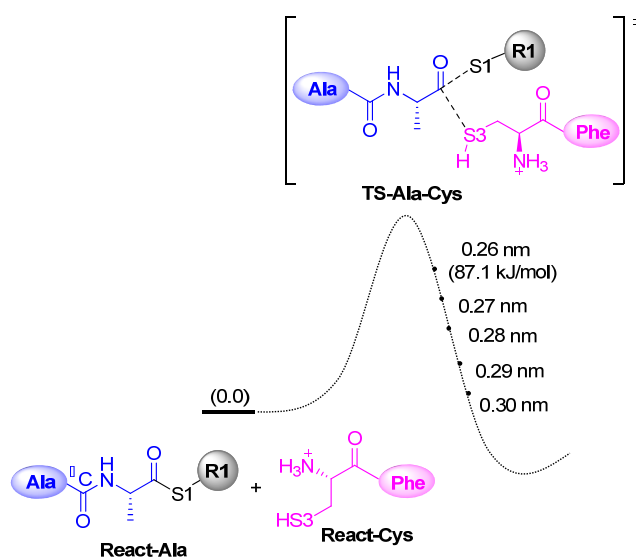


Fig.S4

我们考察了丙氨酸硫酯与半胱氨酸直接发生交换的过程。如 Fig.S4 所示, 在 $\text{pH}=7$ 的反应条件下, 半胱氨酸以 React-Cys 的形式存在。与丙氨酸硫酯直接交换的过渡态为 TS-Ala-Cys, 其中羰基 C—S3 键逐渐形成, C—S1 键断裂。然而我们经过大量的尝试, 该过渡态在放开优化后羰基 C—S3 键总是自动解离。为了得到该过渡态近似的能量, 我们绑定羰基 C—S3 键

并将其逐渐缩短，考察在该过程中能量变化的情况。固定 C—S3 为 0.30,0.29,0.28,0.27 以及 0.26 nm，发现随着 C-S3 键的缩短，体系的能量越来越高。对 0.26 nm 的结构进行能量计算得到其相对于反应底物高出 87.1 kJ/mol，因此我们推测该过程中的过渡态能量必然高于 87.1 kJ/mol，且高于 MPAA 参与的 NCL 反应的能垒（66.6 kJ/mol）。所以硫醇-硫酯的交换是有必要的。

三种底物的两性离子形式和中性形式能量之间的对比

三种底物的两性离子形式和中性形式能量之间的对比。前者的 C-端和 N-端为离子形式 (-COO⁻, -NH₃⁺)，后者的 C-端和 N-端为中性形式(-COOH, -NH₂)。

Substrate	React-Ala	React-Pro	React-Cys
Zwitterion form(eV)	-1407.9763	-1485.3125	-1199.8117
Neutral form(eV)	-1407.9735	-1485.3089	-1199.8061

Gibbs Free Energy Corrections and Electronic Energies in Solvate of related compounds and Transition States

	Thermal Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
S2-Ar (MPAA)	0.083835	-857.2245841
S1-R1	0.112197	-912.8365369
HS1-R1	0.120533	-913.3143023
HS2-Ar	0.092553	-857.6920108
React-Ala	0.288181	-1408.26446
React-Ala (中性形式)	0.283457	-1408.256981
React-Cys	0.225754	-1200.037451
React-Cys (中性形式)	0.223598	-1200.029675
TS-Ala-1	0.389192	-2265.480852
Int-Ala-1	0.257522	-1352.638544
React-Cys-1	0.214177	-1199.57211
Int-Ala-2	0.39492	-1694.982205
Int-Ala-3	0.378573	-1694.530293
Int-Ala-4	0.376822	-1694.531355
TS-Ala-3	0.382704	-1694.515899
Int-Ala-5	0.384327	-1694.516933

Prod-Ala	0.378881	-1694.548243
React-Pro	0.326112	-1485.638656
React-Pro (中性形式)	0.321168	-1485.630072
TS-Pro-1	0.424649	-2342.848882
Int-Pro-1	0.296871	-1430.012937
TS-Pro-2	0.535428	-2629.582465
Int-Pro-2	0.432317	-1772.358511
Int-Pro-3	0.416101	-1771.905074
Int-Pro-4	0.415614	-1771.904954
TS-Pro-3	0.419062	-1771.883067
Int-Pro-5	0.420788	-1771.883323
Prod-Pro	0.414307	-1771.922839
MPAA	0.105196	-858.145646249
React-Ala-OH	0.301684	-1408.67300538
React-Ala-SH	0.296804	-1408.65027743
TS-Ala-Cys-2.6	0.542291	-2608.29705662
TS-Ala-Cys-2.7	-	-2609.0097058(优化)
TS-Ala-Cys-2.8	-	-2609.0131336(优化)
TS-Ala-Cys-2.9	-	-2609.0159197(优化)
TS-Ala-Cys-3.0	-	-2609.0180775(优化)
React-Ala-m06	0.288623	-1408.26747323
S2-Ar-m06	0.084013	-857.225806527
HS2-Ar	0.092930	-857.693289989
S1-R1-m06	0.111987	-912.838139766
HS1-R1-m06	0.121350	-913.315870454
TS-Ala-1-m06	0.399165	-2265.48971595
Int-Ala-1-m06	0.257646	-1352.64175229
React-Cys-m06	0.228418	-1200.03881287
React-Cys-1-m06	0.213975	-1199.57461845
TS-Ala-2-m06	0.502520	-2552.22577823
Int-Ala-3-m06	0.377363	-1694.53440834
TS-Ala-3-m06	0.382906	-1694.52205714
Prod-Ala-m06	0.378034	-1694.55267554
React-Pro-m06	0.323366	-1485.642345
TS-Pro-1-m06	0.434697	-2342.858385
React-Ala-M062X	-	-1408.48645122
React-Pro-M062X	-	-1485.89029293
S2-Ar-M062X	-	-857.354751313
TS-Ala-1-M062X	-	-2265.83001421
Int-Ala-1-M062X	-	-1352.87929969

React-Cys-1-M062X	-	-1199.78562867
TS-Ala-2-M062X	-	-2552.67030964
Int-Ala-4-M062X	-	-1694.85591860
TS-Ala-3-M062X	-	-1694.84175842
TS-Pro-1-M062X	-	-2343.22849411
Int-Pro-1-M062X	-	-1430.28377128
TS-Pro-2-M062X	-	-2630.06469470
Int-Pro-4-M062X	-	-1772.25932078
TS-Pro-3-M062X	-	-1772.23895745
HPO ₄ ²⁻	-0.004268	-643.2383097
H ₂ PO ₄ ⁻	0.007583	-643.7059552
React-Ala-OH	0.301684	-1408.673005
React-Ala-H ₂ O	0.307492	-1484.702059
TS-Ala-1-H ₂ O	0.413752	-2341.922393
H ₂ O	0.003166	-76.43171301
React-P-Ala	0.319398	-2051.988952
Int-P-S12	0.423556	-2909.216583
TS-P-S1	0.422049	-2909.201287
Int-P-S2	0.285959	-1996.354213
Int-P-S2-2.2	-	-2909.825961 (全电子能)
Int-P-S2-2.5	-	-2909.820712 (全电子能)
Int-P-S2-2.7	-	-2909.820104 (全电子能)
Int-P-S2-2.8	-	-2909.819907 (全电子能)
Int-P-S2-2.9	-	-2909.820053 (全电子能)
Int-P-S2-3.0	-	-2909.820584 (全电子能)

Cartesian Coordinates of Intermediates and Transition States

			S-4.31404300	-0.63367200	0.21613100
S2-Ar (MPAA)			C-2.77513200	0.39232100	0.27530600
C 1.40060100	1.19792500	0.17259000	C-1.68034100	-0.29941700	-0.54354000
C 0.04304600	1.21147600	0.50415300	H-2.46286400	0.50208600	1.31755700
C-0.68814800	0.02209700	0.65585300	H-2.99513900	1.37928300	-0.13618400
C 0.00644200	-1.18417200	0.46627000	H-1.50347200	-1.31256300	-0.16831100
C 1.36357500	-1.20200600	0.13482300	H-1.99350000	-0.38042200	-1.59220000
C 2.11236800	-0.01024200	-0.02595700	N 0.70876000	-0.13818900	-0.10087500
H 1.92874800	2.14338300	0.06945200	H 0.65586100	-1.12413200	0.13844500
H-0.45587100	2.16827000	0.65130400	C 2.05046400	0.44212000	-0.06424400
H-0.52225000	-2.12926600	0.58237400	H 2.19023600	1.03958900	-0.97057400
H 1.86258600	-2.15941200	0.00139500	C 2.25394000	1.34491200	1.16457300
S 3.83651200	-0.03052300	-0.44329700	H 1.50325000	2.14134100	1.18029000
C-2.17155800	0.03646000	0.97793500	H 2.16778400	0.76595900	2.09145800
H-2.42881500	-0.83141000	1.59394500	H 3.24531400	1.80768800	1.13171300
H-2.41953700	0.94424200	1.53870400	C 3.09857300	-0.69315500	-0.07269300
C-3.02870700	0.00529400	-0.30376500	O 2.70706100	-1.87076400	0.18755900
O-3.24589700	1.11045300	-0.89521100	O 4.29374100	-0.34950500	-0.31688500
O-3.45094900	-1.12400800	-0.70926900	C-0.39085000	0.50862700	-0.51893100
			O-0.37408000	1.70745700	-0.88325200
			H-5.09779900	0.21730400	0.91363400
S1-R1					
S-4.40377300	-0.60355800	0.27863900			
C-2.78717000	0.29655300	0.36170800	HS2-Ar		
C-1.73589700	-0.24136700	-0.62903100	C 1.35336300	1.19737200	0.19235100
H-2.37770800	0.22607200	1.37806700	C-0.00435000	1.19828900	0.52244600
H-2.94785200	1.36125500	0.15702100	C-0.72511100	0.00230800	0.65817500
H-1.55693700	-1.30435700	-0.43443900	C-0.03661700	-1.20438700	0.45789400
H-2.12348400	-0.14954800	-1.65113200	C 1.32012300	-1.22129600	0.12780500
N 0.64960700	-0.12699600	-0.12812100	C 2.02529100	-0.01640100	-0.00784200
H 0.58260500	-1.12054800	0.07049700	H 1.88203600	2.14254600	0.09804200
C 1.99386600	0.44098900	-0.04032700	H-0.50673500	2.14981800	0.68010400
H 2.15321900	1.07623100	-0.91737000	H-0.56598100	-2.14858400	0.56272300
C 2.18513700	1.29031100	1.22885700	H 1.82323700	-2.17406700	-0.01915100
H 1.43568200	2.08703400	1.27093000	S 3.76626800	-0.09395900	-0.42508100
H 2.08809700	0.67326100	2.12984000	C-2.20682700	0.00997700	0.97918900
H 3.17775300	1.75185800	1.22814300	H-2.46408200	-0.87560900	1.56793400
C 3.03804700	-0.69653500	-0.08137300	H-2.45320800	0.90220000	1.56391200
O 2.64024300	-1.88379500	0.11930000	C-3.05756000	0.01873300	-0.31022800
O 4.23903300	-0.34783700	-0.29058000	O-3.24938400	1.13974000	-0.87713500
C-0.43581400	0.53950900	-0.56184500	O-3.49660700	-1.09463100	-0.73714400
O-0.38768400	1.75261800	-0.88632900	H 3.98249600	1.23859200	-0.45677600

HS1-R1

React-Ala

C-5.34724100	-0.16218700	0.11770600	C-5.44421400	0.04469700	-0.14543900
O-5.67541800	-0.82166700	1.12009400	O-5.76593600	0.56289000	-1.23300400
N-4.12352700	-0.18086100	-0.43019800	N-4.21225400	0.18221800	0.38607200
H-3.94456600	0.36303300	-1.27005200	H-4.01548000	-0.23314900	1.29078600
C-6.35978800	0.77271700	-0.55361100	C-6.41349700	-0.82342700	0.66387900
N-7.71060800	0.13373400	-0.39508700	N-7.65866600	-0.07123900	0.89534700
H-7.89957200	-0.05904900	0.59708300	C-3.14528400	0.94959000	-0.24440700
C-3.02178200	-0.97299400	0.10891400	C-1.80530600	0.33020400	0.16330300
C-1.71101600	-0.25982500	-0.23161400	O-1.65708000	-0.28086400	1.21330400
O-1.58717500	0.43080300	-1.23455100	H-8.30526100	-0.68379300	1.39304000
H-8.44763200	0.75197800	-0.75282400	S-0.48764700	0.61615000	-0.99244500
S-0.39455200	-0.57111700	0.91464800	C 0.92434100	-0.16036600	-0.10496400
C 1.00795900	0.26848800	0.06929800	C 2.19132900	0.01302300	-0.94710500
C 2.27432300	0.08031200	0.90889100	H 0.69320700	-1.21627700	0.04571200
H 0.75921200	1.32541200	-0.04003900	H 1.02885700	0.32606100	0.86833800
H 1.12206800	-0.17672900	-0.92262100	H 2.05466600	-0.43735800	-1.93933900
H 2.14958900	0.54923900	1.89393700	H 2.41895600	1.07320600	-1.09583400
H 2.47922700	-0.98227900	1.07466100	N 4.53549200	-0.01757600	-0.30265900
N 4.61803300	0.05287100	0.27403500	H 4.55850500	0.92076200	-0.68853700
H 4.62240500	-0.89425200	0.64088800	C 5.79512900	-0.58131700	0.16492300
C 5.89714100	0.52270300	-0.25740500	H 5.58980500	-1.21415300	1.03259200
H 5.71279300	0.99766100	-1.22655900	C 6.50182200	-1.42080800	-0.91768900
C 6.56794200	1.54218500	0.67876600	H 5.83344500	-2.22250600	-1.24495800
H 5.90087500	2.39151000	0.85718600	H 6.75814500	-0.79913500	-1.78226800
H 6.81336400	1.08188000	1.64301700	H 7.41568100	-1.87155900	-0.51938800
H 7.49082700	1.91879400	0.22694800	C 6.69499200	0.55614800	0.61621100
C 6.82828000	-0.68909800	-0.49497100	O 6.52571600	1.73308600	0.33476500
O 6.48829000	-1.81085400	-0.01185400	O 7.73419700	0.11536200	1.34401800
O 7.88801600	-0.45639500	-1.14944400	C-6.71563900	-2.11281000	-0.10513700
C-6.37593200	2.15993800	0.08629100	H-7.17712100	-1.89295700	-1.07390800
H-6.58531700	2.09561800	1.15940100	H-5.79899700	-2.68864200	-0.27466700
H-5.40382600	2.64051600	-0.05456900	H-7.40550300	-2.73580700	0.47637100
H-7.13969300	2.78219100	-0.39197500	H-5.91905100	-1.09540400	1.60740300
H-6.17510300	0.84268500	-1.62725700	C-3.18974200	2.43907100	0.15106200
C-3.00591800	-2.40209200	-0.46846200	H-4.17050500	2.84637500	-0.11294200
H-3.96510600	-2.88435300	-0.25661300	H-3.03292700	2.55983000	1.22812700
H-2.85003000	-2.37750800	-1.55203200	H-2.42332500	3.00787900	-0.38452900
H-2.21039800	-2.99547200	-0.00765200	H-3.26526700	0.86455200	-1.32776300
H-3.14170600	-1.02262400	1.19413100	H-7.46751200	0.70710400	1.52772000
H-7.76853000	-0.75872100	-0.90031600	C 3.37407200	-0.70149100	-0.30890000
C 3.47206600	0.75005300	0.24677200	O 3.27101800	-1.85495600	0.15462900
O 3.38009600	1.88898000	-0.26472100	H 8.30868300	0.87352100	1.57770800

React-Ala (中性形式)

React-Cys

C-1.83933700	-0.57359600	-0.42720600	O 0.28242000	2.65181400	-0.85297600
O-1.58082800	-1.64128300	0.16032000	H-4.80186700	-1.94574500	-1.38123600
N-0.98115000	0.43789700	-0.58219000	C-4.13420600	0.46885900	-0.41575300
H-1.27056700	1.28038100	-1.07446400	H-3.70091200	1.42514600	-0.71754000
C-3.23988100	-0.33810300	-1.01301900	H-5.12059500	0.39889100	-0.88545900
N-3.90332800	-1.67555100	-1.13425300	H-3.08565200	-0.44470500	-2.00046200
C 0.37589900	0.46118200	-0.03298400	C 1.30676200	-0.45666200	-0.96093400
C 0.80491200	1.93516900	0.14999200	H 0.88009500	-1.46186300	-1.04455300
O 0.30901300	2.78693600	-0.64839200	H 1.31648300	-0.01445600	-1.96299600
H-4.84293800	-1.58094200	-1.53812200	H 0.32086200	-0.04162200	0.93776000
C-4.10944200	0.62732400	-0.19370600	H-3.37954500	-2.71996800	-1.17193600
H-3.64365600	1.61477600	-0.20732100	S-4.47676100	0.52156000	1.39587000
H-5.08755600	0.71843400	-0.67558500	C 2.71211600	-0.53969000	-0.40733400
H-3.15954200	0.06093400	-2.02761600	C 3.74767600	0.23676600	-0.94854600
C 1.35375400	-0.30149900	-0.97558600	C 3.00695300	-1.40101700	0.66236700
H 0.90442500	-1.28187000	-1.17066800	C 5.04694400	0.15709100	-0.43527000
H 1.39915600	0.23488500	-1.93005000	H 3.53517300	0.90537000	-1.78012800
H 0.35999900	-0.03084900	0.94192500	C 4.30268200	-1.48154600	1.17991600
H-3.35942100	-2.30425700	-1.73745900	H 2.21625900	-2.01549600	1.08805400
S-4.45818500	0.12506500	1.54312500	C 5.32814100	-0.70163100	0.63197700
C 2.74807500	-0.48796700	-0.41788900	H 5.83729100	0.76350900	-0.87081900
C 3.82377500	0.27819600	-0.89165000	H 4.51309600	-2.15627200	2.00608000
C 2.99563700	-1.43965500	0.58558200	H 6.33738000	-0.76729800	1.03052300
C 5.11275800	0.10377500	-0.37589500	O 1.53051600	2.11675500	0.94963700
H 3.65017200	1.01644800	-1.67166000	H-3.25728600	0.95088000	1.79008500
C 4.28053900	-1.61437400	1.10715200	H 1.77972000	3.06269000	0.89160600
H 2.17500300	-2.04920900	0.95860500			
C 5.34533100	-0.84204800	0.62748500	TS-Ala-1		
H 5.93301600	0.70610200	-0.75884600	C 2.05852600	-0.80862200	0.87319200
H 4.45194000	-2.35640200	1.88327900	O 1.58265900	-0.72680800	-0.26369900
H 6.34598000	-0.97951200	1.02954700	C 3.19481700	-1.82466200	1.17223900
O 1.64079800	2.17581200	1.06791700	C 3.63015800	-1.95325500	2.62949300
H-3.98597100	-2.13184800	-0.21663600	H 2.83615200	-2.78267500	0.79875400
H-3.21170200	0.32332300	2.02775500	H 4.13621700	-1.04875600	2.98648000
			H 2.76772500	-2.14875300	3.27077300
React-Cys (中性形式)			N 4.35791600	-1.45224800	0.35132200
C-1.89477200	-0.75811800	-0.26707900	C 4.63265100	-1.95886200	-0.86071800
O-1.57453000	-1.66292100	0.52343400	O 3.99932600	-2.87834300	-1.40985700
N-1.05362000	0.24686600	-0.59637100	C 5.82201000	-1.31248000	-1.58196700
H-1.34643000	0.93113000	-1.28756300	H 6.59127000	-1.00848500	-0.86991800
C-3.27210000	-0.69575000	-0.94344700	N 6.43987600	-2.37309600	-2.44761200
N-3.96632100	-1.97492900	-0.79734200	H 6.82070800	-3.14452300	-1.88687800
C 0.30370400	0.35315500	-0.07941200	C 5.39258700	-0.13511000	-2.45555400
C 0.68217400	1.82456100	-0.04650300	H 4.97566700	0.65644400	-1.82709900

