

Supporting Information

**Mechanism for the Enhanced Reactivity of 4-Mercaptopropyl
Thioesters in Native Chemical Ligation**

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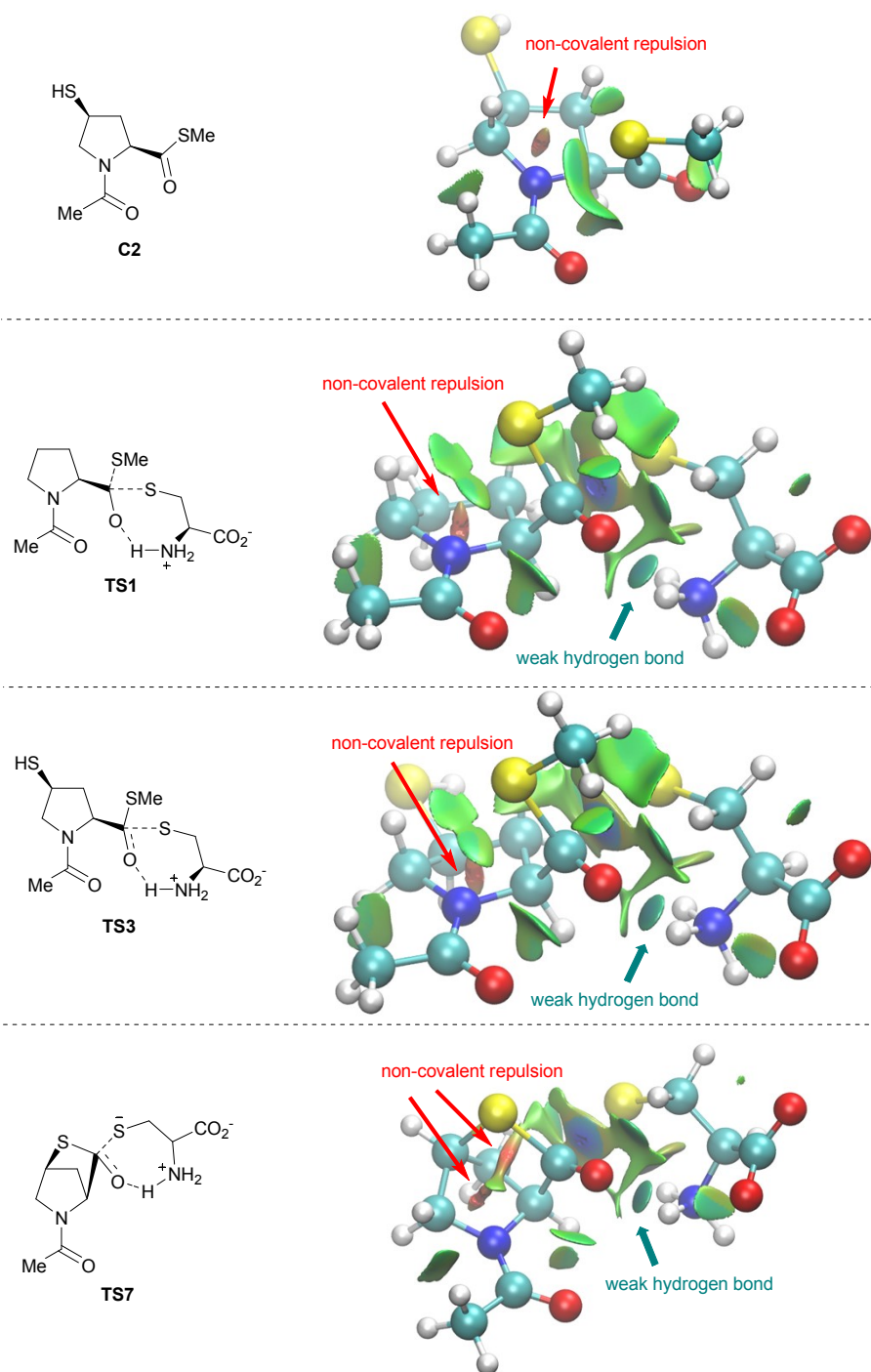


Fig. S1 NCIplot of C2, TS1, TS3 and TS7. Light green areas indicate weak van der Waals interactions. Blue areas indicate typical hydrogen bonds while the blue-green area here indicates a weak hydrogen bond. Red areas indicate relative strong non-covalent repulsion.

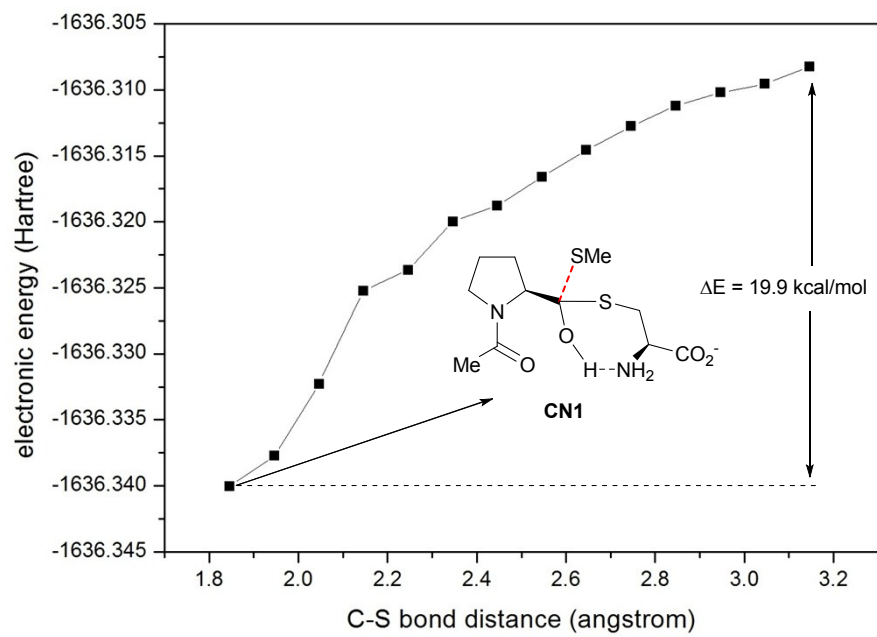
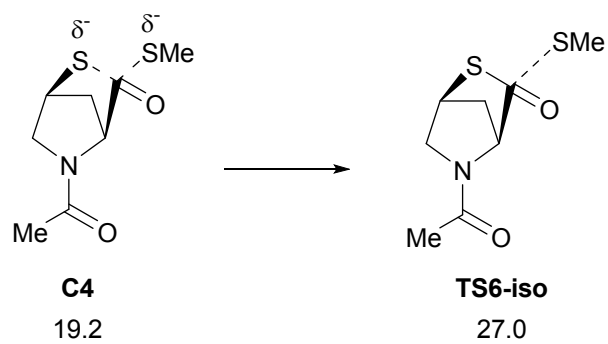


