

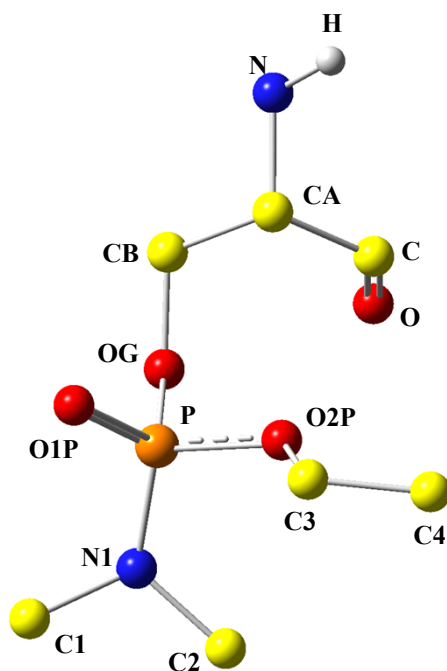
Can hydroxylamine be a more potent nucleophile for the reactivation of tabun-inhibited AChE than prototype oxime drugs? An answer derived from quantum chemical and steered molecular dynamics studies

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```
[ SUN ]
[ atoms ]
  N      N      -0.28000    0
  H      H       0.28000    0
  CA     CH1     0.00000    1
  CB     CH2     0.15000    1
  OG     OA     -0.36000    1
  P      P       0.76000    2
  O1P    OP     -0.63500    2
  O2P    OP     -0.36000    2
  N1     NL     -0.21700    2
  C1     CH3     0.18000    3
  C2     CH3     0.18000    3
  C3     CH2     0.15100    4
  C4     CH3     0.15100    4
  C      C       0.380     5
  O      O      -0.380     5
[ bonds ]
  N      H      gb_2
  N      CA     gb_20
  CA     C      gb_26
  C      O      gb_4
  C      +N     gb_9
  -C     N      gb_9
  CA     CB     gb_26
  CB     OG     gb_17
  P      OG     gb_27
```

```

P      N1      gb_48
P      O1P     gb_23
P      O2P     gb_27
N1     C1      gb_20
N1     C2      gb_20
C3     O2P     gb_19
C3     C4      gb_26

```

[angles]

```

; ai  aj  ak  gromos  type
-C   N   H   ga_31
H    N   CA  ga_17
-C   N   CA  ga_30
N    CA  C   ga_12
CA   C   +N  ga_18
CA   C   O   ga_29
O    C   +N  ga_32
N    CA  CB  ga_12
C    CA  CB  ga_12
CA   CB  OG  ga_12
CB   OG  P   ga_25
OG   P   N1  ga_47
OG   P   O1P ga_13
OG   P   O2P ga_13
N1   P   O1P ga_48
N1   P   O2P ga_47
O1P  P   O2P ga_28
P    N1  C1  ga_49
P    N1  C2  ga_48
C1   N1  C2  ga_48
P    O2P C3  ga_25
O2P  C3  C4  ga_12

```

[impropers]

```

; ai  aj  ak  al  gromos  type
N    -C  CA  H   gi_1
C    CA  +N  O   gi_1
CA   N   C   CB  gi_2
P    OG  N1  O1P gi_2
N1   P   C2  C1  gi_2

```

[dihedrals]

```

; ai  aj  ak  al  gromos  type
-CA  -C   N   CA  gd_4
-C   N   CA  C   gd_19
N    CA  C   +N  gd_20
N    CA  CB  OG  gd_17
CB   CA  C   O   gd_20
C    CA  N   H   gd_14
OG   CB  CA  C   gd_17
CA   CB  OG  P   gd_12
CB   OG  P   O2P gd_9

```

C2	N1	P	OG	gd_9
C3	O2P	P	OG	gd_9
C4	C3	O2P	P	gd_12

GROMOS bond-stretching parameters

```
#define gb_2      0.1000  1.8700e+07
#define gb_20     0.1470  8.7100e+06
#define gb_26     0.1530  7.1500e+06
#define gb_4      0.1230  1.6600e+07
#define gb_9      0.1330  1.1800e+07
#define gb_17     0.1430  8.1800e+06
#define gb_27     0.1610  4.8400e+06
#define gb_48     0.1620  3.0422e+06
#define gb_23     0.1480  8.6000e+06
#define gb_19     0.1435  6.1000e+06
```

GROMOS bond-angle bending parameters

```
#define ga_31     123.00   415.00
#define ga_17     115.00   460.00
#define ga_30     122.00   700.00
#define ga_12     109.50   520.00
#define ga_18     115.00   610.00
#define ga_29     121.00   685.00
#define ga_32     124.00   730.00
#define ga_25     120.00   530.00
#define ga_47     103.00   420.00
#define ga_13     109.60   450.00
#define ga_48     109.60   450.00
#define ga_47     103.00   420.00
#define ga_28     120.00   780.00
#define ga_49     109.50   425.00
```

GROMOS improper (harmonic) dihedral angle parameters

```
#define gi_1      0.0      167.42309
#define gi_2      35.26439  334.84617
```

GROMOS (trigonometric) dihedral torsional angle parameters

```
#define gd_4      180.000   33.5      2
#define gd_19     180.000   1.0       6
#define gd_20     0.000     1.0       6
#define gd_14     0.000     3.77     3
#define gd_17     0.000     5.86     3
#define gd_12     0.000     1.26     3
#define gd_9      0.000     3.14     2
```

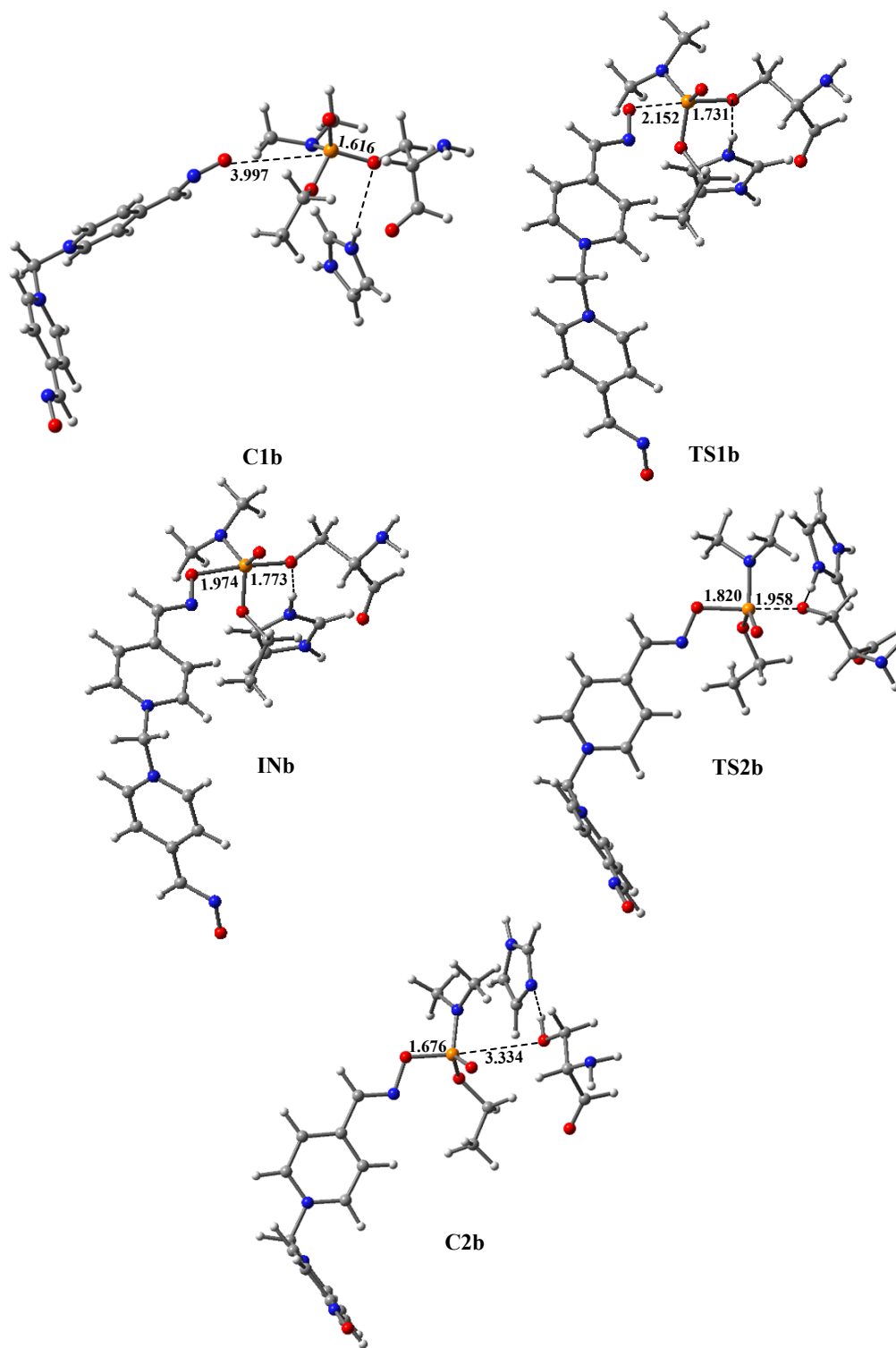
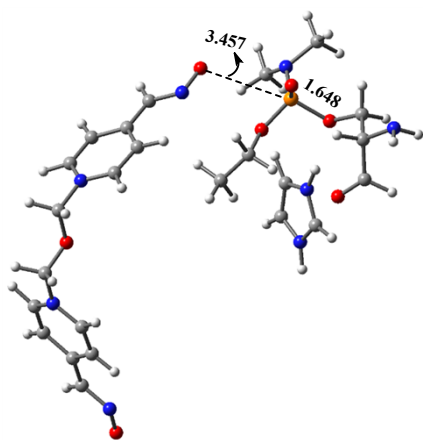
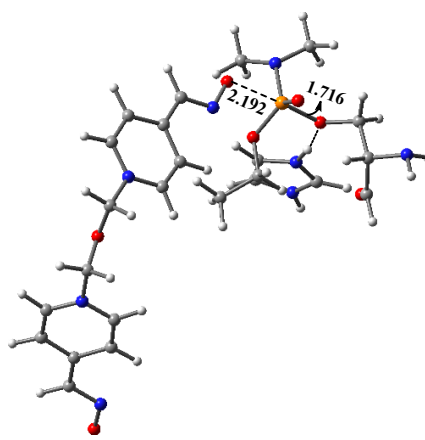


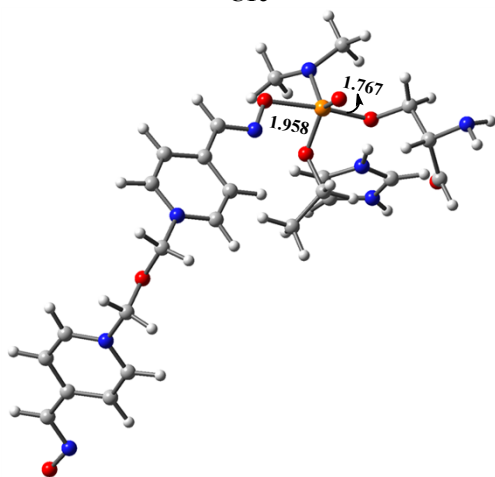
Fig. S1 M05-2X/6-31G* optimized geometries and selected bond distances (Å) for species involved in the reactivation process of tabun-conjugated serine (SUN) molecule with methoxime (MMB4) dianion in aqueous phase (red = oxygen; blue = nitrogen; white = hydrogen; yellow = phosphorus; gray = carbon).



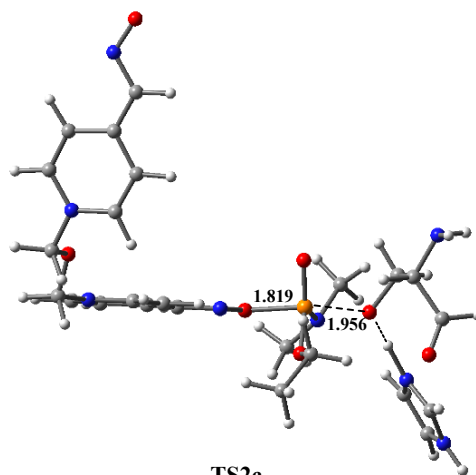
C1c



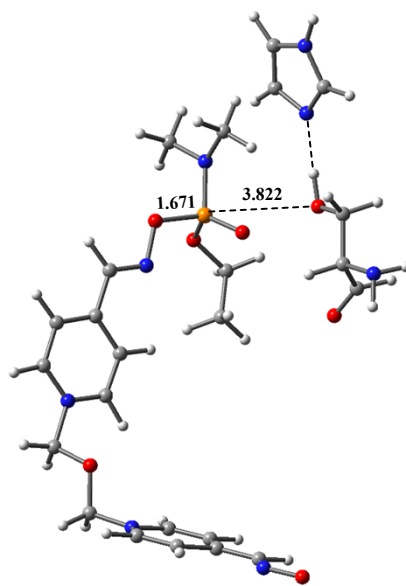
TS1c



INc



TS2c



C2c

Fig. S2 M05-2X/6-31G* optimized geometries and selected bond distances (Å) for species involved in the reactivation process of tabun-conjugated serine (SUN) molecule with Obidoxime dianion in aqueous phase. (red = oxygen; blue = nitrogen; white = hydrogen; yellow = phosphorus; gray = carbon)

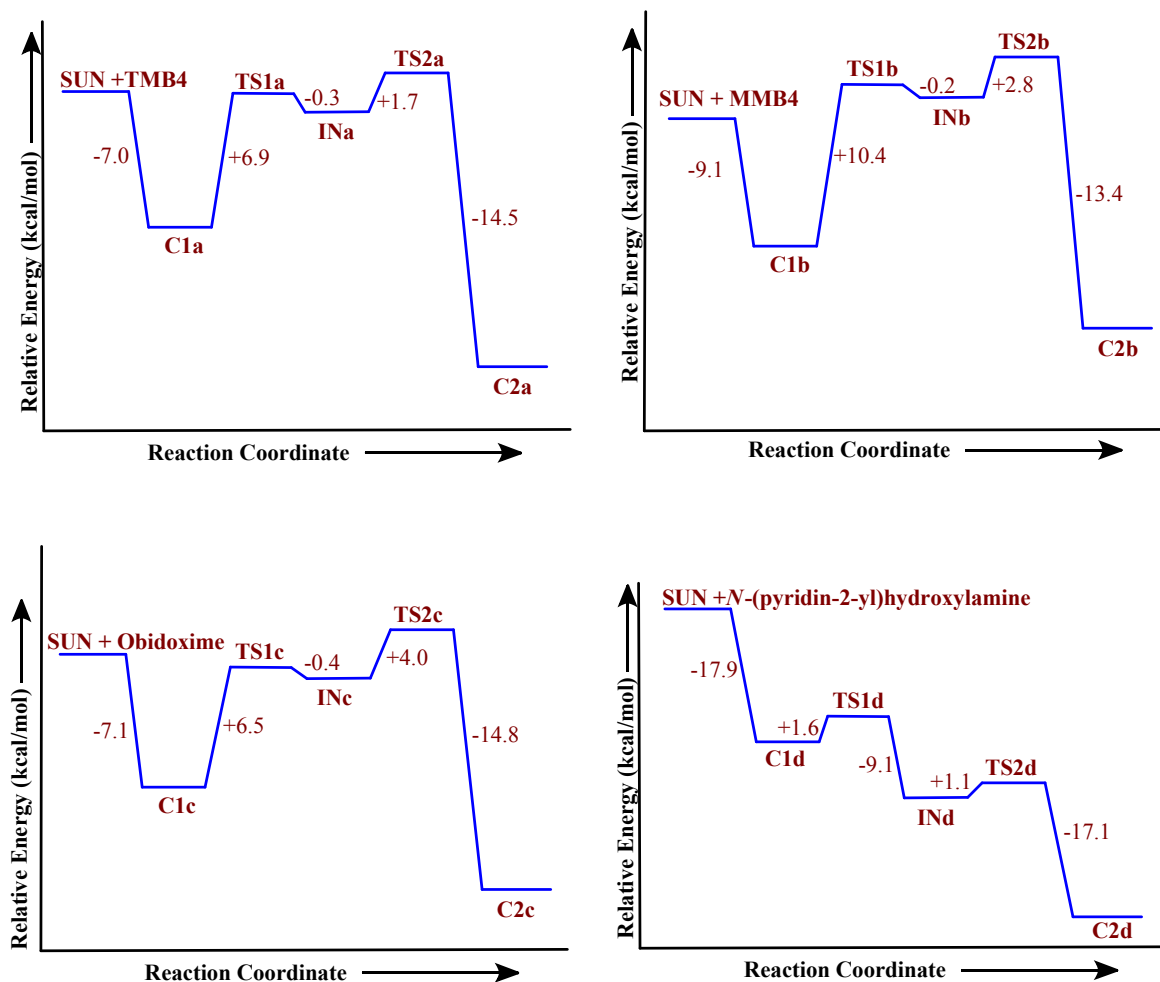


Fig. S3 M05-2X/6-31G* calculated energy profile diagram for the reactivation of tabun-inhibited AChE with oximes and pyridinylhydroxylamine in aqueous phase.

