SUPPORTING INFORMATION

Interaction of cysteine with Li^+ and LiF in presence of $(H_2O)_n$(n=0-6) clusters

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Table S1. Total energy difference (in eV) of Cys conformers with respect to isomer Z(I) using SMD model with B3LYP-D3(BJ) /6-311+G(2d,p) method.

	isomer	ΔE(B3LYP-D3(BJ))
Z-Cys	Z(I)	0.000
	Z(II)	0.060
	Z(III)	0.066
	Z(IV)	0.067
	Z(V)	0.077
	Z(VI)	0.092
N-Cys	N(I)	0.107
	N(V)	0.167
	N(III)	0.173
	N(IV)	0.213
	N(II)	0.223
	N(VI)	0.244
	N(VII)	0.246
	N(IX)	0.246
	N(VIII)	0.248
	N(X)	0.264
	N(XI)	0.274

Table S2. Interaction energy components of Cys·Li^+ $(H_2O)_n$ (n=0-6) complexes. Ordered all atoms in cluster by bonding and then segmented each molecule into a fragment, the units in the output of interaction energy components are all kJ/mol. Frag 1, Frag 2 and Frag 3 represent Cys, Li^+ and water clusters, respectively.

Isomers	Fragments	Electrostatic	Repulsion	Dispersion	Total
N-0A	Frag 1···Frag 2	-242.26	44.11	-12.91	-211.07
N-1A	Frag 1···Frag 2	-231.43	33.6	-11.22	-209.05
	Frag 1···Frag 3	16.73	1.93	-4.88	13.78
	Frag 2···Frag 3	-147.92	39.81	-5.93	-114.04
N-2A	Frag 1···Frag 2	-220.91	28.74	-8.87	-201.04
	Frag 1···Frag 3	25.73	12.08	-16.06	21.75
	Frag 2···Frag 3	-272.26	71.82	-11.25	-211.69
N-3A	Frag 1···Frag 2	-171.52	76.77	-10.04	-104.79
	Frag 1···Frag 3	25.56	48.1	-28.61	45.06
	Frag 2···Frag 3	-387.57	93.62	-15.74	-309.69
Z-4A	Frag 1···Frag 2	-213.37	28.13	-6.19	-191.43
	Frag 1···Frag 3	-21.02	31.08	-29.20	-19.15
	Frag 2···Frag 3	-369.75	77.47	-14.49	-306.76
Z-5A	Frag 1···Frag 2	-210.54	33.74	-6.79	-183.60
	Frag 1···Frag 3	-38.31	30.30	-29.02	-37.03
	Frag 2···Frag 3	-356.29	67.06	-13.68	-302.91
Z-6A	Frag 1···Frag 2	-213.92	36.27	-7.19	-184.84
	Frag 1···Frag 3	-110.62	78.41	-48.73	-80.93
	Frag 2···Frag 3	-297.53	62.11	-13.29	-248.70

Table S3. Interaction energy components of Cys·LiF $(H_2O)_n$ (n=0-6) complexes. Ordered all atoms in cluster by bonding and then segmented each molecule into a fragment, the units in the output of interaction energy components are all kJ/mol. Frag 1, Frag 2 and Frag 3 represent Cys, LiF and water clusters, respectively.

Isomers	Fragments	Electrostatic	Repulsion	Dispersion	Total
N-0A′	Frag 1···Frag 2	-200.38	85.51	-21.72	-136.58
N-1A′	Frag 1···Frag 2	-258.31	87.89	-22.31	-192.74
	Frag 1···Frag 3	-2.48	10.34	-10.73	-2.88
	Frag 2···Frag 3	-78.64	35.67	-6.83	-49.80
N-2A′	Frag 1···Frag 2	-229.77	81.57	-21.28	-169.48
	Frag 1···Frag 3	7.24	11.06	-13.32	4.98
	Frag 2···Frag 3	-171.13	67.32	-15.73	-119.54
N-3A′	Frag 1···Frag 2	-189.17	64.86	-19.28	-143.58
	Frag 1···Frag 3	19.47	7.69	-12.11	15.05
	Frag 2···Frag 3	-227.44	76.37	-20.12	-171.18
N-4A′	Frag 1···Frag 2	-173.72	51.30	-17.35	-139.78
	Frag 1···Frag 3	21.31	8.52	-14.20	15.63
	Frag 2···Frag 3	-276.00	87.77	-23.24	-211.47
Z-5A′	Frag 1···Frag 2	-157.90	54.16	-15.51	-119.25
	Frag 1···Frag 3	-166.60	81.47	-51.55	-136.68
	Frag 2···Frag 3	-202.61	84.99	-19.66	-137.28
Z-6A′	Frag 1···Frag 2	-166.54	54.94	-16.01	-127.61
	Frag 1···Frag 3	-185.28	83.97	-59.62	-160.93
	Frag 2···Frag 3	-204.00	81.10	-19.65	-142.54

Energy decomposition analysis (EDA) is a very important method to study the weak interaction. It can decompose the total interaction energy into various components, so as to further study the nature of weak interaction in the system, which compared with the EDA relied on wavefunction, with the advantages of more affordable and convenient to inspect the intramolecular interaction. The basic principle of the molecular forcefield was to define the following formula from the electrostatic and van der Waals (vdW) interactions (including the exchange-repulsion term and the dispersion term):

$$E_{AB}^{ele} = \frac{q_A q_B}{r_{AB}} \quad (1)$$

$$E_{AB}^{vdW} = E_{AB}^{rep} + E_{AB}^{dis} \quad (2)$$

$$E_{AB}^{rep} = \varepsilon_{AB}\left(\frac{R_{AB}^0}{r_{AB}}\right)^{12} E_{AB}^{dis} = 2\varepsilon_{AB}\left(\frac{R_{AB}^0}{r_{AB}}\right)^6 \quad (3)$$

where A, B, is the atomic label, and q is the atomic charge, and r is the distance between atoms, and ε is the depth of vdW potential well, and R^0 is the nonbond distance between atoms. The electrostatic interaction is merely reflected via the atomic charge. When r ¼ R^0, the vdW interaction between atoms is exactly equal to the potential well depth, where ε and R0are defined in the molecular forcefield. Here we carry out popular AMBER99 forcefield of Multiwfn supported and define the vdW parameter according to the atom type in AMBER forcefield. The parameters are produced by mixing rules with the vdW parameters of atoms in the actual calculation of vdW interaction between atoms. The non-bonded radius parameter R* is stated for each atom, and the non- bond distance parameter between atoms is added by the non-bond radius of the corresponding atoms, as shown in below formula:

$$\varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B} R_{AB}^0 = R_A^* + R_B^* \quad (4)$$

Table S4. Calculated CM5 charge for the three compounds in Cys·$Li^+(H_2O)_n$ (n=0-6) with B3LYP-D3(BJ) /6-311+G(2d,p) method.

Charge	Isomers	Cys	Li^+	H_2O
CM5	N-0A	0.2584	0.7416	0.0000
	N-1A	0.2412	0.6625	0.0963
	N-2A	0.2082	0.6442	0.1477
	N-3A	0.1495	0.3780	0.4725
	Z-4A	0.1308	0.6096	0.2596
	Z-5A	0.1287	0.6069	0.2644
	Z-6A	0.1058	0.5935	0.3007

Table S5. Calculated CM5 for the three compounds in Cys·$LiF(H_2O)_n$ (n=0-6) with B3LYP-D3(BJ) /6-311+G(2d,p) method.

Charge	Isomers	Cys	LiF	H_2O
CM5	N-0A′	-0.0280	0.0280	
	N-1A′	-0.0149	-0.0147	0.0296
	N-2A′	-0.0034	-0.0455	0.0489
	N-3A′	0.0186	-0.0123	-0.0064
	N-4A′	0.0318	-0.0220	-0.0098
	Z-5A′	0.0053	-0.0470	0.0417
	Z-6A′	0.0406	-0.0514	0.0108

Table S6. Optimized Cartesian Coordinates of most stable structure of Cys·$Li^+(H_2O)_n$ (n=0-6) and Cys·$LiF(H_2O)_n$(n=0-6) clusters.

N-0A
1 1

C	-0.41481200	0.69207300	-0.73481300
C	0.83691600	-0.09831600	-1.17317700
C	-1.30631900	-0.20254300	0.11538200
S	1.93947500	-0.61594900	0.21833700
H	0.55807300	-0.97407400	-1.75576700
H	1.45201400	0.53839800	-1.81002500
N	-0.00753700	1.83032100	0.11549200
H	-0.95894500	0.98911000	-1.63605600
O	-2.16681700	-0.91076600	-0.58300100
O	-1.16849300	-0.27719400	1.32668900
H	1.37766400	-1.82093400	0.44654700
H	-0.79294400	2.46315700	0.25491100
H	0.71021300	2.37499200	-0.35702700
H	-2.67536800	-1.49454900	0.00607600
Li	0.44607500	0.70774100	1.78522100

N-1A
1 1

N	0.12356200	-0.16865000	1.71574700
H	0.16141500	0.59209000	2.38925000
C	-1.10650100	-0.06579000	0.91055300
H	-2.02354000	-0.25851300	1.47612400
C	-1.21391600	1.35045800	0.30601800
C	-0.99683000	-1.08542600	-0.21369300
H	-2.09574600	1.43445100	-0.32601300
H	-1.32022700	2.07278300	1.11633400
S	0.27591900	1.88772200	-0.64120100
O	0.07940500	-1.44203700	-0.66057000
H	-0.10185300	1.40696400	-1.84322400
O	-2.16720100	-1.47804200	-0.68097300
H	-2.03526000	-2.08915800	-1.42538600
H	0.12070600	-1.02945100	2.25837300
Li	1.49970200	-0.28479500	0.13824600
O	3.30354500	-0.78047300	-0.08866600
H	3.58681200	-1.56610000	-0.56972400
H	4.10644400	-0.32271600	0.18292900

N-2A
1 1

N	0.41582500	-0.02059200	1.54210300
H	0.06534300	0.79446800	2.03568600
C	-0.69571300	-0.81027600	0.98743700
H	-0.96109500	-1.65307000	1.63649500
C	-1.98522700	0.00846100	0.80785900
C	-0.24701600	-1.40903000	-0.34234800
H	-2.79154100	-0.64171800	0.47562900
H	-2.27670400	0.42881700	1.77128500
S	-1.89319000	1.44441400	-0.34010000
O	0.79927600	-1.12693900	-0.89223500
H	-1.98813300	0.74193600	-1.48749100
O	-1.13792800	-2.25519400	-0.84078100
H	-0.81111100	-2.60962300	-1.68388900
H	0.92759300	-0.57054300	2.22599600
Li	1.79592500	0.36650000	-0.02420500
O	3.61955500	-0.17611000	0.16339200
H	4.00178300	-0.90402700	-0.33860600
H	4.35659700	0.29335000	0.56755000
O	1.33907800	2.10813100	-0.60107500
H	1.69185100	2.71901700	-1.25482300
H	0.37360100	2.21963700	-0.58692700

N-3A
1 1

N	2.68575700	-1.44624300	-0.12019500
H	3.45729700	-1.91026900	0.34282900
C	1.80368700	-0.74635800	0.81638100
H	1.90027800	-1.20732500	1.80484000
C	2.04277300	0.75767500	0.98809400
C	0.35155900	-1.01092600	0.38433200
H	1.35004500	1.15686600	1.72571300
H	3.06748900	0.92966100	1.31240800
O	-0.59469400	-0.39219600	0.82542900
O	0.22759600	-1.96287900	-0.52572200
H	1.16930800	-2.23269000	-0.72698800
H	3.05880900	-0.81454700	-0.82419600
S	1.78254100	1.61515800	-0.63252800
H	2.51924500	2.70979900	-0.36574600
Li	-2.28071100	0.18303000	-0.01017000
O	-3.81419600	0.43243400	1.10920200
H	-3.96829300	1.19407500	1.67694700
H	-4.37113000	-0.27743600	1.44420900
O	-2.52563000	-1.31542800	-1.19573100
H	-3.07749100	-1.49929300	-1.96097200
H	-1.75556100	-1.89767700	-1.24455400
O	-1.59797700	1.87328300	-0.64087400
H	-1.93783900	2.47257100	-1.31194400
H	-0.63988700	2.02428500	-0.59150000

N-4A
1 1

C	1.75346600	-0.76173800	0.76849100
H	2.04707800	-1.25181200	1.69868600
C	2.19691000	0.69994200	0.75996200
C	0.21325400	-0.90580900	0.58587700
H	1.62024000	1.23046200	1.51284200
H	3.25652200	0.80013400	0.99923500
S	1.97821600	1.48851900	-0.88490000
O	-0.13158000	-1.75188800	-0.27931700
H	0.62088500	1.45562000	-0.90031200
O	-0.48483100	-0.15965000	1.28693000
Li	-1.98218800	0.94781100	0.93566900
H	2.54337100	-0.84424400	-1.13762900
H	3.20588700	-2.04712600	-0.15187700
H	1.57164400	-2.13788200	-0.69241500
N	2.36113900	-1.52537900	-0.37975700
O	-3.67043200	0.03522000	0.70023100
H	-4.09476500	-0.49832600	1.37828600
H	-3.51274700	-0.55124700	-0.06532400
O	-2.44672000	-1.11457100	-1.43880200
H	-1.65081300	-1.53702700	-1.02884500
H	-2.70767700	-1.64328300	-2.19902100
O	-1.53870000	1.40386200	-0.97335800
H	-1.86967500	0.59780200	-1.42518900
H	-1.92651100	2.15788500	-1.42933900
O	-2.05990700	2.41285300	2.18907700
H	-1.54535300	2.44877300	3.00153500
H	-2.80099300	3.01549500	2.30749900

N-5A
1 1

N	2.50800300	0.17062900	-1.03361000
H	2.89033800	0.28105500	-2.05009100
C	2.43054200	-1.30588400	-0.64244200
H	1.12679600	0.88040800	-0.94156900
C	1.63827000	-1.76798300	-1.22575800
C	3.36587000	-1.82370100	-0.85912300
H	2.13386900	-1.54997500	1.15392100
H	1.13873100	1.97763000	-0.32720000
S	0.85873700	-1.08210000	1.18591700
O	0.17403700	0.28070000	-1.46169200
H	-1.44098600	-0.35763300	-0.77634400
O	3.39764800	0.43512500	0.80738700
H	4.36881800	1.05424700	-0.43193600
H	2.90939200	1.84093000	0.02826800
L	3.41270000	0.93435300	-0.10150200
O	-2.94692200	1.01233400	-0.68395900
H	-3.32372000	1.37713000	-1.49126600
H	-2.46953900	1.74388200	-0.22698800
O	-1.23635000	2.46428500	0.76762600
H	-0.36012800	2.46383800	0.30255900
H	-1.30330400	3.28132900	1.27114400
O	-1.06944200	-0.27403700	1.20616400
H	-1.09722000	0.68097700	1.40114900
H	-1.88407200	-0.65005400	1.58018200
O	-2.28199700	-2.06144700	-0.96906300
H	-2.45565000	-2.73468500	-1.63087500
H	-2.99280500	-2.08852400	-0.30384400
O	-3.76487100	-1.00023800	1.04929100
H	-4.56873400	-1.11960000	1.56453600
H	-3.86532100	-0.18733000	0.52142500

