Supporting information

for

the manuscript entitled:

Antioxidant and UV-radiation absorption activity of aaptamine derivatives – Potential application for natural organic sunscreens

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List of supporting information

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Table S2: Cartesian coordinates, and thermochemical properties for TSs of **HAT reactions** between three aaptamines derivatives with HOO radical. All calculations were performed in the gas phase and in water at the M05-2X/6-311++G(d,p) level of theory.

Table S3: Cartesian coordinates, and thermochemical properties for TSs of **RAF reactions** between three aaptamines derivatives with HOO radical. All calculations were performed in the gas phase and in water at the M05-2X/6-311++G(d,p) level of theory.

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Table S7: Cartesian coordinates, and thermochemical properties for the complexes between three aaptamines derivatives with **Cu(I)** ion. All calculations were performed in water at the M05-2X/6-311++G(d,p) level of theory.

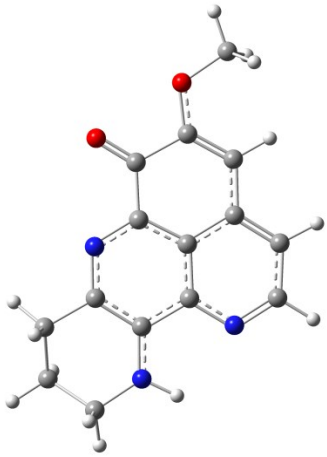
Table S8: Lowest absorption wavelength (nm) of C1−C3 calculated by TD-DFT with different methods of various % HF in exchange correlation.

Table S1: Cartesian coordinates, and thermochemical properties of three aaptamines derivatives. All calculations are performed in the gas phase at the M05-2X/6-311++G(d,p) level of theory.

Compound C1

0 1

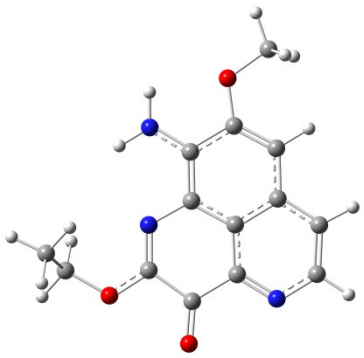
C	0.29937700	0.57206100	-0.01561900
C	-0.97304000	1.16268700	-0.02280400
C	0.41181300	-0.83151400	-0.03892800
C	1.43989700	1.42022900	0.01705900
C	-2.10357200	0.29561000	-0.05789400
C	-1.87089400	-1.09213700	-0.08303600
C	2.76262700	0.83527200	0.02753100
C	-0.11339000	3.26368500	0.02519200
C	2.92159000	-0.50611000	0.00784500
H	3.60838000	1.50688100	0.05184400
H	-0.28388200	4.33394200	0.03982300
O	4.08878900	-1.15187800	0.01577000
C	5.27167300	-0.36988900	0.04732100
H	6.09431200	-1.07637300	0.04857700
H	5.33184300	0.26961800	-0.83520500
H	5.30375100	0.24010000	0.95192700
C	1.75205300	-1.46121700	-0.02679400
O	1.94355400	-2.65185700	-0.04323500
N	-0.65187400	-1.61995600	-0.06743100
C	1.21171700	2.77726200	0.03768600
H	2.03567600	3.47744900	0.06257600
N	-1.18059600	2.50232000	-0.00421100
C	-3.05352000	-2.02490300	-0.11943700
H	-2.78468400	-2.93512400	0.41350100
H	-3.25840100	-2.30704600	-1.15606700
N	-3.34737400	0.81745700	-0.05796400
H	-3.40435100	1.82262300	-0.08956400
C	-4.53516700	-0.01033800	-0.17917700
H	-5.36420200	0.51180800	0.29563300
H	-4.78915000	-0.16228100	-1.23316600
C	-4.28683600	-1.35766400	0.48943600
H	-5.16522700	-1.99043400	0.36890400
H	-4.12986500	-1.19825300	1.55789200



Thermochemistry

Zero-point correction= 0.264703 (Hartree/Particle)
Thermal correction to Energy= 0.280018
Thermal correction to Enthalpy= 0.280962
Thermal correction to Gibbs Free Energy= 0.222313
Sum of electronic and zero-point Energies= -894.004848
Sum of electronic and thermal Energies= -893.989533
Sum of electronic and thermal Enthalpies= -893.988589
Sum of electronic and thermal Free Energies= -894.047238

HF=-894.2695509 (Hartree/Particle)

Compound **C2**				
0 1				
O	-3.36091700	-1.98068300	-0.03052500	
N	0.37717400	3.18955600	0.07731900	
N	1.21692000	-0.92121800	-0.19829000	
C	-0.41006200	0.91360700	-0.01880900	
C	-1.75426500	1.34060800	0.07385300	
C	-0.09111700	-0.46020600	-0.11498500	
C	0.60586900	1.88948300	-0.01040900	
C	-1.10722100	-1.39927300	-0.12868900	
C	-2.79402000	0.36525700	0.07219800	
C	-2.47395100	-0.95580500	-0.02478300	
C	-1.97580200	2.71719300	0.16577000	
C	2.01668000	1.43158800	-0.10553200	
C	-0.89526500	3.58480000	0.16299600	
C	2.17498800	-0.07361900	-0.19856700	
C	-4.74024200	-1.65503800	0.06601200	
H	-3.81922100	0.69382200	0.14962600	
H	-2.98292500	3.10590900	0.23908300	
H	-1.05604500	4.65303500	0.23342800	
H	-5.27292400	-2.59948400	0.04113700	
H	-5.04519400	-1.03529700	-0.77814900	
H	-4.94553200	-1.13755100	1.00408200	
O	2.97574800	2.15715500	-0.10847400	
O	3.44795700	-0.43862900	-0.28926400	
C	3.74225300	-1.84342000	-0.37492300	
H	4.73907800	-1.87684600	-0.80537700	
H	3.03407500	-2.31025200	-1.05702900	
C	3.71519800	-2.49194300	0.99523500	
H	2.71656500	-2.44666000	1.42446900	
H	4.01371600	-3.53742800	0.91114000	
H	4.41145900	-1.98567500	1.66209000	
N	-0.86073500	-2.72622600	-0.26033300	
H	0.09664300	-3.02340900	-0.19684100	
H	-1.60376800	-3.37707400	-0.08863300	

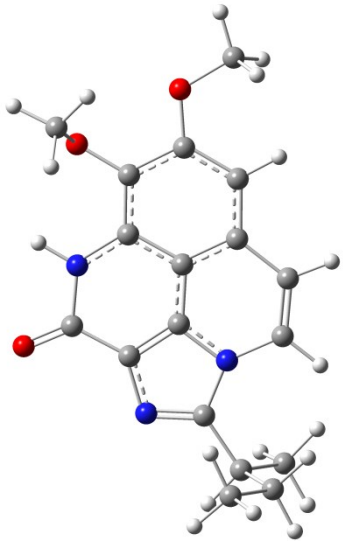
Thermochemistry

Zero-point correction= 0.260503 (Hartree/Particle)
Thermal correction to Energy= 0.277666
Thermal correction to Enthalpy= 0.278610
Thermal correction to Gibbs Free Energy= 0.215844
Sum of electronic and zero-point Energies= -931.131154
Sum of electronic and thermal Energies= -931.113992
Sum of electronic and thermal Enthalpies= -931.113048
Sum of electronic and thermal Free Energies= -931.175813

HF=-931.3916574 (Hartree/Particle)

Compound **C3**				
0 1				
O	-0.44255000	3.81780200	-0.36741000	

C	0.55769700	-0.17784400	-0.16210400
C	-0.76194100	0.26172700	-0.21913100
C	1.52201400	0.83397200	-0.16741500
C	0.84355000	-1.53939400	-0.10268900
C	-1.22109400	1.54604000	-0.28172600
C	-0.24104800	2.62686400	-0.30231400
C	2.18879600	-1.91661400	-0.05301200
C	-1.58425800	-1.95180000	-0.16007200
H	2.45725700	-2.96078600	-0.01531200
H	-2.44083800	-2.60402900	-0.16319900
C	-0.31478800	-2.41813400	-0.10343400
H	-0.17029800	-3.48809000	-0.05938900
C	2.85450600	0.45088800	-0.10267500
O	3.81679600	1.41794000	-0.14358500
C	4.52817000	1.59869900	1.08894700
H	3.82699100	1.83852500	1.88981300
H	5.09090100	0.70132600	1.33455600
H	5.20499600	2.43186600	0.92654600
N	1.09199500	2.14420000	-0.23600300
H	1.79618000	2.86564300	-0.28412300
N	-1.83465500	-0.57964500	-0.21968300
C	-2.95384400	0.26125300	-0.28535700
N	-2.59566700	1.52092400	-0.32171100
C	-4.36846300	-0.22349200	-0.29282500
H	-4.95486500	0.69625100	-0.31336200
C	-4.73039600	-0.98406800	0.99223000
H	-4.21337000	-1.94659600	1.01864200
H	-5.79733900	-1.21325000	0.94984300
C	-4.41514600	-0.19049800	2.25645300
H	-4.75631100	-0.71978200	3.14552000
H	-3.34273800	-0.01752600	2.35471700
H	-4.90213000	0.78491500	2.22890200
C	-4.69267200	-1.03629200	-1.55093200
H	-4.47531500	-0.46002600	-2.44920700
H	-4.11710700	-1.96179300	-1.59441700
H	-5.74991100	-1.30242700	-1.55784500
C	3.17266200	-0.92437800	-0.06138700
O	4.50309500	-1.18842400	-0.03202600
C	4.91351200	-2.54623800	-0.06183800
H	4.54840500	-3.04017100	-0.96350600
H	5.99821500	-2.52614800	-0.07041200
H	4.56329900	-3.07893700	0.82387800

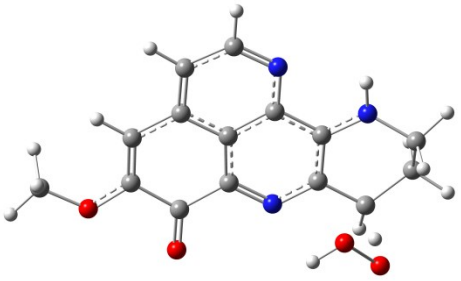


Thermochemistry

Zero-point correction= 0.353912 (Hartree/Particle)
Thermal correction to Energy= 0.375392
Thermal correction to Enthalpy= 0.376336
Thermal correction to Gibbs Free Energy= 0.303763
Sum of electronic and zero-point Energies= -1087.117342
Sum of electronic and thermal Energies= -1087.095862
Sum of electronic and thermal Enthalpies= -1087.094917
Sum of electronic and thermal Free Energies= -1087.167490

HF=-1087.4712538 (Hartree/Particle)

Table S2: Cartesian coordinates, and thermochemical properties for TSs of **HAT** reactions between three aaptamines derivatives with HOO radical. All calculations were performed in the gas phase and in water at the M05-2X/6-311++G(d,p) level of theory.

Compound C1 + HOO in the gas phase	
0 2	
C -0.69116800 0.73100200 -0.10839200	
C 0.50753300 1.45568300 -0.10211500	
C -0.66093300 -0.66615000 -0.33095200	
C -1.90559700 1.42852100 0.12120300	
C 1.71797600 0.73219900 -0.32791300	
C 1.62521000 -0.65821000 -0.57892500	
C -3.15847300 0.70423600 0.12238300	
C -0.55450600 3.41420700 0.32685200	
C -3.18396100 -0.63093200 -0.08105300	
H -4.06357900 1.26870200 0.29285700	
H -0.49202600 4.48170900 0.50220100	
O -4.27515600 -1.39644600 -0.09931700	
C -5.52721400 -0.76174400 0.10922600	
H -6.27102400 -1.54865900 0.05347300	
H -5.55760400 -0.28969700 1.09279900	
H -5.71306500 -0.01796100 -0.66758800	
C -1.92959700 -1.43752300 -0.31237800	
O -1.99404300 -2.63124600 -0.46525900	
N 0.46009800 -1.31976900 -0.55849300	
C -1.81692900 2.78652500 0.33691100	
H -2.70425000 3.37779500 0.51760000	
N 0.58058100 2.78857600 0.11867800	
C 2.85090100 -1.40915200 -0.83562600	
H 2.67721000 -2.31180800 -1.41444700	
H 3.14824000 -1.86134300 0.31294900	
N 2.89517300 1.37165900 -0.31336900	
H 2.86135300 2.34337000 -0.04541400	
C 4.15519900 0.64019300 -0.31124800	
H 4.94030300 1.31583100 -0.64363800	
H 4.38535300 0.29943900 0.70129700	
C 4.04057600 -0.56204600 -1.24202700	
H 4.95901100 -1.14540500 -1.19297900	
H 3.91734200 -0.21568500 -2.27242200	
O 3.33302500 -2.06661200 1.56042300	
O 2.42718700 -1.21115100 2.14274700	
H 1.61956000 -1.73676500 2.21114700	

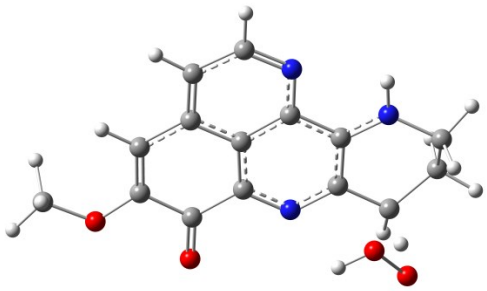
Thermochemistry

Zero-point correction= 0.276082 (Hartree/Particle)
Thermal correction to Energy= 0.294531
Thermal correction to Enthalpy= 0.295475
Thermal correction to Gibbs Free Energy= 0.228025