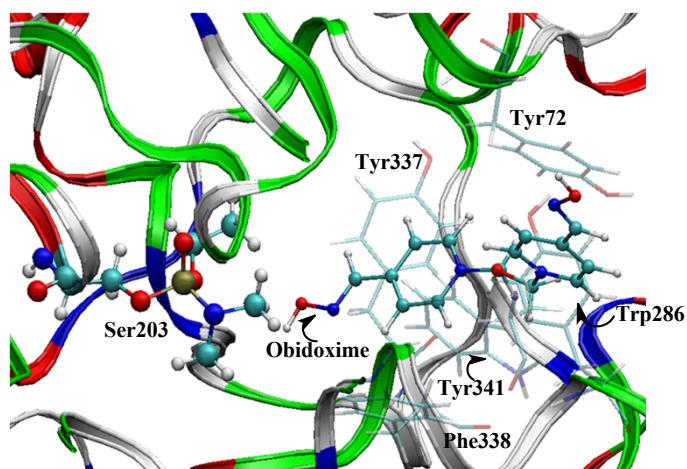


Fig. S4 Stable conformation of tabun-inhibited AChE with obidoxime showing interaction with residues of peripheral anionic site and active site. (Cyan= carbon, blue = nitrogen, white = hydrogen, yellow-grey = phosphorus and red = oxygen) (Residues of peripheral anionic site are shown in tube format).

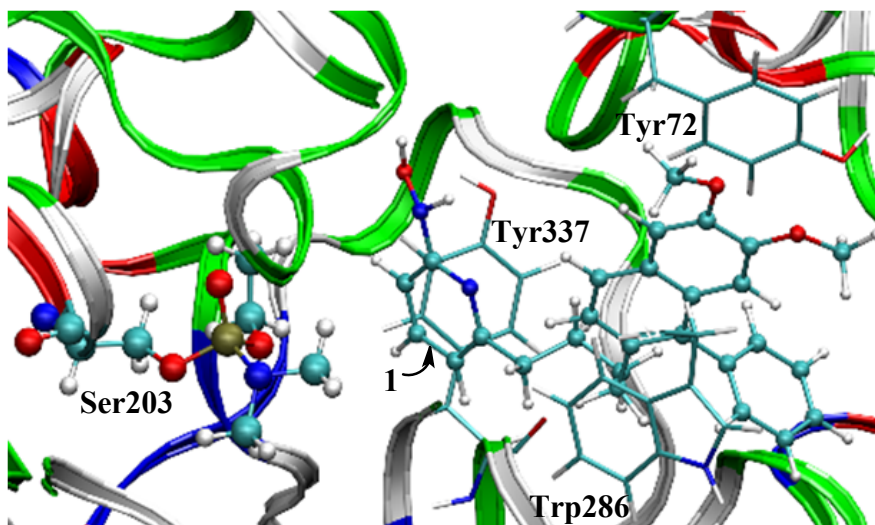
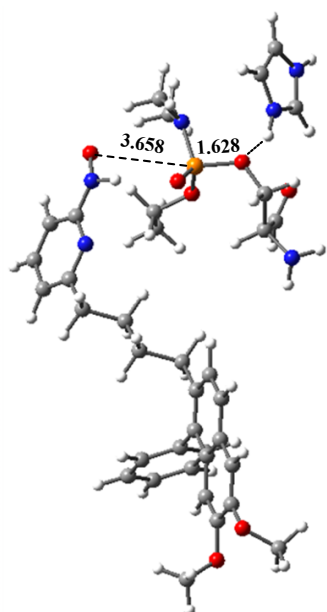
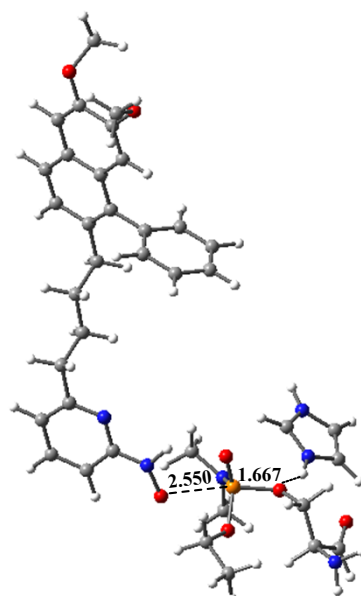


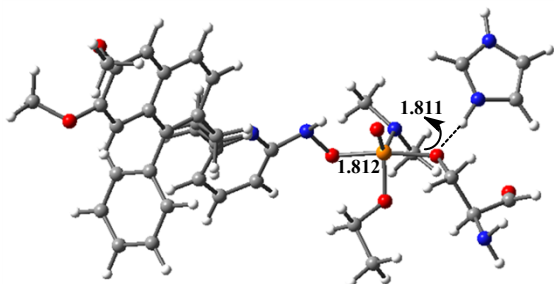
Fig. S5 Stable conformation of tabun-inhibited AChE with **1** showing interaction with residues of peripheral anionic site and active site. (Cyan= carbon, blue = nitrogen, white = hydrogen, yellow-grey = phosphorus and red = oxygen) (Residues of peripheral anionic site are shown in tube format).



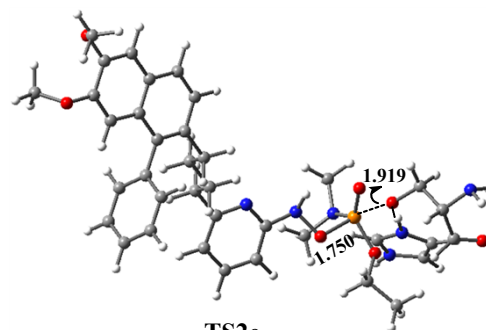
C1e



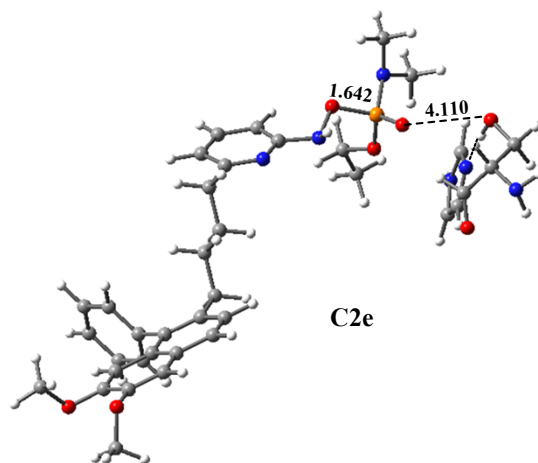
TS1e



INe



TS2e



C2e

Fig. S6 M05-2X/6-31G* optimized geometries and selected bond distances (Å) for species involved in the reactivation process of tabun-conjugated serine (SUN) molecule with anionic form of **1** in aqueous phase. (red = oxygen; blue = nitrogen; white = hydrogen; yellow = phosphorus; gray = carbon)

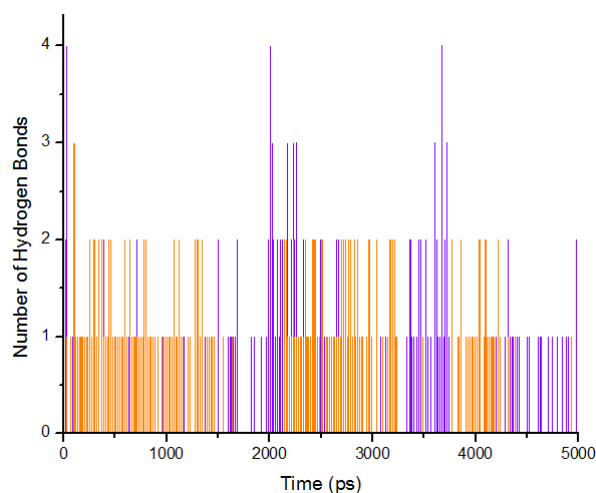
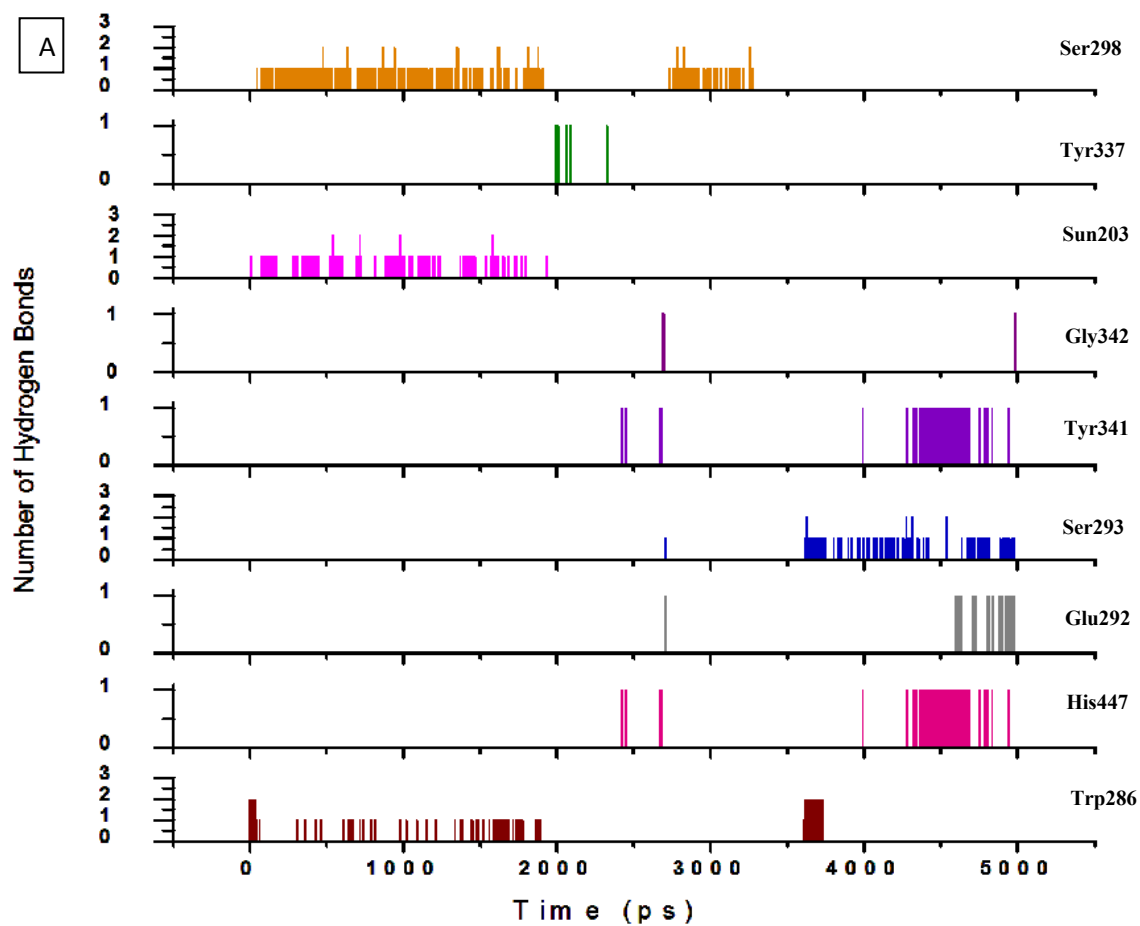


Fig. S7 Temporal evolution of the number of hydrogen bonds formed between amino acid residues of mAChE and drugs for mAChE.TMB4 (violet) and mAChE.1 (orange).



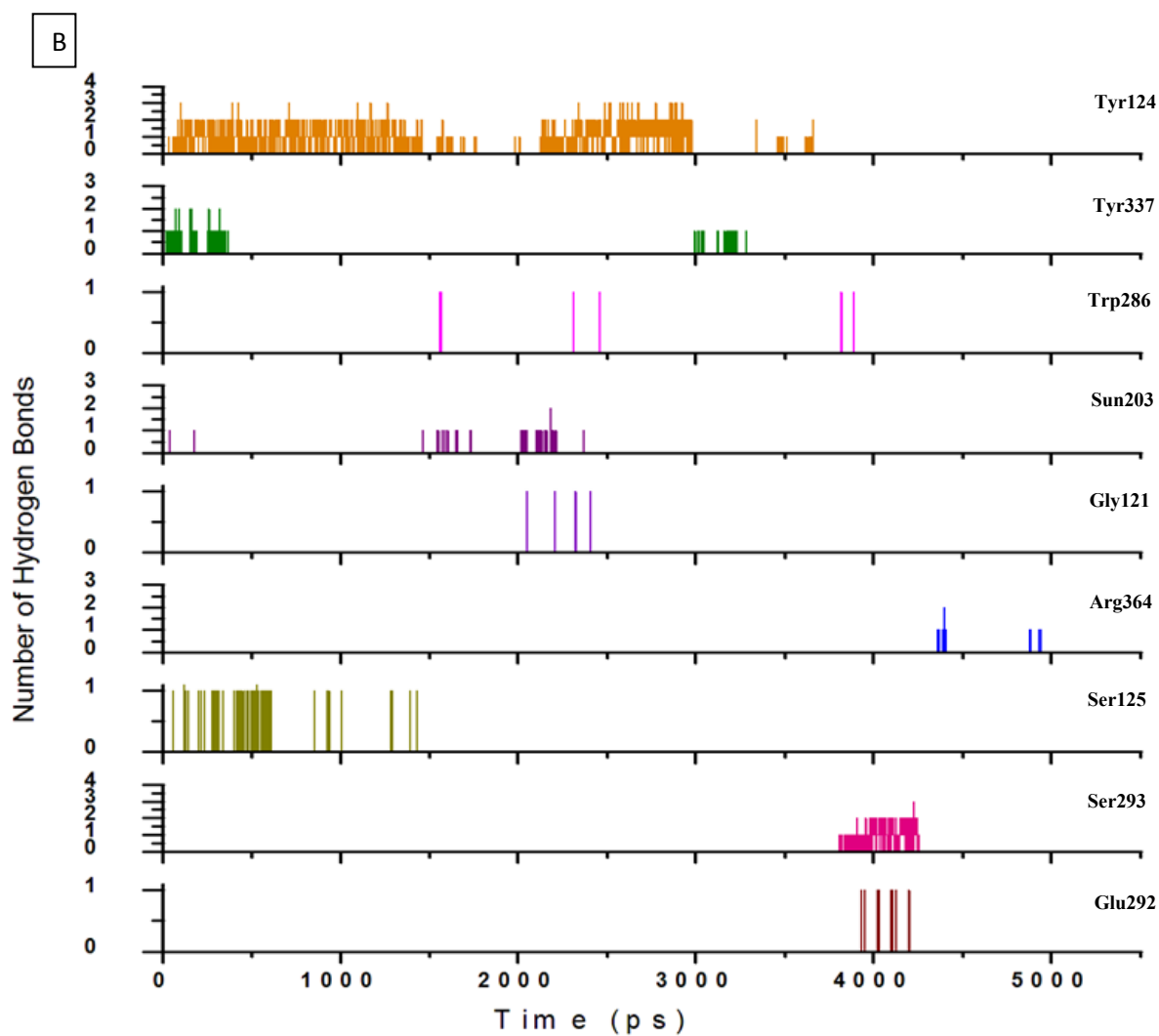


Fig. S8 Number of direct hydrogen bonds as a function of time between amino acid residues of mAChE and TMB4 (A), **1** (B) during the process of leaving the active-site gorge.