Fig. S2 Potential energy scan for the C-SMe bond cleavage on CN1.



Scheme S1 Direct thiolate release on **C4** (free energy in kcal/mol).

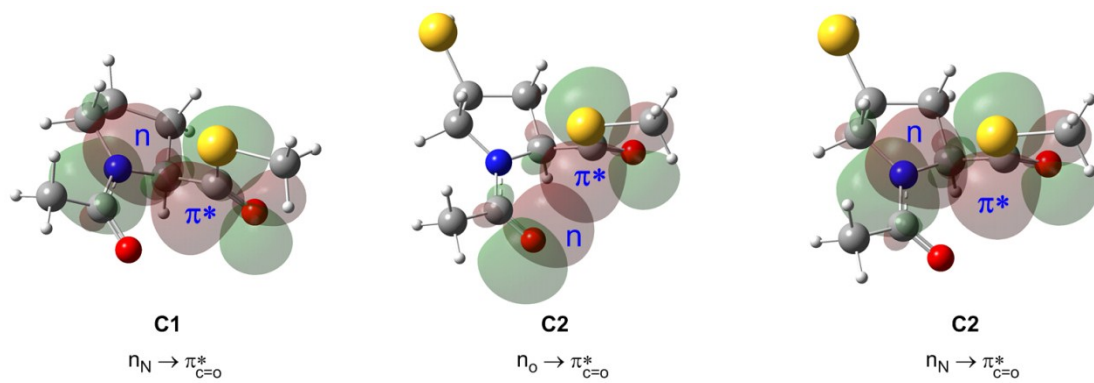


Fig. S3 Orbital overlaps of the $n \rightarrow \pi^*$ interactions in **C1** and **C2**.

Table 1. Calculated Gibbs free energies corrections, solution-phase single point energies and solution-phase Gibbs free energies of all intermediates and transition states (in Hartree).^a

compounds	Gibbs free energy corrections	solution-phase single point energies	solution-phase Gibbs free energies
N1	0.076525	-721.9567939	-721.8772411
H ₂ PO ₄ ⁻	0.008859	-643.7987837	-643.7868969
N2	0.066793	-721.4876619	-721.4178411
H ₃ PO ₄	0.018371	-644.2424875	-644.2210886
C1	0.16732	-916.0876542	-915.9173064
TS1	0.257715	-1637.570798	-1637.310055
CN1	0.259054	-1637.584111	-1637.322029
TS2	0.296301	-2281.82553	-2281.526201
MeSH	0.021885	-438.6836487	-438.6587358
CN2	0.225177	-1199.362015	-1199.13381
C2	0.164024	-1314.275411	-1314.108359
TS3	0.255366	-2035.759727	-2035.501333
CN3	0.255014	-2035.773074	-2035.515032
TS4	0.293339	-2680.015291	-2679.718924
CN4	0.221424	-1597.54972	-1597.325269
C3	0.154785	-1313.800097	-1313.642284
TS5	0.156836	-1313.787892	-1313.628028
C4	0.155946	-1313.788319	-1313.629345
TS6	0.194411	-1958.039228	-1957.841789
TS6-iso	0.154759	-1313.774682	-1313.616896
C5	0.123156	-875.573511	-875.4473272
TS7	0.212776	-1597.063978	-1596.848174
CN5	0.212646	-1597.080926	-1596.865252
TS8	0.252613	-2241.327006	-2241.071365

^aNote that the free energy changes for the deprotonation of thiols **N1** and **C2** were calculated according to the experimental Pka but not the calculated solution-phase Gibbs free energies.

Cartesian coordinates of intermediates, transition states and MECPs

N1

N	-0.16941100	1.60063500	0.06353700
H	-0.02328100	1.67740100	1.08005600
C	-0.26012500	0.17815000	-0.35552800
H	-0.13211400	0.16503700	-1.44731900
C	0.80231000	-0.67560700	0.30473800
C	-1.70459000	-0.30923300	-0.05262100
H	0.66807500	-0.69315500	1.39556400
H	0.67599600	-1.70134300	-0.06023300
S	2.51856300	-0.20231500	-0.09725400
O	-2.56039100	0.59292100	0.06943500
O	-1.86724500	-1.53936400	0.00224300
H	0.58349600	2.11239200	-0.41202900
H	-1.08683600	2.03090900	-0.13766300
H	2.59905500	0.85304300	0.73996500

H₂PO₄⁻

P	-0.00007100	0.09341200	0.12232200
O	-1.27904500	-0.36601800	-0.79456000
H	-1.51571000	-1.28869500	-0.61834300
O	1.27974600	-0.36318600	-0.79468700
H	1.51928400	-1.28496900	-0.61775000
O	-0.00182500	1.59323600	0.12413700
O	0.00081000	-0.71747200	1.39026800