Sum of electronic and zero-point Energies= -1044.902145
Sum of electronic and thermal Energies= -1044.883696
Sum of electronic and thermal Enthalpies= -1044.882752
Sum of electronic and thermal Free Energies= -1044.950201

HF=-1045.1782264 (Hartree/Particle)

Compound C1 + HOO in WATER



0 2

C	-0.69930200	0.72621200	-0.10746300
C	0.49634400	1.45144600	-0.10732200
C	-0.67760800	-0.66952100	-0.32781800
C	-1.91432100	1.42143400	0.12115700
C	1.71219800	0.72232800	-0.32666200
C	1.61460700	-0.68474100	-0.56376100
C	-3.16312700	0.69539900	0.13079400
C	-0.57723600	3.41286700	0.30602000
C	-3.17795000	-0.63854200	-0.07542400
H	-4.07004900	1.25474700	0.30893300
H	-0.52181400	4.48122200	0.46994100
O	-4.27388400	-1.41717000	-0.08690400
C	-5.53229200	-0.77205400	0.14558800
H	-6.27813800	-1.55789900	0.09901200
H	-5.53707200	-0.30548500	1.13007000
H	-5.72003800	-0.02792100	-0.62767000
C	-1.93350900	-1.42065300	-0.32137600
O	-2.00035600	-2.63385000	-0.50427600
N	0.45156700	-1.33260300	-0.55303900
C	-1.83450200	2.78108600	0.32719300
H	-2.72482600	3.36778000	0.50650400
N	0.56259000	2.78552800	0.09864300
C	2.84495900	-1.43370100	-0.80808200
H	2.67660600	-2.35639000	-1.35691700
H	3.15520400	-1.83508200	0.32555900
N	2.88235700	1.34519700	-0.32105900
H	2.87470400	2.33313500	-0.10988700
C	4.15849800	0.63918600	-0.41008400
H	4.89058200	1.32786900	-0.82167800
H	4.47867200	0.35247200	0.59316200
C	4.00902100	-0.59113000	-1.28774800
H	4.93358100	-1.16443700	-1.26108700
H	3.83180500	-0.28682700	-2.32298900
O	3.34166900	-2.05369600	1.62593300
O	2.56833200	-1.08501100	2.21621200
H	1.69443300	-1.48991700	2.31744500

Thermochemistry
Zero-point correction= 0.275373 (Hartree/Particle)
Thermal correction to Energy= 0.293809
Thermal correction to Enthalpy= 0.294754
Thermal correction to Gibbs Free Energy= 0.227777

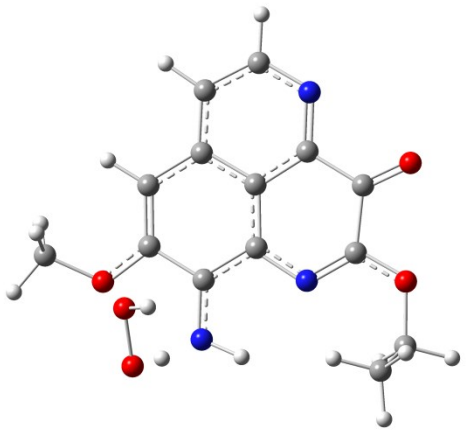
Sum of electronic and zero-point Energies= -1044.946300
Sum of electronic and thermal Energies= -1044.927863
Sum of electronic and thermal Enthalpies= -1044.926919
Sum of electronic and thermal Free Energies= -1044.993896

HF=-1045. 2216729 (Hartree/Particle)

Compound C2 + HOO in the gas phase

0 2

O	-3.45968000	-0.62574200	-0.76549200
N	1.51787100	3.20108000	0.39050900
N	1.23161300	-0.91078700	-0.43929300
C	0.16212600	1.26987700	-0.10101500
C	-1.02872100	2.02989800	-0.01736500
C	0.11124000	-0.11764800	-0.37493700
C	1.39486800	1.91306600	0.11600100
C	-1.14014900	-0.73618000	-0.59562400
C	-2.29307700	1.40154700	-0.22984500
C	-2.34881000	0.07285200	-0.52252100
C	-0.87904400	3.38787700	0.27339000
C	2.63192100	1.09324500	0.03502600
C	0.39070500	3.91337500	0.46239900
C	2.38726100	-0.37416700	-0.25839500
C	-4.70362400	-0.02909500	-0.42410600
H	-3.18876500	1.99954400	-0.16099900
H	-1.74659300	4.02899400	0.35133000
H	0.51159400	4.96575300	0.68609100
H	-5.45046800	-0.80042800	-0.57465800
H	-4.91495900	0.82241400	-1.07259500
H	-4.69014100	0.27935000	0.62171900
O	3.74670300	1.51542300	0.18895600
O	3.50321200	-1.07109600	-0.31683700
C	3.41618100	-2.48714200	-0.58888200
H	4.40630800	-2.73943200	-0.95603100
H	2.68083500	-2.64543500	-1.37454400
C	3.07867100	-3.26172200	0.66840300
H	2.08454700	-3.00520500	1.02799000
H	3.10454300	-4.33001600	0.45295200
H	3.80815400	-3.04793400	1.44798800
N	-1.26018800	-2.03369500	-0.88095500
H	-0.35292200	-2.48892300	-0.84143400
H	-2.04202900	-2.55745000	-0.18442800
O	-2.49444800	-2.92667600	0.96470800
O	-2.52707500	-1.74804300	1.68603500
H	-1.86217400	-1.88303500	2.37065400



Thermochemistry
Zero-point correction= 0.272857 (Hartree/Particle)
Thermal correction to Energy= 0.292706
Thermal correction to Enthalpy= 0.293650
Thermal correction to Gibbs Free Energy= 0.223231

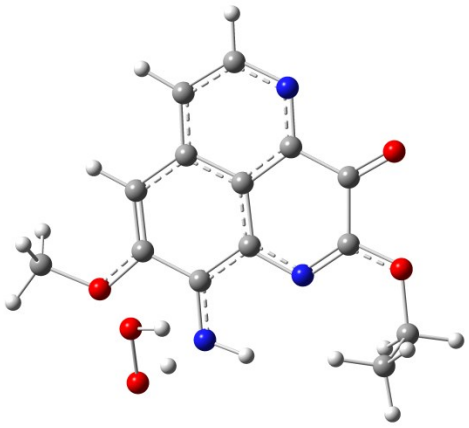
Sum of electronic and zero-point Energies= -1082.025020
Sum of electronic and thermal Energies= -1082.005170
Sum of electronic and thermal Enthalpies= -1082.004226
Sum of electronic and thermal Free Energies= -1082.074646

HF=-1082.2978766 (Hartree/Particle)

Compound C2 + HOO in WATER

0 2

O	-3.48143400	-0.73169400	-0.68915500
N	1.40359900	3.24221000	0.39122300
N	1.22859300	-0.86970300	-0.45964700
C	0.10102100	1.26886700	-0.08077600
C	-1.11068300	1.99233600	0.01994500
C	0.09042800	-0.11600100	-0.36331200
C	1.31417500	1.94489000	0.11558100
C	-1.14979800	-0.76734000	-0.56994100
C	-2.36243100	1.33057900	-0.17486100
C	-2.38149300	0.00199600	-0.46321200
C	-1.00161800	3.35137200	0.30924100
C	2.55833000	1.16498300	0.01069800
C	0.25479100	3.91829300	0.48147100
C	2.36864400	-0.29646000	-0.28918800
C	-4.75106700	-0.07873400	-0.54871000
H	-3.27002800	1.90917200	-0.09432300
H	-1.88702200	3.96501100	0.40014800
H	0.33732100	4.97310300	0.70550000
H	-5.49454300	-0.84423000	-0.74061100
H	-4.84172000	0.72513800	-1.27802200
H	-4.86019000	0.30879800	0.46336200
O	3.67392600	1.62849100	0.15214400
O	3.51288400	-0.94787200	-0.36987200
C	3.48526000	-2.38165300	-0.63120100
H	4.47792600	-2.58746500	-1.01795400
H	2.74385900	-2.57501300	-1.40114400
C	3.21525800	-3.15196000	0.63984800
H	2.22486600	-2.93383400	1.03463200
H	3.27371700	-4.21824000	0.42008200
H	3.96417400	-2.91294500	1.39396400
N	-1.22118400	-2.05677200	-0.90556500
H	-0.30311200	-2.49392900	-0.90632100
H	-1.93533500	-2.61821100	-0.26313300
O	-2.33267200	-3.04475700	1.01591000
O	-2.21202400	-1.90218500	1.77977000
H	-1.37730700	-2.01036500	2.25786800



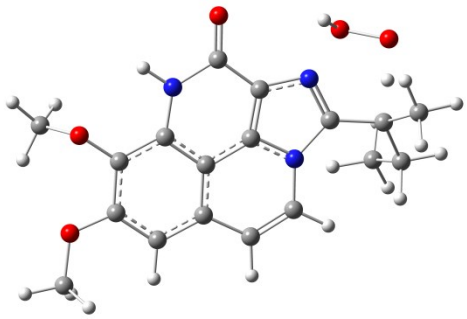
Thermochemistry

Zero-point correction= 0.271787 (Hartree/Particle)
Thermal correction to Energy= 0.291840
Thermal correction to Enthalpy= 0.292784
Thermal correction to Gibbs Free Energy= 0.221711

Sum of electronic and zero-point Energies= -1082.064630
Sum of electronic and thermal Energies= -1082.044577
Sum of electronic and thermal Enthalpies= -1082.043633
Sum of electronic and thermal Free Energies= -1082.114706

HF=-1082.3364166 (Hartree/Particle)

Compound C3 + HOO in the gas phase



0 2

O	-0.27287900	3.65403600	-0.51026200
C	1.02235000	-0.24895600	-0.20192200
C	-0.32469200	0.08408800	-0.30182300
C	1.90799000	0.83321900	-0.20277600
C	1.41078500	-1.58340400	-0.11603100
C	-0.86758800	1.33229400	-0.42659500
C	0.02855600	2.48541400	-0.42663800
C	2.77845900	-1.85617900	-0.02526600
C	-0.97651100	-2.18113100	-0.24431500
H	3.12493700	-2.87609000	0.03334600
H	-1.77567700	-2.89970800	-0.27121900
C	0.32309500	-2.54561600	-0.14646000
H	0.54607800	-3.60167600	-0.09464200
C	3.26271700	0.55496400	-0.09501800
O	4.14673100	1.59272500	-0.12942300
C	4.82665500	1.83983500	1.11064100
H	4.09816600	2.02414500	1.90156700
H	5.46023700	0.99477600	1.36785900
H	5.43186400	2.72638900	0.94925400
N	1.38664200	2.10843700	-0.31094500
H	2.03890500	2.87827300	-0.34415700
N	-1.33462300	-0.83067500	-0.31060900
C	-2.50991200	-0.07651500	-0.44931900
N	-2.22544200	1.21327600	-0.51934400
C	-3.89242300	-0.58022000	-0.51655000
H	-4.47677900	0.25631600	0.29804200
C	-4.22493200	-1.93473500	0.07514200
H	-3.79960200	-2.73638000	-0.53980700
H	-5.30644700	-2.05605200	-0.01037700
C	-3.82829900	-2.07616300	1.54552800
H	-4.12167900	-3.05219800	1.93093500
H	-2.75602100	-1.95978100	1.70082100
H	-4.32751100	-1.30689200	2.13366900
C	-4.59185400	-0.24564300	-1.82114900
H	-4.38420200	0.78270000	-2.10904300
H	-4.24248400	-0.90836300	-2.61905700
H	-5.66872200	-0.37627000	-1.71524800
C	3.68389200	-0.79203000	-0.02245000
O	5.02768900	-0.95243500	0.04441300
C	5.54304400	-2.27528100	0.05151200
H	5.24328800	-2.81051900	-0.85051500
H	6.62255600	-2.17032100	0.07198700

H	5.20971100	-2.81794800	0.93749400
O	-4.95929600	1.12277500	1.00249400
O	-3.90733600	1.57466100	1.76179400
H	-3.40993100	2.13460800	1.14417300

Thermochemistry

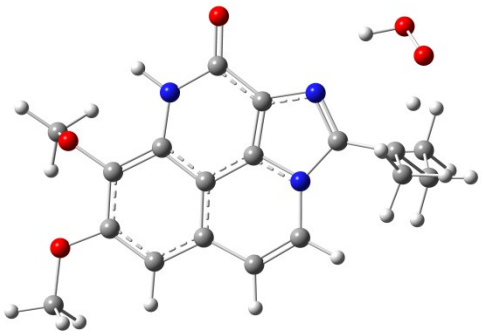
Zero-point correction= 0.365074 (Hartree/Particle)
Thermal correction to Energy= 0.389569
Thermal correction to Enthalpy= 0.390513
Thermal correction to Gibbs Free Energy= 0.310311
Sum of electronic and zero-point Energies= -1238.010903
Sum of electronic and thermal Energies= -1237.986408
Sum of electronic and thermal Enthalpies= -1237.985464
Sum of electronic and thermal Free Energies= -1238.065666

HF=-1238.3759775 (Hartree/Particle)

