Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications.

In silico study on aging and reactivation processes of tabun conjugated AChE

Nellore Bhanu Chandar,[a,b] Rabindranath Lo,[a] Manoj K. Kesharwani [a] and Bishwajit Ganguly [a,b]*

[a] Computation and Simulation Unit (Analytical Discipline and Centralized Instrument Facility), CSIR-Central Salt & Marine Chemicals Research Institute, Bhavnagar, Gujarat, India-364 002.

[b] Academy of Scientific and Innovative Research, CSIR-CSMCRI, Bhavnagar, Gujarat, India-364 002.

E-mail: ganguly@csmcri.org.

Supporting information

P-N Bond breaking

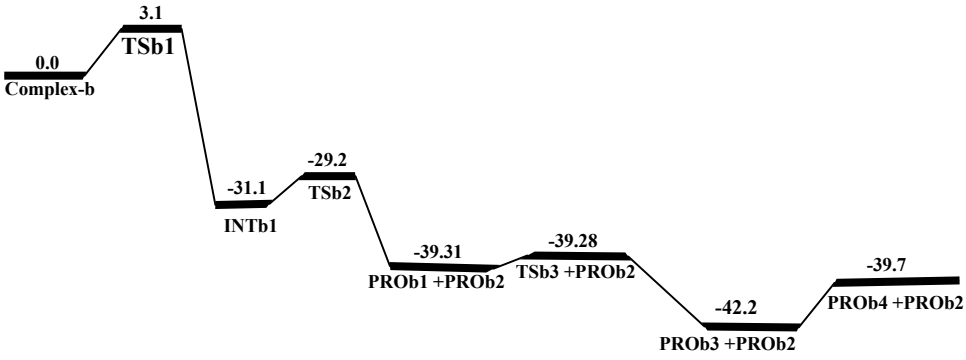


Fig. S1. MP2/6-31+G*//M05-2X/6-31G* calculated energy profile diagram for deamination (P-N anti elimination) of tabun-conjugated AChE in aqueous phase. Relative energies are in kcal/mol.

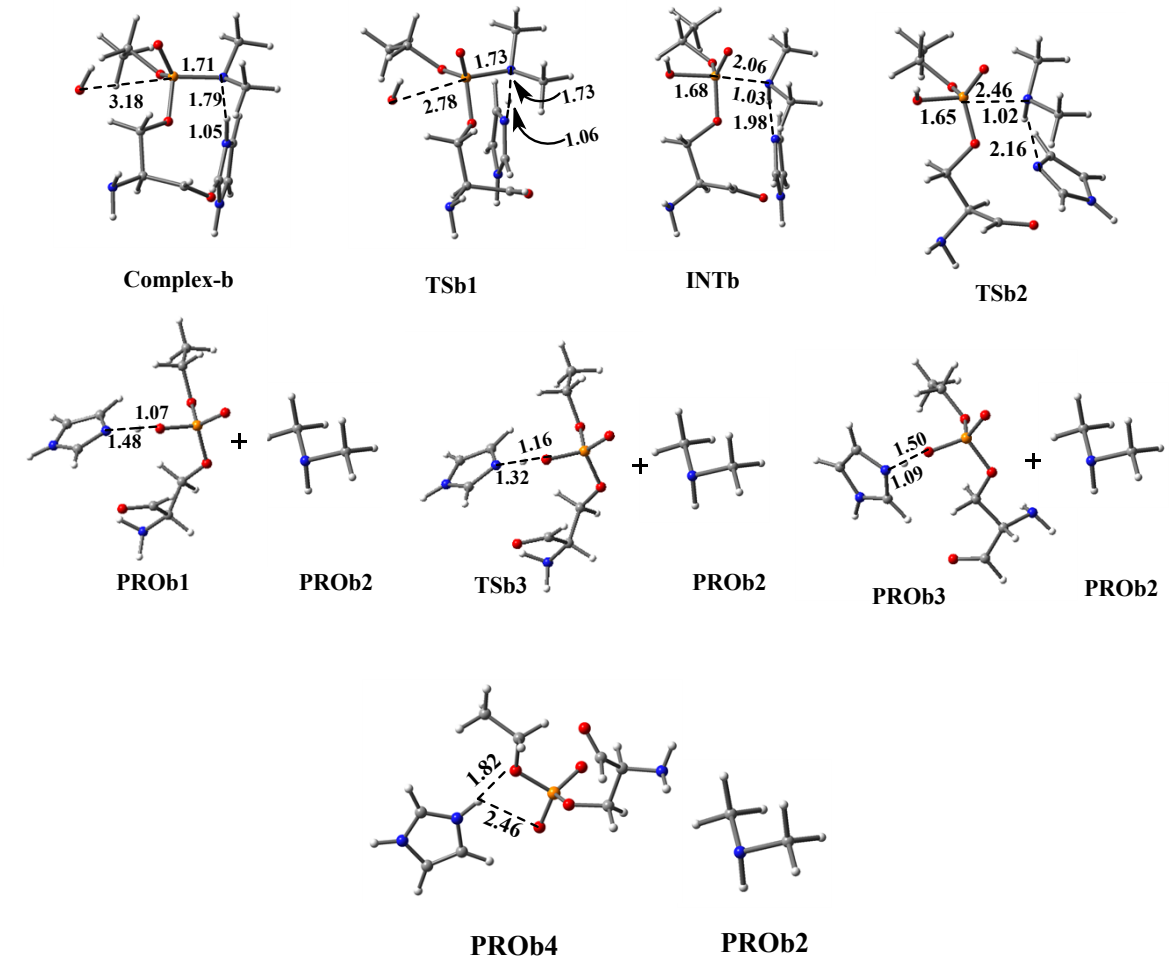
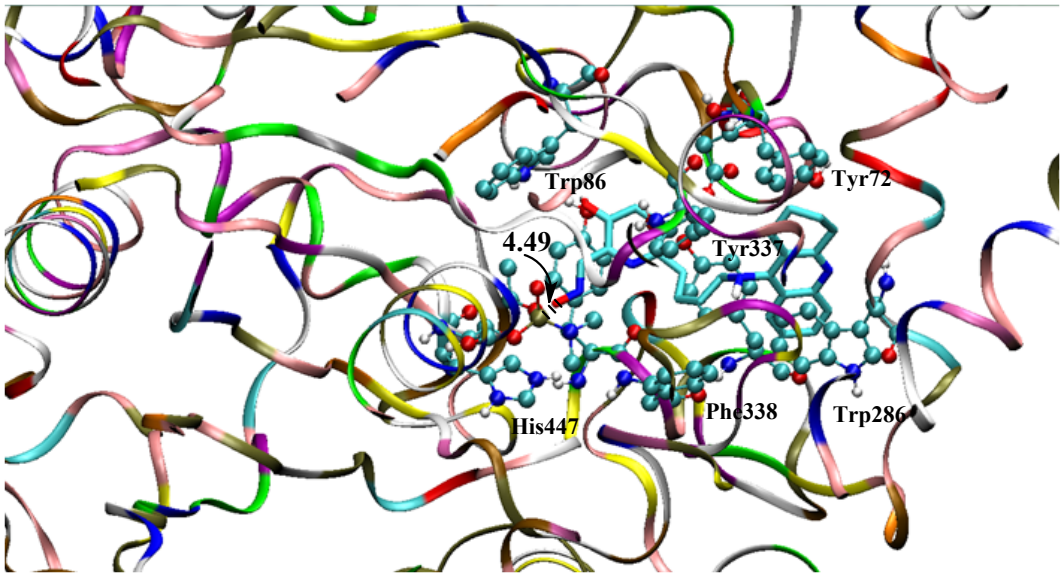


Fig. S2. M05-2X/6-31G* optimized geometries and selected bond distances in Å for species involved in deamination (P-N anti elimination) of tabun-conjugated AChE in aqueous phase (grey= carbon, blue = nitrogen, white = hydrogen, orange= phosphorus and red = oxygen).