N2

N	0.14837800	1.48054500	-0.32623400
H	-0.35239000	1.84211300	0.49782800
C	-0.24375300	0.06856200	-0.50772900
H	-0.15410400	-0.17625400	-1.57266300
C	0.74423800	-0.79533400	0.30448400
C	-1.68097500	-0.16063600	-0.01541000
H	0.43096400	-0.75502600	1.36369300
H	0.59915300	-1.83415200	-0.02709200
S	2.45998500	-0.21391800	0.10121500
O	-2.16824100	0.71930700	0.73142600
O	-2.20328200	-1.24168900	-0.35508100
H	1.21200500	1.41428000	-0.16638100
H	-0.07892000	2.07140600	-1.13000300

H₃PO₄

P	-0.00025100	-0.00030900	0.11143500
O	-0.53342300	-1.32658500	-0.59309800
H	-0.27034000	-2.13914800	-0.12791300
O	1.42259200	0.20169300	-0.57761000
H	1.98828000	0.84073200	-0.11118600
O	-0.00831600	-0.00646300	1.59250400
O	-0.88023800	1.13138000	-0.58529700
H	-1.71910000	1.30284600	-0.12442400

C1

C	-2.05350200	-0.62410200	-0.86483500
C	-0.28620000	-0.81070900	0.79415800
C	-0.55643900	-2.18770300	0.15514000
C	-1.99054600	-2.06336200	-0.36216400
H	-3.07021500	-0.21305200	-0.85892500
H	-1.64611300	-0.53379800	-1.88568800
H	-0.47973000	-0.81135900	1.87795100
H	0.13293900	-2.34139200	-0.68875900
H	-0.41008200	-3.00203600	0.87382600
H	-2.70283400	-2.19502200	0.46507300
C	1.17157600	-0.40415900	0.63087000
O	2.00049400	-0.60252200	1.48408300
S	1.57709400	0.28057100	-0.96073600
C	3.36169500	0.44185900	-0.73250400
H	3.81743900	-0.54029300	-0.55966400
H	3.75642600	0.87638500	-1.65845200
H	3.57468100	1.11106700	0.10947600
N	-1.20052100	0.07881200	0.09635400
C	-1.21964400	1.39752200	0.39921000
O	-0.47927600	1.84863300	1.27304200
C	-2.17624000	2.25611300	-0.38145200
H	-2.03359100	2.11084900	-1.46141300
H	-3.21381200	1.98472100	-0.13800900
H	-2.00367700	3.30514100	-0.11981400
H	-2.22523000	-2.79368400	-1.14584600

TS1

C	3.72892800	-0.30428600	-0.71997900
C	1.32869500	0.08336300	-0.80158600
C	1.70384300	-1.11969800	-1.68580400
C	3.19325400	-0.95254900	-1.98934400
H	4.65615000	0.25734200	-0.88089100
H	3.90998800	-1.05375100	0.07049700

H	0.80419900	0.87633500	-1.35630400	C	-0.37391200	-0.72240000	-0.18944800
H	1.53022100	-2.04285600	-1.11556100	S	-1.39665500	-2.06120700	-0.94425100
H	1.07388900	-1.16186700	-2.58066300	C	-0.13357700	-2.81220000	-1.98995200
H	3.34262600	-0.26829800	-2.83764800	H	0.70333300	-3.16397300	-1.37059900
C	0.44653100	-0.24114400	0.42367400	H	-0.59960900	-3.66850500	-2.49394300
S	1.24696700	-1.46812800	1.51593000	H	0.22408200	-2.09861900	-2.74205200
C	-0.15096500	-1.77495400	2.61169500	N	-2.39327000	0.74692400	0.04994800
H	-0.95765100	-2.23311100	2.02207800	C	-2.26901100	1.97333200	-0.51414600
H	0.18674300	-2.46979900	3.39055600	O	-1.18986900	2.56359300	-0.56104900
H	-0.49212000	-0.84080400	3.07469400	C	-3.52097800	2.60468300	-1.07317600
N	2.63358000	0.59088900	-0.34413700	H	-4.10642600	1.89427100	-1.67058000
C	2.76153500	1.74755700	0.34475700	H	-4.15593500	2.96395100	-0.24959100
O	1.79845200	2.48399900	0.55642300	H	-3.22686300	3.45959900	-1.69115200
C	4.14741000	2.09899900	0.82529500	O	0.19171700	0.01770800	-1.19408400
H	4.59722100	1.26444400	1.38032000	S	0.94064000	-1.51606400	0.91703800
H	4.79983700	2.32742400	-0.03007700	C	2.49363900	-0.88659300	0.21095000
H	4.07731700	2.98182200	1.46928700	C	2.86750300	0.54193100	0.60396100
O	-0.34740400	0.56308900	0.89857300	H	2.45669100	-0.99021700	-0.88340000
S	-1.23385700	-1.77002600	-0.86160400	H	3.26295000	-1.57259900	0.58711400
C	-2.64722800	-0.98132500	-0.04331400	N	1.91472300	1.52265500	0.07618300
C	-3.24462500	0.17942700	-0.84023700	H	2.89914000	0.59131000	1.70392600
H	-2.32068400	-0.57836800	0.93176900	C	4.31399700	0.83793700	0.11793600
H	-3.45723600	-1.69750700	0.15308300	H	2.46320400	2.20053300	-0.46015900
N	-2.14035100	1.05859900	-1.29112900	H	0.81802200	0.71376400	-0.75984600
H	-3.74781600	-0.19587800	-1.74234200	H	1.46311200	2.04125400	0.82892900
C	-4.24096100	0.99568500	0.00076600	O	4.49582000	1.88775000	-0.53757300
H	-2.48788800	1.88830100	-1.78095400	O	5.18249400	-0.00368200	0.43404900
H	-1.58936500	1.35275000	-0.46524000	H	-4.06481900	-1.05477200	2.25577200
H	-1.50083600	0.49168200	-1.87279700				
O	-3.96842000	2.20199100	0.18811500				
O	-5.22473200	0.36123500	0.43330600				
H	3.69139700	-1.90276400	-2.21901800				

