

Reduction Potential of Ru^{III}-Based Complexes with Potential Antitumor Activity and Thermodynamics of their Hydrolysis Reactions and Interactions with Possible Biological Targets: a Theoretical Investigation

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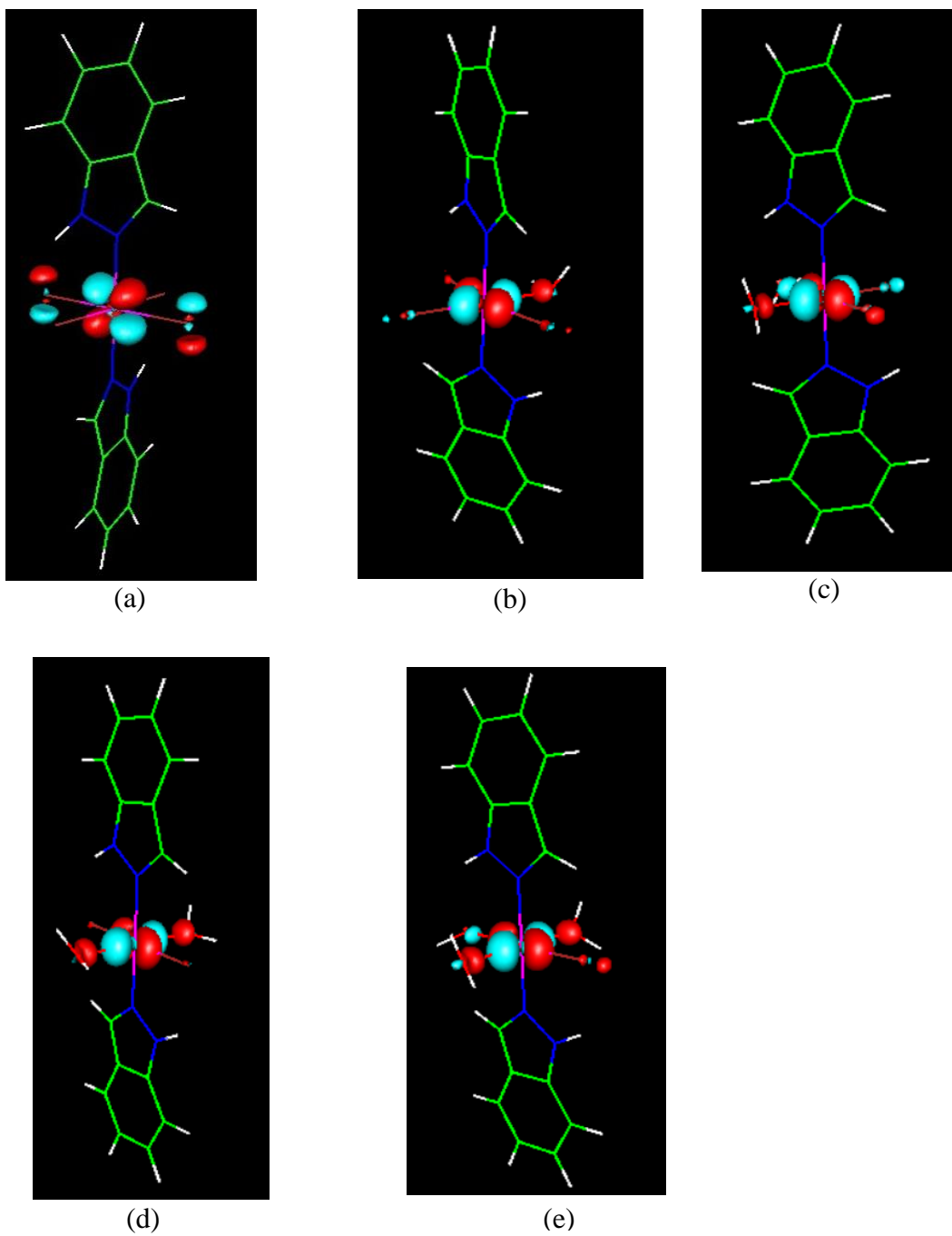
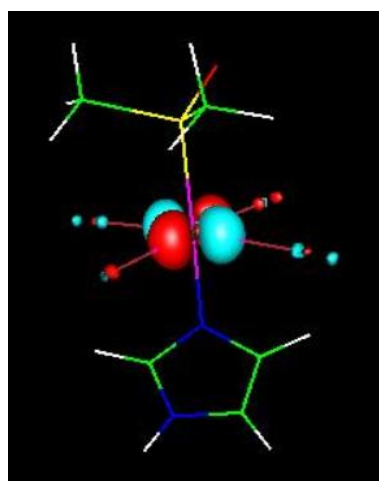
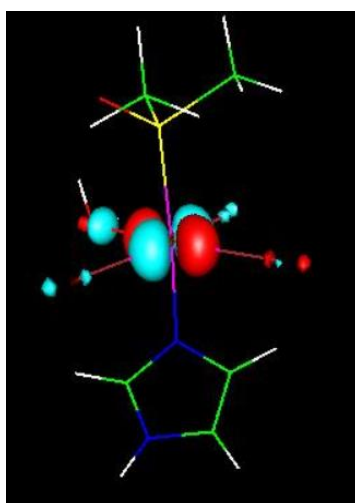


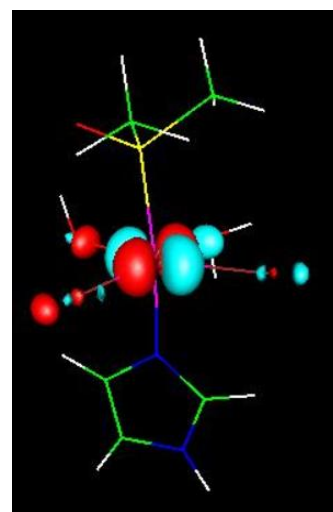
Figure S1. TPSSh/def2-TZVP LUMO orbitals for (a) the KP1019 complex and its (b) mono-, (c) and (d) di-, and (e) tri-water substituted derivatives.



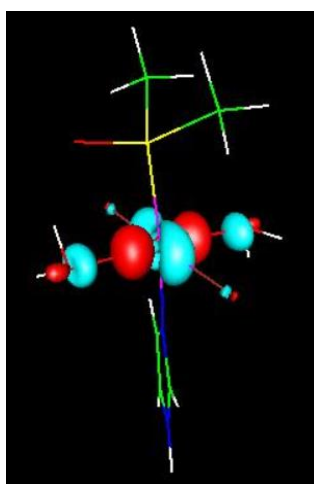
(a)



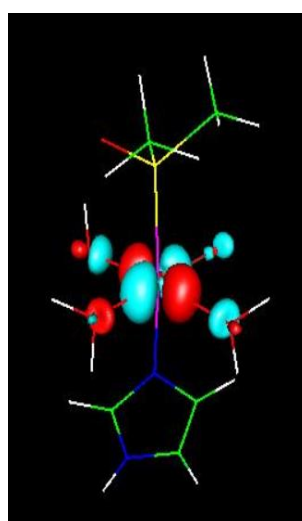
(b)



(c)



(d)



(e)

Figure S2. TPSSh/def2-TZVP LUMO orbitals for (a) the NAMI-A complex and its (b) mono-, (c) and (d) di-, and (e) tri-water substituted derivatives.