H 6.25937200	0.26902100	-2.98922600	Int-Ala-1		
H 4.63419600	-0.44370400	-3.18297100	C-4.49489000	0.21120800	-0.00989600
H 5.73688600	-2.77007800	-3.08366100	O-5.10602000	-0.69558000	0.58181200
S 0.22658900	-2.26359900	2.12245900	N-3.25727900	0.08911200	-0.51342700
C-0.94918600	-2.25033300	0.71564600	H-2.85154700	0.86950500	-1.02299100
C-2.23555600	-1.44612600	0.98682100	C-5.13126000	1.59499700	-0.17842000
H-1.21781400	-3.27973800	0.44655100	N-6.61902300	1.39080400	-0.21181200
H-0.42705300	-1.81422800	-0.14657500	C-2.46561600	-1.13345400	-0.41091200
H-2.76080300	-1.85730800	1.85546000	C-0.99452600	-0.73684000	-0.25838700
H-1.96828300	-0.40790500	1.21892100	O-0.52220500	0.24215800	-0.81120100
N-4.37694500	-1.95721300	-0.06548100	H-7.10489000	2.29452100	-0.24525300
C-5.41626300	-1.95907200	-1.09402900	S-0.04991300	-1.86477200	0.76339000
H-5.36495300	-1.00564900	-1.62899400	C-4.76969700	2.54142100	0.96610300
C-5.22918300	-3.10496900	-2.10430700	H-5.05914200	2.11656200	1.93322500
H-4.23370400	-3.05183500	-2.55663600	H-3.69047700	2.71788600	0.96652500
H-5.33731700	-4.07927300	-1.61310300	H-5.27572800	3.50296400	0.82912900
H-5.97550900	-3.03189400	-2.90174900	H-4.85740700	2.02861000	-1.14235400
C-6.80734900	-2.05444800	-0.42936300	C-2.63748400	-2.03706800	-1.64637800
O-6.87022200	-2.40660000	0.78699600	H-3.69641300	-2.29075200	-1.75623800
O-7.79990600	-1.79067400	-1.17291800	H-2.29771900	-1.52269300	-2.55125000
H 7.20257600	-1.97908300	-3.01032300	H-2.06799100	-2.96435000	-1.52949000
C-3.15416000	-1.41866400	-0.22226900	H-2.79685500	-1.67111900	0.48042300
O-2.77828500	-0.92348000	-1.31322000	H-6.90766000	0.84270200	-1.03076100
H-4.66466600	-2.28513100	0.85132800	C 1.61346600	-1.21755700	0.59242600
C 1.48723700	2.46634400	-0.10738500	C 2.09649900	-0.28502600	1.51891300
C 0.64851700	3.39171100	-0.73031300	C 2.43989300	-1.67031000	-0.44435600
C-0.58849800	3.74489100	-0.16549800	C 3.40345700	0.19234600	1.40210400
C-0.96783900	3.13339400	1.03882900	H 1.45930500	0.07071900	2.32348400
C-0.13947800	2.19671700	1.66349700	C 3.74369600	-1.18350600	-0.55076700
C 1.09743900	1.85828500	1.09603800	H 2.06987700	-2.39263100	-1.16640300
H 2.44388400	2.21540600	-0.55644500	C 4.24666700	-0.25031300	0.37047700
H 0.96051400	3.84972100	-1.66607800	H 3.77015600	0.91985000	2.12175900
H-1.92451000	3.38497200	1.49034200	H 4.37769800	-1.53414000	-1.36120000
H-0.45700800	1.72774600	2.59041900	C 5.67568200	0.24067600	0.27122900
S 2.17991200	0.71746300	1.94585600	H 5.75074800	1.24911300	0.68866500
C-1.47042200	4.78451600	-0.82720400	H 5.98583700	0.26895800	-0.77737700
H-1.39182400	4.69995000	-1.91514700	C 6.63579700	-0.69058500	1.04868300
H-2.51333400	4.62193400	-0.53728600	O 7.17214400	-1.64694400	0.40865300
C-1.06105000	6.21462300	-0.40588900	O 6.81208700	-0.45037600	2.28310500
O-0.30494900	6.86875200	-1.18981800	H-6.93230500	0.88319000	0.62523400
O-1.49374300	6.64071200	0.70973900			
H 4.33060800	-2.78964800	2.72690400	React-Cys-1		
H 4.94989700	-0.70162500	0.69648600	C-1.82966200	-0.73013700	-0.29963200
			O-1.49078500	-1.77655500	0.29273400

N-1.02187300	0.32152900	-0.46641600	C-6.76961800	-2.71699100	-0.80746000
H-1.35096900	1.15030100	-0.95338800	H-6.88891800	-2.40557400	-1.85080100
C-3.22439600	-0.61900400	-0.93789800	H-5.70549600	-2.86358100	-0.60169500
N-3.98013200	-1.84595900	-0.54062200	H-7.28478000	-3.67125700	-0.65549100
C 0.34922300	0.39482300	0.04040800	H-7.22520600	-1.98065000	1.18395600
C 0.73589900	1.88219000	0.20379100	C-5.06280100	2.13904300	1.62225700
O 0.20748500	2.71149800	-0.59755200	H-6.12383200	2.40187300	1.57172600
H-4.68325100	-2.10142500	-1.24034600	H-4.84821800	1.70355300	2.60356300
C-4.05958800	0.60671400	-0.51264900	H-4.47223500	3.05236200	1.50096500
H-3.47554300	1.51229800	-0.69941300	H-4.97095200	1.58180400	-0.46840500
H-4.92832100	0.65526500	-1.18037600	H-9.22843000	-0.86031800	0.58809700
H-3.10315400	-0.64303100	-2.02551400	C 1.50964000	-0.18561100	-0.28403900
C 1.32509900	-0.33814400	-0.92768400	O 1.61682300	-1.20588200	0.42166000
H 0.90871100	-1.33725800	-1.09930500	N 2.51378100	0.63672900	-0.59458300
H 1.31832300	0.19021600	-1.88771300	H 2.34153800	1.45891000	-1.16972300
H 0.38052700	-0.09030300	1.01831900	C 0.12651400	0.21641100	-0.83241600
H-3.34256200	-2.63408600	-0.37272900	N-0.67145900	-1.04709000	-0.95540900
S-4.60156700	0.50261800	1.25040100	C 3.87243300	0.50351300	-0.06391600
C 2.74413100	-0.46513400	-0.41775900	C 4.52761800	1.90348500	-0.04503800
C 3.77633600	0.32054400	-0.95246100	O 4.15336200	2.72836100	-0.93294500
C 3.05983800	-1.38068000	0.60027700	H-0.76654400	-1.50877000	-0.04216100
C 5.08894200	0.20042500	-0.48240800	C-0.54069700	1.21267700	0.12670300
H 3.55010900	1.03058600	-1.74510600	H-0.63570000	0.78777400	1.12987200
C 4.36847600	-1.50152500	1.07588000	H 0.08768700	2.10422000	0.18571200
H 2.27394400	-2.00477900	1.02090300	H 0.21177600	0.63419200	-1.83753900
C 5.38931100	-0.70988100	0.53564900	C 4.69507200	-0.50000200	-0.92607300
H 5.87442900	0.81719900	-0.91246600	H 4.06901200	-1.38984500	-1.05539600
H 4.59259000	-2.21630400	1.86402500	H 4.85042800	-0.05838800	-1.91703200
H 6.40820900	-0.80561800	0.90241400	H 3.80322100	0.12468400	0.95818100
O 1.57493600	2.15755800	1.10985300	H-1.61041900	-0.86685300	-1.32909700
H-4.45869200	-1.59509200	0.36018400	C 6.02084600	-0.90733800	-0.32157300
Int-Ala-2			C 7.22738900	-0.34901200	-0.77029000
C-6.67924100	-0.29190000	-0.07229100	C 6.06844900	-1.86704200	0.70340300
O-7.17970400	0.52414400	-0.86485200	C 8.44969300	-0.73277700	-0.20729500
N-5.54771300	-0.08313200	0.61892900	H 7.20925700	0.39039800	-1.56806300
H-5.23495200	-0.79078100	1.27820300	C 7.28674300	-2.25352100	1.26923400
C-7.33056100	-1.66201800	0.14490800	H 5.14320100	-2.31831500	1.05601700
N-8.80197400	-1.48981100	-0.10200400	C 8.48330300	-1.68572400	0.81588100
C-4.74686400	1.13048100	0.50096900	H 9.37363600	-0.28881100	-0.56985500
C-3.26879700	0.73802900	0.55678400	H 7.30257400	-3.00008300	2.05964800
O-2.86009200	-0.19966200	1.21956100	H 9.43197700	-1.98707100	1.25292100
H-9.28424700	-2.39470800	-0.05168400	O 5.40718500	2.11062200	0.83956200
S-2.19598200	1.81320100	-0.39494300	H-8.96307400	-1.08484900	-1.03270600
			H-0.20934900	-1.70889100	-1.59101200

			C 6.16894700	-1.75293400	0.89192100
Int-Ala-3			C 8.45543700	-0.92856800	-0.47957900
C-6.77608300	-0.33190100	-0.18325000	H 7.09257300	-0.02081200	-1.88349100
O-7.29030000	0.49890700	-0.95298500	C 7.43507400	-2.08476600	1.38245300
N-5.64183100	-0.12899400	0.50149800	H 5.28002900	-2.08239100	1.42622500
H-5.30085000	-0.85732600	1.12342900	C 8.58450500	-1.67205600	0.69790900
C-7.41633700	-1.71103800	0.01064400	H 9.34146100	-0.60689700	-1.02166000
N-8.88943400	-1.54639700	-0.23240300	H 7.52460400	-2.66862500	2.29538700
C-4.84225800	1.08750500	0.39335200	H 9.56985300	-1.93207700	1.07647300
C-3.37704900	0.70669100	0.63452900	O 5.60964800	2.15221200	0.54918200
O-3.06599900	-0.25691000	1.31982500	H-9.05481000	-1.13264100	-1.15834800
H-9.36566100	-2.45487500	-0.19065600	H-0.06400400	-1.36483200	-1.72264600
S-2.21217500	1.81823700	-0.11760100			
C-6.84759800	-2.74779400	-0.95714900	Int-Ala-4		
H-6.96394900	-2.41971100	-1.99572700	C-6.21588700	-0.79850000	0.08216100
H-5.78358000	-2.89310700	-0.75000900	O-7.10832800	0.06769100	0.06615200
H-7.35898200	-3.70676000	-0.82260900	N-4.91680400	-0.54008100	0.29131700
H-7.30846500	-2.04472000	1.04469400	H-4.25017000	-1.30749500	0.29820500
C-5.29021100	2.16093700	1.40438100	C-6.55448300	-2.27007700	-0.18051400
H-6.34732100	2.38911800	1.23747100	N-7.99753100	-2.46382700	0.18710300
H-5.16057700	1.80174600	2.43062600	C-4.39167900	0.80898700	0.48190300
H-4.71301900	3.08123900	1.27325300	C-2.95494300	0.83695300	-0.04941000
H-4.95552000	1.47605600	-0.62202900	O-2.25035000	-0.16301000	-0.06843600
H-9.31858200	-0.92647500	0.46461200	H-8.29514400	-3.42246200	-0.02796200
C 1.53017200	-0.00771400	-0.02637600	S-2.41462600	2.44298000	-0.58403000
O 1.64013400	-0.87106800	0.87175600	C-6.34044700	-2.66217400	-1.64187100
N 2.57385000	0.67489100	-0.52177500	H-6.91620400	-2.01390400	-2.31126300
H 2.42387000	1.36061600	-1.25636800	H-5.27949900	-2.57487500	-1.89187200
C 0.14837700	0.33457200	-0.61791600	H-6.64594200	-3.70214400	-1.79833100
N-0.59947100	-0.85719100	-1.01786200	H-5.97852300	-2.91846400	0.48281000
C 3.95416900	0.52521200	-0.06136100	C-4.42198200	1.23568100	1.96225600
C 4.70455700	1.85726900	-0.28517000	H-5.45125300	1.17670500	2.32916900
O 4.37976400	2.54372400	-1.30139300	H-3.79016200	0.57769100	2.56797400
H-0.68102600	-1.48091200	-0.21399800	H-4.07258700	2.26650400	2.07468000
C-0.60463500	1.14254800	0.45159100	H-5.00888900	1.49574500	-0.10348800
H-0.80208200	0.53043700	1.33587100	H-8.15835800	-2.29446100	1.18703400
H-0.01054000	2.00838100	0.75657800	C 1.66260100	1.65147800	-0.28340700
H 0.29119100	0.95826100	-1.50540900	O 2.35236500	2.28757500	-1.11069500
C 4.65126200	-0.64869700	-0.81116800	N 2.03498500	0.47132500	0.23473100
H 3.98985900	-1.51744100	-0.71820300	H 1.43398600	0.01148400	0.91215000
H 4.70995200	-0.39193300	-1.87498200	C 0.30183100	2.19594100	0.18701100
H 3.93376600	0.30311700	1.00740600	N 0.38895900	3.57147400	0.68116100
C 6.02585300	-1.00300600	-0.28747700	C 3.26402700	-0.24040500	-0.11350100
C 7.18562500	-0.59797600	-0.96592500	C 3.04108400	-1.75262300	0.11446600

O 2.31269600	-2.08766300	1.09760800	H-6.05509700	1.08247600	3.54229200
H 0.86640500	4.14294100	-0.01766100	H-4.55737200	2.01631300	3.71303700
C-0.66301300	2.10387700	-1.00521700	H-3.82756900	1.15927300	1.41639800
H-0.39982000	2.84751300	-1.76363500	H-7.49779400	1.31738800	-1.72899600
H-0.62494400	1.11522000	-1.46948000	C-0.07169500	0.90281900	3.15523400
H-0.06575800	1.56526900	1.00084500	O-0.38357400	2.10667600	3.04905700
C 4.45622800	0.28854800	0.73723300	N 1.17909000	0.46126000	3.32812600
H 4.47837000	1.37652700	0.60818100	H 1.35365400	-0.53783000	3.40011100
H 4.24123800	0.08526700	1.79249200	C-1.14191000	-0.19140700	3.03855100
H 3.47229600	-0.06495600	-1.17095500	N-2.43452600	0.29071200	3.55572600
C 5.80062900	-0.29413800	0.36097200	C 2.36751300	1.31525900	3.34612600
C 6.39906200	-1.29349800	1.14363000	C 3.57806300	0.48332400	2.86338600
C 6.48046100	0.15517100	-0.78361600	O 3.57389400	-0.75601600	3.13413100
C 7.64075200	-1.83470800	0.79244100	H-2.49437300	1.30466500	3.42207900
H 5.88894100	-1.64789200	2.03696800	C-1.36892100	-0.58326700	1.56807900
C 7.71983500	-0.38412800	-1.14008700	H-1.51057900	0.30476800	0.94390300
H 6.03579300	0.93653200	-1.39675600	H-0.52315300	-1.15617500	1.18046400
C 8.30472800	-1.38302800	-0.35251400	H-0.84847600	-1.07514800	3.60801100
H 8.08821900	-2.60673900	1.41380900	C 2.60459100	1.88391300	4.77692700
H 8.23101000	-0.02204100	-2.02890800	H 1.65501900	2.32436000	5.10198300
H 9.27004600	-1.80118500	-0.62668300	H 2.82655700	1.04667000	5.44822500
O 3.62411800	-2.54693600	-0.68013300	H 2.20450100	2.14378200	2.65365900
H-8.59524200	-1.81135300	-0.33577500	C 3.70015500	2.92359800	4.86540900
H 0.97610700	3.58927000	1.51516400	C 4.96103900	2.60407000	5.39193000
			C 3.47435600	4.23736700	4.42154400
TS-Ala-3			C 5.97353700	3.56720000	5.46593700
C-5.52073700	0.23231600	-0.24417100	H 5.15104400	1.59274300	5.74519400
O-4.65141700	0.86955200	-0.86630200	C 4.48325100	5.20219600	4.49082600
N-5.56062100	0.08807100	1.08840100	H 2.49905400	4.50507900	4.01994000
H-6.34630500	-0.41238700	1.49468800	C 5.73875000	4.86940500	5.01340700
C-6.64055100	-0.47562200	-1.01649100	H 6.94358300	3.29962900	5.87792600
N-7.07548600	0.46173200	-2.10990400	H 4.28832500	6.21364900	4.14260800
C-4.56696300	0.62938000	2.01774500	H 6.52388500	5.61911800	5.07107900
C-3.88892200	-0.57355300	2.74389900	O 4.49556900	1.10648200	2.25496900
O-4.55091500	-1.20155800	3.60626100	H-6.26944700	0.73880500	-2.68472600
H-7.76721400	0.01084200	-2.72008200	H-2.55147700	0.08960900	4.55035100
S-2.85509900	-1.64220100	1.54652900			
C-6.16133900	-1.78654000	-1.63578200	Int-Ala-5		
H-5.30525500	-1.61713800	-2.29725600	C 5.95553600	-0.71640600	-0.27872800
H-5.86117500	-2.47798100	-0.84347700	O 5.88579000	-1.30064600	-1.37612400
H-6.97248900	-2.24916600	-2.20769500	N 4.93408800	-0.57021500	0.57454200
H-7.51524500	-0.63814000	-0.38455400	H 5.10454100	-0.12304700	1.47156900
C-5.25935700	1.59162100	2.98855700	C 7.27501300	-0.06541000	0.15927800
H-5.70166100	2.41932500	2.42462500	N 8.38148200	-0.87405900	-0.45858100

C 3.58068200	-1.07611600	0.34674100	H-9.21686500	-1.92913800	-0.69983000
C 2.60898300	0.05457600	0.80171700	O-5.28811700	2.20019700	-0.95983300
O 2.67900300	0.42003900	2.02718400	H 8.21284200	-0.98669100	-1.46676300
H 9.28879600	-0.41352400	-0.32634500	H 0.78711000	-0.99801800	1.25546800
S 2.71839300	1.53155200	-0.50870900			
C 7.38254400	1.38656300	-0.30395400	Int-Ala-6		
H 7.27306200	1.46269000	-1.39104900	C 5.54530900	-0.68263700	0.06120800
H 6.59762400	1.98086200	0.17173300	O 5.41363900	0.52477300	-0.19110100
H 8.35286700	1.80087700	-0.01052800	N 4.68554200	-1.62578200	-0.36721400
H 7.40427800	-0.13824500	1.24113300	H 4.84035300	-2.59735800	-0.11317900
C 3.35931000	-2.38827900	1.11052800	C 6.70999400	-1.18812500	0.91502100
H 4.10874200	-3.12145400	0.79421300	N 7.87026900	-0.26764200	0.66470700
H 3.45143600	-2.23742500	2.19111000	C 3.51622800	-1.29976600	-1.16154100
H 2.37042400	-2.80978700	0.89739300	C 2.45916800	-0.62535200	-0.29408000
H 3.47202000	-1.24756300	-0.72515800	O 2.35344200	-0.66470200	0.89632800
H 8.43522600	-1.81376400	-0.04839700	H 8.66915300	-0.52800200	1.25456700
C-1.15170500	0.18982300	-0.28685200	S 2.24286700	3.25077300	-0.00554200
O-1.25000300	-0.80833600	-1.02768400	C 6.37004100	-1.19019700	2.40480400
N-2.18688500	0.91713400	0.14566200	H 6.07664900	-0.19004700	2.74133300
H-2.02408400	1.71330100	0.75744700	H 5.54396600	-1.88210900	2.59085300
C 0.22756500	0.69009000	0.15524900	H 7.23798700	-1.52556100	2.98210000
N 1.11535400	-0.46999300	0.43946500	H 7.02587000	-2.18008000	0.58673500
C-3.58129000	0.67736400	-0.22770600	C 2.94399500	-2.56777900	-1.81910000
C-4.34812200	2.01624600	-0.13358100	H 3.71997400	-3.01641000	-2.44570100
O-3.99368000	2.81905700	0.78211600	H 2.62895300	-3.29019600	-1.05952300
H 1.11156700	-1.10731200	-0.36766900	H 2.08929100	-2.32733700	-2.45740200
C 0.93133400	1.48927300	-0.94480800	H 3.81063000	-0.58943900	-1.94107800
H 0.78990200	1.00857300	-1.91714500	H 8.17365000	-0.29969700	-0.31618700
H 0.53285900	2.50491400	-0.98790600	C-0.92876300	0.50616000	-0.68353900
H 0.16145300	1.27223000	1.07591600	O-1.02587300	-0.48109200	-1.44503200
C-4.20698200	-0.40114400	0.70447600	N-1.95267100	1.11968900	-0.10229000
H-3.53679900	-1.26793900	0.67945100	H-1.79454900	1.90729700	0.52306200
H-4.20361700	-0.01102000	1.72846400	C 0.48721200	1.04255700	-0.34980200
H-3.60272300	0.32062500	-1.25929400	N 1.42142600	0.13043900	-1.10235200
C-5.60579000	-0.82841000	0.31672300	C-3.35596300	0.71988000	-0.24670000
C-6.72446900	-0.36656300	1.02680500	C-4.24064500	1.95998000	0.02213900
C-5.81420700	-1.70139700	-0.76428600	O-3.78953500	2.82356100	0.83400000
C-8.01802800	-0.75889500	0.66529400	H 1.88516600	0.60774500	-1.88993300
H-6.58061300	0.30512100	1.87053400	C 0.71539300	2.51159000	-0.71941400
C-7.10454900	-2.09430700	-1.13076600	H 0.70048100	2.64635300	-1.80512400
H-4.95793800	-2.07826800	-1.32005500	H-0.09543700	3.11250800	-0.30287700
C-8.21293700	-1.62219000	-0.41747200	H 0.66635300	0.87884400	0.71517100
H-8.87115500	-0.39042000	1.22980400	C-3.67810500	-0.43718200	0.74381700
H-7.24475600	-2.77186900	-1.96956800	H-2.92626300	-1.21662100	0.57548900