Compound C3 + HOO in WATER

0 2

O	-0.42187000	3.56035900	-0.34279200
C	1.08201300	-0.27671100	-0.15463100
C	-0.27758400	-0.00778300	-0.19606300
C	1.91356000	0.84510700	-0.18007000
C	1.52785700	-1.59744300	-0.09886700
C	-0.87891800	1.21601000	-0.26285700
C	-0.03783700	2.38715500	-0.28802400
C	2.90656000	-1.81101100	-0.06516700
C	-0.83324400	-2.30627000	-0.13169000
H	3.29990700	-2.81516800	-0.02579600
H	-1.61346300	-3.04999000	-0.13398500
C	0.48366100	-2.61082700	-0.08978400
H	0.76133000	-3.65439300	-0.05197300
C	3.28092800	0.62232800	-0.14356600
O	4.15065000	1.68160500	-0.20361700
C	4.62355200	2.09523700	1.09808900
H	3.78039700	2.41746900	1.70837300
H	5.14893400	1.27373100	1.58143800
H	5.30138800	2.92560200	0.92634100
N	1.32258400	2.09975200	-0.24493800
H	1.93490500	2.90632600	-0.25700900
N	-1.23932000	-0.96516600	-0.18301700
C	-2.44895700	-0.27513300	-0.24209400
N	-2.24465500	1.02679600	-0.29381700
C	-3.77591600	-0.94953900	-0.26292700
H	-4.56787100	0.05847000	-0.32353200
C	-4.15403800	-1.69334200	1.00412200
H	-3.56592400	-2.61683600	1.04668500
H	-5.19769400	-1.99695100	0.90742700
C	-3.94798100	-0.88256900	2.27824600
H	-4.24402900	-1.46623300	3.14928900
H	-2.90122800	-0.60022000	2.40301100
H	-4.54607000	0.02842400	2.25835600



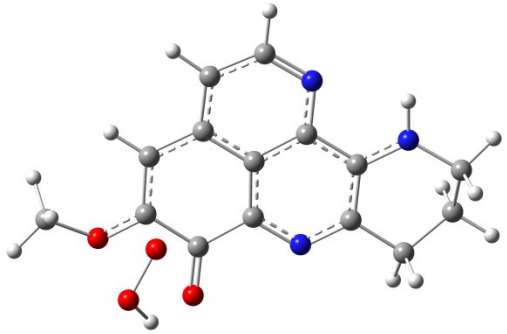
C	-4.07577000	-1.67379600	-1.55759300
H	-3.90210500	-1.02798700	-2.41779400
H	-3.43001900	-2.55211500	-1.65155800
H	-5.11138800	-2.01255500	-1.56237600
C	3.76177300	-0.70441100	-0.08953500
O	5.11356600	-0.80400300	-0.07129900
C	5.68556400	-2.11584300	-0.00004900
H	5.40349600	-2.70136700	-0.87414200
H	6.75940800	-1.96296000	0.01287400
H	5.36962800	-2.61863200	0.91311400
O	-5.20108200	1.10885700	-0.55022800
O	-4.73782600	2.03535900	0.36910900
H	-3.78870100	2.11135100	0.12903200

Thermochemistry

Zero-point correction= 0.363780 (Hartree/Particle)
Thermal correction to Energy= 0.388226
Thermal correction to Enthalpy= 0.389170
Thermal correction to Gibbs Free Energy= 0.309512
Sum of electronic and zero-point Energies= -1238.050826
Sum of electronic and thermal Energies= -1238.026380
Sum of electronic and thermal Enthalpies= -1238.025436
Sum of electronic and thermal Free Energies= -1238.105095

HF=-1238.4146061 (Hartree/Particle)

Table S3: Cartesian coordinates, and thermochemical properties for TSs of **RAF reactions** between three aaptamines derivatives with HOO radical. All calculations were performed in the gas phase and in water at the M05-2X/6-311++G(d,p) level of theory.

Compound C1 + HOO in the gas phase				RAF reaction
0 2				
C	0.10913800	0.71320200	-0.14913000	
C	1.41673200	1.19063600	0.03342400	
C	-0.10120900	-0.67167500	-0.28492100	
C	-0.95524500	1.66676700	-0.19875200	
C	2.47332700	0.23488300	0.07218000	
C	2.14117800	-1.12481600	-0.07987900	
C	-2.28443600	1.22484800	-0.42028800	
C	0.73417600	3.36209800	0.12700800	
C	-2.57541800	-0.14783700	-0.42061100	
H	-3.07702300	1.95182600	-0.50887700	
H	0.99477000	4.40745300	0.24194200	
O	-3.74151400	-0.64508600	-0.82196800	
C	-4.90594800	0.13805900	-0.55808300	
H	-5.74767300	-0.52997900	-0.70247000	
H	-4.88164300	0.49300000	0.47132700	
H	-4.97399800	0.97079300	-1.25887100	
C	-1.47457200	-1.18704100	-0.44478500	
O	-1.77007500	-2.35884100	-0.50238600	
N	0.89467400	-1.54468400	-0.25651400	
C	-0.61189800	3.00410300	-0.06016800	
H	-1.37199100	3.77231400	-0.09131900	
N	1.72807700	2.50269900	0.17540700	
C	3.24506600	-2.14916100	-0.04816100	
H	2.96341000	-2.97308900	-0.70133200	
H	3.33027400	-2.55456900	0.96398100	
N	3.74509800	0.64975500	0.23868800	
H	3.87180900	1.63798100	0.38683100	
C	4.85449900	-0.28016300	0.36602800	
H	5.75912900	0.22106300	0.02595700	
H	4.99677500	-0.56306700	1.41381400	
C	4.57466500	-1.52389000	-0.46983800	
H	5.38997900	-2.23550600	-0.34660400	
H	4.53114900	-1.23990000	-1.52297000	
O	-2.64441900	-0.41602200	1.48867900	
O	-3.49219100	-1.46575700	1.64490000	
H	-3.01463600	-2.22714500	1.26758800	

Thermochemistry

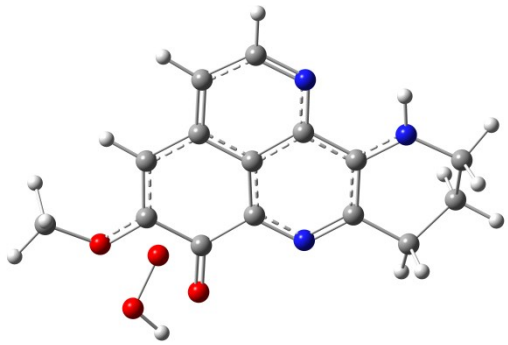
Zero-point correction= 0.280650 (Hartree/Particle)
Thermal correction to Energy= 0.298568
Thermal correction to Enthalpy= 0.299512
Thermal correction to Gibbs Free Energy= 0.234739

Sum of electronic and zero-point Energies= -1044.907342
Sum of electronic and thermal Energies= -1044.889424
Sum of electronic and thermal Enthalpies= -1044.888480
Sum of electronic and thermal Free Energies= -1044.953254

HF=-1045.1879922 (Hartree/Particle)

Compound C1 + HOO in WATER

RAF reaction



0 2

C	0.09434800	0.70787600	-0.15102600
C	1.39361000	1.19980300	0.04191200
C	-0.10787500	-0.67435700	-0.29546500
C	-0.97980600	1.64978000	-0.21204000
C	2.46291100	0.25189000	0.09205000
C	2.14132100	-1.12582600	-0.06907800
C	-2.30534300	1.19492900	-0.42603400
C	0.67871400	3.36825900	0.11495200
C	-2.57143100	-0.18188700	-0.42362700
H	-3.10486100	1.91472400	-0.51279200
H	0.92165500	4.41732300	0.22229200
O	-3.74317700	-0.70356300	-0.76872600
C	-4.90736100	0.13484300	-0.63784300
H	-5.75617400	-0.52725300	-0.76644000
H	-4.92383900	0.58685900	0.35222700
H	-4.90568000	0.89812200	-1.41345600
C	-1.45589600	-1.18969400	-0.49258000
O	-1.73312400	-2.37177400	-0.65912500
N	0.90657100	-1.54722300	-0.26229200
C	-0.66040400	2.99182800	-0.08067500
H	-1.43200500	3.74750900	-0.12584700
N	1.68287400	2.51725700	0.17815200
C	3.26127900	-2.12643400	-0.01545500
H	2.99108300	-2.98917500	-0.62146700
H	3.38324600	-2.46935800	1.01598700
N	3.71846200	0.65857500	0.27863100
H	3.86546600	1.64949300	0.39913800
C	4.86161900	-0.24993600	0.32481600
H	5.72358700	0.28502200	-0.06557800
H	5.06946200	-0.52360500	1.36098300
C	4.56540900	-1.49306000	-0.49464300
H	5.39085200	-2.19453200	-0.38990100
H	4.48009700	-1.22129700	-1.54848200
O	-2.57828200	-0.40395400	1.55064000
O	-3.42124200	-1.45454300	1.80043000
H	-2.87820200	-2.25149400	1.69455100

Thermochemistry

Zero-point correction= 0.280097 (Hartree/Particle)
Thermal correction to Energy= 0.298187
Thermal correction to Enthalpy= 0.299131
Thermal correction to Gibbs Free Energy= 0.233816

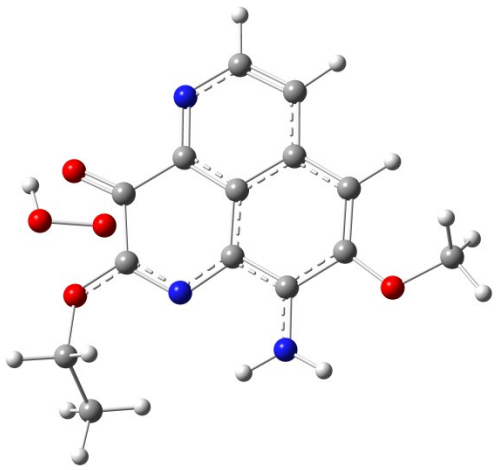
Sum of electronic and zero-point Energies= -1044.948341
Sum of electronic and thermal Energies= -1044.930251
Sum of electronic and thermal Enthalpies= -1044.929307
Sum of electronic and thermal Free Energies= -1044.994622

HF=-1045.2284382 (Hartree/Particle)

Compound C2 + HOO in the gas phase	RAF reaction

0 2

O	3.72680700	-1.89126500	0.21499800
N	-0.16611900	3.13675800	-0.45715800
N	-0.84532200	-1.02177400	-0.26305000
C	0.67662700	0.89680200	-0.20516000
C	2.00348100	1.36474000	-0.13692400
C	0.39001600	-0.50219900	-0.15032500
C	-0.35796300	1.83250900	-0.35920900
C	1.46365300	-1.40358800	-0.01200200
C	3.07619900	0.42876800	0.01465000
C	2.80863700	-0.90480800	0.07462000
C	2.19314500	2.74612200	-0.22812500
C	-1.75480200	1.32016400	-0.39460300
C	1.09389800	3.57390100	-0.38910600
C	-1.87396600	-0.17866600	-0.24147100
C	5.09201500	-1.50718400	0.31499700
H	4.08646400	0.80354900	0.07718200
H	3.18802800	3.16812800	-0.17954700
H	1.22837500	4.64532100	-0.46680900
H	5.65415300	-2.42823200	0.42300900
H	5.24570000	-0.87374500	1.18938900
H	5.40714100	-0.98403000	-0.58860000
O	-2.73766100	2.01814600	-0.44934100
O	-3.10142900	-0.61608800	-0.46134100
C	-3.40891000	-1.96153400	-0.04092900
H	-4.43777500	-1.90569800	0.30394300
H	-2.76447200	-2.21118100	0.79955200
C	-3.26322300	-2.93423900	-1.19267100
H	-2.23062800	-2.97403300	-1.53311300
H	-3.57167900	-3.93041100	-0.87271300
H	-3.89584900	-2.62832700	-2.02485800
N	1.24785900	-2.72689300	0.03692900
H	0.29502100	-3.04883600	0.02174900
H	2.01486100	-3.35765200	0.17677900
O	-1.88411600	0.22669700	1.67341400
O	-3.17510600	0.51177400	1.96691300
H	-3.33508500	1.38967200	1.57737100



Thermochemistry

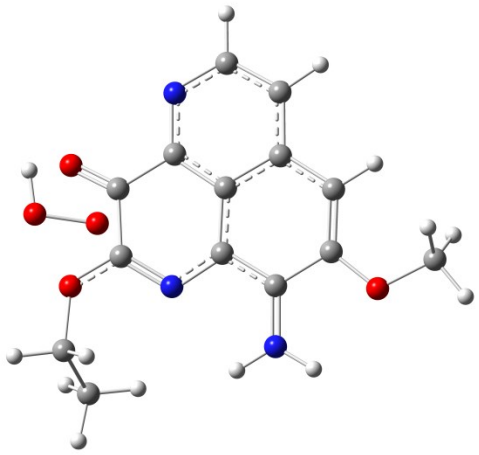
Zero-point correction= 0.276791 (Hartree/Particle)
Thermal correction to Energy= 0.296529
Thermal correction to Enthalpy= 0.297473
Thermal correction to Gibbs Free Energy= 0.228689

Sum of electronic and zero-point Energies= -1082.035081
Sum of electronic and thermal Energies= -1082.015344
Sum of electronic and thermal Enthalpies= -1082.014400
Sum of electronic and thermal Free Energies= -1082.083184

HF=-1082.3118724 (Hartree/Particle)