N-6A
1 1

N	-2.51451400	0.38933000	0.92279000
H	-3.09165400	0.94685700	1.66699100
C	-2.66329700	-1.09606200	1.22029100
H	-1.06741600	0.94883200	0.95040800
C	-2.21980100	-1.27723800	2.19731000
C	-3.71866400	-1.37015400	1.28123400
H	-1.93770800	-2.26864700	0.01077700
H	-0.94903700	2.06944700	0.40140200
S	-0.64998400	-1.95589000	0.25166200
O	-0.18615100	0.24113000	1.47932900
H	1.41847300	-0.21564300	0.66485500
O	-2.44382200	0.37527500	-1.20531700
H	-4.03083000	0.54225300	-0.56099700
H	-2.91832000	1.80175100	-0.50505100
Li	-3.05070800	0.78842200	-0.42689300
O	3.03061700	0.95431800	0.97108000
H	3.38038100	1.08657600	1.85849600
H	2.63398100	1.81200400	0.68435000
O	1.49421400	2.80997600	-0.16938900
H	0.55472400	2.67390700	0.15062300
H	1.59249100	3.72935200	-0.43523700
O	1.21647300	0.36944500	-1.30944000

H	1.35488300	1.33569100	-1.21864600
H	2.04052300	0.00826200	-1.68162900
O	1.92075200	-2.05125400	0.38769900
H	2.05507600	-2.79608700	0.98062600
H	2.69442400	-1.99426100	-0.20227500
O	3.75828700	-0.71258400	-1.14028100
H	4.57689500	-0.82297200	-1.63454600
H	3.92109600	-0.06241200	-0.43288000
O	-1.34550700	0.04820400	-2.35686600
H	-1.42952500	-0.86772100	-2.64343200
H	-0.41454400	0.14635800	-2.06547600

Z-0A
1 1

C	-2.49309000	-0.59028600	0.27823000
H	-3.14487000	-1.45351000	0.12239800
C	-3.12010300	0.66721300	-0.32029400
C	-1.11284400	-0.93798700	-0.31169500
H	-3.11032800	0.57197000	-1.40364500
H	-4.15442100	0.78497700	0.00539400
S	-2.25433100	2.20189700	0.19209100
O	-0.24882200	-1.38821300	0.49853500
H	-1.16423100	2.01944700	-0.58176500
O	-0.91718500	-0.78261100	-1.53230700
Li	0.80656700	-1.55207100	-1.13236200
H	-2.03825800	0.55064000	1.93462400
H	-3.06183400	-0.72524600	2.33787300
H	-1.42316900	-1.01317300	1.97085900
N	-2.26674200	-0.44625500	1.76245000

Z-1A
1 1

C	0.11868700	0.59613600	0.78881700
H	0.46674900	1.00894100	1.73866300
C	-1.18242400	-0.17645600	0.98632500
C	1.26389100	-0.25644900	0.19871000
H	-0.96167900	-1.07390500	1.55945200
H	-1.91605700	0.41392000	1.53688300
S	-1.98717100	-0.62152900	-0.60213400
O	2.00631700	0.32181100	-0.64793100
H	-1.09602500	-1.57254700	-0.95165700
O	1.39862700	-1.43041200	0.58543500
Li	2.97183600	-1.41968100	-0.59146600
H	-0.76004300	1.44819700	-0.87240400
H	-0.32617200	2.62380600	0.25455400
H	0.86854900	1.81089400	-0.66080500
N	-0.05064400	1.74184900	-0.17698500
O	4.36830700	-2.50679300	-1.20532200
H	4.54833300	-3.40480100	-0.90489400
H	5.04958900	-2.29354300	-1.85249200

Z-2A
1 1

C	-0.93708200	0.96059600	0.58151500
H	-0.88019000	1.54917000	1.50003400
C	-1.48205400	-0.43294600	0.87729100
C	0.47712300	0.95805600	-0.06812200
H	-0.73683100	-0.97212000	1.45656000
H	-2.40518800	-0.38739300	1.45690600
S	-1.90068300	-1.36887000	-0.64550700

O	0.63154300	1.78878600	-0.99332000
H	-0.62892900	-1.53905800	-1.06350600
O	1.29806500	0.14402700	0.40278900
Li	3.08596400	0.00287800	-0.15863100
H	-2.24971100	1.01069600	-1.01516500
H	-2.51918300	2.30220300	0.03442000
H	-1.11556500	2.25405700	-0.95741900
N	-1.80886200	1.70956400	-0.39309800
O	4.32025100	-1.30643400	0.42815400
H	4.27055500	-1.80585300	1.24995700
H	5.11400800	-1.60695100	-0.02663600
O	3.23172700	1.26081500	-1.51855300
H	2.34055300	1.67066800	-1.56015600
H	3.84593400	1.79294500	-2.02899000

Z-3A
1 1

C	-1.24806300	0.39664400	1.12583300
H	-1.32585500	0.51171800	2.20880900
C	-1.73486800	-0.98315100	0.69095000
C	0.22231100	0.66445900	0.69345000
H	-1.04270800	-1.72353800	1.08321700
H	-2.73263500	-1.19909000	1.07554600
S	-1.85648200	-1.13694200	-1.13588100
O	0.42271100	1.79265300	0.17707900
H	-0.52605700	-1.08691800	-1.38282800
O	1.02282900	-0.27033500	0.86985300
Li	2.50998600	-0.54770300	-0.29534700
H	-2.39295600	1.13879600	-0.42724400
H	-2.81851100	1.85828600	1.03939300
H	-1.31883000	2.22171500	0.27104700
N	-2.04789600	1.49836300	0.47853400
O	3.79450800	-1.49130300	0.75142700
H	3.58189500	-1.60067900	1.68441900
H	4.67351900	-1.85860700	0.61974200
O	2.71821400	1.24176200	-1.11155200
H	1.96930300	1.70055600	-0.66266200
H	3.46902300	1.84231600	-1.10493600
O	1.70743300	-1.12148700	-2.02582100
H	1.94819000	-0.32924900	-2.52661300
H	1.84076100	-1.87890500	-2.60512000

Z-4A
1 1

C	1.75346600	-0.76173800	0.76849100
H	2.04707800	-1.25181200	1.69868600
C	2.19691000	0.69994200	0.75996200
C	0.21325400	-0.90580900	0.58587700
H	1.62024000	1.23046200	1.51284200
H	3.25652200	0.80013400	0.99923500
S	1.97821600	1.48851900	-0.88490000
O	-0.13158000	-1.75188800	-0.27931700
H	0.62088500	1.45562000	-0.90031200
O	-0.48483100	-0.15965000	1.28693000
Li	-1.98218800	0.94781100	0.93566900
H	2.54337100	-0.84424400	-1.13762900
H	3.20588700	-2.04712600	-0.15187700
H	1.57164400	-2.13788200	-0.69241500
N	2.36113900	-1.52537900	-0.37975700

O	-3.67043200	0.03522000	0.70023100
H	-4.09476500	-0.49832600	1.37828600
H	-3.51274700	-0.55124700	-0.06532400
O	-2.44672000	-1.11457100	-1.43880200
H	-1.65081300	-1.53702700	-1.02884500
H	-2.70767700	-1.64328300	-2.19902100
O	-1.53870000	1.40386200	-0.97335800
H	-1.86967500	0.59780200	-1.42518900
H	-1.92651100	2.15788500	-1.42933900
O	-2.05990700	2.41285300	2.18907700
H	-1.54535300	2.44877300	3.00153500
H	-2.80099300	3.01549500	2.30749900

Z-5A
1 1

C	2.50800300	0.17062900	-1.03361000
H	2.89033800	0.28105500	-2.05009100
C	2.43054200	-1.30588400	-0.64244200
C	1.12679600	0.88040800	-0.94156900
H	1.63827000	-1.76798300	-1.22575800
H	3.36587000	-1.82370100	-0.85912300
S	2.13386900	-1.54997500	1.15392100
O	1.13873100	1.97763000	-0.32720000
H	0.85873700	-1.08210000	1.18591700
O	0.17403700	0.28070000	-1.46169200
Li	-1.44098600	-0.35763300	-0.77634400
H	3.39764800	0.43512500	0.80738700
H	4.36881800	1.05424700	-0.43193600
H	2.90939200	1.84093000	0.02826800
N	3.41270000	0.93435300	-0.10150200
O	-2.94692200	1.01233400	-0.68395900
H	-3.32372000	1.37713000	-1.49126600
H	-2.46953900	1.74388200	-0.22698800
O	-1.23635000	2.46428500	0.76762600
H	-0.36012800	2.46383800	0.30255900
H	-1.30330400	3.28132900	1.27114400
O	-1.06944200	-0.27403700	1.20616400
H	-1.09722000	0.68097700	1.40114900
H	-1.88407200	-0.65005400	1.58018200
O	-2.28199700	-2.06144700	-0.96906300
H	-2.45565000	-2.73468500	-1.63087500
H	-2.99280500	-2.08852400	-0.30384400
O	-3.76487100	-1.00023800	1.04929100
H	-4.56873400	-1.11960000	1.56453600
H	-3.86532100	-0.18733000	0.52142500

Z-6A
1 1

C	-2.51451400	0.38933000	0.92279000
H	-3.09165400	0.94685700	1.66699100
C	-2.66329700	-1.09606200	1.22029100
C	-1.06741600	0.94883200	0.95040800
H	-2.21980100	-1.27723800	2.19731000
H	-3.71866400	-1.37015400	1.28123400
S	-1.93770800	-2.26864700	0.01077700
O	-0.94903700	2.06944700	0.40140200
H	-0.64998400	-1.95589000	0.25166200
O	-0.18615100	0.24113000	1.47932900
Li	1.41847300	-0.21564300	0.66485500

H	-2.44382200	0.37527500	-1.20531700
H	-4.03083000	0.54225300	-0.56099700
H	-2.91832000	1.80175100	-0.50505100
N	-3.05070800	0.78842200	-0.42689300
O	3.03061700	0.95431800	0.97108000
H	3.38038100	1.08657600	1.85849600
H	2.63398100	1.81200400	0.68435000
O	1.49421400	2.80997600	-0.16938900
H	0.55472400	2.67390700	0.15062300
H	1.59249100	3.72935200	-0.43523700
O	1.21647300	0.36944500	-1.30944000
H	1.35488300	1.33569100	-1.21864600
H	2.04052300	0.00826200	-1.68162900
O	1.92075200	-2.05125400	0.38769900
H	2.05507600	-2.79608700	0.98062600
H	2.69442400	-1.99426100	-0.20227500
O	3.75828700	-0.71258400	-1.14028100
H	4.57689500	-0.82297200	-1.63454600
H	3.92109600	-0.06241200	-0.43288000
O	-1.34550700	0.04820400	-2.35686600
H	-1.42952500	-0.86772100	-2.64343200
H	-0.41454400	0.14635800	-2.06547600

N-0A′
0 1

N	-1.32333600	1.92283200	-0.29864400
H	-1.53860900	1.43783600	-1.16689600
C	-0.74339700	0.96601000	0.62812600
H	-0.60582500	1.46635300	1.59781500
C	-1.70214500	-0.20160500	0.87486400
C	0.65573900	0.47598800	0.24056800
H	-1.34472500	-0.83866800	1.67929300
H	-2.67786700	0.20267600	1.14127100
S	-1.99838400	-1.24369000	-0.61538300
O	1.33100800	1.09924000	-0.59879800
H	-0.82519500	-1.90564600	-0.55911500
O	1.07103400	-0.58182300	0.85967700
H	2.07436300	-0.83479900	0.52693500
H	-0.62873200	2.62438900	-0.53386800
F	3.24922600	-0.94806100	-0.03457000
Li	3.02036200	0.41368400	-0.99525000

N-1A′
0 1

N	1.68585100	-1.62758900	-0.82605000
H	0.95216900	-2.16820900	-1.27107700
C	1.20817300	-1.14124700	0.46318300
H	1.40139600	-1.84728700	1.28692400
C	1.90068500	0.17496400	0.84641400
C	-0.31360000	-0.94827200	0.43376600
H	1.47735400	0.56100700	1.77055400
H	2.97209300	0.01706900	0.97336700
S	1.66160900	1.47388700	-0.43815200
O	-0.82915300	-0.18441800	1.27646600
H	1.75236600	0.57446100	-1.44951500
O	-0.95095100	-1.57178300	-0.47679600
H	-2.15214100	-1.14747100	-0.49990900
H	2.51224300	-2.20407100	-0.72465100
F	-3.08866100	-0.58890400	-0.44519400

Li	-2.37011700	0.67966800	0.59450200
O	-1.56455100	2.26078700	-0.10350000
H	-0.60647600	2.06595200	-0.16728000
H	-1.80651400	2.66920800	-0.93984000

N-2A′
0 1

N	2.33714300	-1.58274300	-0.55548000
H	1.72301000	-2.16561100	-1.11261000
C	1.61569900	-1.07832600	0.60709800
H	1.68507700	-1.74863900	1.47900900
C	2.17659900	0.28018500	1.05465300
C	0.11848800	-0.94744400	0.31148600
H	1.58121900	0.67457700	1.87486900
H	3.21321700	0.17357900	1.37552200
S	2.11449200	1.52504900	-0.30055000
O	-0.58068000	-0.23012900	1.04031300
H	2.44134200	0.60749600	-1.24344900
O	-0.31106900	-1.59978200	-0.71067500
H	-1.40039200	-1.28469700	-0.92824400
H	3.15227500	-2.11852100	-0.28383400
F	-2.46798300	-0.77202400	-1.08087800
Li	-2.10781300	0.59891500	0.14574800
O	-1.17554500	2.15833500	-0.50810700
H	-0.21302400	1.99841200	-0.46369100
H	-1.34700500	2.51037800	-1.38631900
O	-3.94368800	0.21770600	0.80751700
H	-3.84023300	-0.49141400	0.14587600
H	-4.02893800	-0.22119800	1.65887900