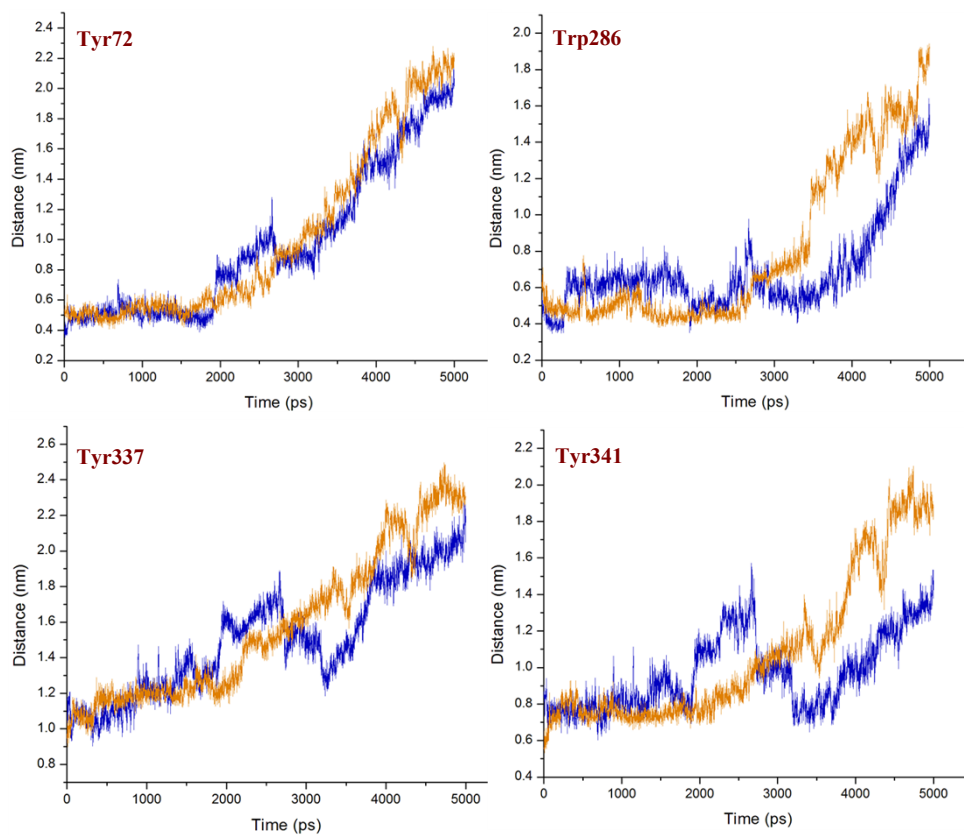


Fig. S9 Center of mass distances between the peripheral moiety of the drugs and the hydrophobic aromatic residues of mAChE as indicated in the plots. In all the plots, the SMD pulling results shown by blue lines are for the mAChE.TMB4, and the orange lines are for the mAChE.1 complexes.

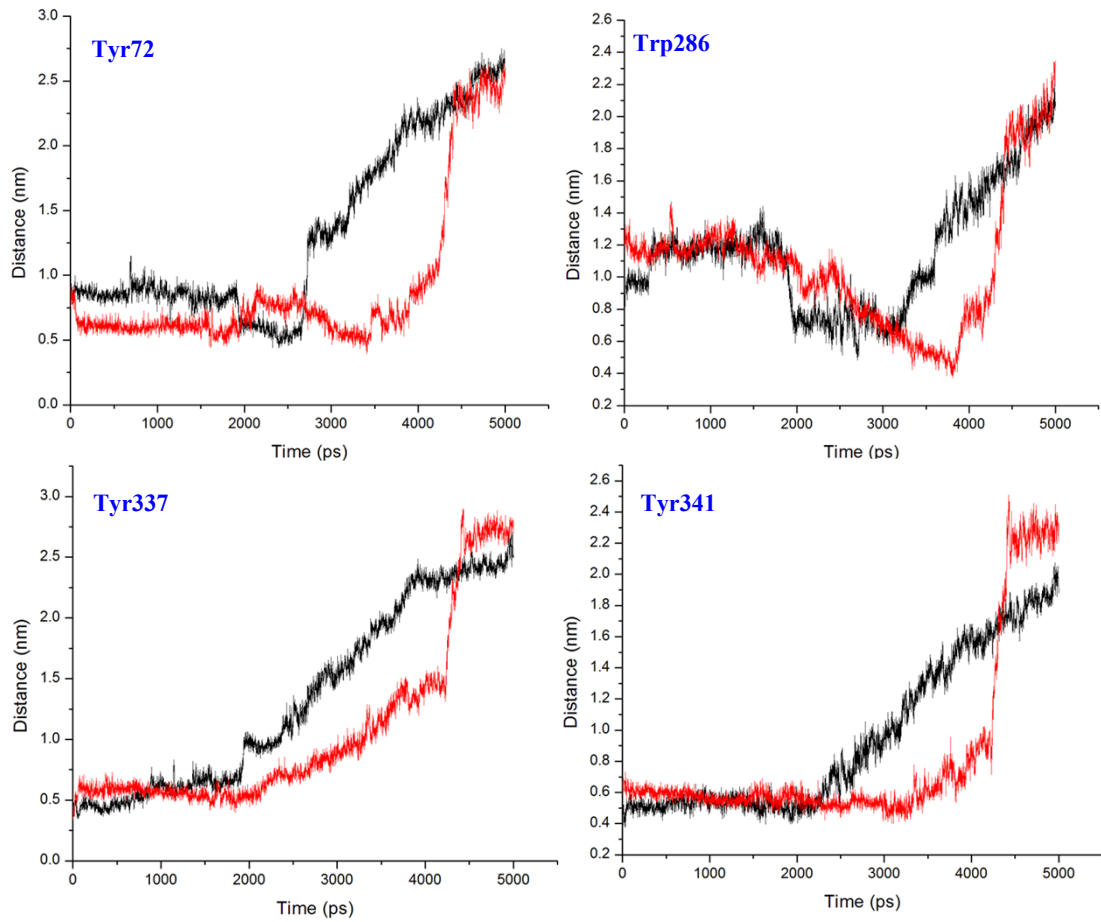


Fig. S10 Center of mass distances between the active ring of the drugs and the hydrophobic aromatic residues of mAChE as indicated in the plots. In all the plots, the SMD pulling results shown by black lines are for the mAChE.TMB4, and the red lines are for the mAChE.1 complexes.

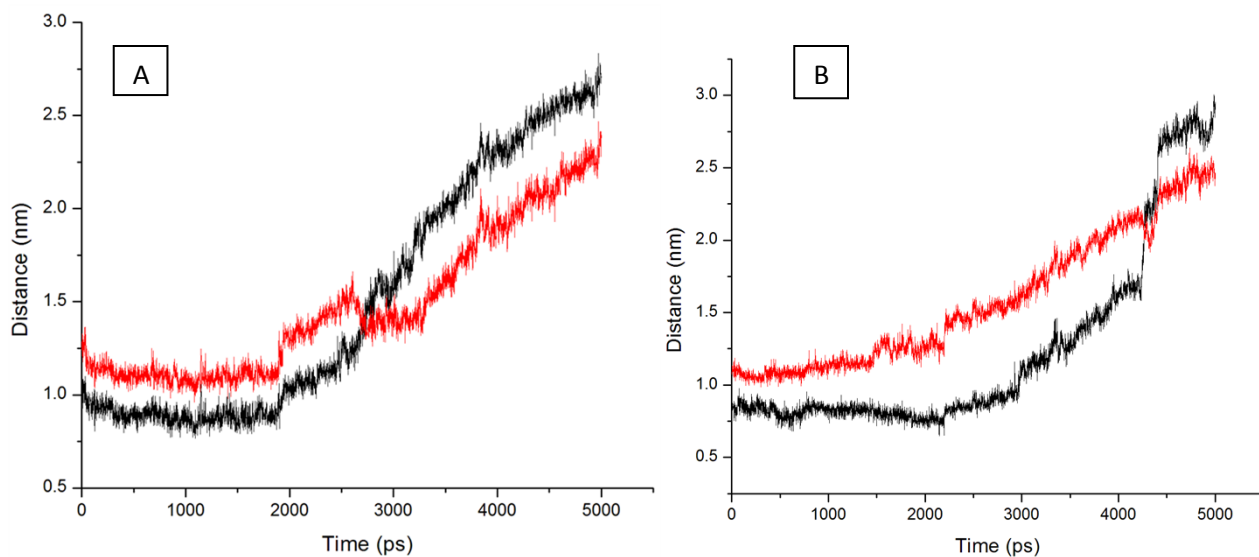


Fig. S11 Temporal spatial distance during SMD pulling between the center of mass of active-site SUN 203 and (A) the N1 atom (black line) and the N2 atom (red line) of the two pyridinium rings of TMB4 that was initially close to active triad and the peripheral site, respectively. (B) the N1 atom (black line) of the pyridine ring and C1 atom (red line) of the peripheral site of the drug candidate **1**.

Table S1: Calculated toxicity limit of the studied reactivators.

	Toxicity limit
TMB4	71%
MMB4	47%
Obidoxime	47%
<i>N</i> -(pyridin-2-yl)hydroxylamine	64%
phenyltetrahydroisoquinoline pyridinealdoxime compound ^a	71%

^a Compound **1d** from ref 16.