CN1

C	-3.65816600	0.12482400	0.44908000
C	-1.26854600	0.12128700	0.75215000
C	-1.92006200	-0.68976500	1.89562900
C	-3.39263400	-0.26343300	1.90123100
H	-4.49676500	0.81931000	0.33759000
H	-3.85826000	-0.76179600	-0.17418400
H	-0.61890300	0.91977500	1.13813600
H	-1.83539000	-1.76587200	1.68757000
H	-1.41976100	-0.49894800	2.85227500
H	-3.53255000	0.62024300	2.54066500

TS2

C	3.82158300	-1.65286200	0.04811600
C	2.18949100	-0.17709100	-0.93571200
C	1.97683400	-1.57618900	-1.54068300
C	3.25012800	-2.36070800	-1.18170900
H	4.91333800	-1.73019400	0.10020800
H	3.38728000	-2.04690100	0.97751300
H	2.33794900	0.58532500	-1.72059200
H	1.08242100	-2.03962600	-1.10376500
H	1.82649300	-1.51872800	-2.62602900
H	3.97494400	-2.29521600	-2.00539200
C	1.00861200	0.39187000	-0.14001800
S	0.69231700	-1.66688600	1.43991900
C	-0.16802700	-0.64157000	2.66498100
H	-1.25280600	-0.63312600	2.49004200

H	0.01607600	-1.01122800	3.68398700	C	2.94377200	-1.76601000	-0.11173400
H	0.20956600	0.39157200	2.60225800	C	4.16908100	-0.88492700	0.13188600
N	3.40943700	-0.26202600	-0.15230900	H	4.20352200	1.30608900	0.33175000
C	4.16421500	0.83774100	0.07567700	H	3.31629800	0.45960500	1.62931800
O	3.82714600	1.95088500	-0.33099500	H	2.03825900	-0.81895400	-1.87840900
C	5.44757200	0.63480300	0.84148100	H	2.53295300	-2.11219300	0.84940900
H	5.29011500	0.00997500	1.73024300	H	3.13880200	-2.64266200	-0.73954400
H	6.19066500	0.13520900	0.20212700	H	4.73160000	-0.75637700	-0.80399700
H	5.83423400	1.61615800	1.13579300	C	0.50235900	-1.16357200	-0.48442500
O	1.13638800	1.28273900	0.68988400	O	-0.20601700	-1.71867300	-1.28212000
S	-0.52237900	0.26070100	-1.12984500	N	2.32610300	0.50159700	-0.24210500
C	-1.59997000	1.38433800	-0.19673400	C	1.53323300	1.57477700	-0.40854500
C	-1.56523700	2.82639800	-0.66989300	O	0.49050900	1.48846800	-1.07467200
H	-1.33264500	1.30978200	0.86733800	C	1.95230700	2.84523500	0.27087700
H	-2.62292000	1.00807400	-0.30930900	H	2.01599000	2.68080400	1.35669600
N	-0.20924600	3.42720100	-0.54770800	H	2.94377200	3.16556200	-0.07819200
H	-1.85924000	2.88378000	-1.72641200	H	1.21588800	3.62590200	0.05479500
C	-2.55881300	3.71118300	0.13414000	S	-0.05330000	-0.76383600	1.17443100
H	-0.36465600	4.36956300	-0.14139300	C	-1.84096200	-0.96379700	0.90366000
H	0.39011600	2.86679500	0.08816500	C	-2.42537200	0.04006200	-0.07681900
H	0.27551100	3.50419100	-1.44815800	H	-2.29741900	-0.85548700	1.89788500
O	-2.10704200	4.79903500	0.55372900	H	-2.04627000	-1.97512800	0.53623300
O	-3.70679900	3.25402600	0.26055800	N	-2.04525500	1.44005500	0.23500100
H	-0.70896000	-2.39190800	0.50435100	H	-2.05111500	-0.16265500	-1.08991700
O	-1.47486600	-2.87830200	-0.07407900	C	-3.97473600	-0.04672500	-0.14130400
P	-2.89093600	-2.22322400	-0.03780000	H	-2.03133800	1.61666700	1.24799100
O	-3.17517500	-1.69363300	-1.53036900	H	-1.12044000	1.68378500	-0.17163400
O	-3.81456600	-3.53299900	0.07575900	H	-2.79398500	2.03167200	-0.16243300
O	-3.16244400	-1.18338700	0.99523000	O	-4.57022100	1.04296900	-0.27574600
H	-3.61042400	-0.82607900	-1.53464600	O	-4.45946000	-1.18950000	-0.08631800
H	-4.76221100	-3.32858300	0.01294800	H	4.84506400	-1.29407500	0.89191700
H	3.04938800	-3.42215100	-0.98894900				

MeSH

S	-0.66148100	-0.08731200	0.00000300
C	1.15305000	0.01931200	0.00000700
H	1.52239800	0.52782400	0.89846700
H	1.52537400	-1.01270100	-0.00009900
H	1.52239100	0.52790600	-0.89841100
H	-0.90476700	1.23808900	-0.00004300

CN2

C	3.55829400	0.44751900	0.55400700
C	1.94982200	-0.80070500	-0.78130100

C2

C	-1.57037400	0.85571000	-0.42204900
C	0.04961800	-0.16623100	1.07704000
C	-1.11020200	-1.14408300	0.80958500
C	-2.26128300	-0.21713100	0.41961100
H	-2.12309400	1.80279800	-0.42873000
H	-1.43400300	0.51697400	-1.46462600
H	0.12856200	0.10467300	2.14069700
H	-0.86572100	-1.79239000	-0.04528800
H	-1.33228800	-1.77306600	1.67937700
H	-2.68550500	0.25385700	1.31635100
S	-3.60268700	-1.00239500	-0.52636300