H-3.53987200	-0.06146400	1.76386800	H-1.99902000	1.64670800	1.22263100
H-3.51294900	0.37880600	-1.27176900	C 0.38396600	0.90606400	0.68029200
C-5.06183900	-1.02999000	0.59361600	N 1.46023500	-0.00341200	0.31617900
C-6.08229900	-0.72076600	1.50555900	C-3.38301900	0.61566600	0.00418900
C-5.35175700	-1.91170400	-0.46089100	C-4.29796800	1.83926100	0.24211300
C-7.36068900	-1.27274600	1.36826200	O-4.06934500	2.53781600	1.27607300
H-5.87332300	-0.04320100	2.33071000	H 1.90777800	2.00980000	-1.75884100
C-6.62803600	-2.46336100	-0.60401600	C 0.68558400	2.36911600	0.28867400
H-4.56998600	-2.17043000	-1.17230300	H-0.10593600	3.01903900	0.67095700
C-7.63876200	-2.14459500	0.31076100	H 1.61971600	2.67700800	0.76209800
H-8.13664400	-1.02154900	2.08728600	H 0.27135900	0.89300000	1.77085700
H-6.83255800	-3.14502600	-1.42609500	C-3.93210600	-0.65220500	0.72407300
H-8.63122700	-2.57469300	0.20198200	H-3.17022500	-1.43230500	0.61555900
O-5.35846200	2.00370100	-0.56631400	H-4.02329900	-0.42693900	1.79268200
H 7.61415800	0.70498600	0.87789600	H-3.31931400	0.41949400	-1.06812200
H 3.13815700	2.59801300	-0.78199100	C-5.25221700	-1.15785300	0.18535200
H 0.76559400	-0.57036600	-1.54886200	C-6.45693600	-0.88497300	0.85144800
			C-5.29904900	-1.91590200	-0.99658800
Prod-Ala			C-7.67720700	-1.35093200	0.35010300
C 5.92762300	-0.98914500	-0.24850700	H-6.43816600	-0.30217200	1.77001400
O 5.82403100	-1.84731800	-1.14460500	C-6.51603300	-2.38158000	-1.50280800
N 4.93631500	-0.63329000	0.57827400	H-4.37381600	-2.14623600	-1.52108200
H 5.11913700	0.05130200	1.30759500	C-7.71119000	-2.09969400	-0.83071600
C 7.24333300	-0.22463700	-0.06265800	H-8.59894100	-1.12968700	0.88284000
N 8.35069200	-1.15337200	-0.47183900	H-6.53069800	-2.96915200	-2.41765600
C 3.58288700	-1.18483100	0.50589200	H-8.65798600	-2.46440100	-1.22106800
C 2.61734400	-0.09871500	0.99026100	O-5.22153600	2.03913200	-0.59921800
O 2.90553800	0.61573400	1.96944700	H 8.17698700	-1.51788700	-1.41721300
H 9.25339700	-0.66427500	-0.47151500	H 1.27979400	-0.62481300	-0.46820000
S 0.77935900	2.71222300	-1.51703000			
C 7.29595500	1.03914200	-0.91825400	React-Pro		
H 7.14912100	0.80317300	-1.97775400	C-1.54200100	0.52774100	-0.05114500
H 6.50980300	1.72899800	-0.59907000	O-1.42865800	0.07244700	1.07739300
H 8.26340300	1.53659400	-0.79223500	C-4.87219000	1.63760200	0.70046200
H 7.40993800	0.01275300	0.98988400	C-2.80455600	1.23224300	-0.55362400
C 3.43659100	-2.45225600	1.36368200	C-2.85518000	2.70203500	-0.06384100
H 4.15197900	-3.20800500	1.02434800	C-4.35427400	2.96368500	0.14130800
H 3.62966200	-2.23133100	2.41873000	H-5.93091000	1.47244000	0.49421200
H 2.42617700	-2.86335700	1.26724600	H-4.70415500	1.56299100	1.78056000
H 3.37887900	-1.42635100	-0.53959100	H-2.83474900	1.18230700	-1.64737600
H 8.42382200	-1.95830300	0.16183500	H-2.32271500	2.79419900	0.88902100
C-0.91393900	0.37327900	0.04785300	H-2.39004600	3.37385900	-0.78839100
O-0.88360500	-0.51534400	-0.82705600	H-4.54320900	3.79558400	0.82521700
N-2.04233800	0.93761500	0.49509900	H-4.84020400	3.18195700	-0.81637000

N-4.03772200	0.63694300	-0.00783300	H-2.50292800	2.76651000	0.93322200
C-4.30911400	-0.65809800	-0.22855900	H-2.58748200	3.36473700	-0.73655300
O-3.54645100	-1.39809100	-0.88459500	H-4.75715000	3.68880300	0.88031100
C-5.58908700	-1.24650300	0.37478600	H-5.03061800	3.08666100	-0.76951800
H-6.43771100	-0.57376100	0.24203900	N-4.14406400	0.56040600	-0.00544700
N-5.91204600	-2.47816400	-0.42270000	C-4.37517900	-0.74676100	-0.26576600
H-6.10188100	-2.25398600	-1.40655700	O-3.55481300	-1.40710800	-0.94016300
C-5.42265400	-1.63204400	1.84505800	C-5.65139000	-1.38267200	0.29397800
H-5.24176100	-0.73907900	2.44900000	H-6.46148300	-0.64775100	0.20123900
H-6.33722100	-2.11259200	2.20848200	N-5.95945300	-2.61308100	-0.45130700
H-4.57942700	-2.31931300	1.97338400	H-6.08057600	-2.38818700	-1.43923000
H-5.12265600	-3.13576600	-0.40604200	C-5.47837400	-1.72106300	1.78219200
S-0.22236600	0.52627600	-1.24413100	H-5.31805200	-0.82387300	2.38788700
C 1.14711900	-0.17568700	-0.23738000	H-6.38542300	-2.21695000	2.14778700
C 2.40600200	-0.27286900	-1.10619600	H-4.63055000	-2.40003300	1.92764000
H 0.83952300	-1.16024900	0.12020200	S-0.30704900	0.63606600	-1.20279500
H 1.31146400	0.48068400	0.62149400	C 1.06730100	-0.06040300	-0.20044700
H 2.22410700	-0.93566000	-1.96133600	C 2.32529400	-0.15461400	-1.06979300
H 2.68248700	0.71030700	-1.49909500	H 0.76265300	-1.04633400	0.15511800
N 4.69724200	-0.15992600	-0.29834800	H 1.23221500	0.59326500	0.66035700
C 5.91721600	-0.54693600	0.41000000	H 2.14115400	-0.80861600	-1.93172300
H 5.63335200	-0.96085700	1.38239900	H 2.60844000	0.82971900	-1.45527200
C 6.72344400	-1.60159400	-0.36708700	N 4.65766900	-0.12694500	-0.37312500
H 6.10845600	-2.48724200	-0.55604600	C 5.86782800	-0.59096000	0.29162800
H 7.06209300	-1.20107000	-1.32963200	H 5.58464900	-1.03193600	1.25209500
H 7.60025700	-1.90850600	0.21200800	C 6.63254500	-1.64353100	-0.53457600
C 6.78019700	0.71063400	0.65813900	H 5.96470600	-2.48355100	-0.74676500
O 6.52042200	1.75588900	-0.01093700	H 6.97719100	-1.21713000	-1.48266900
O 7.71172800	0.59039200	1.50890900	H 7.49595000	-2.01556600	0.02427100
H-6.73816700	-2.94777900	-0.03402200	C 6.75185700	0.60995600	0.57899700
C 3.56025100	-0.87154600	-0.31190500	O 6.58180900	1.73003100	0.12140400
O 3.43694200	-1.97013500	0.27641900	O 7.77609200	0.29221700	1.38853300
H 4.72571100	0.75314500	-0.74249100	H-6.86667000	-2.94683800	-0.12514800
			C 3.47588400	-0.76852200	-0.28471400
			O 3.32702100	-1.81165300	0.38334800
React-Pro (中性形式)			H 4.71753100	0.73096500	-0.91166100
C-1.64602300	0.54315600	-0.02887100	H 8.33946400	1.08164400	1.52378300
O-1.52282300	0.06263400	1.08806100			
C-5.00436800	1.51960500	0.72442200	TS-Pro-1		
C-2.93014400	1.20585200	-0.53024200	C-0.93009200	-1.55311000	-0.64446200
C-3.03047200	2.66739400	-0.02198900	O-0.52822400	-1.22381600	0.47818900
C-4.53751500	2.87296500	0.18584000	C-3.36163300	-3.94564100	-1.33015400
H-6.05949300	1.32432900	0.52731400	C-1.10869400	-3.04638300	-1.02479200
H-4.82786500	1.43795100	1.80326100	C-1.34716100	-3.35460000	-2.52114700
H-2.94369800	1.17107800	-1.62529200			

C-2.54741100	-4.31669700	-2.56982900	C-1.13887100	3.37004200	-0.53962100
H-4.00476700	-4.75357400	-0.98306200	C-1.25959600	2.14612000	-1.20192100
H-3.98308800	-3.06096900	-1.50945000	C-1.98224400	1.09362700	-0.61940200
H-0.22545600	-3.55559900	-0.63741300	H-3.13877200	0.48524600	1.10185500
H-1.57004400	-2.43684700	-3.07208400	H-2.90347000	2.64577000	2.27235700
H-0.44937500	-3.78529600	-2.96828700	H-0.57583100	4.17558200	-1.00577300
H-3.13246000	-4.21372700	-3.48854800	H-0.79131500	2.00798000	-2.17213000
H-2.21344600	-5.35759200	-2.49094700	S-2.18990100	-0.44156400	-1.51087600
N-2.30872500	-3.62253200	-0.34067300	C-1.62600700	4.91959300	1.40611800
C-2.24760500	-4.04866100	0.93355700	H-1.73469700	4.78875400	2.48871400
O-1.23056300	-3.93987500	1.64888900	H-0.64833600	5.36805800	1.20879400
C-3.51209000	-4.66379600	1.55335800	C-2.73041800	5.89431000	0.93574600
H-3.92359400	-5.45386600	0.92377900	O-2.37931600	6.90263100	0.24772200
N-3.07832500	-5.34771300	2.81943800	O-3.92669800	5.62161900	1.26547600
H-2.41393700	-6.10632100	2.62871500			
C-4.57758100	-3.62030100	1.88734400	Int-Pro-1		
H-4.95513600	-3.16211100	0.96978200	C 1.06347900	-0.74240600	-0.13159500
H-5.41912400	-4.09491200	2.40323500	O 0.81994500	-0.14079900	0.89875500
H-4.16338100	-2.83273100	2.52631500	C 4.46679800	-1.21049900	0.88976100
H-2.61092900	-4.68430600	3.44862500	C 2.44714900	-1.28342800	-0.49496000
S 1.16471100	-1.30482700	-2.11490900	C 2.69898300	-2.66790000	0.15551600
C 2.23948300	-0.65955100	-0.77869400	C 4.20542400	-2.65359800	0.45485000
C 2.85501600	0.72126100	-1.08802300	H 5.49720400	-0.89322500	0.72159600
H 3.04643800	-1.37376800	-0.57332800	H 4.21610500	-1.05793100	1.94537000
H 1.62629300	-0.58999000	0.13051800	H 2.53576000	-1.34193200	-1.58521900
H 3.43708400	0.66930500	-2.01430200	H 2.12884100	-2.75159400	1.08715200
H 2.05245300	1.45318600	-1.23084200	H 2.39458300	-3.47681700	-0.51196200
N 5.05653400	1.12364700	-0.12350600	H 4.48300400	-3.37088500	1.23186200
C 6.05947900	1.51539700	0.86539700	H 4.77790500	-2.88182700	-0.45126500
H 5.73827400	2.45570000	1.32516300	N 3.53222100	-0.44016300	0.03430900
C 6.23017400	0.45570300	1.96831700	C 3.62092700	0.84357900	-0.34674600
H 5.27161700	0.25857200	2.45845200	O 2.79748000	1.36521200	-1.12700400
H 6.60788600	-0.48446000	1.54947300	C 4.76244300	1.69308300	0.22177900
H 6.93744100	0.80943100	2.72515200	H 5.71227700	1.15821900	0.17337400
C 7.40865900	1.77277600	0.15685500	N 4.91301700	2.87723400	-0.69104100
O 7.54591600	1.37104500	-1.03784100	H 5.18068300	2.59279300	-1.64062500
O 8.29888400	2.35676600	0.84512700	C 4.48476700	2.18669000	1.64183600
H-3.89049600	-5.74581500	3.30460100	H 4.42819100	1.33942600	2.32975400
C 3.72627000	1.20131000	0.05894500	H 5.29816100	2.84035900	1.97408200
O 3.22112200	1.61985400	1.12979400	H 3.53985400	2.73891400	1.68492300
H 5.42266700	0.83287100	-1.02486400	H 4.02788000	3.39366400	-0.76576000
C-2.57426100	1.28874000	0.63761800	H 5.63317300	3.51437500	-0.33231200
C-2.44291200	2.51360500	1.29619600	C-2.39705600	-1.37786700	0.29889900
C-1.72945200	3.57475100	0.71761200	C-3.58729300	-0.90913800	0.85863000

C-4.08997300	0.36057300	0.53382200	C-3.96010900	2.45685600	0.41214500
C-3.36087000	1.15778900	-0.36325200	C-3.33475500	3.69472200	0.18934300
C-2.16772800	0.70310500	-0.92763300	C-2.13447100	3.71141500	-0.53728100
C-1.68363100	-0.56858600	-0.59440800	C-1.57779900	2.53133000	-1.03707100
H-2.02601800	-2.36477900	0.56008600	C-2.21594100	1.30250100	-0.81720500
H-4.13037700	-1.53963900	1.55799800	H-3.91856500	0.32809800	0.09030300
H-3.72951700	2.14728000	-0.62314300	H-4.88733400	2.41865700	0.97926400
H-1.61838600	1.33528100	-1.61937200	H-1.62650800	4.65629100	-0.71407600
S-0.17901200	-1.17393900	-1.35718100	H-0.64837400	2.56825100	-1.59787300
C-5.39685800	0.85932200	1.10675600	S-1.55141700	-0.19549500	-1.53577300
H-5.58176000	0.38095300	2.07648900	C-3.96718000	4.97739900	0.68754600
H-5.35045200	1.93999600	1.26572100	H-4.49298200	4.79397200	1.62877100
C-6.61484000	0.53882000	0.20661000	H-3.19047200	5.72967000	0.86128100
O-7.35363800	1.50816400	-0.14968800	C-4.96789500	5.54642400	-0.34552900
O-6.81127600	-0.67712000	-0.10030300	O-4.48345500	6.11781300	-1.37091800
			O-6.20780100	5.39491700	-0.11451300
TS-Pro-2			C 3.06443200	1.12035900	1.91369100
C-0.67970200	-0.96301900	-0.07923200	O 2.20076800	1.87500400	2.40452100
O-0.85131300	-0.46590400	1.04920400	N 4.23322100	1.54533600	1.42036000
C-2.36512900	-3.76316400	-0.97203400	H 4.89174200	0.88129300	1.02182400
C-0.42819600	-2.48782600	-0.22940400	C 2.84907800	-0.39842900	1.88326100
C-0.15322400	-3.01613700	-1.65820300	N 1.54492800	-0.68551300	2.56191600
C-1.22540100	-4.09185300	-1.93970600	C 4.62264300	2.95216300	1.32683200
H-2.96664300	-4.63355600	-0.71240600	C 5.63597000	3.10789000	0.17028700
H-3.02893000	-2.98965800	-1.37318200	O 6.37383200	2.11056600	-0.09512400
H 0.37495800	-2.73383700	0.46587000	H 1.47984300	-1.68440800	2.78642700
H-0.20669400	-2.20775500	-2.38986300	C 2.86731600	-1.03018800	0.48268500
H 0.85805800	-3.42405600	-1.71868200	H 3.88967400	-0.94875400	0.09826300
H-1.56304600	-4.08402400	-2.98004300	H 2.67345600	-2.10397900	0.60324600
H-0.83533300	-5.09080600	-1.71627000	H 3.62191300	-0.87026700	2.49980700
N-1.64449600	-3.23371800	0.20516400	C 5.22366200	3.44092700	2.67846400
C-1.86556000	-3.53043000	1.49751600	H 4.52105600	3.13665300	3.46249900
O-1.09841600	-3.19790700	2.42480900	H 6.16350700	2.90486300	2.85361900
C-3.15765300	-4.28180000	1.85136200	H 3.73122000	3.54024800	1.09779100
H-3.32444600	-5.13289200	1.19113600	H 1.45740100	-0.15052600	3.43276600
N-2.95462100	-4.86827400	3.22019600	S 1.70217900	-0.29067500	-0.73713700
H-2.19856400	-5.56262700	3.22178200	C 5.45363400	4.93409900	2.76482300
C-4.37823400	-3.36181200	1.86948000	C 6.74526700	5.47463800	2.67499500
H-4.56098800	-2.96624100	0.86691400	C 4.37262500	5.81351300	2.94540100
H-5.26590600	-3.92137700	2.18309600	C 6.95493700	6.85585400	2.75777700
H-4.22337100	-2.52124700	2.55446500	H 7.59409800	4.80768800	2.53995200
H-2.69666000	-4.13559400	3.89266700	C 4.57639400	7.19386100	3.02633200
H-3.81271500	-5.32769300	3.54640300	H 3.36421300	5.41268400	3.02644100
C-3.41333300	1.27334000	-0.08663200	C 5.87003200	7.72084100	2.93219400

H 7.96458900	7.25322700	2.68673100	C 5.16828600	-2.39815900	1.01678300
H 3.72684600	7.85774300	3.16737200	C 6.65005600	-2.01994700	1.15790800
H 6.02993500	8.79418000	2.99748400	H 7.56602800	-0.05667400	0.77918400
O 5.67185000	4.23136000	-0.41042100	H 6.40800400	-0.07848600	2.13007200
H 0.71929100	-0.45798000	1.96570300	H 4.71658700	-1.70330500	-1.01441500
			H 4.65694100	-2.29363000	1.97995600
Int-Pro-2			H 5.00956300	-3.41251400	0.64467800
C-1.61981400	0.11689300	-0.07846200	H 7.09527400	-2.41082300	2.07669200
O-1.68011400	0.93238800	0.86054500	H 7.22292000	-2.39859400	0.30406400
N-2.65737400	-0.56202300	-0.57281800	N 5.51644400	-0.18721800	0.20719900
H-2.51723600	-1.20736100	-1.34707200	C 5.30724800	0.93495700	-0.49732800
C-0.25902900	-0.19231700	-0.73235500	O 4.36085400	1.05087200	-1.30409000
N 0.56768000	1.05395300	-0.61999300	C 6.25099600	2.11897000	-0.26687000
C-4.01877700	-0.49450100	-0.03923600	H 7.28921000	1.79084000	-0.20889100
C-4.71298600	-1.85164700	-0.29781600	N 6.16035700	2.98697800	-1.49041000
O-4.39861000	-2.46648100	-1.36179700	H 6.50697300	2.49967400	-2.32502600
H 0.68424400	1.32360900	0.36489200	C 5.86929200	2.93813000	0.96587300
C 0.40871700	-1.37344800	-0.01377300	H 5.95337700	2.32109200	1.86438200
H 0.55589700	-1.15563900	1.04773100	H 6.54770100	3.79106600	1.07153900
H-0.24722400	-2.24248400	-0.10175100	H 4.83996200	3.30417100	0.88694000
H-0.37758100	-0.39653000	-1.79824100	H 5.18379400	3.25058700	-1.67079100
C-4.79491400	0.67992000	-0.70425800	H 6.71376700	3.84249700	-1.36484300
H-4.17946200	1.57763900	-0.57589400			
H-4.86611200	0.47897200	-1.77908200	Int-Pro-3		
H-3.95474700	-0.32149800	1.03656700	C-1.69819200	-0.29342200	0.08184200
H 1.49927300	0.93520200	-1.03667600	O-1.78794100	0.30975500	1.17430300
C-6.17351300	0.92414600	-0.13058500	N-2.75982600	-0.78180500	-0.57835500
C-7.32432300	0.49242000	-0.80770100	H-2.62317400	-1.26000000	-1.46410000
C-6.32979500	1.59378500	1.09447200	C-0.32864300	-0.50321700	-0.59094200
C-8.59853200	0.71879900	-0.27565300	N 0.37069000	0.76318300	-0.81655600
H-7.22072500	-0.02399200	-1.75963800	C-4.14599400	-0.65867000	-0.12971900
C-7.60041200	1.82062900	1.63093800	C-4.96535800	-1.83436600	-0.70597300
H-5.44843800	1.94265300	1.62902100	O-4.63105600	-2.26757600	-1.85045100
C-8.74076800	1.38243500	0.94711100	H 0.47530300	1.25052800	0.07427300
H-9.47771400	0.37834100	-0.81731900	C 0.49028000	-1.44875500	0.30037100
H-7.70106400	2.34304600	2.57922000	H 0.70877600	-0.98589700	1.26674900
H-9.72976200	1.56066900	1.36175500	H-0.06752300	-2.37227800	0.47876000
O-5.56044100	-2.23457300	0.55912700	H-0.48616700	-0.97587600	-1.56487800
H 0.11282600	1.83813000	-1.10429500	C-4.73535200	0.71105300	-0.58109200
S 2.01459100	-1.89762000	-0.72731800	H-4.02061300	1.47976700	-0.26639300
C 3.17010700	-0.99354600	0.30834200	H-4.77294300	0.72378700	-1.67637100
O 2.82189200	-0.22308700	1.18498800	H-4.15996200	-0.71337500	0.96051900
C 6.63176100	-0.49036900	1.13993400	C-6.09957400	1.03209100	-0.01153300
C 4.62737900	-1.34540400	0.01705600	C-7.26187000	0.88216800	-0.78342700

C-6.22926400	1.50087300	1.30656400	C 0.49877500	2.08711100	-0.07638300
C-8.52054700	1.18985200	-0.25492500	N 0.65383500	3.53233400	0.11734000
H-7.18039600	0.52555000	-1.80808800	C 3.51942900	-0.29570200	0.02703400
C-7.48439800	1.80767600	1.83984700	C 3.42971300	-1.66859700	0.72995500
H-5.33802100	1.63228100	1.91701200	O 2.80460000	-1.71479000	1.83299400
C-8.63645500	1.65296900	1.05955100	H 1.05662100	3.93677000	-0.72971700
H-9.40805600	1.07004200	-0.87161800	C-0.55559800	1.79002400	-1.15130000
H-7.56249200	2.17315700	2.86098000	H-0.31830300	2.32977300	-2.07291300
H-9.61295500	1.89555700	1.47112600	H-0.59067000	0.72164400	-1.38082400
O-5.92944500	-2.26039900	-0.00506500	H 0.18072300	1.65033100	0.87399800
H-0.20665900	1.36088000	-1.40861000	C 4.74460100	0.51658000	0.54279800
S 2.08686900	-1.96611500	-0.43708200	H 4.66432500	1.51973600	0.10914900
C 3.25489700	-0.92149300	0.41314600	H 4.65566000	0.61974600	1.63016000
O 2.94366300	-0.07404700	1.23482100	H 3.62112200	-0.45137600	-1.04894400
C 6.73555900	-0.33509100	1.09274800	C 6.08805300	-0.08204000	0.18904100
C 4.70839900	-1.26764000	0.07602000	C 6.84468600	-0.77331800	1.14756900
C 5.30094300	-2.26524400	1.10379100	C 6.61000500	0.04454200	-1.10940200
C 6.78029200	-1.86130700	1.18018400	C 8.08700400	-1.32794500	0.82038600
H 7.65389900	0.09675600	0.69140300	H 6.45776700	-0.87645600	2.15921400
H 6.52727500	0.11690700	2.06884400	C 7.84934100	-0.50995200	-1.44186600
H 4.75818300	-1.67578500	-0.93911900	H 6.04167500	0.58473000	-1.86395100
H 4.81966700	-2.12538100	2.07823200	C 8.59322100	-1.19958700	-0.47690100
H 5.14651600	-3.29822700	0.78493100	H 8.65793900	-1.85763400	1.57921700
H 7.26122900	-2.20303000	2.10074900	H 8.23665900	-0.39898900	-2.45187100
H 7.33192800	-2.26934300	0.32569200	H 9.55892700	-1.62794000	-0.73333000
N 5.59665500	-0.09588500	0.17226500	O 4.01450700	-2.64101400	0.16910700
C 5.37021400	0.97662300	-0.60041700	H 1.33122700	3.69709400	0.86264800
O 4.42281000	1.02890900	-1.41195000	S-2.25591700	2.30515000	-0.70009600
C 6.29218600	2.18918200	-0.44026300	C-2.89967000	0.80576900	0.01948900
H 7.33731700	1.88711600	-0.36752600	O-2.27217600	-0.23896400	0.09976100
N 6.17812600	2.98594300	-1.70956400	C-5.66217400	-0.62932100	1.84241900
H 6.53844200	2.46339500	-2.51641400	C-4.30337100	0.99039800	0.59921100
C 5.89615100	3.06972000	0.74485900	C-4.24775400	1.29794400	2.11641800
H 5.98906900	2.50608800	1.67691700	C-5.53550600	0.65960200	2.65589100
H 6.55909500	3.93965400	0.80126200	H-6.69384300	-0.97172400	1.74579400
H 4.86061900	3.41241300	0.64446100	H-5.06135500	-1.43723500	2.27378300
H 5.19348100	3.20808900	-1.90295800	H-4.81645700	1.79289800	0.05794000
H 6.70485200	3.86388700	-1.63408500	H-3.37060500	0.81517700	2.56131600
			H-4.18376600	2.37287600	2.29819600
Int-Pro-4			H-5.48617600	0.45956500	3.72968500
C 1.81424700	1.42381600	-0.51858100	H-6.39487700	1.31132000	2.46188300
O 2.39740600	1.80066100	-1.55956000	N-5.11161700	-0.23949200	0.51914000
N 2.27976000	0.44243600	0.26953600	C-5.37771100	-0.78527700	-0.67718400
H 1.77208800	0.19130900	1.11266900	O-4.93192500	-0.31149300	-1.74296700