MP2/6-31+G/M05-2X/6-31G* calculated Cartesian coordinates of all stationary points, including electronic energies and imaginary frequencies of transition states geometries. (All energies are given in Hartree).**

Tabun

E= -1252.22947

N	-0.01818000	4.18777300	-1.22194800
C	-0.41469000	2.92313600	-0.64008500
C	0.76780500	1.96694700	-0.43593200
O	0.27238000	0.69833000	0.05901000
C	-1.07848300	3.16073600	0.69950300
O	-1.06650700	4.23477900	1.25496300
O	2.32503400	0.25609900	1.58901700
P	1.37608700	-0.35053300	0.62274100
N	0.35543500	-1.56638900	1.12392800
C	-0.39739300	-1.26556500	2.35024800
C	0.90764300	-2.92770400	1.12074800
O	2.04759600	-0.92089000	-0.70739300
C	3.48378800	-1.16158500	-0.77389300
C	3.85381500	-1.25801900	-2.23523200
C	-3.57671300	-2.54433900	-0.88783200
N	-4.26008600	-1.35193100	-0.81259900
C	-2.26320100	-2.24606600	-0.70252000
C	-3.40552800	-0.35781200	-0.59180000
N	-2.18975500	-0.88453600	-0.52259100
H	-1.55359400	2.28534100	1.16681300
H	0.51525300	4.72040800	-0.54418100
H	0.57071600	4.03485100	-2.03221300
H	-1.14118600	2.42612100	-1.29107200
H	1.47345300	2.38011600	0.28547800
H	1.27203500	1.79464600	-1.38730500
H	-1.33063300	-0.36105600	-0.35476400
H	-3.65710300	0.68255100	-0.48738000
H	-1.38824100	-2.86903900	-0.68561600
H	-5.25967000	-1.23733200	-0.90747800
H	-4.07493900	-3.47974600	-1.06328200
H	3.62182700	-0.32407500	-2.74743800
H	4.92294600	-1.45231000	-2.32777900
H	3.30872500	-2.07075400	-2.71522900
H	3.69386900	-2.09037300	-0.24386500
H	3.99537400	-0.34163000	-0.27517600
H	0.22317500	-1.37493200	3.24409900
H	-0.78693000	-0.24886200	2.30833100
H	-1.24004000	-1.95469600	2.41354200
H	1.65212800	-3.07310700	1.90952900
H	0.08675700	-3.62495200	1.29071400
H	1.35258100	-3.14251700	0.15162700

TMB4

E= -947.66047

C	2.95495000	-0.41619400	-1.18176600
C	3.05829300	-1.33914600	0.97252300
C	4.14121400	-0.57078700	1.28181600
C	4.69126000	0.33796400	0.33151500
C	5.80950300	1.12744800	0.64601000
N	6.30113800	1.96643800	-0.27701500
O	7.30117600	2.63978300	0.06886000
C	4.03310700	0.37709100	-0.93497400
N	2.46648100	-1.27627400	-0.24718200
C	-2.95518300	-0.41602200	-1.18221300
C	-3.05795400	-1.33906200	0.97204700
C	-4.14086100	-0.57078700	1.28163600
C	-4.69119700	0.33794900	0.33152300
C	-5.80941800	1.12738200	0.64627100
N	-6.30137900	1.96625800	-0.27666900
O	-7.30142700	2.63949200	0.06941900
C	-4.03334700	0.37717300	-0.93512100
N	-2.46643600	-1.27610000	-0.24779500
C	1.25536400	-2.05676600	-0.52951200
C	-1.25529900	-2.05651500	-0.53031400
H	2.62222700	-2.03505500	1.67498000
H	2.43694900	-0.40877600	-2.13044100
H	4.58254600	-0.66348900	2.26413400
H	6.28235900	1.06673200	1.62244300
H	4.39387300	1.03859800	-1.70694300
H	-2.62169800	-2.03499100	1.67436600
H	-2.43739000	-0.40844700	-2.13099900
H	-4.58189800	-0.66362900	2.26407500
H	-6.28200700	1.06671200	1.62283700
H	-4.39432600	1.03869100	-1.70697900
H	1.30190800	-2.96709600	0.06625800
H	1.28159400	-2.34124100	-1.58097100
H	-1.28127100	-2.34026000	-1.58197600
H	-1.30209000	-2.96724500	0.06482800
C	0.00000600	-1.24905000	-0.20849100
H	0.00024400	-0.32727500	-0.79555700
H	-0.00027000	-0.97373500	0.84864100

C1a

E= -2199.89937

N	-6.85589600	1.84875600	3.45678900
C	-5.80197400	1.67660800	2.47133500
C	-6.45492700	1.25339900	1.14853700
O	-5.47444000	0.96282100	0.13998300
C	-4.96333900	2.91341300	2.23481100
O	-3.87079100	2.89181900	1.70563400
O	-4.97208600	-1.24341700	1.35030800
P	-4.83312500	-0.55153900	0.04504100
N	-5.53445800	-1.28731500	-1.25548600

C -6.99734900 -1.28789800 -1.23863600
C -4.94569800 -1.20918500 -2.59005300
O -3.36588500 -0.20219300 -0.46281700
C -2.30136200 -0.09714800 0.53480800
C -1.01184300 0.15897400 -0.20873300
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H -5.14072600 0.86446400 2.77710800
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H -5.37184600 -2.01290700 -3.19181000
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H -1.05831700 1.09334900 -0.76911200
H -0.81085600 -0.66314400 -0.89592300
C -2.31678300 3.38594000 -2.89704000
N -2.17647600 4.30914200 -1.88538100
C -3.09853600 2.39039300 -2.40052600
C -2.84259700 3.90189000 -0.80897800
N -3.40880500 2.73969100 -1.10667800
H -3.44101400 1.47348800 -2.84274700
H -2.90967100 4.40645000 0.13749500
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H -1.85575800 3.51463400 -3.85888500
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N 3.11952700 -3.41439500 0.58295200
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C 7.06028100 0.51327800 1.44749400
C 7.58418400 1.69396600 1.01792900
C 8.29979000 1.76803000 -0.21543400
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C 8.86505900 2.95501200 -0.70984500
H 9.40458400 2.96981400 -1.65281900
N 8.73407400 4.08631400 -0.00276300
O 9.26118600 5.11074800 -0.49828900
C 8.41546000 0.54217700 -0.93284800

H 8.94561700 0.51067700 -1.87428500
N 7.19911600 -0.63598500 0.73293600
H -1.64891100 5.16881900 -1.94124300
C 4.48200600 -3.28221300 1.11436300
H 4.41792800 -3.31913400 2.20087500
H 5.05183500 -4.14882500 0.78207100
C 6.55405500 -1.87365300 1.18875300
H 7.16743600 -2.70910000 0.85401100
H 6.55961900 -1.86796700 2.27782700
C 5.13166100 -1.98279500 0.64433100
H 4.53910500 -1.13099800 0.98633600
H 5.15551700 -1.95853900 -0.44797100

TS1a

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N	3.89459000	0.83347100	3.98407100	O	-2.24473600	-0.09997800	-0.58740700
C	4.21626300	2.67065800	2.83450500	C	-1.46070400	0.61303900	0.40278900
C	3.99119500	0.47424000	2.70650600	C	-0.30007300	1.25973200	-0.31980700
N	4.18518300	1.57941300	2.00019900	H	-4.79131800	0.61662000	4.90065400
H	4.36558500	3.66697200	2.46097200	H	-3.46751200	0.32675200	2.92253600
H	3.94509400	-0.52580200	2.30333300	H	-5.08699600	-1.31675200	2.00698900
H	4.29973400	1.60550300	0.98821700	H	-6.14925800	0.02087800	1.50956500
H	3.98034900	2.70355200	5.04412700	H	-5.66641400	2.44388800	2.97029700
H	8.18679300	2.45989500	-2.46481700	H	-6.05604200	-2.52624000	-1.83909100
H	6.11538600	-3.42065100	0.07823900	H	-6.06565900	-0.83645000	-1.28122600
H	3.74544500	0.19217300	4.74984800	H	-4.20310400	-0.58951800	-3.03133800
C	-4.28398800	-2.59526100	1.28824300	H	-4.18012400	-2.33464700	-3.33595700
C	-4.57128300	-1.97026500	-0.96618400	H	-2.70805200	-1.52604900	-2.77709400
C	-3.22894900	-1.91342400	-1.15910600	H	-2.10163400	1.34925100	0.89034900
C	-2.32503800	-2.20740300	-0.08949100	H	-1.10948700	-0.10139500	1.14647900
H	-5.27756300	-1.75589100	-1.75574000	H	0.33200200	1.79098700	0.39355600
H	-4.76379500	-2.86907100	2.21672200	H	-0.65654700	1.97339600	-1.06393800
H	-2.84249200	-1.64905200	-2.13074800	H	0.29501800	0.49551100	-0.82126500
C	-0.93157600	-2.17515300	-0.23183800	C	-3.55753000	3.45451500	-2.85381600
H	-0.27324400	-2.40473800	0.60178000	N	-4.30505700	4.19721600	-1.96853400
N	-0.40833100	-1.86886700	-1.42894500	C	-3.39032600	2.23261500	-2.28054800
O	0.84240900	-1.87122900	-1.49989400	C	-4.58465900	3.46392500	-0.89398600
C	-2.93017600	-2.55311900	1.15468400	N	-4.03841000	2.26845700	-1.06700200
H	-2.31540400	-2.79450100	2.01008600	H	-2.86226000	1.35832100	-2.61237000
N	-5.10879600	-2.30717300	0.24372600	H	-5.13381400	3.78863900	-0.02953700
C	-6.56050100	-2.33241200	0.40281800	H	-4.11451300	1.48301000	-0.40103200
H	-6.78805200	-2.76535100	1.37265300	H	-3.21421300	3.85401200	-3.79017800
H	-7.00287400	-2.94758900	-0.37589200	H	-6.17134400	0.33933600	4.08652300
C	-6.90815800	-0.09279700	1.30898500	H	-5.88086500	-2.17139300	-0.12269400
C	-7.86586500	-0.62302900	-0.78145000	C	3.99352400	-3.49698700	-0.50615600
C	-8.37620600	0.62872400	-0.90397600	C	3.27667400	-1.73896200	0.88397300
C	-8.15923700	1.61136700	0.11470000	C	1.98544100	-1.90036900	0.47888700
H	-8.02009600	-1.38434800	-1.53265200	C	1.65259500	-2.90000200	-0.47285600
H	-6.32788700	-0.44605600	2.14983300	H	3.56769300	-0.98635900	1.60294200
H	-8.95210400	0.88243600	-1.77995600	H	4.82814900	-4.09070600	-0.84987800
C	-8.65302700	2.91519100	0.04432900	H	1.21601500	-1.26529900	0.88981400
H	-8.46956300	3.63456800	0.83696400	C	0.32445400	-3.10259500	-0.94570700
N	-9.37166900	3.28550800	-1.03512500	H	0.10574800	-3.89158000	-1.65919500
O	-9.77959600	4.46489300	-1.03595300	N	-0.62367400	-2.30549100	-0.51141400
C	-7.39219600	1.17383100	1.24091900	O	-1.79068600	-2.53302900	-0.97946600
H	-7.19215900	1.85340400	2.05719800	C	2.71531800	-3.70352400	-0.94652100
N	-7.13321700	-0.99656000	0.31057700	H	2.53296200	-4.48621200	-1.66870500
				N	4.27344200	-2.52450400	0.39449000
				C	5.65360700	-2.31341000	0.85795300
				H	6.28151800	-3.05893600	0.37925600
				H	5.69783300	-2.44513100	1.93513300

TS1b

E= -2121.53768

C 6.35608800 -0.64783600 -0.77519300
C 6.29394000 -0.03775800 1.50718800
C 6.69405200 1.22511800 1.21551400
C 6.94565100 1.62054400 -0.13856100
H 6.10440700 -0.36407300 2.51978100
H 6.20697200 -1.43415600 -1.50179700
H 6.82453700 1.93677700 2.01540500
C 7.35249200 2.90355600 -0.50184900
H 7.53674600 3.16918300 -1.53851700
N 7.51788300 3.83517600 0.46151500
O 7.87859800 4.96133800 0.06702400
C 6.75672900 0.60010600 -1.12552100
H 6.93649100 0.81650200 -2.16897500
N 6.11804800 -0.97978800 0.52967000
H -4.59556700 5.15555700 -2.09872800

INb

E= -2121.53822

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C -5.06402800 -0.27236500 1.70677900
O -4.30504400 -0.07099300 0.53524400
C -4.78834800 2.03121900 2.52372500
O -4.04392300 2.73523800 1.87301000
O -2.95268900 -2.01313600 1.27377500
P -3.15224100 -1.29430700 -0.02857900
N -4.15536600 -1.87204100 -1.25910500
C -5.59401200 -1.84771400 -1.03060200
C -3.81760900 -1.59023200 -2.65126200
O -2.21324600 -0.07345900 -0.58048300
C -1.49173800 0.70367900 0.40284900
C -0.34386000 1.38362600 -0.31169900
H -4.84146100 0.71349000 4.88384700
H -3.45685700 0.41211100 2.93105300
H -5.01173100 -1.30791400 2.03753800
H -6.10920200 -0.01712300 1.49704100
H -5.75924200 2.42379500 2.87984500
H -6.05579600 -2.54691400 -1.73083300
H -6.03077300 -0.85473700 -1.18187700
H -4.24037700 -0.63222900 -2.97912300
H -4.23307700 -2.37670700 -3.28565400
H -2.73997700 -1.57012000 -2.78090500
H -2.17357300 1.42382500 0.85684100
H -1.12232800 0.03146200 1.17779200
H 0.24939000 1.96077700 0.39939600
H -0.71519000 2.06125300 -1.08193800
H 0.29550700 0.63550900 -0.78232100
C -3.65890100 3.36391200 -2.89525100
N -4.46305600 4.07403000 -2.03338700
C -3.44025000 2.15774800 -2.30550300
C -4.72628300 3.33519800 -0.95775600
N -4.11508000 2.16859500 -1.10613100
H -2.85941300 1.30962700 -2.61664400
H -5.31003900 3.64104700 -0.10928000
H -4.16192900 1.38002500 -0.42947400
H -3.31717000 3.77263900 -3.82822000

H -6.18025400 0.32340800 4.04752000
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C 3.96387700 -3.48007000 -0.52415300
C 3.29731600 -1.70094400 0.86141500
C 1.99501700 -1.84557900 0.47682100
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H 3.61242400 -0.94672800 1.56787600
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H 1.24113200 -1.19394300 0.89123100
C 0.28682400 -3.03491700 -0.90676000
H 0.05069500 -3.82358400 -1.61514500
N -0.63069200 -2.23543200 -0.45295700
O -1.82394900 -2.46018600 -0.90831900
C 2.67240800 -3.66889400 -0.94414500
H 2.46502600 -4.45323000 -1.65768200
N 4.26902200 -2.50716700 0.36284800
C 5.66308900 -2.32092700 0.81119200
H 6.27158100 -3.06871200 0.31173700
H 5.71532800 -2.47213500 1.88536100
C 6.38576300 -0.65058300 -0.80576500
C 6.32351300 -0.05918100 1.48321800
C 6.73817800 1.20108800 1.20345300
C 6.99846700 1.60553000 -0.14691700
H 6.12800800 -0.39231100 2.49244600
H 6.23147500 -1.42950800 -1.53928000
H 6.87483100 1.90404700 2.00993800
C 7.42224300 2.88577500 -0.49697500
H 7.61292300 3.15939300 -1.53034100
N 7.59820200 3.80589300 0.47674500
O 7.97544800 4.92997300 0.09409100
C 6.80065900 0.59564900 -1.14365300
H 6.98644700 0.81905700 -2.18457900
N 6.13983900 -0.99142200 0.49630700
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TS2b

E= -2121.53310