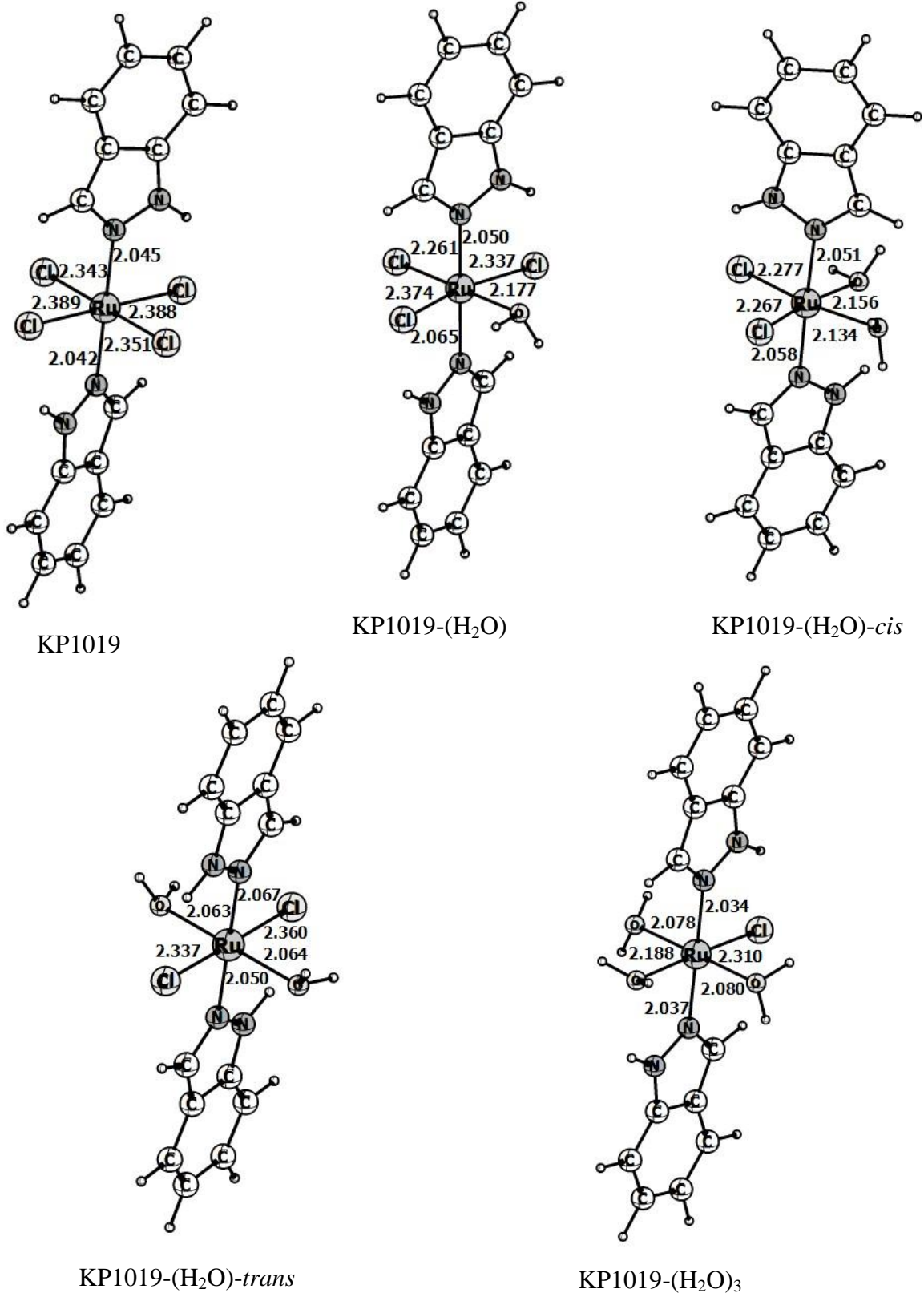


Figure S3. TPSSh/def2-TZVP optimized structures for the KP1019 complex in the +3 formal oxidation state and its mono- (KP1019-(H₂O)), di- (KP1019-(H₂O)₂-*cis*, KP1019-(H₂O)₂-*trans*) and tri- (KP1019-(H₂O)₃) water substituted derivatives.

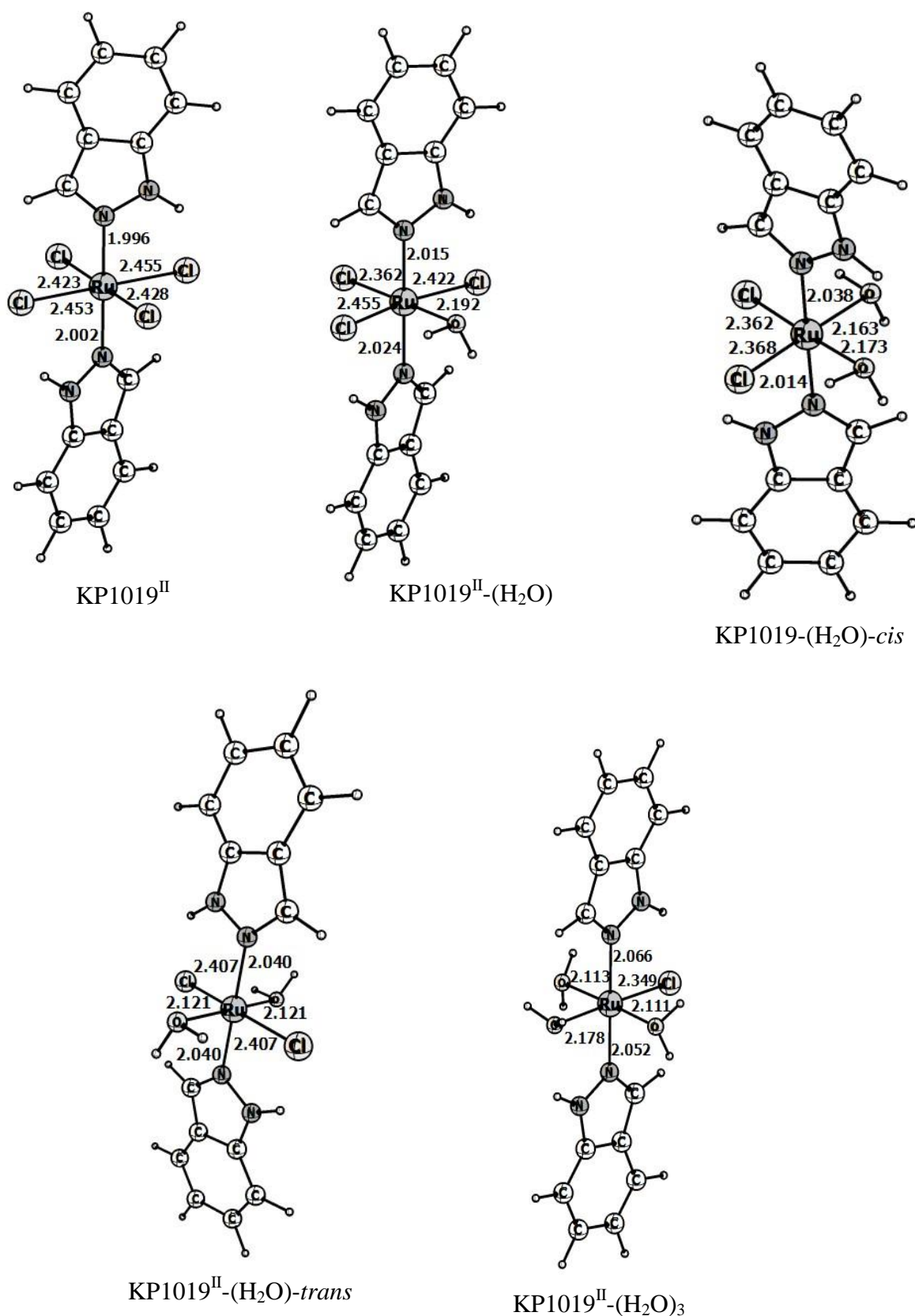


Figure S4. TPSSh/def2-TZVP optimized structures for the KP1019 complex in the +2 formal oxidation state and its mono- (KP1019^{II}-(H₂O)), di- (KP1019^{II}-(H₂O)₂-*cis*, KP1019^{II}-(H₂O)₂-*trans*) and tri- (KP1019^{II}-(H₂O)₃) water substituted derivatives.

TPSSh/def2-TZVP optimized Cartesian coordinates of all species studied in this work, with ruthenium in the +2 and +3 oxidation states

NAM^{III}

44	0.415435000	0.568854000	-0.062975000
17	-1.831427000	1.047832000	0.537443000
17	0.994738000	0.550732000	2.266866000
17	-0.199033000	0.441514000	-2.313031000
17	2.622291000	-0.075586000	-0.627422000
16	0.945883000	2.773814000	-0.190153000
6	2.617239000	3.009022000	0.443572000
6	0.059353000	3.659673000	1.105138000
8	0.833775000	3.582033000	-1.422724000
7	-0.052558000	-1.449806000	0.101052000
6	0.353788000	-2.483339000	-0.706772000
6	-0.799530000	-1.959972000	1.055821000
6	-0.163164000	-3.649403000	-0.227646000
7	-0.893081000	-3.298239000	0.892681000
1	3.281907000	2.522249000	-0.266369000
1	2.797840000	4.083886000	0.500312000
1	2.682946000	2.514099000	1.412915000
1	0.457290000	4.675106000	1.145115000
1	-0.989666000	3.648575000	0.816722000
1	0.195087000	3.113378000	2.038831000
1	0.983534000	-2.290505000	-1.556435000
1	-1.269053000	-1.393344000	1.840602000
1	-0.086295000	-4.668889000	-0.562993000
1	-1.412209000	-3.922963000	1.484809000

NAM^{III}-(H₂O)

Ru	0.477703	0.473973	0.380304
Cl	-1.589728	0.920954	1.352813
Cl	1.695652	0.249291	2.314674
Cl	2.218144	-0.058819	-1.123336
S	0.906110	2.669813	0.204535
C	2.651727	3.074876	0.161516
C	0.397562	3.625958	1.631158
O	0.260558	3.260208	-1.008974
N	-0.001045	-1.542619	0.413122
C	0.854697	-2.595354	0.642336
C	-1.212438	-2.042352	0.260208
C	0.141455	-3.754633	0.624486

N	-1.164117	-3.382902	0.381949
H	3.076756	2.522678	-0.674105
H	2.752256	4.152369	0.029228
H	3.092674	2.730443	1.097477
H	0.643590	4.672473	1.450327
H	-0.674442	3.471280	1.736916
H	0.919055	3.221554	2.499308
H	1.904405	-2.426604	0.801300
H	-2.106825	-1.468933	0.090497
H	0.430363	-4.781698	0.759400
H	-1.952854	-4.003198	0.302839
O	-0.575131	0.714310	-1.480404
H	-0.549630	1.700789	-1.578693
H	0.106384	0.390692	-2.100793

NAMI^{III}-(H₂O)₂-cis

Ru	0.46923236635964	0.52122453254032	0.14676030812667
Cl	-1.73756166309227	0.99540965974816	0.15428287908670
Cl	0.97118448932544	0.54746412765996	2.38728612250499
S	0.88988492519987	2.74096414775230	-0.10936069091011
C	2.50586861031484	3.25817400307303	0.47060674661829
C	-0.17070431111965	3.84358595950224	0.81669637766027
O	0.80410845400442	3.07926642432591	-1.56335237876327
N	-0.00398184902429	-1.51119545529105	0.16843213691494
C	-0.59502664468585	-2.19410563275562	-0.87988055170838
C	0.05506837929563	-2.35167439321295	1.19349350348611
C	-0.88245991011690	-3.46083517322127	-0.47562999039997
N	-0.46154430496166	-3.53742088281891	0.83083941896331
H	3.24294582270213	2.69574926486030	-0.10177758233135
H	2.61326013976316	4.32404973356170	0.26845515163611
H	2.58141121698001	3.03906021477881	1.53636638873946
H	0.12743488742878	4.86600715683718	0.58499411350342
H	-1.18970774391680	3.63895455319457	0.49561191388735
H	-0.05539580987577	3.61203939259849	1.87634791315815
H	-0.80614471451466	-1.71143767738362	-1.81763237078559
H	0.42760071155491	-2.11464878388758	2.17581227627190
H	-1.34320792473286	-4.28945073831781	-0.98423065743679
H	-0.54118965457923	-4.34499504974884	1.43077688199589
O	0.42516420140931	0.52413849615483	-1.96560211647384
H	0.48355888722791	1.50548096397586	-2.17150560663642
H	1.18204779265069	0.10319094652629	-2.40044614787570
O	2.50840835898333	-0.14631049942009	-0.13710484380333