H	-4.08034900	-1.74469300	0.49289800
C	1.39268300	-0.77750700	0.69556100
O	2.11678100	-1.30766500	1.50038800
S	1.75143500	-0.74114100	-1.04677900
C	3.31195100	-1.64925900	-1.01261400
H	3.16166500	-2.65713400	-0.60800500
H	3.66066900	-1.71209600	-2.05016500
H	4.04840300	-1.10680900	-0.40779800
N	-0.28679500	0.99004200	0.26012700
C	0.55943600	2.04865700	0.21041200
O	1.59137300	2.04693200	0.87830800
C	0.17223600	3.18017800	-0.69950400
H	0.00447000	2.80675400	-1.71980300
H	-0.76071500	3.64773300	-0.35317500
H	0.97585900	3.92355000	-0.70017400

TS3

C	3.39219800	0.26913200	-0.28068000
C	0.98391300	0.16683900	-0.62733500
C	1.59666600	-1.24082000	-0.71348100
C	3.06881900	-1.01069000	-1.04491200
H	4.25777200	0.79936300	-0.69372700
H	3.58354100	0.05553500	0.78716700
H	0.44473500	0.45752400	-1.54183600
H	1.51222600	-1.73085000	0.26670200
H	1.08103200	-1.86456400	-1.45123500
H	3.19837100	-0.82151300	-2.11919300
S	4.19271100	-2.35566200	-0.54911900
H	3.67869600	-3.28393200	-1.38160400
C	0.00371400	0.39127100	0.54551600
S	0.82076100	0.11749400	2.15273300
C	-0.64851300	0.15922500	3.19644400
H	-1.27694700	-0.70684400	2.94520900
H	-0.31275100	0.09408800	4.23867300
H	-1.19985900	1.09559700	3.04630600
N	2.16284600	1.03475300	-0.45524500
C	2.07408400	2.38686700	-0.45513000
O	1.01097800	2.95887800	-0.68571200
C	3.34348000	3.14803800	-0.16953100
H	3.81915600	2.78653400	0.75253600
H	4.05990700	3.02030300	-0.99396100
H	3.09559200	4.20993800	-0.07028000
O	-0.95771900	1.14564300	0.46819000
S	-1.26406400	-1.90386700	0.27292400

C	-2.87388000	-1.09422600	0.47530500
C	-3.52141400	-0.68956900	-0.84841700
H	-2.74649700	-0.17686000	1.07724600
H	-3.58888600	-1.73626100	1.00785900
N	-2.51371300	0.02236400	-1.66990100
H	-3.82185300	-1.58394500	-1.41260200
C	-4.74839900	0.21653400	-0.64293800
H	-2.91959300	0.38555000	-2.53767200
H	-2.12525800	0.80848600	-1.11921700
H	-1.72378300	-0.62231000	-1.83706200
O	-4.72384100	1.33596300	-1.19989700
O	-5.65117900	-0.25657400	0.07730100

CN3

C	3.19279600	0.64685900	0.11984100
C	0.89410900	0.25623000	-0.47782200
C	1.79261500	-0.68456200	-1.31072300
C	3.18970700	-0.06127400	-1.23557300
H	3.93758500	1.44721300	0.17366600
H	3.38297700	-0.06761000	0.93938200
H	0.22811700	0.85589400	-1.11385700
H	1.81556200	-1.68859600	-0.86351800
H	1.43762700	-0.78143400	-2.34350600
H	3.31037900	0.69712500	-2.02058000
S	4.57432600	-1.24032000	-1.34157900
H	4.34862000	-1.61513700	-2.61700100
C	-0.03239800	-0.48241500	0.51951100
S	1.00254200	-1.48258500	1.67491000
C	-0.31696500	-2.13926800	2.71479100
H	-1.03155100	-2.70143400	2.09734600
H	0.15222300	-2.81838000	3.43799400
H	-0.82886900	-1.33146600	3.25148800
N	1.83059400	1.16408900	0.19204500
C	1.49595200	2.45427900	0.45421100
O	0.37018600	2.89090000	0.22446800
C	2.57349500	3.33760500	1.03185800
H	3.09546300	2.84986600	1.86516800
H	3.31670900	3.57791500	0.25717000
H	2.10614600	4.26675200	1.37414500
O	-0.80883200	0.37216100	1.25506200
S	-1.08092800	-1.65947600	-0.52735900
C	-2.77627800	-1.11342600	-0.16128400
C	-3.24462200	0.13664000	-0.90573900
H	-2.87808100	-0.97746400	0.92544400

H	-3.40794300	-1.96158200	-0.45438800
N	-2.48717200	1.32706400	-0.50863400
H	-3.13062700	-0.05093400	-1.98497300
C	-4.76725100	0.32516600	-0.65614600
H	-3.17757900	2.01934400	-0.20422000
H	-1.44041100	0.86797400	0.60512300
H	-1.99307700	1.73232900	-1.30315300
O	-5.14654100	1.44218600	-0.24034200
O	-5.48846600	-0.66716600	-0.89652600