Compound C2 + HOO in WATER

RAF reaction



0 2

O	3.77859800	-1.81579300	0.23463000
N	-0.25670100	3.08834900	-0.52074300
N	-0.83653700	-1.06913200	-0.20886800
C	0.63993700	0.87333600	-0.21738700
C	1.95698400	1.37588900	-0.15314900
C	0.38857200	-0.52584300	-0.13165800
C	-0.41699700	1.77213600	-0.39987700
C	1.49572800	-1.40512300	0.01052300
C	3.06064600	0.47310000	0.01289300
C	2.83744700	-0.86251400	0.08849600
C	2.11299800	2.75324900	-0.26737000
C	-1.78384500	1.22081800	-0.46735800
C	0.99105700	3.55460200	-0.44800300
C	-1.87273600	-0.25266700	-0.24945700
C	5.14447300	-1.38245700	0.31854500
H	4.05800500	0.88293600	0.06708300
H	3.09631900	3.20060400	-0.22385600
H	1.10974500	4.62570800	-0.54073600
H	5.73102500	-2.28744400	0.42932400
H	5.27687900	-0.73743800	1.18588600
H	5.42499700	-0.85863400	-0.59420500
O	-2.78764800	1.89069500	-0.66153800
O	-3.10527100	-0.71976500	-0.37610000
C	-3.36259900	-2.10172300	0.00047600
H	-4.38935400	-2.08757400	0.35410600
H	-2.70064000	-2.36108000	0.82267800
C	-3.20558800	-3.02836400	-1.18189800
H	-2.17490200	-3.05692100	-1.52912600
H	-3.50083400	-4.03422700	-0.88119600
H	-3.85181900	-2.71089900	-1.99985900
N	1.32416800	-2.71504200	0.07685900
H	0.39128300	-3.09714700	0.01978100
H	2.11757100	-3.32944100	0.17563400
O	-1.86268700	0.39402000	1.74215900
O	-3.14310400	0.77558400	2.04427400
H	-3.16034900	1.73778300	1.92769300

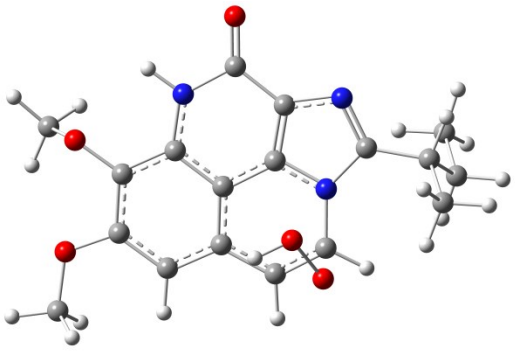
Thermochemistry

Zero-point correction= 0.275748 (Hartree/Particle)
Thermal correction to Energy= 0.295676
Thermal correction to Enthalpy= 0.296620
Thermal correction to Gibbs Free Energy= 0.227051

Sum of electronic and zero-point Energies= -1082.077981
Sum of electronic and thermal Energies= -1082.058053
Sum of electronic and thermal Enthalpies= -1082.057109
Sum of electronic and thermal Free Energies= -1082.126677

HF=-1082.3537289 (Hartree/Particle)

Compound C3 + HOO in the gas phase				RAF reaction
0 2				
O	-0.19936400	3.89014700	-0.81149600	
C	0.68427700	-0.03851200	0.05617900	
C	-0.62421200	0.43124800	-0.02302500	
C	1.67682800	0.91735600	-0.16016400	
C	0.93090000	-1.38445200	0.34688400	
C	-1.04173600	1.69907900	-0.29841800	
C	-0.03087400	2.72333600	-0.54382800	
C	2.27416600	-1.79471600	0.42013000	
C	-1.52730900	-1.72480300	0.32242700	
H	2.51145500	-2.82520400	0.63346700	
H	-2.38215900	-2.30088700	0.63180100	
C	-0.22828900	-2.19696600	0.55103400	
H	-0.12169400	-3.24508700	0.78655300	
C	3.00093500	0.50254600	-0.07028500	
O	3.98417400	1.41215300	-0.31353700	
C	4.77845100	1.76515200	0.82996900	
H	4.13402900	2.14959900	1.62165300	
H	5.33890900	0.90258900	1.18069300	
H	5.45722700	2.54238900	0.49343800	
N	1.28879400	2.21099700	-0.44089800	
H	2.01253600	2.88623500	-0.63813900	
N	-1.72240900	-0.35519200	0.15482300	
C	-2.81673900	0.49926700	-0.05623600	
N	-2.41804200	1.71944700	-0.30976800	
C	-4.24752000	0.08288300	0.06131100	
H	-4.79653500	1.00958000	-0.11252500	
C	-4.58767900	-0.40662600	1.47763800	
H	-4.09455400	-1.36256200	1.67218700	
H	-5.66045200	-0.60865500	1.50573900	
C	-4.21683200	0.60181500	2.56082600	
H	-4.53918200	0.25719600	3.54292000	
H	-3.13888500	0.76495800	2.59516200	
H	-4.68673300	1.56611400	2.36422600	
C	-4.65099900	-0.93598500	-1.00967700	
H	-4.41662600	-0.56181100	-2.00529800	
H	-4.12831300	-1.88315700	-0.88548600	
H	-5.72380900	-1.12145100	-0.94881800	
C	3.28218400	-0.85832900	0.20422500	
O	4.60462700	-1.15741000	0.23079300	
C	4.97642700	-2.51081500	0.44243300	
H	4.56428600	-3.15067100	-0.33921000	
H	6.06008600	-2.52948900	0.39596900	



H	4.64443400	-2.85683600	1.42261400
O	-1.72005200	-2.38947300	-1.51381200
O	-1.23232500	-1.40188900	-2.31978400
H	-0.36077900	-1.71671200	-2.59189400

Thermochemistry

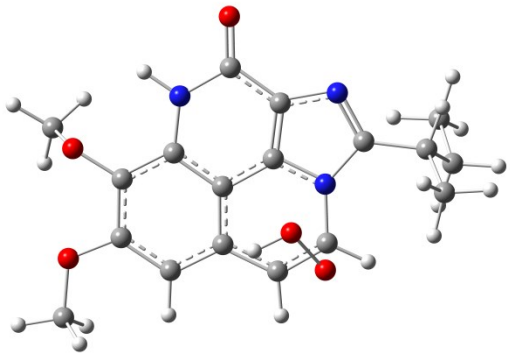
Zero-point correction= 0.369971 (Hartree/Particle)
Thermal correction to Energy= 0.394431
Thermal correction to Enthalpy= 0.395375
Thermal correction to Gibbs Free Energy= 0.315115
Sum of electronic and zero-point Energies= -1238.017449
Sum of electronic and thermal Energies= -1237.992989
Sum of electronic and thermal Enthalpies= -1237.992045
Sum of electronic and thermal Free Energies= -1238.072305

HF=-1238.3874198 (Hartree/Particle)

Compound C3 + HOO in WATER | RAF reaction

0 2

O	-0.23731800	3.85790800	-0.85262100
C	0.69148200	-0.05311500	0.05111400
C	-0.61775900	0.40002300	-0.03823200
C	1.67529200	0.90601500	-0.17675500
C	0.94481200	-1.39637400	0.35504500
C	-1.03138100	1.66464200	-0.33194600
C	-0.02770900	2.67150600	-0.57563000
C	2.28515500	-1.79999700	0.44007200
C	-1.51165100	-1.75254900	0.32162400
H	2.52714500	-2.82672300	0.66728300
H	-2.36523900	-2.34015600	0.61351800
C	-0.21190400	-2.21652700	0.54905200
H	-0.09821100	-3.26266000	0.79090600
C	2.99952500	0.49422500	-0.08853400
O	4.00865700	1.38362400	-0.33891600
C	4.58035700	1.95021100	0.86399700
H	3.81396600	2.50235400	1.40656600
H	4.99307400	1.15969400	1.48738800
H	5.36765400	2.62194200	0.53698900
N	1.27702600	2.20041800	-0.47571300
H	2.00101600	2.89054100	-0.63492200
N	-1.71328000	-0.38019000	0.14951200
C	-2.81136900	0.46552000	-0.06630700
N	-2.41262000	1.68667000	-0.34498400
C	-4.24143400	0.05324300	0.06550700
H	-4.80089500	0.96219200	-0.15957600
C	-4.58643800	-0.36592700	1.50316300
H	-4.05490000	-1.28534300	1.75729100
H	-5.65145500	-0.60503600	1.51888500
C	-4.28225900	0.71862900	2.52988800
H	-4.61010700	0.41312300	3.52355000
H	-3.21239300	0.92865100	2.58101400



H	-4.79568900	1.64717200	2.27325600
C	-4.64509800	-1.02618700	-0.94326700
H	-4.34573000	-0.75289800	-1.95524500
H	-4.20060100	-1.98932300	-0.69690800
H	-5.72904700	-1.14047700	-0.92253400
C	3.28779300	-0.85733100	0.21458400
O	4.61144900	-1.14533300	0.25453200
C	4.98940800	-2.49354200	0.56030500
H	4.60035300	-3.17678600	-0.19367700
H	6.07398100	-2.50122300	0.54394300
H	4.62927300	-2.77305500	1.54959000
O	-1.64857000	-2.38591700	-1.57312800
O	-1.10086700	-1.39960400	-2.34974200
H	-0.18781300	-1.68050100	-2.51210200

Thermochemistry

Zero-point correction= 0.369248 (Hartree/Particle)
Thermal correction to Energy= 0.393573
Thermal correction to Enthalpy= 0.394517
Thermal correction to Gibbs Free Energy= 0.315029
Sum of electronic and zero-point Energies= -1238.061792
Sum of electronic and thermal Energies= -1238.037468
Sum of electronic and thermal Enthalpies= -1238.036523
Sum of electronic and thermal Free Energies= -1238.116012

HF=-1238.4310406 (Hartree/Particle)

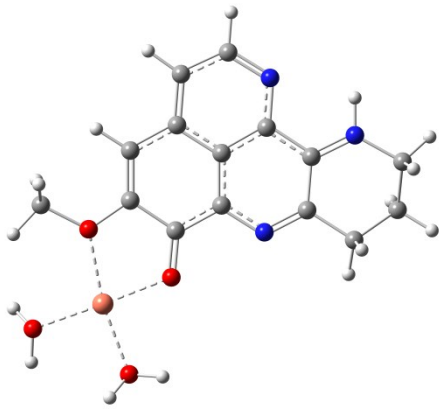
Table S4: NBO analysis investigated at the transition states (TSs) of FHT reactions between **C1**−**C3** compounds and HOO• radical

Reactions	**Donor NBO (i)**	**Acceptor NBO (j)**	**E(2), kcal mol^{-1}**
C1@C19H + HOO•	σ(1) C19–H	σ*(1) O34–O35	7.7
	π(1) O34–O35	σ*(1) C19–H	44.8
	LP(2) O34	σ*(1) C19–H	27.2
	LP(3) O34	σ*(1) C19–H	255.8
	LP(1) O35	σ*(1) C19–H	324.3
C2@N14H + HOO•	σ*(1) N14–H	σ*(1) O34–O35	5.5
C3@C21H + HOO•	σ*(1) C21–H	σ*(1) O44–O45	1293.7
	LP(1) O45	σ*(1) C21–C24	77.5
	LP(1) O44	σ*(1) C21–C24	5.6

Table S5: NPA charges, atomic spin densities (ASD), natural electron configuration (NEC) calculated at the transition states (TSs) for shifting-H, donor and acceptor of **C1** – **C3**.

Atom	NPA charges	ASD	NEC
C1@C19H + HOO•			
C19	-0.3535	0.41185	$2S^{1.02}2p^{3.31}$
H	0.3255	-0.03654	$1S^{0.67}$
O34	-0.3245	0.42642	$2S^{1.81}2p^{4.49}$
C2@N14H + HOO•			
N14	-0.6605	0.26019	$2S^{1.39}2p^{4.25}$
H	0.4294	-0.01012	$1S^{0.61}$
O34	-0.3943	0.32787	$2S^{1.82}2p^{4.56}$
C3@C21H + HOO•			
C21	-0.1832	0.46482	$2S^{0.96}2p^{3.20}$
H	0.3494	-0.05014	$1S^{0.64}$
O44	-0.3245	0.41883	$2S^{1.80}2p^{4.51}$

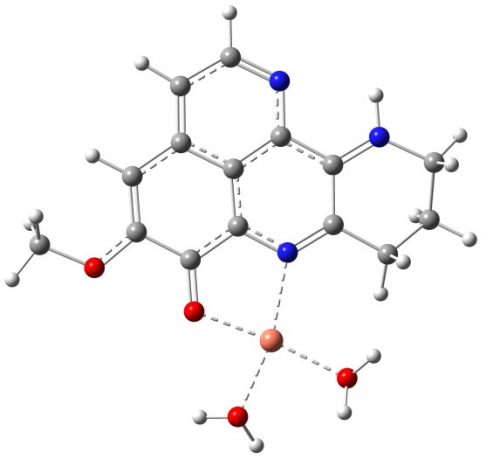
Table S6: Cartesian coordinates, and thermochemical properties for the complexes between three aaptamines derivatives with **Cu(II) ion**. All calculations were performed in water at the M05-2X/6-311++G(d,p) level of theory.