C-6.22905100	-2.05825200	-0.71952500	C 2.60064000	-0.62619400	-1.04540100
H-7.07985900	-1.99039200	-0.04070100	O 3.31131800	-1.34078100	-1.79580400
N-6.81045900	-2.14279500	-2.10266200	C 5.43129400	1.37722000	-1.04996500
H-7.43323700	-1.35098200	-2.30106400	C 3.07766200	0.81977900	-0.71046200
C-5.40943800	-3.31796800	-0.44080200	C 3.24683600	1.67983000	-1.99113800
H-5.01541400	-3.28763600	0.57861000	C 4.59891200	2.39087100	-1.83238400
H-6.04489600	-4.20457200	-0.53771700	H 6.26547100	1.83046400	-0.51584700
H-4.57012600	-3.39887400	-1.14007100	H 5.81902500	0.58484000	-1.70067800
H-6.06467100	-2.13073600	-2.80926000	H 2.38709500	1.27724200	0.00120400
H-7.34854500	-3.01038200	-2.21012400	H 3.27618300	1.03328100	-2.87384900
			H 2.41221200	2.37647800	-2.10608400
TS-Pro-3			H 5.05673700	2.64438600	-2.79297700
C-1.19364600	-0.43610900	-0.93019800	H 4.49095400	3.30991300	-1.24515600
O-1.10745000	0.79727700	-0.75778200	N 4.43817300	0.80912500	-0.11205500
N-2.25224400	-1.16365900	-0.55667400	C 4.62891000	0.53103100	1.18839700
H-2.27340900	-2.16269800	-0.74377800	O 3.70084100	0.22082400	1.96163800
C-0.05841100	-1.20973500	-1.63057000	C 6.06529600	0.55636500	1.73116100
N 1.01080600	-0.25220200	-1.97656700	H 6.59568400	1.45891100	1.42584400
C-3.42603900	-0.62169800	0.13061600	N 5.95716800	0.63878500	3.22749900
C-4.07543000	-1.75470700	0.95733500	H 5.48527200	1.50089000	3.52387600
O-4.04887900	-2.92001900	0.45718500	C 6.85557800	-0.69489800	1.35005800
H 0.67438600	0.70034400	-1.79587100	H 6.98098300	-0.74122200	0.26507200
C 0.56564600	-2.32317400	-0.76456400	H 7.84983200	-0.66443000	1.80789200
H-0.18519300	-2.88239300	-0.20237300	H 6.33454700	-1.59970900	1.68167200
H 1.10942600	-3.02749800	-1.40004300	H 5.40963100	-0.14879200	3.59468500
H-0.46452900	-1.64907700	-2.54782700	H 6.88997000	0.61866700	3.65551800
C-4.43167400	-0.02405300	-0.89697700			
H-3.86328300	0.66353000	-1.53336900	Int-Pro-5		
H-4.79699100	-0.83752000	-1.53380400	C 1.34908500	0.32853100	-0.23538600
H-3.09209400	0.16855400	0.80584400	O 1.30116300	-0.56183300	0.63828500
C-5.59693500	0.71263800	-0.27344200	N 2.46628900	0.95881400	-0.61084600
C-6.86260600	0.11496600	-0.17216500	H 2.42316100	1.67508100	-1.33171600
C-5.43374000	2.01879600	0.21764300	C 0.06522700	0.79534000	-0.93084000
C-7.93673300	0.80025500	0.40642700	N-0.89395400	-0.34935600	-0.95060200
H-7.00785500	-0.89448600	-0.55117600	C 3.78524100	0.74280100	-0.01478500
C-6.50310100	2.70673200	0.79813800	C 4.61718000	2.03499300	-0.18326000
H-4.46153500	2.50126700	0.13904100	O 4.36951400	2.75423500	-1.19820900
C-7.76021500	2.09849400	0.89567000	H-0.65878300	-0.98388300	-0.17475400
H-8.90962400	0.31940500	0.47373200	C-0.60393600	1.98878100	-0.18324300
H-6.35665200	3.71809500	1.16974000	H 0.07215500	2.42533300	0.55526700
H-8.59370500	2.63323700	1.34414000	H-0.87103100	2.76430000	-0.90345400
O-4.60986300	-1.43090500	2.05748600	H 0.27357700	1.07521000	-1.96380100
H 1.29573200	-0.33047600	-2.95308500	C 4.48349000	-0.47425900	-0.69126200
S 1.71075100	-1.50102200	0.39701900	H 3.76601700	-1.30211900	-0.66488200

H 4.66126600	-0.22606400	-1.74389700	C-1.16083400	0.61863900	-0.66381100
H 3.65349500	0.53679900	1.04958600	O-1.20233200	-0.37898700	-1.41630700
C 5.77572300	-0.90856400	-0.03507300	N-2.21560200	1.18075400	-0.08577300
C 7.01885600	-0.57956100	-0.59668800	H-2.09609100	1.98847300	0.52235000
C 5.75667800	-1.66075200	1.15145600	C 0.21858900	1.25220500	-0.34769100
C 8.21238200	-0.98557900	0.01050600	N 1.21333400	0.35074900	-1.03076900
H 7.05175100	-0.00100200	-1.51746500	C-3.59897800	0.72441100	-0.24905000
C 6.94615300	-2.06669700	1.76330000	C-4.53655800	1.93494500	-0.02852700
H 4.80188000	-1.93421700	1.59611800	O-4.13862700	2.83330500	0.77340100
C 8.18000300	-1.72915300	1.19449100	H 1.73122800	0.82880200	-1.78227100
H 9.16502600	-0.72176500	-0.44246100	C 0.34071600	2.70311700	-0.83035000
H 6.91022400	-2.65087700	2.67971100	H 0.33741500	2.74802100	-1.92340200
H 9.10573500	-2.04724200	1.66741800	H-0.53041200	3.26053700	-0.47995900
O 5.50238200	2.26286700	0.69117400	H 0.39744700	1.18053600	0.72724500
H-0.80710400	-0.86873000	-1.82994100	C-3.89873200	-0.42427300	0.75775100
S-2.08940400	1.36008800	0.68077800	H-3.11525700	-1.17815600	0.61953400
C-2.43682900	0.19511800	-0.83659800	H-3.79550200	-0.02499800	1.77301100
O-2.76478400	0.79302900	-1.92186500	H-3.71963200	0.35584600	-1.26945000
C-5.49190900	-1.23315700	-1.37961300	C-5.25724300	-1.06880600	0.59029000
C-3.27104500	-1.05614200	-0.40862200	C-6.30602500	-0.78030300	1.47645300
C-3.27086000	-2.14423400	-1.51931900	C-5.49634200	-1.97478500	-0.45644100
C-4.74783600	-2.52152100	-1.72967700	C-7.56281800	-1.37537100	1.32134300
H-6.53224000	-1.40048200	-1.10494000	H-6.13649600	-0.08439300	2.29535900
H-5.45949900	-0.51379000	-2.20504700	C-6.75121900	-2.56899800	-0.61775000
H-2.89738800	-1.44333500	0.54204800	H-4.69225400	-2.21804700	-1.14817800
H-2.86522400	-1.73285600	-2.44904900	C-7.79089600	-2.26979400	0.27084700
H-2.65491100	-2.99906700	-1.22771700	H-8.36155400	-1.13911300	2.02022500
H-4.95645300	-2.85099600	-2.75180300	H-6.91638100	-3.26814000	-1.43398800
H-5.04952100	-3.31845700	-1.04056300	H-8.76664200	-2.73291100	0.14741600
N-4.70459500	-0.71133700	-0.24036700	O-5.64085500	1.92336300	-0.64379900
C-5.19090900	-0.31753900	0.95150900	H 0.60279100	-0.36329700	-1.51746800
O-4.47340700	-0.13030200	1.95356700	S 1.77566200	3.64246700	-0.16268900
C-6.69939100	-0.04377200	1.06167800	C 2.19332300	-0.40377900	-0.15460600
H-7.28171600	-0.90992700	0.74173800	O 2.02817700	-0.41330300	1.03055500
N-7.00138300	0.12373200	2.52470700	C 4.91358400	-2.72758800	-0.12134600
H-6.75870400	-0.71696900	3.06090300	C 3.23160800	-1.15898600	-0.95693400
C-7.14042200	1.21664000	0.31704400	C 2.77615900	-2.61880500	-1.23298800
H-7.00095400	1.08839000	-0.75891500	C 4.10350100	-3.39170700	-1.23668300
H-8.20309600	1.40665400	0.50238700	H 5.99085900	-2.81083400	-0.27335800
H-6.55826800	2.08487400	0.64480300	H 4.65817700	-3.13361900	0.86300000
H-6.46295000	0.90287200	2.92152800	H 3.42476300	-0.62761500	-1.89501200
H-8.00069400	0.31627900	2.65888400	H 2.13347100	-2.97071800	-0.41932700
			H 2.22511500	-2.68610500	-2.17293500
			H 3.95881100	-4.45976500	-1.05468100

Int-Pro-6

H 4.61425600	-3.26605800	-2.19756400	H-8.81996700	1.13370200	-0.92153300
N 4.48409300	-1.31014000	-0.20761500	H-6.88726100	2.31910100	2.74096400
C 5.11828000	-0.20944500	0.23066700	H-8.96507600	2.05356700	1.39026900
O 4.66184400	0.93495800	0.03408300	O-5.42319100	-2.24493400	0.04928000
C 6.41800900	-0.38742600	1.01826900	H 0.97919100	0.58606300	0.83715100
H 7.05425500	-1.14748300	0.56299200	C 2.38883000	0.48062000	-0.64396400
N 7.17439400	0.90628600	0.90347900	O 2.74777500	0.02089400	-1.74341400
H 7.39506500	1.12937000	-0.07450500	C 5.46839800	2.36805600	-0.41309400
C 6.17078100	-0.69994400	2.49489600	C 3.23253100	1.50713500	0.11945000
H 5.66712800	-1.66529900	2.59270000	C 3.13102200	2.91600700	-0.50610200
H 7.12616100	-0.75669300	3.02684400	C 4.50316000	3.53879400	-0.21515300
H 5.54636200	0.07249700	2.95643600	H 6.38690900	2.47005000	0.16762000
H 6.62085700	1.68568700	1.27974800	H 5.72829600	2.23874000	-1.46949700
H 8.05674500	0.85156900	1.42585700	H 2.92058900	1.52828900	1.16930100
H 2.75019700	2.97440500	-0.82173000	H 2.97711800	2.83158400	-1.58782600
			H 2.29675900	3.47721800	-0.07877200
Prod-Pro			H 4.73673300	4.37449400	-0.88051700
S 0.78627200	-2.80209500	1.24733400	H 4.55108800	3.89486400	0.82023100
C-1.13847800	-0.37031700	0.00002400	N 4.67665700	1.20499600	0.05856800
O-1.20734900	0.33745900	1.02498400	C 5.13737900	0.01891900	0.47924200
N-2.20810500	-0.88912100	-0.61641600	O 4.38702900	-0.87071100	0.93483600
H-2.08599600	-1.45362000	-1.45334000	C 6.64165200	-0.25568900	0.36751000
C 0.22014100	-0.71250800	-0.63746200	H 7.22704800	0.59257800	0.72569000
N 1.21261600	0.18104600	-0.06476500	N 6.94256400	-1.38866000	1.30785700
C-3.58750000	-0.71337800	-0.16143300	H 6.73274700	-1.13879600	2.28131000
C-4.43297700	-1.90607500	-0.66184700	C 7.07010900	-0.65439100	-1.04520400
O-4.09137600	-2.43760400	-1.76185300	H 6.90516000	0.17477500	-1.73768900
H 1.91889400	-2.12130500	1.52897000	H 8.13791400	-0.89757600	-1.05402300
C 0.59989600	-2.20249000	-0.48298500	H 6.50026100	-1.52269700	-1.39337400
H-0.17531300	-2.82837600	-0.93302400	H 6.37417500	-2.21195900	1.07508600
H 1.52960200	-2.38912100	-1.02386900	H 7.93426800	-1.64767500	1.24938100
H 0.15794000	-0.51940800	-1.71473900			
C-4.15782400	0.63995000	-0.68239500	MPAA		
H-3.41979500	1.40959400	-0.43020600	C-1.36787400	-1.21825900	0.10783500
H-4.22032900	0.58904000	-1.77539900	C-0.01125700	-1.21859300	0.43745700
H-3.59008400	-0.70604300	0.93048000	C 0.68016100	-0.01961700	0.65888300
C-5.50197100	1.02547200	-0.10516000	C-0.02322300	1.18700200	0.54490700
C-6.67940900	0.88262900	-0.85493300	C-1.37954800	1.20123400	0.21411600
C-5.59765100	1.54838900	1.19546100	C-2.06105500	-0.00444000	-0.00768900
C-7.92023500	1.24934400	-0.32201300	H-1.87894400	-2.16365600	-0.05394600
H-6.62332300	0.48486800	-1.86603900	H 0.51196600	-2.16765900	0.52595500
C-6.83498000	1.91384400	1.73328700	H 0.48959200	2.12992600	0.72083300
H-4.69411400	1.67502100	1.78860800	H-1.90067200	2.15212100	0.13642300
C-8.00259500	1.76533800	0.97511800	S-3.79975400	0.07078800	-0.42608500

C 2.16179900	-0.03377200	1.00302100	C -3.11215800	3.10941300	0.30049100
H 2.42424900	0.86313100	1.57444200	H -3.99894600	3.65321600	-0.03906700
H 2.40727600	-0.91470500	1.60096800	H -3.10135100	3.07765200	1.39396000
C 3.01482300	-0.09285200	-0.25086900	H -2.22436500	3.63910200	-0.05352800
O 3.48841700	-1.12037400	-0.71314300	H -3.17078400	1.75468800	-1.38333400
O 3.24036700	1.07021900	-0.90606700	H -6.61925000	-1.48557600	-1.56875400
H-3.99619800	-1.26092500	-0.53141600	C 3.09458900	-0.76900400	-0.25693500
H 2.82556200	1.82619200	-0.44818000	O 2.90030400	-1.84580400	0.34825200
			H -1.10764900	-0.01884800	1.60278500
React-Ala-OH			React-Ala-SH		
C -4.65720400	-0.24740300	-0.24810300	C-4.87734700	-0.06018000	-0.16626000
O -3.92892200	-0.88973200	-1.01901100	O-4.30963100	-0.77539300	-1.00423100
N -4.36137500	1.00101600	0.16008700	N-4.34986200	1.10483000	0.26267800
H -4.96605300	1.47196900	0.82725500	H-4.80342500	1.62617800	1.00873500
C -5.94121600	-0.84994300	0.32289900	C-6.20473700	-0.47250600	0.47004600
N -6.40790500	-1.89316000	-0.65011800	N-6.89044700	-1.38818800	-0.50225300
H -5.68724200	-2.61288400	-0.78899800	H-6.27899100	-2.17548400	-0.75358500
C -3.16154700	1.68959900	-0.29090200	C-3.06554100	1.56649300	-0.22281100
C -1.91133600	0.92739300	0.11763900	C-1.99034800	0.54357100	0.14353100
O -1.91985700	0.45267400	1.31682100	O-1.86113700	-0.14645800	1.09229600
H -7.25721900	-2.35086800	-0.29835600	H-7.75222600	-1.76829000	-0.09239400
S -0.63086000	0.84952700	-0.99402300	S-0.59142100	0.37804700	-1.26580900
C 0.73455900	0.03066300	-0.05374400	C 0.83439500	-0.16506600	-0.22630500
C 1.95234900	-0.06081500	-0.97881100	C 2.09553800	-0.26469800	-1.08565100
H 0.39401300	-0.96369700	0.24766300	H 0.52807300	-1.13957100	0.16124900
H 0.95209700	0.64412800	0.82581800	H 0.93575400	0.54693500	0.59567500
H 1.71254600	-0.65765400	-1.86742000	H 1.93094600	-0.94838300	-1.92709900
H 2.26369000	0.93349800	-1.31105400	H 2.37281600	0.71305200	-1.48951400
N 4.29318000	-0.17573600	-0.33899700	N 4.40554500	-0.19985800	-0.33508600
H 4.37791000	0.73675700	-0.77802200	H 4.46595000	0.67043400	-0.85591000
C 5.51362500	-0.68396900	0.28761300	C 5.62039800	-0.58188400	0.38499600
H 5.25000700	-1.08373000	1.27157100	H 5.32924600	-0.93737200	1.37778000
C 6.16687900	-1.79954600	-0.54597600	C 6.38739100	-1.69810000	-0.34241000
H 5.46027200	-2.62079400	-0.70375400	H 5.74525300	-2.57515200	-0.47365700
H 6.48378200	-1.41977500	-1.52425400	H 6.72281900	-1.36038500	-1.32990800
H 7.04352700	-2.19469000	-0.02349400	H 7.26380000	-1.99704500	0.24137900
C 6.50376200	0.48520800	0.49781100	C 6.51495500	0.66560600	0.56792900
O 6.27924900	1.57627600	-0.10763200	O 6.26592800	1.68832300	-0.13856300
O 7.49318000	0.24633000	1.25189500	O 7.45497000	0.55866300	1.41055900
C -5.72030600	-1.48656800	1.69478900	C-5.99878600	-1.19005700	1.80464200
H -4.93012700	-2.24396200	1.65259100	H-5.35902600	-2.07019300	1.68176500
H -5.43418800	-0.71569700	2.41529000	H-5.52994900	-0.50749700	2.51875500
H -6.64835200	-1.95332500	2.04091100	H-6.96652500	-1.50115200	2.21114300
H -6.72945800	-0.09490500	0.36655000			

H-6.85416500	0.39628100	0.59280000	H 1.03560000	1.07977900	-1.43106000
C-2.70507800	2.92396100	0.39778900	H -0.63354900	0.50859400	-1.50318100
H-3.46773600	3.64891400	0.09901400	H 1.01429000	-1.15072100	-2.27905400
H-2.67340000	2.85359300	1.48888600	C 5.17322800	-2.41012900	-0.72291400
H-1.73636400	3.27773700	0.03534400	H 4.40610400	-3.18057900	-0.58538800
H-3.09489900	1.64531900	-1.31464400	H 5.37183200	-2.33319100	-1.79798500
H-7.13823400	-0.89869200	-1.37025500	H 4.40465200	-1.09960400	0.83788100
C 3.23561900	-0.84665200	-0.25098000	H -0.04784700	-2.93660600	-1.36722300
O 3.06259400	-1.87437600	0.43901800	S 0.11743900	0.95021900	0.75380600
H-0.31419900	1.70553300	-1.36972400	C 6.43236300	-2.81945100	0.00898800
			C 7.69269200	-2.69056500	-0.59365200
TS-Ala-Cys-2.6			C 6.36294600	-3.35055800	1.30795800
C 0.46276700	4.62248500	0.16318800	C 8.85528600	-3.07989900	0.08084800
O 0.95315900	4.77753500	1.29462200	H 7.76274100	-2.28452300	-1.60053200
N -0.71726400	4.02894800	-0.07907300	C 7.52153200	-3.73778300	1.98706600
H -1.04998500	3.97229600	-1.03778700	H 5.39285600	-3.46564100	1.78731800
C 1.20773600	5.11350300	-1.08627100	C 8.77355300	-3.60326900	1.37512900
N 2.28572900	6.04802600	-0.62081400	H 9.82228700	-2.97416000	-0.40494200
H 2.93976700	5.56783300	0.00921300	H 7.44709100	-4.14793300	2.99135400
C -1.61150700	3.54093000	0.96158400	H 9.67499000	-3.90763100	1.90108800
C -2.17853400	2.17201500	0.53508500	O 6.35964900	0.43025900	0.22282100
O -2.39469300	1.90029400	-0.64105100	H -0.15908700	-2.30153100	0.15079000
H 2.81565800	6.40815400	-1.42279800	H -1.15550800	-1.73388700	-1.07372300
C 1.82751800	3.98276900	-1.90548700	S -3.01909300	1.29881800	1.89370100
H 2.50939800	3.38169300	-1.29460300	C -3.73277400	-0.12408100	0.97874200
H 1.03702400	3.33625800	-2.29544000	C -5.13247900	0.15479500	0.41226600
H 2.37846200	4.39702400	-2.75637200	H -3.76250800	-0.94478200	1.70135500
H 0.53246000	5.70956600	-1.70455800	H -3.03174500	-0.39303400	0.18422300
C -2.76378200	4.53944000	1.18897200	H -5.83303600	0.35900600	1.22776900
H -2.33564000	5.51274900	1.44937700	H -5.10187400	1.03348800	-0.24044800
H -3.36792100	4.64863900	0.28200500	N -6.65824800	-1.70922300	0.03475700
H -3.41200000	4.21718900	2.00858900	C -7.29880900	-2.82358400	-0.66391700
H -1.03428000	3.43815500	1.88096200	H -7.34116500	-2.57794900	-1.72988000
H 1.89677500	6.84714300	-0.10711600	C -6.52462500	-4.14134000	-0.48742900
C 2.10369900	-1.40970900	-0.41688600	H -5.49169300	-4.02660000	-0.83112900
O 2.01493700	-2.14635700	0.58403500	H -6.51076900	-4.44820300	0.56494400
N 3.23859500	-0.87671700	-0.87223000	H -6.99560700	-4.93546500	-1.07516800
H 3.23034700	-0.29380100	-1.70643800	C -8.75091000	-2.97909000	-0.15607800
C 0.83463100	-1.04166000	-1.20652600	O -9.08614700	-2.36047900	0.89874500
N -0.20833100	-2.06347800	-0.85029300	O -9.49933100	-3.74435600	-0.83424100
C 4.54678500	-1.06710900	-0.24427300	C -5.60662000	-1.01945700	-0.43325700
C 5.44641100	0.13752000	-0.60170000	O -5.02418200	-1.31357000	-1.50370600
O 5.22228500	0.72407300	-1.70394700	H -7.13674700	-1.39292000	0.87322900
C 0.32163800	0.38636900	-0.98132500	H -0.57015300	-0.11831100	1.20928100