TS4

C	-3.82098200	-0.12599600	0.25963800
C	-1.81538600	-0.86482800	-0.85747900
C	-2.14102800	0.54908100	-1.36488200
C	-3.60212100	0.78101500	-0.95587100
H	-4.86603300	-0.44407400	0.34293700
H	-3.51498000	0.37635600	1.19035900
H	-1.73569600	-1.58642200	-1.68932200
H	-1.48722400	1.28576000	-0.88054500
H	-2.01072100	0.63291300	-2.45125800
H	-4.27281600	0.45357600	-1.76039800
S	-4.02100700	2.50336000	-0.52875200
H	-4.03567700	2.97021700	-1.79342500
C	-0.46341400	-1.01408200	-0.15056700
S	-0.89395000	0.87631800	1.64152500
C	0.38173500	0.17838400	2.72717100
H	1.36752400	0.62314600	2.53246800
H	0.13134400	0.34812700	3.78434800
H	0.44481300	-0.90931900	2.56214000
N	-2.94305600	-1.25609800	-0.02636800
C	-3.25018400	-2.56533700	0.14943600
O	-2.55987200	-3.45887800	-0.33813200
C	-4.48409000	-2.87128000	0.95969500
H	-4.51079800	-2.28618300	1.88822700
H	-5.38524900	-2.62762800	0.37757700
H	-4.48909100	-3.94175900	1.19017000
O	-0.20559100	-1.94680200	0.59797700
S	0.84858500	-0.22575600	-1.13903400
C	2.32113000	-0.84310500	-0.27562200
C	2.88470300	-2.14736800	-0.81146600
H	2.07966800	-0.92873600	0.79376800
H	3.09051600	-0.06960900	-0.38191500
N	1.95186500	-3.28933200	-0.61101200
H	3.09111100	-2.05842900	-1.88571400

C	4.22416800	-2.49254700	-0.09920200
H	2.51478500	-4.00259400	-0.10454300
H	1.13113800	-3.01191400	-0.03726700
H	1.61024600	-3.68765400	-1.49178800
O	4.29430400	-3.63049200	0.41465900
O	5.08745100	-1.60009000	-0.11550700
H	-0.00980400	2.18473500	0.72469700
O	0.42584300	2.98062300	0.14170300
P	1.98516900	3.00959200	0.08710100
O	2.38512500	2.76194300	-1.45184700
O	2.25542100	4.57924800	0.29505000
O	2.73788200	2.12104800	1.01761400
H	3.11138300	2.12442100	-1.54308400
H	3.19660000	4.81002500	0.23063600

CN4

C	2.91674400	-0.91771200	-0.27635000
C	1.37535700	0.37764600	1.09493700
C	2.51971300	1.27412400	0.59323100
C	3.64706800	0.27525200	0.33850100
H	3.45042600	-1.86319600	-0.12224400
H	2.75533100	-0.77188000	-1.35882700
H	1.38483300	0.27231600	2.19007000
H	2.23836400	1.75084000	-0.35864500
H	2.78158900	2.05507100	1.31629600
H	4.09751900	-0.03263000	1.29149500
S	4.96190300	0.85916900	-0.77525300
H	5.47519100	1.76798200	0.07823600
C	0.00396100	0.94365500	0.74808900
O	-0.70219500	1.48083200	1.55916300
N	1.64156700	-0.90166600	0.44213300
C	0.71673500	-1.88186100	0.43343500
O	-0.35614200	-1.73190200	1.03371900
C	1.04557200	-3.12185600	-0.34273200
H	1.24936300	-2.86546300	-1.39267300
H	1.94625700	-3.60086500	0.06679200
H	0.20099200	-3.81580900	-0.28472600
S	-0.44960800	0.80342700	-0.98105000
C	-2.22457800	1.16589300	-0.82123500
C	-2.98985300	0.12600400	-0.01986100
H	-2.59929700	1.21980200	-1.85361900
H	-2.36140300	2.14646800	-0.35273100
N	-2.72306000	-1.26031400	-0.47533000
H	-2.69117600	0.16969200	1.03673300

C	-4.52360800	0.37138000	-0.06483800
H	-2.59241600	-1.30868600	-1.49410500
H	-1.88821900	-1.66369300	-0.00663400
H	-3.57685100	-1.79958900	-0.25056300
O	-5.23107100	-0.65734500	-0.10634300
O	-4.88802300	1.55801700	-0.02037400

C3

C	-1.59338400	0.81195100	-0.44265000
C	0.01926100	-0.16944100	1.07729100
C	-1.13968600	-1.14915200	0.80165800
C	-2.31595300	-0.25060000	0.38892100
H	-2.14812800	1.75708700	-0.50002400
H	-1.43545700	0.43023500	-1.46654800
H	0.09541300	0.10154900	2.14175500
H	-0.89388500	-1.79281700	-0.05745000
H	-1.35930200	-1.78895600	1.66522000
H	-2.67030600	0.25773500	1.30544600
S	-3.67263800	-1.08650200	-0.46937600
C	1.36258300	-0.77246000	0.70073200
O	2.08882000	-1.31065800	1.50039500
S	1.72854600	-0.72760000	-1.04361200
C	3.28826700	-1.63705000	-1.00855100
H	3.13745400	-2.64617000	-0.60696800
H	3.64011000	-1.69826000	-2.04523400
H	4.02514000	-1.09828000	-0.40079700
N	-0.31726200	0.98611900	0.25743400
C	0.52152900	2.04285900	0.21011800
O	1.54994100	2.06200100	0.89031700
C	0.14034700	3.16681900	-0.71477800
H	-0.01125400	2.78513300	-1.73456300
H	-0.80047600	3.63156100	-0.38669000
H	0.93914000	3.91569300	-0.71051400

TS5

C	1.72560600	1.44858500	-0.08133600
C	0.24944000	-0.13154900	0.97029600
C	-0.01571700	1.26605900	1.51562100
C	0.35419400	2.04549500	0.24947200
H	2.52990900	1.92015900	0.50941000
H	1.96537500	1.54061000	-1.14838800
H	0.30178800	-0.93438800	1.71965700
H	-1.05737700	1.41255100	1.82223600
H	0.66018100	1.49176200	2.35506300

H	0.38875100	3.13505300	0.37379100
S	-0.86927400	1.54173400	-1.01410700
C	-0.80331900	-0.52348000	-0.09776800
O	-0.54234400	-1.37803000	-0.96138700
N	1.54332600	0.04640400	0.31783800
C	2.37238800	-0.97610500	0.03726900
O	2.13823000	-2.13349800	0.39521700
C	3.62223600	-0.61646300	-0.72679100
H	3.35893100	-0.31175400	-1.75042900
H	4.14943500	0.22327200	-0.25344300
H	4.27764400	-1.49290800	-0.76783600
S	-2.47697500	-0.67189000	0.75495400
C	-3.44797200	-0.89730900	-0.74511200
H	-4.47948900	-1.14143400	-0.46184600
H	-3.43895800	0.03210400	-1.33508600
H	-3.02771800	-1.71652300	-1.34209400