H	3.02113953962862	0.13479726128483	0.64043408084543
H	2.44430402979125	-1.11324985331702	-0.05131728727421

NAM^{III}-(H₂O)₂-trans

Ru	0.53630152713778	0.48182645890397	0.41542735121187
Cl	-1.34983739252989	0.95058116411276	1.68496572570863
Cl	2.45349306885337	-0.03715223182809	-0.74769890403597
S	0.97439852050810	2.72907138186137	0.17488740087922
C	2.70848015252338	3.17365783996104	0.15123497592767
C	0.35598827311096	3.82055656394556	1.45311669540697
O	0.36486418274712	3.16933095602821	-1.11974059973436
N	0.05015095292487	-1.55185430799107	0.44483933213876
C	0.90254502946986	-2.63604572813428	0.31161218542628
C	-1.17698815828539	-2.03774337156074	0.58497997302464
C	0.16963893571086	-3.78104502636354	0.38075514979226
N	-1.13412096028854	-3.37916446535571	0.54807229848730
H	3.18087526854648	2.55930665752206	-0.61157667414282
H	2.76945728358519	4.23451894320597	-0.09236419980938
H	3.13813712969135	2.95765387026933	1.13000256608421
H	0.54875761749728	4.84086700906427	1.12122173834616
H	-0.71045658528163	3.62703846710713	1.54810540204509
H	0.86943150642683	3.60296292078055	2.39003278361774
H	1.95666871741792	-2.50503522836128	0.14106792048409
H	-2.07162449608683	-1.45569815800104	0.72353007647259
H	0.45216370743387	-4.81752989866605	0.31977729881379
H	-1.93504254942628	-3.98812854101643	0.62762033457287
O	-0.46688931876710	0.77383094838685	-1.35504798589065
H	-0.29644146406281	1.74936104046808	-1.56785523433473
H	-0.09491833782938	0.23869842965549	-2.07409959014974
O	1.49263716721254	0.16638152565542	2.27113017493113
H	0.81497517212221	0.42353189015129	2.92584467071899
H	1.60048193763789	-0.79316260080111	2.38757786200737

NAM^{III}-(H₂O)₃

Ru	0.51952444142924	0.49013329972747	0.47068662608838
Cl	2.38613953599897	-0.01926816207050	-0.65295924220379
S	1.00983541395285	2.77217770780391	0.23823832497578
C	2.72359537705987	3.25060700123208	0.03078032417917
C	0.51486806624533	3.79839375401436	1.62256565494694
O	0.25037219067235	3.21612700617176	-0.97264496205652
N	0.00059323937023	-1.53309129679109	0.49025810471202
C	0.87991996411726	-2.58903108500709	0.68456836581507

C	-1.20552759715810	-2.06884657852137	0.30612349836937
C	0.18276191788991	-3.75767094871158	0.62834688442218
N	-1.12031115305117	-3.40421431219753	0.38998095201071
H	3.12817532737272	2.66769701167746	-0.79368614061444
H	2.71718454402576	4.31634688883136	-0.20444985870065
H	3.27044275087552	3.05298341870585	0.95359256968176
H	0.65227423498193	4.83646461301206	1.31641355851185
H	-0.53349157105396	3.59646859172875	1.83459236289916
H	1.13282006328912	3.55538025395000	2.48800209038343
H	1.94084691799290	-2.43882287317848	0.78832259820460
H	-2.11839707394094	-1.53861118334280	0.09164956993568
H	0.49764516818520	-4.78353129426990	0.72085013894882
H	-1.89401881085574	-4.04730178094644	0.27729029724680
O	-0.57319337714052	0.87201612686299	-1.21448282929278
H	-0.36109704768469	1.84352298863170	-1.45564224111620
H	-0.43552913895811	0.29519958693125	-1.98334451230584
O	1.37478695744243	0.11707839101663	2.33137192274012
H	2.30928455616082	0.35157798215699	2.45541305167436
H	1.28723827361340	-0.81914484780099	2.58365183308798
O	-1.30174757793176	0.94951485785394	1.48166067771064
H	-2.00598663901919	1.40231630167035	0.99023472848478
H	-1.72090364088161	0.31132045685888	2.07928652226062

NAMI^{II}

44	0.432828000	0.594747000	-0.094656000
17	-1.909332000	1.022237000	0.527186000
17	1.004558000	0.554709000	2.322604000
17	-0.200482000	0.354521000	-2.425327000
17	2.706239000	-0.108147000	-0.692746000
16	0.938115000	2.727984000	-0.206832000
6	2.599675000	2.987407000	0.480050000
6	0.041212000	3.625321000	1.093772000
8	0.878335000	3.620271000	-1.402709000
7	-0.026899000	-1.414998000	0.091171000
6	0.341014000	-2.455393000	-0.723832000
6	-0.751324000	-1.909586000	1.068439000
6	-0.175849000	-3.617458000	-0.227557000
7	-0.867297000	-3.254814000	0.919113000
1	3.277765000	2.459368000	-0.188665000
1	2.794961000	4.063740000	0.505879000
1	2.624922000	2.519444000	1.465920000
1	0.426252000	4.648491000	1.142804000

1	-1.008119000	3.596921000	0.804061000
1	0.177833000	3.070186000	2.023801000
1	0.944426000	-2.256405000	-1.592303000
1	-1.190656000	-1.321906000	1.856416000
1	-0.122228000	-4.640929000	-0.559927000
1	-1.390859000	-3.866987000	1.518693000

NAMI^{III}-(H₂O)

Ru	0.41496971089848	0.53371053888423	0.03318066421142
Cl	-1.88457591728687	0.99172067543112	0.60446468645821
Cl	1.06436419171600	0.43120226983565	2.34440005513352
Cl	2.53551972609647	-0.09673603289402	-1.01404809525560
S	0.87922321196082	2.63999217272874	-0.11149660530405
C	2.58062684355977	3.04290113348739	0.32503360347075
C	0.04002437480815	3.66021558286788	1.11242586423033
O	0.62928975858318	3.28134119824849	-1.45366543379290
N	-0.06996739548659	-1.49452684042585	0.10685880579966
C	0.35228252405052	-2.55106972095938	-0.66467823261179
C	-0.87002627121431	-1.98254006615300	1.03165986922111
C	-0.21456799037150	-3.70172523734994	-0.20326329843804
N	-0.98632868978760	-3.32208730788766	0.87756647209369
H	3.20353431869562	2.46580540223199	-0.35637665769175
H	2.73975990665114	4.11738224451129	0.21435941288715
H	2.73601363933146	2.69334711142910	1.34712823087293
H	0.36964675579005	4.69592956284474	1.01073470616273
H	-1.02460721452554	3.54299013898848	0.91790867447818
H	0.27773392542669	3.23374757555472	2.08868840949386
H	1.04961326592565	-2.39219508984682	-1.46853529643030
H	-1.36290018277078	-1.39293800005999	1.78552693347928
H	-0.14525039876874	-4.72530763014731	-0.52838142262477
H	-1.54841020723926	-3.92818344992370	1.44926353966822
O	-0.09425036517433	0.65139546338292	-2.07691241856433
H	-0.12079025270440	1.63200706954485	-2.16090672630569
H	0.82168673983592	0.43013253567609	-2.35933395764183

NAMI^{II}-(H₂O)₂-cis

Ru	0.50014721600934	0.55771312357041	0.09871298162497
Cl	-1.81445423262943	1.04820293515237	0.15769479985821
Cl	1.14082161967089	0.48955924478304	2.40447015771960
S	0.97617085721046	2.67342615382737	-0.16556495750919
C	2.63912824264806	3.12790627915809	0.35427260440178
C	0.02511637411771	3.81552607580596	0.84359670817092

O	0.84917787520047	3.12577309981809	-1.59422415399638
N	0.02322981186758	-1.47475967781722	0.14339631423532
C	0.03789803591444	-2.35708529008910	-0.91820988818691
C	-0.40887736876233	-2.14407627039308	1.19502337417122
C	-0.38842339796134	-3.57908338548004	-0.49110886627634
N	-0.66563610135254	-3.42336063034995	0.84780819999279
H	3.32221659369525	2.52571408883145	-0.24272115898865
H	2.79214037932984	4.18967058915420	0.15887287018986
H	2.74448626135386	2.88430708782789	1.41259453942622
H	0.32470854337015	4.83681288266910	0.60715985603169
H	-1.01860573837231	3.62931526747934	0.59604265848381
H	0.20755415846372	3.56251200770374	1.88865773855963
H	0.32889128398201	-2.03433870902705	-1.90310431866278
H	-0.52860552655129	-1.73244979892408	2.18275277516372
H	-0.52278322358206	-4.51672620888636	-1.00089381331502
H	-1.01905860408093	-4.13589363815587	1.46513680490609
O	0.09527740035249	0.55432701965417	-2.00449171127557
H	-0.87893826759749	0.66116710251897	-1.92115261516008
H	0.40339752503483	1.47119942744792	-2.22787248198631
O	2.57692992655300	-0.06829505183158	-0.05923253688019
H	2.69762543313995	-0.01169478781408	0.92217247215443
H	2.52616320497563	-1.02113623763368	-0.23043236385284