			C 7.76690500	-2.66817300	-0.62981200
TS-Ala-Cys-2.7			C 6.45570300	-3.33480500	1.28234200
C 0.33901100	4.66647000	0.14244400	C 8.93594700	-3.06089400	0.03145900
O 0.81378400	4.83849300	1.27848600	H 7.82705500	-2.25800100	-1.63566700
N-0.81860300	4.03508900	-0.10927200	C 7.62079600	-3.72527100	1.94835900
H-1.14651000	3.97443700	-1.06915600	H 5.49040900	-3.45094600	1.77102900
C 1.08766100	5.17638400	-1.09625900	C 8.86676300	-3.58914500	1.32447400
N 1.98168800	6.29175600	-0.63706700	H 9.89811400	-2.95391500	-0.46357100
H 2.62298300	5.96410600	0.09595000	H 7.55615600	-4.13896400	2.95186600
C-1.70420000	3.53110900	0.93116000	H 9.77318200	-3.89592200	1.84036400
C-2.23641500	2.14589900	0.52204000	O 6.44459000	0.44520400	0.23002600
O-2.40336900	1.83086800	-0.64921700	H-0.07778400	-2.29718800	0.14762600
H 2.54049400	6.64808200	-1.42078300	H-1.07381600	-1.72532500	-1.07513800
C 1.92850800	4.09635900	-1.77331300	S-3.03671500	1.26484400	1.88812900
H 2.62718200	3.63812100	-1.06546800	C-3.68774300	-0.20867000	1.00861700
H 1.27225500	3.32136500	-2.17806600	C-5.07698800	0.00754000	0.39533300
H 2.49392600	4.53260400	-2.60376000	H-3.71593700	-0.99948400	1.76446100
H 0.38537700	5.61938200	-1.80551500	H-2.95854200	-0.49226500	0.24563200
C-2.88187700	4.50326800	1.14802800	H-5.79456800	0.28719900	1.17264400
H-2.47896200	5.48858200	1.40311300	H-5.03839000	0.82138200	-0.33774800
H-3.48519300	4.59102200	0.23811500	N-6.71135100	-1.76540400	0.03322700
H-3.52525400	4.17058600	1.96733700	C-7.34497000	-2.91947700	-0.60395700
H-1.12651400	3.45048200	1.85251400	H-7.18817600	-2.83965000	-1.68415300
H 1.44177400	7.07297400	-0.24658200	C-6.74845900	-4.24927200	-0.11010800
C 2.18304200	-1.39038400	-0.41073500	H-5.66712600	-4.26651700	-0.27969000
O 2.09918600	-2.13892200	0.58177000	H-6.93601500	-4.38637300	0.96130300
N 3.31523500	-0.84621500	-0.86038900	H-7.19580400	-5.08783900	-0.65304200
H 3.30406600	-0.25662400	-1.68980200	C-8.86738900	-2.88211200	-0.34219800
C 0.91260900	-1.02084400	-1.19691200	O-9.30336500	-2.10496800	0.55964300
N-0.12543100	-2.05150400	-0.85156000	O-9.57188900	-3.66551900	-1.04640100
C 4.62601700	-1.04390100	-0.24020400	C-5.53340500	-1.24350000	-0.34231300
C 5.52708800	0.16092500	-0.59281300	O-4.83298100	-1.74118000	-1.25490800
O 5.30012500	0.75573000	-1.69000000	H-7.26818400	-1.29806700	0.74269500
C 0.39145900	0.40221700	-0.95852100	H-0.54554200	-0.11342300	1.21032500
H 1.10730300	1.10345900	-1.39333100			
H-0.55815500	0.52527800	-1.49004700	TS-Ala-Cys-2.8		
H 1.09370500	-1.11909700	-2.27030800	C 0.21779100	4.76236200	0.12213800
C 5.24694200	-2.38438200	-0.73280100	O 0.75404700	4.95067200	1.22816700
H 4.48060000	-3.15521400	-0.59320100	N-0.94893900	4.12513100	-0.05661200
H 5.43573300	-2.30054600	-1.80913600	H-1.31502700	4.02086800	-0.99861600
H 4.48942100	-1.08448800	0.84239200	C 0.89971300	5.25083700	-1.16254600
H 0.04126500	-2.91965400	-1.37483200	N 1.78935800	6.39733600	-0.77712100
S 0.16937600	0.94781300	0.78043000	H 2.46164300	6.10548200	-0.05673200
C 6.51257300	-2.79864100	-0.01515800	C-1.73230800	3.55970000	1.03430200

C-2.29971400	2.20429000	0.58031900	O 6.42663300	0.45808700	0.21222900
O-2.45955900	1.92375200	-0.59899800	H-0.08721300	-2.27842600	0.14901000
H 2.31340300	6.73566000	-1.59230400	H-1.08528500	-1.71866200	-1.07746500
C 1.73340400	4.16151100	-1.83430200	S-3.05162100	1.25162900	1.91507000
H 2.47356900	3.74856300	-1.14078300	C-3.70480500	-0.18499200	0.97675700
H 1.07736700	3.35545600	-2.17334600	C-5.11234000	0.04699700	0.40912500
H 2.25040700	4.57162800	-2.70826900	H-3.70587100	-1.01250400	1.69235300
H 0.15982400	5.65550600	-1.85625500	H-2.98937500	-0.41819100	0.18371000
C-2.87262200	4.51210700	1.44992500	H-5.82156800	0.22162500	1.22368800
H-2.43841000	5.48468400	1.70246400	H-5.11253600	0.92915600	-0.23968300
H-3.59064300	4.64487000	0.63374400	N-6.58032100	-1.85785500	0.01647400
H-3.40076200	4.13233200	2.32898700	C-7.18532300	-2.98862300	-0.68766000
H-1.06499400	3.41341000	1.88492200	H-7.22228700	-2.74520800	-1.75424200
H 1.24967000	7.18242700	-0.39415300	C-6.38030500	-4.28632600	-0.50079700
C 2.17660400	-1.39888400	-0.43439600	H-5.34705000	-4.14615600	-0.83383900
O 2.09413200	-2.14649500	0.55896300	H-6.36995600	-4.59123400	0.55218600
N 3.30883200	-0.85564300	-0.88517100	H-6.82516900	-5.09294600	-1.09185700
H 3.29793300	-0.26385200	-1.71303500	C-8.63861500	-3.17961800	-0.19511900
C 0.90484400	-1.02965700	-1.21871000	O-8.99957100	-2.57105100	0.85706900
N-0.13826300	-2.04829900	-0.85371900	O-9.36150700	-3.96102900	-0.88243700
C 4.61678900	-1.04271300	-0.25569600	C-5.54341000	-1.14002400	-0.44157100
C 5.51349000	0.16439000	-0.61210400	O-4.94194600	-1.41720600	-1.50583200
O 5.28755800	0.75184800	-1.71349100	H-7.07306800	-1.55555800	0.85182400
C 0.39350800	0.39878100	-0.98894800	H-0.55556800	-0.07651100	1.18334600
H 1.10899900	1.09252100	-1.43639100			
H-0.55958400	0.52273800	-1.51372600	TS-Ala-Cys-2.9		
H 1.07895200	-1.14204400	-2.29187000	C 0.23013500	4.79369400	0.14008100
C 5.24954100	-2.38398000	-0.73130900	O 0.76921600	4.97340100	1.24621700
H 4.48228500	-3.15583100	-0.60292900	N-0.94623300	4.17508600	-0.03909900
H 5.45903800	-2.30511500	-1.80414700	H-1.30718800	4.06638700	-0.98255100
H 4.47321200	-1.07502500	0.82635300	C 0.91931500	5.27025600	-1.14458200
H 0.01981600	-2.92552600	-1.36421400	N 1.82003400	6.40941000	-0.76300400
S 0.20023100	0.95477700	0.75054200	H 2.48630800	6.11465400	-0.03818100
C 6.50140700	-2.79327900	0.01316300	C-1.71816300	3.58740500	1.04702300
C 7.76777900	-2.66744800	-0.57729100	C-2.27478300	2.23329000	0.57859700
C 6.41864000	-3.32182700	1.31244800	O-2.42272200	1.95592300	-0.60190900
C 8.92314700	-3.05688800	0.10952600	H 2.35112900	6.73702000	-1.57799000
H 7.84855600	-2.26371900	-1.58428000	C 1.74295100	4.16763300	-1.80778000
C 7.56990400	-3.70916800	2.00377800	H 2.47946800	3.75335300	-1.11109600
H 5.44373000	-3.43478900	1.78245100	H 1.08005700	3.36428400	-2.14047200
C 8.82809500	-3.57741300	1.40403100	H 2.26316700	4.56594000	-2.68522200
H 9.89502700	-2.95325600	-0.36690100	H 0.18516700	5.67859000	-1.84221400
H 7.48495200	-4.11730700	3.00806200	C-2.86298000	4.52409400	1.48471300
H 9.72397900	-3.88167500	1.93945500	H-2.43405400	5.49478000	1.75282200

H-3.58431900	4.66691900	0.67314400	N-6.54889900	-1.82112300	0.01410700
H-3.38590600	4.12504600	2.35839700	C-7.17607500	-2.93813500	-0.69246300
H-1.04332200	3.43359100	1.89102200	H-7.21411700	-2.68904200	-1.75777400
H 1.28734500	7.20262500	-0.38696100	C-6.39246800	-4.25014300	-0.51549200
C 2.10132300	-1.52634000	-0.35514900	H-5.35876200	-4.12633500	-0.85365800
O 2.08502600	-2.10506400	0.74771700	H-6.38159100	-4.55960300	0.53615500
N 3.20423400	-1.11024600	-0.98175800	H-6.85424300	-5.04638100	-1.10763800
H 3.13049900	-0.64212900	-1.88263200	C-8.63001500	-3.10658300	-0.19353200
C 0.77914800	-1.21670300	-1.07762100	O-8.97621700	-2.49355400	0.86104200
N-0.26372600	-2.12839300	-0.49725500	O-9.36831700	-3.87565400	-0.87827800
C 4.55078500	-1.16338300	-0.40763100	C-5.50150000	-1.11937300	-0.44506400
C 5.41227100	-0.08028800	-1.09746600	O-4.90691700	-1.40457100	-1.51098800
O 5.11762200	0.21555300	-2.29537100	H-7.03627200	-1.51164200	0.85005200
C 0.33739100	0.25161300	-0.99317800	H-0.36294000	0.11877400	1.32252800
H 1.01761700	0.84600400	-1.60832100			
H-0.66452700	0.34817700	-1.42319800	TS-Ala-Cys-3.0		
H 0.85404800	-1.47529000	-2.13683100	C-0.11238500	5.01945800	0.14933200
C 5.17317700	-2.57996800	-0.58809400	O 0.50909500	5.23188300	1.20561200
H 4.42608000	-3.30141700	-0.23937000	N-1.20308200	4.24601400	0.05434800
H 5.32864300	-2.75690800	-1.65842100	H-1.63431300	4.11206300	-0.85594300
H 4.47706800	-0.93782200	0.65895000	C 0.35741200	5.64818300	-1.16774100
H-0.12739000	-3.09070900	-0.82983200	N 1.10541500	6.90129600	-0.81268000
S 0.36831400	1.04307500	0.66484800	H 1.87712000	6.69092200	-0.16708500
C 6.46651600	-2.79279700	0.16778200	C-1.77476600	3.52110100	1.18176300
C 7.70313500	-2.78563400	-0.49488400	C-2.32004200	2.18111000	0.66636600
C 6.45335700	-3.00749300	1.55619600	O-2.48335300	1.94710400	-0.52080900
C 8.89679100	-2.98065900	0.20882500	H 1.49816600	7.33786700	-1.65499500
H 7.73107500	-2.62645300	-1.57070600	C 1.26749600	4.71891700	-1.96840500
C 7.64311500	-3.19989100	2.26418100	H 2.13867300	4.41607800	-1.37762100
H 5.50266900	-3.02641100	2.08525700	H 0.71104200	3.82449500	-2.26215100
C 8.87108300	-3.18627200	1.59189100	H 1.60812700	5.22514300	-2.87786600
H 9.84419300	-2.97309400	-0.32466600	H-0.49942500	5.96244800	-1.76724900
H 7.61175900	-3.36621900	3.33827500	C-2.88089000	4.34143200	1.87659000
H 9.79727200	-3.33897500	2.14019200	H-2.46989700	5.31610700	2.15705700
O 6.36388900	0.40917900	-0.42396100	H-3.73419700	4.49323800	1.20720800
H-0.20022500	-2.16207300	0.52889900	H-3.22739600	3.84210400	2.78574000
H-1.21083500	-1.83173700	-0.76481400	H-0.97412600	3.32868900	1.89968600
S-2.97294400	1.23871200	1.90632100	H 0.49600600	7.58725200	-0.35201400
C-3.63971900	-0.18552700	0.95852200	C 2.18506000	-1.52768700	-0.40425800
C-5.05053000	0.06026200	0.40576300	O 2.17124100	-2.10612400	0.69876200
H-3.63991800	-1.01723100	1.66938000	N 3.28578000	-1.09856800	-1.02600800
H-2.93051600	-0.41805300	0.16003900	H 3.21141000	-0.63161500	-1.92740100
H-5.74952100	0.23893400	1.22832900	C 0.86240800	-1.23544600	-1.13253600
H-5.04989700	0.94464800	-0.24011900	N-0.17433200	-2.14974700	-0.54587500

C 4.62900300	-1.13446200	-0.44268900	C-5.38145300	-1.29028800	-0.43939200
C 5.48444100	-0.04669900	-1.13246600	O-4.77592000	-1.54703300	-1.50633700
O 5.19402700	0.24156800	-2.33328700	H-6.90981800	-1.73689400	0.84526900
C 0.40878200	0.22997200	-1.05993400	H-0.29907700	0.13620300	1.25636600
H 1.07877100	0.82334200	-1.68734800			
H-0.59684100	0.31398800	-1.48378800	React-Ala-m06		
H 0.94166500	-1.50340000	-2.18916600	C 5.32952500	-0.18255600	-0.06491300
C 5.26792900	-2.54551900	-0.60886100	O 5.68893100	-0.93581900	-0.97636100
H 4.52223000	-3.27324300	-0.27058100	N 4.08905400	-0.14483800	0.43780500
H 5.44393100	-2.72422300	-1.67571900	H 3.87357000	0.48909300	1.20590900
H 4.54530500	-0.90312200	0.62191000	C 6.29768900	0.83058700	0.52304400
H-0.01904300	-3.11711700	-0.85463500	N 7.67055400	0.25914200	0.39385400
S 0.45277200	1.03839400	0.59067700	H 7.88048900	0.05311000	-0.59225500
C 6.54971100	-2.74272600	0.17041900	C 3.01180100	-0.96461400	-0.08910100
C 7.79870000	-2.71093900	-0.46775700	C 1.70037500	-0.26769600	0.22395100
C 6.51290900	-2.96584300	1.55707800	O 1.56600500	0.45300700	1.19778700
C 8.98142600	-2.88951400	0.25848000	H 8.37150400	0.92502000	0.73942800
H 7.84498300	-2.54497900	-1.54191500	S 0.39744700	-0.65073700	-0.90349800
C 7.69158200	-3.14243300	2.28741400	C -0.98760000	0.20782700	-0.07695800
H 5.55239600	-3.00437700	2.06696300	C -2.24703100	0.00213100	-0.90041400
C 8.93211100	-3.10349500	1.63967300	H -0.73292500	1.26962900	0.00568300
H 9.93895500	-2.86217600	-0.25593200	H -1.09976800	-0.20858200	0.93139200
H 7.64193000	-3.31576300	3.35971600	H -2.12623600	0.44594700	-1.90046900
H 9.84986600	-3.24336200	2.20528400	H -2.45628500	-1.06597300	-1.04456700
O 6.42789600	0.45410200	-0.45573700	N -4.58477000	0.01920000	-0.28256300
H-0.12567100	-2.15950800	0.48136700	H -4.62022700	-0.92511500	-0.66016000
H-1.12157900	-1.87305700	-0.83288600	C -5.83350900	0.53536300	0.25659300
S-2.91923900	1.09025200	1.96037400	H -5.62397700	1.00858300	1.22564200
C-3.53992500	-0.32164100	0.96383800	C -6.46838100	1.55770200	-0.67992600
C-4.96315700	-0.11153700	0.42883900	H -5.77436700	2.38286400	-0.88040000
H-3.50298700	-1.17654700	1.64580100	H -6.73458800	1.08762000	-1.63682400
H-2.82950900	-0.50025700	0.15276100	H -7.37881900	1.97550400	-0.23435300
H-5.66081100	0.02738700	1.25985700	C -6.81340900	-0.62035000	0.49061800
H-4.99747300	0.78425300	-0.20019800	O -6.57719100	-1.72204400	-0.07453500
N-6.41328400	-2.02296400	0.00640000	O -7.81455800	-0.35481100	1.20859600
C-7.00858500	-3.14715100	-0.71615100	C 6.23124300	2.13793700	-0.24124200
H-7.04162800	-2.88946900	-1.77944600	H 6.42443400	1.96908100	-1.30908000
C-6.19671300	-4.44225300	-0.54188000	H 5.23730300	2.58442800	-0.13106600
H-5.16271800	-4.29119400	-0.86786900	H 6.97052600	2.84716100	0.14886000
H-6.18958900	-4.75995800	0.50734400	H 6.11568900	0.98132600	1.59227200
H-6.63355200	-5.24412300	-1.14526800	C 2.99787700	-2.35897300	0.53455300
C-8.46296600	-3.35315400	-0.23316100	H 3.97086500	-2.83964700	0.38004100
O-8.83173200	-2.76302700	0.82684200	H 2.80415600	-2.29344000	1.61287400
O-9.17868500	-4.12773100	-0.93538700	H 2.22682400	-2.98764600	0.07400900

H	3.14063000	-1.04642400	-1.17659000	S	-4.29930700	-0.64848100	0.29820000
H	7.77258900	-0.61659400	0.92130100	C	-2.68092000	0.21581200	0.41088800
C	-3.42488400	0.68918500	-0.24919400	C	-1.74468500	-0.11366800	-0.75372200
O	-3.31150900	1.81492700	0.26683700	H	-2.17458100	-0.05325200	1.35206900
S2-Ar-m06							
C	1.37753800	1.19580300	0.16922400	H	-2.21277900	0.19871800	-1.69794200
C	0.02661200	1.20961700	0.50497100	N	0.62249600	-0.10864100	-0.23411100
C	-0.69792800	0.02385800	0.66681500	H	0.52928500	-1.11535200	-0.12474100
C	-0.00800900	-1.17916800	0.47890700	C	1.95163300	0.43726400	-0.01487600
C	1.34259100	-1.19710900	0.14308900	H	2.16093600	1.16897600	-0.80697700
C	2.08646200	-0.00911300	-0.02428400	C	2.06276200	1.11787000	1.34568300
H	1.90898200	2.14235100	0.05777700	H	1.30656000	1.90560300	1.44903900
H	-0.47816200	2.16759600	0.65028600	H	1.91123700	0.38636100	2.15187900
H	-0.53991000	-2.12534000	0.60388600	H	3.05260300	1.57321600	1.47093600
H	1.84642600	-2.15596700	0.01054100	C	2.99589900	-0.68049500	-0.10204900
S	3.80023300	-0.03027100	-0.44184800	O	2.59976500	-1.87129800	0.01662000
C	-2.17065500	0.03907400	0.98256100	O	4.19271600	-0.31065100	-0.24507700
H	-2.43510600	-0.83074700	1.59839700	C	-0.43973400	0.62184500	-0.61141600
H	-2.42494600	0.95114900	1.53939700	O	-0.36669800	1.85382400	-0.79809900
C	-2.98577400	0.00312900	-0.31131400	HS1-R1-m06			
O	-3.19199100	1.10316100	-0.90031900	S	-4.31805800	-0.62476500	0.17242700
O	-3.37126400	-1.12581600	-0.73099700	C	-2.82316000	0.44035900	0.20029900
HS2-Ar							
C	1.33480400	1.19900600	0.18151200	C	-1.66624000	-0.34703500	-0.38789900
C	-0.01630300	1.20616700	0.51583900	H	-2.60456600	0.73370100	1.23407600
C	-0.73368700	0.01653300	0.66795400	H	-3.01646500	1.34359100	-0.38729500
C	-0.05410200	-1.19062100	0.47689700	H	-1.50514000	-1.27821800	0.17194000
C	1.29621800	-1.21353700	0.14367500	H	-1.89528600	-0.62998100	-1.42727500
C	1.99989300	-0.01502400	-0.00532400	N	0.71940200	-0.16105600	-0.04120900
H	1.86855800	2.14323600	0.07276200	H	0.68445600	-1.14240200	0.22582100
H	-0.52225300	2.16090200	0.66617900	C	2.04743800	0.42882900	-0.09970800
H	-0.59003800	-2.13319300	0.59701400	H	2.13957500	0.98555700	-1.04250200
H	1.80182200	-2.16962700	0.00504000	C	2.29876700	1.37071000	1.07271300
S	3.72860400	-0.10230600	-0.42549100	H	1.52935400	2.15061400	1.11690200
C	-2.20425400	0.03164000	0.98347300	H	2.28259500	0.81396300	2.02009500
H	-2.46881000	-0.84439200	1.58896200	H	3.27604700	1.85708600	0.97196900
H	-2.45614200	0.93914600	1.54735900	C	3.10490600	-0.68105500	-0.09235000
C	-3.01384400	0.01072800	-0.31754500	O	2.74339500	-1.84197800	0.24043300
O	-3.20398900	1.11695300	-0.89748300	O	4.27725500	-0.32702900	-0.39026200
O	-3.40703700	-1.11188400	-0.74273600	C	-0.39857200	0.47285100	-0.42283600
H	3.94504700	1.23090700	-0.42659100	O	-0.40200600	1.65569200	-0.80867100
S1-R1-m06							
H	-5.16543700	0.28829000	0.69259000				