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O 3.94835100 0.97689700 -0.54316500
C 4.72877000 3.34579200 0.92922500
O 4.52660700 2.86661500 2.02549100
O 1.78572400 0.67206500 -1.74335800
P 2.59528200 -0.35684900 -1.01596000
N 3.86035200 -1.25536900 -1.67343200
C 4.43856700 -0.73857700 -2.91010200
C 3.87031700 -2.71371700 -1.61112600
O 2.51518300 -0.64708900 0.57008700
C 2.07070100 0.38882400 1.47370900
C 1.38308200 -0.29417400 2.63655500
H 3.52043800 5.40602000 -0.32059000
H 2.73386600 3.19528600 0.20340400
H 3.37425800 2.29335500 -2.00475800
H 5.09364000 2.36057300 -1.54645200
H 5.71250600 3.78929200 0.68324500

H 3.87678600 -1.06760800 -3.79166200
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H 4.68318700 4.81730400 -1.29491900
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H 8.05028200 -0.29534900 2.87475400

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H 6.00141800 3.35836800 -0.27545700
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H 5.63115000 -0.12682700 -2.14672200
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H 5.43362100 -2.30602100 -0.92577100
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H 0.35474300 -0.17666700 2.37732400
H 0.37935000 1.04977000 1.09202900
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C 6.40221600 -1.10420800 1.47928500
C 7.78938100 -0.98105200 -0.15537400
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H 8.34595000 -0.66153300 -1.02086000
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C -3.66656200 -1.43821900 0.89491400
C -2.38209700 -1.39589500 0.41471800
C -1.95754700 -2.36916500 -0.50139100
H -4.04575100 -0.71653600 1.60285700
H -4.88151600 -4.08470100 -0.66861100
H -1.71127200 -0.61892900 0.74900800
C -0.59107700 -2.37673000 -1.03713800
H -0.29191100 -3.14435300 -1.74436500
N 0.20999500 -1.47041400 -0.64168800
O 1.44860900 -1.60574400 -1.22202800
C -2.86290800 -3.35194600 -0.90324200
H -2.58516700 -4.12018800 -1.61024800
N -4.52164100 -2.40451100 0.49137100
C -5.89670900 -2.43253900 1.05940400
H -5.81742400 -2.57769400 2.13233100
H -6.41226500 -3.27861600 0.61573400

C2b

E= -2121.55976

C -6.86383600 -0.30632900 1.78711600
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C -7.63930400 0.23217700 -0.80289200
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N -8.95815500 2.68625900 -1.31568300
O -9.53428400 3.77754900 -1.47652200
C -7.50362900 0.86281300 1.53578000
H -7.69617400 1.53657500 2.35841800
N -6.59704600 -1.20250800 0.78608200
H 8.73926800 -2.82060500 0.23157800

Obidoxime

E= -983.51304

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C 2.86610800 -1.36914300 1.05686600
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C1c

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P -4.58651500 -0.60862900 -0.11190900
N -5.18887400 -1.19180100 -1.53186000
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C -2.11904800 -0.22925300 0.65769300
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H -6.96030200 -1.89366800 -2.37952500
H -7.01843700 -0.17416200 -1.92885100
H -4.66365000 -0.01605600 -3.22790600
H -4.86768000 -1.75435100 -3.50200200
H -3.42680600 -1.17991300 -2.65588500
H -2.44598900 0.54730100 1.35053800
H -2.13553800 -1.19990000 1.14732800
H -0.01629900 0.07463000 0.87664800
H -0.74566200 1.04752000 -0.41165800
H -0.48610100 -0.69440800 -0.64899500
C -1.73348500 3.47841400 -2.50254800
N -1.67779400 4.31645100 -1.41160100
C -2.59269100 2.47766300 -2.17225500
C -2.46794800 3.85347100 -0.44772400
N -3.03167800 2.73865200 -0.89465100
H -2.91174200 1.61123600 -2.72087300
H -2.62215500 4.28641100 0.52367200
H -3.69201600 2.16945400 -0.36316400
H -1.16738300 3.66241300 -3.39689800
H -7.32394500 2.36279400 3.18939600
H -7.09456500 -1.44386300 -0.68024300
C 3.12042500 -3.79091400 -0.67614200
C 2.11412400 -3.14099200 1.35392800
C 0.87830600 -3.16613500 0.78972900
C 0.71155300 -3.51851300 -0.58696300
H 2.27589000 -2.87160500 2.38759000
H 4.04690700 -4.01375900 -1.18547900
H 0.01599700 -2.91749200 1.38872600
C -0.53418600 -3.56023500 -1.22450000
H -0.62494800 -3.82823200 -2.27337500
N -1.64070500 -3.26850300 -0.51740100
O -2.72061700 -3.32923200 -1.14446700
C 1.91128600 -3.83033700 -1.29673900
H 1.86788100 -4.10391100 -2.34152100
N 3.23152400 -3.46562100 0.64188600
C 7.33189400 -0.48375800 -0.40150300
C 6.49343500 0.60194800 1.51562900

C	6.79557100	1.82164100	1.00035000
C	7.40661200	1.93897100	-0.28901700
H	6.02650900	0.47765500	2.48197100
H	7.50329900	-1.43054800	-0.89298100
H	6.57278300	2.71023600	1.56973700
C	7.74759800	3.16483500	-0.86949500
H	8.21063500	3.21604700	-1.85073600
N	7.49841300	4.30211200	-0.19434800
O	7.83008800	5.36109400	-0.76971500
C	7.65674200	0.70776000	-0.96976100
H	8.11192400	0.71282700	-1.95006700
N	6.77054300	-0.55011700	0.83807200
H	-1.12293100	5.15759800	-1.34010800
C	4.54524800	-3.32940900	1.23215600
H	4.45487200	-3.43210300	2.31406000
H	5.19201900	-4.11634200	0.83984100
C	6.33524400	-1.82546600	1.36249400
H	7.02309600	-2.59968800	1.01887700
H	6.34640600	-1.78026900	2.45238800
O	5.02965000	-2.05240900	0.87302100

TS1c

E= -2235.74171

N	-5.31493800	0.30945100	4.20961300
C	-4.59914200	0.53601400	2.95218200
C	-5.44160600	0.05262300	1.78454900
O	-4.72752100	0.17608500	0.55943400
C	-4.25101800	2.00351500	2.83328700
O	-4.66505600	2.74312400	1.96447400
O	-3.60077700	-1.96323100	1.14364800
P	-3.79614600	-1.11836100	-0.07313400
N	-4.82568700	-1.55258600	-1.32411000
C	-6.25537900	-1.37939500	-1.08660700
C	-4.45244300	-1.28151000	-2.70962700
O	-2.68476000	-0.08719700	-0.65403900
C	-1.81417300	0.55836700	0.30288300
C	-0.55505500	0.96778100	-0.42868400
H	-4.70251600	0.45209900	5.00431600
H	-3.67569600	-0.04754600	2.97172600
H	-5.71663900	-0.98301300	1.97257700
H	-6.34663400	0.65655400	1.69303000
H	-3.63271200	2.40253800	3.65578000
H	-6.79243700	-2.00120900	-1.80492000
H	-6.57836700	-0.33950000	-1.20507200
H	-4.74972300	-0.27076300	-3.01534300
H	-4.96491000	-1.99580600	-3.35767100
H	-3.38141400	-1.39945500	-2.83643800
H	-2.33434000	1.42338000	0.72011600
H	-1.59267900	-0.14197800	1.10817900
H	0.13700400	1.45189200	0.26201100
H	-0.78875500	1.66779700	-1.23219800
H	-0.07585800	0.08673000	-0.85617400
C	-3.81805800	3.70244200	-2.68982400
N	-4.58403500	4.44735700	-1.82214600
C	-3.70837200	2.46508800	-2.13545900
C	-4.92859900	3.70029000	-0.77581400

N	-4.40717800	2.49458000	-0.94996900
H	-3.19317700	1.58132700	-2.46383200
H	-5.51096800	4.01868700	0.06857800
H	-4.52962100	1.69900300	-0.29706300
H	-3.42433400	4.11070500	-3.60223300
H	-6.08280400	0.96626600	4.30338400
H	-6.52253800	-1.71998100	-0.08707300
C	3.13147700	-4.19317300	-0.75560600
C	2.60807400	-2.49153800	0.78282900
C	1.31172900	-2.46198100	0.36295800
C	0.87460800	-3.33290500	-0.66995000
H	2.98982000	-1.84354300	1.55837600
H	3.89875800	-4.84086100	-1.15273600
H	0.61585300	-1.77781600	0.82382900
C	-0.46561700	-3.34593600	-1.15102900
H	-0.77030500	-4.05061100	-1.91933500
N	-1.32172800	-2.48336600	-0.65197600
O	-2.50723800	-2.54909400	-1.11953300
C	1.84311000	-4.20896600	-1.21433000
H	1.57819800	-4.89720600	-2.00410800
N	3.50679700	-3.35224900	0.23555700
C	7.72123300	-0.04778500	-0.47537000
C	6.26945600	0.63956600	1.25167800
C	6.43212800	1.94505300	0.91857100
C	7.28530400	2.32041400	-0.16896400
H	5.62845400	0.31911500	2.06065400
H	8.18451800	-0.88360100	-0.97922200
H	5.91405800	2.70647800	1.48004700
C	7.49523900	3.64767300	-0.55533900
H	8.14931600	3.89909100	-1.38532300
N	6.87160900	4.63189600	0.11957300
O	7.10150400	5.79453100	-0.27649900
C	7.92492100	1.24209600	-0.85484700
H	8.58099400	1.44376900	-1.68968100
N	6.91615600	-0.35807500	0.57844000
H	-4.84432700	5.41523900	-1.94509500
C	4.88805900	-3.30129100	0.69947100
H	4.89596700	-3.38015600	1.78865000
H	5.42733900	-4.14114000	0.26270200
O	5.40181700	-2.06187400	0.27793600
C	6.62726200	-1.73551400	0.90608700
H	7.44117100	-2.36085800	0.54049500
H	6.54196200	-1.83360600	1.98957000

INc

E= -2235.74273

N	-6.34120500	-1.30583800	3.46185500
C	-5.43868400	-0.58902000	2.55588400
C	-5.96489000	-0.64782100	1.13236700
O	-5.04730900	-0.05174300	0.23321000
C	-5.28010500	0.83321300	3.04515200
O	-5.65137500	1.81808900	2.44019800
O	-3.84696600	-2.20667100	0.25994700
P	-3.84317100	-1.00455900	-0.64063900
N	-4.66490000	-0.94344600	-2.11775200
C	-4.12240400	-0.12814500	-3.20112600

C	-6.12075500	-0.90337500	-2.08625200
O	-2.82394000	0.27483900	-0.51175300
C	-2.31396700	0.60376100	0.79437800
C	-1.00756800	1.34408700	0.60088700
H	-5.91923800	-1.41660200	4.37687200
H	-4.46522400	-1.08393400	2.57585200
H	-6.13470900	-1.69360300	0.88399600
H	-6.90960000	-0.10221200	1.05676000
H	-4.86039600	0.93201100	4.06147000
H	-4.47357200	0.90943600	-3.13535100
H	-4.45660100	-0.53770600	-4.15724300
H	-6.48536100	-1.20698300	-3.06982700
H	-6.51302800	0.09343900	-1.85646800
H	-6.50840000	-1.61005900	-1.35439800
H	-3.04684100	1.21938200	1.31991900
H	-2.16069000	-0.31540800	1.36177800
H	-0.57746900	1.60571900	1.56890600
H	-1.16863800	2.26269500	0.03450100
H	-0.30200600	0.71604400	0.05571400
C	-4.19480200	4.44067600	-1.32627900
N	-5.25211700	4.71220000	-0.48807100
C	-3.95383100	3.10614900	-1.21438600
C	-5.64178300	3.59067200	0.11557000
N	-4.86675200	2.60619400	-0.31382400
H	-3.21780800	2.47482400	-1.67721500
H	-6.43236500	3.50029800	0.83699700
H	-4.95763800	1.60399600	-0.02336800
H	-3.71657300	5.20432200	-1.91142300
H	-7.19877400	-0.77931300	3.59287700
H	-3.03746500	-0.13983200	-3.17554600
C	3.19388200	-3.39496300	-0.96221200
C	2.31055400	-2.36474600	0.95911000
C	1.10117200	-2.18611100	0.34703100
C	0.91041000	-2.62691600	-0.98096000
H	2.50848000	-2.04183000	1.97048500
H	4.06099200	-3.85299600	-1.41438000
H	0.29375900	-1.71352900	0.88532000
C	-0.34286400	-2.47040800	-1.67265500
H	-0.45639700	-2.83996800	-2.68758800
N	-1.31773600	-1.88118800	-1.05322500
O	-2.41845400	-1.78079200	-1.73710900
C	2.00380600	-3.24033300	-1.62369500
H	1.91823200	-3.59649500	-2.64012400
N	3.33561400	-2.97308100	0.31367100
C	4.63599800	-3.07931700	0.96708600
H	5.14227800	-3.96658800	0.58499400
H	4.47394400	-3.17804500	2.04096900
C	7.92218900	-0.62648800	-0.38539600
C	7.09138700	0.49854800	1.51377600
C	7.59264000	1.68146300	1.07600900
C	8.31067600	1.75830300	-0.16051700
H	6.54010900	0.40678700	2.43846200
H	8.00245700	-1.57060200	-0.90474200
H	7.44820200	2.57195700	1.66732900
C	8.85475900	2.94523800	-0.66002600
H	9.39321500	2.96834500	-1.60294900
N	8.70622200	4.08180200	0.04646100

O	9.21560600	5.10589300	-0.45622700
C	8.44594500	0.52777000	-0.87515000
H	8.97201000	0.50382200	-1.81893200
N	7.26249500	-0.65749100	0.80705300
H	-5.67103100	5.61882800	-0.33942800
C	6.62033200	-1.87513600	1.24260300
H	6.54768000	-1.86741100	2.33056400
H	7.21690000	-2.72784300	0.91663500
O	5.33433700	-1.90201900	0.64895800

TS2c

E= -2235.73497

N	3.45177100	4.75680500	-0.52510400
C	3.66890000	3.45765100	0.10001500
C	4.19794600	2.48059100	-0.95934300
O	4.28047000	1.16867300	-0.44845100
C	4.67057700	3.50775000	1.22809500
O	4.59338700	2.87029200	2.25762600
O	2.16788500	0.65800400	-1.66121800
P	3.12323600	-0.30114400	-1.01983000
N	4.49406500	-0.95794800	-1.75092100
C	4.96648900	-0.26674000	-2.94687900
C	4.69992200	-2.40195200	-1.81367600
O	3.11319700	-0.72724100	0.53786300
C	2.49190800	0.13372700	1.51749200
C	1.98577800	-0.75245400	2.63546900
H	3.10078500	5.42096700	0.15554600
H	2.72602500	3.06451700	0.48176300
H	3.50627200	2.50306700	-1.79858100
H	5.18966400	2.80378900	-1.30034400
H	5.53752100	4.17043100	1.04297300
H	4.41580200	-0.57447700	-3.84302700
H	6.02244500	-0.50111300	-3.09983200
H	5.76709100	-2.58050900	-1.96579300
H	4.14618000	-2.87339900	-2.63066800
H	4.40470900	-2.86398700	-0.87484600
H	3.22941900	0.85412200	1.86605300
H	1.66972800	0.67388600	1.04569200
H	1.51839600	-0.14404100	3.41132200
H	2.81053100	-1.30981400	3.08153300
H	1.25193200	-1.46184800	2.25081300
C	8.40050900	-0.54272200	0.81914200
N	8.10145500	0.23109700	1.91460900
C	7.35798600	-0.37963000	-0.04462400
C	6.92308700	0.83471900	1.70864900