C4

C	1.71925300	1.45251600	-0.09629600
C	0.25001600	-0.12338500	0.96806800
C	-0.01449900	1.27504200	1.51147600
C	0.34463900	2.04154500	0.23450000
H	2.52148200	1.93954100	0.48431400
H	1.95377700	1.53302700	-1.16552300
H	0.29402000	-0.93136400	1.71142700
H	-1.05444700	1.42102100	1.82386500
H	0.66769600	1.51089600	2.34269400
H	0.36190800	3.13362500	0.33400100
S	-0.88081800	1.49414500	-1.01035100
C	-0.79753600	-0.49249800	-0.11849400
O	-0.53550500	-1.37075100	-0.96817500
N	1.54819800	0.05437300	0.32208100
C	2.38012300	-0.96704200	0.04603300
O	2.15298100	-2.12241200	0.41488800
C	3.62559800	-0.60812500	-0.72547400
H	3.35740200	-0.31856000	-1.75229100
H	4.14795700	0.24136900	-0.26433600
H	4.28720800	-1.48029300	-0.75728500
S	-2.47305700	-0.66993700	0.76069400
C	-3.45422800	-0.88953400	-0.73372000
H	-4.47990600	-1.15454600	-0.44753000
H	-3.46759400	0.04551900	-1.31494100
H	-3.02490200	-1.69397400	-1.34469800

TS6

C	2.89847700	-1.79215100	0.21634600
C	1.86019000	0.06054200	-0.91561300
C	1.03424400	-1.20085600	-1.11973600
C	1.36816300	-1.83256300	0.23465600
H	3.30821500	-2.63470600	-0.36403700
H	3.33075900	-1.80697400	1.22494200
H	1.99065700	0.74354500	-1.76087100
H	-0.03250500	-1.01049500	-1.26801300
H	1.42938300	-1.80672700	-1.94742600
H	0.94402600	-2.82265600	0.43152500
S	0.75787100	-0.60881600	1.46919200
C	1.29960500	0.79499800	0.32362700
O	1.76988700	1.81804000	0.79663900
N	3.13878100	-0.51012800	-0.46569900
C	4.28452000	0.20685400	-0.43648800
O	4.35267200	1.33707000	-0.91917500
C	5.46787100	-0.46748000	0.20682700
H	5.31780600	-0.50971300	1.29606800
H	5.58804700	-1.49690000	-0.15665600
H	6.36894600	0.11584300	-0.00994400
S	-0.80044400	1.50604700	-0.63399300
C	-1.26143300	2.20400000	0.97531200
H	-2.08868800	2.91910700	0.87158800
H	-1.57292600	1.41090500	1.67334800
H	-0.39390500	2.72879500	1.40439400
H	-1.77991700	-0.06648900	-0.30174300
O	-2.44210600	-0.84860700	-0.06156200
P	-3.92248200	-0.32908700	-0.07036100
O	-4.18201300	0.02863400	-1.61516300
O	-4.71586200	-1.69378600	0.20650500
O	-4.29975100	0.78043600	0.84688200
H	-4.86450300	0.71104300	-1.72383400
H	-5.57091700	-1.53743800	0.64020700

C5

C	-0.20829800	-1.64114300	-0.13739000
C	0.26584700	0.36491700	1.10132300
C	1.27846600	-0.71287600	1.46101800
C	1.28437100	-1.38468200	0.08378700
H	-0.52819700	-2.54161900	0.40846700
H	-0.46793600	-1.75334500	-1.19700400
H	-0.11762500	1.01527200	1.89238600
H	2.25169300	-0.30791100	1.76160900

H	0.88990000	-1.38933600	2.23427500
H	1.92997600	-2.25878000	-0.04378700
S	1.82065300	-0.02676800	-1.04974700
C	0.93695300	1.16286600	-0.02297500
O	0.86630700	2.34014000	-0.23741900
N	-0.78846200	-0.41957600	0.44420200
C	-1.94629700	0.17570600	0.05169300
O	-2.19854400	1.33384900	0.37002300
C	-2.87781400	-0.66410000	-0.77773100
H	-2.49372000	-0.71708800	-1.80795100
H	-2.95224800	-1.68850900	-0.39022400
H	-3.86452100	-0.18939700	-0.79042500

TS6-iso

C	1.80193200	1.48010500	0.15427000
C	0.28146400	-0.23750700	0.88685600
C	-0.13909800	1.10289400	1.46739600
C	0.34946000	1.94617800	0.28773500
H	2.44475400	1.99046400	0.88901300
H	2.20751300	1.64246600	-0.85275500
H	0.20754200	-1.13270400	1.50971800
H	-1.22200600	1.14164000	1.62277800
H	0.41832900	1.34137300	2.38433900
H	0.22328800	3.03078700	0.36555900
S	-0.61409200	1.28806100	-1.14337300
C	-0.47377800	-0.40090000	-0.44051400
O	-0.56372200	-1.39535700	-1.11837100
N	1.66696800	0.04875500	0.46741900
C	2.52146300	-0.93416900	0.10071600
O	2.23084300	-2.12162600	0.23815400
C	3.84026000	-0.48769100	-0.47352800
H	3.68374700	-0.10056600	-1.49164300
H	4.28832600	0.31537900	0.12658900
H	4.51646700	-1.34797500	-0.51741000
S	-2.98289300	-0.66219900	0.89554600
C	-3.65163400	-0.44910100	-0.78193300
H	-2.89862400	-0.69858500	-1.55334500
H	-4.51985300	-1.10401700	-0.96978000
H	-3.98387400	0.58367100	-0.98401300