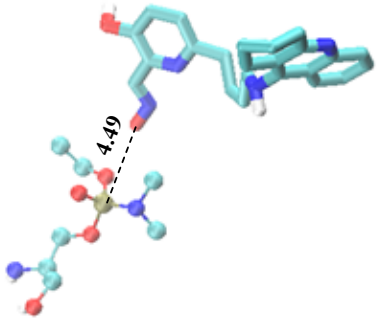
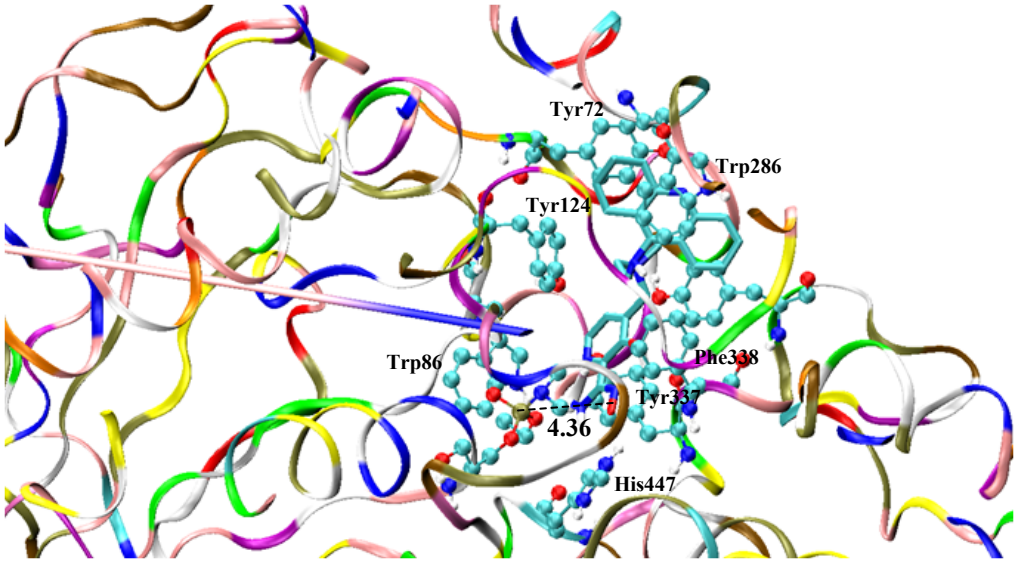


Fig. S3. Stable conformation of aldoxime based reactivator (molecule 12 from reference 23) with tabun-inhibited AChE showing interactions in the active site gorge. (red = oxygen, cyan = carbon, blue = nitrogen, white = hydrogen) (surrounding aromatic residues and SUN are shown in CPK and molecule 12 shown in tube format). SUN and reactivator are shown separately for clarity, distance is given in Å)



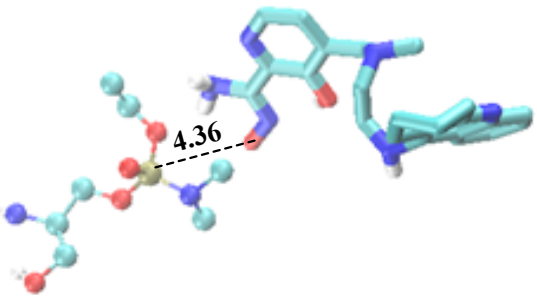


Fig. S4. Stable conformation of amidoxime based reactivator (molecule 8 from reference 23) with tabun-inhibited AChE showing interactions in the active site gorge. (red = oxygen, cyan = carbon, blue = nitrogen, white = hydrogen) (surrounding aromatic residues and SUN are shown in CPK and molecule 8 shown in tube format). SUN and reactivator are shown separately for clarity, distance is given in Å)

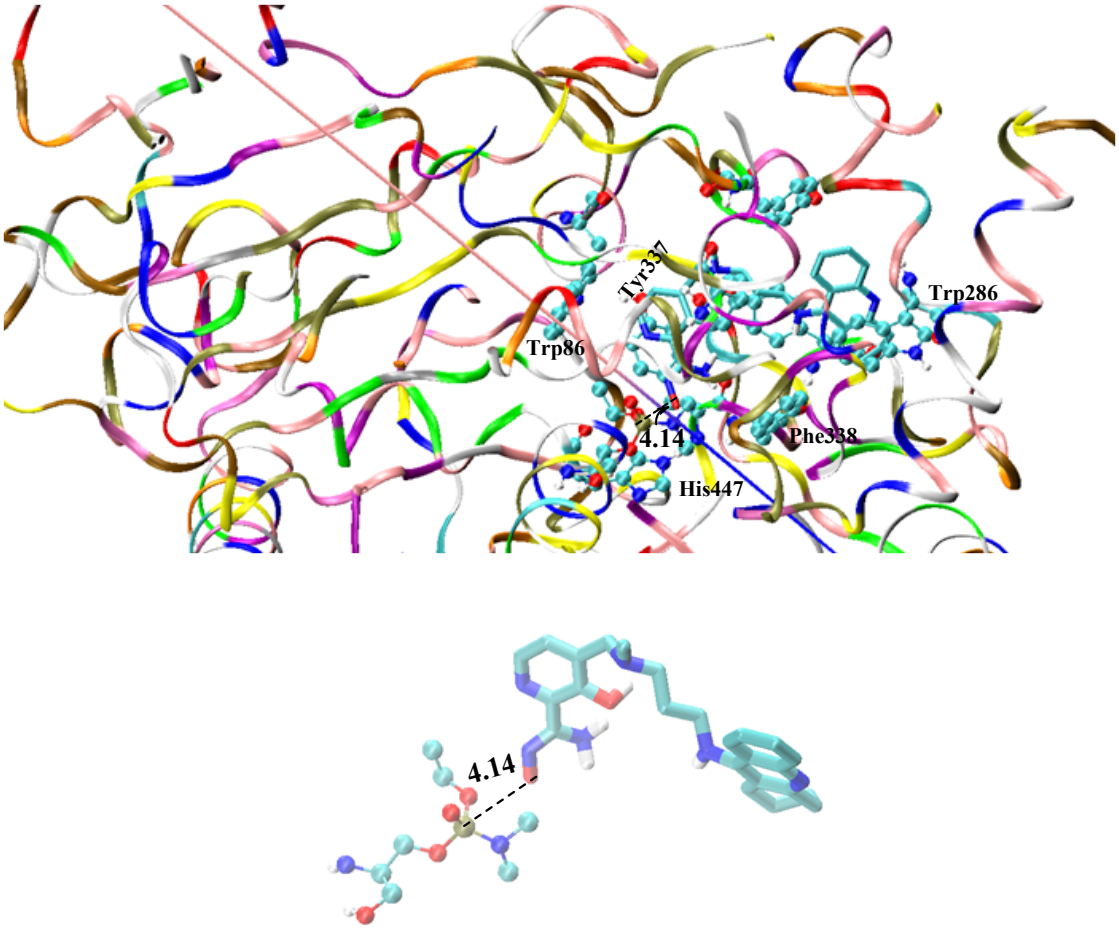


Fig. S5. Stable conformation of amidoxime based reactivator (molecule 9 from reference 23) with tabun-inhibited AChE showing interactions in the active site gorge. (red = oxygen, cyan = carbon, blue = nitrogen, white = hydrogen) (surrounding aromatic residues and SUN are shown in CPK and molecule 9 shown in tube format). SUN and reactivator are shown separately for clarity, distance is given in Å)

O-dealkylation

Complex-a

Charge=0, spin multiplicity=1

Energy= -1327.94991628 Ha

N	0.20851500	4.01451100	-0.36416600
C	0.51147800	2.58791000	-0.41870100
C	-0.38214800	1.95414700	-1.47667000
O	-0.08644300	0.54500000	-1.56199800
C	1.96832300	2.34578800	-0.76335700
O	2.74608800	1.72842900	-0.07228500
O	-2.54122100	-0.29867400	-1.43532800
P	-1.15391500	-0.49170900	-0.94330000
N	-0.34075400	-1.91835900	-1.22269700
C	-0.06098000	-2.22356000	-2.63373500
C	-0.83596900	-3.09039700	-0.48893300
O	-1.00728400	-0.33466900	0.64912900

C	-2.15541600	0.06433300	1.48410300
C	-2.99734100	-1.12005400	1.88739300
H	0.71494200	4.44999400	0.39795600
H	0.30855700	2.13198900	0.55114400
H	-1.42965300	2.12545300	-1.22835900
H	-0.18338100	2.37815000	-2.46114500
H	2.30034100	2.82438700	-1.70397600
H	0.69328800	-3.01013200	-2.66923000
H	0.33106100	-1.33974900	-3.13209000
H	-0.95662800	-2.57113300	-3.15733800
H	-0.08187600	-3.87460400	-0.55709100
H	-1.77494400	-3.46711700	-0.90641600
H	-0.98307300	-2.83785400	0.55919800
H	-1.69465600	0.54815600	2.34235400
H	-2.77861200	0.78606500	0.96413000
H	-3.87971800	-0.66665900	2.34847500
H	-2.47308300	-1.79505000	2.56570100
H	-3.31910600	-1.67299000	1.00170400
C	2.55530500	-0.61135600	2.33641200
C	2.47626000	-1.19659500	0.20863300
N	1.73849900	-0.87085100	1.26110700
H	2.16630500	-0.32061800	3.29473500
H	2.09465300	-1.43527000	-0.76805600
H	0.72256500	-0.76506300	1.22868900
H	0.50768100	4.47484500	-1.21855000
O	-4.76458000	1.38496900	2.10494100
H	-4.00857300	1.51992200	2.69373200
C	3.83214700	-0.80582600	1.91203800
H	4.77214600	-0.72165200	2.42526100
H	4.53054500	-1.38119400	-0.01647100
N	3.74909900	-1.17258900	0.58809200