N	6.45082400	0.48205600	0.52516500
H	7.19220600	-0.81238000	-1.01451200
H	6.44540800	1.50453300	2.40335300
H	5.35716500	0.83100200	0.02565000
H	9.30187400	-1.12479000	0.75628200
H	4.33041200	5.13149500	-0.86979300
H	4.87064700	0.80970400	-2.82834400
C	-3.15680600	-4.04672400	-0.30171200
C	-2.79281500	-2.05888800	0.90056700
C	-1.53666700	-1.92957400	0.37149900
C	-1.05882200	-2.89631100	-0.53338800

H -3.21978400 -1.34558200 1.59022600
H -3.84604200 -4.84610800 -0.52838000
H -0.92266200 -1.08565300 0.64690200
C 0.26295100 -2.80332300 -1.13382900
H 0.59014200 -3.55982900 -1.84135200
N 1.00964300 -1.81137400 -0.80874200
O 2.19194000 -1.81319700 -1.41572600
C -1.90206200 -3.96673300 -0.85985000
H -1.58651100 -4.73294000 -1.55303500
N -3.58005800 -3.10812300 0.56540200
C -6.58114700 0.68335900 1.44533900
C -8.16177000 -0.30018200 -0.00423700
C -8.51773800 0.91416300 -0.49606400
C -7.89321600 2.10947700 -0.01535100
H -8.60854400 -1.22116000 -0.34970600
H -5.82666700 0.50827500 2.19913800
H -9.27883800 0.97725500 -1.25777700
C -8.21725500 3.38665300 -0.48103900
H -7.72219900 4.27299300 -0.09501800
N -9.16480300 3.51703200 -1.42955400
O -9.40406200 4.68506600 -1.80204500
C -6.89393800 1.92493100 0.99127300
H -6.37608500 2.77914800 1.40372900
N -7.21381600 -0.42742800 0.97042200
H 8.66898000 0.33513600 2.74192800
C -4.92927700 -3.16938800 1.14256000
H -4.83857000 -3.15177800 2.23011300
H -5.39332500 -4.10003100 0.81994000
C -6.77304000 -1.73192900 1.40346000
H -7.56426300 -2.45412500 1.20811900
H -6.55118200 -1.69950000 2.47117600
O -5.60278700 -2.03831500 0.66268200

C2c

E= -2235.76384

N 2.55786400 4.41456100 -0.47154800
C 3.07735300 3.39881000 0.44449300
C 4.47735900 2.99466900 0.00434500
O 5.02424600 2.16684000 1.00949100
C 3.14459400 3.92177600 1.86191900
O 2.55139200 3.45084400 2.80756700
O 2.62918500 0.31456300 -0.71448500
P 3.14425300 -0.95220200 -0.15156600
N 4.67018800 -1.36439700 -0.59647700
C 5.10820500 -1.02167700 -1.95082800
C 5.26496400 -2.59317800 -0.06958700
O 3.06524500 -1.14566300 1.42272500
C 2.79620500 -0.00031600 2.29414100
C 1.30678500 0.24234800 2.39427600
H 1.60545600 4.65568600 -0.22169000
H 2.43013900 2.52272800 0.42263000
H 4.40166600 2.48238800 -0.95849700
H 5.08463000 3.90156200 -0.13491100
H 3.76637500 4.83048100 1.98317900
H 6.19464500 -0.93074600 -1.94375100
H 4.67472800 -0.06757300 -2.24149000

H 6.34975000 -2.48879300 -0.10387300
H 4.97138000 -3.46518500 -0.66138200
H 4.95930600 -2.73754900 0.96442200
H 3.21867200 -0.29134100 3.25304900
H 3.33451100 0.86519200 1.91508400
H 1.12810600 1.08107800 3.06759200
H 0.79837200 -0.64350500 2.77745800
H 0.89811100 0.49117300 1.41427200
C 8.81269700 -0.36357500 -1.01007400
N 8.58967100 0.59411300 -1.96708400
C 7.99282500 -0.02798100 0.03328500
C 7.66707600 1.45530100 -1.48487300
N 7.28339800 1.10895800 -0.27369500
H 7.87392900 -0.53174900 0.97827500
H 7.31082700 2.30421000 -2.04487600
H 5.85323100 1.77827300 0.64449500
H 9.51408700 -1.16625900 -1.15262200
H 3.10452200 5.26721100 -0.39471300
H 4.81814100 -1.79144600 -2.67293100
C -3.30255200 -4.26990200 -0.47638900
C -3.07499500 -2.31111900 0.80397200
C -1.73685200 -2.23397100 0.50875100
C -1.15779000 -3.21312100 -0.31085300
H -3.58838800 -1.58809700 1.41959000
H -3.97340200 -5.03605700 -0.83408100
H -1.14530800 -1.42427300 0.90906100
C 0.26737400 -3.17387200 -0.66500600
H 0.69694900 -3.96601800 -1.27078100
N 0.95798700 -2.19129400 -0.24675800
O 2.27188700 -2.28573300 -0.65394000
C -1.96208200 -4.24243200 -0.80102900
H -1.56107800 -5.01709600 -1.43811800
N -3.82846100 -3.31938400 0.31347600
C -6.67272400 0.61458900 1.13254800
C -8.08211300 -0.13816500 -0.60458400
C -8.29023900 1.13259500 -1.03372000
C -7.67290600 2.23982800 -0.36735700
H -8.52756100 -0.99529500 -1.08829600
H -6.04786700 0.33052900 1.96728700
H -8.92744400 1.30800500 -1.88615100
C -7.85123700 3.56899800 -0.75863800
H -7.36668600 4.38491100 -0.23039500
N -8.64332700 3.84096000 -1.81421100
O -8.75824600 5.04880900 -2.10972500
C -6.84281000 1.90649100 0.74887400
H -6.34041700 2.68714200 1.30235000
N -7.29526200 -0.40882000 0.47894400
H 9.03599600 0.65076200 -2.86869900
C -5.26193000 -3.34176500 0.66296900
H -5.34331300 -3.44856900 1.74611100
H -5.71444200 -4.19686200 0.16422000
O -5.78149400 -2.12205400 0.21945500
C -7.00528100 -1.77210700 0.85017100
H -7.81828100 -2.41091400 0.50936700
H -6.90683300 -1.83801300 1.93421800

***N*-(pyridin-2-yl)hydroxylamine**

E= -377.20692

C	0.50494300	-0.25550300	-0.00000300
C	-1.65981600	-1.03600800	-0.00000200
C	-1.31503700	1.32139800	0.00000800
H	-2.31858200	-1.90220100	-0.00000500
H	-1.69010000	2.33957700	0.00001300
N	1.80631300	-0.51330900	-0.00000400
H	2.06760900	-1.49344200	-0.00001100
O	2.77386800	0.42403200	-0.00000200
C	-2.21554300	0.23841800	0.00000500
H	-3.28685300	0.38007400	0.00000700
N	-0.35765800	-1.31582400	-0.00000600
C	0.03943700	1.09809400	0.00000500
H	0.77249400	1.88927300	0.00000800

C1d

E= -1629.45129

N	1.50599300	4.25397800	-0.89105400
C	1.22550400	2.92887400	-0.33553400
C	1.88285200	1.89069700	-1.23089400
O	1.78918800	0.56203800	-0.68402600
C	1.73848700	2.86121600	1.08944900
O	2.79063800	2.34963400	1.40729600
O	-0.53942300	0.08309500	-1.68590300
P	0.34156700	-0.13201700	-0.50771900
N	0.82765200	-1.70702000	-0.17503000
C	0.52372900	-2.66930200	-1.25478200
C	0.49800900	-2.25814200	1.15377400
O	-0.13827700	0.52171400	0.86758900
C	-1.56068400	0.48111700	1.23291300
C	-1.64984600	0.84619600	2.69565200
H	0.91427200	4.95660700	-0.46359300
H	0.14338100	2.79220100	-0.32520900
H	1.42548000	1.91542800	-2.21858600
H	2.94892500	2.09229800	-1.31707000
H	1.13203600	3.40494400	1.83277200
H	-0.54458300	-2.89237100	-1.23933600
H	1.11171100	-3.57029200	-1.07383900
H	1.05854700	-3.18673900	1.27208400
H	-0.57349700	-2.45288800	1.22176500
H	0.80893400	-1.56236900	1.93013600
H	-2.07595100	1.20611700	0.60225800
H	-1.93738900	-0.52310600	1.02297500
H	-2.69769300	0.84784400	3.00103500
H	-1.23176400	1.83697000	2.88013500
H	-1.11247900	0.11776800	3.30466600
C	5.80800000	-2.01827000	0.69607300
N	6.31313400	-1.10512500	-0.20174400
C	4.46529000	-1.80263700	0.75221200
C	5.32157800	-0.35714300	-0.68013100
N	4.19606500	-0.76551100	-0.11160300
H	3.68690200	-2.28841200	1.31727800
H	5.42051000	0.43642100	-1.39927000
H	3.25109700	-0.37090000	-0.30444300
H	6.43655400	-2.72546700	1.20515700

H	2.46881800	4.51629100	-0.70746200
H	0.81396800	-2.25034200	-2.21676000
H	7.28435000	-1.00707300	-0.46073500
C	-4.87225400	-1.17175400	0.61713000
C	-4.17022800	-0.70756900	-0.53361000
C	-5.79025300	0.87602200	-0.92963800
C	-6.06150500	-0.56240600	0.94760500
H	-4.44640400	-1.98263500	1.18694300
H	-6.12977500	1.69562500	-1.55877100
H	-6.61234100	-0.89768100	1.81990500
N	-3.03261100	-1.29436200	-0.92257500
H	-2.44548500	-0.75511400	-1.55076200
O	-2.37436200	-2.17570000	-0.11565300
C	-6.55841600	0.49093300	0.16295900
H	-7.48763600	0.99188000	0.39427500
N	-4.63276000	0.32404200	-1.29131800

TS1d

E= -1629.44860

N	2.09586900	4.24721800	-0.55417400
C	2.15372800	2.87615400	-0.07295800
C	1.71786500	1.93989700	-1.20841400
O	1.65039600	0.58951800	-0.75589200
C	3.52063200	2.44307000	0.41150400
O	3.70350900	1.51014800	1.16606800
O	-0.54510600	-0.30138000	-1.74466300
P	0.14408900	-0.06948500	-0.44407200
N	0.75918400	-1.38090300	0.38382200
C	0.17350300	-2.69908500	0.14369800
C	1.07843200	-1.13903900	1.79058700
O	-0.34261600	1.14359100	0.48781000
C	-1.66651400	1.72522400	0.37884300
C	-1.52702600	3.21049200	0.63932800
H	2.28045300	4.89438500	0.20322000
H	1.44582100	2.74065000	0.74456900
H	0.75162100	2.28497300	-1.57829400
H	2.43255100	1.97364200	-2.03297800
H	4.37457300	3.01990500	0.01224800
H	-0.71465000	-2.84914500	0.75431600
H	0.93436600	-3.45147300	0.36870200
H	1.73053000	-1.94205300	2.13940500
H	0.17394500	-1.11858700	2.40569900
H	1.61189300	-0.19372800	1.89601100
H	-2.05309300	1.52475900	-0.61965400
H	-2.30391100	1.21873000	1.09571600
H	-2.50753300	3.68640400	0.57906700
H	-0.86616400	3.67864700	-0.09275700
H	-1.11990100	3.38788300	1.63633800
C	5.64487300	-2.29506900	0.21777200
N	4.73792300	-3.04810400	-0.49320400
C	5.04677400	-1.09594900	0.45382200
C	3.62571000	-2.34313800	-0.68503600
N	3.79804200	-1.15829500	-0.11760200
H	5.38419700	-0.21708900	0.97073700
H	2.74440200	-2.67118500	-1.20562300
H	3.08387400	-0.42049000	-0.13687700

H 6.61368500 -2.67189100 0.48875100
H 2.80715500 4.41018100 -1.25998300
H -0.10786400 -2.78249000 -0.90479600
H 4.88215800 -3.99229900 -0.82102500
C -4.71439700 -0.69925000 1.12881300
C -4.18989300 -0.78316300 -0.19559900
C -6.28689700 -0.47029900 -1.08600400
C -6.06624400 -0.49745700 1.28376500
H -4.03575000 -0.79859600 1.96144800
H -6.89097000 -0.37811400 -1.98585200
H -6.48692600 -0.42859900 2.28118200
N -2.89406800 -1.01932700 -0.40136900
H -2.51841600 -0.87859400 -1.33261800
O -1.97849900 -0.98886400 0.60123400
C -6.89879600 -0.37943100 0.15838100
H -7.96405900 -0.21941900 0.24521000
N -4.98485000 -0.66144300 -1.29440800

INd

E= -1629.46315

N 2.19491900 4.07842200 -0.97247800
C 2.23300700 2.80675400 -0.26148600
C 1.63126500 1.70848400 -1.15320600
O 1.51169900 0.50352900 -0.44286700
C 3.62581900 2.36222700 0.11189400
O 3.89840100 1.66159500 1.06486400
O -0.50485200 -0.32799900 -1.59643600
P -0.15790000 -0.11824800 -0.13612000
N 0.63390600 -1.32375200 0.78778200
C -0.05904900 -2.59220400 0.97123400
C 1.28023500 -0.88259800 2.02286900
O -0.40513300 1.31060200 0.64238000
C -1.66855900 1.99072000 0.56760900
C -1.38125600 3.47697100 0.65986600
H 2.59319800 4.81533500 -0.40178500
H 1.62143500 2.85974100 0.63867100
H 0.66383100 2.06826900 -1.50778700
H 2.26951500 1.55406400 -2.03267100
H 4.41888500 2.68787700 -0.58872300
H -0.79859600 -2.55717800 1.77633700
H 0.69000300 -3.35380500 1.20802600
H 1.96884600 -1.66438700 2.35478100
H 0.55096500 -0.70720000 2.82444600
H 1.84655400 0.02917500 1.84770100
H -2.16439500 1.74508900 -0.37328100
H -2.30794400 1.65680900 1.38271700
H -2.31291200 4.04297000 0.60337700
H -0.72537300 3.79341200 -0.15305900
H -0.89196000 3.71025500 1.60711100
C 5.36872400 -2.38494800 -0.15246000
N 4.35979600 -3.24221200 -0.52800000
C 4.79507000 -1.15763000 -0.01716000
C 3.21439200 -2.56548600 -0.61413800
N 3.46012700 -1.30099900 -0.31165500
H 5.20817100 -0.21098100 0.28010400
H 2.25495400 -2.97323500 -0.87668600

H 2.70961700 -0.55229000 -0.31993300
H 6.38087600 -2.71745200 -0.01405300
H 2.75904000 4.02746100 -1.81548600
H -0.56879100 -2.87975300 0.05266800
H 4.45916900 -4.23058200 -0.70768100
C -4.45967600 -0.40138400 0.93663000
C -3.94453100 -0.87559000 -0.28380600
C -6.00592300 -0.78724900 -1.27134800
C -5.81174800 -0.11667200 1.00372200
H -3.79978100 -0.27496600 1.78074500
H -6.59151100 -0.95077600 -2.17051900
H -6.23951300 0.25335200 1.92761100
N -2.62416000 -1.26250200 -0.41330700
H -2.24391600 -1.09470000 -1.34381300
O -1.76886600 -0.64918400 0.51157800
C -6.61811200 -0.31101300 -0.12007200
H -7.67804100 -0.10009100 -0.10490300
N -4.70341300 -1.06515000 -1.37222000

TS2d

E= -1629.46136

N -3.43444100 -3.72472800 -0.54961500
C -2.82508600 -2.45526400 -0.14082000
C -2.33438300 -1.73390100 -1.39345100
O -1.64359900 -0.53543900 -1.11692400
C -3.85891300 -1.62015100 0.57410300
O -3.85756400 -1.35174200 1.75641500
O 0.42208500 -1.90582700 -1.04912300
P 0.16467900 -0.55106100 -0.43619100
N 0.28974100 0.90834800 -1.29953000
C 0.32740000 0.80023800 -2.75134800
C 1.12741500 1.98020300 -0.78474500
O -0.59102500 -0.31082700 0.98939000
C 0.02521400 -0.32753800 2.29326500
C -1.08316100 -0.10431400 3.30092600
H -3.77131200 -4.22982600 0.26246600
H -1.99081300 -2.64848100 0.53216600
H -1.67576200 -2.40751300 -1.93632500
H -3.19506700 -1.49044500 -2.02860400
H -4.69815800 -1.29311000 -0.07184000
H 1.33779100 0.58206900 -3.11825300
H 0.00094000 1.74598200 -3.19447200
H 0.81319300 2.91189900 -1.26363600
H 2.19228900 1.82442700 -0.98779600
H 0.98524400 2.08691600 0.28952000
H 0.51672100 -1.28747600 2.44857300