N-3A′
0 1

N	2.84808400	-1.62389300	-0.39205000
H	2.24358200	-2.27952400	-0.87159200
C	2.14460400	-0.99222400	0.71782000
H	2.24823700	-1.54376700	1.66542800
C	2.68993400	0.42447400	0.96818700
C	0.64314600	-0.89864200	0.46364400
H	2.13361200	0.90085500	1.77269500
H	3.74475500	0.37473200	1.23984000
S	2.51153800	1.50068400	-0.51286000
O	-0.06385900	-0.21096600	1.19675900
H	2.90145800	0.52175100	-1.36235600
O	0.21033300	-1.56595200	-0.56852000
H	-0.79002500	-1.29036500	-0.76096600
H	3.67822100	-2.10794500	-0.07329600
F	-1.97742700	-0.64745000	-0.94742700
Li	-1.69172400	0.58924200	0.44779700
O	-4.51119900	-0.77312400	-0.32966700
H	-3.61886100	-0.84897400	-0.73991900
H	-4.66299900	-1.62106400	0.09812800
O	-3.38110200	1.07664200	1.23232000
H	-3.98959100	0.46344800	0.74981900
H	-3.71217100	1.96607100	1.07946300
O	-0.90742500	1.81790300	-0.92442700
H	0.06289900	1.82941700	-0.88120200
H	-1.13000700	1.09546900	-1.53246000

N-4A′
0 1

N	2.90353100	-1.30220200	-1.22620400
H	2.26810900	-1.62256900	-1.94646600
C	2.26211900	-1.33860300	0.08257500
H	2.35252100	-2.31820200	0.58014800
C	2.89488300	-0.30441800	1.02731700
C	0.76177700	-1.08080400	-0.01103800
H	2.37392900	-0.30827000	1.98245600
H	3.94590900	-0.54523400	1.19040200
S	2.77207000	1.40590200	0.36298400
O	0.11012700	-0.80567500	0.98877100
H	3.05998700	1.01755900	-0.90096400
O	0.26095800	-1.17771300	-1.21684400
H	-0.72612300	-0.88617400	-1.19383000
H	3.73710800	-1.87708300	-1.24049900
F	-2.01192700	-0.27513200	-0.95872000
Li	-1.49724900	0.34932700	0.75783900
O	-0.62109900	2.07394600	0.59683300
H	0.34077300	2.00044900	0.50101300
H	-0.96625000	2.38889000	-0.26528500
O	-3.04109500	0.03704400	1.87199300
H	-3.55921700	-0.63424800	1.36684500
H	-2.96809100	-0.27876600	2.77596900
O	-4.04324100	-1.61119500	0.01999600
H	-4.85470800	-1.33401200	-0.41514100
H	-3.31372900	-1.23207300	-0.52100100
O	-1.96210500	2.24929600	-1.77055100
H	-2.84266000	2.61549600	-1.64571800
H	-2.06733300	1.28074600	-1.65199300

N-5A′
0 1

N	-3.50530700	-1.47723100	0.72472400
H	-2.91060300	-2.21074800	1.08988700
C	-2.96991900	-0.95083400	-0.52521600
H	-3.30078800	-1.51875400	-1.40995000
C	-3.42289000	0.50250700	-0.74052100
C	-1.44663700	-1.01187200	-0.56388700
H	-2.97679900	0.89891700	-1.65025900
H	-4.50924100	0.54294200	-0.82660500
S	-2.89520400	1.60235700	0.63565700
O	-0.81772900	-0.39557900	-1.41528800
H	-3.17583800	0.67781600	1.58330800
O	-0.90035900	-1.75515400	0.36565100
H	0.12164000	-1.64695900	0.31862600
H	-4.44080200	-1.84297700	0.59568900
F	1.48113000	-1.18413400	0.18245800
Li	1.00808700	0.21844400	-0.94513300
O	0.50360100	1.82854600	0.11125200
H	-0.42600400	1.85098200	0.38475000
H	1.04695800	1.66872800	0.91553300
O	4.45098400	0.69263100	-0.01897400
H	4.43436100	-0.29968300	0.04213800
H	5.37248900	0.95918100	-0.07850400
O	3.98137100	-1.90604500	0.18228000
H	4.13504800	-2.29959100	1.04641900
H	3.00274000	-1.79259000	0.12349400
O	2.29878900	0.79231500	1.86232000
H	2.01082100	-0.05129300	1.46606300
H	3.14045000	0.96637400	1.40887500

O	2.45596100	1.18662100	-1.84310500
H	3.27190100	1.05676100	-1.31542300
H	2.12835900	2.05442400	-1.57544600

N-6A′
0 1

N	-3.80779700	-1.07200000	0.93130700
H	-3.31435800	-1.85185200	1.34794400
C	-3.27645100	-0.77192100	-0.39302100
H	-3.72370700	-1.39223900	-1.18793000
C	-3.55156300	0.69102900	-0.77198300
C	-1.77973300	-1.05105300	-0.47698600
H	-3.10066200	0.91575800	-1.73622600
H	-4.62715800	0.86060600	-0.83232400
S	-2.83381900	1.87425900	0.43897500
O	-1.09523900	-0.55983200	-1.36400100
H	-3.17272000	1.11204500	1.50456800
O	-1.31796100	-1.84906900	0.45611400
H	-0.29959900	-1.89750600	0.37679000
H	-4.79517500	-1.29317700	0.88590200
F	1.13212400	-1.61364700	0.22188000
Li	0.81280500	-0.18718600	-0.99442900
O	0.55327400	1.45023500	0.13009000
H	-0.37908700	1.70851800	0.21191000
H	0.84392800	1.12957300	1.02266400
O	4.18315100	0.41553500	1.12018500
H	4.15375900	-0.42581100	0.61068500
H	5.04562000	0.46153600	1.54199600
O	3.61411700	-1.78907000	-0.35040100
H	4.00274700	-2.66713800	-0.38206600
H	2.65958900	-1.89370300	-0.09149000
O	1.59896200	0.16262500	2.21465300
H	1.42078600	-0.64668100	1.69971400
H	2.54868300	0.31854600	2.06923300
O	3.11200400	2.23034800	-0.79021400
H	3.58169700	1.76889400	-0.07394200
H	2.20184000	2.31497400	-0.45991900
O	2.35250900	0.00451700	-2.14194500
H	2.73630100	0.86517000	-1.85086600
H	2.99368500	-0.66278800	-1.85235000

Z-0A′
0 1

C	0.51371000	0.52830100	0.55746200
H	1.11440400	0.84007900	1.41689400
C	-0.89533000	0.19029800	1.02189400
C	1.24179100	-0.70505800	-0.08191400
H	-0.85129300	-0.65168400	1.70565200
H	-1.36266800	1.03539900	1.53230400
S	-2.02034300	-0.23254300	-0.36958900
O	2.16633300	-0.42405300	-0.90479300
H	-1.38633800	-1.37861600	-0.67767700
O	0.86209700	-1.80724900	0.29403800
H	0.04313300	2.49568800	0.05633700
H	1.50751900	2.02815900	-0.74987400
H	-0.09461300	1.43358200	-1.18444500
N	0.48916800	1.69188800	-0.38436600
F	2.69628500	2.44293500	-1.19609900
Li	3.25176400	0.84425000	-1.43917800

Z-1A′
0 1

C	-0.08234200	-0.60396500	0.62123100
H	-0.10046700	-1.48348800	1.27022900
C	-1.25945700	-0.63818700	-0.34405500
C	1.26727400	-0.55082700	-0.15592800
H	-1.22998900	0.23366700	-0.99574800
H	-1.17754000	-1.52903800	-0.95990800
S	-2.90436800	-0.68027200	0.49972900
O	2.11681300	0.25868700	0.31674100
H	-3.19501500	0.62758500	0.35340700
O	1.34497300	-1.21910700	-1.19772200
F	0.21066100	2.34980100	-0.21002400
Li	1.80801700	1.80943500	-0.76596500
H	-0.99446100	0.63429600	2.03017900
H	0.68457600	0.66796900	2.04157900
H	-0.05829700	1.53951100	0.71381800
N	-0.15026300	0.62770000	1.45998500
O	2.25069800	1.02907400	-2.47234000
H	1.72766900	1.13369000	-3.27190500
H	2.15267700	0.08363800	-2.20854500

Z-2A′
0 1

C	-0.52935600	-0.33084500	0.92456800
H	-1.12202500	-0.83042000	1.69510400
C	-0.98667700	-0.75864700	-0.46137300
C	0.98462000	-0.62636900	1.16644200
H	-0.33569100	-0.32674800	-1.21654200
H	-0.93031000	-1.84154500	-0.53226800
S	-2.72253000	-0.26957500	-0.85513100
O	1.52775300	0.15104800	1.99320700
H	-2.41283600	0.90452000	-1.44121900
O	1.49866200	-1.53662800	0.49088800
F	0.61405100	1.88798500	-0.83782300
Li	2.26547300	1.32153000	-0.86418500
H	-1.64799100	1.43041200	1.17777900
H	-0.13153400	1.38462900	1.93551400
H	-0.14512900	1.61562600	0.21272900
N	-0.67416700	1.14585800	1.10056400
O	2.60592900	-0.41026800	-1.66351700
H	2.14014500	-0.72647200	-2.44245300
H	2.31016700	-0.99344200	-0.92134300
O	3.47234700	1.31367100	0.63510500
H	4.24515400	0.74893000	0.53897600
H	2.90660200	0.87018600	1.31895800

Z-3A′
0 1

C	-0.97474700	-0.90060500	-0.54490400
H	-1.50192400	-1.52365300	-1.27102000
C	-1.70220000	0.43231700	-0.36617700
C	0.49246100	-0.67322300	-1.02175900
H	-1.04099700	1.16240600	0.09142200
H	-1.98192700	0.80797700	-1.34714300
S	-3.23821800	0.34359500	0.64242500
O	1.34379400	-1.44094800	-0.51355600
H	-2.59093700	0.39914500	1.82635800
O	0.65799700	0.28044000	-1.81054600

F	-0.29858900	0.09220100	2.35445400
Li	1.14229400	0.97523500	1.92378500
H	-1.72515300	-2.17243900	0.95373700
H	-0.06021900	-2.27638500	0.62117500
H	-0.62667900	-0.92973400	1.55646800
N	-0.87421800	-1.66081300	0.73719800
O	2.53182100	1.90908400	-1.06480200
H	3.06904900	2.31870300	-1.74741300
H	1.91609300	1.25209900	-1.50674200
O	2.72744900	0.21781600	1.13859900
H	3.03232700	0.83122900	0.44721900
H	2.43667800	-0.55803800	0.61398300
O	1.02197000	2.66136700	1.01148100
H	1.52852500	2.61223000	0.16817400
H	0.24595000	3.20522300	0.85795300

Z-4A′
0 1

C	-1.04640300	-1.46589400	0.01691400
H	-1.57966900	-2.41111300	-0.11451900
C	-1.57879200	-0.41832300	-0.94923900
C	0.48129500	-1.71243400	-0.17047900
H	-0.95732300	0.47223600	-0.93607400
H	-1.54282800	-0.83328800	-1.95231700
S	-3.30611700	0.12029500	-0.57767300
O	1.09294800	-2.00648900	0.88455300
H	-2.95362800	1.38913700	-0.27784300
O	0.91552100	-1.55078700	-1.32705200
F	-0.08664500	1.18669300	1.73946500
Li	1.59684000	1.22611800	1.17524600
H	-2.20143300	-1.06268700	1.72560600
H	-0.63990500	-1.69822700	1.99440600
H	-0.79788300	-0.06956800	1.60658000
N	-1.22163800	-1.05565900	1.44681200
O	2.98513600	0.02782300	-1.60272300
H	3.57543900	-0.15395000	-2.33840600
H	2.29009900	-0.68590600	-1.59318900
O	2.97398900	-0.09293900	1.17651200
H	3.33168100	-0.05857200	0.27073400
H	2.48850100	-0.94731800	1.19347000
O	1.67253000	2.15336100	-0.49263400
H	2.06237300	1.55361400	-1.15792100
H	0.77514700	2.41010500	-0.76299600
O	-1.07017400	2.68392300	-0.13995200
H	-1.26018500	3.59346000	0.10718200
H	-0.78409800	2.22334100	0.68632400

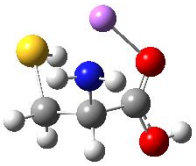
Z-5A′
0 1

C	1.19578800	0.84822100	-0.71881400
H	1.75924000	1.61590000	-1.25581300
C	1.65274800	-0.54554400	-1.15326500
C	-0.31973700	1.05251600	-1.00828700
H	0.96270900	-1.30399700	-0.79718700
H	1.66214700	-0.58569900	-2.23852500
S	3.32635200	-1.01904000	-0.53394600
O	-0.89997500	1.96306600	-0.35563400
H	2.85341200	-1.93027900	0.34320000
O	-0.81851800	0.27251900	-1.83846100
F	-0.13869600	-0.46990900	2.02703600

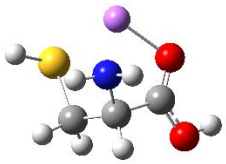
Li	-1.81859000	-0.60669100	1.50794800
H	2.41909200	0.80741800	0.93765800
H	1.28785100	2.07221800	0.98535400
H	0.79895100	0.46034400	1.32686200
N	1.45058900	1.07324300	0.73823800
O	-3.19092600	-0.78763400	-1.50364200
H	-3.73364600	-0.91407800	-2.28598900
H	-2.36444200	-0.31029100	-1.78362000
O	-3.00873800	0.71945800	0.81254700
H	-3.43117000	0.28320100	0.05072100
H	-2.40245500	1.36808100	0.39223700
O	-2.07516300	-2.24004800	0.53973400
H	-2.45199400	-2.00278500	-0.32912700
H	-1.19451400	-2.63075100	0.40682300
O	0.67400200	-2.70769400	1.01318200
H	0.79196500	-3.41620200	1.65247000
H	0.44228500	-1.89873500	1.53543300
O	0.65832900	3.70508400	0.95410300
H	-0.06241800	3.28964100	0.42709200
H	0.23597200	4.05727600	1.74319100