TSa

Charge=0, spin multiplicity=1

Energy= -1327.93429447 Ha

N	0.47466100	3.84220700	-0.75639700
C	0.68548500	2.39746700	-0.73278700
C	-0.31137700	1.75365800	-1.68772100
O	-0.10054500	0.33290100	-1.71158800
C	2.09783700	2.04078400	-1.15181100
O	2.88882300	1.43067700	-0.46910700
O	-2.56662700	-0.43834800	-1.50162900
P	-1.19792300	-0.57337900	-0.92423500
N	-0.43439200	-2.06424600	-1.04611100
C	-0.24617100	-2.55295200	-2.41738500
C	-0.98431500	-3.10153300	-0.16645800
O	-1.06970300	-0.19926700	0.59531500
C	-2.37366800	0.55002000	1.42622900
C	-2.99255900	-0.65110700	2.08565000
H	1.06439500	4.29325600	-0.06672200
H	0.51656300	2.01843900	0.27562700
H	-1.32683200	2.00621700	-1.37831900
H	-0.16249100	2.11812900	-2.70521800
H	2.38843300	2.42771100	-2.14740100
H	0.43862300	-3.40143300	-2.39110900
H	0.19392500	-1.76869600	-3.02978300
H	-1.19047800	-2.87782300	-2.86732400
H	-0.29033400	-3.94271300	-0.15009100
H	-1.96012700	-3.45956800	-0.51333400
H	-1.08589000	-2.71054300	0.84389400
H	-1.76841400	1.20679400	2.02039000
H	-2.88613900	0.98905000	0.59316600

H	-3.78667200	-0.30930800	2.74049100
H	-2.24380900	-1.19530200	2.66362700
H	-3.40058300	-1.32577000	1.33087600
C	2.33386500	-0.25768300	2.38507800
C	2.30884300	-1.33401200	0.46036100
N	1.55046600	-0.70985000	1.35025500
H	1.92652500	0.28487900	3.21833600
H	1.95010800	-1.77445000	-0.45378400
H	0.54061400	-0.54099400	1.21626500
H	0.73338600	4.22458500	-1.66100900
O	-3.88205800	1.91295900	2.36089800
H	-3.53416300	2.73499900	1.98686300
C	3.60911900	-0.64106000	2.10970700
H	4.52594300	-0.50165900	2.65197200
H	4.34929800	-1.71689900	0.42752000
N	3.56005100	-1.31255100	0.90972300

PROa1

Charge=0, spin multiplicity=1

Energy= -1173.47796913 Ha

N	-3.46210500	-2.46465200	0.21027600
C	-2.26938900	-1.64298000	0.00054300
C	-2.34983700	-0.43008200	0.91904100
O	-1.13764200	0.32166300	0.87213000
C	-1.02256400	-2.44482200	0.30806400
O	-0.25750600	-2.87299500	-0.52741100
O	-2.16874100	1.95136700	-0.83427900
P	-0.88773500	1.26854200	-0.45445600
N	0.28732600	2.28635600	0.23449000
C	-0.20471800	3.15133500	1.30551400
C	1.08270100	3.03390800	-0.74009000
O	-0.17134600	0.43334400	-1.51309700
H	-3.46581300	-3.24531800	-0.43623000
H	-2.22259700	-1.33270400	-1.04342600
H	-3.20257500	0.18804000	0.63987800
H	-2.47066900	-0.75945100	1.95325900
H	-0.88480000	-2.68853200	1.37910700
H	0.64739000	3.59571800	1.82352200
H	-0.77537200	2.55808400	2.01767300
H	-0.84006400	3.95901300	0.92259700
H	1.94610500	3.47038800	-0.23359900
H	0.51217200	3.84745600	-1.20642400
H	1.43347700	2.35822100	-1.51754300
C	2.65825800	-1.77636900	-0.72497200
C	2.54117200	0.00925800	0.54987800
N	1.95065300	-0.63230400	-0.44681900
H	2.34867700	-2.46502000	-1.48902800
H	2.18814200	0.93261300	0.97871400
H	1.05212600	-0.26829800	-0.92874600
H	-3.45912900	-2.85795900	1.14687700
C	3.71405700	-1.81859500	0.13342200
H	4.50653800	-2.53387800	0.25529200
H	4.24820300	-0.42918700	1.65850800
N	3.61526900	-0.69144000	0.91766400

Ethanol

Charge=0, spin multiplicity=1

Energy= -154.53639405 Ha

C	1.17261400	-0.40335000	0.00000000
H	1.13819900	-1.03949000	0.88560500
H	2.11555400	0.14513100	0.00000000
H	1.13819900	-1.03949000	-0.88560500
O	-1.19552700	-0.22140600	0.00000000
H	-1.94293100	0.38896300	0.00000000
C	0.00000000	0.55609500	0.00000000

H	0.03975600	1.19983200	-0.88468200
H	0.03975600	1.19983200	0.88468200

P-N anti deamination

Complex-b

Charge=0, spin multiplicity=1

Energy= -1327.95557380 Ha

N	4.33193300	-0.23860200	-1.23170600
C	3.06755100	0.28494500	-0.73003800
C	2.20814400	-0.89187900	-0.27993900
O	0.91508300	-0.34135600	0.08583400
C	3.24439000	1.22253900	0.44328300
O	2.57309600	2.21020400	0.65885700
O	0.14218900	-2.65740700	1.05040900
P	-0.25947200	-1.30190500	0.59379200
N	-0.88010100	-0.26946100	1.80431400
C	0.09963200	0.08290900	2.84503400
C	-2.13296600	-0.76261600	2.39915000
O	-1.47480600	-1.20389600	-0.42694800
C	-1.95953300	-2.39028400	-1.13891300
C	-3.08024000	-1.91908200	-2.03684600
H	4.91826900	0.51948800	-1.56146300
H	2.54431400	0.81413700	-1.52807100
H	2.03256000	-1.61765300	-1.09197100
H	2.64432700	-1.37173500	0.60103800
H	4.04782800	0.93074300	1.14490300
H	-0.36112400	0.80521800	3.51864200
H	0.97370200	0.53866000	2.38515700
H	0.40334700	-0.79508400	3.42350400
H	-2.53769600	0.01488300	3.04690200
H	-1.96439600	-1.66647300	2.99292900
H	-2.85194500	-0.97515100	1.61054600
H	-1.09639500	-2.78539400	-1.68401000
H	-2.31913400	-3.09910900	-0.39201900
H	-3.49577700	-2.76955100	-2.58004100
H	-2.70710700	-1.19468900	-2.76204300
H	-3.87986500	-1.45405400	-1.45746900
C	-2.30636500	3.47805900	-1.15225900
C	-2.57336700	2.44125400	-0.31335700
C	-0.38316300	2.71141700	-0.36249900
N	-1.36461200	1.99101700	0.16323700
H	-3.50562100	1.99295700	-0.02153400
H	0.67260400	2.57934000	-0.17240700
H	-1.21837900	1.17904900	0.81209000
H	-2.95370200	4.11044400	-1.73145400
H	4.84273000	-0.69796800	-0.48380400
O	0.86134400	-2.74406700	-2.01421800
H	0.83688300	-3.22892100	-1.17867600
H	-0.42169300	4.30939400	-1.69198000
N	-0.93741700	3.62256500	-1.16139000

TSb1

Charge=0, spin multiplicity=1

Energy= -1327.95058741 Ha

N	4.33921400	-0.36411000	-1.33557500
C	3.09761600	0.17910500	-0.79848600
C	2.21352400	-0.98464800	-0.36229200
O	0.94327600	-0.41738900	0.02904400
C	3.32247900	1.08046100	0.39481900
O	2.69776500	2.09137000	0.63969200
O	0.01387600	-2.71987900	0.99411400

