

Supporting Information:

Exploiting the role of stereoelectronic effects to design the antagonists of human complement C3a receptor.

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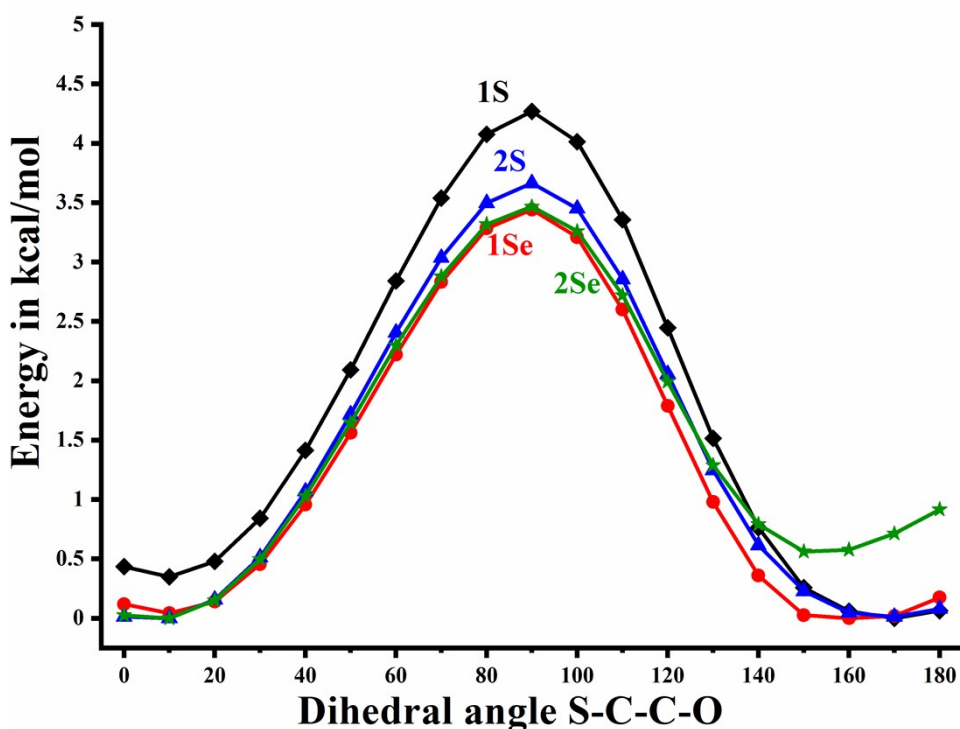


Figure S1: Variation in energy with dihedral angle X–C–C–O (X = S, Se) reveals barriers to rotation from low energy conformations. **1S** (black) shows preferred dihedral angle 180°, **1Se** (red), **2S** (blue) shows no preference, and **2Se** (green) shows preference for 0°.