H 0.77703000 0.45714500 2.35362600
H -0.67347200 -0.12762500 4.31231800
H -1.84751700 -0.87353100 3.20123200
H -1.55122100 0.86795600 3.13653000
C -3.88567200 3.16973600 0.64993100
N -3.17876000 3.65404300 -0.42470800
C -3.63865500 1.82867600 0.68591800
C -2.53218800 2.63576100 -1.00757000
N -2.79776900 1.51819600 -0.35706400
H -3.99364400 1.08010400 1.37271700

H	-1.89049900	2.72438400	-1.86663100
H	-2.27446600	0.45436300	-0.68532300
H	-4.48326200	3.80654700	1.27657700
H	-4.24131300	-3.55280800	-1.14286200
H	-0.34951800	0.01423900	-3.07723800
H	-3.14498000	4.61533400	-0.72805900
C	4.14861600	0.67272600	0.94421700
C	3.98362300	-0.28614900	-0.06779400
C	6.23934900	-0.56087800	-0.29395200
C	5.44142700	0.99714400	1.31935300
H	3.28372500	1.12605500	1.40362600
H	7.04650600	-1.07540900	-0.80449200
H	5.60809600	1.73036700	2.09871100
N	2.72865600	-0.61801200	-0.56010000
H	2.66636400	-1.58193200	-0.87248700
O	1.70926300	-0.38298100	0.37241200
N	5.00472100	-0.89958600	-0.67475900
C	6.52180700	0.37541800	0.69135600
H	7.54384900	0.60272700	0.95956600

C2d

E= -1629.49134

N	3.46479300	-3.68315200	-1.57284500
C	2.91194300	-2.65927200	-0.70258300
C	3.93388100	-2.08617100	0.31021100
O	3.35719400	-1.16863700	1.21287800
C	2.40351900	-1.50779400	-1.52383200
O	2.67671600	-1.36085700	-2.69948600
O	-0.25168500	-1.97234600	0.47214500
P	-0.72785700	-0.63928300	0.91463400
N	-0.40091400	-0.08617800	2.44137300
C	-0.87339400	-0.91819800	3.55303100
C	0.92046900	0.50291800	2.69012500
O	-0.24429400	0.51557200	-0.07119400
C	-0.86498800	1.83149400	-0.03115200
C	0.11412200	2.82163700	-0.61814500
H	4.07509400	-3.23751100	-2.24970800
H	2.06583100	-3.04724200	-0.12871300
H	4.33271700	-2.92537500	0.88486200
H	4.76481700	-1.63622000	-0.24700100
H	1.80641900	-0.76008400	-0.98608400
H	-0.92422900	-0.29822300	4.44844300
H	-0.19887200	-1.75850400	3.74280900
H	1.68122700	-0.26380300	2.85394700
H	0.84727000	1.13809000	3.57351400
H	1.22233200	1.11447300	1.84206500
H	-1.78099700	1.77689600	-0.61821400
H	-1.11332600	2.07342900	1.00275900
H	-0.34114300	3.81268900	-0.63976200
H	0.37914600	2.53544000	-1.63570800
H	1.02549600	2.86608800	-0.02056900
C	3.72957800	3.07141500	-1.50559100
N	3.88195900	3.50308500	-0.21257800
C	3.53316000	1.72069500	-1.41671100
C	3.77798900	2.42859300	0.59832800
N	3.56531500	1.32916400	-0.09718000

H	3.36326000	1.01398100	-2.21246400
H	3.86602300	2.49387500	1.67049700
H	3.38358800	-0.28146900	0.78762400
H	3.77186400	3.74380100	-2.34382400
H	4.03497500	-4.32210200	-1.02973800
H	-1.87098300	-1.29616200	3.33857200
H	4.04776700	4.45178400	0.08361100
C	-4.50684600	0.85949800	0.04880200
C	-4.15455600	-0.37144900	-0.50827400
C	-6.08647600	-0.51115500	-1.70420000
C	-5.72991800	1.39852600	-0.32516400
H	-3.85569800	1.35719600	0.75073900
H	-6.68846600	-1.08789100	-2.39699900
H	-6.04650900	2.34888500	0.08490500
N	-2.90575400	-0.98285000	-0.26776100
H	-3.01566900	-1.99164700	-0.21491200
O	-2.36705100	-0.54545900	0.97213400
N	-4.91722500	-1.05481200	-1.35704300
C	-6.54163600	0.71012600	-1.22371600
H	-7.49943700	1.10067700	-1.53652800

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E= -1376.09058307

C	-7.94579600	0.54519000	-0.36049500
C	-7.33644000	-0.72141700	-0.08840500
C	-5.32496600	-0.00262500	-0.97745900
C	-7.17789600	1.51409000	-0.95488400
H	-8.98034300	0.68697800	-0.09056700
H	-7.61271400	2.48364100	-1.17532500
N	-8.03820100	-1.69306200	0.48051200
H	-7.54190800	-2.56274500	0.64261700
O	-9.33340100	-1.60141400	0.84112800
C	-5.83257900	1.25901800	-1.28250000
H	-5.20863700	2.00654500	-1.75299100
N	-6.03188000	-0.97694400	-0.40017800
C	-3.87603400	-0.32741400	-1.25905900
H	-3.45315400	0.42085400	-1.93464700
C	-3.04474300	-0.38211400	0.02729200
H	-3.11840700	0.58119000	0.54317400
H	-3.47803100	-1.13390000	0.69298100
C	-1.57715400	-0.70476200	-0.23972900
H	-1.14768200	0.05246200	-0.90361600
H	-1.49769900	-1.66431500	-0.76175900
C	-0.74942400	-0.76152600	1.05190600
H	-0.83329900	0.19380800	1.57255800
H	-1.16881600	-1.52855500	1.70912900
C	0.69788800	-1.08557700	0.77110600
C	1.64802300	-0.10370200	0.56025400
C	1.07070800	-2.45145700	0.65583800
C	2.99530400	-0.46326300	0.24100800
C	1.29027100	1.34329100	0.65853900
C	2.35102200	-2.82184500	0.34652000
H	0.31223000	-3.20851600	0.82055900
C	3.34729300	-1.83648300	0.13171500
C	4.00493700	0.51230200	0.01995900
C	1.25980000	1.98495700	1.89991200

C	0.99597700	2.07975700	-0.49236500	H	-3.56638000	0.81501900	3.06954000
H	2.62110100	-3.86806800	0.26581600	H	-5.20490200	1.44491400	2.80862700
C	4.68680400	-2.19194900	-0.17257300	C	-9.35686900	-3.05125400	-0.09077200
C	5.28928400	0.14570600	-0.28257900	N	-9.09407100	-3.58278600	1.15234200
H	3.77270000	1.56695700	0.08331000	C	-8.16195600	-2.63499100	-0.58980900
C	0.93053500	3.33486300	1.99024300	C	-7.79120800	-3.49776100	1.40970300
H	1.49235000	1.41877400	2.79404300	N	-7.21490600	-2.92578200	0.36267300
C	0.66770900	3.43038700	-0.40331900	H	-7.90139900	-2.15388900	-1.51513400
H	1.02778600	1.58874500	-1.45790200	H	-7.28838200	-3.82612900	2.30119300
C	5.64200300	-1.23311700	-0.37417500	H	-6.21235900	-2.73538800	0.28553500
H	4.96795300	-3.23568500	-0.24442700	H	-10.34943300	-3.01642300	-0.50018700
O	6.24642500	1.11139300	-0.46827100	H	-2.06061900	-4.40280700	1.05480900
C	0.63315900	4.06007000	0.83850500	H	-5.87998600	0.08287300	-3.23414500
H	0.90787600	3.81946100	2.95818000	H	-9.77872000	-3.97705600	1.78166400
H	0.43948600	3.98900000	-1.30226600	C	-3.28839600	4.79410900	-0.07972900
O	6.92577200	-1.59751800	-0.69183900	C	-3.02602700	3.73780500	-0.99976000
C	6.66665600	1.24212400	-1.83358500	C	-0.74384500	4.01496800	-0.75322900
H	0.37751500	5.10969400	0.90840900	C	-2.21315600	5.44936500	0.47484300
C	7.86516300	-1.35870500	0.36581600	H	-4.31426900	5.04067600	0.14364700
H	7.41269500	2.03240400	-1.84909900	H	-2.38070000	6.25912500	1.17716700
H	7.10239100	0.31045600	-2.19159000	N	-4.03073900	3.08741300	-1.59692700
H	5.81704800	1.52302800	-2.45861900	H	-3.77648700	2.19674700	-2.01329300
H	7.58737900	-1.93880900	1.24766700	O	-5.31904400	3.21214500	-1.16409700
H	8.83179600	-1.69063200	-0.00404200	C	-0.90247400	5.07162800	0.14198600
H	7.90370400	-0.29867700	0.61232400	H	-0.04098400	5.56563300	0.57013300
H	-3.81813900	-1.29855700	-1.75931200	N	-1.76024800	3.35762900	-1.31687900

C1e

E= -2628.34444259

N	-1.72423100	-3.46940300	0.84438300	H	0.09982700	1.44155000	-0.79174600
C	-2.83649100	-2.52371500	0.75594800	C	2.25640900	1.55700900	-0.83698100
C	-3.54915900	-2.76256500	-0.56717000	H	3.04474700	2.24331400	-0.51066500
O	-4.76420100	-1.99679000	-0.69208900	H	2.33918800	1.47628300	-1.92623900
C	-3.75136200	-2.70214500	1.94907200	C	2.50387100	0.17829200	-0.20941700
O	-4.86187500	-3.19058800	1.89554200	H	2.43999400	0.26093900	0.87678200
O	-3.65367500	0.05612100	-1.78944400	H	1.71277100	-0.50493000	-0.53191500
P	-4.69167400	-0.37508100	-0.81501600	C	3.84316200	-0.38335700	-0.62155400
N	-6.25139600	0.03365500	-1.16036300	C	4.98824100	-0.19955200	0.13074500
C	-6.51709900	0.57340900	-2.50107700	C	3.92926800	-1.06366300	-1.86549200
C	-7.10834500	0.62980800	-0.13118600	C	6.24406300	-0.69989700	-0.33702000
O	-4.42467100	-0.00386900	0.71863600	C	4.93900400	0.52403400	1.43688100
C	-3.99766300	1.36536800	1.02919400	C	5.11896100	-1.54630400	-2.33818700
C	-4.15789400	1.54919500	2.51997400	H	3.02188400	-1.19690600	-2.44401100
H	-1.07834800	-3.20419800	1.57799600	C	6.30798000	-1.37684000	-1.58557500
H	-2.42371400	-1.51485000	0.79138600	C	7.44446300	-0.53741300	0.40500900
H	-2.88110500	-2.52150900	-1.39182800	C	4.58288300	-0.14919000	2.60898400
H	-3.85725500	-3.80403500	-0.64212200	C	5.26185800	1.88213000	1.50736900
H	-3.30495100	-2.43578500	2.92066300	H	5.16787000	-2.06555900	-3.28793600
H	-6.32613400	1.64921500	-2.49461200	C	7.55242200	-1.88196200	-2.04271800
H	-7.55946000	0.36825600	-2.75310200	C	8.63644900	-1.02582600	-0.06025200
H	-8.14863900	0.42871000	-0.39402100	H	7.43694600	-0.01898500	1.35446500
H	-6.93654900	1.70775400	-0.08657500	C	4.53948600	0.52472300	3.82670100
H	-6.90577000	0.17985500	0.83841200	H	4.33670000	-1.20334400	2.55969600
H	-2.95608200	1.45778200	0.72009600	C	5.21979100	2.55698600	2.72508400
H	-4.61152600	2.06524600	0.45328200	H	5.54855800	2.40631100	0.60328200
H	-3.81891100	2.54882900	2.79729300	C	8.69382700	-1.71811300	-1.30511900

H	7.60985500	-2.41081000	-2.98640000
O	9.77366500	-0.87458900	0.69267100
C	4.85711800	1.87990600	3.88702500
H	4.25936300	-0.00799800	4.72671100
H	5.47003100	3.60968600	2.76542900
O	9.89112000	-2.19216100	-1.77715600
C	10.69874600	0.07519800	0.14444100
H	4.82371500	2.40427200	4.83351200
C	10.38522900	-3.32484500	-1.04845300
H	11.54557700	0.10428900	0.82524800
H	11.02733000	-0.23652400	-0.84616000
H	10.23205400	1.06060000	0.09168800
H	9.67740000	-4.15251700	-1.12293100
H	11.32629600	-3.60192200	-1.51657700
H	10.55007100	-3.06629100	-0.00343000
H	0.72082700	3.40935400	-2.18537500

TS1e

E= -2628.33469673

N	8.34372900	-2.24896100	-3.14224000
C	7.94031700	-1.74908600	-1.82959900
C	6.45129700	-1.97917700	-1.62653800
O	6.00921800	-1.36489900	-0.41266700
C	8.76322000	-2.38784700	-0.73157300
O	8.30217900	-2.96036400	0.23378300
O	3.81467000	-0.21171400	-1.09413300
P	5.15790200	0.06506800	-0.51060900
N	5.25644500	0.37106100	1.12601300
C	4.12196600	1.00699500	1.79358200
C	6.54770600	0.85904600	1.60541000
O	6.25300300	0.81956000	-1.41226500
C	5.89914100	1.58319100	-2.59325000
C	6.94412300	1.29078900	-3.65071200
H	9.26848200	-1.91455000	-3.38643500
H	8.12554300	-0.67278300	-1.80062600
H	5.90801400	-1.58234500	-2.48440400
H	6.23750800	-3.04538800	-1.54357700
H	9.85431400	-2.34515000	-0.88646100
H	4.15941000	2.08980400	1.68152700
H	4.14817600	0.72216200	2.84908000
H	6.59983900	0.70327400	2.68451600
H	6.67334000	1.92518400	1.39217400
H	7.35814700	0.30034900	1.13747900
H	4.90224200	1.28709200	-2.91499700
H	5.86384700	2.62796100	-2.30812700
H	6.72251300	1.86457100	-4.55257400
H	6.96202000	0.23007200	-3.90796600
H	7.93618400	1.57807400	-3.29756000
C	6.31305500	-3.68979600	4.01341000
N	5.14563000	-2.96081500	3.97428200
C	6.94979700	-3.45658200	2.83420800
C	5.06844600	-2.30341500	2.81963000
N	6.15482900	-2.59298000	2.11835800
H	7.88334400	-3.81511800	2.44367900
H	4.27381000	-1.65198600	2.50523400
H	6.33786400	-2.22853700	1.17445300

H	6.58156700	-4.29533100	4.85922900
H	8.37975500	-3.26284600	-3.14710700
H	3.19538400	0.64888300	1.34828800
H	4.44844800	-2.92238000	4.70393200
C	2.69977700	4.53803100	0.38701100
C	2.21430900	3.36143500	-0.25902800
C	0.02464100	4.05351800	0.00476100
C	1.77866700	5.45764600	0.82851500
H	3.76486100	4.66595100	0.49890900
H	2.11679000	6.36222600	1.32285400
N	3.06254200	2.45724000	-0.74485000
H	2.70267700	1.55709500	-1.04150100
O	4.39780700	2.49915200	-0.50774700
C	0.40484100	5.23402200	0.64081500
H	-0.33899800	5.94372800	0.97642200
N	0.88483400	3.13132500	-0.43529500
C	-1.43788700	3.72459200	-0.18228000
H	-1.59789000	3.38214100	-1.20860700
C	-1.90160400	2.62886600	0.78395400
H	-1.27618100	1.74408600	0.63562300
H	-1.73996200	2.96512100	1.81360800
C	-3.37083200	2.26505100	0.58839000
H	-3.53420100	1.93072200	-0.44125000
H	-3.99493400	3.15294500	0.73537400
C	-3.83112700	1.16054900	1.55007600
H	-3.22203200	0.26963900	1.38918300
H	-3.66035300	1.49086300	2.57865500
C	-5.29591600	0.84357000	1.36841200
C	-5.74024600	-0.12863000	0.49154600
C	-6.24460300	1.62841300	2.07686700
C	-7.14256000	-0.34649700	0.30993900
C	-4.77302800	-0.96431000	-0.28115200
C	-7.59084100	1.44344300	1.91753600
H	-5.87903300	2.38916200	2.75739100
C	-8.07483200	0.45021800	1.02950400
C	-7.64454900	-1.33668600	-0.57755400
C	-4.17432100	-2.08329300	0.30472300
C	-4.46591600	-0.64812200	-1.60762500
H	-8.30233000	2.04784000	2.46753900
C	-9.46524400	0.22539200	0.85773900
C	-8.99128300	-1.52923700	-0.73464600
H	-6.96693500	-1.95553900	-1.15028400
C	-3.27727800	-2.86517400	-0.41819100
H	-4.41378500	-2.33477800	1.33116700
C	-3.57003300	-1.43040900	-2.33217700
H	-4.93472600	0.21326800	-2.06879200