P	-0.27777700	-1.35101700	0.48884000
N	-0.80358200	-0.29941200	1.76063600
C	0.22178100	-0.06451200	2.78839800
C	-2.05759700	-0.75461400	2.37996400
O	-1.54047100	-1.09705800	-0.45029200
C	-2.22162300	-2.19242700	-1.13123000
C	-3.23154600	-1.56049100	-2.06232700
H	4.94552000	0.38709700	-1.64451200
H	2.57515200	0.74375400	-1.57237800
H	1.99971100	-1.68837400	-1.17659600
H	2.65206700	-1.49596900	0.50056800
H	4.11930400	0.73880200	1.08135400
H	-0.18045800	0.62996100	3.52638600
H	1.10353100	0.37996100	2.33270500
H	0.49958800	-0.99444100	3.29534400
H	-2.39314300	0.00314700	3.08853900
H	-1.91771800	-1.70030400	2.91358900
H	-2.81915300	-0.88184300	1.61317800
H	-1.43432900	-2.74145600	-1.64983800
H	-2.71206700	-2.80279200	-0.37040800
H	-3.79396600	-2.34003100	-2.57909700
H	-2.72508000	-0.94635300	-2.80824300
H	-3.93510800	-0.93229400	-1.51261700
C	-2.20725700	3.54982900	-0.96258200
C	-2.46141800	2.47947300	-0.16214200
C	-0.27350800	2.72558700	-0.26382200
N	-1.24649100	1.99383700	0.25979200
H	-3.39079800	2.02919900	0.13648100
H	0.78567200	2.57200600	-0.11441300
H	-1.09243400	1.13881700	0.87439100
H	-2.86311300	4.21511800	-1.49327400
H	4.84375100	-0.86659400	-0.61158500
O	0.51565300	-2.61711000	-1.85484400
H	0.61262700	-3.29458900	-1.17370100
H	-0.32863900	4.38244800	-1.52091400
N	-0.83767900	3.67882100	-1.00643700

INTb1

Charge=0, spin multiplicity=1

Energy= -1328.00448329Ha

N	0.42353000	3.99362700	1.27134400
C	0.57204900	2.72549800	0.56541400
C	-0.81206300	2.08454400	0.46275600
O	-0.64849200	0.86776400	-0.26226100
C	1.03723400	3.03312200	-0.83823400
O	1.92221600	2.44373900	-1.41837300
O	-2.57629900	-0.33834100	-1.84464200
P	-1.86729500	-0.20611800	-0.52068700
N	-0.28092500	-1.28262200	-1.27848900
C	0.31104000	-0.63542500	-2.46245400
C	-0.67453900	-2.65964700	-1.61930200
O	-1.78895100	-1.38061500	0.60777600
C	-2.83640000	-1.67015300	1.55430300
C	-2.57094900	-0.97625500	2.87451500
H	-0.02423000	3.83031500	2.16687100
H	1.26588100	2.00879500	1.01764500
H	-1.19697900	1.89084400	1.46410700
H	-1.49874500	2.75882800	-0.04996000
H	0.49110500	3.86193100	-1.32023700
H	1.13578500	-1.24120100	-2.84436300
H	0.67855300	0.34924700	-2.19060400
H	-0.46279200	-0.54525000	-3.22202100
H	0.17556300	-3.19948200	-2.04169300

H	-1.47774500	-2.60913600	-2.35221100
H	-1.02531700	-3.16673300	-0.72576400
H	-3.80067400	-1.38337300	1.14283400
H	-2.81169000	-2.75325300	1.67368400
H	-3.31627400	-1.27860800	3.61300100
H	-2.62176900	0.10424800	2.74511600
H	-1.58279600	-1.24664000	3.24943100
C	4.26938500	-1.92525800	1.12887200
C	2.96311000	-2.31191500	1.00151500
C	3.10087200	-0.37255700	0.09131400
N	2.24084500	-1.33628000	0.35436400
H	2.50481900	-3.22816100	1.33603400
H	2.87701000	0.55652100	-0.41133400
H	0.44787500	-1.31810700	-0.55445800
H	5.12855800	-2.40058000	1.56761700
H	1.33740000	4.37831100	1.48185400
O	-3.01685000	0.70207300	0.31210100
H	-3.70539300	0.91076500	-0.33211400
H	5.15970300	-0.11222300	0.45839100
N	4.33657100	-0.68672200	0.54270400

TSb2

Charge=0, spin multiplicity=1

Energy= -1328.00216540 Ha

N	-0.95307500	3.29210600	-1.93708400
C	-0.76392800	2.37393700	-0.81651100
C	0.71382900	2.02606300	-0.72828300
O	0.87649600	1.21359800	0.44437300
C	-1.22043500	3.00643900	0.48165600
O	-2.11593500	2.58674500	1.18163000
O	2.64508800	-0.15950500	1.88923700
P	2.12584200	0.19621400	0.54185400
N	0.20664200	-1.19230700	1.21881000
C	-0.44099500	-0.64486300	2.40383600
C	0.62930700	-2.56847400	1.43266700
O	1.97223200	-0.84683000	-0.67172200
C	3.14537400	-1.29780700	-1.39708300
C	2.71923500	-2.47782400	-2.24144000
H	-1.94075700	3.46488100	-2.08394900
H	-1.33838900	1.46238000	-0.98422000
H	1.01179000	1.48581300	-1.62638900
H	1.32671600	2.92443600	-0.63305400
H	-0.69905800	3.94658700	0.74228800
H	-1.27456400	-1.27003100	2.75013600
H	-0.81664300	0.35250100	2.17981200
H	0.29802900	-0.57259900	3.20355700
H	-0.19685000	-3.21985500	1.74575200
H	1.39516100	-2.57854000	2.21015700
H	1.06200300	-2.96116600	0.51335500
H	3.51281000	-0.47706300	-2.00854600
H	3.92026000	-1.57980000	-0.68316300
H	3.56638000	-2.83256600	-2.83008400
H	1.91978400	-2.18529400	-2.92285400
H	2.36453900	-3.29526900	-1.61330800
C	-4.20802700	-2.21912600	-0.72996900
C	-2.88852300	-2.14512000	-1.08470000
C	-3.30202800	-0.36337900	0.03547300
N	-2.33033100	-0.98192400	-0.60522600
H	-2.31276400	-2.85686800	-1.65369500
H	-3.21544100	0.58837100	0.53726500
H	-0.45251300	-1.14748000	0.44442400
H	-4.96966500	-2.95655600	-0.91204000
H	-0.52279000	4.19001600	-1.73670000
O	3.28689300	1.14123400	-0.15067800
H	3.89155100	1.44599500	0.53992100

H	-5.33185300	-0.80501900	0.39554200
N	-4.45272500	-1.07317300	-0.01630300

PROb1

Charge=0, spin multiplicity=1

Energy= -1193.33907113Ha

N	2.61429700	-1.64735200	1.62687800
C	1.48363000	-2.19889000	0.90104800
C	0.23332200	-1.43265500	1.34345600
O	-0.93302700	-1.91785200	0.65376400
C	1.64513600	-2.14973200	-0.61047200
O	2.56619200	-1.56881000	-1.14325900
O	-2.78698900	-1.70688800	-1.07463600
P	-1.67934000	-0.98059200	-0.41606400
O	-2.12205100	0.25493100	0.51866400
C	-2.85083900	1.33266100	-0.12562800
C	-3.42435900	2.21541300	0.95906600
H	3.38786100	-2.30135600	1.58520400
H	1.34116500	-3.24795800	1.17442800
H	0.07820200	-1.59689400	2.40640500
H	0.37364600	-0.36440300	1.17341500
H	0.88941200	-2.67869700	-1.20633100
H	-2.16099800	1.88064400	-0.76955200
H	-3.63996400	0.89964600	-0.74077200
H	-3.96770000	3.04625600	0.50793300
H	-2.63101200	2.61971700	1.58893800
H	-4.11056800	1.64568800	1.58544000
C	1.83692500	3.23106700	0.45439000
C	0.70556400	2.47954000	0.31804300
C	2.20383300	1.57622100	-0.95472200
N	0.94877200	1.45250100	-0.56536700
H	-0.25135000	2.60321200	0.79549600
H	2.71925800	0.92070200	-1.63509500
H	2.05689200	4.10422200	1.04171400
H	2.93403800	-0.82112300	1.12868000
O	-0.58902200	-0.40900300	-1.39021700
H	0.03061700	0.39341300	-1.03509700
H	3.72297700	2.94543600	-0.49172800
N	2.77086400	2.64050800	-0.36061600

PROb2

Charge=0, spin multiplicity=1

Energy= -134.67915381 Ha

N	0.00005900	0.58073300	-0.15615000
C	1.20062700	-0.22663700	0.02023500
C	-1.20069800	-0.22661000	0.02023000
H	1.22778700	-0.76798600	0.97760800
H	2.08563100	0.40695500	-0.04501000
H	1.25444100	-0.96716600	-0.78109600
H	-1.22812800	-0.76732500	0.97794000
H	-1.25421300	-0.96768700	-0.78061300
H	-2.08560000	0.40703100	-0.04573400
H	0.00009500	1.31053200	0.54716400