Compound C1 – Cu(II) complex at O14O15				
2 2				
C	-1.37135300	1.06195300	0.00000300	
C	-2.77044700	1.03713000	-0.01272900	
C	-0.64468900	-0.14620700	-0.02304000	
C	-0.72764500	2.32483000	0.03631000	
C	-3.40632400	-0.25174800	-0.07055800	
C	-2.56396300	-1.42922100	-0.09835400	
C	0.70764600	2.37978000	0.02553800	
C	-2.92306700	3.30661400	0.06064900	
C	1.40183400	1.22378300	-0.01023600	
H	1.19376100	3.34395600	0.03879600	
H	-3.54883200	4.18848900	0.08751000	
O	2.76134500	1.13470800	-0.05433700	
C	3.52244900	2.36086300	-0.10974200	
H	4.55851600	2.06373700	-0.20840500	
H	3.20768200	2.93246000	-0.97954400	
H	3.36482000	2.92047700	0.80911200	
C	0.77182400	-0.09855500	-0.00822900	
O	1.52171500	-1.12600100	0.00195700	
N	-1.26587100	-1.35662600	-0.06372900	
C	-1.52759600	3.45013000	0.06853200	
H	-1.08901200	4.43800100	0.09728800	
N	-3.53984100	2.13926600	0.01805400	
C	-3.24474000	-2.76336900	-0.18959000	
H	-2.59916700	-3.51880500	0.25269200	
H	-3.37846400	-3.01113500	-1.24676800	
N	-4.71478500	-0.35016900	-0.10258900	
H	-5.23619800	0.51835600	-0.10041500	
C	-5.45087100	-1.61611000	-0.12789300	
H	-6.37689800	-1.45967900	0.41849000	
H	-5.69672000	-1.85613700	-1.16315700	
C	-4.60927900	-2.71380700	0.49290700	
H	-5.12728900	-3.66346500	0.37804900	
H	-4.48591900	-2.51775100	1.55940300	
Cu	3.48020800	-0.80265200	0.02216500	
O	5.44784700	-0.41554200	0.04096400	
O	3.85144800	-2.79833900	0.02765300	
H	5.66692800	0.26497000	0.68954300	
H	5.96885000	-1.19118800	0.28425900	
H	3.08164700	-3.29274400	-0.28024000	
H	4.57224900	-3.02493600	-0.57287000	
Thermochemistry				
Zero-point correction=		0.319161 (Hartree/Particle)		

Thermal correction to Energy= 0.340569
Thermal correction to Enthalpy= 0.341514
Thermal correction to Gibbs Free Energy= 0.270080
Sum of electronic and zero-point Energies= -1242.809494
Sum of electronic and thermal Energies= -1242.788085
Sum of electronic and thermal Enthalpies= -1242.787141
Sum of electronic and thermal Free Energies= -1242.858574

HF=-1243.1286548 (Hartree/Particle)

Compound C1 – Cu(II) complex at O14N1



2 2

C	0.24409900	1.72191400	-0.02774900
C	-1.04319400	2.26061600	-0.05052600
C	0.42247200	0.33647500	-0.01690200
C	1.36407100	2.59148600	-0.01480700
C	-2.14286900	1.33564700	-0.06180700
C	-1.86105800	-0.08424500	-0.00803300
C	2.69042400	2.03156800	0.01403800
C	-0.24230400	4.38617200	-0.05199500
C	2.86735400	0.68622100	0.02330800
H	3.53120200	2.70947300	0.02853400
H	-0.44382300	5.44899600	-0.06018600
O	4.04672800	0.04259200	0.05333700
C	5.22995100	0.85288400	0.09265900
H	6.06021800	0.15589900	0.11682300
H	5.28632900	1.47563600	-0.79921900
H	5.22962500	1.47046700	0.99000000
C	1.72140400	-0.22785100	0.00388800
O	1.89398200	-1.47923200	0.01039200
N	-0.62954400	-0.52395000	-0.00088400
C	1.09411000	3.94420400	-0.02705300
H	1.89542300	4.67012700	-0.01606400
N	-1.29105400	3.58453200	-0.06410400
C	-3.01329800	-1.04040700	0.03859200
H	-2.72096300	-1.90285300	0.63277500
H	-3.22647000	-1.37828900	-0.98034900
N	-3.38090400	1.77184000	-0.12298800
H	-3.50639700	2.77512400	-0.17768300
C	-4.56079700	0.90642600	-0.12298600
H	-5.36836800	1.46300200	0.34353700
H	-4.83873000	0.69018600	-1.15545800
C	-4.25044500	-0.37083900	0.63071200
H	-5.10394100	-1.04173300	0.56583200
H	-4.07752200	-0.13688600	1.68221900
Cu	0.19831300	-2.53978400	-0.01749900
O	-1.39417700	-3.81222400	-0.21222400
O	1.38326500	-4.19285600	-0.01776500
H	-2.06757600	-3.45734500	-0.80545300
H	-1.11027600	-4.64672300	-0.60653800
H	2.24219200	-3.98954100	0.37288000

H	1.02059800	-4.92662900	0.49368400

Thermochemistry

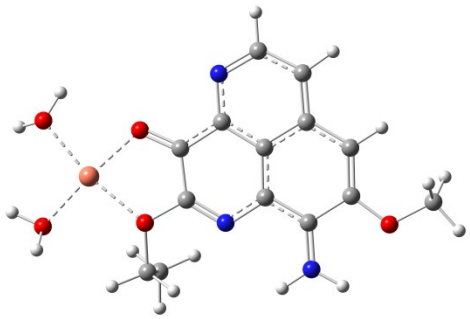
Zero-point correction= 0.319201 (Hartree/Particle)
Thermal correction to Energy= 0.340688
Thermal correction to Enthalpy= 0.341632
Thermal correction to Gibbs Free Energy= 0.270240
Sum of electronic and zero-point Energies= -1242.814621
Sum of electronic and thermal Energies= -1242.793134
Sum of electronic and thermal Enthalpies= -1242.792190
Sum of electronic and thermal Free Energies= -1242.863582

HF=-1243.1338219 (Hartree/Particle)

Compound C2 – Cu(II) complex at O17O18

2 2

O	-5.11494300	-1.43593300	-0.07433700
N	-0.44876400	2.95229500	0.12588300
N	-0.40727000	-1.22273700	-0.23496800
C	-1.64162400	0.84031000	-0.00953800
C	-2.89053800	1.51175300	0.08958000
C	-1.58569000	-0.55403800	-0.12609600
C	-0.45928500	1.60356000	0.01355900
C	-2.78775300	-1.30238600	-0.13902700
C	-4.10923300	0.74740600	0.07063600
C	-4.06095300	-0.60034100	-0.04045800
C	-2.85773100	2.88286400	0.19917000
C	0.78294100	0.90106400	-0.07878800
C	-1.61540100	3.55220400	0.21186300
C	0.67899100	-0.53736300	-0.21923400
C	-6.42194400	-0.84607700	-0.00703900
H	-5.04823300	1.27512100	0.14735100
H	-3.77235900	3.45451400	0.27560200
H	-1.60394400	4.63075900	0.29773800
H	-7.11850600	-1.67534600	-0.05548100
H	-6.56950900	-0.17658600	-0.85315300
H	-6.53828000	-0.30794300	0.93239800
O	1.92538600	1.44541800	-0.04221300
O	1.90004800	-1.13337600	-0.35384500
C	2.01333300	-2.57475800	-0.10649800
H	2.91851900	-2.85984100	-0.63067200
H	1.15927800	-3.05516000	-0.57076600
C	2.10081400	-2.82883500	1.37697500
H	1.19466500	-2.50099900	1.88516300
H	2.22459600	-3.89865200	1.54621500
H	2.95838200	-2.30664500	1.80025000
N	-2.79613300	-2.61325800	-0.24052400
H	-1.92445300	-3.11859000	-0.30834900
H	-3.67025900	-3.11741700	-0.24761000
Cu	3.47868100	0.19637500	-0.15210300
O	4.73095600	1.78589400	0.03906400
O	4.93021700	-1.18260000	-0.16071900



H	4.33115400	2.46477200	0.59683300
H	5.56816200	1.54978800	0.45682600
H	5.80134800	-0.76870500	-0.11614400
H	4.92398700	-1.70545600	-0.97217300

Thermochemistry

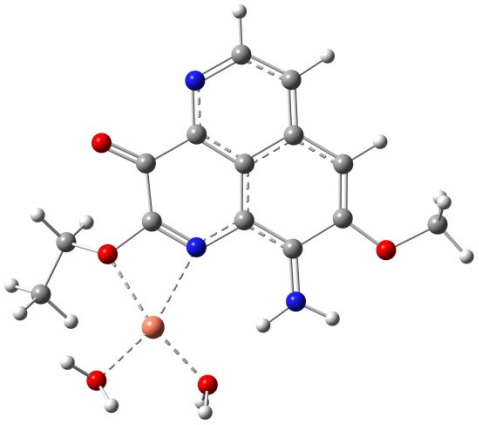
Zero-point correction= 0.313888 (Hartree/Particle)
Thermal correction to Energy= 0.337378
Thermal correction to Enthalpy= 0.338322
Thermal correction to Gibbs Free Energy= 0.261315
Sum of electronic and zero-point Energies= -1279.931023
Sum of electronic and thermal Energies= -1279.907532
Sum of electronic and thermal Enthalpies= -1279.906588
Sum of electronic and thermal Free Energies= -1279.983595

HF=-1280.2449103 (Hartree/Particle)

Compound C2 – Cu(II) complex at O18N1

2 2

O	-3.41276800	-2.78117100	0.19037300
N	-1.88041500	3.41167500	-0.20339500
N	0.44418700	-0.03863700	-0.04448100
C	-1.72260500	0.99980300	-0.06313800
C	-3.13606600	0.89328500	-0.01548000
C	-0.91949900	-0.15865200	-0.02400700
C	-1.15438400	2.28250400	-0.15578700
C	-1.51400900	-1.43017500	0.06111400
C	-3.74379000	-0.40285400	0.07389600
C	-2.96929500	-1.51226200	0.10909900
C	-3.86595800	2.06640200	-0.05983300
C	0.29694800	2.40617000	-0.22447100
C	-3.19617300	3.29253800	-0.15266400
C	0.99748100	1.12050100	-0.11462300
C	-4.83305400	-2.97889700	0.25098900
H	-4.82117800	-0.46570800	0.10918600
H	-4.94647400	2.04327700	-0.02484400
H	-3.76931100	4.20941000	-0.18641500
H	-4.97557200	-4.05184700	0.31178900
H	-5.30161600	-2.58510700	-0.64967500
H	-5.23806400	-2.49260500	1.13726500
O	0.91874600	3.45661400	-0.37550200
O	2.36444600	1.07356200	-0.16149800
C	3.07625100	1.86660500	0.87299000
H	2.40195400	1.95693800	1.72181900
H	3.26933200	2.84064800	0.43888400
C	4.34038500	1.14057300	1.23983000
H	5.01302300	1.07212900	0.38637900
H	4.83987400	1.70159500	2.02984000
H	4.11543100	0.13903500	1.60857600
N	-0.83531400	-2.56406700	0.10534400
H	0.17499200	-2.59418100	0.07792900
H	-1.34260100	-3.43354000	0.16888500



Cu	2.45937500	-1.07033200	-0.18893100
O	4.35645400	-1.34428500	-0.83011200
O	2.15219900	-3.03057500	0.06055300
H	4.68874600	-0.54778700	-1.26304100
H	4.38564500	-2.04542500	-1.49376300
H	2.54043700	-3.33749900	0.89059400
H	2.57426800	-3.53890300	-0.64470900

Thermochemistry

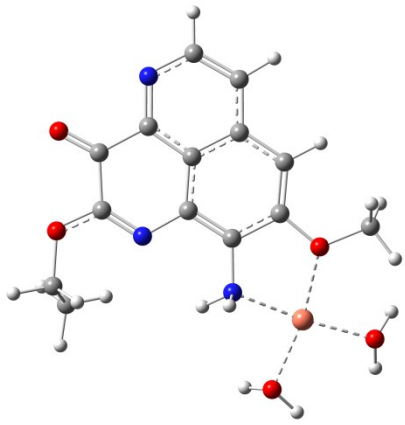
Zero-point correction= 0.313436 (Hartree/Particle)
Thermal correction to Energy= 0.337003
Thermal correction to Enthalpy= 0.337947
Thermal correction to Gibbs Free Energy= 0.260570
Sum of electronic and zero-point Energies= -1279.910889
Sum of electronic and thermal Energies= -1279.887322
Sum of electronic and thermal Enthalpies= -1279.886378
Sum of electronic and thermal Free Energies= -1279.963756

HF=-1280.2243256 (Hartree/Particle)

Compound C2 – Cu(II) complex at N14 O15

2 2

O	2.45741400	-1.36536400	-0.35784100
N	-3.82448100	-2.21427200	0.29322000
N	-1.46603700	1.22027500	-0.32854900
C	-1.65340900	-1.22418400	-0.02377800
C	-1.02303600	-2.48527200	0.05057100
C	-0.89379300	-0.04373500	-0.24519700
C	-3.04827700	-1.16001200	0.10602500
C	0.46329100	-0.16513400	-0.38238400
C	0.39017200	-2.58355000	-0.06371900
C	1.09659100	-1.43610300	-0.26539800
C	-1.85682800	-3.59462400	0.25212300
C	-3.68477900	0.17154900	0.02776600
C	-3.22135800	-3.41117500	0.36288700
C	-2.73285300	1.32728600	-0.19782700
C	3.21127000	-2.59687100	-0.28295900
H	0.86533000	-3.54839800	0.02510300
H	-1.43572700	-4.58819200	0.31845600
H	-3.86879300	-4.26340100	0.51529400
H	4.24563600	-2.31316800	-0.43323400
H	2.87848600	-3.26094900	-1.07681700
H	3.06850400	-3.04861700	0.69595900
O	-4.87526500	0.36610900	0.13221500
O	-3.37005400	2.48340300	-0.25666400
C	-2.58828800	3.70091400	-0.42456700
H	-3.31063100	4.41658300	-0.80329600
H	-1.82575100	3.51814200	-1.17635500
C	-2.00497700	4.15044100	0.89475700
H	-1.28798300	3.42865000	1.28100800
H	-1.49262900	5.10101500	0.74419200