TS-Ala-1-m06			C 1.44292000	2.37294400	-1.27086000
C-2.41201200	-0.62783300	-0.77573200	C 0.32389000	1.75431100	-1.81951300
O-1.91557400	-0.66100700	0.34322900	C-0.85861100	1.66468700	-1.08130200
C-3.65357600	-1.46500100	-1.11990100	H-1.83956500	2.16297700	0.77683100
C-4.05585100	-1.50639000	-2.57618900	H 0.17399300	3.22189800	1.76057200
H-3.45535100	-2.47252600	-0.73995100	H 2.36867700	2.42393700	-1.84637400
H-4.42986500	-0.53356400	-2.92506300	H 0.37100800	1.32566700	-2.82065800
H-3.20284000	-1.79390400	-3.20082400	S-2.27354100	0.88392000	-1.82452900
N-4.74932400	-0.90431700	-0.32015200	C 2.62221200	3.56246700	0.60840700
C-4.93400200	-1.20385100	0.97883000	H 2.59417800	3.49426400	1.70338300
O-4.47813900	-2.20023100	1.54612900	H 3.53135800	3.06611900	0.24551000
C-5.72932300	-0.16994000	1.75535900	C 2.65107800	5.03970300	0.19785600
H-6.61160600	0.15984900	1.19629700	O 3.34366900	5.35161400	-0.81073400
N-6.22069300	-0.82248700	3.00184900	O 1.94920600	5.84073200	0.87763800
H-6.83275200	-1.62198800	2.79896400	H-4.85782900	-2.23969000	-2.72035100
C-4.82964600	0.99686300	2.11917300	H-5.13646800	-0.01979800	-0.64993500
H-4.51462500	1.52274000	1.21030300			
H-5.36403900	1.70902200	2.75881800	Int-Ala-1-m06		
H-3.93314900	0.64097100	2.64547400	C 4.66332700	0.02682200	-0.08971300
H-5.43034100	-1.17688200	3.55672000	O 5.12276800	-0.66243800	-1.00619500
S-0.75394300	-2.35759700	-2.05980700	N 3.42151800	-0.09660700	0.39773800
C 0.52321800	-2.15887100	-0.77226200	H 3.13224700	0.47203600	1.19188200
C 1.82019300	-1.51876800	-1.27051800	C 5.49168500	1.14284000	0.52710000
H 0.76035100	-3.13252300	-0.31529800	N 6.92680900	0.79416300	0.31442600
H 0.09590200	-1.53017000	0.02712100	C 2.48212900	-1.07495500	-0.12325300
H 2.31075700	-2.17556900	-2.00194000	C 1.07450400	-0.55625500	0.10127400
H 1.59160600	-0.56504500	-1.76945700	O 0.77125500	0.11978000	1.06408200
N 3.81437000	-1.99574900	0.02609200	H 7.53549300	1.55635100	0.63510900
C 4.79034900	-1.85405800	1.09441500	S -0.07380900	-1.09630900	-1.14962300
H 5.00020800	-0.78448900	1.23294000	C 5.20020600	2.47344600	-0.13733500
C 4.28395200	-2.44333900	2.40707800	H 5.35699500	2.40721800	-1.22207300
H 3.33249700	-1.98256900	2.69846100	H 4.16235200	2.76683600	0.05153600
H 4.12702800	-3.52638600	2.30611400	H 5.85538700	3.25201200	0.27064700
H 5.00974500	-2.27137100	3.21094100	H 5.33414300	1.19660900	1.60945800
C 6.09761200	-2.55029800	0.70161600	C 2.62357500	-2.42759200	0.57131000
O 6.06527200	-3.38459200	-0.24300400	H 3.64973100	-2.79413600	0.45217900
O 7.10851400	-2.25628600	1.39550900	H 2.40472600	-2.32891300	1.64231700
H-6.74372900	-0.15305700	3.57852300	H 1.93982600	-3.16707400	0.13779800
C 2.73100800	-1.21407400	-0.11092200	H 2.67174600	-1.18583900	-1.19909100
O 2.46493300	-0.29578000	0.68991300	H 7.19219900	-0.06057000	0.81870700
H 4.01413300	-2.70978700	-0.67020400	C -1.60910800	-0.49396100	-0.46808200
C-0.91439200	2.21274400	0.20348600	C -2.04859200	0.79357900	-0.77887800
C 0.21493200	2.81328200	0.75013300	C -2.37273700	-1.32301400	0.35386800
C 1.40756800	2.89790500	0.02381700	C -3.25955500	1.24521200	-0.26587900

H -1.44520100	1.43948700	-1.41579500	H 4.23509500	-2.49073400	1.78467200
C -3.58296800	-0.85996600	0.85915900	H 6.17719300	-1.07998300	1.12815700
H -2.02361000	-2.32582300	0.59680700	O 1.61311700	2.25372400	0.94275800
C -4.04317000	0.42493500	0.55318400	H -3.81050400	-2.23233500	0.17494100
H -3.60501300	2.25176500	-0.50360700	H -5.04851600	-0.49506100	1.61068300
H -4.18360800	-1.50506100	1.50100800			
C -5.38333800	0.89538500	1.04204700	React-Cys-1-m06		
H -5.36406500	1.97843100	1.21422800	C -1.85343000	-0.69103600	-0.29807200
H -5.64203200	0.38746100	1.97928400	O -1.54801600	-1.73284000	0.30192000
C -6.44355900	0.56933800	-0.01920500	N -1.02488600	0.34643500	-0.45107600
O -6.96816000	-0.57803900	0.02446200	H -1.30634900	1.15767200	-0.99797500
O -6.68751800	1.45449100	-0.88486400	C -3.22174000	-0.53765800	-0.94933500
H 7.11019600	0.63202400	-0.68504000	N -4.00334100	-1.75768100	-0.62159800
			C 0.34280500	0.35402000	0.04501400
React-Cys-m06			C 0.81659800	1.80533500	0.19473500
C -1.77463800	-0.66798400	-0.39106400	O 0.40723400	2.62756900	-0.66994700
O -1.39818900	-1.69775900	0.18275900	H -4.76808900	-1.90082000	-1.28846300
N -1.02069100	0.42058800	-0.55633400	C -4.02821100	0.66703100	-0.46311800
H -1.37875200	1.23661700	-1.05142200	H -3.44879400	1.57922800	-0.65105900
C -3.18549300	-0.57771500	-0.96382600	H -4.92560200	0.73615900	-1.09533100
N -3.81509200	-1.91875700	-0.80512200	H -3.08956400	-0.50699400	-2.03886800
C 0.34573500	0.51101100	-0.06388700	C 1.26662900	-0.40638500	-0.92682900
C 0.73698200	1.98603500	0.08053000	H 0.83814900	-1.40889800	-1.06990800
O 0.18214500	2.80562400	-0.70063800	H 1.23615900	0.10750300	-1.89925900
H -4.78763700	-1.90445400	-1.13724500	H 0.35890700	-0.13503200	1.02705700
C -4.05303700	0.49857900	-0.33144700	H -3.41352200	-2.59622500	-0.57800900
H -3.65819300	1.48024100	-0.61192000	S -4.48457100	0.50159800	1.30679800
H -5.06953700	0.44050200	-0.73785300	C 2.68132200	-0.51352600	-0.43832900
H -3.13009500	-0.38923500	-2.04348500	C 3.68373400	0.31116900	-0.95533000
C 1.31170700	-0.20207900	-1.03264100	C 3.01183200	-1.41871900	0.57564200
H 0.85196300	-1.16479600	-1.29812800	C 4.98835900	0.23740700	-0.46997700
H 1.38032400	0.39202000	-1.95651400	H 3.43321900	1.02238800	-1.74464400
H 0.39134900	0.02708900	0.92012800	C 4.31311300	-1.49465200	1.06533000
H -3.30391000	-2.63173900	-1.33992500	H 2.23570000	-2.07024600	0.98231700
S -4.11222700	0.47376800	1.49731900	C 5.30598400	-0.66467900	0.54354900
C 2.67436200	-0.44222000	-0.45224800	H 5.75767200	0.88814300	-0.88381000
C 3.77227100	0.34083000	-0.81597100	H 4.55439200	-2.20491700	1.85509700
C 2.85772100	-1.46185400	0.48823000	H 6.32445000	-0.72464800	0.92462700
C 5.02646300	0.11446000	-0.25126900	O 1.60722200	2.05405100	1.14172900
H 3.63767300	1.13992300	-1.54719700	H -4.40950700	-1.57023300	0.32888000
C 4.10815300	-1.69164400	1.05531400			
H 2.00345800	-2.08028600	0.77301700	TS-Ala-2-m06		
C 5.19753500	-0.90201100	0.68676500	C -1.23821700	4.65009100	0.32038000
H 5.87305200	0.73395900	-0.54477700	O -1.06619500	4.95529700	1.50620500

N -2.01993900	3.64880900	-0.09956700	C 5.68430800	0.58276800	-0.15133700
H -2.04104000	3.42299700	-1.09303900	O 5.55561800	1.38238800	-1.11831100
C -0.53479100	5.41859800	-0.78790600	C 0.76869600	1.03678100	-0.91899800
N -0.08568200	6.72025800	-0.21324400	H 1.60211900	1.66448000	-1.25970500
H 0.54709000	6.56617200	0.58258000	H -0.10040600	1.30385300	-1.54602500
C -2.59981200	2.67638400	0.80956400	H 1.22205400	-0.60303900	-2.27794500
C -2.45918200	1.29491000	0.19890200	C 5.39796100	-1.81235700	-0.88253400
O -2.48132800	1.11438700	-1.00459200	H 4.63988100	-2.60467600	-0.96096600
H 0.41547100	7.27110200	-0.92022900	H 5.62842000	-1.47849900	-1.90554300
C 0.66829400	4.66647000	-1.32028400	H 4.56877700	-0.92414200	0.91810400
H 1.35733300	4.40650600	-0.50555200	H 0.21198700	-2.23113500	-0.59446800
H 0.34255600	3.74294700	-1.81123800	S 0.38753200	1.31514800	0.84367200
H 1.19937000	5.27813000	-2.05933300	C 6.63324400	-2.35198100	-0.22335600
H -1.23679100	5.65757300	-1.59385900	C 7.90154700	-2.08161100	-0.74237100
C -4.08291600	2.96090300	1.04364100	C 6.53353200	-3.12098300	0.94108300
H -4.19555300	3.98777000	1.41260700	C 9.04775500	-2.56580500	-0.11366100
H -4.65182700	2.85598200	0.10978300	H 7.98657300	-1.47711500	-1.64731900
H -4.50320900	2.27952100	1.79236300	C 7.67540500	-3.60418300	1.57472400
H -2.05668000	2.72071500	1.75863300	H 5.54563000	-3.33893700	1.35229000
H -0.87615300	7.27881900	0.12999900	C 8.93747400	-3.32781300	1.04773500
C -5.41014000	-0.65865200	1.22716600	H 10.02918500	-2.34823900	-0.53325700
C -6.53588400	-1.27541900	0.68983400	H 7.58208500	-4.20195000	2.48051800
C -6.43916000	-2.07549200	-0.45274100	H 9.83129000	-3.70778400	1.54050200
C -5.18309300	-2.25098700	-1.04263300	O 6.53263200	0.66850400	0.77454500
C -4.04878900	-1.65404100	-0.50218200	H -0.33595400	-0.84221400	0.18763500
C -4.15998300	-0.84570500	0.63207100	H -0.83424100	-1.18064700	-1.38222100
H -5.50201700	-0.03062400	2.11278000			
H -7.50908300	-1.12921400	1.16024000	Int-Ala-3-m06		
H -5.09226800	-2.87275300	-1.93405000	C -6.79976300	-0.21562700	-0.09569500
H -3.07700100	-1.81928600	-0.96525600	O -7.31783600	0.72708600	-0.70362600
S -2.71032600	-0.09572700	1.38173000	N -5.58429100	-0.17396400	0.46406000
C -7.64667800	-2.78291700	-1.00040200	H -5.22784200	-0.98783800	0.96285600
H -8.55444200	-2.21388700	-0.76358700	C -7.51292500	-1.55263600	0.02113600
H -7.56380400	-2.88513300	-2.08942100	N -8.96860200	-1.29946900	-0.18598400
C -7.74562400	-4.17725800	-0.36716000	C -4.73915800	1.00459800	0.39249900
O -7.20577900	-5.13595300	-0.98653100	C -3.29833900	0.56183800	0.57775300
O -8.32597500	-4.26226100	0.75070800	O -3.00612400	-0.47271900	1.14879600
C 2.34431000	-0.93897900	-0.47640800	H -9.49436500	-2.18029500	-0.13796200
O 2.27520500	-1.92197600	0.27659100	S -2.12522200	1.73013900	-0.05069200
N 3.47829100	-0.28025500	-0.73175400	C -7.02528500	-2.52922800	-1.03062800
H 3.48949800	0.51408300	-1.36849000	H -7.12986700	-2.09824700	-2.03533700
C 1.10509900	-0.42676100	-1.20041700	H -5.97039800	-2.76762500	-0.85950300
N -0.04350400	-1.24672000	-0.73225500	H -7.59988900	-3.46159800	-0.98120300
C 4.75273800	-0.63513000	-0.12482700	H -7.40316700	-1.96453300	1.03016700

C -5.10363500	2.02729000	1.46734100	C -6.10234900	1.51867800	0.62861800
H -6.16446600	2.28736400	1.37661800	N -6.17224000	2.91253200	1.15805200
H -4.92655800	1.60903300	2.46667100	C -3.32896100	-1.04472500	1.05937500
H -4.51446600	2.94482900	1.35716300	C -3.16087400	-1.71442400	-0.32023600
H -4.86028200	1.45357900	-0.60300300	O -3.76287300	-2.76711700	-0.56354100
H -9.35225300	-0.65748900	0.51785800	H -7.10283500	3.31646100	0.99795900
C 1.54608800	-0.13184800	-0.13495100	S -2.95233900	-0.52294200	-1.73893300
O 1.69077000	-1.06785700	0.66900700	C -6.41906100	1.53285000	-0.85297200
N 2.55897100	0.63709700	-0.55707500	H -5.67895000	2.13135200	-1.40091500
H 2.38569100	1.38648500	-1.22388300	H -6.40496600	0.51108400	-1.24752400
C 0.16144300	0.23103300	-0.67165200	H -7.41680000	1.95343300	-1.02506400
N -0.60558800	-0.92350500	-1.10284000	H -6.83581200	0.92945600	1.18862300
C 3.92651100	0.49253000	-0.08434400	C -3.36865700	-2.06354700	2.18145700
C 4.66677900	1.82507400	-0.25222000	H -3.45288900	-1.55009100	3.14607200
O 4.36336500	2.52285000	-1.25830300	H -4.23260300	-2.73054900	2.06723600
H -0.66574900	-1.58547800	-0.32717200	H -2.46601800	-2.68471300	2.20319000
C -0.54867900	0.97231300	0.45584400	H -2.53759700	-0.30580400	1.22801900
H -0.75799300	0.29606600	1.29538000	H -5.97779900	2.94928500	2.16624100
H 0.07319200	1.79512100	0.82861500	C 0.82600900	-0.66553200	-0.25425000
H 0.28097900	0.90800300	-1.52876700	O 0.87924700	-0.68617700	0.98483700
C 4.65312500	-0.61984300	-0.86568800	N 1.80444300	-0.19895600	-1.03642200
H 4.00958300	-1.51103200	-0.83800800	H 1.70022600	-0.22827400	-2.04919300
H 4.73521500	-0.30774100	-1.91776400	C -0.43125900	-1.12169300	-0.98299000
H 3.89811200	0.22788100	0.98043300	N -1.17987700	-2.07939600	-0.17571300
C 6.00784000	-0.94899200	-0.31003100	C 3.05799200	0.33164800	-0.52378800
C 7.17465700	-0.50295900	-0.93596900	C 3.67439500	1.27324300	-1.56613800
C 6.12042400	-1.69093900	0.87064200	O 3.50984900	0.96488400	-2.77792000
C 8.42744400	-0.78916700	-0.39542700	H -0.85550400	-2.04813200	0.79515500
H 7.09643600	0.07992700	-1.85562600	C -1.32386500	0.09853400	-1.24724600
C 7.36915900	-1.97826700	1.41527500	H -1.40050400	0.73864900	-0.35707400
H 5.21317400	-2.04596800	1.36406900	H -0.92498400	0.70484400	-2.06812100
C 8.52797500	-1.52710900	0.78243400	H -0.17147600	-1.58258900	-1.94308300
H 9.32736800	-0.43455200	-0.89639600	C 4.02930800	-0.82206100	-0.20747700
H 7.43905600	-2.55921900	2.33407300	H 3.49784400	-1.52255100	0.45254500
H 9.50578100	-1.75107700	1.20656100	H 4.24654900	-1.35513000	-1.14521200
O 5.54639900	2.09948600	0.60522200	H 2.84574200	0.89357800	0.39485000
H -9.13141200	-0.87702100	-1.10948800	C 5.30111800	-0.36640600	0.44541000
H -0.10030500	-1.40105200	-1.84908800	C 6.49169800	-0.27257100	-0.27947400
TS-Ala-3-m06			C 5.30399800	0.00334800	1.79474000
C -4.68949100	1.01155500	0.86549000	C 7.66189400	0.17968700	0.32829700
O -3.73885300	1.79927400	0.87350800	H 6.49716800	-0.55651600	-1.33343600
N -4.59072600	-0.31595600	1.02893300	C 6.46985000	0.45689600	2.40591000
H -5.44413700	-0.87240000	0.99667500	H 4.37760600	-0.06931000	2.36826200
			C 7.65338100	0.54656900	1.67271900

H	8.58263000	0.24361600	-0.25015000	C	3.84537900	-0.71536500	-0.73083600
H	6.45727000	0.73912100	3.45787400	H	3.07568200	-1.47922100	-0.54943100
H	8.56702600	0.89871500	2.14958500	H	3.86718500	-0.52279200	-1.81387500
O	4.32810800	2.25691400	-1.13169100	H	3.37963600	0.41618800	1.06317000
H	-5.47756500	3.50993900	0.69001000	C	5.18273500	-1.20761300	-0.26155800
H	-1.08393300	-3.03378800	-0.52219700	C	6.32821400	-1.02903500	-1.04133300
Prod-Ala-m06				C	5.30934700	-1.82505000	0.98747200
C	-6.03310500	-0.98394400	0.16372000	C	7.57452000	-1.45668100	-0.58616800
O	-6.01844800	-1.79605100	1.09651300	H	6.23726400	-0.54637900	-2.01637300
N	-4.94590700	-0.55854700	-0.48631700	C	6.55232300	-2.25107400	1.44764100
H	-5.04079400	0.09936400	-1.25868900	H	4.41887300	-1.97103300	1.60227300
C	-7.33793500	-0.34683400	-0.28890200	C	7.69011400	-2.06772000	0.66083500
N	-8.44222400	-1.27607400	0.09109700	H	8.45702300	-1.31167900	-1.20787500
C	-3.60263600	-1.00134000	-0.15443200	H	6.63570800	-2.73049300	2.42226100
C	-2.63169000	0.03133800	-0.70234000	H	8.66210500	-2.40401200	1.01895700
O	-2.92442900	0.72482700	-1.68488900	O	5.30634200	1.92203200	0.45272700
H	-9.35575700	-0.85435700	-0.11386900	H	-8.40209900	-1.48540100	1.09779900
S	-0.53060700	2.73617100	1.64058100	H	-1.25219200	-0.52405900	0.70842100
C	-7.55926900	0.99318500	0.38324800	React-Pro-m06			
H	-7.53392400	0.88872300	1.47587800	C	-1.62925000	0.58433500	-0.06496000
H	-6.77644800	1.69620000	0.07984500	O	-1.55168300	-0.02739900	0.98512900
H	-8.52786800	1.41169400	0.08597200	C	-4.92734100	1.47474900	0.79463400
H	-7.36532400	-0.25098000	-1.37924000	C	-2.88519300	1.30902300	-0.51720300
C	-3.29648100	-2.36595000	-0.76355600	C	-2.97578600	2.68300400	0.16741400
H	-4.04060700	-3.09745000	-0.42812200	C	-4.47033800	2.86682300	0.39802200
H	-3.32654300	-2.31132300	-1.85958700	H	-5.99033400	1.29846700	0.60210200
H	-2.30577700	-2.71874200	-0.45307700	H	-4.71433900	1.26619100	1.85378100
H	-3.51467800	-1.05327700	0.93861000	H	-2.88940300	1.40294100	-1.61280600
H	-8.38163800	-2.17095500	-0.40997200	H	-2.45074800	2.64607800	1.13297400
C	0.94184400	0.38838400	0.03970500	H	-2.51826600	3.46699500	-0.44385400
O	0.94155900	-0.49593000	0.90735400	H	-4.69112300	3.61071500	1.17008500
N	2.05405600	0.94684300	-0.44993900	H	-4.96793200	3.17231900	-0.53228700
H	1.99339800	1.63968100	-1.19385900	N	-4.09326600	0.61721400	-0.06627400
C	-0.36107000	0.93815900	-0.53338700	C	-4.25955600	-0.68037900	-0.35085600
N	-1.44351800	0.08909900	-0.08296200	O	-3.50821500	-1.30185400	-1.11756900
C	3.39379200	0.57678600	-0.02238700	C	-5.36290700	-1.42233200	0.37833300
C	4.36027700	1.72187600	-0.35256800	H	-6.26734900	-0.82034700	0.50066700
O	4.15124800	2.34772900	-1.42758200	N	-5.74128300	-2.59056600	-0.46976600
H	-1.61347500	1.98971700	1.95365400	H	-6.16403300	-2.29279100	-1.35759500
C	-0.58264200	2.40410300	-0.15662600	C	-4.84039600	-1.92251600	1.71216400
H	0.19904600	3.02983400	-0.60188400	H	-4.58529800	-1.07673100	2.36051000
H	-1.53960400	2.74495100	-0.56555400	H	-5.60280400	-2.52491200	2.21936200
H	-0.30879300	0.88761600	-1.63204200	H	-3.93915800	-2.53258100	1.56398200