Z-6A′
0 1

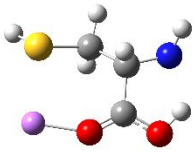
C	1.31680700	0.90248000	-0.69954500
H	1.81851000	1.72653400	-1.21135200
C	1.92447900	-0.43151100	-1.12411800
C	-0.20838100	1.01343800	-0.99225700
H	1.29886200	-1.25555900	-0.80733500
H	1.99095200	-0.45943300	-2.20950500
S	3.60527900	-0.75004400	-0.43501800
O	-0.74167800	2.10074100	-0.65261800
H	3.15891300	-1.62541200	0.49447900
O	-0.78158400	0.02270000	-1.49616800
F	-0.19122500	-0.38172200	1.92864700
Li	-1.90363400	-0.35459100	1.50839600
H	2.47093100	0.90252800	1.00674500
H	1.32071600	2.14751300	0.98487400
H	0.82910100	0.52937300	1.33031300
N	1.50343500	1.14400000	0.76880800
O	-3.49142000	-0.10189500	-1.33924200
H	-3.98386200	-0.04759500	-2.16217600
H	-2.53409800	0.00475800	-1.55994500
O	-2.79731500	1.26703300	0.94371800
H	-3.40310900	0.96410800	0.24460500
H	-2.13244500	1.76897700	0.42821000
O	-2.84879600	-1.82860100	0.74425100
H	-3.36061400	-1.43638700	0.01514900
H	-2.17171000	-2.37054100	0.27569000
O	0.78202600	3.79310100	0.76613800
H	0.11440900	3.41454400	0.15040700
H	0.28465600	4.25145600	1.44983900
O	1.19744400	-2.45609100	1.27885700
H	0.65778200	-1.72049000	1.66629700
H	1.24046500	-3.14671300	1.94628300
O	-0.77568900	-2.77348800	-0.71926000
H	-0.03449600	-2.82284200	-0.08757300
H	-0.68519400	-1.90425800	-1.14447200



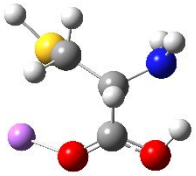
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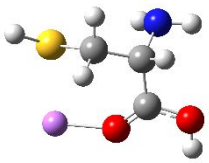
N0-B
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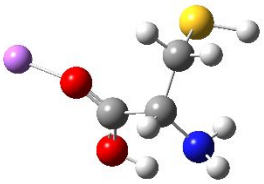
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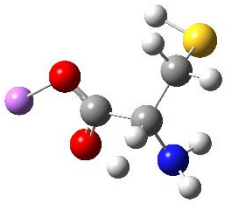
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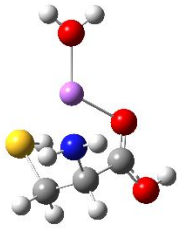
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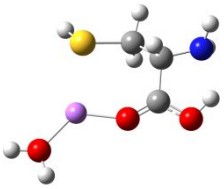
N0-F
0.667



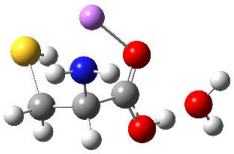
N0-G
0.719



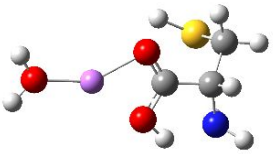
N1-A
0.000



N1-B
0.291



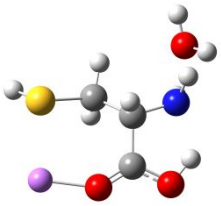
N1-C
0.327



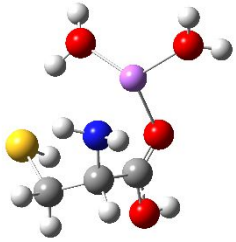
N1-D
0.514



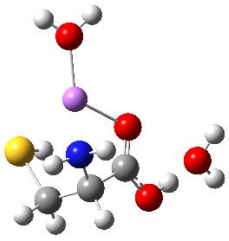
N1-D
0.928



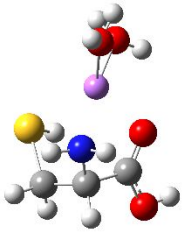
N1-E
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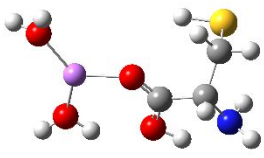
N2-A
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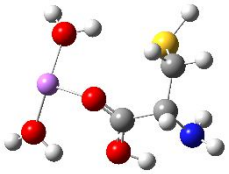
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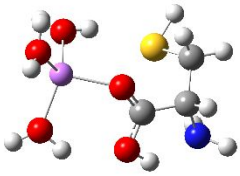
N2-C
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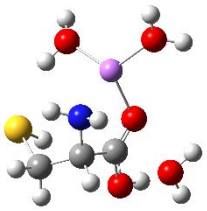
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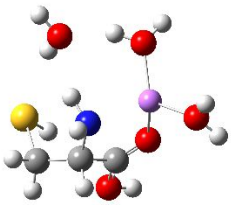
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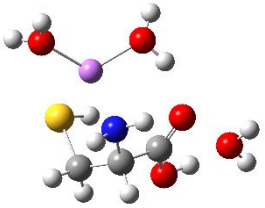
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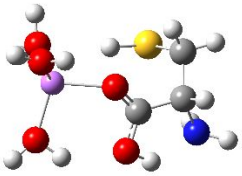
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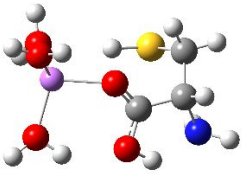
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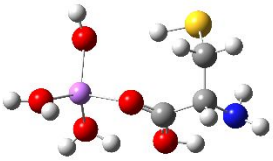
N3-D
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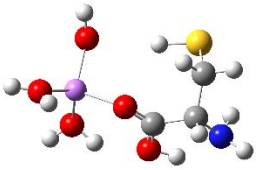
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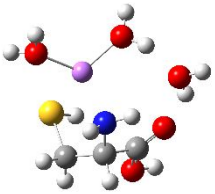
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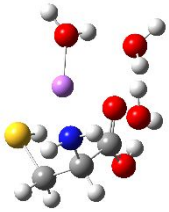
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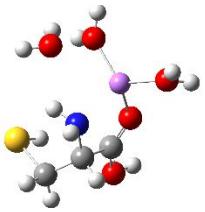
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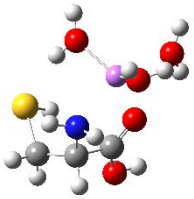
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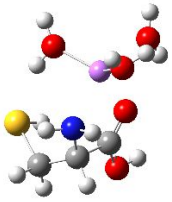
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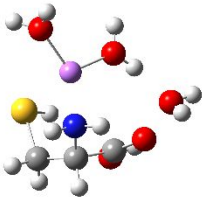
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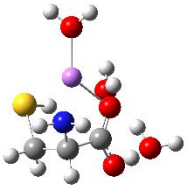
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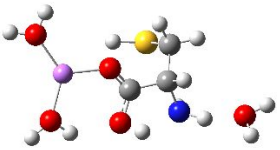
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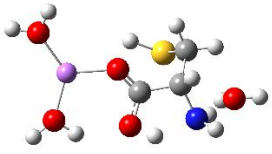
N3-N
0.187



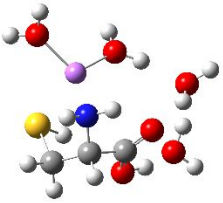
N3-O
0.256



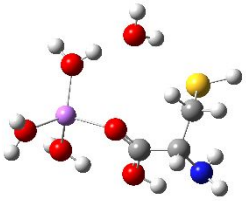
N3-P
0.376



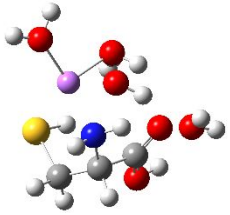
N3-Q
0.409



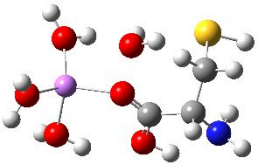
N4-A
0.092



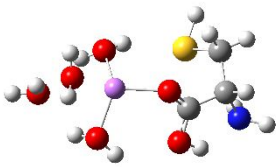
N4-B
0.121



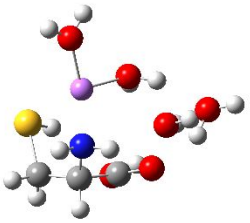
N4-C
0.129



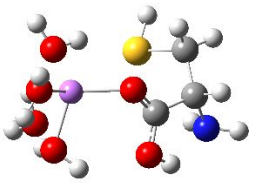
N4-D
0.154



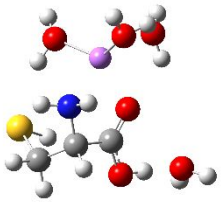
N4-E
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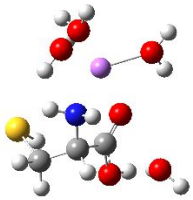
N4-F
0.182



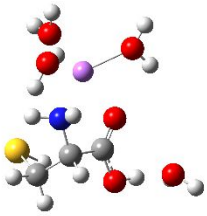
N4-G
0.191



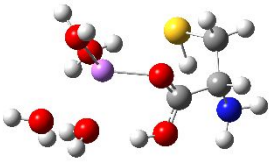
N4-H
0.223



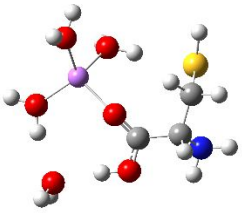
N4-I
0.223



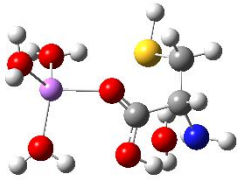
N4-J
0.231



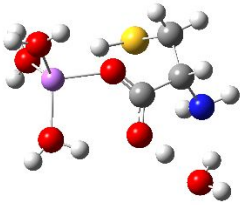
N4-K
0.302



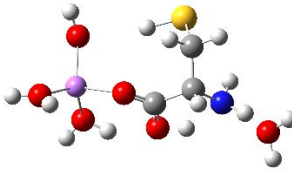
N4-L
0.302



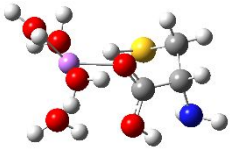
N4-M
0.304



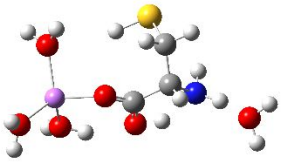
N4-N
0.318



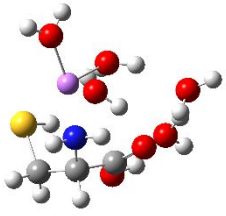
N4-O
0.338



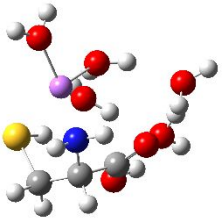
N4-P
0.362



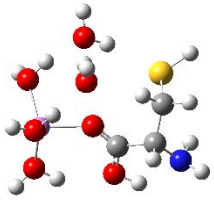
N4-Q
0.363



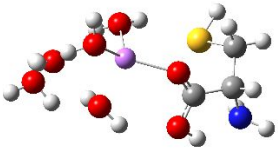
N5-A
0.052



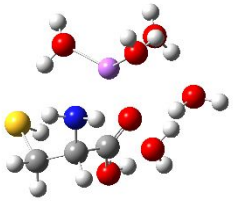
N5-B
0.052



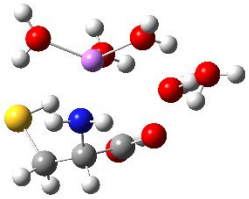
N5-C
0.142



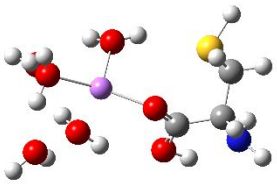
N5-D
0.143



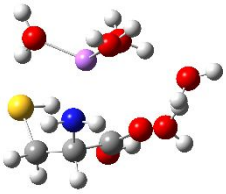
N5-E
0.172



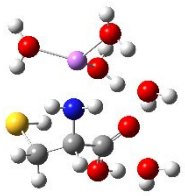
N5-F
0.185



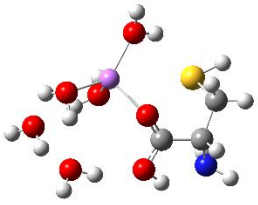
N5-G
0.186



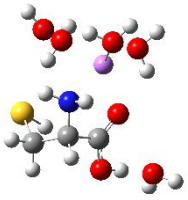
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0.203



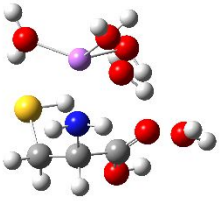
N5-I
0.219



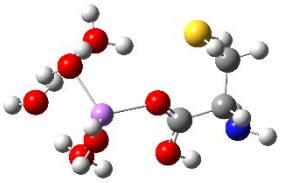
N5-J
0.222



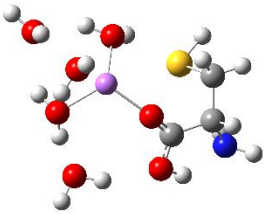
N5-K
0.222



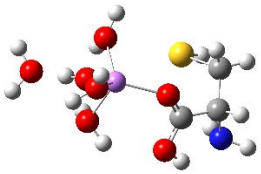
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0.247



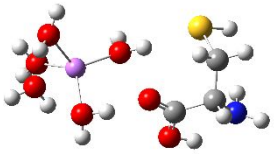
N5-M
0.257



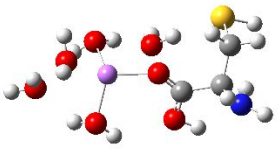
N5-N
0.264



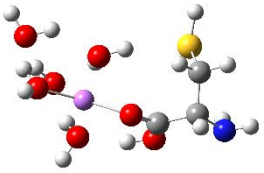
N5-O
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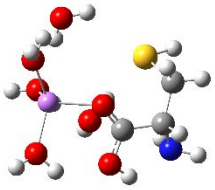
N5-P
0.300