PROb3

Charge=0, spin multiplicity=1

Energy= -1193.34375076Ha

N	3.50505600	0.47430200	1.36147400
C	2.97922000	0.95308300	0.08449600
C	1.64304500	0.31988400	-0.24438900
O	1.80999900	-1.08218900	-0.43877300
C	2.82865900	2.46158500	0.11737300
O	1.78356500	3.05141100	-0.06327500

O	0.79149900	-3.32742200	-1.04313300
P	0.43728500	-1.92564200	-0.68542000
O	-0.18306400	-1.80404700	0.82148800
C	-1.51397500	-2.31318900	1.01756400
C	-2.09624300	-1.64906900	2.24679000
H	4.44938800	0.81256500	1.50795200
H	3.70195700	0.69695600	-0.69535800
H	0.94428400	0.49852700	0.57850100
H	1.24287100	0.76791500	-1.15515800
H	3.74366000	3.01449300	0.38578600
H	-2.11824700	-2.09418000	0.13418100
H	-1.46165500	-3.39677800	1.13884000
H	-3.10164600	-2.02645200	2.43858400
H	-2.14877300	-0.56881000	2.10176600
H	-1.47416000	-1.85485500	3.11857300
C	-3.56859300	2.06176900	-0.04106600
C	-3.18696500	0.85254200	-0.53609100
C	-1.37606800	2.08199600	-0.33937300
N	-1.82334400	0.89064700	-0.71187000
H	-3.76898600	-0.01895900	-0.77692800
H	-0.35030400	2.41871300	-0.35026100
H	-4.53233600	2.44966000	0.23304700
H	2.93912000	0.82490900	2.12753300
O	-0.46924100	-1.12222400	-1.61350400
H	-1.22167200	0.06440500	-1.08471500
H	-2.36077800	3.75645300	0.40799500
N	-2.41864600	2.80708400	0.06992700

P-N rearrangement deamination process

Complex-c

Charge=0, spin multiplicity=1

Energy= -1327.95269170 Ha

C	-1.60223900	2.32852500	0.23514800
H	-1.93540400	1.87929600	1.17447000
C	-1.58106900	1.25211700	-0.83648000
H	-1.20730500	1.65906600	-1.77626100
H	-2.59433200	0.82379000	-0.95860700
O	-0.63202400	0.20051800	-0.48306300
P	-1.06603200	-1.02187800	0.50223600
N	-1.30019400	-2.40388500	-0.37039500
C	-0.19613500	-3.28554100	-0.73963900
H	0.52372500	-3.36188100	0.06993300
H	0.30399400	-2.94345500	-1.65350300
H	-0.60946300	-4.27633100	-0.93513100
C	-2.35510700	-2.35402500	-1.39282400
H	-3.11103100	-1.57330900	-1.17559300
H	-2.83429400	-3.33516700	-1.44026300
H	-1.91009100	-2.14303700	-2.37334400
O	-2.16227400	-0.62740600	1.42368300
O	0.34898800	-1.32518300	1.20130000
C	0.77871300	-0.41376500	2.24579500
H	0.02440600	-0.40926500	3.03163100
H	0.85457700	0.58977300	1.82206900
C	2.11756200	-0.89758400	2.75387700
H	2.85482200	-0.90198200	1.95028400
H	2.02763900	-1.90737400	3.15444300
H	2.46828400	-0.23624000	3.54685500
H	1.23591900	0.58028400	-0.69772400
C	-0.25597600	2.97636700	0.46450900
O	0.76084900	2.69682800	-0.13916500
N	4.34912500	0.74059400	-0.96715400
H	5.23699500	1.22105800	-0.99687500
C	4.16492900	-0.61769900	-1.09360900
C	3.17412200	1.33916400	-0.79440400
H	3.00189200	2.39052400	-0.65655700

N	2.23899300	0.39831500	-0.80727000
C	2.82593800	-0.83217000	-0.99117800
H	2.25474100	-1.74077300	-1.02369200
H	-0.25570200	3.80256400	1.19541800
N	-2.56745700	3.36090400	-0.14925800
H	-2.76023700	3.98368800	0.62637400
H	-2.19958300	3.92733300	-0.90625500
H	4.98416700	-1.29692300	-1.24061500
O	-4.29402200	-0.05394700	-0.91721900
H	-4.00305900	-0.17378900	-0.00352300

TSc1

Charge=0, spin multiplicity=1

Energy= -1327.94700240 Ha

C	-1.77340500	2.32676600	0.12837800
H	-1.97323700	1.80879000	1.07470000
C	-1.64981500	1.28109900	-0.97080400
H	-1.22840600	1.72570000	-1.87368300
H	-2.60280000	0.75846000	-1.16746700
O	-0.71796500	0.22885400	-0.59823300
P	-1.12276100	-0.98831600	0.39740100
N	-1.02807700	-2.42177900	-0.42772900
C	-0.33313300	-3.54830500	0.18727400
H	-0.45633600	-3.53332400	1.26794000
H	0.73933100	-3.55309000	-0.03686300
H	-0.77139800	-4.47132500	-0.19648400
C	-1.10860100	-2.45423600	-1.88304700
H	-1.87195300	-1.73774600	-2.17560700
H	-1.42228900	-3.45631600	-2.18480900
H	-0.14003000	-2.24200700	-2.35168900
O	-2.18724400	-0.69411000	1.40053700
O	0.31157700	-1.09344500	1.18847700
C	0.55690700	-0.16684400	2.25977700
H	-0.24349000	-0.25225800	2.99395900
H	0.55271100	0.85107900	1.86003900
C	1.90476500	-0.50001500	2.86368300
H	2.69410000	-0.41111000	2.11572400
H	1.90359100	-1.52057900	3.24822700
H	2.12519200	0.18256000	3.68550900
H	1.09947900	0.67193300	-0.59130400
C	-0.50736400	3.11831900	0.34812900
O	0.58636100	2.79213400	-0.06626000
N	4.21043900	0.81347000	-0.92683100
H	5.10121200	1.28593000	-0.98226900
C	4.01151100	-0.54526500	-1.02998700
C	3.04316900	1.42420900	-0.73720600
H	2.88300500	2.47942800	-0.61350800
N	2.10228500	0.49144100	-0.71571800
C	2.67295400	-0.74584200	-0.89472000
H	2.08637000	-1.64589600	-0.89176400
H	-0.63873400	4.04988100	0.92096500
N	-2.85570600	3.28279600	-0.09317100
H	-2.80599500	3.64029300	-1.04209500
H	-3.74426400	2.80158800	-0.01761200
H	4.82220000	-1.23307400	-1.18414900
O	-3.42784000	-0.84499600	-1.18049300
H	-3.69046100	-0.78248800	-0.25571100

INTc1

Charge=0, spin multiplicity=1

Energy= -1327.97056893 Ha

C	-1.90195500	2.35611100	0.01636600
H	-2.54331200	1.72703500	0.64114900
C	-1.22276600	1.45798600	-1.00510500
H	-0.40847600	2.00162900	-1.49232200
H	-1.94204900	1.13498400	-1.75077100

O	-0.61560500	0.34575700	-0.35630000
P	-1.37318500	-1.05679600	0.25591300
N	-1.21011400	-2.42263500	-0.77883700
C	-0.36698100	-3.54031200	-0.38270900
H	-0.48855400	-3.74972400	0.67709900
H	0.69820800	-3.36732600	-0.57694800
H	-0.68333900	-4.42011300	-0.95178900
C	-1.06945900	-2.14108400	-2.20107100
H	-1.76553200	-1.36050100	-2.49448200
H	-1.29575600	-3.04638600	-2.77179700
H	-0.04689500	-1.82928600	-2.46258200
O	-2.09992600	-1.17731700	1.58760400
O	0.25218300	-1.35774000	0.89162000
C	0.60647300	-0.73025800	2.10828600
H	-0.16466600	-0.91295500	2.85760000
H	0.67954000	0.35881800	1.97423100
C	1.93977800	-1.28526300	2.58465300
H	2.73344300	-1.08262100	1.86342200
H	1.86732200	-2.36686900	2.71569100
H	2.22221200	-0.83961800	3.54111000
H	1.05146900	0.30527300	-0.28913400
C	-0.90211900	3.01793500	0.93943600
O	0.30134900	2.89028500	0.86415300
N	3.99597900	1.32064500	-0.80484800
H	4.72486300	2.01733100	-0.85711000
C	4.14514000	-0.02318900	-1.06331300
C	2.73235500	1.57056500	-0.46111700
H	2.31615100	2.52411800	-0.19022500
N	2.07047600	0.42458400	-0.49165700
C	2.92248800	-0.58634900	-0.86218500
H	2.58769100	-1.60477900	-0.93630900
H	-1.35204100	3.68497800	1.69231300
N	-2.72470300	3.42913200	-0.53559900
H	-2.21851500	3.90502700	-1.27542500
H	-3.55454400	3.03295900	-0.96075800
H	5.08701300	-0.44897800	-1.35631300
O	-2.79062000	-0.54402300	-0.62579000
H	-3.50468800	-0.90569800	-0.08849600