TS7

C	3.50528000	-0.24665600	0.24570600
C	1.36948900	-0.24907500	-0.86558600
C	2.07029900	-1.57798300	-1.09452500

C	2.80138800	-1.60706000	0.25076500
H	4.43203000	-0.28790900	-0.34852100
H	3.74300400	0.10943500	1.25615600
H	0.82916400	0.20684400	-1.69921300
H	1.37280300	-2.40909900	-1.23528700
H	2.78061500	-1.51783900	-1.93106700
H	3.45982300	-2.46111000	0.43920000
S	1.43327000	-1.56270400	1.48751100
C	0.49440800	-0.41625900	0.38971600
O	-0.26605400	0.41702400	0.85284600
N	2.48887500	0.59246500	-0.40863500
C	2.36685100	1.93637200	-0.30447700
O	1.37452000	2.52525200	-0.73250900
C	3.51201400	2.65901200	0.35309300
H	3.47953500	2.47813900	1.43825700
H	4.48128200	2.30171700	-0.01930800
H	3.40820000	3.73288700	0.16551900
S	-1.24394000	-1.97362900	-0.87618400
C	-2.55687100	-1.19094500	0.09917900
C	-3.18042900	0.03968700	-0.58458500
H	-2.13761200	-0.86467000	1.06590200
H	-3.37666700	-1.88873500	0.31892400
N	-2.11293000	0.81488400	-1.25343400
H	-3.88362900	-0.28037100	-1.36460300
C	-3.90374900	0.92087300	0.44699200
H	-1.50576300	1.23355900	-0.53000500
H	-1.53218200	0.11859600	-1.76973800
H	-2.48174100	1.55046600	-1.86214200
O	-3.38167900	2.02595200	0.71172300
O	-4.92701900	0.41929400	0.95687800

CN5

C	-3.39759000	0.15574900	0.20111800
C	-1.09595700	-0.09882900	0.84135900
C	-1.95048600	-1.12113700	1.58620900
C	-2.98309800	-1.29063400	0.46816800
H	-4.14786500	0.49524100	0.93354800
H	-3.79610300	0.29881200	-0.81171100
H	-0.30680000	0.40077500	1.41595600
H	-1.41151200	-2.04276900	1.83331300
H	-2.39565800	-0.68966100	2.49367900
H	-3.81530300	-1.97680600	0.65624200
S	-1.96534500	-1.89549800	-0.94143200
C	-0.52199500	-0.83430500	-0.40620500

O	-0.12748300	0.00049400	-1.41755200
N	-2.11675800	0.85058300	0.39445500
C	-1.87259600	2.14932300	0.12593700
O	-0.77329200	2.66798000	0.32776900
C	-3.03570000	2.93442800	-0.42393300
H	-3.27494300	2.58167600	-1.43797500
H	-3.93246400	2.80206000	0.19675800
H	-2.76163400	3.99373700	-0.46277900
S	0.82920300	-2.01336600	0.11205900
C	2.35838000	-1.13644400	-0.34559400
C	2.64064400	0.20361600	0.33341700
H	2.38819100	-1.01183100	-1.43859900
H	3.14394300	-1.85167500	-0.06742500
N	1.80253600	1.26604600	-0.22459700
H	2.45302100	0.09258300	1.41257300
C	4.15667700	0.52299700	0.18030400
H	0.63051400	0.59651700	-1.03299700
H	1.33172400	1.80941000	0.49858600
H	2.42958300	1.90670800	-0.71801700
O	4.46355800	1.58390300	-0.40653200
O	4.94390000	-0.32587100	0.65195600

TS8

C	1.06230400	3.15686800	0.23891500
C	-0.15043400	1.34292600	-0.77043400
C	1.33858000	1.16265700	-1.02535200
C	1.85054900	1.84322200	0.25046900
H	1.55164200	3.90961500	-0.40085600
H	0.93663200	3.57521700	1.24592600
H	-0.80172900	1.16921900	-1.63861600
H	1.63757900	0.11142000	-1.12437900
H	1.64481100	1.70732300	-1.93124900
H	2.93546000	1.98902000	0.28589200
S	1.26679700	0.79371600	1.63176000
C	-0.65476400	0.42255100	0.36588900
O	-1.65824500	0.73261700	1.02979800
N	-0.21960300	2.73057200	-0.33992700
C	-1.36236800	3.44401100	-0.39594100
O	-2.39735900	2.97890400	-0.87943900
C	-1.28975200	4.84559400	0.15049000
H	-0.45567100	5.39978700	-0.30210200
H	-2.23471700	5.35895800	-0.05544200
H	-1.11966900	4.81386000	1.23665100
S	-0.48478900	-1.36698600	-0.14350300

C	-2.08197100	-1.99559600	0.44728000
C	-3.26236600	-1.76376000	-0.48246300
H	-2.27898200	-1.56446100	1.43900500
H	-1.96068800	-3.07876000	0.56516800
N	-3.58080900	-0.31926100	-0.65235300
H	-3.04339900	-2.17916200	-1.47496600
C	-4.54206200	-2.47249700	0.04908000
H	-3.06435800	0.26553800	0.04048100
H	-3.35296200	0.03756000	-1.58610200
H	-4.60474800	-0.25224200	-0.49000300
O	-5.57708000	-1.77065200	0.09576900
O	-4.41096700	-3.66758700	0.36080900
H	2.34312300	-0.80874800	1.20531400
O	2.93429700	-1.62293200	0.99016000
P	3.93183300	-1.40258100	-0.20662900
O	5.06357200	-2.51230500	0.01010500
O	3.12536100	-2.00066300	-1.45485300
O	4.44676400	-0.02179500	-0.40214300
H	5.79947100	-2.19462200	0.55966200
H	3.52440800	-1.76822100	-2.31034500