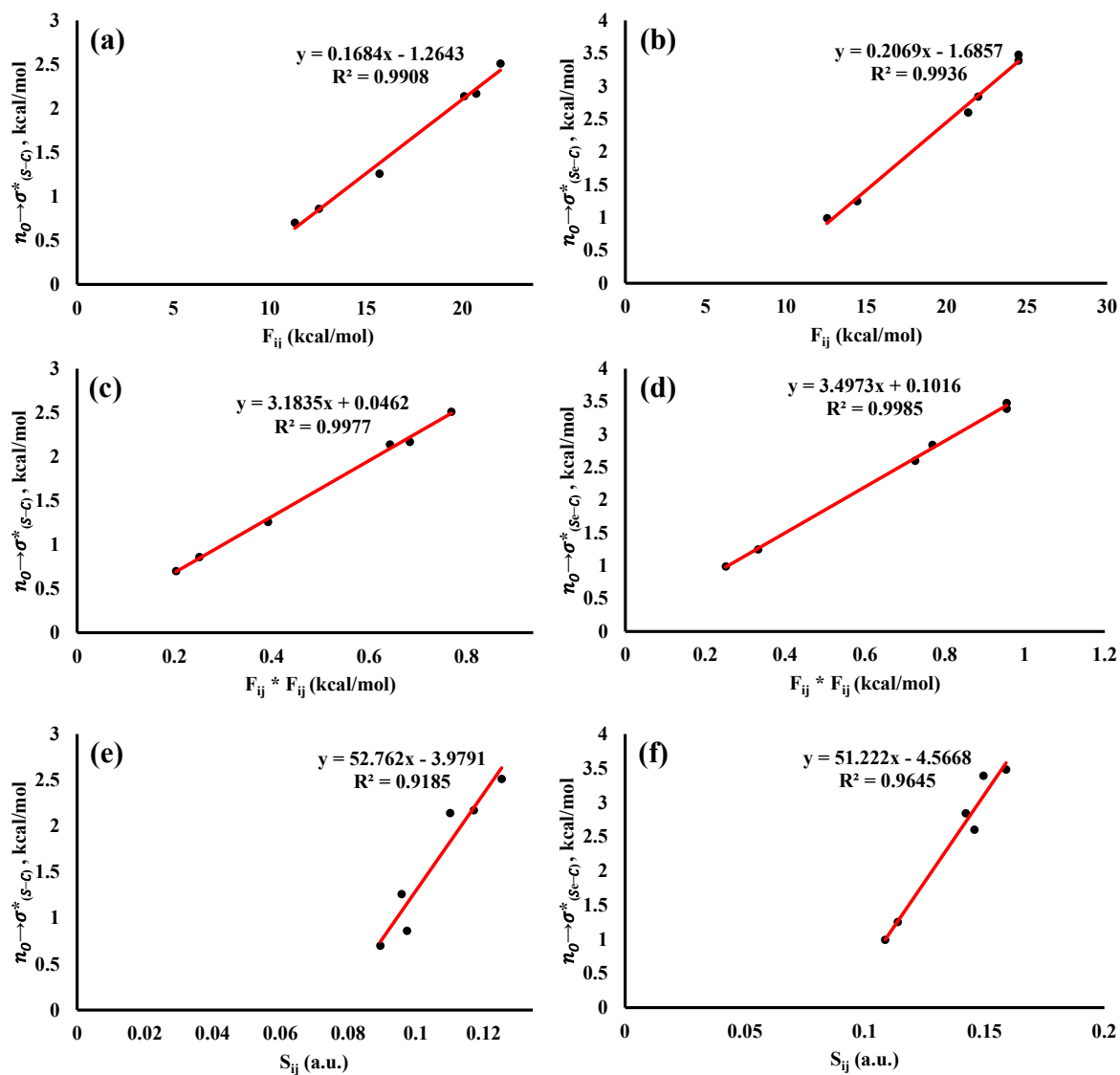


Figure S2: Correlations of energies of interactions a) $n_{O \rightarrow \sigma^* C-S}$ with the corresponding Fock matrix elements (F_{ij}). b) $n_{O \rightarrow \sigma^* C-Se}$ with the corresponding Fock matrix elements (F_{ij}). c) $n_{O \rightarrow \sigma^* C-S}$ with the square of corresponding Fock matrix elements ($F_{ij} * F_{ij}$). d) $n_{O \rightarrow \sigma^* C-Se}$ with the the square of corresponding Fock matrix elements ($F_{ij} * F_{ij}$). e) $n_{O \rightarrow \sigma^* C-S}$ with the corresponding overlap matrix elements (S_{ij}). f) $n_{O \rightarrow \sigma^* C-Se}$ with the corresponding overlap matrix elements (S_{ij}).