H	-2.79725500	4.29766900	1.62786000
N	1.32096600	0.95280500	-0.61953300
H	0.90107300	1.80622400	-0.25877400
H	1.45149500	1.08810000	-1.62296300
Cu	3.23520700	0.55842800	0.04080600
O	5.07195000	-0.04614200	0.64608000
O	3.67533700	2.55021300	0.01114100
H	5.00527100	-0.77359000	1.27763700
H	5.53796100	0.66531700	1.10256500
H	3.07280800	3.05132800	0.57512000
H	4.56064200	2.71427400	0.35965500

Thermochemistry

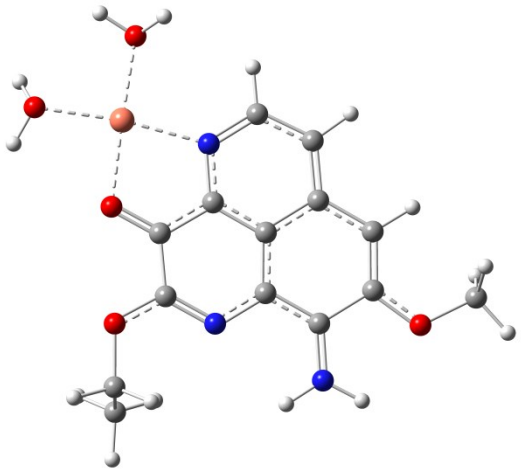
Zero-point correction= 0.315588 (Hartree/Particle)
Thermal correction to Energy= 0.338742
Thermal correction to Enthalpy= 0.339686
Thermal correction to Gibbs Free Energy= 0.263558
Sum of electronic and zero-point Energies= -1279.914238
Sum of electronic and thermal Energies= -1279.891084
Sum of electronic and thermal Enthalpies= -1279.890140
Sum of electronic and thermal Free Energies= -1279.966268

HF=-1280.2298261 (Hartree/Particle)

Compound C2 – Cu(II) complex at O17 N1

2 2

O	5.01844000	-1.00923400	0.03007700
N	-1.33353700	-1.43441800	-0.02768700
N	1.23709400	1.81155700	-0.24548000
C	0.92392200	-0.57944900	-0.08157600
C	1.44335800	-1.89966000	0.02666100
C	1.74296400	0.54940200	-0.14976800
C	-0.45635500	-0.40534100	-0.11034700
C	3.14294200	0.36558800	-0.10582600
C	2.86741900	-2.07793000	0.06101300
C	3.67794600	-0.99325700	0.00039100
C	0.52920400	-2.93069600	0.09761700
C	-1.00957000	0.90270700	-0.22337700
C	-0.85302500	-2.65785700	0.07290700
C	-0.04416700	1.99028100	-0.27996300
C	5.66360000	-2.28851800	0.13563900
H	3.26696100	-3.07754600	0.13988900
H	0.85752200	-3.95694300	0.17993500
H	-1.56686600	-3.46634900	0.14151200
H	6.72656600	-2.07674100	0.14691200
H	5.40794800	-2.90306000	-0.72600300
H	5.36410800	-2.77836600	1.06074100
O	-2.25934000	1.08140000	-0.25600600
O	-0.60487900	3.20274700	-0.37906500
C	0.25836500	4.36669300	-0.29417100
H	-0.33839300	5.16290800	-0.72814000



H	1.13725100	4.19777600	-0.91047400
C	0.61321500	4.66923200	1.14404700
H	1.19069100	3.86172700	1.59065700
H	1.21108900	5.58040600	1.17737900
H	-0.29140100	4.82761900	1.73042300
N	3.98800900	1.37096700	-0.15553700
H	3.63908400	2.31606800	-0.22505000
H	4.98258400	1.20427800	-0.11686700
Cu	-3.24618600	-0.67932100	-0.02949900
O	-5.02536900	0.28750200	-0.06616100
O	-4.14639000	-2.45639100	0.39841100
H	-4.90927700	1.22820600	0.11569700
H	-5.64101400	-0.04387700	0.59912700
H	-5.10662800	-2.38290100	0.33115900
H	-3.89037800	-3.14502400	-0.22802800

Thermochemistry

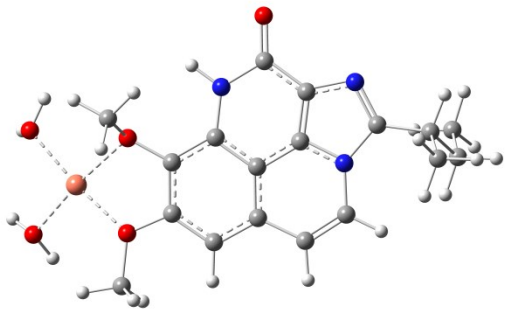
Zero-point correction= 0.314541 (Hartree/Particle)
Thermal correction to Energy= 0.337883
Thermal correction to Enthalpy= 0.338827
Thermal correction to Gibbs Free Energy= 0.262731
Sum of electronic and zero-point Energies= -1279.938240
Sum of electronic and thermal Energies= -1279.914898
Sum of electronic and thermal Enthalpies= -1279.913954
Sum of electronic and thermal Free Energies= -1279.990050

HF=-1280.2527811 (Hartree/Particle)

Compound C3 – Cu(II) complex at O14 O15

2 2

O	-1.65970800	3.78023200	0.05236900
C	-0.81502600	-0.24615400	-0.20640600
C	-2.11355500	0.24496300	-0.16514000
C	0.19311800	0.72516300	-0.17818200
C	-0.60398800	-1.62511900	-0.26453900
C	-2.50645800	1.55029000	-0.09854200
C	-1.48484000	2.56177000	-0.03870200
C	0.71510800	-2.08111100	-0.28576500
C	-3.04713900	-1.92350700	-0.25451100
H	0.93469700	-3.13747700	-0.30645000
H	-3.93463300	-2.53274300	-0.27414600
C	-1.80125200	-2.44749300	-0.28620800
H	-1.70102100	-3.52215000	-0.33194200
C	1.49564000	0.25238000	-0.25108500
O	2.59246800	1.10028000	-0.27161200
C	2.76808500	1.77381300	-1.56782600
H	2.93476400	1.01612200	-2.32918100
H	1.88419800	2.36360200	-1.78865100
H	3.63712500	2.41159800	-1.44849700
N	-0.18390600	2.05463500	-0.08641500
H	0.53911300	2.75905100	-0.00965200



N	-3.22394900	-0.53599000	-0.19377400
C	-4.30400100	0.35181000	-0.14243100
N	-3.88490000	1.59766700	-0.08493200
C	-5.73618200	-0.07117700	-0.16604500
H	-6.29639100	0.86235300	-0.09981800
C	-6.11060100	-0.92806000	1.05265900
H	-5.59767500	-1.89035200	1.00537400
H	-7.17897500	-1.13910200	0.97944500
C	-5.80544300	-0.23575100	2.37578000
H	-6.15029500	-0.83725900	3.21678300
H	-4.73320100	-0.07167000	2.49902600
H	-6.30217700	0.73503600	2.42598800
C	-6.09812800	-0.76267400	-1.48486500
H	-5.84918500	-0.13003900	-2.33688900
H	-5.57708700	-1.71348400	-1.59734800
H	-7.16960600	-0.96234000	-1.50363900
C	1.72887500	-1.13162300	-0.27807300
O	3.06218400	-1.46080800	-0.27919000
C	3.43453800	-2.85209900	-0.41720400
H	2.98065000	-3.25037800	-1.32061600
H	4.51395600	-2.85477900	-0.50473000
H	3.11347000	-3.40098100	0.46452200
Cu	4.34818300	0.03844600	0.29259900
O	5.44138700	1.69574400	0.64553000
O	5.89374300	-1.13861100	0.88656000
H	4.88298500	2.48313100	0.61493800
H	5.83715700	1.67768200	1.52594000
H	5.58389500	-1.88842100	1.41024300
H	6.50712600	-0.65373200	1.45303500

Thermochemistry

Zero-point correction= 0.408647 (Hartree/Particle)
Thermal correction to Energy= 0.435957
Thermal correction to Enthalpy= 0.436901
Thermal correction to Gibbs Free Energy= 0.352643
Sum of electronic and zero-point Energies= -1435.908484
Sum of electronic and thermal Energies= -1435.881174
Sum of electronic and thermal Enthalpies= -1435.880230
Sum of electronic and thermal Free Energies= -1435.964488

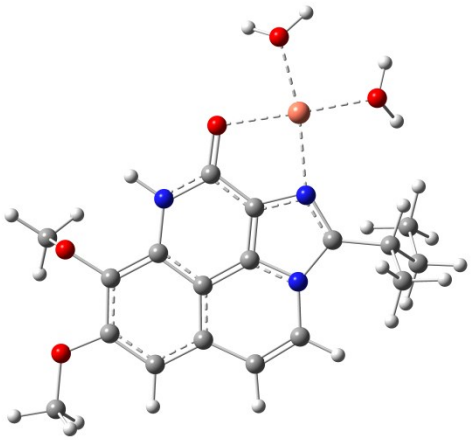
HF=-1436.3171307 (Hartree/Particle)

Compound C3 – Cu(II) complex at O18N19

2 2

O	1.01132600	-2.63573400	-0.15733400
C	-1.62100700	0.53043600	-0.12276900
C	-0.24917400	0.66516200	-0.15170300
C	-2.10050600	-0.78671200	-0.10822000
C	-2.40260800	1.68344600	-0.12357800
C	0.61447300	-0.36700800	-0.16497200
C	0.16753000	-1.69992300	-0.14617200
C	-3.78563000	1.51012300	-0.11138200

C	-0.29639300	3.00342900	-0.16981100
H	-4.44366200	2.36548900	-0.11645400
H	0.24489300	3.93418300	-0.17458300
C	-1.64928500	2.93451300	-0.14117500
H	-2.19197200	3.86896700	-0.13021200
C	-3.47652700	-0.94313400	-0.09422000
O	-4.02377800	-2.19701200	-0.12303000
C	-4.42284100	-2.67253400	1.18400400
H	-3.55145000	-2.72120500	1.83591000
H	-5.17694300	-2.01103100	1.60548700
H	-4.83476400	-3.66505800	1.03169600
N	-1.18782000	-1.85275600	-0.11872900
H	-1.56235200	-2.79539000	-0.10089900
N	0.46462600	1.81538800	-0.18484700
C	1.81067300	1.43167800	-0.22416900
N	1.89481300	0.10637700	-0.20928100
C	2.96764300	2.36746300	-0.28713900
H	3.84122100	1.72056600	-0.37582500
C	3.10521600	3.17931000	1.00954500
H	2.24713900	3.84647200	1.11605000
H	3.98791600	3.81074200	0.89703200
C	3.24632800	2.29289400	2.24134300
H	3.44473200	2.89238600	3.12952700
H	2.33620300	1.71811800	2.42300300
H	4.07132300	1.58760900	2.11516700
C	2.89750000	3.26558800	-1.52575900
H	2.79461400	2.67202600	-2.43383900
H	2.06288600	3.96333200	-1.46866300
H	3.81741700	3.84573100	-1.59278300
C	-4.30123100	0.20715600	-0.10115200
O	-5.62513700	-0.07008900	-0.10668700
C	-6.54353900	1.03114200	-0.11593100
H	-6.40397200	1.63251600	-1.01324300
H	-7.53122300	0.58306700	-0.11857200
H	-6.41227500	1.64075500	0.77701200
Cu	2.93854100	-1.72772600	-0.15509300
O	4.78641500	-0.91303500	0.00775600
O	3.64038700	-3.61361600	-0.31900400
H	4.78184100	-0.13246300	0.57740300
H	5.40985700	-1.53278300	0.40746200
H	3.05715700	-4.23762100	0.13053700
H	4.51493300	-3.72770400	0.07244700



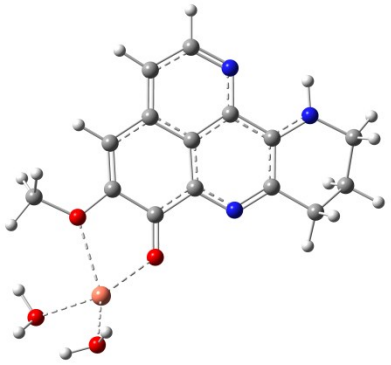
Thermochemistry

Zero-point correction= 0.407539 (Hartree/Particle)
Thermal correction to Energy= 0.435540
Thermal correction to Enthalpy= 0.436484
Thermal correction to Gibbs Free Energy= 0.350086
Sum of electronic and zero-point Energies= -1435.912648
Sum of electronic and thermal Energies= -1435.884647
Sum of electronic and thermal Enthalpies= -1435.883703

Sum of electronic and thermal Free Energies= -1435.970101

HF=-1436.320187 (Hartree/Particle)

Table S7: Cartesian coordinates, and thermochemical properties for the complexes between three aaptamines derivatives with **Cu(I) ion**. All calculations were performed in water at the M05-2X/6-311++G(d,p) level of theory.