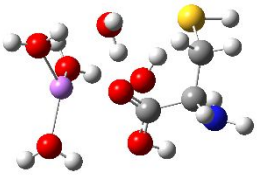
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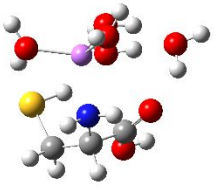
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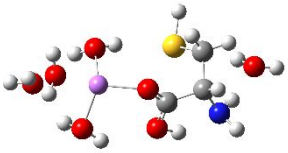
N5-S
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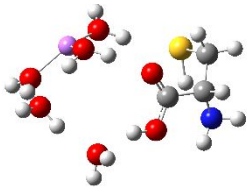
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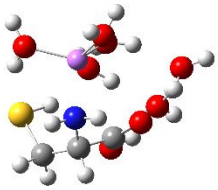
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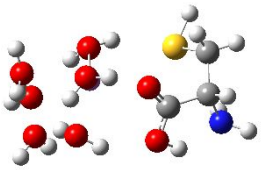
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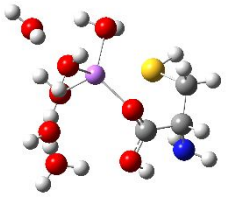
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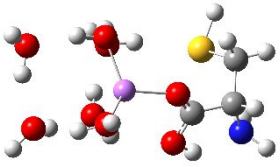
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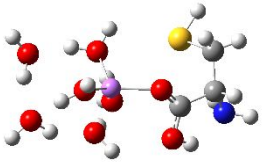
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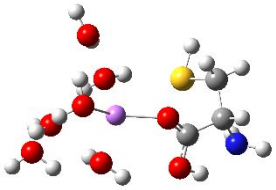
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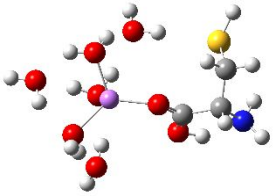
N6-D
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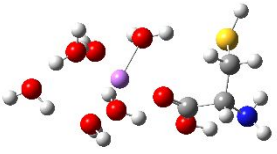
N6-E
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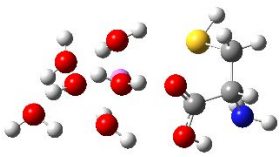
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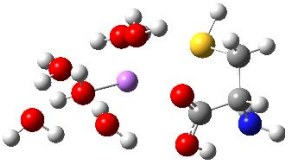
N6-G
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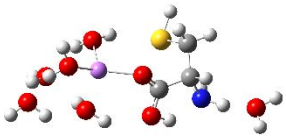
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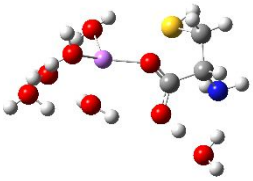
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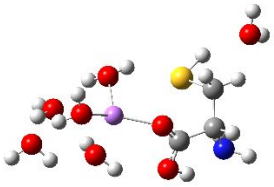
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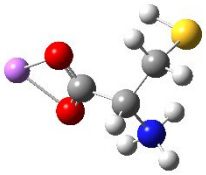
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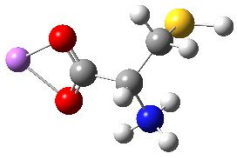
N6-L
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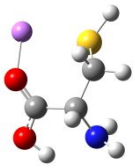
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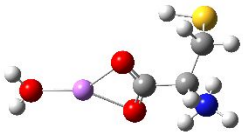
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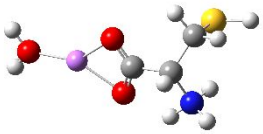
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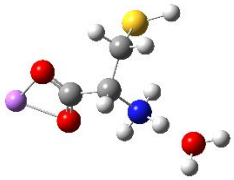
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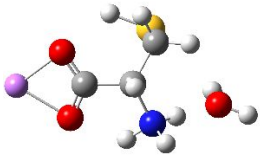
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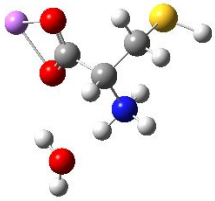
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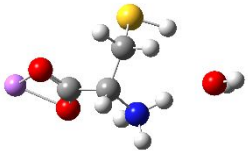
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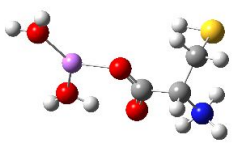
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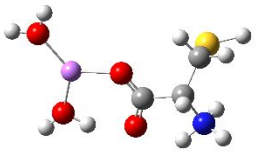
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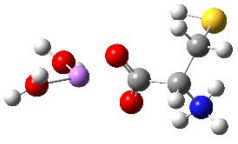
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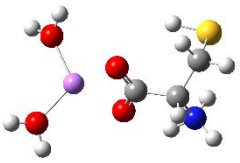
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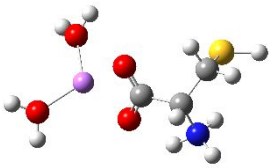
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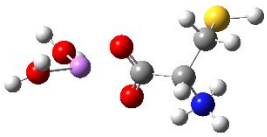
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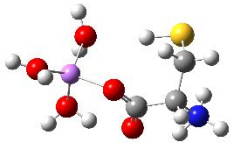
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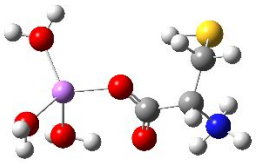
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0.267



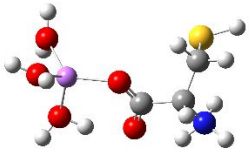
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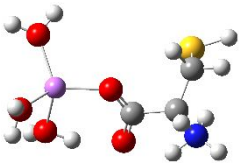
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0.009



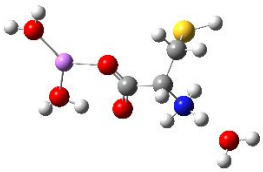
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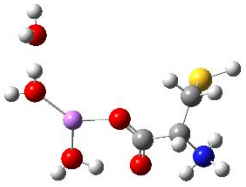
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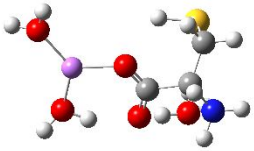
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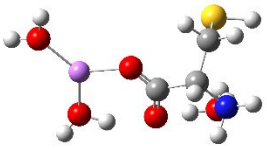
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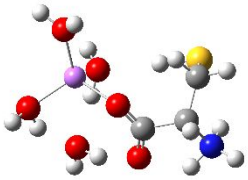
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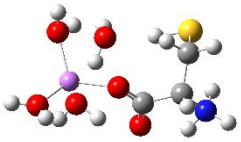
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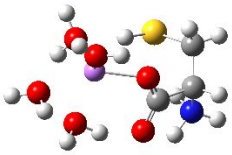
Z3-H
0.211



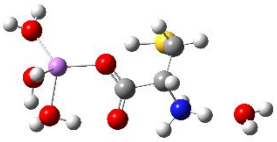
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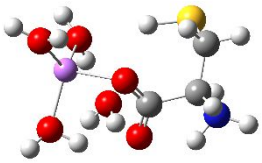
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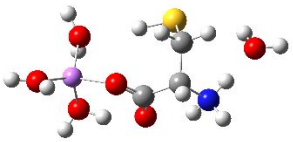
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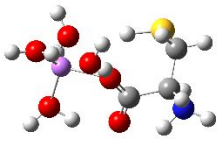
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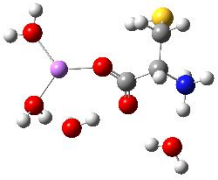
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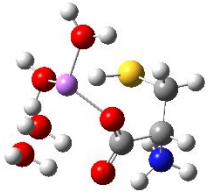
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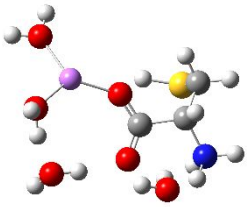
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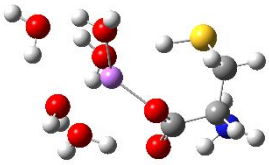
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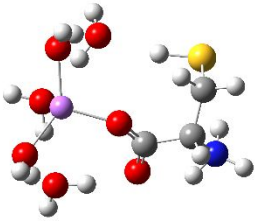
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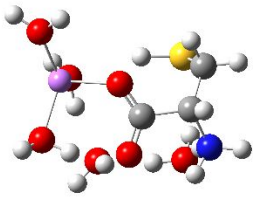
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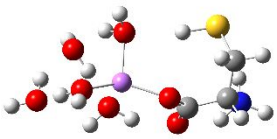
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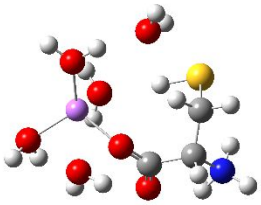
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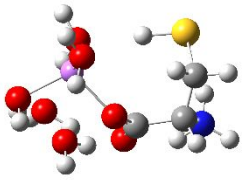
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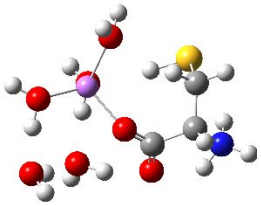
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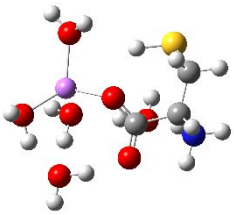
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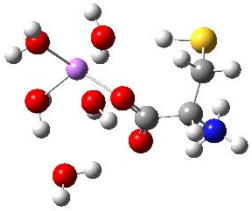
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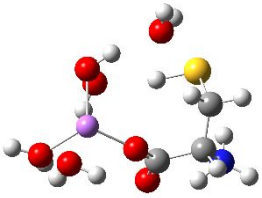
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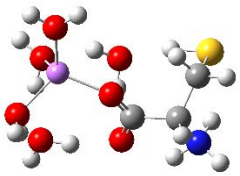
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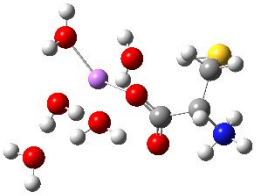
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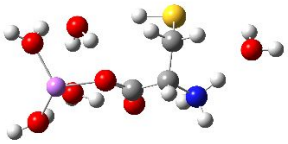
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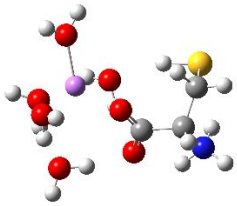
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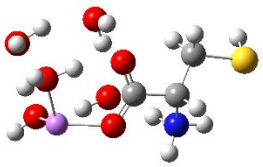
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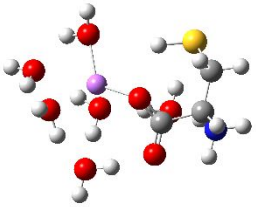
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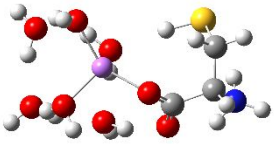
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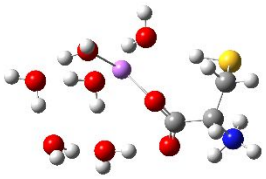
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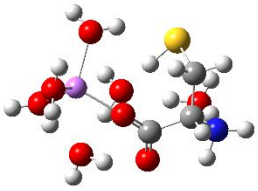
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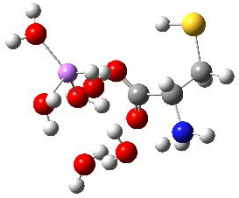
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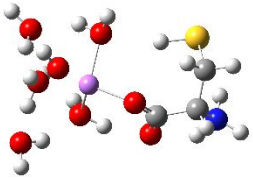
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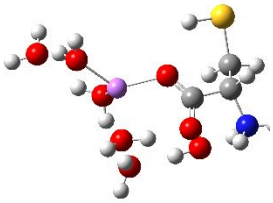
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0.090



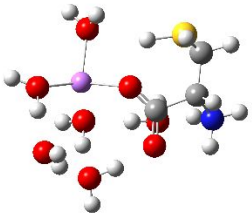
Z6-E
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Z6-F
0.126



Z6-G
0.129



Z6-H
0.166

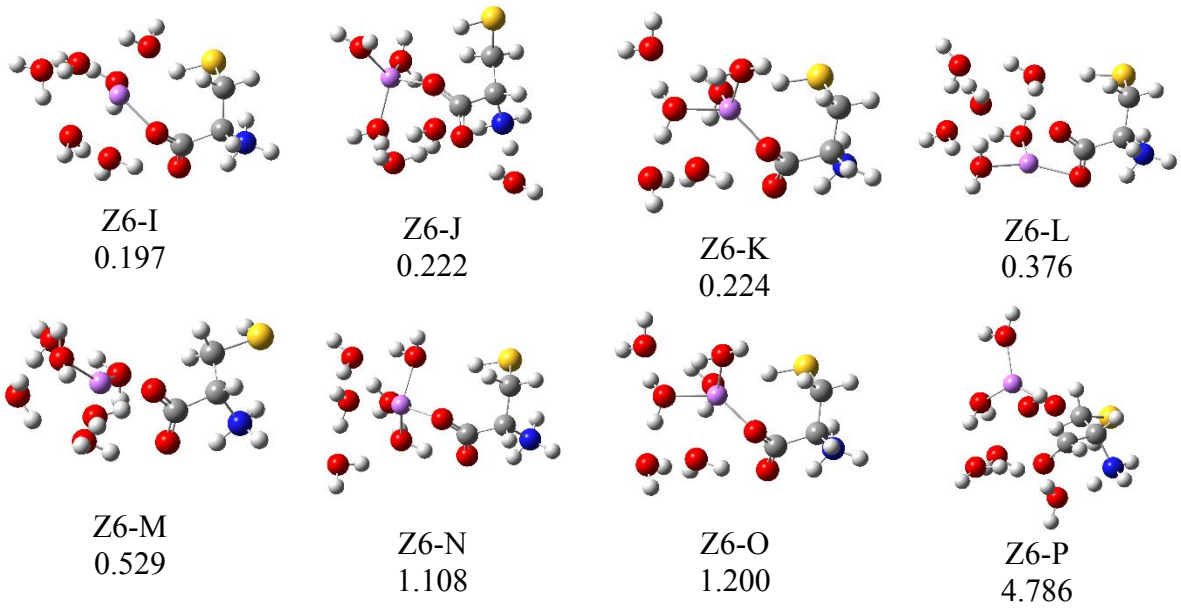
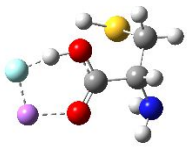
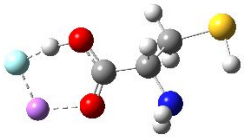


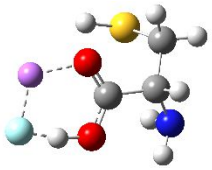
Figure S1. B3LYP-D3 (BJ)/6-311G (d, p) optimized structures of $Cys \cdot Li^{+}(H_2O)_n$(n=0-6) clusters. C in gray, N in blue, O in red, H in white, and S in yellow are used for all the structures. All of the structures are real minima based on the frequency calculation. Relative energies (eV) including zero-point energy are shown at B3LYP-D3 (BJ)/6-311+G (2d, p) level of theory.