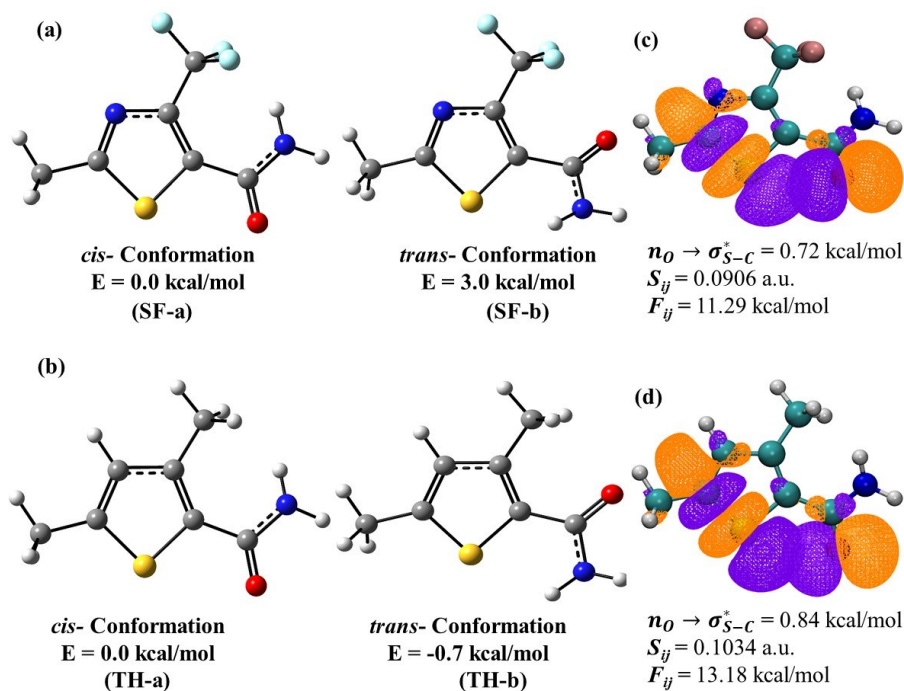


Figure S3: The geometries of cis and trans conformation and electronic energies of (a) 2-methyl-4-(trifluoromethyl)thiazole-5-carboxamide (SF) and (b) 3,5-dimethylthiophene-2-carboxamide (TH) and orbital overlapping ($n_O \rightarrow \sigma_{S-C}^*$) of (c) SF-a and (d) TH-a.

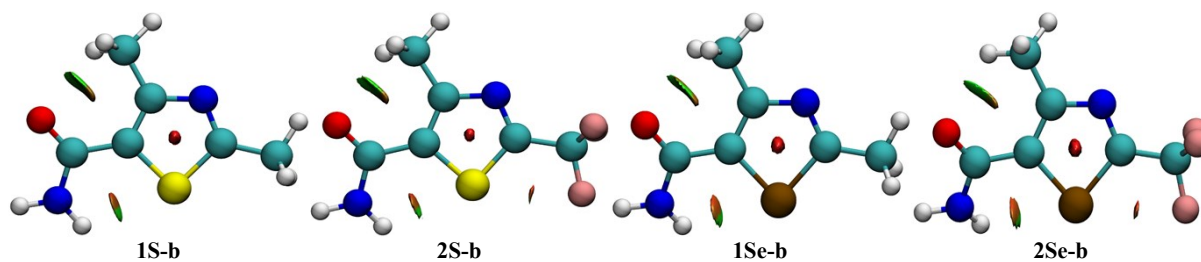


Figure S4: NCI plots showing the non-covalent van der Waals interaction between thiazole/selenazole ring and the amide moiety using the color-filled RDG iso-surface. The green and light brown color represents van der Waals (vdW), and red color represents ring current.

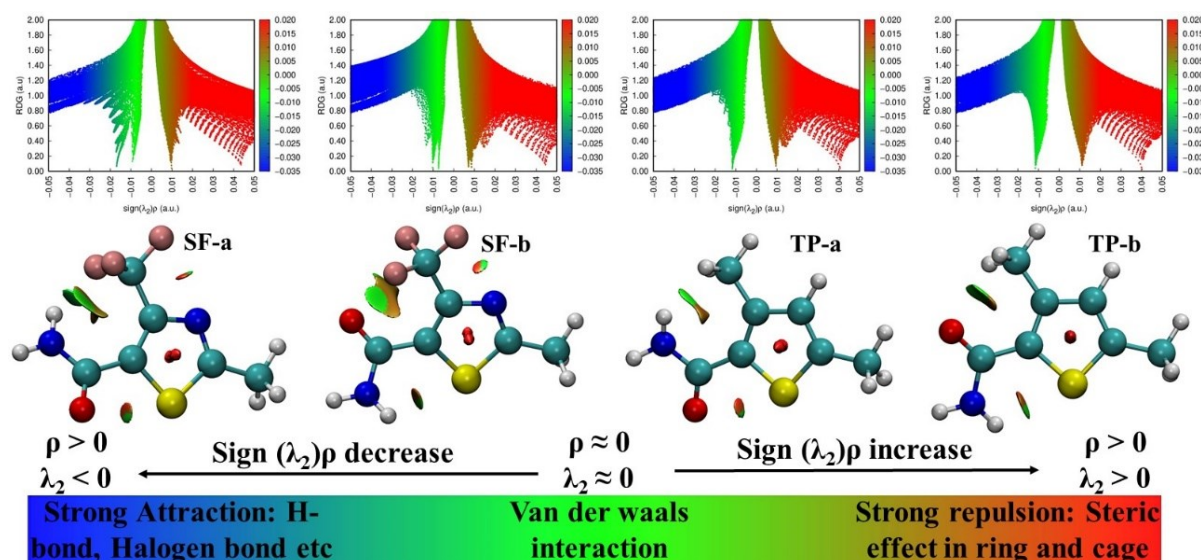


Figure S5: NCI plots showing the non-covalent van der Waals interaction between thiazole and thiophene rings and the amide moiety using the color-filled RDG iso-surface as well as scatter graph. The blue, green, and red circles represent hydrogen (H) bond, van der Waals (VdW), and steric repulsive interactions, respectively. (C-cyan, N-blue, O-red, S-yellow, Se-brown, H-white, F-pink)