Compound C1 – Cu(I) complex at O14O15				
1 1				
C	-1.45002400	1.04228300	-0.03919800	
C	-2.84887500	0.98467500	-0.08057300	
C	-0.70044700	-0.14568300	0.02604500	
C	-0.82510600	2.31758000	-0.06605800	
C	-3.45769500	-0.31290700	-0.06794000	
C	-2.59797000	-1.45943500	-0.00652300	
C	0.61268600	2.39933500	-0.03372500	
C	-3.04119700	3.25113700	-0.15791000	
C	1.35093700	1.26884200	0.02125600	
H	1.07029500	3.37744900	-0.05821200	
H	-3.67963600	4.12380800	-0.20227600	
O	2.69607300	1.21617400	0.05049400	
C	3.41081800	2.45959000	0.04436500	
H	4.46202700	2.19312000	0.07136800	
H	3.18587300	3.01425900	-0.86559200	
H	3.14520800	3.04417800	0.92421500	
C	0.73708200	-0.07966300	0.06798500	
O	1.46680200	-1.08823700	0.13988600	
N	-1.29277200	-1.35732300	0.04714900	
C	-1.64483700	3.42329600	-0.12551800	
H	-1.22832600	4.42090500	-0.14764400	
N	-3.64048400	2.07789600	-0.13827400	
C	-3.23787900	-2.81851400	-0.01363800	
H	-2.58537800	-3.51669500	0.50672900	
H	-3.33226900	-3.15762700	-1.04933400	
N	-4.77468100	-0.44040200	-0.11560600	
H	-5.31374100	0.41238600	-0.17568500	
C	-5.47211600	-1.72583900	-0.08961700	
H	-6.42188400	-1.57132100	0.41549200	
H	-5.67518000	-2.04404400	-1.11353500	
C	-4.62274000	-2.75958300	0.62589500	
H	-5.11398300	-3.72839200	0.56179800	
H	-4.53409900	-2.49041000	1.67997900	
Cu	3.52236200	-1.04047100	-0.01252300	
O	5.13110400	-0.50568000	1.37466200	
O	4.85414600	-2.03430600	-1.35983800	
H	5.00892700	0.42107900	1.60739800	
H	5.95343300	-0.53116400	0.87383000	
H	4.66193300	-1.83320600	-2.28147600	
H	5.74301900	-1.69615700	-1.20749600	

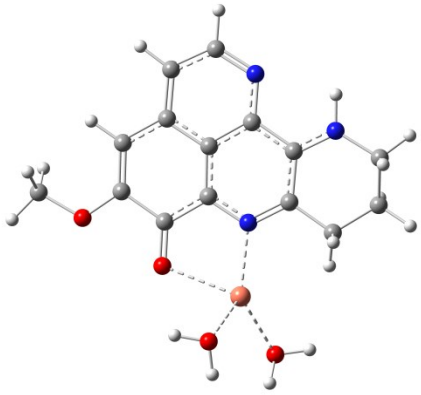
Thermochemistry

Zero-point correction=	0.314525 (Hartree/Particle)
Thermal correction to Energy=	0.338162

Thermal correction to Enthalpy= 0.339106
Thermal correction to Gibbs Free Energy= 0.261548
Sum of electronic and zero-point Energies= -1242.974189
Sum of electronic and thermal Energies= -1242.950551
Sum of electronic and thermal Enthalpies= -1242.949607
Sum of electronic and thermal Free Energies= -1243.027165

HF=-1243.2887131 (Hartree/Particle)

Compound C1 – Cu(I) complex at O14N1



1 1

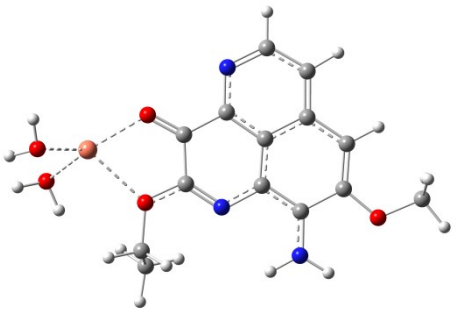
C	1.12610100	1.31833200	-0.01245200
C	0.27878500	2.43139400	-0.07474100
C	0.58619200	0.02688900	0.03768800
C	2.53150300	1.52405400	0.00216400
C	-1.13348700	2.18940000	-0.09129300
C	-1.58704500	0.83516700	-0.04483600
C	3.41335400	0.38367900	0.06921000
C	2.03475000	3.87673500	-0.10961900
C	2.90861600	-0.87008800	0.11983200
H	4.47778900	0.56780900	0.07846800
H	2.39142200	4.89773700	-0.14816600
O	3.62807000	-2.00440600	0.18572100
C	5.05518000	-1.87071400	0.20620000
H	5.44362200	-2.88163200	0.26102400
H	5.39893800	-1.38394900	-0.70592000
H	5.36461400	-1.29983000	1.08107900
C	1.44778500	-1.13213400	0.10982400
O	1.01529200	-2.29093400	0.15921700
N	-0.74433600	-0.17491700	0.02313700
C	2.97308000	2.82696400	-0.04847000
H	4.02977000	3.05607400	-0.04113200
N	0.72893200	3.70524100	-0.12310300
C	-3.06227200	0.56784300	-0.07289100
H	-3.25439600	-0.36892900	0.45257300
H	-3.37765700	0.43770800	-1.11210900
N	-1.99400500	3.19716100	-0.15092000
H	-1.60486900	4.12801000	-0.20045200
C	-3.44642200	3.02583800	-0.16140000
H	-3.88109800	3.89118600	0.33163600
H	-3.79907300	3.00555800	-1.19389100
C	-3.82152000	1.73754700	0.54873800
H	-4.89492600	1.58288100	0.46167500
H	-3.57229600	1.82033400	1.60802000
Cu	-1.37449800	-2.14241400	0.04482100
O	-2.72804600	-3.33278300	1.15905800
O	-1.39087200	-3.46676500	-1.73787600
H	-3.52860200	-2.82945300	1.34175700
H	-3.01165200	-4.06702400	0.60356300
H	-0.46585900	-3.69302500	-1.88213400
H	-1.81260000	-4.29217100	-1.47628800

Thermochemistry

Zero-point correction= 0.314179 (Hartree/Particle)
Thermal correction to Energy= 0.338127
Thermal correction to Enthalpy= 0.339071
Thermal correction to Gibbs Free Energy= 0.260729
Sum of electronic and zero-point Energies= -1242.985658
Sum of electronic and thermal Energies= -1242.961709
Sum of electronic and thermal Enthalpies= -1242.960765
Sum of electronic and thermal Free Energies= -1243.039108

HF=-1243.2998364 (Hartree/Particle)

Compound C2 – Cu(I) complex at O17O18



1 1

O	-5.13189600	-1.43181300	-0.23369100
N	-0.52480100	2.96418000	0.31978400
N	-0.42088300	-1.19411900	-0.20043800
C	-1.69421600	0.86000800	0.05744800
C	-2.94883500	1.51873600	0.14687300
C	-1.62099200	-0.53124000	-0.11988500
C	-0.52225400	1.63058800	0.14880800
C	-2.80255600	-1.27987300	-0.20850900
C	-4.15437300	0.74997100	0.05079900
C	-4.08156700	-0.59308800	-0.12319500
C	-2.92986100	2.89010600	0.32391300
C	0.75185300	0.94647100	0.05458700
C	-1.70197300	3.56095500	0.40417800
C	0.66773600	-0.52025600	-0.11238400
C	-6.44268300	-0.85154500	-0.18330100
H	-5.10293900	1.26125900	0.11807200
H	-3.85274400	3.44866800	0.40047700
H	-1.69348900	4.63379200	0.54374800
H	-7.13347800	-1.67914900	-0.29927200
H	-6.56554600	-0.13928100	-0.99807500
H	-6.59757800	-0.36251200	0.77748000
O	1.85217800	1.51850600	0.10659300
O	1.87738400	-1.09810100	-0.17823100
C	1.96237600	-2.54398700	-0.26704100
H	2.96948100	-2.71847500	-0.63431500
H	1.24283200	-2.88748200	-1.00597000
C	1.74968600	-3.19020900	1.08304100
H	0.74228800	-3.01537300	1.45505800
H	1.89950100	-4.26574600	0.98377500
H	2.46765700	-2.80872500	1.80889100
N	-2.80076700	-2.59889900	-0.36999900
H	-1.92429100	-3.09316500	-0.42366500
H	-3.66889800	-3.10554100	-0.42674000
Cu	3.64219000	0.46819200	-0.12693300
O	5.23722200	0.66549900	-1.51611700
O	4.78318700	-0.70981500	1.33357000

H	5.39519000	1.58659900	-1.74774600
H	6.04253200	0.37206700	-1.07657600
H	5.66375700	-0.85298100	0.97042300
H	4.37873800	-1.58368500	1.36107200

Thermochemistry

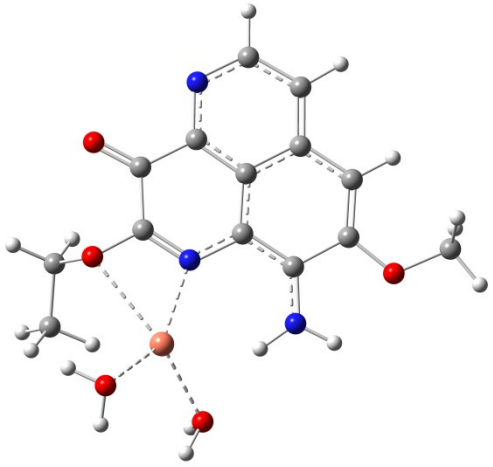
Zero-point correction= 0.309500 (Hartree/Particle)
Thermal correction to Energy= 0.335238
Thermal correction to Enthalpy= 0.336182
Thermal correction to Gibbs Free Energy= 0.253404
Sum of electronic and zero-point Energies= -1280.097308
Sum of electronic and thermal Energies= -1280.071571
Sum of electronic and thermal Enthalpies= -1280.070626
Sum of electronic and thermal Free Energies= -1280.153405

HF=-1280.4068089 (Hartree/Particle)

Compound C2 – Cu(I) complex at O18N1

1 1

O	-3.04835200	-2.95812600	0.10584000
N	-2.10001200	3.35048700	-0.10212800
N	0.56139600	0.12231100	-0.13220400
C	-1.71194200	0.95897500	-0.05402300
C	-3.10996300	0.72281500	-0.00827800
C	-0.79522400	-0.11730800	-0.05776600
C	-1.27356400	2.29324900	-0.09858500
C	-1.27679200	-1.43516400	0.03380800
C	-3.59753800	-0.62180000	0.03924500
C	-2.72012400	-1.65164100	0.05528700
C	-3.94859700	1.82398800	-0.01168600
C	0.15956700	2.54829000	-0.15371900
C	-3.40057700	3.10844700	-0.05898400
C	1.00178400	1.33507700	-0.17429400
C	-4.44452100	-3.28589700	0.14492000
H	-4.66428100	-0.78593700	0.06729500
H	-5.02169900	1.69477800	0.02154700
H	-4.05618200	3.96901600	-0.06096200
H	-4.48859500	-4.36859800	0.18052600
H	-4.93906900	-2.91681600	-0.75244500
H	-4.90189000	-2.85936700	1.03645900
O	0.67790700	3.66253300	-0.20377200
O	2.33168200	1.52218400	-0.32435000
C	3.03015700	2.07021400	0.84434200
H	2.28904600	2.36914700	1.58294600
H	3.56546600	2.94900200	0.49621900
C	3.96212200	1.01514100	1.38814000
H	4.70666600	0.74047800	0.64096200
H	4.47690700	1.40519900	2.26713400
H	3.40153700	0.12227900	1.67679100
N	-0.51801900	-2.52319900	0.10206500
H	0.48495600	-2.48766400	0.20232400
H	-0.96902100	-3.42106800	0.18374400



Cu	2.27683600	-1.08186600	-0.27394600
O	4.01650600	-1.22442400	-1.51113700
O	2.53354300	-2.98428900	0.74658500
H	4.45574000	-0.36772900	-1.46955900
H	4.61796600	-1.83710200	-1.07398800
H	2.75192400	-2.81728700	1.66990300
H	3.31970600	-3.39077000	0.36563000

Thermochemistry

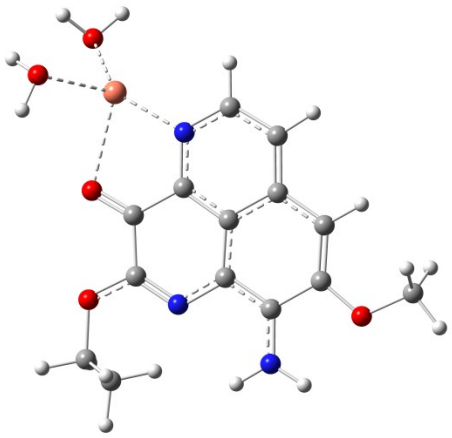
Zero-point correction= 0.310034 (Hartree/Particle)
Thermal correction to Energy= 0.335211
Thermal correction to Enthalpy= 0.336156
Thermal correction to Gibbs Free Energy= 0.255668
Sum of electronic and zero-point Energies= -1280.094813
Sum of electronic and thermal Energies= -1280.069635
Sum of electronic and thermal Enthalpies= -1280.068691
Sum of electronic and thermal Free Energies= -1280.149179

HF=-1280.4048464 (Hartree/Particle)