TSc2

Charge=0, spin multiplicity=1

Energy= -1327.96100609 Ha

C	-3.25741000	-0.36886300	0.29881300
H	-2.96981500	-0.46003900	1.34726900
C	-2.20724500	-1.09798300	-0.55586600
H	-2.43848600	-0.97932800	-1.61895600
H	-2.26188600	-2.15908000	-0.30995100
O	-0.92408000	-0.58162800	-0.25886000
P	0.39382900	-1.66801200	-0.14265800
N	2.00217900	-2.02104200	-0.70483300
C	3.00594800	-2.20129000	0.33325300
H	2.57210400	-2.75745300	1.16243900
H	3.39590300	-1.24948500	0.71220700
H	3.83772800	-2.78049600	-0.08096900
C	2.53454500	-1.18962500	-1.77689500
H	1.77402500	-1.02734700	-2.53885100
H	3.38811800	-1.69297200	-2.24085000
H	2.88623900	-0.21288200	-1.41673800
O	0.02584000	-2.73732400	0.87494600
O	1.10533400	-0.31000100	0.73440200
C	0.52761700	0.01255500	1.99896500
H	0.06809800	-0.88263300	2.42151100
H	-0.26163700	0.76399400	1.88328600

C	1.62196100	0.52760600	2.91881700
H	2.07611500	1.43461500	2.51545000
H	2.40264800	-0.22664300	3.03148900
H	1.21453600	0.75974900	3.90524700
H	-0.05761400	1.15348000	-0.18146200
C	-3.25472400	1.09264800	-0.06023300
O	-2.50037700	1.91217400	0.41995200
N	0.79908800	4.11105000	-0.78060700
H	0.62903700	5.07736700	-1.01854900
C	2.02955400	3.54467500	-0.53526500
C	-0.15045700	3.18845400	-0.64502500
H	-1.20885500	3.34105300	-0.75203700
N	0.43681800	2.04436500	-0.31769100
C	1.79771700	2.23651000	-0.24443700
H	2.45582300	1.43206300	0.02046300
H	-3.98596500	1.38656000	-0.83361100
N	-4.61196000	-0.88360000	0.10912800
H	-4.79574400	-0.99403800	-0.88410600
H	-4.67313900	-1.81322200	0.50889100
H	2.94131300	4.11070900	-0.58469600
O	-0.16317200	-2.22501200	-1.70580500
H	0.48774500	-2.89299600	-1.95943300

INTc2

Charge=0, spin multiplicity=1

Energy= -1327.97119234 Ha

C	0.67665800	2.88021700	-0.50290800
H	-0.37372300	3.03357800	-0.23879700
C	0.78714500	1.48199200	-1.09425300
H	1.84600000	1.24691500	-1.26536100
H	0.27876500	1.47316900	-2.06191900
O	0.24616200	0.53707500	-0.20543900
P	-1.41749200	-0.02610200	-0.51030000
N	-2.86649500	-1.08340000	-0.77310300
C	-4.12316000	-0.48335500	-0.35750800
H	-4.22362300	0.50339000	-0.80022900
H	-4.19724200	-0.38746200	0.73836200
H	-4.95612700	-1.11262900	-0.68932100
C	-2.79333300	-2.43223800	-0.21981700
H	-1.82394000	-2.88703400	-0.42993500
H	-3.56706800	-3.05971200	-0.67526100
H	-2.94045600	-2.44661100	0.86860600
O	-2.00407400	1.29365900	-0.96559400
O	-1.45421300	-0.45268500	1.09212400
C	-0.78555900	0.26327000	2.13623000
H	-0.83199600	1.33590700	1.94192100
H	0.26588100	-0.02100700	2.16616400
C	-1.49176600	-0.08594100	3.43282300
H	-1.45032200	-1.16193200	3.61065900
H	-2.53973500	0.21523800	3.38790900
H	-1.01721800	0.42339800	4.27358500
H	1.00990200	-1.30367900	-0.85546500
C	1.47661500	3.03399700	0.77025900
O	2.20101700	2.19225500	1.25684800
N	3.62394000	-2.90892000	-0.17626700
H	4.25600800	-3.69427800	-0.23215200
C	3.81716800	-1.77090800	0.57508400
C	2.46582200	-2.82008400	-0.82776700
H	2.05584600	-3.56201200	-1.48909800
N	1.91499700	-1.65796100	-0.51147200
C	2.73050500	-0.97856000	0.36269200
H	2.46048100	-0.00168300	0.73155100
H	1.39351000	4.03217800	1.23316200

N	1.09423800	3.97922600	-1.37472500
H	1.98341000	3.74759900	-1.80634900
H	0.42728400	4.07900200	-2.13114700
H	4.69342900	-1.63105600	1.18087200
O	-0.62517000	-1.03565400	-1.62009200
H	-1.32378000	-1.53990500	-2.06608000

TSc3

Charge=0, spin multiplicity=1

Energy= -1327.95740549 Ha

N	1.00686600	3.79319500	-1.83311000
C	0.34103600	2.89780000	-0.88427400
C	0.79696300	1.46501500	-1.13009800
O	0.31730300	0.61823400	-0.10744600
C	0.68624600	3.28082100	0.53645800
O	-0.09278000	3.73209700	1.34773700
O	-1.96694000	0.79205200	-1.12330700
P	-1.14236100	-0.28531300	-0.46508800
N	-2.39143700	-1.79737400	-0.80985800
C	-3.66501900	-1.45897600	-1.42079200
C	-2.57056900	-2.79091400	0.23918500
O	-1.32550400	-0.58836700	1.13484500
C	-1.10467500	0.44039500	2.11540700
C	-1.93799100	0.08528700	3.33061000
H	0.67734300	4.74361700	-1.70726100
H	-0.73867200	2.95201800	-1.00962500
H	0.47169000	1.14857600	-2.12293100
H	1.89500300	1.43354700	-1.11332600
H	1.76041700	3.17294700	0.78903800
H	-4.14967000	-2.36196300	-1.80818500
H	-3.51171500	-0.75584000	-2.23488800
H	-4.34804700	-0.99585200	-0.69569100
H	-3.06041400	-3.68149600	-0.17001100
H	-3.18199900	-2.41037300	1.06579500
H	-1.60188800	-3.08473500	0.64399600
H	-0.04382100	0.48363500	2.36165400
H	-1.39413800	1.40801200	1.70613400
H	-1.78949100	0.82685100	4.11748600
H	-1.65002700	-0.89352300	3.71715500
H	-2.99729000	0.05731300	3.07118000
C	4.25547200	-2.35792800	0.17170900
N	3.95566700	-1.25359100	0.93652500
C	3.17604200	-2.56873400	-0.62987400
C	2.74238300	-0.80552600	0.61564100
N	2.25641400	-1.59069300	-0.33420200
H	2.99197600	-3.32166800	-1.37437200
H	2.22775800	0.04070500	1.03526600
H	1.30211500	-1.47527000	-0.75907500
H	5.18852900	-2.88268800	0.26307000
H	2.00764700	3.80631000	-1.65762700
O	-0.23368000	-1.34291200	-1.33818700
H	-1.17477500	-1.96558100	-1.46368200
H	4.55578600	-0.83789000	1.63375400

PROc3 (PROb4)

Charge=0, spin multiplicity=1

Energy= -1193.33973214 Ha

N	-4.87841900	-1.07654100	-0.16669400
C	-3.57851800	-0.40341400	-0.17195300
C	-2.50744600	-1.41218100	-0.55985800
O	-1.23383000	-0.77371200	-0.65238900
C	-3.58655400	0.74769900	-1.15345200
O	-3.49938600	1.91670100	-0.84941300
O	-1.13838700	-0.78171900	1.90874900
P	-0.27228600	-0.77431200	0.68754100