NAMI^{II}-(H₂O)₂-trans

Ru	0.53266641338621	0.51659450902823	0.41898044341090
Cl	-1.35548223780927	0.90416270723438	1.87024186229988
Cl	2.39350105475726	-0.06189045389187	-0.96658211435807
S	0.93684047320743	2.66297586696186	0.16943874062867
C	2.67631698183168	3.12064973986514	0.11670317113531
C	0.38819638586239	3.76373266140681	1.48434718626073
O	0.31933572772868	3.20971997234296	-1.08902656575928
N	0.06425762241700	-1.52413650190505	0.46208541924686
C	0.90572637751498	-2.60935649380404	0.31690511638204
C	-1.16080397827146	-1.99985124006082	0.59709497152598
C	0.16954034547021	-3.75485784585570	0.37155500860736
N	-1.13495381565992	-3.34776040716195	0.54704724193492
H	3.12913969621916	2.48970479260979	-0.64562858177314
H	2.75009810586066	4.17931777362670	-0.13434920961637
H	3.12054402185015	2.90151535057107	1.08818423703270
H	0.59648463457402	4.78780455303895	1.17348882274371
H	-0.67922930076062	3.58972185760560	1.60517611687188
H	0.91135497497001	3.51023661896470	2.40670856581777

H	1.95761861396085	-2.46701295796931	0.13809405263036
H	-2.04342643954145	-1.40231555427748	0.74885223626476
H	0.44337976984284	-4.79240173142109	0.29499339357272
H	-1.93985365256324	-3.94889963897856	0.61290111372658
O	-0.42918299633854	0.68079157637491	-1.45390094031837
H	-0.39622234022289	1.66676794156136	-1.58742796017718
H	0.29971720094926	0.34637264379982	-2.01667679374375
O	1.44647318571629	0.29512795380388	2.35307006021209
H	0.59052296735379	0.45380717360288	2.82322955458019
H	1.61056709569454	-0.65390435807317	2.46191357886075

NAM^{III}-(H₂O)₃

Ru	0.59582637876627	0.52717905476412	0.42175910409311
Cl	-1.27685759220248	0.89368630761885	1.77516700064422
S	0.89609507306813	2.73106016530382	0.22012344912468
C	2.59962122075305	3.28015321694093	0.01026359707433
C	0.42211366636088	3.77034620684604	1.60518139045450
O	0.14991222107509	3.23859265972808	-0.97932322129042
N	0.14828222771891	-1.51084654005229	0.42790929758025
C	0.96341836531098	-2.62509105610457	0.54155735745634
C	-1.09190498903006	-1.96160455408879	0.31125864084313
C	0.19720322131232	-3.75197565633271	0.48999922571183
N	-1.09262039485427	-3.30768259587649	0.34439259977393
H	2.97159200395373	2.81376944148295	-0.90161524933083
H	2.60345368466455	4.36437252783860	-0.10494540951597
H	3.18815234569840	2.97517792938485	0.87634509778950
H	0.52453346490507	4.80752918913107	1.28624479061594
H	-0.61050810534916	3.52218439944998	1.84317248177311
H	1.06888138068721	3.54928887862437	2.45525980293368
H	2.03039046192083	-2.55341735766639	0.68034569413752
H	-1.97061232641010	-1.34598339501502	0.22269783910689
H	0.44869035693119	-4.79662958049805	0.54778718390291
H	-1.91366213902673	-3.89052203146686	0.27526391517695
O	-0.48899462660836	0.75022118230498	-1.36512828190680
H	-0.52296310993501	1.75007607930042	-1.44594489136895
H	-0.00161975332057	0.45432958906531	-2.14879150313458
O	1.53377945776106	0.27167027642675	2.32522936370037
H	0.76812795659338	0.61052248259049	2.84676175809932
H	1.53151593349599	-0.67631235321366	2.53522863255150
O	2.27455069922676	-0.00416863440625	-0.85749687000402
H	3.16639152897345	0.22595219328885	-0.56103747987685
H	2.27511375255946	-0.96257931636937	-1.00127639611559

KP1019^{III}

44	0.888781000	-1.318675000	-0.781652000
17	-1.351449000	-1.257895000	-0.098671000
6	1.160852000	1.497617000	0.455694000
6	1.174261000	2.851616000	0.043273000
1	1.248491000	1.051396000	1.431752000
6	1.024534000	2.807105000	-1.367829000
1	0.754233000	1.003079000	-2.572076000
6	1.286143000	4.093938000	0.684826000
6	0.984288000	3.968865000	-2.148325000
6	1.244504000	5.241969000	-0.082879000
1	1.401682000	4.150057000	1.761477000
6	1.096109000	5.176772000	-1.484580000
1	0.867569000	3.922988000	-3.224541000
1	1.327686000	6.212212000	0.394012000
1	1.066194000	6.098641000	-2.055177000
6	0.175407000	-4.111106000	-1.872418000
6	1.115089000	-5.455215000	-0.333085000
6	0.357032000	-5.473151000	-1.533458000
1	-0.332808000	-3.646499000	-2.700164000
6	1.494209000	-6.631359000	0.324315000
6	-0.029601000	-6.703316000	-2.084927000
6	1.096605000	-7.826595000	-0.245760000
1	2.074394000	-6.605824000	1.238878000
6	0.341296000	-7.865795000	-1.436732000
1	-0.610359000	-6.739281000	-2.999745000
1	1.372578000	-8.758821000	0.235148000
1	0.049137000	-8.826613000	-1.845895000
7	1.015621000	0.714692000	-0.598898000
7	0.763631000	-3.347999000	-0.967783000
7	0.943536000	1.497061000	-1.697155000
7	1.338073000	-4.151667000	-0.046763000
1	1.742616000	-3.670861000	0.758620000
17	3.135449000	-1.378337000	-1.470874000
17	0.223486000	-1.061217000	-3.060870000
17	1.595787000	-1.587227000	1.484047000

KP1019^{III}-(H₂O)

44	0.938489000	-1.345771000	-0.773282000
17	-1.257585000	-1.241548000	-0.247593000
6	1.214193000	1.492841000	0.445647000

6	1.167740000	2.849947000	0.049108000
1	1.326497000	1.049419000	1.420545000
6	0.995128000	2.818129000	-1.355598000
1	0.783152000	1.041445000	-2.590119000
6	1.250235000	4.086598000	0.710412000
6	0.906993000	3.985285000	-2.125240000
6	1.159741000	5.237301000	-0.043491000
1	1.378599000	4.132566000	1.785221000
6	0.992636000	5.183556000	-1.445188000
1	0.772412000	3.951104000	-3.199299000
1	1.217681000	6.204373000	0.441235000
1	0.925180000	6.111246000	-2.001465000
6	0.195537000	-4.133096000	-1.847184000
6	1.065245000	-5.504938000	-0.295345000
6	0.322702000	-5.498075000	-1.501120000
1	-0.292946000	-3.664129000	-2.684088000
6	1.399670000	-6.691280000	0.369211000
6	-0.096168000	-6.713681000	-2.065260000
6	0.971594000	-7.868314000	-0.210722000
1	1.966788000	-6.686599000	1.291682000
6	0.231071000	-7.883460000	-1.413270000
1	-0.664424000	-6.729263000	-2.987547000
1	1.209727000	-8.809449000	0.271162000
1	-0.082161000	-8.834884000	-1.826080000
7	1.087317000	0.707944000	-0.614292000
7	0.807753000	-3.383991000	-0.944378000
7	0.954957000	1.506985000	-1.702806000
7	1.332855000	-4.207212000	-0.006564000
1	1.764917000	-3.761375000	0.797474000
17	0.724149000	-1.145313000	-3.128725000
17	1.789730000	-1.565944000	1.391971000
8	3.033544000	-1.486200000	-1.349216000
1	2.949305000	-1.384738000	-2.317474000
1	3.488775000	-0.695642000	-1.023265000

KP1019^{III}-(H₂O)₂-cis

44	0.861988000	-1.322142000	-0.764124000
17	-0.204649000	-1.486681000	1.229123000
6	0.936386000	1.523690000	0.420771000
6	1.037219000	2.874528000	0.021092000
1	0.870796000	1.090710000	1.405319000
6	1.075779000	2.844126000	-1.391833000

1	1.085619000	1.104622000	-2.655886000
6	1.105700000	4.106184000	0.696160000
6	1.178226000	4.005022000	-2.165527000
6	1.208712000	5.251219000	-0.061290000
1	1.080289000	4.148414000	1.777853000
6	1.243123000	5.197803000	-1.473182000
1	1.207094000	3.976141000	-3.247519000
1	1.266054000	6.215738000	0.427092000
1	1.325704000	6.123566000	-2.029626000
6	0.113163000	-4.134176000	-1.796516000
6	1.176200000	-5.487577000	-0.361066000
6	0.313823000	-5.494503000	-1.484666000
1	-0.489901000	-3.688543000	-2.572391000
6	1.614261000	-6.665545000	0.256316000
6	-0.134785000	-6.718133000	-2.015327000
6	1.155710000	-7.846601000	-0.287235000
1	2.271716000	-6.652152000	1.115926000
6	0.292394000	-7.876087000	-1.407777000
1	-0.797445000	-6.746126000	-2.871363000
1	1.464856000	-8.784399000	0.158246000
1	-0.037111000	-8.834539000	-1.788923000
7	0.912562000	0.731761000	-0.640502000
7	0.784578000	-3.364035000	-0.941008000
7	0.986483000	1.528781000	-1.747572000
7	1.423601000	-4.180476000	-0.077193000
8	-1.060809000	-1.266222000	-1.688867000
1	-1.411823000	-0.362426000	-1.637925000
1	-1.659196000	-1.806736000	-1.143134000
1	2.031242000	-3.764062000	0.614191000
8	1.630208000	-1.082459000	-2.764212000
1	1.511453000	-1.886076000	-3.296148000
17	3.053780000	-1.435810000	-0.157087000
1	2.591377000	-1.024247000	-2.592606000