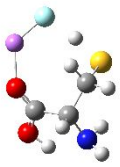
N-0A′
0.000



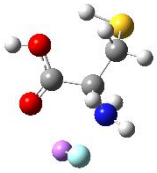
N-0B′
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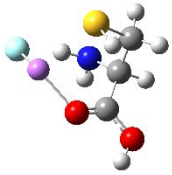
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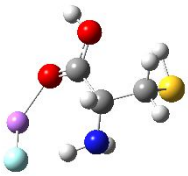
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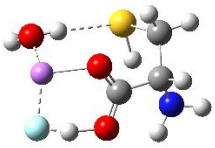
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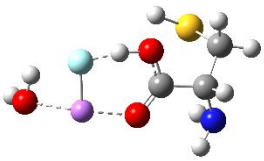
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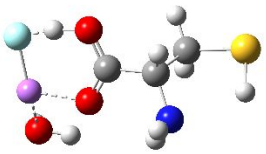
N-0G′
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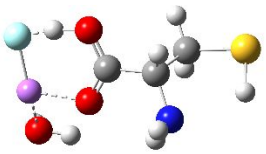
N-1A′
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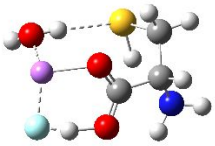
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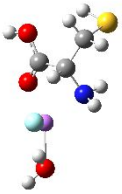
N-1C′
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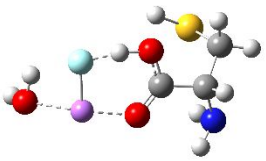
N-1D′
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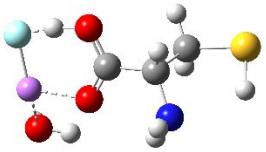
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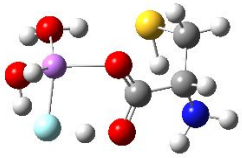
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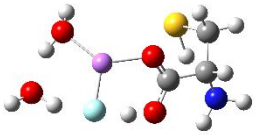
N-1G′
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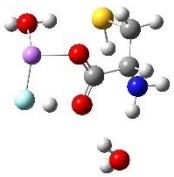
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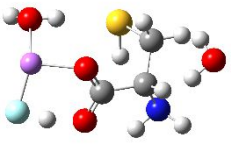
N-2A′
0.000



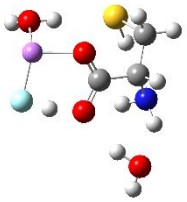
N-2B′
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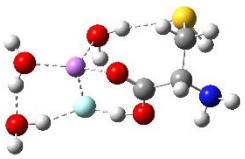
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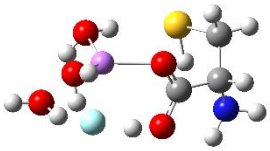
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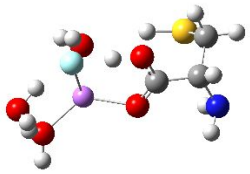
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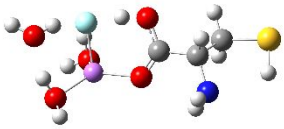
N-3A′
0.000



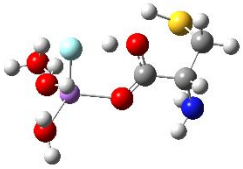
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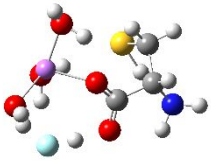
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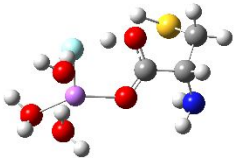
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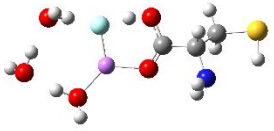
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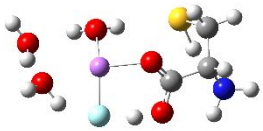
N-3F′
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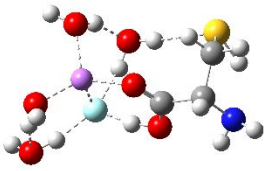
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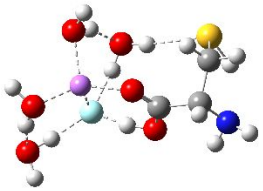
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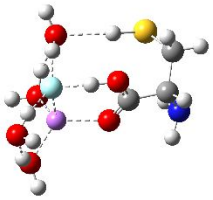
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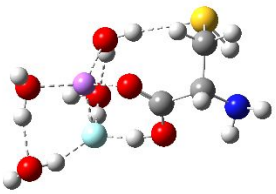
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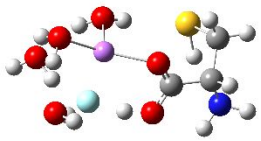
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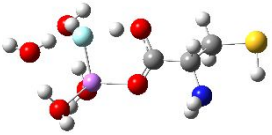
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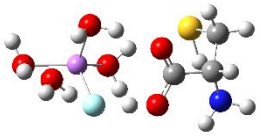
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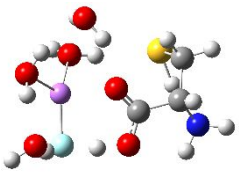
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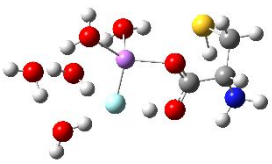
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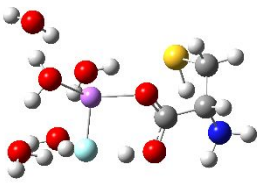
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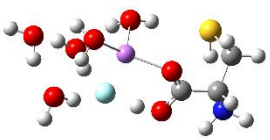
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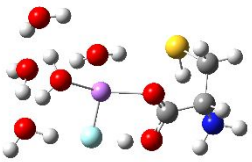
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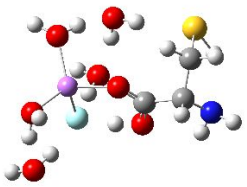
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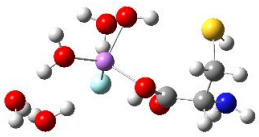
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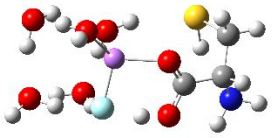
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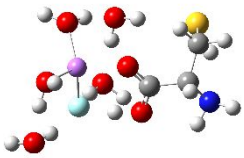
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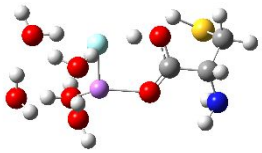
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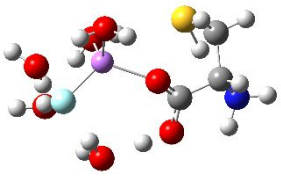
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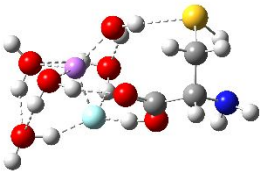
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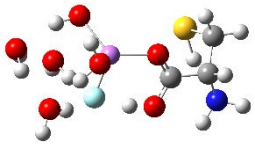
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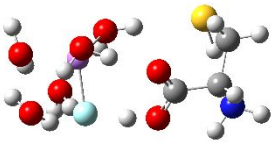
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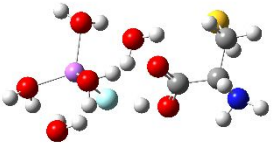
N-5K′
0.176



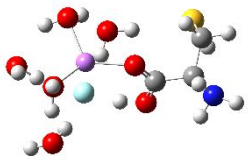
N-5L′
0.186



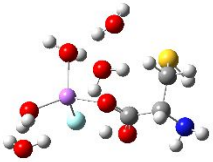
N-5M′
0.199



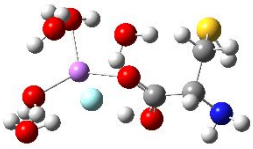
N-5N′
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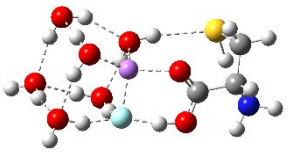
N-5O′
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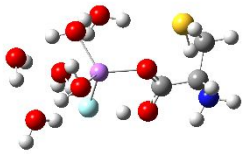
N-5P′
0.286



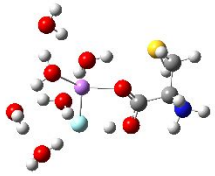
N-5Q′
0.405



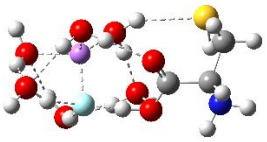
N-6A′
0.008



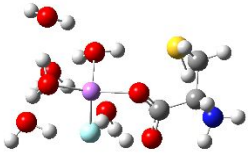
N-6B′
0.077



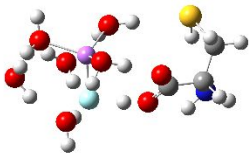
N-6C′
0.180



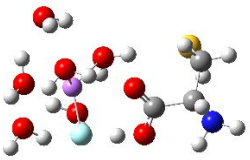
N-6D′
0.189



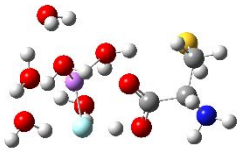
N-6E′
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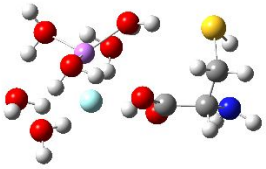
N-6F′
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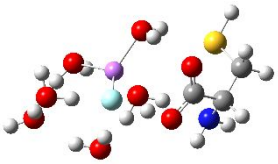
N-6G′
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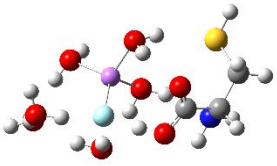
N-6H′
0.221



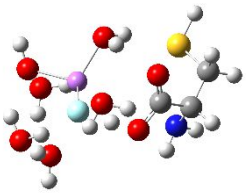
N-6I′
0.262



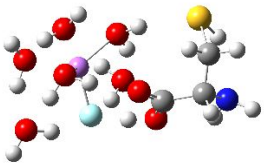
N-6J′
0.300



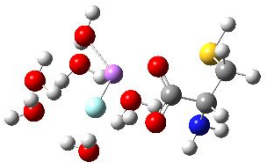
N-6K′
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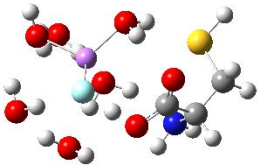
N-6L′
0.313



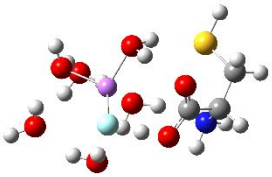
N-6M′
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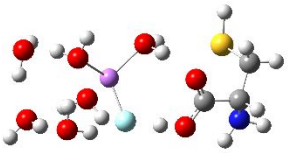
N-6N′
0.320



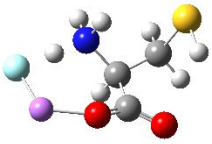
N-6O′
0.385



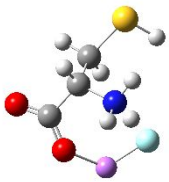
N-6P′
0.456



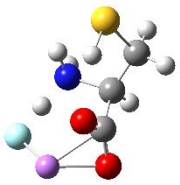
N-6Q′
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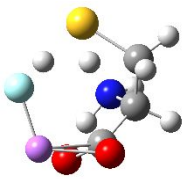
Z-0A′
0.077



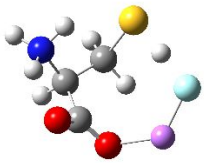
Z-0B′
0.152



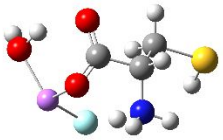
Z-0C′
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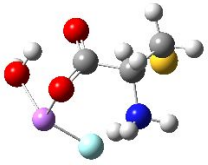
Z-0D′
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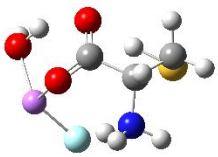
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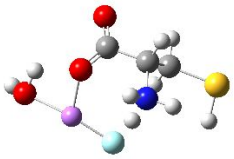
Z-1A′
0.121



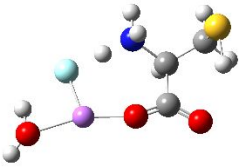
Z-1B′
0.182



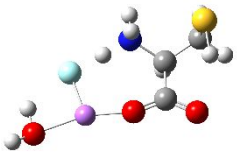
Z-1C′
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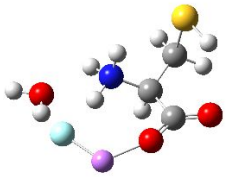
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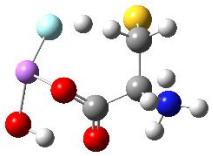
Z-1E′
0.233



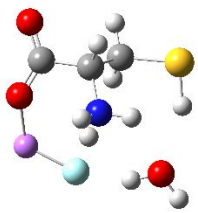
Z-1F′
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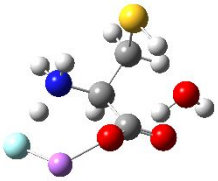
Z-1G′
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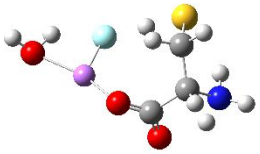
Z-1H′
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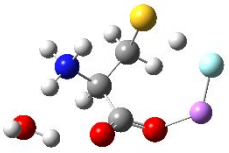
Z-1I′
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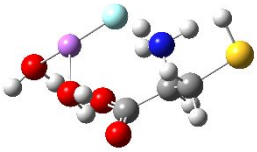
Z-1J′
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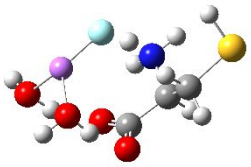
Z-1K′
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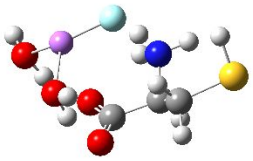
Z-1L′
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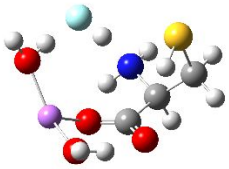
Z-2A′
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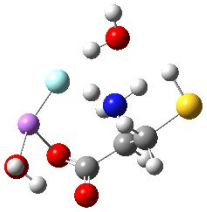
Z-2B′
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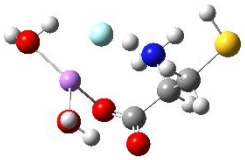
Z-2C′
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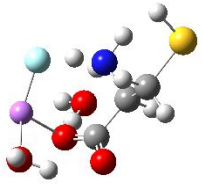
Z-2D′
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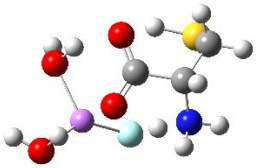
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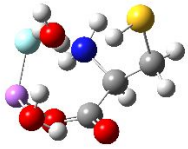
Z-2F′
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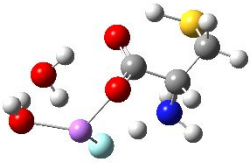
Z-2G′
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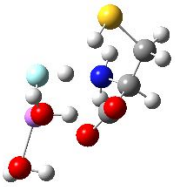
Z-2H′
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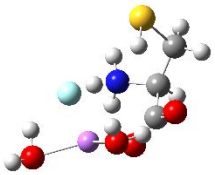
Z-2I′
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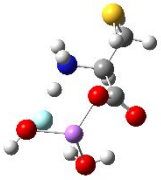
Z-2J′
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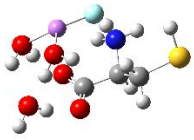
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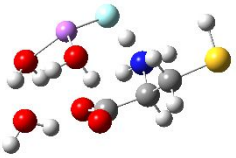
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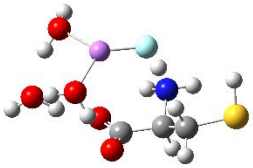
Z-2M′
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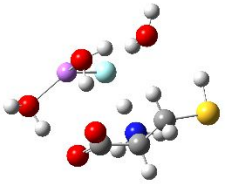
Z-3A′
0.049