O	0.43847500	0.69527100	0.46575300
C	-0.39116900	1.87101700	0.40842200
C	0.44796900	3.06992500	0.79644400
H	-5.59729600	-0.44160800	0.16131700
H	-3.35840300	-0.01805100	0.82282400
H	-2.50576000	-2.22127400	0.17035600
H	-2.72395800	-1.83103700	-1.54555400
H	-3.74175800	0.44844000	-2.20840000
H	-0.78486500	1.96744700	-0.60270300
H	-1.22975800	1.74009500	1.09369000
H	-0.15790600	3.97654500	0.76063100
H	1.28623100	3.19070800	0.10826400
H	0.83836800	2.94954700	1.80743900
C	4.97000900	-1.09062000	-0.55053400
N	5.20375000	0.25744700	-0.70759800
C	3.65928700	-1.21652800	-0.20821900
C	4.08260700	0.93429100	-0.47121400
N	3.13835200	0.05524400	-0.16735800
H	3.03437800	-2.06243000	0.01074200
H	3.96919600	2.00239800	-0.52028300
H	2.16267800	0.28660000	0.06164200
H	5.74143000	-1.82437800	-0.69440300
H	-5.13877500	-1.35096700	-1.10953800
O	0.85599700	-1.74791400	0.51331500
H	6.08464400	0.67945600	-0.96353400

Reactivation process

Complex-d

Charge=0, spin multiplicity=1

Energy= -1797.72420949 Ha

N	-4.95047800	-3.54452700	0.23487700
C	-4.13559400	-2.51055000	-0.40200700
C	-3.18511800	-1.92792500	0.62492500
O	-2.52679200	-0.78986700	0.02641900
C	-3.39132300	-3.09790600	-1.58655100
O	-2.18777500	-3.21820300	-1.64322500
O	-0.23772500	-1.52640300	1.01095200
P	-1.01888400	-0.38170700	0.47750300
N	-0.55561700	0.45462600	-0.87305100
C	0.68632000	1.23269200	-0.76480000
C	-0.74235600	-0.13686100	-2.19885500
O	-1.23187100	0.82006800	1.51603700
C	-0.85897400	0.68401400	2.91971300
C	-1.80360100	-0.24846500	3.64802700
C	-4.49445500	3.67106600	-1.45649400
N	-3.29651800	3.95447200	-0.83946000
C	-4.64960200	2.32209600	-1.39031200
C	-2.73311700	2.82919500	-0.41099300
N	-3.54269100	1.82984200	-0.73832500
H	-4.03877000	-3.49099700	-2.38904700
H	-5.73478400	-3.79740800	-0.35431800
H	-4.40454500	-4.38615300	0.38592500
H	-4.80582900	-1.72665200	-0.76363400
H	-2.43258200	-2.65860600	0.91791100
H	-3.74462600	-1.59468100	1.49698300
H	-3.34655600	0.85089400	-0.52450100
H	-1.80031000	2.73160200	0.11605900
H	-5.43696200	1.68341500	-1.74592700
H	-2.89536500	4.87454100	-0.72493500
H	-5.11683300	4.43773100	-1.87944100
H	-1.71168000	-1.26723600	3.26940600
H	-1.55843400	-0.25767900	4.71164800
H	-2.83656000	0.08512800	3.53556400

H	-0.93316000	1.69783000	3.30702400
H	0.18254200	0.37603200	2.95790300
H	0.57714700	2.15144100	-1.34550700
H	0.90432000	1.47695400	0.27630900
H	1.53134800	0.66314300	-1.16298300
H	-0.72333200	0.67007700	-2.93286500
H	0.05417200	-0.84774300	-2.43971300
H	-1.70116900	-0.64339100	-2.25522600
O	2.17020600	1.27595400	2.18579000
N	3.01178100	0.49756500	1.52934900
C	3.77734800	1.07398000	0.64811900
C	4.67927800	0.25057700	-0.16032800
C	4.74661300	-1.15477700	0.03652400
C	6.37734800	-1.22146900	-1.72542600
C	6.23571500	0.15428300	-1.85377200
N	5.40899600	0.87585200	-1.09189400
C	5.61729900	-1.88447500	-0.76501000
H	6.80723200	0.70125200	-2.59528100
H	7.06297900	-1.76438700	-2.36226800
H	5.68308400	-2.95618600	-0.62491900
O	3.99764900	-1.76903900	0.96509700
H	3.42978500	-1.01923000	1.39381200
N	3.75624900	2.45428600	0.46070500
H	3.94667700	2.71933800	-0.49486900
H	2.87920000	2.80884600	0.82380300

TSd1

Charge=0, spin multiplicity=1

Energy= -1797.71984352 Ha

N	4.72355600	3.38629400	0.56688300
C	3.78501000	2.50251900	-0.11771500
C	2.81200600	1.77720900	0.79848600
O	2.10186500	0.81168300	0.02508700
C	3.07529500	3.35700400	-1.15006800
O	1.87675500	3.50144800	-1.22364800
O	0.02831400	1.28267200	1.36074800
P	0.67324300	0.14831100	0.64307400
N	0.25195400	-0.48306500	-0.83642800
C	-0.27916800	-1.82237400	-1.03200000
C	-0.17798500	0.48453800	-1.84248700
O	1.36322600	-1.05292300	1.46867600
C	1.07228400	-1.24611000	2.87811200
C	1.99675700	-0.39688200	3.72567600
C	4.45311100	-2.87030300	-2.29994800
N	3.93941700	-3.47795400	-1.17719600
C	4.07436100	-1.56535200	-2.23466400
C	3.27204900	-2.58447000	-0.45036000
N	3.34565900	-1.41929900	-1.07796700
H	3.75848600	3.89486600	-1.82829100
H	4.22578600	3.96517200	1.23528200
H	5.39259400	2.83837400	1.09437300
H	4.37286600	1.76753400	-0.67864500
H	2.10552500	2.48208800	1.23607600
H	3.36830800	1.27980800	1.59808800
H	2.90152500	-0.55030600	-0.73320300
H	2.75803600	-2.76111600	0.47768100
H	4.25976400	-0.74361900	-2.90194200
H	4.04587100	-4.45189800	-0.93238400
H	5.02972800	-3.40793900	-3.02971700
H	1.80989700	0.66226200	3.54271500
H	1.82038200	-0.60187900	4.78335800
H	3.04113700	-0.61713200	3.49911100
H	1.23434300	-2.30798400	3.05524900
H	0.02484100	-1.01066400	3.03788600
H	0.09635500	-2.19116800	-1.99136500

H	0.06205500	-2.47676800	-0.23625400
H	-1.37185600	-1.83050800	-1.04528200
H	0.07447400	0.09814700	-2.83292900
H	-1.25781400	0.65659700	-1.79196600
H	0.34406700	1.43004700	-1.69957500
O	-1.30233600	-1.07897200	1.36286800
N	-2.28879300	-0.37590800	0.82165400
C	-3.40569800	-0.99975700	0.61347000
C	-4.50000200	-0.25597400	-0.02273900
C	-4.33043800	1.11011200	-0.37095100
C	-6.57771800	1.05733500	-1.22014900
C	-6.64541400	-0.28138600	-0.85146900
N	-5.63256600	-0.92410200	-0.26606700
C	-5.40233100	1.76036000	-0.97660500
H	-7.54459600	-0.85951100	-1.03164400
H	-7.42485900	1.53924600	-1.68966100
H	-5.29480000	2.80294500	-1.24793400
O	-3.18441400	1.76572800	-0.13644000
H	-2.55429900	1.07064700	0.31363200
N	-3.59849700	-2.32245300	0.99057100
H	-4.26341700	-2.80203700	0.40166200
H	-2.69815200	-2.78035700	1.06154100