KP1019^{III}-(H₂O)₂-trans

44	0.904697000	-1.354817000	-0.824269000
17	0.904945000	-1.515437000	1.530119000
6	1.033019000	1.503324000	0.358075000
6	1.075675000	2.850272000	-0.043280000
1	1.034570000	1.068783000	1.344118000
6	1.044562000	2.818909000	-1.460156000
1	0.960497000	1.045538000	-2.718790000

6	1.138880000	4.085033000	0.632364000
6	1.075163000	3.986885000	-2.234278000
6	1.168874000	5.230635000	-0.126190000
1	1.164030000	4.125989000	1.714246000
6	1.137320000	5.177568000	-1.541489000
1	1.050899000	3.959418000	-3.316043000
1	1.218612000	6.197092000	0.359354000
1	1.162970000	6.107015000	-2.097427000
6	0.758756000	-4.186842000	-2.011523000
6	0.748886000	-5.509623000	-0.197903000
6	0.707645000	-5.534787000	-1.614137000
1	0.752654000	-3.747046000	-2.994496000
6	0.712256000	-6.677675000	0.573484000
6	0.627768000	-6.766933000	-2.292002000
6	0.633335000	-7.866491000	-0.121829000
1	0.743858000	-6.652913000	1.655255000
6	0.591666000	-7.914816000	-1.536564000
1	0.594197000	-6.803851000	-3.373684000
1	0.601833000	-8.796827000	0.432333000
1	0.528901000	-8.879179000	-2.024517000
7	0.980500000	0.707840000	-0.712826000
7	0.825554000	-3.399743000	-0.938373000
7	0.985692000	1.507819000	-1.813331000
7	0.822949000	-4.200872000	0.158874000
17	0.906917000	-1.160948000	-3.153544000
8	2.965148000	-1.442597000	-0.787811000
1	3.401551000	-0.664131000	-1.167295000
1	3.277767000	-1.548724000	0.127299000
8	-1.159016000	-1.333874000	-0.782853000
1	-1.473360000	-1.420388000	0.133728000
1	-1.563222000	-0.540756000	-1.167500000
1	0.852619000	-3.753227000	1.067967000

KP1019^{III}-(H₂O)₃

44	0.979356000	-1.314286000	-0.801056000
17	0.940054000	-1.469706000	1.503020000
6	1.062252000	1.536843000	0.372015000
6	1.113037000	2.873693000	-0.035080000
1	1.034842000	1.110020000	1.361494000
6	1.128050000	2.839068000	-1.455411000
1	1.085826000	1.099321000	-2.721448000
6	1.149968000	4.113649000	0.644408000

6	1.176594000	3.998420000	-2.230936000
6	1.198287000	5.253885000	-0.117065000
1	1.140476000	4.154759000	1.726124000
6	1.210759000	5.193422000	-1.534226000
1	1.188233000	3.975371000	-3.312996000
1	1.228175000	6.223610000	0.362754000
1	1.249560000	6.121126000	-2.092538000
6	0.882281000	-4.142795000	-1.996841000
6	0.810959000	-5.469446000	-0.197674000
6	0.820581000	-5.484493000	-1.620903000
1	0.908513000	-3.721576000	-2.987376000
6	0.751849000	-6.640553000	0.560078000
6	0.767758000	-6.714272000	-2.319886000
6	0.701720000	-7.823386000	-0.154733000
1	0.743787000	-6.630646000	1.642134000
6	0.709116000	-7.863108000	-1.575119000
1	0.772798000	-6.741608000	-3.402147000
1	0.653570000	-8.759368000	0.388643000
1	0.666399000	-8.825637000	-2.068331000
7	1.048221000	0.719352000	-0.698945000
7	0.908212000	-3.344302000	-0.909182000
7	1.088047000	1.520155000	-1.805676000
7	0.866432000	-4.161653000	0.173749000
8	-1.096857000	-1.265533000	-0.855958000
1	-1.433728000	-0.357315000	-0.780224000
1	-1.482627000	-1.752516000	-0.105319000
1	0.872966000	-3.727042000	1.091919000
8	1.027732000	-1.079917000	-2.976400000
1	0.252712000	-1.384734000	-3.474861000
1	1.809036000	-1.429434000	-3.434359000
8	3.057480000	-1.388831000	-0.813907000
1	3.440259000	-0.506017000	-0.678600000
1	3.400221000	-1.938956000	-0.086755000

KP1019^{II}

44	0.882746000	-1.318939000	-0.779623000
17	-1.434638000	-1.257932000	-0.076079000
6	1.068158000	1.469223000	0.476999000
6	1.118195000	2.816347000	0.058926000
1	1.070314000	1.022937000	1.457210000
6	1.088641000	2.762546000	-1.368191000
1	0.877235000	0.935580000	-2.566779000

6	1.174664000	4.068872000	0.690097000
6	1.107932000	3.919039000	-2.152471000
6	1.192981000	5.217264000	-0.089182000
1	1.198615000	4.137325000	1.773163000
6	1.158924000	5.143470000	-1.494081000
1	1.080387000	3.862433000	-3.235116000
1	1.233241000	6.191382000	0.389597000
1	1.169746000	6.060217000	-2.076017000
6	0.090545000	-4.076196000	-1.832494000
6	1.167351000	-5.413643000	-0.372726000
6	0.305400000	-5.433427000	-1.511829000
1	-0.487045000	-3.606799000	-2.610739000
6	1.598435000	-6.587689000	0.249672000
6	-0.118756000	-6.670808000	-2.020792000
6	1.156197000	-7.796066000	-0.278884000
1	2.252136000	-6.556311000	1.114245000
6	0.308634000	-7.837068000	-1.401319000
1	-0.775542000	-6.713807000	-2.883816000
1	1.472874000	-8.725824000	0.184509000
1	-0.017675000	-8.799293000	-1.785772000
7	1.014057000	0.669272000	-0.584668000
7	0.755639000	-3.301235000	-0.979195000
7	1.047535000	1.451529000	-1.692660000
7	1.418537000	-4.111301000	-0.114946000
1	1.835708000	-3.611137000	0.680083000
17	3.203093000	-1.386723000	-1.489766000
17	0.206658000	-1.018481000	-3.118604000
17	1.614129000	-1.634204000	1.543035000

KP1019^{II}-(H₂O)

44	0.959094000	-1.349090000	-0.797943000
17	-1.314663000	-1.244874000	-0.165808000
6	1.191099000	1.444083000	0.458132000
6	1.161354000	2.803889000	0.068584000
1	1.260777000	0.984421000	1.429806000
6	1.044514000	2.781863000	-1.347343000
1	0.834179000	0.993179000	-2.584551000
6	1.214093000	4.039112000	0.732415000
6	0.982429000	3.954247000	-2.107001000
6	1.148013000	5.200887000	-0.016932000
1	1.298258000	4.080913000	1.812669000
6	1.034762000	5.157411000	-1.420331000

1	0.887844000	3.924236000	-3.186257000
1	1.182510000	6.164125000	0.480305000
1	0.981449000	6.087222000	-1.976321000
6	0.208580000	-4.117953000	-1.877561000
6	1.068354000	-5.463096000	-0.291757000
6	0.336210000	-5.477605000	-1.510330000
1	-0.272270000	-3.654579000	-2.721997000
6	1.396006000	-6.638809000	0.391009000
6	-0.068807000	-6.706131000	-2.052178000
6	0.979285000	-7.834433000	-0.170359000
1	1.952342000	-6.614446000	1.320613000
6	0.254026000	-7.870252000	-1.377918000
1	-0.628564000	-6.741121000	-2.980285000
1	1.215606000	-8.765809000	0.332999000
1	-0.054589000	-8.828348000	-1.781970000
7	1.105250000	0.661104000	-0.612642000
7	0.810174000	-3.350830000	-0.977663000
7	1.031463000	1.474057000	-1.704043000
7	1.333478000	-4.163045000	-0.025388000
1	1.715422000	-3.671284000	0.788895000
17	0.659354000	-1.092086000	-3.220621000
17	1.791534000	-1.609802000	1.461770000
8	3.033609000	-1.474147000	-1.495199000
1	2.765945000	-1.304623000	-2.426878000
1	3.432910000	-0.654550000	-1.172865000

KP1019^{II}-(H₂O)₂-cis

44	0.798735000	-1.295357000	-0.816784000
17	-0.269895000	-1.460559000	1.283460000
6	0.974064000	1.525555000	0.406444000
6	1.076775000	2.877510000	-0.003964000
1	0.932897000	1.088998000	1.390275000
6	1.074939000	2.837645000	-1.419583000
1	0.997998000	1.074387000	-2.657925000
6	1.180167000	4.114258000	0.651094000
6	1.168622000	3.993630000	-2.201070000
6	1.272927000	5.258222000	-0.116192000
1	1.188959000	4.166767000	1.733299000
6	1.265415000	5.196149000	-1.525224000
1	1.164113000	3.953245000	-3.283681000
1	1.354768000	6.224579000	0.366749000
1	1.340057000	6.115995000	-2.093478000

6	0.137296000	-4.094213000	-1.922235000
6	1.085900000	-5.409987000	-0.371225000
6	0.339377000	-5.451094000	-1.575844000
1	-0.376714000	-3.671443000	-2.772481000
6	1.493467000	-6.569680000	0.294895000
6	-0.017646000	-6.693047000	-2.123942000
6	1.128675000	-7.775895000	-0.272317000
1	2.065229000	-6.524909000	1.213296000
6	0.379658000	-7.839191000	-1.465658000
1	-0.593361000	-6.750948000	-3.040186000
1	1.424964000	-8.698179000	0.213250000
1	0.112459000	-8.808570000	-1.869084000
7	0.908730000	0.733302000	-0.650282000
7	0.700137000	-3.297409000	-1.011141000
7	0.965261000	1.523900000	-1.756940000
7	1.262657000	-4.094799000	-0.078770000
8	-1.273175000	-1.119273000	-1.413157000
1	-1.558910000	-1.033946000	-0.468815000
1	-1.567865000	-2.010610000	-1.654043000
1	1.791069000	-3.633162000	0.649951000
8	1.735216000	-1.091326000	-2.766763000
1	1.631661000	-1.933028000	-3.234613000
17	3.089492000	-1.460959000	-0.239598000
1	2.630259000	-1.154012000	-2.336136000