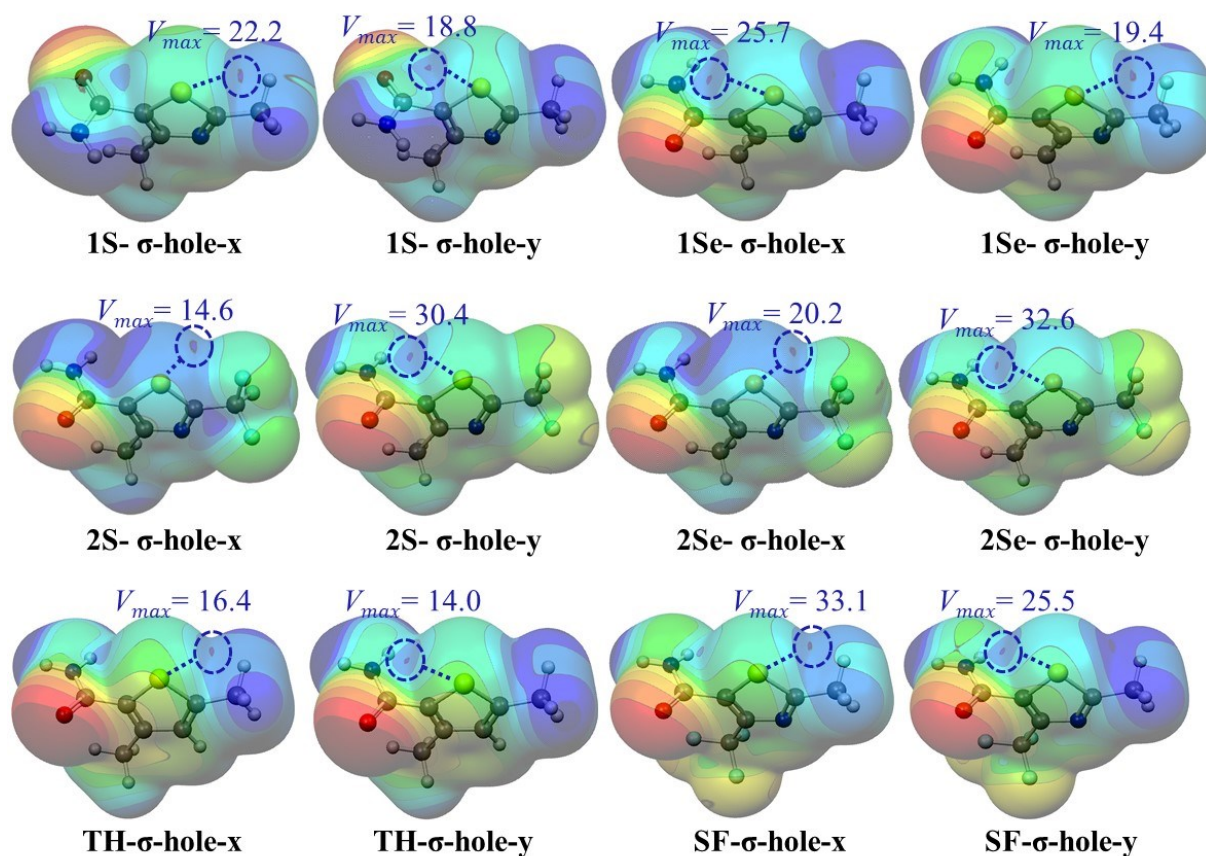


Figure S6: Molecular electrostatic potential (MESP) surface computed at the CBS-QB3 method showing the locations of the σ -Holes at 0.001 a.u. isodensity surface. V_{max} values are in kcal/mol unit. Minimum potential kept constant in all the structures at -37.65 kcal/mol. Blue and light blue colors indicate the positive potential, and green, yellow and red color indicate the negative potentials.