Compound C2 – Cu(I) complex at O17N13

1 1

O	4.99711900	-1.21943100	-0.02573300
N	-1.37307600	-1.36993700	0.01978200
N	1.36339400	1.78514100	-0.18132500
C	0.91208300	-0.60328600	-0.04433800
C	1.38406200	-1.94117300	0.02109700
C	1.80141800	0.48184400	-0.11013900
C	-0.46963100	-0.37624100	-0.04035500
C	3.17857100	0.23955100	-0.10236600
C	2.79368200	-2.18400100	0.02788200
C	3.65289000	-1.13408700	-0.02942900
C	0.43186700	-2.94607300	0.07871400
C	-0.95833500	0.99339700	-0.09852800
C	-0.92581200	-2.61992300	0.07548800
C	0.10329400	2.02706700	-0.17962800
C	5.57482800	-2.53048100	0.05064700
H	3.14655600	-3.20283700	0.08068900
H	0.72936500	-3.98426400	0.12889700
H	-1.67145300	-3.40061400	0.12279400
H	6.64803800	-2.37674800	0.04442500
H	5.27261200	-3.12141900	-0.81286100
H	5.26836300	-3.01910800	0.97446900
O	-2.15280400	1.29385400	-0.08493000
O	-0.39534300	3.26764600	-0.26478500
C	0.53535600	4.37885900	-0.30494900
H	-0.04361500	5.18722000	-0.74121900
H	1.35643200	4.12344100	-0.96975500
C	1.01350400	4.73746200	1.08384500
H	1.57797200	3.92271900	1.53325900
H	1.66050900	5.61291200	1.02059200



H	0.16577600	4.98046900	1.72384300
N	4.07788500	1.21889900	-0.15963400
H	3.76822300	2.17645200	-0.20642200
H	5.06175000	1.00708600	-0.15115500
Cu	-3.35393900	-0.84153600	0.06316200
O	-4.68203200	-0.28566100	-1.60118800
O	-4.98269900	-1.01757100	1.41173200
H	-4.31095000	0.51361400	-1.98963700
H	-5.52303800	-0.01088500	-1.22084500
H	-5.80057200	-1.05951600	0.90494800
H	-4.95974800	-1.83088600	1.92611900

Thermochemistry

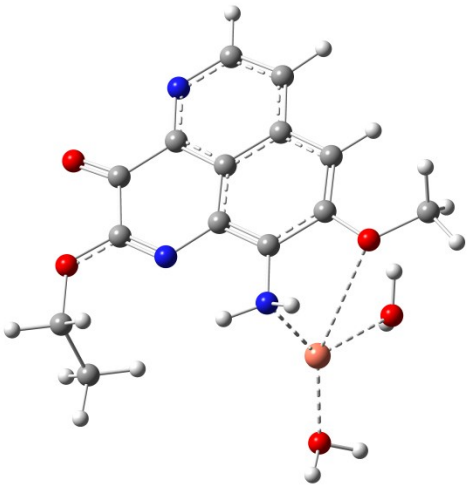
Zero-point correction= 0.309304 (Hartree/Particle)
Thermal correction to Energy= 0.335240
Thermal correction to Enthalpy= 0.336185
Thermal correction to Gibbs Free Energy= 0.252701
Sum of electronic and zero-point Energies= -1280.105587
Sum of electronic and thermal Energies= -1280.079650
Sum of electronic and thermal Enthalpies= -1280.078706
Sum of electronic and thermal Free Energies= -1280.162190

HF=-1280.4148909 (Hartree/Particle)

Compound C2 – Cu(I) complex at N14 O15

1 1

O	2.57740800	-1.62293600	-1.25687400
N	-3.41570500	-2.16284400	0.85418500
N	-1.22898900	1.07773500	-0.69437500
C	-1.35938500	-1.29152600	-0.05433600
C	-0.73379300	-2.55535300	0.05411400
C	-0.65362600	-0.17918100	-0.57067600
C	-2.69249300	-1.16170300	0.36201100
C	0.65847000	-0.33935300	-0.95710100
C	0.62120000	-2.70873600	-0.35639600
C	1.29191400	-1.62700400	-0.84806000
C	-1.50698500	-3.59700900	0.57074600
C	-3.32212400	0.16391900	0.25140900
C	-2.81952000	-3.35484300	0.94917400
C	-2.44100200	1.24091800	-0.32290300
C	3.32426100	-2.83651100	-1.09162800
H	1.08995000	-3.67715600	-0.26881400
H	-1.08818900	-4.58830000	0.67768800
H	-3.41929300	-4.16080500	1.34941600
H	4.32664300	-2.61216900	-1.43898300
H	2.88660600	-3.63207200	-1.69277400
H	3.34363200	-3.12022000	-0.03957700
O	-4.46610100	0.41167800	0.58488600
O	-3.07550500	2.40592900	-0.42091400
C	-2.33997800	3.54814600	-0.93737000
H	-3.11920400	4.22689300	-1.26950600



H	-1.75231800	3.22308400	-1.79181200
C	-1.48750200	4.17680900	0.14099200
H	-0.71360100	3.49421000	0.48670300
H	-1.00712900	5.06691100	-0.26626100
H	-2.10642600	4.47497800	0.98660900
N	1.43361600	0.73696400	-1.38536000
H	0.87030900	1.53258300	-1.66191900
H	2.11315600	0.48431600	-2.09401100
Cu	2.59614000	1.13428400	0.32623700
O	3.17325300	-0.46342900	1.68441900
O	3.40711700	2.73143200	1.41912000
H	2.73443600	-1.30194700	1.50311700
H	2.93465600	-0.24480800	2.59137700
H	3.80511900	3.39673100	0.84823200
H	4.12513100	2.40771600	1.97355700

Thermochemistry

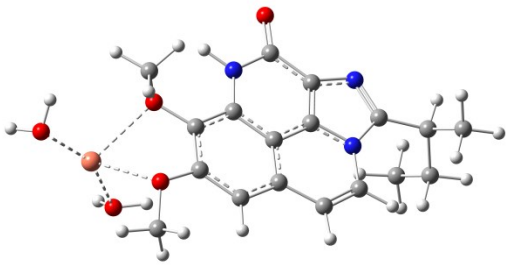
Zero-point correction= 0.310317 (Hartree/Particle)
Thermal correction to Energy= 0.335900
Thermal correction to Enthalpy= 0.336844
Thermal correction to Gibbs Free Energy= 0.253992
Sum of electronic and zero-point Energies= -1280.095919
Sum of electronic and thermal Energies= -1280.070335
Sum of electronic and thermal Enthalpies= -1280.069391
Sum of electronic and thermal Free Energies= -1280.152243

HF=-1280.4062353 (Hartree/Particle)

Compound C3 – Cu(I) complex at O14 O15

1 1

O	-1.58671400	3.81229100	0.08847300
C	-0.74410500	-0.19452300	-0.41059900
C	-2.03939600	0.28610700	-0.28202200
C	0.26039100	0.77537000	-0.35852700
C	-0.52226400	-1.56420900	-0.56182200
C	-2.42919800	1.58367400	-0.11204300
C	-1.40769500	2.59720600	-0.05870600
C	0.80030000	-1.99719800	-0.67164300
C	-2.96428900	-1.87912600	-0.45706900
H	1.02575800	-3.04644000	-0.78808300
H	-3.84878100	-2.49286500	-0.47524900
C	-1.71835300	-2.39065800	-0.58301600
H	-1.61944800	-3.45982300	-0.70410400
C	1.56985000	0.33375400	-0.46948500
O	2.61197500	1.22216000	-0.36283600
C	3.12949000	1.65461900	-1.64460200
H	3.54081300	0.80282700	-2.18301700
H	2.32991000	2.12046100	-2.21903000
H	3.90763700	2.38043000	-1.42838700
N	-0.11339300	2.09994000	-0.19058500
H	0.62146700	2.79582000	-0.15925100
N	-3.14734200	-0.49844100	-0.29808300



C	-4.22451000	0.37857000	-0.12626700
N	-3.80544900	1.62125300	-0.01713100
C	-5.65579200	-0.04636300	-0.07659500
H	-6.20753300	0.88106100	0.08270500
C	-5.94703200	-0.97281800	1.11357700
H	-5.44694800	-1.93237000	0.97012900
H	-7.01970900	-1.17479900	1.10696600
C	-5.54004100	-0.36322100	2.44998200
H	-5.82914500	-1.01207800	3.27676800
H	-4.46013300	-0.21298400	2.50453600
H	-6.02172400	0.60580000	2.59403400
C	-6.11341500	-0.66215600	-1.40245100
H	-5.91793700	0.01457500	-2.23430400
H	-5.60994900	-1.60830400	-1.60063700
H	-7.18549000	-0.85486200	-1.35809400
C	1.82152200	-1.04556000	-0.62550400
O	3.14081800	-1.35694900	-0.71243300
C	3.51510400	-2.73918700	-0.61667500
H	3.15831200	-3.28927300	-1.48575700
H	4.59996100	-2.74193600	-0.59436600
H	3.11853800	-3.17176700	0.30084900
Cu	4.41398200	0.01604500	0.77086400
O	6.14620600	0.65739300	-0.13372900
O	3.32710000	-0.77435000	2.36389600
H	5.95179100	1.33582000	-0.78958900
H	6.74945400	1.07101900	0.49273300
H	2.39106600	-0.82208200	2.13824800
H	3.37140000	-0.22286200	3.15225300

Thermochemistry

Zero-point correction= 0.404045 (Hartree/Particle)
Thermal correction to Energy= 0.433605
Thermal correction to Enthalpy= 0.434549
Thermal correction to Gibbs Free Energy= 0.343220
Sum of electronic and zero-point Energies= -1436.085084
Sum of electronic and thermal Energies= -1436.055524
Sum of electronic and thermal Enthalpies= -1436.054580
Sum of electronic and thermal Free Energies= -1436.145909

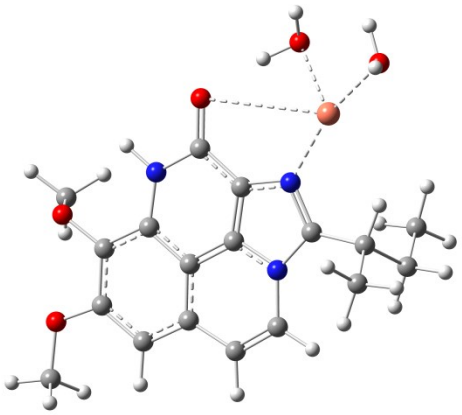
HF=-1436.489129 (Hartree/Particle)

Compound C3 – Cu(I) complex at O18N19

1 1

O	0.62373400	-2.95751800	-0.31870300
C	-1.70452500	0.44271100	-0.16153300
C	-0.31998000	0.49147400	-0.19256900
C	-2.26043200	-0.83785500	-0.19708500
C	-2.44016900	1.62654100	-0.09766900
C	0.53841500	-0.56742500	-0.24832300
C	-0.01571800	-1.89471800	-0.27748700
C	-3.83028400	1.52066000	-0.07380700
C	-0.30191600	2.85489400	-0.09845900

H	-4.44174600	2.40876300	-0.02930300
H	0.28228200	3.75881500	-0.07104500
C	-1.65309300	2.84947000	-0.06339000
H	-2.16061200	3.80172800	-0.00738700
C	-3.64303500	-0.93329400	-0.17216400
O	-4.24762200	-2.16182600	-0.24330400
C	-4.62854300	-2.67792500	1.05265600
H	-3.74120400	-2.80129900	1.67264900
H	-5.33362700	-1.99994900	1.52978000
H	-5.09662700	-3.64037500	0.87100500
N	-1.39999000	-1.92592200	-0.25734700
H	-1.81250100	-2.85127400	-0.26934100
N	0.40310200	1.64195000	-0.17112200
C	1.73570500	1.25550600	-0.21662500
N	1.82420500	-0.06300800	-0.26417700
C	2.90638900	2.18058500	-0.21414000
H	3.77207100	1.51681900	-0.27755100
C	3.01351200	2.96211700	1.10348800
H	2.18002600	3.66193800	1.18917300
H	3.92373900	3.56126500	1.04495000
C	3.06572400	2.04786600	2.32196600
H	3.23572300	2.62320500	3.23187400
H	2.13153500	1.49638900	2.44454800
H	3.87434800	1.32065000	2.22203500
C	2.90486000	3.10249500	-1.43662200
H	2.84315200	2.52565400	-2.35931700
H	2.07202100	3.80463900	-1.40969800
H	3.83029900	3.67803500	-1.44898500
C	-4.41268500	0.24872700	-0.11407100
O	-5.75086300	0.03938500	-0.10722100
C	-6.60662300	1.18724900	-0.03599500
H	-6.45680300	1.82629600	-0.90511600
H	-7.61774400	0.79468800	-0.03388600
H	-6.41998700	1.74243600	0.88230700
Cu	3.54670100	-1.08682700	-0.18460600
O	3.15930700	-3.12625300	0.81036500
O	5.55177800	-1.51393200	-0.44103100
H	2.27046200	-3.15123700	0.40922400
H	3.69407700	-3.73272200	0.28877700
H	5.86805500	-1.33100100	-1.33211400
H	5.68122700	-2.45992500	-0.31035200



Thermochemistry

Zero-point correction= 0.403684 (Hartree/Particle)
Thermal correction to Energy= 0.433386
Thermal correction to Enthalpy= 0.434331
Thermal correction to Gibbs Free Energy= 0.342231
Sum of electronic and zero-point Energies= -1436.097728
Sum of electronic and thermal Energies= -1436.068026
Sum of electronic and thermal Enthalpies= -1436.067081
Sum of electronic and thermal Free Energies= -1436.159181

HF=-1436.501412 (Hartree/Particle)

Table S8: Lowest absorption wavelength (nm) of **C1**–**C3** calculated by TD-DFT with different methods of various % HF in exchange correlation.

Method	%HF	Absorption / nm		
		C1	C2	C3
B3LYP	20	471	482	332
B98	22	465	476	327
M06	27	461	472	329
PBE0	25	459	470	322
CAM-B3LYP*	19/65	427	439	298
M05-2X	56	423	435	292
Exp. (ref.[4])		398	402	350

*19 % HF at short-range and 65 % HF at long-range