KP1019^{II}-(H₂O)₂-trans

44	0.896404000	-1.315196000	-0.794108000
17	0.333047000	-1.492639000	1.539512000
6	1.111834000	1.507367000	0.444382000
6	1.142679000	2.861175000	0.035175000
1	1.117405000	1.068131000	1.428498000
6	1.058829000	2.821689000	-1.379228000
1	1.007109000	1.027430000	-2.614547000
6	1.226236000	4.099908000	0.691037000
6	1.057453000	3.985090000	-2.158062000
6	1.224391000	5.247832000	-0.074484000
1	1.289498000	4.150705000	1.771697000
6	1.140848000	5.187767000	-1.482220000
1	0.986970000	3.946324000	-3.238134000
1	1.286708000	6.216035000	0.407770000
1	1.139031000	6.111960000	-2.048287000
6	0.679000000	-4.137983000	-2.032518000

6	0.730848000	-5.452211000	-0.208829000
6	0.646554000	-5.491731000	-1.623190000
1	0.673798000	-3.698885000	-3.016696000
6	0.730921000	-6.615526000	0.570162000
6	0.560913000	-6.730433000	-2.278867000
6	0.645596000	-7.818156000	-0.105502000
1	0.801623000	-6.576693000	1.650218000
6	0.561420000	-7.878254000	-1.513187000
1	0.496920000	-6.781326000	-3.359477000
1	0.646290000	-8.742293000	0.460663000
1	0.497418000	-8.846407000	-1.995325000
7	1.014867000	0.713471000	-0.617674000
7	0.777288000	-3.344077000	-0.970588000
7	0.977893000	1.509021000	-1.717880000
7	0.813586000	-4.139608000	0.129669000
17	1.460626000	-1.138582000	-3.127658000
8	3.005003000	-1.462163000	-0.621739000
1	3.197384000	-1.410605000	-1.584190000
1	3.315781000	-0.622566000	-0.251069000
8	-1.212336000	-1.169308000	-0.965813000
1	-1.404907000	-1.222257000	-0.003448000
1	-1.520872000	-2.009417000	-1.337310000
1	0.785511000	-3.657970000	1.026357000

KP1019^{II}-(H₂O)₃

44	0.951105000	-1.298097000	-0.833758000
17	0.881626000	-1.494586000	1.505488000
6	1.046420000	1.551290000	0.385047000
6	1.116393000	2.903248000	-0.021909000
1	1.009698000	1.117499000	1.371273000
6	1.136739000	2.866700000	-1.435610000
1	1.080423000	1.115338000	-2.690010000
6	1.168648000	4.139754000	0.645327000
6	1.205861000	4.026890000	-2.214733000
6	1.237273000	5.284199000	-0.118430000
1	1.155617000	4.187508000	1.727209000
6	1.255089000	5.225229000	-1.529847000
1	1.221903000	3.993253000	-3.296978000
1	1.279440000	6.251819000	0.365569000
1	1.310551000	6.149820000	-2.091628000
6	0.872580000	-4.164806000	-2.048335000
6	0.804698000	-5.472831000	-0.232934000

6	0.822911000	-5.516765000	-1.647526000
1	0.900521000	-3.762506000	-3.047853000
6	0.756095000	-6.633305000	0.549762000
6	0.790563000	-6.755963000	-2.311103000
6	0.726118000	-7.833606000	-0.130568000
1	0.741717000	-6.593300000	1.631497000
6	0.742730000	-7.897594000	-1.542900000
1	0.802839000	-6.810030000	-3.392977000
1	0.687687000	-8.757415000	0.433763000
1	0.716780000	-8.867708000	-2.023261000
7	1.027215000	0.745900000	-0.674985000
7	0.883408000	-3.357476000	-0.989351000
7	1.080310000	1.548151000	-1.780423000
7	0.842091000	-4.155916000	0.109180000
8	-1.157932000	-1.211886000	-0.928911000
1	-1.419819000	-0.350483000	-0.566475000
1	-1.508990000	-1.864952000	-0.301744000
1	0.840422000	-3.683045000	1.011262000
8	1.019169000	-1.049925000	-2.996408000
1	0.242682000	-1.417905000	-3.444239000
1	1.795567000	-1.469101000	-3.397185000
8	3.061883000	-1.350222000	-0.826824000
1	3.361970000	-0.510933000	-0.442389000
1	3.342906000	-2.030680000	-0.193698000

KP1019-Cys

44	0.796024000	-1.510479000	-1.084448000
17	-0.442654000	-1.650397000	1.008572000
6	-0.303154000	1.328086000	-0.800456000
6	0.181487000	2.654220000	-0.756857000
6	1.591897000	2.541429000	-0.928917000
6	-0.384169000	3.927035000	-0.590624000
6	2.429052000	3.659997000	-0.937866000
6	0.445262000	5.036911000	-0.598703000
6	1.836243000	4.904029000	-0.768959000
6	0.033311000	-4.487781000	-1.249515000
6	2.027755000	-5.457471000	-0.857713000
6	0.656427000	-5.749075000	-1.112345000
6	2.975408000	-6.463063000	-0.650619000
6	0.242908000	-7.089662000	-1.150879000
6	2.532737000	-7.778401000	-0.699424000
6	1.182424000	-8.088529000	-0.946551000

7	0.705507000	0.485197000	-0.991364000
7	0.932518000	-3.519931000	-1.101149000
7	1.844415000	1.220606000	-1.082614000
7	2.137136000	-4.109929000	-0.886911000
17	2.918191000	-1.411576000	0.151318000
16	2.248060000	-1.411598000	-3.025020000
6	1.761113000	-0.200819000	-4.319970000
6	0.384037000	-0.456154000	-4.973130000
6	0.323262000	-0.115032000	-6.503205000
7	0.021380000	-1.898222000	-4.850379000
8	-0.019787000	-1.089127000	-7.243365000
8	0.612704000	1.049200000	-6.821979000
1	-1.298157000	0.928760000	-0.701940000
1	2.703573000	0.677793000	-1.114042000
1	-1.455436000	4.037988000	-0.459445000
1	3.499324000	3.559716000	-1.078079000
1	0.018814000	6.027357000	-0.475242000
1	2.458370000	5.793255000	-0.775060000
1	-0.991473000	-4.213584000	-1.436822000
1	4.014722000	-6.223411000	-0.456263000
1	-0.796764000	-7.340366000	-1.334292000
1	3.242254000	-8.584401000	-0.540651000
1	0.874432000	-9.129241000	-0.972731000
1	2.873812000	-3.461408000	-0.589577000
1	2.543760000	-0.258086000	-5.081379000
1	1.768497000	0.814538000	-3.924579000
1	-0.377685000	0.109080000	-4.438079000
1	0.847339000	-2.374412000	-4.422953000
1	-0.743745000	-2.009519000	-4.154703000
17	-1.392553000	-1.645467000	-2.183501000
1	-0.187859000	-2.150777000	-5.845516000

KP1019-GSH

44	1.355393000	-1.736818000	-1.986591000
17	1.281784000	-0.452104000	0.073318000
17	1.411905000	-3.045431000	-4.061570000
17	3.715671000	-1.097440000	-2.286967000
6	1.491861000	0.719448000	-3.832007000
6	-0.670182000	1.341000000	-3.932390000
6	0.627340000	1.670608000	-4.421117000
1	2.557963000	0.570161000	-3.897416000
6	-1.810876000	2.058424000	-4.303424000

6	0.763210000	2.752566000	-5.305588000
6	-1.640524000	3.118354000	-5.182879000
1	-2.786766000	1.800168000	-3.908540000
6	-0.367940000	3.462057000	-5.678912000
1	1.739586000	3.031669000	-5.689713000
1	-2.505156000	3.699034000	-5.488643000
1	-0.275372000	4.303904000	-6.358673000
6	2.579855000	-3.543493000	0.159661000
6	2.836863000	-4.917080000	0.357526000
1	2.812924000	-2.680564000	0.759867000
6	2.296183000	-5.564564000	-0.794253000
6	3.465808000	-5.699106000	1.339600000
6	2.376842000	-6.946457000	-0.975557000
6	3.549725000	-7.072996000	1.157771000
1	3.884571000	-5.234911000	2.226664000
6	3.013330000	-7.690700000	0.013286000
1	1.958622000	-7.420152000	-1.856995000
1	4.036090000	-7.685705000	1.911436000
1	3.099031000	-8.767185000	-0.103188000
7	1.939438000	-3.363532000	-0.996144000
7	1.743528000	-4.589445000	-1.549982000
7	-0.505630000	0.280637000	-3.110136000
7	0.791251000	-0.107333000	-3.062062000
1	-1.148644000	-0.378234000	-2.629746000
1	1.431514000	-4.549330000	-2.529396000
6	-2.684671000	3.612578000	2.549744000
6	-3.024486000	5.047213000	1.989819000
8	-2.058989000	5.766482000	1.685478000
6	-1.502909000	2.870371000	1.924973000
6	-1.677550000	2.283514000	0.505109000
6	-2.536259000	1.025663000	0.440507000
8	-3.782510000	1.095954000	0.405628000
8	-4.261801000	5.314198000	1.992420000
7	-3.961984000	2.833739000	2.540924000
7	-1.882060000	-0.144358000	0.465832000
6	-2.544306000	-1.441040000	0.352266000
6	-3.299668000	-1.914065000	1.617339000
8	-3.999481000	-2.927547000	1.545344000
6	-1.514581000	-2.502458000	-0.079792000
16	-0.950067000	-2.382799000	-1.824419000
7	-3.152408000	-1.202645000	2.754136000
6	-3.955107000	-1.436221000	3.943089000