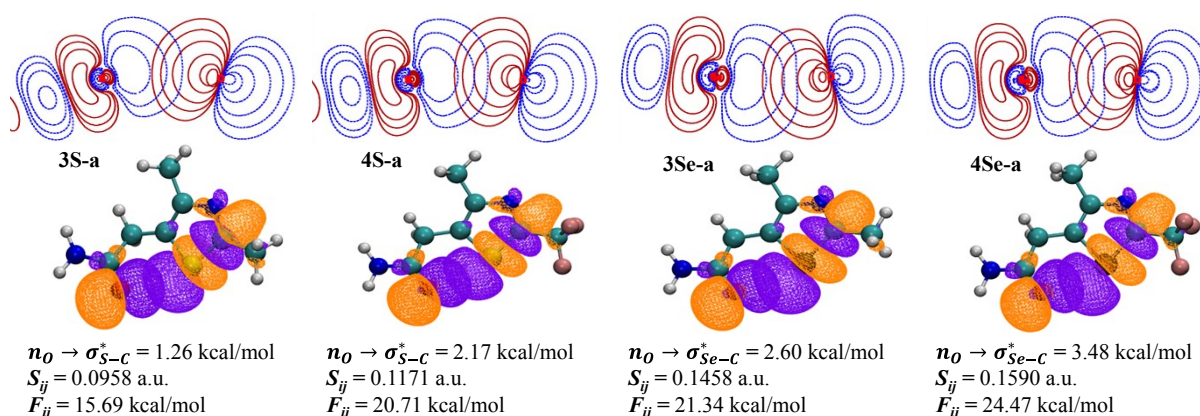


Figure S7: n to σ^* interaction between n_O of amide group and σ^* orbital of C-X bond in 3S-a, 4S-a, 3Se-1, 4Se-a. The top diagram of each scaffold shows contour lines and 3D visualize the orbital overlap of the same interaction along with the interaction energy, overlap and fock matrix elements mentioned at the bottom of the structures.

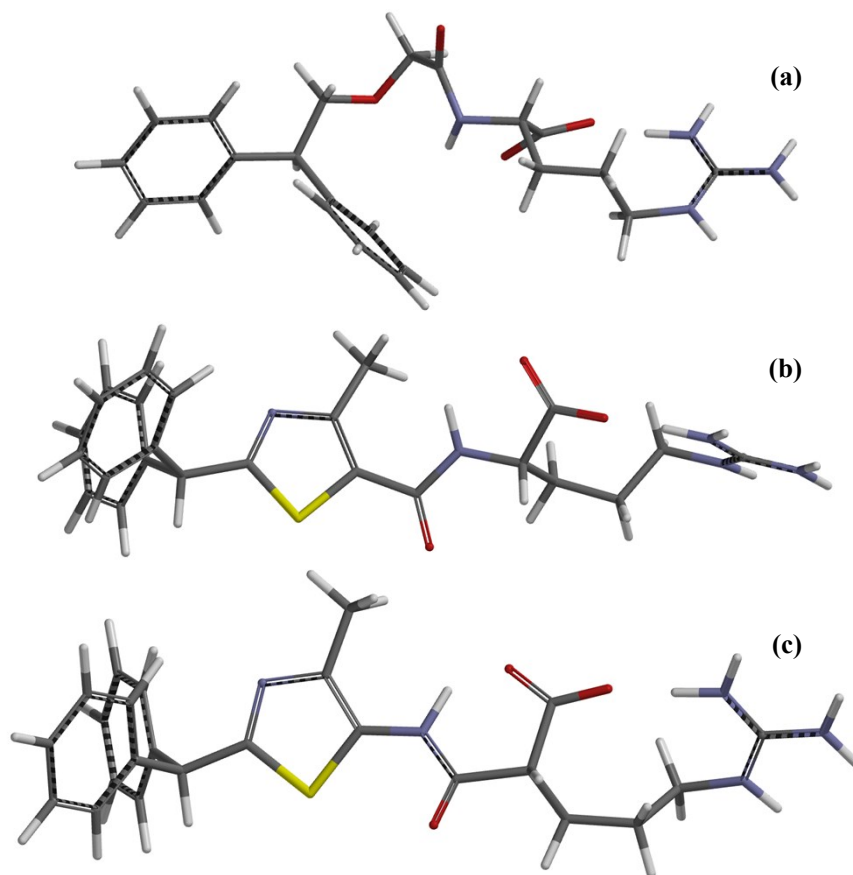
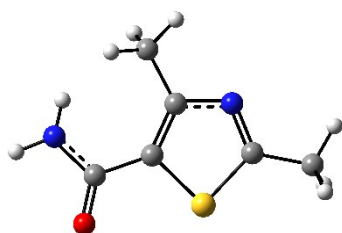


Figure S8: Minimized geometries of a) SB290157 b) L-1 c) L-2 at Merck Molecular Force Field (MMFF).

Coordinates:

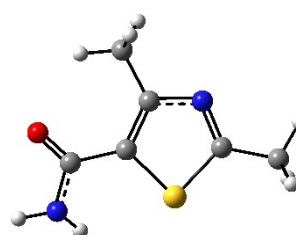
1S-a



Electronic Energy: -815.0962211 a.u.