H -4.90869500	-3.15137200	-0.69611700	C -5.61528300	1.61255000	1.17877500
S -0.26842600	0.82085300	-1.16929600	H -5.43006100	1.71231800	0.10355800
C 1.04616200	-0.02507800	-0.22367300	H -6.44595800	2.27689200	1.44424800
C 2.34806500	0.07943200	-0.99845200	H -4.71232000	1.93438800	1.71640500
H 0.74664400	-1.06921000	-0.08360600	H -5.44539100	0.38230700	3.54503100
H 1.13083300	0.45243300	0.75999600	S -0.41508500	-2.55783500	-1.31670000
H 2.24229900	-0.39193100	-1.98757600	C 0.96459900	-2.07213000	-0.22938400
H 2.62205500	1.12865600	-1.16824500	C 2.20184900	-1.58599400	-0.98424000
N 4.65203200	-0.03676200	-0.26961600	H 1.25222500	-2.91276800	0.42188600
C 5.83819800	-0.59269000	0.36305300	H 0.60357200	-1.26798900	0.43531100
H 5.54482800	-1.02236900	1.33082200	H 2.57846600	-2.37890800	-1.64479800
C 6.48033800	-1.67586600	-0.49673600	H 1.92950000	-0.72477800	-1.61156100
H 5.75848800	-2.46969300	-0.72332000	N 4.36018800	-1.91284700	0.06679200
H 6.83846900	-1.25244700	-1.44533000	C 5.47595200	-1.65625200	0.96164000
H 7.33179900	-2.12744500	0.02553400	H 5.70684900	-0.58191400	0.93293400
C 6.85516300	0.52428500	0.62589700	C 5.14710400	-2.06175800	2.39451500
O 6.68328300	1.63132600	0.04798000	H 4.24343400	-1.54694600	2.74255100
O 7.81646300	0.22521600	1.38414300	H 4.97118200	-3.14478400	2.45575000
H -6.41570500	-3.19063100	0.01969200	H 5.97181300	-1.80414700	3.06913300
C 3.45938100	-0.64786700	-0.27738000	C 6.71680700	-2.41781500	0.48009100
O 3.26643300	-1.75408400	0.25703300	O 6.57237000	-3.28995000	-0.41914600
H 4.75271000	0.89965700	-0.65571700	O 7.79803500	-2.12723000	1.05957400
			H -7.05038900	0.69569000	3.22275600
TS-Pro-1-m06			C 3.26718100	-1.13717800	-0.01920400
C -2.06045100	-0.80038000	-0.24321200	O 3.11769500	-0.11440200	0.67824800
O -1.50833400	-0.62525200	0.83524900	H 4.47027300	-2.70261800	-0.56438500
C -5.35971000	-0.81153000	-1.18044200	C -0.70081800	2.23956100	0.25943200
C -3.25389600	-1.75101700	-0.41216200	C 0.43504900	2.92596400	0.67737000
C -3.55573500	-2.23623000	-1.83493100	C 1.60221100	2.92023700	-0.09345800
C -5.05517000	-2.02676800	-2.03630900	C 1.59994700	2.22482000	-1.30600100
H -6.40963100	-0.74152400	-0.88251300	C 0.47236900	1.52657900	-1.72615700
H -5.07932100	0.12265300	-1.69091400	C -0.68166000	1.51938500	-0.93841600
H -3.08460600	-2.57589700	0.29090700	H -1.60314200	2.25196400	0.87032000
H -2.98403100	-1.64719000	-2.56344300	H 0.42068600	3.47183600	1.62174600
H -3.25322700	-3.28041200	-1.96144600	H 2.50527200	2.20575700	-1.91535300
H -5.32453400	-1.86912800	-3.08617700	H 0.49141900	0.96701000	-2.66152900
H -5.62222400	-2.89014300	-1.66326800	S -2.09912400	0.59713400	-1.48664500
N -4.49025800	-1.03141300	-0.01589100	C 2.82949700	3.66189600	0.35765200
C -4.75816700	-0.73325400	1.26468300	H 2.84896900	3.71813800	1.45338900
O -4.06022700	-1.10287300	2.21923700	H 3.72892600	3.13442600	0.01467500
C -5.95029500	0.17521800	1.52753800	C 2.81911000	5.08230800	-0.21920400
H -6.85216500	-0.16346600	1.00890200	O 3.42047400	5.27167800	-1.31322800
N -6.25686100	0.08861900	2.98618100	O 2.17661800	5.96064200	0.42231200
H -6.48833200	-0.87118900	3.26998000			

HPO ₄ ²⁻			C	6.50376200	0.48520800	0.49781100	
P	0.12979600	-0.01646500	0.00014400	O	6.27924900	1.57627600	-0.10763200
O	0.38180800	-0.81288400	1.30350500	O	7.49318000	0.24633000	1.25189500
O	-1.52398100	0.36094500	-0.00547300	C	-5.72030600	-1.48656800	1.69478900
O	0.38291800	-0.84829400	-1.28116400	H	-4.93012700	-2.24396200	1.65259100
O	0.77342600	1.38748300	-0.01792400	H	-5.43418800	-0.71569700	2.41529000
H	-2.06030500	-0.45103200	0.00629100	H	-6.64835200	-1.95332500	2.04091100
H ₂ PO ₄ ⁻			H	-6.72945800	-0.09490500	0.36655000	
C	-3.11215800	3.10941300	0.30049100	H	-3.99894600	3.65321600	-0.03906700
P	0.00010400	0.08956100	0.11839500	H	-3.10135100	3.07765200	1.39396000
O	0.00038600	-0.67033600	1.43281700	H	-2.22436500	3.63910200	-0.05352800
O	-1.29647500	-0.38386300	-0.78480100	H	-3.17078400	1.75468800	-1.38333400
O	1.29578500	-0.38436100	-0.78555600	H	-6.61925000	-1.48557600	-1.56875400
O	0.00031600	1.60154000	0.07712800	C	3.09458900	-0.76900400	-0.25693500
H	-1.51619900	-1.32321000	-0.64553000	O	2.90030400	-1.84580400	0.34825200
H	1.51454700	-1.32403700	-0.64710100	H	-1.10764900	-0.01884800	1.60278500
React-Ala-OH			React-Ala-H ₂ O				
C	-4.65720400	-0.24740300	-0.24810300	C	5.31857200	-0.29850500	-0.18991400
O	-3.92892200	-0.88973200	-1.01901100	O	5.66914300	-1.27922600	-0.86977400
N	-4.36137500	1.00101600	0.16008700	N	4.11174700	-0.16330400	0.37811600
H	-4.96605300	1.47196900	0.82725500	H	3.92672000	0.64592300	0.96469700
C	-5.94121600	-0.84994300	0.32289900	C	6.27653400	0.88108900	0.01096400
N	-6.40790500	-1.89316000	-0.65011800	N	7.66074600	0.30275200	0.10901900
H	-5.68724200	-2.61288400	-0.78899800	H	7.85090100	-0.30125500	-0.70104600
C	-3.16154700	1.68959900	-0.29090200	C	3.04889100	-1.15708400	0.24861800
C	-1.91133600	0.92739300	0.11763900	C	1.70809000	-0.42312300	0.33105500
O	-1.91985700	0.45267400	1.31682100	O	1.55683000	0.54696800	1.06554200
H	-7.25721900	-2.35086800	-0.29835600	H	8.36569200	1.04881200	0.12890000
S	-0.63086000	0.84952700	-0.99402300	S	0.42840100	-1.12074300	-0.67025300
C	0.73455900	0.03066300	-0.05374400	C	-1.00881200	-0.09161100	-0.16049700
C	1.95234900	-0.06081500	-0.97881100	C	-2.21742000	-0.41288900	-1.04357000
H	0.39401300	-0.96369700	0.24766300	H	-0.72252700	0.95497800	-0.26744300
H	0.95209700	0.64412800	0.82581800	H	-1.22133000	-0.30205500	0.89086900
H	1.71254600	-0.65765400	-1.86742000	H	-1.99474300	-0.17323700	-2.09127700
H	2.26369000	0.93349800	-1.31105400	H	-2.47624700	-1.47499900	-0.99257200
N	4.29318000	-0.17573600	-0.33899700	N	-4.58025300	-0.19033900	-0.49940400
H	4.37791000	0.73675700	-0.77802200	H	-4.61960400	-1.20161000	-0.58937100
C	5.51362500	-0.68396900	0.28761300	C	-5.82849300	0.45319300	-0.08849400
H	5.25000700	-1.08373000	1.27157100	H	-5.59598700	1.17144400	0.70398200
C	6.16687900	-1.79954600	-0.54597600	C	-6.50394500	1.19826700	-1.25281500
H	5.46027200	-2.62079400	-0.70375400	H	-5.81910900	1.93908800	-1.67793800
H	6.48378200	-1.41977500	-1.52425400	H	-6.79659200	0.50038900	-2.04577100
H	7.04352700	-2.19469000	-0.02349400				

H -7.39825200	1.71969000	-0.89783900	H-1.59048200	-2.89733000	0.12856200
C -6.78394200	-0.60858300	0.50228500	H-0.71189300	-1.40251300	-0.20298200
O -6.51330500	-1.83249900	0.31150200	H-3.09228600	-1.63925900	1.72706100
O -7.79520000	-0.16323300	1.12225700	H-2.21987200	-0.14859200	1.33295500
C 6.21864500	1.86784100	-1.15378500	N-4.61981800	-1.46389800	-0.26788500
H 6.45022700	1.36872300	-2.10091500	C-5.60883900	-1.33154700	-1.33660700
H 5.21576300	2.29892600	-1.21876700	H-5.60929000	-0.29029900	-1.67438600
H 6.93428500	2.68063000	-0.99118800	C-5.29006000	-2.24282100	-2.53440900
H 6.08417400	1.38622100	0.95911900	H-4.28071700	-2.04225700	-2.90723600
C 3.12354600	-2.22804800	1.35258100	H-5.35084500	-3.29913700	-2.24694100
H 4.09230300	-2.73358700	1.29600400	H-5.99991600	-2.06165900	-3.34778400
H 3.01488300	-1.77013600	2.34115000	C-7.01588300	-1.65313100	-0.78563400
H 2.33484000	-2.97532300	1.21884300	O-7.10332000	-2.23055400	0.33971400
H 3.15228900	-1.63348200	-0.72941400	O-7.99261300	-1.33203100	-1.52742000
H 7.77416000	-0.26661500	0.95643400	H 7.36993800	-2.22712900	-2.54313900
C -3.40593500	0.44580800	-0.62676700	C-3.40984400	-0.87634700	-0.26995600
O -3.27510900	1.67635500	-0.43545400	O-3.01317900	-0.16816100	-1.22822300
O -0.22547400	2.68983700	1.93235400	H-4.92358600	-1.98209600	0.55056500
H 0.30780200	1.93702500	1.60757300	C 1.67460800	2.63875800	0.22884100
H -1.06920400	2.60482700	1.45652500	C 0.95345200	3.67655700	-0.36499900
			C-0.32189800	4.03217500	0.10217800
TS-Ala-1-H ₂ O			C-0.85918900	3.31250300	1.18094500
C 1.89369400	-0.76842900	0.91753800	C-0.14837100	2.26852500	1.77779000
O 1.44900300	-0.56441600	-0.21849700	C 1.12530300	1.92416400	1.30323700
C 2.92176200	-1.90104500	1.17698600	H 2.66152600	2.38255200	-0.14570000
C 3.25442800	-2.19273000	2.63918000	H 1.38775900	4.21644700	-1.20283700
H 2.51542000	-2.78883000	0.69593200	H-1.84809400	3.56639400	1.55594500
H 3.81318500	-1.37149700	3.10218700	H-0.58530500	1.72119300	2.60785700
H 2.34107600	-2.36552900	3.21310700	S 2.05380300	0.62848200	2.11529700
N 4.15618000	-1.54934300	0.45245600	C-1.09560700	5.17631200	-0.51686900
C 4.60638300	-2.16103700	-0.65113300	H-0.79694500	5.29734700	-1.56482400
O 4.08416900	-3.16075000	-1.18252400	H-2.16721800	4.96126800	-0.48971100
C 5.85159200	-1.52816500	-1.28221400	C-0.83810500	6.52468600	0.19629900
H 6.53968400	-1.17118100	-0.51350600	O 0.34532200	6.98514900	0.16740800
N 6.57153700	-2.61482700	-2.02754400	O-1.82450500	7.09410600	0.75842900
H 6.92226500	-3.34299600	-1.39459100	H 3.87611300	-3.09269500	2.69425800
C 5.48729800	-0.40309100	-2.25055600	H 4.68885600	-0.75665100	0.80170700
H 5.00056800	0.40856400	-1.70315900	O 1.41704200	-2.64125900	-2.15702900
H 6.39387200	-0.00781500	-2.72119200	H 1.31426300	-1.91803900	-1.49867800
H 4.80548800	-0.76235900	-3.02880100	H 2.30265700	-2.99226500	-1.93538200
H 5.93705800	-3.06605100	-2.69829400			
S-0.14496800	-2.25061300	1.97981100	H ₂ O		
C-1.27606600	-1.94251400	0.56910300	O 0.00000000	0.00000000	0.11933500
C-2.52915000	-1.12476400	0.94117700	H 0.00000000	0.76701600	-0.47734000

H 0.0000000	-0.76701600	-0.47734000	O-4.07890800	-0.29959600	-1.90231000
			P 4.04383400	2.73339100	-0.17851500
React-P-Ala			O 4.61035100	1.54061300	0.58209700
C 3.55340900	-2.01191000	0.14279500	O 2.41547000	2.75905300	-0.02699300
O 2.98695500	-3.12072700	0.17702800	O 4.29838500	2.50203400	-1.79207200
N 3.18141700	-0.94217700	0.86090800	O 4.52631600	4.13626800	0.11661500
H 3.68761000	-0.05087200	0.74009100	H 2.00015900	1.86494000	0.02194700
C 4.75058800	-1.80180400	-0.79073300	H 4.27635800	1.55745000	-2.03058400
N 5.56235800	-3.06740000	-0.75308000			
H 4.95892600	-3.87930200	-0.93835500	Int-P-S12		
C 1.97685600	-0.93647100	1.68381600	C 1.02490000	-0.82738800	1.18148200
C 0.76780800	-0.50628300	0.83516600	O 1.03652300	-0.56885800	-0.07617500
O 0.79810000	0.46762900	0.08896900	C 2.40105500	-1.24959700	1.80055500
H 6.30287300	-3.04454800	-1.46354600	C 2.42487900	-1.57267800	3.29760600
S-0.67161700	-1.50705900	1.05806100	H 2.69961200	-2.13707800	1.23712500
C-1.90512600	-0.59420100	0.04339800	H 2.17160400	-0.69908200	3.90716600
C-3.25381200	-1.31540900	0.13339700	H 1.72901500	-2.38069100	3.54128400
H-1.54309800	-0.55982500	-0.98572200	N 3.39267700	-0.21418200	1.49570000
H-1.97579800	0.42537700	0.43185300	C 4.51253800	-0.41068100	0.80113600
H-3.16537100	-2.33475900	-0.26365000	O 4.91464600	-1.52405400	0.39244900
H-3.58533300	-1.39092100	1.17376400	C 5.33453600	0.84071000	0.47949600
N-5.46303300	-0.32788800	-0.09121500	H 5.18051400	1.61883200	1.22869000
H-5.56150100	-0.51630200	0.90217300	N 6.78362300	0.44664200	0.56402100
C-6.59072300	0.37204000	-0.70667400	H 7.05386000	0.20527000	1.52521600
H-6.19518700	1.19664600	-1.30881900	C 5.03078600	1.36148000	-0.92461800
C-7.41903600	-0.55286300	-1.61438100	H 3.98497600	1.67520900	-0.97990700
H-6.78320400	-0.99587800	-2.38760200	H 5.66300500	2.22758700	-1.14711500
H-7.87639000	-1.36251100	-1.03390700	H 5.20579600	0.58495900	-1.67679400
H-8.21400800	0.01580700	-2.10653100	H 6.96079900	-0.37578600	-0.02750800
C-7.47810500	0.98339700	0.40271000	S -0.21545800	-2.21062500	1.71357800
O-7.26503500	0.63476200	1.60288500	C -1.52917700	-2.02165300	0.45426400
O-8.37860100	1.78686900	0.01644300	C -2.72961500	-1.18323100	0.91766200
C 4.30205600	-1.53869100	-2.22775500	H -1.85145200	-3.03818000	0.20473900
H 3.71817900	-2.38133000	-2.61382500	H -1.06720200	-1.59035200	-0.43766000
H 3.67940800	-0.64076100	-2.26588700	H -3.12644800	-1.57459800	1.85975700
H 5.17571900	-1.38298500	-2.86908300	H -2.40971300	-0.15047000	1.09516900
H 5.39971100	-1.00330600	-0.42998900	N -5.05321800	-1.49671500	0.26412200
C 2.13079700	0.01834900	2.87530700	C -6.24192800	-1.48677600	-0.58582400
H 2.96915400	-0.30689800	3.49916900	H -6.17555800	-0.62375200	-1.25507300
H 2.31392500	1.04320900	2.53899900	C -6.34660600	-2.76794000	-1.43167400
H 1.22261300	0.00856900	3.48593000	H -5.44666400	-2.89310300	-2.04229600
H 1.81360400	-1.95264000	2.04960900	H -6.45675700	-3.64894800	-0.78848200
H 6.00325200	-3.20622800	0.16377600	H -7.21134500	-2.71286300	-2.10064800
C-4.30182900	-0.59679000	-0.70682300	C -7.50547500	-1.31494700	0.28765800

O -7.39947700	-1.48869700	1.53895900	C 5.63879800	0.22065500	-0.07400600
O -8.57647400	-1.03469500	-0.33027700	H 6.18168300	0.82901400	0.65234800
H 7.38789800	1.21285800	0.24602000	N 6.64436100	-0.72095600	-0.67407100
C -3.81896000	-1.15264800	-0.14178100	H 7.07265600	-1.32387700	0.03840700
O -3.56815300	-0.82099100	-1.32480100	C 5.04025700	1.09884500	-1.17352400
H -5.21494000	-1.71203200	1.24293000	H 4.34361300	1.81592000	-0.73079000
C 1.08954100	2.68522500	0.24419500	H 5.83600800	1.65782400	-1.67699600
C 0.76797200	3.68323500	-0.67840700	H 4.50391400	0.49328900	-1.91146000
C -0.54792200	4.15365900	-0.81235700	H 6.20258700	-1.33178300	-1.37261500
C -1.53689400	3.57908500	0.00115400	S-0.24724900	-1.69016000	2.84035900
C -1.22428600	2.56819300	0.91335400	C-1.24510800	-1.88244600	1.31113900
C 0.09717000	2.10646600	1.05622100	C-2.64341200	-1.23941300	1.39323900
H 2.12110000	2.35884500	0.33537100	H-1.35395200	-2.94816200	1.07356900
H 1.55463300	4.10717500	-1.29876000	H-0.68937900	-1.42355900	0.48304200
H -2.56684800	3.91848100	-0.08528800	H-3.20434800	-1.66864100	2.23036400
H -2.01269600	2.13677000	1.52377800	H-2.53212500	-0.16432400	1.57953800
S 0.47646500	0.88084900	2.29480200	N-4.55751700	-2.11624400	0.15929500
C -0.88555800	5.26976400	-1.78119200	C-5.44393300	-2.35709600	-0.97741700
H -0.21323900	5.22632600	-2.64409000	H-5.46007700	-1.45197100	-1.59216600
H -1.91493100	5.15521600	-2.13391100	C-4.96031900	-3.53489800	-1.84193300
C -0.74033100	6.65502800	-1.11212200	H-3.93601400	-3.35685100	-2.18499200
O 0.41424800	7.18616100	-1.10649100	H-4.97713200	-4.46951200	-1.26891200
O -1.77857700	7.17021600	-0.59171000	H-5.60337600	-3.65029500	-2.72020300
H 3.43031100	-1.90515100	3.57837400	C-6.88346700	-2.61462600	-0.47926600
H 3.15068700	0.73458600	1.77556000	O-7.06097900	-2.86350700	0.75124600
P 2.62238500	-3.41020800	-2.03803700	O-7.79179900	-2.58063200	-1.36325400
O 2.54759700	-4.22346500	-0.75210100	H 7.39326500	-0.19261800	-1.13709800
O 4.01660800	-2.53611400	-2.04124400	C-3.41657800	-1.40502700	0.09638000
O 1.43889900	-2.28735000	-2.07060200	O-2.99549300	-0.91376400	-0.97951300
O 2.57113500	-4.12252500	-3.37961400	H-4.89471200	-2.44123600	1.05986400
H 4.25945700	-2.19751900	-1.14587000	C 0.58410100	3.09159900	0.13130800
H 1.34551000	-1.73204500	-1.23618600	C-0.22635100	3.80649900	-0.75165200
			C-1.58615200	4.02332700	-0.47471700
TS-P-S1			C-2.11804900	3.48473100	0.70694300
C 1.49742200	0.14926100	1.65180600	C-1.31841500	2.75636600	1.59138900
O 1.20111400	-0.02383000	0.46668700	C 0.04098700	2.56003300	1.31038500
C 2.71898000	-0.56533500	2.28486800	H 1.63651200	2.94820900	-0.09660300
C 2.86550300	-0.44772500	3.79959800	H 0.20565700	4.20623600	-1.66570400
H 2.64040700	-1.60977500	1.98993200	H-3.17070300	3.63115800	0.93778200
H 3.11064100	0.57422700	4.11010800	H-1.75180100	2.34364600	2.49789600
H 1.94186600	-0.75545500	4.29517200	S 1.07093300	1.72108500	2.50738300
N 3.91901700	-0.02087900	1.62419500	C-2.45257000	4.84724700	-1.40357300
C 4.57318400	-0.62713200	0.62565400	H-2.08493700	4.75287400	-2.43159000
O 4.35675600	-1.79863300	0.25557900	H-3.48444200	4.48748800	-1.37073100