6	-4.266271000	-0.138411000	4.736468000
8	-5.072144000	-0.259622000	5.673860000
8	-3.647502000	0.911485000	4.367291000
1	-2.442390000	3.771490000	3.605308000
1	-1.177149000	2.072002000	2.599370000
1	-0.699866000	3.609428000	1.881850000
1	-0.682355000	2.052030000	0.117525000
1	-2.136188000	3.028154000	-0.150220000
1	-4.011011000	2.143999000	3.337257000
1	-4.057716000	2.291662000	1.654920000
1	-0.852012000	-0.153694000	0.378844000
1	-3.322385000	-1.368925000	-0.412749000
1	-0.639927000	-2.448422000	0.572832000
1	-1.991374000	-3.474289000	0.049426000
1	-2.681705000	-0.307678000	2.731826000
1	-4.889448000	-1.914760000	3.645893000
1	-3.446964000	-2.128877000	4.625688000
1	-4.666405000	3.598009000	2.543025000

KP1019-GN3

44	0.144509000	-0.618125000	0.028840000
17	0.196811000	-1.037663000	-2.370141000
6	-2.814366000	-0.086609000	-0.663697000
6	-4.069349000	-0.728249000	-0.553192000
6	-3.798746000	-1.939482000	0.136701000
6	-5.382842000	-0.441515000	-0.953215000
6	-4.803599000	-2.867001000	0.431149000
6	-6.377781000	-1.356081000	-0.660903000
6	-6.088709000	-2.555530000	0.021757000
7	-1.871482000	-0.827865000	-0.096938000
7	-2.470361000	-1.933927000	0.407686000
6	2.999499000	0.389105000	0.599716000
6	4.221452000	-1.352687000	-0.123656000
6	4.332201000	-0.060746000	0.456202000
6	5.341216000	-2.140708000	-0.405710000
6	5.605245000	0.455013000	0.742644000
6	6.582296000	-1.603548000	-0.108160000
6	6.714954000	-0.319273000	0.456649000
7	2.158652000	-0.527404000	0.138859000
7	2.897374000	-1.570819000	-0.310985000
17	0.095126000	-0.416682000	2.445895000
1	-2.553648000	0.844282000	-1.136267000

1	-1.825729000	-2.665733000	0.713564000
1	-5.611780000	0.478460000	-1.479155000
1	-4.584721000	-3.789542000	0.955288000
1	-7.399558000	-1.151260000	-0.961129000
1	-6.893691000	-3.251360000	0.231878000
1	2.367474000	-2.410847000	-0.535673000
1	2.613481000	1.303754000	1.015456000
1	5.240843000	-3.126827000	-0.843396000
1	5.716233000	1.440429000	1.181466000
1	7.474299000	-2.184738000	-0.314697000
1	7.706715000	0.063248000	0.671098000
17	0.320337000	-3.013368000	0.325752000
7	0.418945000	3.584127000	-1.321568000
6	0.604092000	2.232846000	-1.183406000
7	1.485873000	1.651902000	-2.031116000
6	-0.819604000	2.318951000	0.545657000
6	-1.089681000	3.686529000	0.433771000
6	-0.424839000	4.451616000	-0.570087000
8	-0.454858000	5.640623000	-0.852014000
7	-1.962400000	4.091188000	1.422571000
6	-2.193751000	2.997092000	2.104522000
7	-1.544351000	1.895544000	1.611055000
7	-0.015840000	1.525021000	-0.239956000
1	0.942400000	4.061388000	-2.042635000
1	1.663525000	2.160630000	-2.884730000
1	1.292503000	0.643833000	-2.187388000
1	-2.831112000	2.929134000	2.972925000
1	-1.346423000	0.986089000	2.067243000

KP1019-GN7

44	-1.669717000	-0.615248000	0.242534000
6	-2.512700000	0.919843000	2.775811000
6	-2.405701000	0.787782000	4.179321000
6	-1.669675000	-0.412231000	4.379479000
6	-2.821218000	1.529588000	5.295137000
6	-1.334015000	-0.873637000	5.656023000
6	-2.491049000	1.074229000	6.558908000
6	-1.752086000	-0.113939000	6.735145000
7	-1.902241000	-0.099252000	2.186303000
7	-1.424103000	-0.915280000	3.149136000
17	-3.449377000	-2.215866000	0.476454000
6	-0.478483000	-1.367187000	-2.488521000

6	-2.338541000	-1.967224000	-3.599098000
6	-0.928472000	-1.842832000	-3.741375000
6	-3.150986000	-2.413046000	-4.645279000
6	-0.329024000	-2.175553000	-4.965356000
6	-2.529002000	-2.727104000	-5.843436000
6	-1.134076000	-2.611135000	-6.003170000
7	-1.512723000	-1.208450000	-1.666505000
7	-2.634357000	-1.550603000	-2.343639000
1	-3.004168000	1.656199000	2.161105000
1	-0.799044000	-1.652445000	2.809180000
1	-3.388261000	2.445595000	5.168087000
1	-0.764068000	-1.784930000	5.792155000
1	-2.805390000	1.635721000	7.432291000
1	-1.504955000	-0.440961000	7.739733000
1	-3.454913000	-1.679040000	-1.744551000
1	0.519078000	-1.183705000	-2.127614000
1	-4.223917000	-2.503893000	-4.524276000
1	0.744902000	-2.093426000	-5.095414000
1	-3.129772000	-3.072927000	-6.677650000
1	-0.687701000	-2.871736000	-6.956827000
17	-3.275464000	1.062990000	-0.436921000
17	0.019716000	-2.245883000	0.840859000
7	3.006016000	1.328309000	1.776558000
6	3.557490000	2.183753000	0.877244000
7	4.860028000	2.596817000	1.109698000
6	1.718831000	2.002825000	-0.339051000
6	1.055121000	1.097204000	0.489874000
6	1.675290000	0.761930000	1.743493000
8	1.304406000	0.162550000	2.728936000
7	-0.174344000	0.769317000	-0.084536000
6	-0.252669000	1.488080000	-1.188650000
7	0.872411000	2.243762000	-1.378555000
7	2.939439000	2.582956000	-0.201148000
1	3.526426000	1.045720000	2.596464000
1	5.098560000	2.775909000	2.075521000
1	5.120074000	3.356996000	0.496528000
1	-1.115327000	1.508163000	-1.832352000
1	1.057313000	2.861220000	-2.151622000

NAMI-Cys

44	0.359239000	0.571026000	-0.120135000
16	-1.681657000	1.359952000	-1.203776000

6	-2.977823000	0.075103000	-1.402382000
6	-3.984968000	0.076102000	-0.241176000
6	-4.956290000	-1.153178000	-0.199352000
7	-3.191202000	0.004235000	1.025720000
8	-5.919793000	-1.130187000	-0.983895000
8	-4.629460000	-2.041901000	0.647935000
17	-0.503611000	0.986495000	2.225616000
17	2.417935000	-0.292774000	0.936168000
16	1.118835000	2.650962000	-0.187269000
6	2.211491000	2.932177000	1.233068000
6	-0.164043000	3.832980000	0.318757000
8	1.800804000	3.313320000	-1.333652000
7	-0.237885000	-1.426731000	0.037459000
6	-0.444341000	-2.357141000	-0.953696000
6	-0.312661000	-2.062050000	1.189140000
6	-0.669267000	-3.576479000	-0.386057000
7	-0.582037000	-3.372460000	0.977088000
1	-2.528357000	-0.916070000	-1.496997000
1	-3.531603000	0.275499000	-2.320786000
1	-4.546659000	1.009771000	-0.252544000
1	-3.314054000	-1.005332000	1.280991000
1	-3.564763000	0.583482000	1.770797000
1	3.076983000	2.292328000	1.072939000
1	2.477986000	3.992821000	1.249653000
1	1.686505000	2.611001000	2.133510000
1	0.304235000	4.818147000	0.390339000
1	-0.929361000	3.807520000	-0.456322000
1	-0.589601000	3.493809000	1.263789000
1	-0.359779000	-2.057401000	-1.984507000
1	-0.161859000	-1.597794000	2.149578000
1	-0.897008000	-4.541164000	-0.805262000
1	-0.734613000	-4.060056000	1.693317000
17	1.196815000	-0.005338000	-2.300943000
1	-2.203174000	0.322193000	0.883315000

NAMI-GSH

6	-2.675220000	3.434254000	2.334334000
6	-2.909674000	4.817521000	1.691884000
8	-2.038488000	5.548679000	1.270247000
6	-1.540888000	2.651404000	1.660889000
6	-1.855124000	2.085963000	0.258685000
6	-2.676379000	0.799752000	0.269899000