INTd

Charge=0, spin multiplicity=1

Energy= -1797.72804537 Ha

N	-4.55733700	-3.09775600	0.11382400
C	-3.95974900	-1.79073500	-0.15703100
C	-2.71743800	-1.82134500	-1.04865800
O	-1.99935000	-0.60464800	-1.01976200
C	-5.05669600	-0.91705600	-0.72160100
O	-4.91934000	-0.15717200	-1.65575600
O	0.13358200	-1.86085100	-0.85580200
P	-0.38204900	-0.62001400	-0.16944500
N	-0.18316300	0.93879100	-0.79387600
C	0.41177800	2.05544600	-0.08666500
C	-0.42592200	1.22090500	-2.19817800
O	-1.29912500	-0.66615300	1.21577900
C	-0.89898200	-1.22481000	2.47910300
C	-0.61312600	-2.71033700	2.37262400
C	-4.06964000	3.56917700	0.20102500
N	-3.33314400	3.22718100	1.31242500
C	-3.91161500	2.54917000	-0.68678000
C	-2.74725900	2.04674500	1.10790900
N	-3.08828600	1.61955300	-0.09749600
H	-6.03220800	-1.03208300	-0.21986900
H	-4.65049800	-3.61428900	-0.75541800
H	-3.93146100	-3.63912400	0.69886700
H	-3.67435200	-1.34418000	0.80298000
H	-3.02487600	-2.03185300	-2.07928900
H	-2.07444900	-2.63854900	-0.71813800
H	-2.72071500	0.70931000	-0.52653300
H	-2.10668800	1.52082500	1.79299700
H	-4.32328800	2.40024500	-1.66777000
H	-3.24341400	3.77449200	2.15574400
H	-4.62964600	4.48428900	0.14365500
H	0.23453300	-2.88465100	1.71166800
H	-0.38699500	-3.11831700	3.35983000
H	-1.48305900	-3.23433400	1.97130100
H	-1.75370800	-1.04841100	3.13362800
H	-0.03985400	-0.68721600	2.87165900
H	-0.17678600	2.95700800	-0.29177300
H	0.40920400	1.87952300	0.98523100
H	1.44430800	2.23935100	-0.40672300
H	-1.27420600	1.90378000	-2.33450900

H	0.46273300	1.69428500	-2.63032400
H	-0.63034400	0.30500900	-2.74348700
O	1.02304400	-0.37304300	0.92449100
N	2.19603000	-0.34756900	0.21538300
C	3.18907300	0.10722000	0.89994300
C	4.50588200	0.14289400	0.22263200
C	4.67650100	-0.39658000	-1.07137100
C	6.98352300	0.25110300	-0.91221700
C	6.71378500	0.76272300	0.35636000
N	5.50512000	0.70679600	0.90774000
C	5.95404600	-0.33434000	-1.63140000
H	7.49510700	1.22936900	0.94398900
H	7.98136000	0.31323800	-1.32476800
H	6.10909300	-0.74621100	-2.62011300
O	3.68089100	-0.95932700	-1.77276400
H	2.85062200	-0.89344300	-1.20637800
N	3.12416400	0.50460600	2.20316800
H	3.89074900	1.08819300	2.50074900
H	2.20330500	0.76122100	2.52263700

TSd2

Charge=0, spin multiplicity=1

Energy= -1797.72530942 Ha

N	-4.67240700	-2.94982300	0.07819000
C	-4.05266400	-1.65019300	-0.17890100
C	-2.81220000	-1.69986400	-1.06948600
O	-2.06029700	-0.49866300	-1.03888800
C	-5.14088500	-0.76609200	-0.74884300
O	-5.02141000	-0.08641200	-1.74421700
O	0.08631900	-1.79698100	-0.99993700
P	-0.32993200	-0.60809900	-0.18074900
N	-0.13203400	0.96420300	-0.73225200
C	0.38496400	2.05587900	0.07001400
C	-0.40825800	1.33167400	-2.10938600
O	-1.26864500	-0.74184700	1.17034300
C	-0.88792500	-1.40853800	2.38995100
C	-0.59541400	-2.87917000	2.16520600
C	-4.00927000	3.52549800	0.29278500
N	-3.37697400	3.11086400	1.44133700
C	-3.81645800	2.53012700	-0.61840300
C	-2.82401400	1.91157000	1.22257000
N	-3.07908400	1.53659600	-0.01887500
H	-6.09397900	-0.80586300	-0.19533700
H	-4.76340200	-3.46138200	-0.79405500
H	-4.06584100	-3.50302500	0.67228100
H	-3.77026700	-1.21743600	0.78771300
H	-3.11996100	-1.90543100	-2.10002200
H	-2.17923000	-2.52296300	-0.73577000
H	-2.64588600	0.53648700	-0.52947500
H	-2.25541300	1.34541200	1.93865600
H	-4.15948900	2.44297500	-1.63348500
H	-3.33101300	3.61985700	2.31087900
H	-4.52828700	4.46449600	0.23107600
H	0.27249600	-3.00033400	1.51850900
H	-0.39767900	-3.36711400	3.12151700
H	-1.45209400	-3.36778300	1.69706500
H	-1.75521200	-1.28768600	3.03967400
H	-0.03897700	-0.90148500	2.84104400
H	-0.27532400	2.92461800	-0.03289900
H	0.42507000	1.77629700	1.11915300
H	1.39111400	2.34714700	-0.25282600
H	-1.28075400	1.99154500	-2.18512500
H	0.45892300	1.86148000	-2.51770600
H	-0.59016300	0.44565000	-2.71003400
O	1.05897200	-0.47874900	0.89412800

N	2.23361700	-0.39973800	0.17719000
C	3.21803100	0.02950400	0.89181300
C	4.53831800	0.12309000	0.22393200
C	4.72618200	-0.33540400	-1.09699300
C	7.02178600	0.33490400	-0.88248600
C	6.73519800	0.76673000	0.41247100
N	5.52407500	0.66011700	0.94930700
C	6.00692200	-0.22179600	-1.64272400
H	7.50493500	1.20932900	1.03291500
H	8.02138900	0.43608200	-1.28269000
H	6.17446900	-0.57174400	-2.65293200
O	3.74612800	-0.87006500	-1.84136200
H	2.91154500	-0.85358900	-1.28533300
N	3.14788200	0.35138500	2.21088400
H	3.91494400	0.90794400	2.55440700
H	2.22712400	0.55701900	2.56390000

PROd

Charge=0, spin multiplicity=1

Energy= -1797.75064833 Ha

N	-4.80428400	-2.36499800	1.41102300
C	-4.34721800	-1.42177200	0.38966100
C	-3.28538400	-1.96584600	-0.55848900
O	-2.83616300	-0.99926400	-1.48798500
C	-5.60843100	-0.97801100	-0.32490500
O	-5.87463200	-1.22790700	-1.47871400
O	0.28618000	-2.14508000	-0.21169900
P	0.20644200	-0.68276500	0.01318100
N	0.26816200	0.22597600	-1.34449000
C	0.18574600	1.67976200	-1.26920400
C	0.05683300	-0.34657600	-2.66790500
O	-1.03330900	-0.13700500	0.87060600
C	-1.08956000	-0.24981000	2.31790300
C	-0.91273400	-1.67309800	2.80872800
C	-4.95564100	3.21703000	-0.20271200
N	-3.93341500	3.39002800	0.69544100
C	-4.59538800	2.13069400	-0.95270900
C	-3.01274500	2.42694100	0.46665300
N	-3.37959800	1.64566800	-0.52773500
H	-6.32715500	-0.44618700	0.32189500
H	-4.95898300	-3.27451600	0.98822000
H	-4.09215400	-2.48733700	2.12077800
H	-3.95463500	-0.53859900	0.90307400
H	-3.71164300	-2.79572000	-1.12815500
H	-2.45259300	-2.35225200	0.03843800
H	-2.78278000	-0.13026300	-1.03840700
H	-2.10221900	2.33586100	1.03541900
H	-5.13425100	1.66957100	-1.76418400
H	-3.87658800	4.10675800	1.40149200
H	-5.81624500	3.86174300	-0.22449400
H	0.08931000	-2.04402700	2.59534600
H	-1.06777300	-1.69673800	3.88848600
H	-1.63675300	-2.33816200	2.33697600
H	-2.07421000	0.13289800	2.57751300
H	-0.33269500	0.41116500	2.73778500
H	-0.82979900	2.02490600	-1.47734400
H	0.48183600	2.02086000	-0.27822600
H	0.87259300	2.11275400	-1.99908300
H	-0.93109600	-0.08371700	-3.04993800
H	0.82389800	0.03223400	-3.34681200
H	0.13433600	-1.42878500	-2.60890700
O	1.39601300	-0.08983800	0.98572600

N	2.66900300	-0.41060300	0.45694700	H	7.66106600	2.08428300	0.36608900
C	3.50624900	0.55245500	0.68848700	H	8.53519300	0.11184400	-0.89257400
C	4.90123800	0.35430000	0.21353400	H	6.95592600	-1.76218900	-1.43331100
C	5.29607400	-0.79958500	-0.48786400	O	4.47544600	-1.81810400	-0.79054700
C	7.49741400	0.15214000	-0.59118800	H	3.58044000	-1.61423800	-0.42275100
C	7.01062700	1.25660200	0.11239200	N	3.22364700	1.70868700	1.30270000
N	5.74661000	1.34968700	0.50186800	H	3.99558100	2.31901800	1.51750100
C	6.63234500	-0.88294400	-0.89209000	H	2.33905500	1.82308000	1.76633000

The End