C	-0.51730000	-0.10150400	-0.00072600
C	0.03139500	1.16246900	0.04249400
C	1.92354600	-0.00167600	-0.01901900
S	0.75561100	-1.28769400	-0.03708800
N	1.40483300	1.19628000	0.02869600
C	-1.90659100	-0.61758900	0.01445300
O	-2.14201100	-1.79732300	0.22160900
N	-2.91093400	0.29694100	-0.19176800
H	-2.72874300	1.16696600	-0.66309100
H	-3.83409300	-0.09733600	-0.29402100
C	3.39820100	-0.26079400	-0.05003700
C	-0.69259500	2.47726200	0.12462800
H	-0.01008200	3.22773800	0.52249600

1S-b

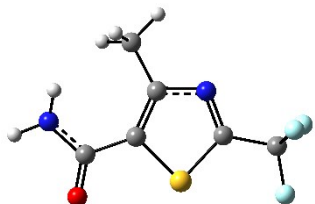


Electronic Energy: -815.0963456 a.u.

C	-0.53223600	-0.05171700	0.02191400
C	0.07306200	1.18286300	-0.05570600
C	1.92704200	-0.05299400	-0.00124400
S	0.69902900	-1.29229200	0.09757700
N	1.44974400	1.15351600	-0.07179100
C	-1.98646600	-0.35357500	0.04357000
O	-2.82818900	0.48743700	0.31221500
N	-2.32980100	-1.65668300	-0.22870200
H	-1.70939600	-2.26115500	-0.74293300
H	-3.31893800	-1.83948600	-0.30519900
C	3.38777000	-0.37947800	0.01826300
C	-0.60115400	2.51774800	-0.12521200

H	-1.01089300	2.82247000	-0.86668700
H	-1.57241800	2.42081300	0.76788800
H	3.71336000	-0.88254400	0.79210000
H	3.69355200	-0.77324500	-0.96974800
H	3.91839300	0.69527100	0.00234200

2S-a

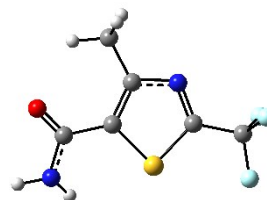


Electronic Energy: -1112.4882609 a.u.

C	1.38217100	-0.08752500	0.00320700
C	0.90154900	1.20883800	0.04798400
C	-1.01472500	0.12609500	0.00284000
S	0.06601300	-1.21443700	-0.02260000
N	-0.46437400	1.30528700	0.04460500
C	2.74620300	-0.68231200	0.00863000
O	2.90429700	-1.87435200	0.21160500
N	3.79438900	0.17176500	-0.20277000
H	3.66296500	1.07192100	-0.63170800
H	4.70077100	-0.26187200	-0.29388600
C	-2.51088600	-0.05177600	-0.01737100
C	1.69450100	2.48294100	0.11866100
H	1.04612200	3.27897500	0.48260400
H	2.55254800	2.39223400	0.78719900
H	2.05583700	2.78492400	-0.87147500
F	-2.83127300	-1.36424600	-0.03418500
F	-3.05926900	0.51622600	-1.10439300
F	-3.08854700	0.49720700	1.06296500

H	-0.44640200	3.05504700	0.81615600
H	-0.14469800	3.11546600	-0.91792600
H	-1.67104600	2.41698000	-0.28568200
H	3.67067300	-0.88657800	0.94472300
H	3.66456600	-1.02968500	-0.81589900
H	3.94856400	0.55166000	-0.05824400

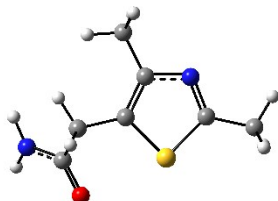
2S-b



Electronic Energy: -1112.4878444 a.u.

C	1.39456900	-0.04591900	-0.01402400
C	0.88914300	1.23775300	0.07198100
C	-1.02020900	0.13006700	0.01144000
S	0.08804400	-1.19289800	-0.09731100
N	-0.48171000	1.30614300	0.09026800
C	2.82782100	-0.45583700	-0.05291200
O	3.71161100	0.31580500	-0.37900400
N	3.08079900	-1.76485300	0.26953200
H	2.43259700	-2.30528100	0.81946300
H	4.05399300	-2.02754300	0.31362200
C	-2.51251300	-0.07959700	-0.00902600
C	1.66557000	2.51488100	0.14428500
H	1.25120800	3.14916000	0.93099900
H	2.72264600	2.33030600	0.31465100
H	1.56411400	3.05733800	-0.80088200
F	-2.80177400	-1.39752200	-0.09968500
F	-3.09041700	0.38935400	1.10795900
F	-3.08403800	0.53692600	-1.05470800

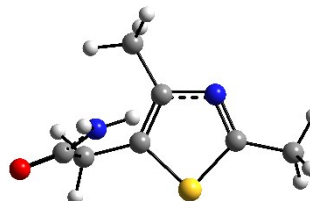
3S-a



Electronic Energy: -854.3129731 a.u.