C	-9.92258900	-0.73889500	0.00141000
H	-10.18300500	0.81839400	1.41154300
O	-9.44460600	-2.50865600	-1.58217300
C	-2.97300900	-2.53978900	-1.73819200
H	-2.81839500	-3.72791600	0.04807300
H	-3.33898700	-1.17346600	-3.35825000
O	-11.27091000	-0.92387900	-0.16992200
C	-10.04666100	-1.99310000	-2.77782900
H	-2.27596300	-3.14770500	-2.30075200
C	-11.75694700	-2.14496600	0.40521000
H	-10.36016800	-2.85665000	-3.35863700

H	-10.90877900	-1.37291500	-2.53650800
H	-9.31418100	-1.41343800	-3.34250400
H	-11.58235000	-2.14369900	1.48266000
H	-12.82488700	-2.17261000	0.20502100
H	-11.26916100	-3.00470100	-0.05179500
H	-2.04228900	4.62300500	-0.03246200

INe

E= -2628.34834477

N	-6.50179000	-0.49843400	4.49637000
C	-7.03337500	-0.37389000	3.14498800
C	-6.07258700	-1.05605100	2.15731800
O	-6.47706900	-0.82589400	0.83309300
C	-8.38761000	-1.01595100	2.96733900
O	-9.22169300	-0.66461000	2.15858800
O	-4.23116600	-0.84831400	-0.18646000
P	-5.37119900	0.15069400	-0.21761300
N	-6.63564800	0.04447900	-1.36809500
C	-6.28439700	0.19493600	-2.77380100
C	-7.87980100	0.74351200	-1.05040200
O	-5.55682000	1.33136700	0.91300700
C	-4.46746600	2.19369900	1.27925000
C	-4.67616300	2.58169300	2.73038700
H	-7.11952300	-0.04805700	5.16207200
H	-7.09530600	0.67598900	2.86032700
H	-5.07276900	-0.66323000	2.35038000
H	-6.04738900	-2.13580900	2.35155800
H	-8.57158300	-1.89371900	3.61629700
H	-6.20072300	1.24225500	-3.07844900
H	-7.06549700	-0.28681200	-3.36944000
H	-8.67433100	0.35045700	-1.69073700
H	-7.79752300	1.82290500	-1.23252100
H	-8.15395300	0.57404000	-0.01204900
H	-3.52050700	1.66811000	1.14456900
H	-4.46241000	3.06672900	0.62952900
H	-3.87119300	3.23976000	3.06268900
H	-4.69424900	1.69575800	3.36743300
H	-5.62444200	3.10899900	2.84797500
C	-9.84749000	-3.68535100	-1.09747500
N	-8.86155400	-3.66455200	-2.05761100
C	-9.41249300	-2.88231400	-0.08766300
C	-7.86584400	-2.87665700	-1.65130200
N	-8.18075900	-2.39766700	-0.45881900
H	-9.87347600	-2.59889700	0.84103900
H	-6.96493400	-2.66039700	-2.19644300
H	-7.54229700	-1.74718600	0.08568400
H	-10.75183500	-4.25281500	-1.21816600
H	-6.45092800	-1.47666900	4.76462400
H	-5.33530900	-0.29696300	-2.98127800
H	-8.88206000	-4.15898400	-2.93750600
C	-2.59288400	3.26386900	-1.73793000
C	-2.31519500	1.88819400	-1.82240800
C	-0.05783000	2.26346500	-2.05559600
C	-1.52410900	4.13828500	-1.81433800
H	-3.61139700	3.59978900	-1.62212100
H	-1.69487400	5.20624900	-1.75114800

N	-3.32455500	0.94257800	-1.84212100
H	-3.05826400	0.06404300	-1.39953800
O	-4.50997200	1.37927800	-1.23354100
C	-0.22947800	3.64336000	-1.97805400
H	0.62389500	4.30484700	-2.04260500
N	-1.07819900	1.39959700	-1.97516600
C	1.31401500	1.65214700	-2.18635400
H	2.03137700	2.41516800	-2.49751500
C	1.77639400	1.01690500	-0.86946000
H	1.80897500	1.78553900	-0.09040600
H	1.03488200	0.27595800	-0.55723000
C	3.14728600	0.35814700	-0.99597700
H	3.88523300	1.09847500	-1.32088600
H	3.11422600	-0.41707000	-1.76873800
C	3.61474000	-0.26490300	0.32675500
H	3.66125100	0.51210200	1.09147100
H	2.87458000	-1.00054100	0.65395100
C	4.95533100	-0.94298400	0.17811600
C	6.14815000	-0.28028000	0.40030700
C	4.98015100	-2.29041000	-0.27078100
C	7.39370400	-0.95202700	0.19072400
C	6.16143000	1.14122000	0.85892000
C	6.15776500	-2.95364600	-0.48403300
H	4.03559200	-2.79384400	-0.44358200
C	7.39577000	-2.30136800	-0.25752000
C	8.64330000	-0.31174400	0.41080600
C	6.00614900	1.45263400	2.21265700
C	6.34488700	2.17964500	-0.05854800
H	6.16054100	-3.98273900	-0.82304100
C	8.63159900	-2.97094700	-0.45165000
C	9.82404900	-0.97485900	0.20684600
H	8.68241800	0.71757800	0.74117300
C	6.02227400	2.77781100	2.63971100
H	5.86917500	0.65029900	2.92792700
C	6.36251000	3.50545200	0.36768500
H	6.47559100	1.94225700	-1.10781600
C	9.82131300	-2.33396700	-0.22538900
H	8.64349800	-4.00348400	-0.77915500
O	11.01374400	-0.33584700	0.45006900
C	6.19974300	3.80698300	1.71766400
H	5.89821300	3.00581700	3.69082900
H	6.50305400	4.30055400	-0.35362000
O	11.00552300	-2.99156500	-0.44172800
C	11.74994800	-0.02873000	-0.74226200
H	6.21274200	4.83733900	2.04950500
C	11.71167900	-3.30737900	0.76654200
H	12.65766300	0.47444900	-0.41946300
H	12.00057200	-0.93989500	-1.28355000
H	11.16450600	0.63674700	-1.37927500
H	11.10282400	-3.96232200	1.39238900
H	12.61807700	-3.82513600	0.46373300
H	11.96482100	-2.39894700	1.31115400
H	1.28542600	0.88257000	-2.96238300

TS2e

E= -2628.34834477

N	-7.52165000	-4.04462300	2.23472900	H	1.42023400	0.06105900	0.14799900
C	-7.39172600	-2.68307300	1.73823400	C	3.45399200	0.33638900	-0.52249500
C	-7.12793900	-2.74113700	0.22036600	H	4.10504600	1.15716300	-0.83992000
O	-7.00552100	-1.47055100	-0.38280800	H	3.37204600	-0.35003400	-1.37175900
C	-8.62801400	-1.84004200	1.95478200	C	4.11064900	-0.39410400	0.65700900
O	-9.70226300	-2.32205000	2.25681400	H	4.20554100	0.29537600	1.49738600
O	-4.58224600	-1.60866000	0.05944300	H	3.45707300	-1.21048700	0.97721900
P	-5.44913100	-0.38339300	-0.10167100	C	5.45904300	-0.95764300	0.27858100
N	-5.89062400	0.28176600	-1.61093700	C	6.63320200	-0.25000700	0.45615400
C	-5.68703700	-0.58174500	-2.77058600	C	5.50220500	-2.23467400	-0.34208900
C	-5.57800100	1.67644500	-1.89640700	C	7.87984500	-0.80688600	0.02906800
O	-6.34948300	0.26399400	1.10029300	C	6.62509800	1.10174500	1.09174500
C	-5.84973200	1.12833400	2.14315200	C	6.68043100	-2.78695400	-0.76481900
C	-6.94356900	1.24907800	3.18378500	H	4.57155400	-2.77447300	-0.47640600
H	-7.44751000	-4.03574300	3.24624600	C	7.90067700	-2.08707000	-0.58916800
H	-6.53775400	-2.18817400	2.20447300	C	9.11135500	-0.11762500	0.19647900
H	-6.21198100	-3.30358200	0.06115300	C	6.62147900	1.23228600	2.48338700
H	-7.96154100	-3.26624500	-0.25892800	C	6.63658000	2.25547800	0.30280000
H	-8.52481400	-0.76278400	1.76278400	H	6.69783600	-3.76394600	-1.23304600
H	-4.65383600	-0.53335100	-3.13366700	C	9.13932700	-2.64393000	-1.00003800
H	-6.35109000	-0.26410500	-3.57966800	C	10.29409100	-0.67105300	-0.21631200
H	-6.17330900	1.98615000	-2.76047300	H	9.13410400	0.86307600	0.65247900
H	-4.52222600	1.83603100	-2.13402800	C	6.61808200	2.49263100	3.07526200
H	-5.85144100	2.30544200	-1.05119800	H	6.61787300	0.34039100	3.09867100
H	-4.94496500	0.70069100	2.57061600	C	6.63466300	3.51669300	0.89385400
H	-5.60388900	2.09962100	1.71726400	H	6.64935600	2.15884000	-0.77651200
H	-6.62780800	1.93647200	3.97021200	C	10.31248300	-1.96292100	-0.82019000
H	-7.15516800	0.28001700	3.63800200	H	9.16730000	-3.62461700	-1.45936500
H	-7.85967800	1.63440500	2.73371200	O	11.46909600	0.00932500	-0.01816300
C	-11.18741500	0.35888200	-1.34131100	C	6.62408800	3.63744800	2.28134400
N	-10.34600000	1.08351800	-2.15082900	H	6.61257400	2.58023000	4.15440200
C	-10.38907600	-0.50514300	-0.65232200	H	6.64160300	4.40245500	0.27128900
C	-9.08930300	0.66710300	-1.94993800	O	11.49662800	-2.50890400	-1.24595300
N	-9.08652600	-0.29627900	-1.04640800	C	12.04839900	0.51236100	-1.23029800
H	-10.65052700	-1.23800700	0.09129300	H	6.62211500	4.61746500	2.74124400
H	-8.21925100	1.06037200	-2.44344200	C	12.35183000	-2.92547000	-0.17194800
H	-8.06413300	-0.87539800	-0.69058400	H	12.96045600	1.02821600	-0.94151500
H	-12.25002100	0.51957000	-1.32731700	H	12.28149300	-0.30447700	-1.91175400
H	-8.47075000	-4.35294900	2.04143200	H	11.36157600	1.21401500	-1.70709500
H	-5.92782400	-1.60861200	-2.50984300	H	11.85343800	-3.69225400	0.42385900
H	-10.62093100	1.81294700	-2.79108400	H	13.24322200	-3.34038100	-0.63518700
C	-2.49743600	2.86573600	-0.25984900	H	12.61815200	-2.07731200	0.45705200
C	-2.14911200	1.54059300	-0.56087600	H	1.34010300	0.92300600	-2.19172800
C	0.03631800	2.09968300	-0.98957100				
C	-1.49728000	3.81950700	-0.34365800				
H	-3.50890100	3.10967400	0.02605500	C2e			
H	-1.71988300	4.85543700	-0.11912600	E=	-2628.37682410		
N	-3.09717200	0.52514700	-0.58894200	N	6.58769600	5.04874800	-0.93526000
H	-2.72009000	-0.37839300	-0.32012700	C	6.90605100	3.63349200	-0.84976500
O	-4.20567100	0.80444100	0.22298900	C	8.42219100	3.34859300	-0.70797800
N	-0.91652600	1.16178000	-0.90789100	O	8.72953200	1.97282200	-0.73169000
C	-0.20766500	3.44388500	-0.71728900	C	6.22274300	3.02464500	0.34247400
H	0.59140300	4.16906900	-0.79118300	O	5.73646400	3.68920800	1.23730500
C	1.41622500	1.60979100	-1.34473800	O	5.37414800	0.77084900	-1.97720700
H	2.04101300	2.45218600	-1.65033800	P	5.58017600	-0.58171600	-1.40376300
C	2.07326600	0.88036400	-0.16636700	N	6.90922400	-1.48156000	-1.80619000
H	2.15618700	1.56718900	0.68214000	C	7.11003600	-1.75681300	-3.23204100

C	8.16414700	-1.24684200	-1.08332200	C	-7.57169100	0.85032400	0.08210300
O	5.54585700	-0.55784600	0.18882700	C	-6.22235300	-0.90602400	1.28226200
C	5.35363700	-1.78809100	0.94299700	C	-6.45284700	2.60590000	-1.20481400
C	5.90948500	-1.57126500	2.33124900	H	-4.32517100	2.54396900	-1.20803900
H	6.70766900	5.46319500	-0.01699300	C	-7.65109100	2.00465600	-0.74428800
H	6.55394900	3.09744300	-1.73500000	C	-8.78247200	0.25921500	0.53434000
H	8.92466300	3.82497300	-1.55283300	C	-5.99706800	-0.80167400	2.65777800
H	8.78374300	3.82707100	0.21045900	C	-6.40043100	-2.17284900	0.71896400
H	6.23172700	1.92852200	0.39560700	H	-6.51472500	3.48728000	-1.83199700
H	7.74479400	-2.63820900	-3.32686000	C	-8.92254300	2.53985300	-1.07613100
H	7.59303600	-0.91679900	-3.73976700	C	-9.99898800	0.78766500	0.19315300
H	8.72347100	-0.41119300	-1.50965900	H	-8.76301600	-0.62560700	1.15630200
H	8.76565300	-2.15468700	-1.14137600	C	-5.94011800	-1.94290500	3.45348000
H	7.95792000	-1.02705000	-0.03779900	H	-5.86357700	0.17885800	3.09921400
H	4.28370600	-1.99075000	0.96507800	C	-6.34534200	-3.31488300	1.51417000
H	5.86345800	-2.60214600	0.42669900	H	-6.58481200	-2.25772100	-0.34556300
H	5.73268300	-2.46173600	2.93587300	C	-10.07346100	1.95534800	-0.62229200
H	5.42131200	-0.72133100	2.80752100	H	-8.99305100	3.42707200	-1.69368900
H	6.98248200	-1.37977300	2.29367100	O	-11.14910400	0.20705900	0.66512500
C	8.10514400	0.84563200	4.14877200	C	-6.11394300	-3.20191900	2.88296500
N	9.12764500	0.01971900	3.75577100	H	-5.76248900	-1.84864200	4.51733300
C	7.74938500	1.54220400	3.02709000	H	-6.48328200	-4.29033500	1.06507100
C	9.35476000	0.23724400	2.44255300	O	-11.29343800	2.47402200	-0.97479100
N	8.53648900	1.15437600	1.96616100	C	-11.90672100	-0.46557400	-0.35064700
H	6.97796700	2.28665100	2.91652100	H	-6.07080000	-4.08920000	3.50166300
H	10.11563700	-0.28466200	1.88579300	C	-11.97696400	3.11463200	0.11172200
H	8.64754900	1.63638500	0.18975000	H	-12.78079000	-0.88013300	0.14481200
H	7.73498200	0.86032900	5.15840300	H	-12.21403100	0.23425800	-1.12641700
H	7.24206400	5.50821900	-1.55913900	H	-11.31173500	-1.27048900	-0.78597100
H	6.15525700	-1.96743000	-3.70974700	H	-11.38101800	3.94925400	0.48531100
H	9.62600400	-0.63162600	4.34132300	H	-12.91526400	3.48417400	-0.29369300
C	2.54010200	-3.38024800	-0.95862700	H	-12.17113700	2.40491200	0.91451600
C	2.18689500	-2.11349900	-1.42613000	H	-1.46692900	-1.57611400	-2.65922400
C	-0.05053000	-2.59884100	-1.44720100				
C	1.50386100	-4.27529100	-0.73324000				
H	3.57288000	-3.64768200	-0.79813200				
H	1.72298600	-5.27330600	-0.37581100				
N	3.13726000	-1.08826400	-1.62416300				
H	2.88155400	-0.52900800	-2.43297800				
O	4.42085900	-1.64413100	-1.87759500				
N	0.94021900	-1.72569800	-1.67319400				
C	0.18915300	-3.88732800	-0.97243100				
H	-0.63547000	-4.56696700	-0.80611600				
C	-1.44751800	-2.09829900	-1.69940700				
H	-2.13715600	-2.94285700	-1.76138300				
C	-1.90409900	-1.13692500	-0.59441200				
H	-1.88383400	-1.65744400	0.36834900				
H	-1.18903800	-0.31191300	-0.52738000				
C	-3.30546800	-0.59015400	-0.85197600				
H	-4.01883500	-1.41753500	-0.92007800				
H	-3.32782500	-0.07135600	-1.81597500				
C	-3.76175500	0.37327500	0.25239700				
H	-3.74775200	-0.14817600	1.21070700				
H	-3.04833400	1.19935400	0.32025800				
C	-5.13718400	0.92786200	-0.03030100				
C	-6.28979400	0.31703600	0.42749300				
C	-5.23920900	2.07994400	-0.85493200				