C-2.42939400	6.34817200	-1.02911400	H-3.47280200	1.02414600	-1.64792300
O-1.34597600	6.98038900	-1.22862000	H-4.53328700	-1.43643600	1.71968300
O-3.48797200	6.85473800	-0.54374400	C-5.47238900	0.62525600	0.18457100
H 3.67524500	-1.10293400	4.13733000	H-5.37674000	1.62383700	-0.25184900
H 4.17919000	0.93667400	1.84865700	H-5.73346200	0.72612300	1.24219900
P 1.99208500	-2.83646300	-2.25447300	C-6.61326300	-0.12824400	-0.53967600
O 1.72589900	-3.78206600	-1.09267600	O-7.30672200	-0.94199900	0.14554500
O 3.59597900	-2.47836300	-2.31503100	O-6.77108000	0.10046300	-1.77872300
O 1.27440800	-1.38961100	-1.96435100	H 6.69389600	-1.02529800	-1.51524000
O 1.59787500	-3.23283800	-3.66452200	P 0.70524700	3.16261200	0.37464900
H 3.94754400	-2.23449900	-1.42330100	O 1.12644700	2.66814800	-0.99920800
H 1.34192200	-1.08665800	-1.02782500	O 1.42405700	2.25294700	1.53930200
			O-0.90508200	2.86938100	0.58502900
Int-P-S2			O 0.92567000	4.60439900	0.78049500
C 4.37015800	-1.12490500	-0.37413000	H 1.29798100	1.28989100	1.38808200
O 4.65687200	-2.16721500	-0.98763900	H-1.19015800	2.03835600	0.15948600
N 3.29204700	-0.97873300	0.41358300			
H 3.16583500	-0.10536000	0.91832800	Int-P-S2-2.2		
C 5.25360900	0.11993000	-0.51703500	C-1.02716300	-0.69259900	-1.18937700
N 6.65968500	-0.36706200	-0.72641700	O-0.94539500	-0.51493800	0.06614800
C 2.32027800	-2.04365500	0.64642500	C-2.37070200	-1.25911500	-1.74112400
C 0.91099200	-1.45659900	0.52983500	C-2.42709700	-1.60653000	-3.23090500
O 0.59115100	-0.40613300	1.06581700	H-2.57469400	-2.15164700	-1.14744200
H 7.28701400	0.41926800	-0.93094300	H-2.25757100	-0.72643300	-3.86033000
S-0.22190300	-2.45923600	-0.41663100	H-1.68809300	-2.36906700	-3.49036700
C 4.83676800	0.98875500	-1.70236800	N-3.43396100	-0.29169700	-1.42707100
H 4.84738400	0.41211100	-2.63358500	C-4.56628800	-0.57675100	-0.78591700
H 3.82749800	1.37570700	-1.53731800	O-4.89091000	-1.71628900	-0.38139500
H 5.51957500	1.83957100	-1.79826200	C-5.50400000	0.60762300	-0.52156100
H 5.26080600	0.69940600	0.40771300	H-5.41526100	1.36137500	-1.30623100
C 2.50028500	-2.68705400	2.03117400	N-6.90822800	0.07533900	-0.59795500
H 3.50563300	-3.11512500	2.09488800	H-7.14588300	-0.22929300	-1.54970500
H 2.37873400	-1.94131800	2.82349600	C-5.26753700	1.22189400	0.85667200
H 1.76936500	-3.48803300	2.18312700	H-4.25973000	1.64384600	0.89989300
H 2.47256200	-2.79526600	-0.12991600	H-5.98664700	2.02815600	1.03584200
H 7.02006600	-0.85666600	0.10139900	H-5.36665700	0.46844100	1.64540300
C-1.75115100	-1.54214800	-0.23019900	H-7.01426100	-0.73558600	0.02548600
C-2.05087000	-0.49638400	-1.11224700	S 0.36713000	-2.26532900	-1.83935200
C-2.65032900	-1.88466200	0.78762600	C 1.63356900	-2.03580400	-0.54103000
C-3.24778300	0.20849800	-0.96553800	C 2.85102800	-1.21492600	-0.99497700
H-1.35657200	-0.22875600	-1.90344900	H 1.95303200	-3.03263900	-0.21650000
C-3.84304600	-1.17236400	0.92263800	H 1.14010400	-1.55693200	0.31201300
H-2.42110300	-2.69487800	1.47381600	H 3.27715800	-1.64282300	-1.90798900
C-4.16044400	-0.11843300	0.05017900	H 2.53501100	-0.19093100	-1.22703800

N 5.16159400	-1.47276200	-0.27293200	C 2.69304900	-0.84606800	1.99407500
C 6.33248900	-1.38049100	0.59742300	C 2.77538900	-0.97900600	3.51439400
H 6.22265500	-0.48730500	1.22044700	H 2.87242600	-1.80925700	1.51661400
C 6.46569000	-2.61019300	1.51242900	H 2.73723000	-0.00222000	4.00922100
H 5.55556100	-2.74048600	2.10665600	H 1.96004100	-1.59582100	3.89937400
H 6.62951900	-3.51925700	0.92192200	N 3.75326500	0.06559200	1.52625700
H 7.30904700	-2.48313300	2.19849400	C 4.70099700	-0.24393200	0.63788000
C 7.60702600	-1.20601300	-0.26032300	O 4.91116500	-1.39293900	0.19412100
O 7.52592600	-1.41564100	-1.50808900	C 5.55725500	0.92908600	0.15074800
O 8.66113400	-0.88395700	0.36628100	H 5.71233500	1.65573300	0.95042700
H-7.58393500	0.79426700	-0.31447400	N 6.91229000	0.37800700	-0.19103400
C 3.91174100	-1.13276200	0.08934300	H 7.38232000	-0.01309900	0.63432700
O 3.62782000	-0.76224300	1.25365300	C 4.95592200	1.59919800	-1.08366700
H 5.35280200	-1.70647700	-1.24215500	H 3.98227900	2.02672700	-0.82913100
C-1.20780300	2.74385700	-0.30276200	H 5.60883400	2.40932300	-1.42519100
C-0.91631300	3.75790700	0.61122300	H 4.82141800	0.87724500	-1.89641500
C 0.39997500	4.21000700	0.79987000	H 6.82924000	-0.37441800	-0.88632200
C 1.41936900	3.60501600	0.04942100	S -0.03425300	-2.21731800	2.26028700
C 1.13652800	2.57713600	-0.85448200	C -1.20978600	-2.21267100	0.85593900
C-0.18236200	2.13454500	-1.04547400	C -2.53421900	-1.49655900	1.16901800
H-2.23817100	2.42735500	-0.43649200	H -1.41122000	-3.24989300	0.56216200
H-1.72486600	4.20713500	1.18335500	H -0.71262500	-1.72731400	0.00703100
H 2.44875800	3.93066300	0.18091100	H -2.99197200	-1.92954400	2.06460900
H 1.94622300	2.11585300	-1.41284200	H -2.33048300	-0.44026400	1.38495500
S-0.51910100	0.87384300	-2.27006100	N -4.76905100	-1.92940600	0.31080900
C 0.70574500	5.33702500	1.76617400	C -5.88944800	-1.94442600	-0.62766500
H 0.01252100	5.29587100	2.61234300	H -5.79493100	-1.07657300	-1.28765000
H 1.72689400	5.23217900	2.14453400	C -5.90316300	-3.22223700	-1.48451100
C 0.56754200	6.71571300	1.08137400	H -4.95627200	-3.32673900	-2.02408200
O-0.58478600	7.25090900	1.06659500	H -6.04442900	-4.10907700	-0.85550400
O 1.60990600	7.22050700	0.55966900	H -6.71496200	-3.18018200	-2.21770500
H-3.41937900	-2.00673200	-3.46622800	C -7.21705900	-1.80553700	0.15222400
H-3.28272000	0.66565800	-1.73757900	O -7.19526100	-1.97285000	1.40906400
P-2.51952900	-3.38127200	2.10134500	O -8.24861200	-1.55311500	-0.53988000
O-2.39514900	-4.20832600	0.82894500	H 7.51261600	1.11397200	-0.58058700
O-3.96568700	-2.59658300	2.09350700	C -3.51806500	-1.53579000	0.01098300
O-1.40793000	-2.18490800	2.11330700	O -3.17974700	-1.20588500	-1.15151100
O-2.41998700	-4.06232900	3.45619700	H -5.01134900	-2.12122400	1.27793600
H-4.23308400	-2.30096600	1.19013600	C 0.77319900	2.82931600	0.13780500
H-1.31785700	-1.66723600	1.25954100	C 0.18024000	3.68044700	-0.79536200
			C -1.19864500	3.94752000	-0.76203200
Int-P-S2-2.5			C -1.97117100	3.31910700	0.22604400
C 1.35336500	-0.32084100	1.40712600	C -1.38817100	2.45138700	1.15402500
O 1.18323600	-0.31653000	0.16964500	C -0.00816200	2.20188900	1.12133800

H	1.84425400	2.65165600	0.09995300	H	-1.33457300	-2.88805800	1.07268800
H	0.79871900	4.15026600	-1.55632700	H	-0.66935800	-1.37227100	0.45768500
H	-3.04244000	3.50233400	0.26766000	H	-3.19286100	-1.59361100	2.19902900
H	-2.00835200	1.96875400	1.90407100	H	-2.51882400	-0.09748400	1.53171400
S	0.72893300	1.17393800	2.38541900	N	-4.53501100	-2.07048100	0.12662700
C	-1.82987600	4.91436200	-1.74296900	C	-5.41938500	-2.32027400	-1.00983900
H	-1.29320400	4.87394700	-2.69701800	H	-5.43902200	-1.41780500	-1.62844400
H	-2.87424800	4.64113000	-1.91726000	C	-4.93044900	-3.49948200	-1.86943800
C	-1.76966200	6.36840500	-1.21996000	H	-3.90673300	-3.31865600	-2.21274800
O	-0.64839300	6.96261400	-1.28007800	H	-4.94389900	-4.43207300	-1.29304200
O	-2.83597100	6.87365600	-0.75028900	H	-5.57267600	-3.62058300	-2.74752300
H	3.72340000	-1.45593700	3.78499200	C	-6.85818300	-2.58166800	-0.51142400
H	3.68300100	1.03612100	1.82339000	O	-7.03559200	-2.82390400	0.72043400
P	2.63139600	-3.05646800	-2.20996300	O	-7.76579800	-2.55721700	-1.39636800
O	2.64146300	-3.95300500	-0.98008000	H	7.39204300	-0.16231900	-1.14596200
O	4.06047000	-2.24821500	-2.30631100	C	-3.39639000	-1.35607500	0.06094800
O	1.51295000	-1.87631400	-2.03117800	O	-2.97348500	-0.87226200	-1.01743400
O	2.39819900	-3.65536400	-3.58495200	H	-4.87379200	-2.38910300	1.02892100
H	4.36784300	-1.92639000	-1.42464200	C	0.61279800	3.09504900	0.12279700
H	1.50340300	-1.44202000	-1.13722500	C	-0.19534800	3.81486400	-0.75859700
				C	-1.54978100	4.05140100	-0.47246900
				C	-2.07868400	3.52781300	0.71733200
Int-P-S2-2.7				C	-1.28118700	2.79501300	1.60004200
C	1.48655100	0.13112400	1.65383900	C	0.07368500	2.57791000	1.31035100
O	1.20793000	-0.01843500	0.45700700	H	1.66138800	2.93695800	-0.11267600
C	2.72016800	-0.57543200	2.27520800	H	0.23452400	4.20303600	-1.67870300
C	2.87600400	-0.46768100	3.79010900	H	-3.12740600	3.68964100	0.95590500
H	2.65153200	-1.61883700	1.97360900	H	-1.71273200	2.39443200	2.51283200
H	3.11357100	0.55427100	4.10635200	S	1.10190200	1.73173900	2.50294500
H	1.96011800	-0.78733700	4.29256400	C	-2.41315900	4.88037400	-1.39984900
N	3.91337800	-0.01731000	1.61336100	H	-2.04684600	4.78515400	-2.42824600
C	4.57716500	-0.61895600	0.61912100	H	-3.44676900	4.52548400	-1.36659500
O	4.37729500	-1.79543100	0.25385700	C	-2.38303900	6.38062500	-1.02370200
C	5.63431200	0.23800100	-0.08280100	O	-1.29669400	7.00821200	-1.22239000
H	6.17166600	0.85277000	0.64230600	O	-3.43918500	6.89156800	-0.53748400
N	6.64849200	-0.69599000	-0.68046000	H	3.69471600	-1.11735000	4.11699000
H	7.08287300	-1.29207300	0.03406700	H	4.15862300	0.94545700	1.83237200
C	5.02831800	1.10806800	-1.18448200	P	1.99571400	-2.83501800	-2.24146400
H	4.32433000	1.81922900	-0.74377900	O	1.73568100	-3.77527700	-1.07375100
H	5.81886800	1.67378900	-1.68865200	O	3.59916500	-2.47590300	-2.31088100
H	4.49842600	0.49576400	-1.92153700	O	1.27758700	-1.38831500	-1.95618100
H	6.21170100	-1.31378400	-1.37592900	O	1.59675700	-3.24029900	-3.64784700
S	-0.23491600	-1.59493900	2.81455100	H	3.95501500	-2.23009600	-1.42136300
C	-1.22954900	-1.81786900	1.29008300	H	1.34420000	-1.08027000	-1.02005700
C	-2.62844100	-1.17492500	1.35896300				

			C -1.63830600	3.98989500	-0.47440500		
Int-P-S2-2.9			C -2.15741500	3.43596800	0.70578800		
C	1.51960200	0.18238000	1.64336700	C -1.34132200	2.72291000	1.58755000	
O	1.20421900	-0.01646200	0.47075200	C	0.02126800	2.55803200	1.30374500
C	2.72587200	-0.54481400	2.28910000	H	1.60803300	2.98571200	-0.10208400
C	2.86357700	-0.41648900	3.80344000	H	0.14827900	4.21771200	-1.66568800
H	2.63155700	-1.59033900	2.00266500	H	-3.21293900	3.55794100	0.93752400
H	3.11896500	0.60481400	4.10786400	H	-1.76456300	2.29771600	2.49307100
H	1.93160500	-0.70978600	4.29209000	S	1.07011100	1.73622000	2.49711000
N	3.93579000	-0.02243300	1.62934600	C	-2.52437500	4.79504000	-1.40096500
C	4.57984000	-0.64008900	0.63071500	H	-2.16422700	4.69913600	-2.43152100
O	4.34023700	-1.80551500	0.25744100	H	-3.55038700	4.42026100	-1.35685300
C	5.66301400	0.18929300	-0.06347500	C	-2.51986300	6.29907600	-1.03804700
H	6.21341200	0.78713200	0.66592200	O	-1.44672500	6.94462500	-1.24953200
N	6.65392600	-0.76881700	-0.66132800	O	-3.58266800	6.79487000	-0.55090200
H	7.07123800	-1.37880100	0.05166300	H	3.66248700	-1.07906400	4.15224700
C	5.08451500	1.07944800	-1.16423500	H	4.21674900	0.92815500	1.85813600
H	4.39773800	1.80728100	-0.72366200	P	1.98309400	-2.83793200	-2.26092500
H	5.89222000	1.62579200	-1.66239700	O	1.70774600	-3.78312700	-1.10110800
H	4.54183700	0.48432900	-1.90604900	O	3.58889800	-2.48795700	-2.31526700
H	6.20343000	-1.37212900	-1.36096400	O	1.27224700	-1.38685600	-1.97110900
S	-0.26655600	-1.74583700	2.86877400	O	1.59111500	-3.22940200	-3.67278100
C	-1.26273900	-1.92254000	1.33404200	H	3.93850900	-2.24598700	-1.42231000
C	-2.66632700	-1.29247300	1.42560200	H	1.34122000	-1.08639400	-1.03486300
H	-1.36498200	-2.98526400	1.07982600				
H	-0.71323800	-1.44815200	0.51059400	Int-P-S2-3.0			
H	-3.22103600	-1.73554600	2.25971700	C	1.54690500	0.23330800	1.63983100
H	-2.56392800	-0.21852200	1.62373900	O	1.20458500	-0.00720200	0.48642100
N	-4.58411100	-2.16117300	0.19190800	C	2.72075100	-0.52030500	2.31322000
C	-5.47284500	-2.39706300	-0.94397000	C	2.84535500	-0.36308100	3.82565400
H	-5.48735000	-1.49063600	-1.55680700	H	2.58670600	-1.56782700	2.04900800
C	-4.99338300	-3.57444700	-1.81133000	H	3.12816700	0.65696300	4.11064600
H	-3.96904700	-3.39832900	-2.15530500	H	1.89850100	-0.61656800	4.30718700
H	-5.01179300	-4.50998600	-1.23985800	N	3.96232900	-0.05907200	1.66919200
H	-5.63779700	-3.68681300	-2.68901600	C	4.56180800	-0.67368000	0.64207800
C	-6.91245700	-2.65171400	-0.44458100	O	4.18702800	-1.76106500	0.16066800
O	-7.08917100	-2.90349700	0.78544100	C	5.77654000	0.05586900	0.06004500
O	-7.82187900	-2.61256400	-1.32731500	H	6.36921100	0.50462800	0.86018400
H	7.41217600	-0.25317900	-1.12346200	N	6.65277100	-0.98032700	-0.58385100
C	-3.44237700	-1.45093700	0.12967400	H	6.98802700	-1.67134500	0.09747700
O	-3.02351300	-0.95527700	-0.94519600	C	5.38143000	1.10594300	-0.97755800
H	-4.91962900	-2.48956800	1.09184200	H	4.77525200	1.88145100	-0.50144600
C	0.55291300	3.10545200	0.12696100	H	6.27900300	1.57765400	-1.39110700
C	-0.27394700	3.80525200	-0.75279500	H	4.80289300	0.65658600	-1.79139200

H 6.14243200	-1.48947500	-1.31681000	C-1.69349400	3.89957400	-0.54193100
S-0.30562900	-1.73562100	2.94037700	C-2.18671200	3.35245800	0.65252500
C-1.29854200	-1.93101200	1.40358300	C-1.34064100	2.69255500	1.54718400
C-2.71099600	-1.32108000	1.49564700	C 0.02596400	2.57426500	1.26054300
H-1.38796500	-2.99585200	1.15246800	H 1.59127800	3.03461200	-0.15912600
H-0.75776700	-1.45230300	0.57672200	H 0.07991300	4.17499400	-1.74281500
H-3.25370600	-1.76438900	2.33755900	H-3.24586200	3.43608600	0.88457800
H-2.62380300	-0.24386200	1.68365800	H-1.74454300	2.27050600	2.46287300
N-4.62835900	-2.22251800	0.28563200	S 1.10877600	1.80093200	2.45775200
C-5.52310000	-2.47896500	-0.84097400	C-2.61583300	4.64080200	-1.48633600
H-5.54869900	-1.57988800	-1.46418200	H-2.25568400	4.53042400	-2.51541100
C-5.04063400	-3.66243700	-1.69854300	H-3.62468300	4.22403800	-1.42647300
H-4.01992400	-3.48263900	-2.05125300	C-2.67508900	6.15398800	-1.16821600
H-5.04840200	-4.59203500	-1.11715700	O-1.63372200	6.84000300	-1.40892500
H-5.69003500	-3.78895300	-2.57057100	O-3.75556200	6.61684500	-0.68759800
C-6.95749900	-2.73898000	-0.32943900	H 3.61944000	-1.04200200	4.19826000
O-7.12490500	-2.97600000	0.90482400	H 4.36621200	0.81098700	2.00741100
O-7.87229600	-2.71912400	-1.20722400	P 1.90820400	-2.55818900	-2.54315200
H 7.47190300	-0.53618500	-1.01546000	O 1.64579700	-3.67318200	-1.54188500
C-3.49327600	-1.50297100	0.20699800	O 3.49764900	-2.14213400	-2.49408200
O-3.08579200	-1.01743700	-0.87688300	O 1.12767600	-1.19216400	-2.07319800
H-4.95523300	-2.54176000	1.19201700	O 1.56631500	-2.75228100	-4.00767500
C 0.53325100	3.11829000	0.07185600	H 3.81759800	-2.02131500	-1.56625800
C-0.32311500	3.76609400	-0.81972300	H 1.22827900	-0.98328200	-1.11734400