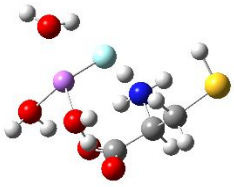
Z-3B′
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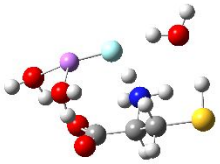
Z-3C′
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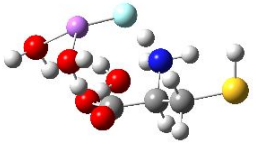
Z-3D′
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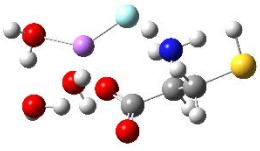
Z-3E′
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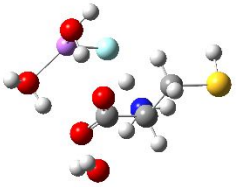
Z-3F′
0.128



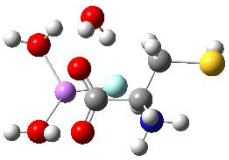
Z-3G′
0.151



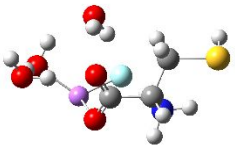
Z-3H′
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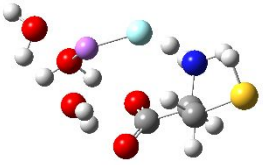
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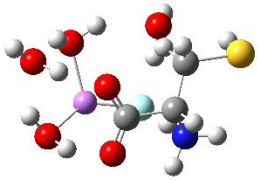
Z-3J′
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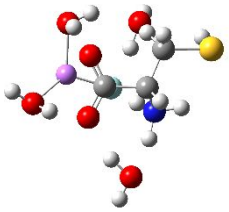
Z-3K′
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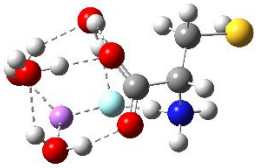
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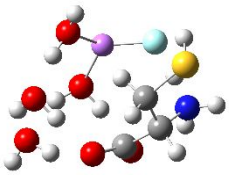
Z-4A′
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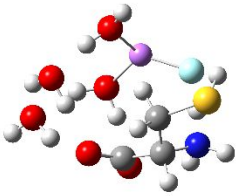
Z-4B′
0.048



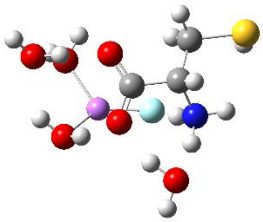
Z-4C′
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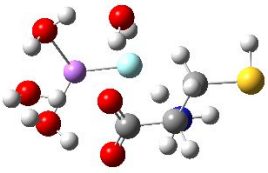
Z-4D′
0.062



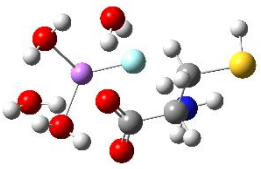
Z-4E′
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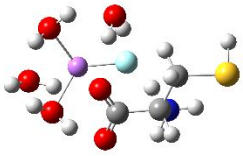
Z-4F′
0.070



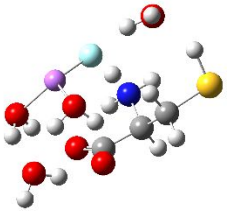
Z-4G′
0.072



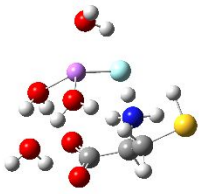
Z-4H′
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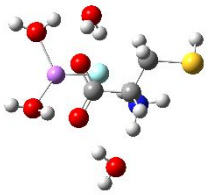
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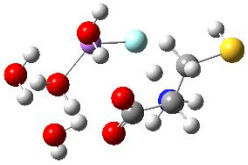
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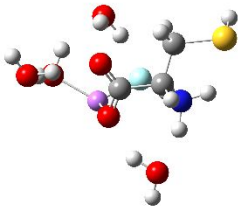
Z-4K′
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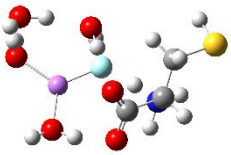
Z-4L′
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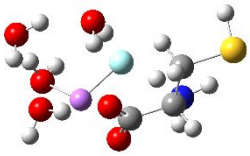
Z-4M′
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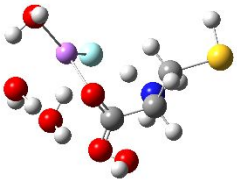
Z-4N′
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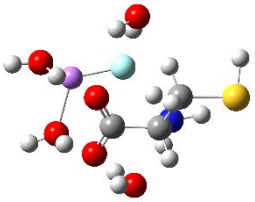
Z-4O′
0.281



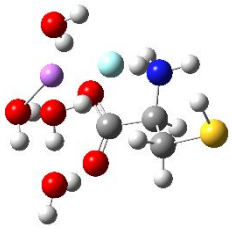
Z-4P′
0.329



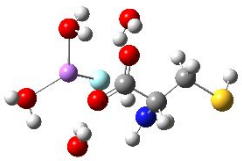
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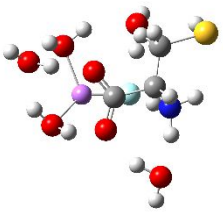
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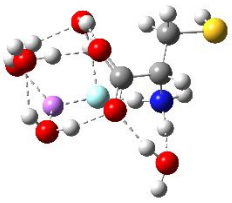
Z-4S′
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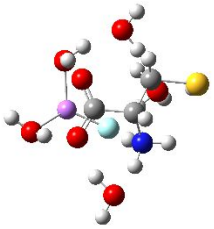
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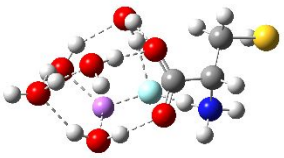
Z-5A′
0.000



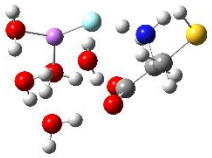
Z-5B′
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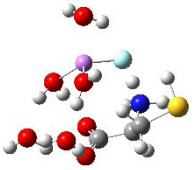
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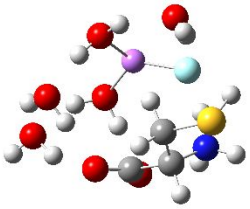
Z-5D′
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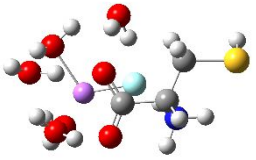
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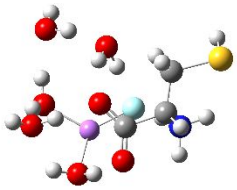
Z-5F′
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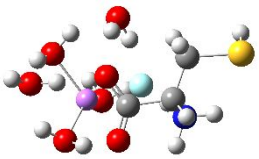
Z-5G′
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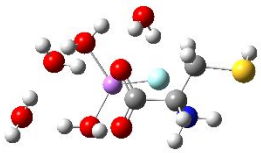
Z-5H′
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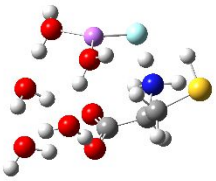
Z-5I′
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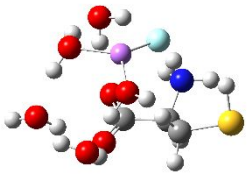
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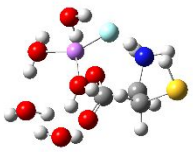
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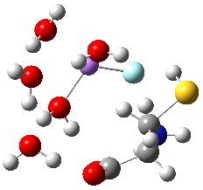
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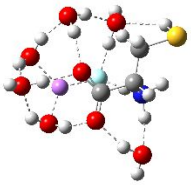
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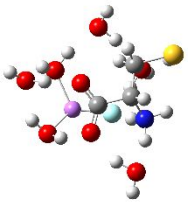
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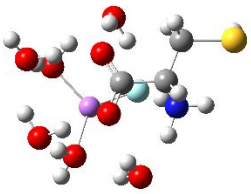
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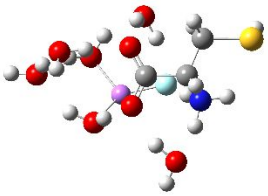
Z-6A′
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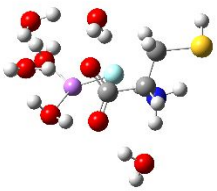
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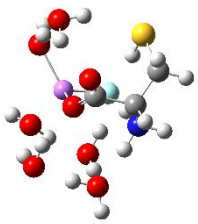
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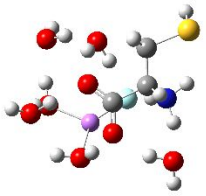
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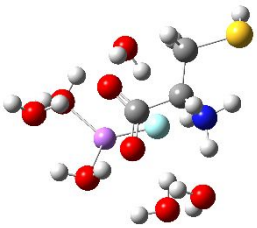
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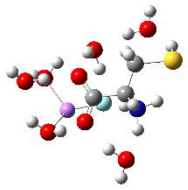
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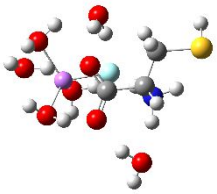
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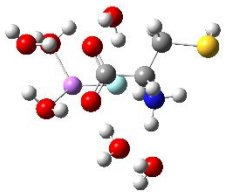
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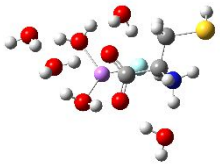
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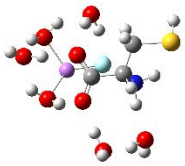
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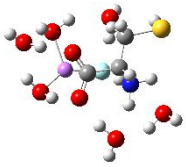
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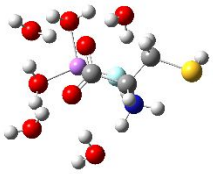
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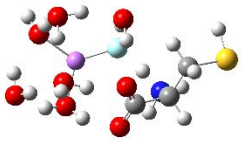
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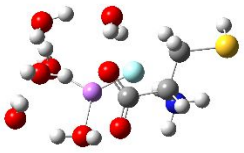
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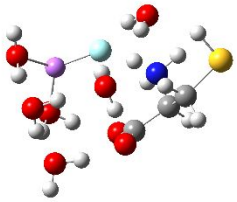
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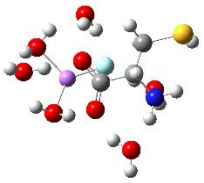
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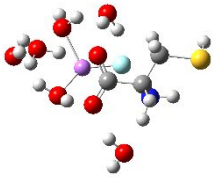
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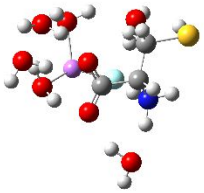
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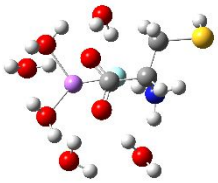
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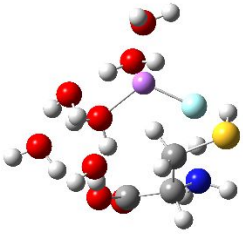
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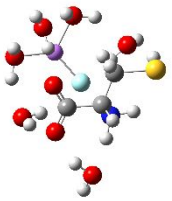
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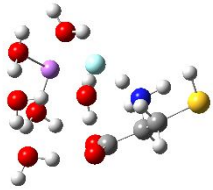
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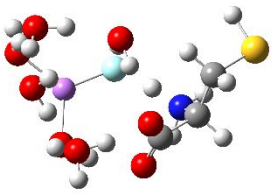
Z-6W′
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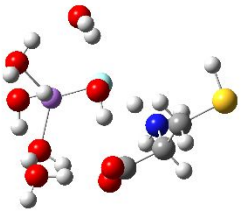
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0.263



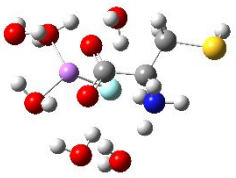
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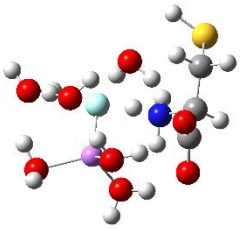
Z-6Z′
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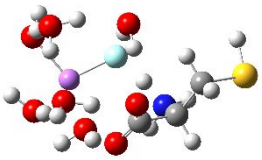
Z-6ZA′
0.282



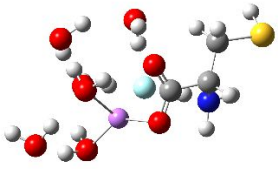
Z-6ZB′
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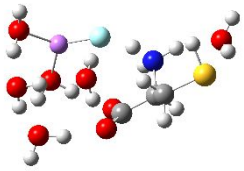
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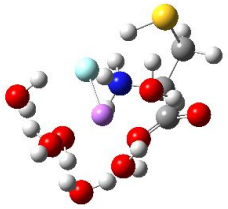
Z-6ZD′
0.306



Z-6ZE′
0.315

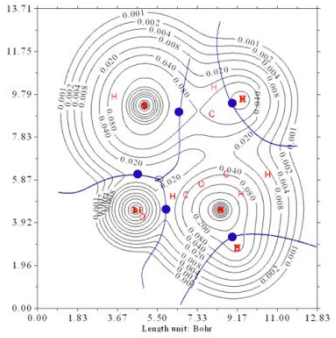


Z-6ZF′
0.326

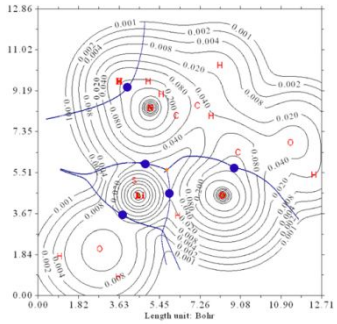


Z-6ZG′
0.452

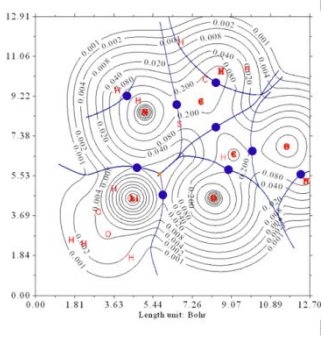
Figure S2. B3LYP-D3 (BJ)/6-311G (d, p) optimized structures of Cys·LiF$(H_2O)_n$(n=0-6) clusters. C in gray, N in blue, O in red, H in white, and S in yellow are used for all the structures. All of the structures are real minima based on the frequency calculation. Relative energies (eV) including zero-point energy are shown at B3LYP-D3 (BJ)/6-311+G (2d, p) level of theory.