C	-2.18595100	-0.37387600	0.12751600
C	-0.75619600	1.32104500	-0.02135900
C	0.11740300	0.32114100	-0.36146500
S	-0.72128400	-1.20905100	-0.33223800
N	-2.04495800	0.91125300	0.25537200
C	1.56049600	0.42269600	-0.76259500
H	1.87450300	1.46668600	-0.71094300
H	1.68820300	0.10663000	-1.80516100
C	2.49018700	-0.48048800	0.05885400
N	3.57093900	0.14025000	0.61095100

3S-b

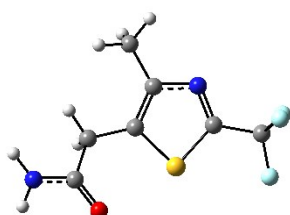


Electronic Energy: -854.316761 a.u.

C	-2.24705100	-0.21466800	0.12977500
C	-0.55090200	1.19809400	-0.16276800
C	0.12070900	0.05335100	-0.50924900
C	1.54714700	-0.12632400	-0.93579200
H	1.88618800	0.75808800	-1.48260300
H	1.65016100	-0.95914100	-1.63451400
C	2.61014900	-0.36992900	0.15539800
O	3.74923600	-0.66003200	-0.15197100
N	2.19764000	-0.20806600	1.44074800
C	-3.62651900	-0.70024000	0.45148600

O	2.28958000	-1.67390100	0.17157200
C	-0.46944800	2.79179500	0.07280100
C	-3.46931500	-1.10377100	0.38255300
H	-0.68075400	3.15300300	1.08332400
H	0.56553100	3.03668100	-0.16896300
H	-1.11931600	3.34718700	-0.60941000
H	-3.77729900	-1.69316600	-0.48531400
H	-3.37921900	-1.78652600	1.23230000
H	-4.24435700	-0.37019800	0.60469800
H	4.20077600	-0.41390100	1.17024800
H	3.69092300	1.13785900	0.59036400

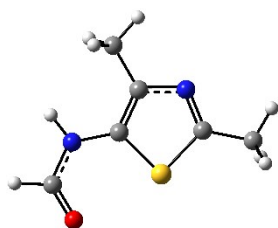
4S-a



Electronic Energy: -1151.707232 a.u.

C	1.34327900	0.14201700	-0.03512700
C	-0.26189400	1.64357400	0.00235400
C	-1.03484700	0.52492000	-0.22163500
C	-2.51535600	0.48615700	-0.45957000
H	-2.72401400	0.52253600	-1.53787200
H	-2.96775800	1.38414000	-0.03165500
C	-3.21979100	-0.77120800	0.05890600
O	-2.67188000	-1.85650700	0.09173400
N	-4.51705700	-0.59099700	0.42667800
C	2.73948000	-0.40314700	0.07856300
C	-0.74696000	3.06153200	0.10768000
H	-1.73908900	3.12869400	0.55974200
H	-0.04887600	3.63470200	0.71823400
H	-0.79572400	3.53906300	-0.87678300
N	1.08374800	1.40564100	0.11491300
H	-4.96579200	0.30851300	0.41863200
H	-5.04513200	-1.39751500	0.72131100
S	-0.02445500	-0.88548000	-0.29843400
F	3.24899300	-0.22900300	1.31270400
F	3.57856900	0.19202000	-0.78735000
F	2.75714800	-1.73034800	-0.18187600

5S-a

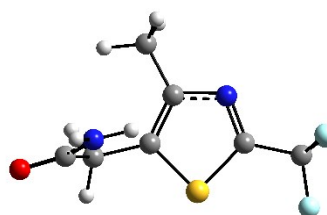


Electronic Energy: -815.0782887 a.u.