8	-3.903069000	0.794766000	0.123752000
8	-4.206140000	5.151034000	1.700547000
7	-3.980817000	2.771638000	2.465694000
7	-1.950717000	-0.320725000	0.487024000
6	-2.508613000	-1.665483000	0.450171000
6	-3.070244000	-2.180454000	1.799731000
8	-3.622111000	-3.282577000	1.835237000
6	-1.439917000	-2.635172000	-0.075648000
16	-1.030003000	-2.238423000	-1.811200000
7	-2.913534000	-1.372054000	2.856178000
6	-3.473333000	-1.593666000	4.177566000
6	-3.543960000	-0.256499000	4.976646000
8	-3.978358000	-0.353548000	6.136975000
8	-3.146891000	0.777861000	4.358041000
44	1.140277000	-1.723336000	-2.184903000
17	1.326856000	-0.426803000	-0.153303000
16	1.988021000	-3.533580000	-1.107273000
6	3.362774000	-3.025244000	-0.057747000
6	2.915978000	-4.541329000	-2.280098000
8	1.155943000	-4.458341000	-0.301108000
7	0.484086000	-0.007783000	-3.170096000
6	0.993905000	1.262115000	-3.033268000
6	-0.516017000	0.059234000	-4.021197000
6	0.278404000	2.116160000	-3.817593000
7	-0.673902000	1.333954000	-4.441425000
17	0.922392000	-2.830461000	-4.310000000
1	-2.338937000	3.660681000	3.352994000
1	-1.244818000	1.838213000	2.327058000
1	-0.690021000	3.331867000	1.574208000
1	-0.905937000	1.883999000	-0.244875000
1	-2.403998000	2.820167000	-0.336075000
1	-3.937778000	2.119045000	3.261079000
1	-4.611088000	4.303018000	2.100102000
1	-4.170853000	2.200939000	1.639034000
1	-0.933490000	-0.252554000	0.427884000
1	-3.363952000	-1.656766000	-0.230512000
1	-0.532429000	-2.582742000	0.525373000
1	-1.830410000	-3.650622000	-0.026437000
1	-2.576503000	-0.421440000	2.737268000
1	-4.475999000	-2.020149000	4.091702000
1	-2.868290000	-2.309210000	4.743405000
1	2.929043000	-2.415179000	0.731864000

1	3.825878000	-3.931055000	0.337778000
1	4.041174000	-2.421601000	-0.661223000
1	3.435664000	-5.319478000	-1.717895000
1	2.183365000	-4.956149000	-2.969402000
1	3.594667000	-3.878589000	-2.817474000
1	1.827945000	1.444186000	-2.379654000
1	-1.113262000	-0.775886000	-4.342463000
1	0.349109000	3.176430000	-3.986019000
1	-1.391053000	1.656926000	-5.067238000
17	3.410637000	-1.086242000	-2.806643000

NAMI-GN3

7	3.214504000	0.829048000	-1.781090000
6	2.019987000	0.208548000	-1.558487000
7	1.549368000	-0.485681000	-2.675666000
6	2.118474000	1.007761000	0.528803000
6	3.317907000	1.701003000	0.351618000
6	3.977563000	1.654041000	-0.918118000
8	5.013228000	2.170392000	-1.313855000
7	3.713671000	2.291976000	1.531368000
6	2.784517000	1.937901000	2.387482000
7	1.791234000	1.179247000	1.834962000
7	1.392713000	0.284923000	-0.391728000
44	-0.575864000	-0.465788000	0.065495000
16	-0.258814000	-2.501724000	-0.750887000
7	-1.060423000	1.395454000	0.855736000
6	-0.838048000	2.565160000	0.291794000
6	-1.765345000	1.632115000	2.014465000
6	-1.958891000	2.973891000	2.155119000
17	-2.820079000	-1.118616000	0.612985000
17	0.048717000	-1.171650000	2.324539000
7	-1.362802000	3.551770000	1.051445000
6	-0.653574000	-3.772653000	0.462637000
6	-1.546424000	-2.895178000	-1.953212000
8	1.027734000	-2.955048000	-1.383703000
1	3.570400000	0.709045000	-2.720540000
1	1.551782000	-1.491002000	-2.435282000
1	0.551362000	-0.241240000	-2.772365000
1	2.771043000	2.203981000	3.433834000
1	1.072478000	0.591418000	2.294857000
1	-0.350181000	2.716271000	-0.655076000
1	-2.079811000	0.806907000	2.628350000

1	-2.461871000	3.558689000	2.905003000
1	-1.330049000	4.532875000	0.833870000
1	0.085970000	-3.684326000	1.255037000
1	-1.646622000	-3.549857000	0.854208000
1	-0.594372000	-4.739825000	-0.039159000
1	-1.406232000	-3.928249000	-2.276332000
1	-2.508264000	-2.719212000	-1.470655000
1	-1.423766000	-2.194566000	-2.777177000
17	-1.356757000	0.480686000	-2.032262000

NAMI-GN7

44	0.137732000	0.238586000	0.080964000
7	0.552190000	2.265536000	-0.019579000
6	0.370126000	3.366586000	0.819285000
6	1.216945000	2.716627000	-1.061497000
6	0.992328000	4.477097000	0.244804000
6	-0.354223000	3.572220000	2.047388000
7	1.507969000	4.043583000	-0.937757000
7	1.126990000	5.749003000	0.705480000
7	-0.137724000	4.933127000	2.498048000
8	-1.098910000	2.888724000	2.716658000
6	0.539660000	5.919483000	1.855877000
7	0.538226000	7.178776000	2.446827000
16	2.134763000	-0.360015000	-0.660848000
6	2.980212000	-1.436333000	0.511191000
6	1.970335000	-1.541317000	-2.015789000
8	3.163292000	0.629570000	-1.125384000
7	-1.776580000	0.648288000	0.748207000
6	-2.776913000	1.374447000	0.148729000
6	-2.268485000	0.149135000	1.860323000
6	-3.897964000	1.319424000	0.921414000
17	-0.713217000	0.455264000	-2.195741000
7	-3.557152000	0.531643000	2.003526000
17	-0.437558000	-2.103395000	0.257321000
1	1.519124000	2.115908000	-1.897689000
1	2.043971000	4.600738000	-1.581787000
1	-0.666274000	5.148167000	3.332994000
1	1.198396000	7.786531000	1.979504000
1	0.676379000	7.175404000	3.449397000
1	2.273391000	-2.219852000	0.786759000
1	3.884389000	-1.821272000	0.035188000
1	3.201639000	-0.822213000	1.381466000

1	2.970995000	-1.858787000	-2.316228000
1	1.345479000	-2.361737000	-1.661704000
1	1.450825000	-1.008472000	-2.810894000
1	-2.606163000	1.839793000	-0.806341000
1	-1.707645000	-0.446772000	2.559467000
1	-4.880565000	1.742873000	0.804966000
1	-4.147013000	0.305965000	2.784769000
17	0.902575000	0.262550000	2.382992000

Glutathione (GSH)

6	2.949523000	-0.162211000	1.070682000
6	4.304316000	-0.455486000	0.322999000
8	4.773122000	-1.587178000	0.475446000
6	1.814437000	-1.115439000	0.696709000
6	1.542985000	-1.248344000	-0.818890000
6	0.111755000	-1.701330000	-1.110302000
8	-0.188350000	-2.805970000	-1.555222000
8	4.734340000	0.537974000	-0.340799000
7	2.644932000	1.284495000	0.759636000
7	-0.795935000	-0.733245000	-0.819037000
6	-2.240526000	-0.868716000	-0.890265000
6	-2.817805000	0.532090000	-0.579933000
8	-3.707712000	0.705211000	0.243287000
6	-2.820739000	-1.942229000	0.036211000
16	-2.330876000	-1.820487000	1.788341000
7	-2.212460000	1.542079000	-1.269934000
6	-1.956518000	2.834538000	-0.637155000
6	-0.526877000	2.905583000	-0.023713000
8	-0.193331000	3.964500000	0.506619000
8	0.171480000	1.832314000	-0.147375000
1	3.132026000	-0.243448000	2.143713000
1	0.900794000	-0.807281000	1.213160000
1	2.093845000	-2.093746000	1.091134000
1	2.233567000	-1.961900000	-1.264525000
1	1.693230000	-0.281620000	-1.310496000
1	2.787445000	1.878689000	1.571554000
1	3.455953000	1.449731000	0.072107000
1	1.676365000	1.517265000	0.374468000
1	-0.438874000	0.157980000	-0.447873000
1	-2.527561000	-1.157135000	-1.912649000
1	-3.908624000	-1.924833000	-0.030486000
1	-2.452966000	-2.912602000	-0.296256000

1	-1.419284000	1.230792000	-1.816985000
1	-2.065711000	3.642903000	-1.363786000
1	-2.697406000	2.983030000	0.147370000
1	-2.989825000	-0.674579000	2.022238000

Cysteine (CysH)

6	0.346224000	0.599632000	0.727431000
6	1.274117000	-0.456342000	0.088159000
8	1.256921000	-1.622640000	0.394461000
6	-1.040765000	0.007611000	1.002532000
16	-2.057494000	-0.201561000	-0.499709000
8	2.120059000	0.057810000	-0.810516000
7	0.369012000	1.818797000	-0.087687000
1	0.809568000	0.832994000	1.692960000
1	-1.346599000	-1.218522000	-1.014640000
1	-0.939906000	-0.952758000	1.505085000
1	-1.618264000	0.679534000	1.639472000
1	0.234581000	2.650006000	0.477286000
1	-0.390705000	1.774647000	-0.768148000
1	1.858223000	1.013539000	-0.868684000

Guanine (GN)

7	-1.196342000	0.885143000	-0.056168000
6	-2.348592000	0.126192000	-0.011435000
6	-1.617496000	2.119967000	-0.055675000
6	-3.478606000	0.939532000	0.013761000
6	-2.525503000	-1.298085000	0.002124000
7	-2.993626000	2.217044000	-0.013569000
7	-4.789019000	0.598685000	0.065620000
7	-3.931846000	-1.596546000	0.047217000
8	-1.730743000	-2.217034000	-0.023428000
6	-4.960417000	-0.699511000	0.069697000
1	-0.991155000	2.998239000	-0.085424000
1	-3.553187000	3.055577000	-0.005069000
1	-4.131968000	-2.587417000	-0.001429000
7	-6.237265000	-1.208222000	0.035284000
1	-6.941707000	-0.512400000	0.234124000
1	-6.396700000	-2.094271000	0.491996000