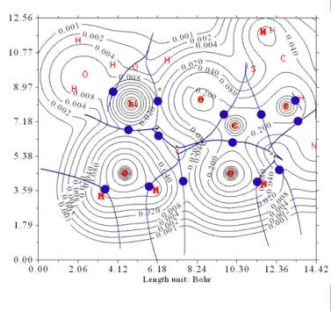
N-0A



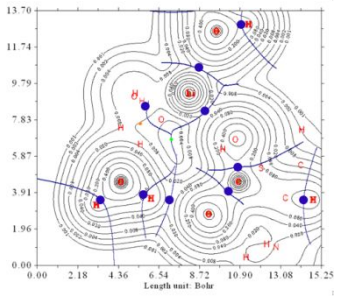
N-1A



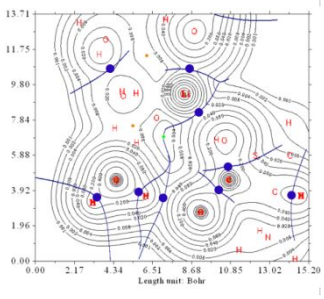
N-2A



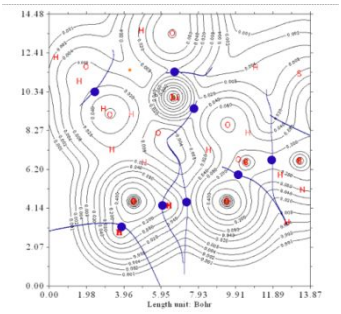
N-3A



Z-4A

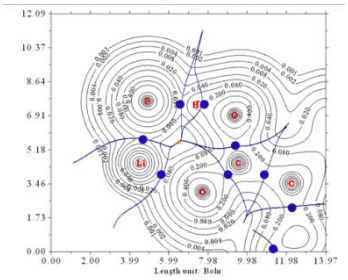


Z-5A

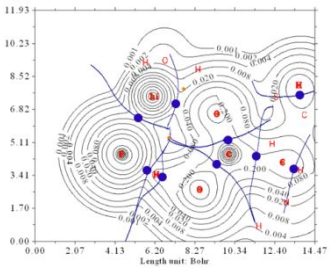


Z-6A

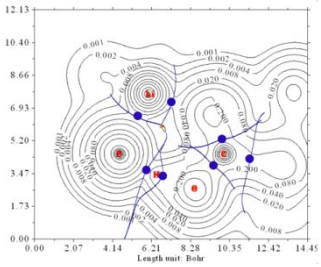
Figure S3. The 2D electron density (ρ_{BCP}) map of the $Cys{\cdot}Li^{+}(H_2O)_n$(n = 0-6) isomers are calculated at B3LYP/ 6-311+G(2d,p) level of theory



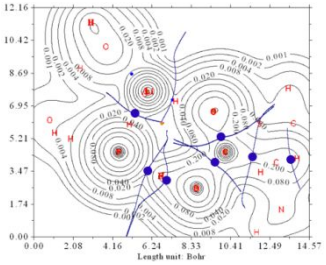
N-0A′



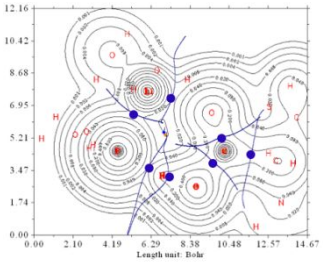
N-1A′



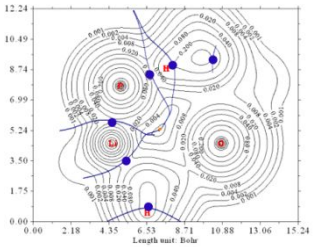
N-2A′



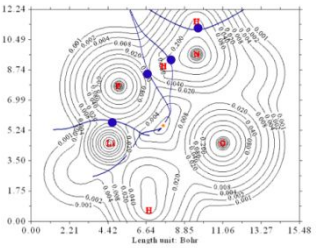
N-3A′



N-4A′

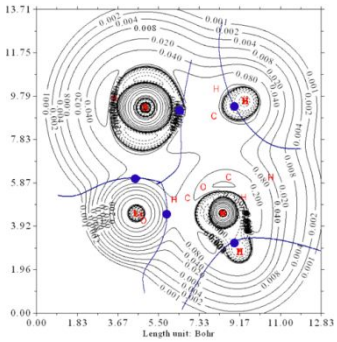


Z-5A′

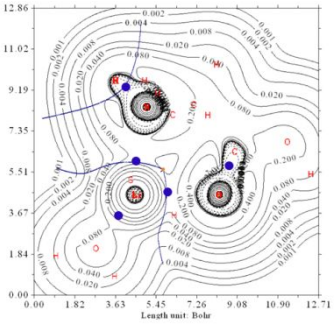


Z-6A′

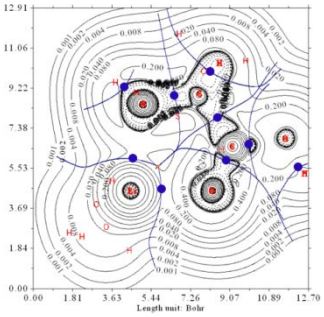
Figure S4. The 2D electron density (ρ_{BCP}) map of the Cys·LiF$(H_2O)_n$(n = 0-6) isomers are calculated at B3LYP/ 6-311+G(2d,p) level of theory



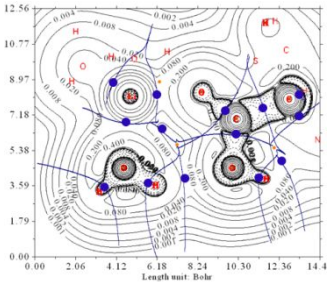
N-0A



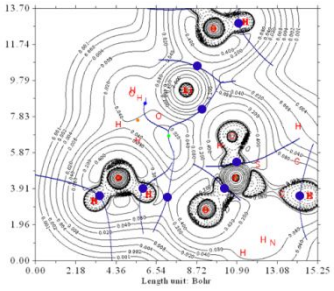
N-1A



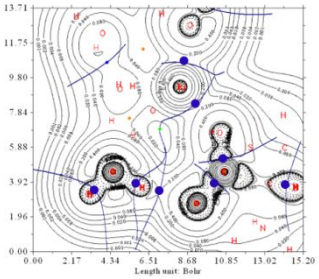
N-2A



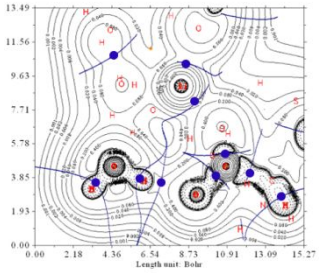
N-3A



Z-4A

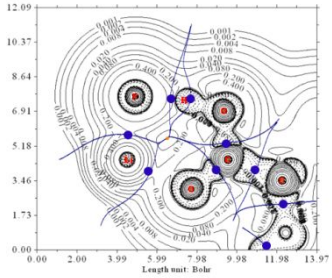


Z-5A

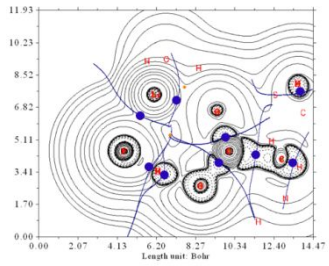


Z-6A

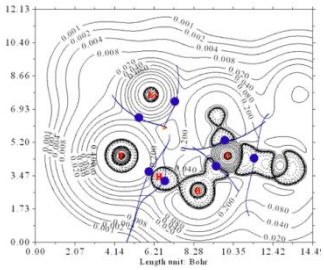
Figure S5. The 2D Laplacian of electron density ($\nabla^2\rho_{BCP}$) map of the Cys·$Li^+(H_2O)_n$(n = 0-6) isomers are calculated at B3LYP/ 6-311+G(2d,p) level of theory



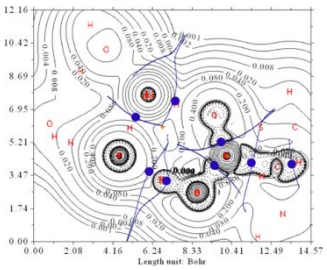
N-0A′



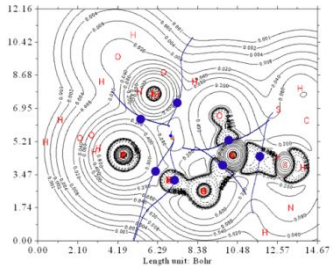
N-1A′



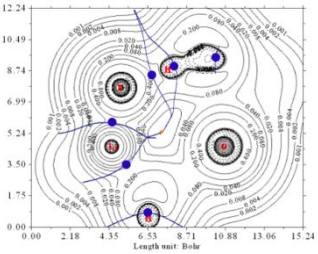
N-2A′



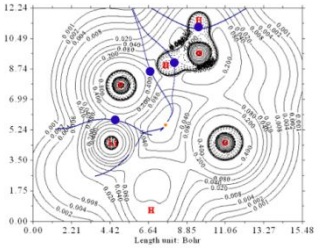
N-3A′



N-4A′



Z-5A′



Z-6A′

Figure S6. The 2D laplacian of electron density ($\nabla^2\rho_{BCP}$) map of the Cys·LiF$(H_2O)_n$(n = 0-6) isomers are calculated at B3LYP/ 6-311+G(2d,p) level of theory

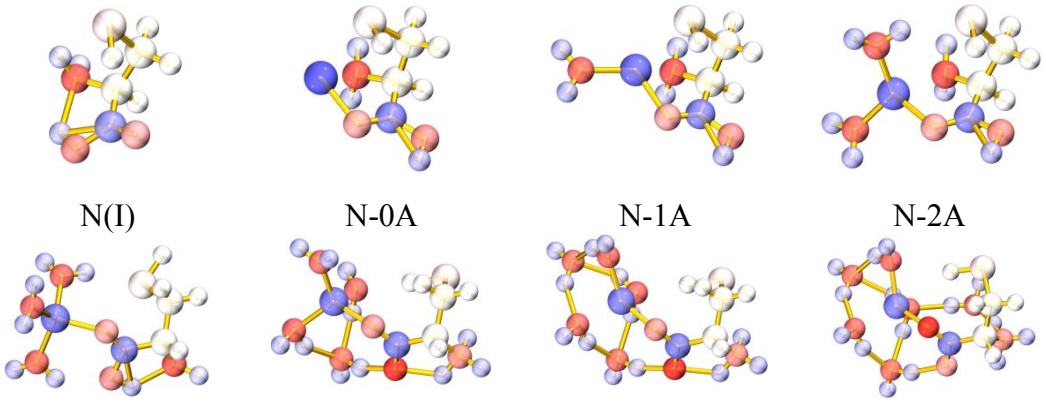


Figure S7. NPA charge calculation of Cys·$Li^{+}(H_2O)_n$(n = 0-6), blue represents a positive charge, red represents a negative charge, and shades represent the size of the charge

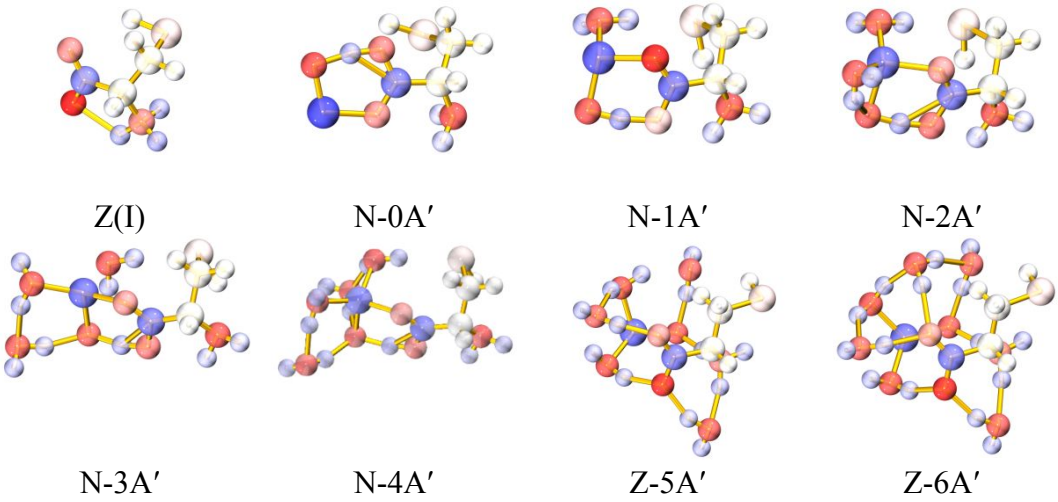


Figure S8. NPA charge calculation of Cys·$LiF(H_2O)_n$(n = 0-6) isomers, blue represents a positive charge, red represents a negative charge, and shades represent the size of the charge