C	-0.49069700	0.37480600	-0.00000800
C	0.48539100	1.33798900	0.00000800

C	0.00958300	2.58958500	-0.14118400
H	-0.57762800	3.24188000	-0.79325300
H	-0.04728500	3.00821300	0.86786800
H	1.05051400	2.61990800	-0.46375400
N	-1.87462000	1.02667200	0.19224400
H	1.23568800	-0.01965700	1.66784100
H	2.86281100	-0.37597200	2.17834200
H	-4.23426400	0.15766200	0.73863600
H	-4.09013400	-1.18787100	-0.41038100
H	-3.61863000	-1.41897000	1.27552000
S	-0.97194600	-1.30333400	-0.38030500

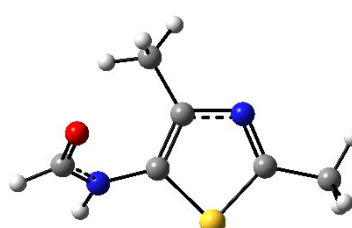
4S-b



Electronic Energy: -1151.709066 a.u.

C	1.36297300	0.10908600	0.07621700
C	-0.46893400	1.33041700	0.20769100
C	-1.01785100	0.11744700	0.56539800
C	-2.43727400	-0.21255400	0.91960500
H	-2.88720600	0.62071700	1.46552000
H	-2.48555000	-1.06729500	1.59740400
C	-3.42215700	-0.53721900	-0.22496300
O	-4.56065000	-0.86938600	0.03305800
N	-2.94434700	-0.40789300	-1.49075000
C	2.81379600	-0.21180900	-0.16377100
C	-1.19251700	2.63956000	0.10062400
H	-0.73029800	3.37862700	0.75997800
H	-1.12591800	3.02874500	-0.91901600
H	-2.24654200	2.54891300	0.36277600
N	0.87741300	1.30149900	-0.06511400
H	-1.98565800	-0.17007900	-1.68086700
H	-3.56167700	-0.63022600	-2.25543800
S	0.22024000	-1.10273400	0.55735400
F	3.62024100	0.51660900	0.62382900
F	3.05702000	-1.51705500	0.09172400
F	3.16991000	0.02540500	-1.43847000

5S-b

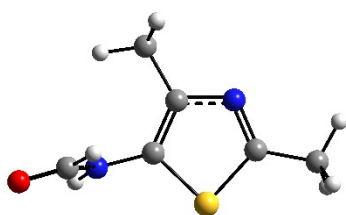


Electronic Energy: -815.0763542 a.u.

C	0.40337800	-0.30775000	0.39469200
C	0.05127900	1.00620500	0.25302300

C	1.79927500	-0.45540200	0.00001700
S	0.21623900	-1.21600300	-0.00002600
N	1.76921500	0.84396100	0.00001400
N	-1.86930400	0.60827500	0.00001000
H	-2.16392700	1.57413900	-0.00017400
C	-2.84361200	-0.35288000	-0.00002900
H	-3.85583400	0.08691000	-0.00010300
O	-2.63450200	-1.54626700	-0.00000900
C	0.25189300	2.82192800	0.00006200
C	3.05843200	-1.26650400	0.00001100
H	1.21620000	3.32894200	-0.00073400
H	-0.30213500	3.15411400	-0.88544100
H	-0.30074800	3.15425300	0.88638000
H	3.90603800	-0.58098100	0.00022500
H	3.12646200	-1.90838800	0.88301200
H	3.12665600	-1.90806500	-0.88321100

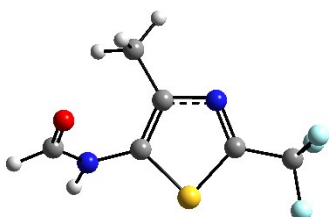
5S-c



Electronic Energy: -815.0763115 a.u.

C	0.38141600	-0.04965800	-0.28151900
C	-0.23281900	1.15693700	-0.07849300
C	-2.04050300	-0.13248000	0.10146000
S	-0.81034200	-1.33889600	-0.19368500
N	-1.59099000	1.08698200	0.13751800
N	1.74171600	-0.30972200	-0.50877700
H	2.06879000	-0.50803500	-1.44700700
C	2.69047600	-0.41904400	0.48628600
H	2.25724900	-0.23629000	1.48644200
O	3.85275900	-0.67481800	0.28807000
C	0.43578000	2.49643900	-0.08410400
C	-3.48062300	-0.49711000	0.28856500
H	0.34806300	2.97187700	0.89697700
H	1.49222600	2.41334500	-0.33938900
H	-0.05334900	3.15448500	-0.80700800
H	-4.04477400	0.41767500	0.46974700
H	-3.88559000	-0.99234400	-0.59814900
H	-3.61665100	-1.17116900	1.13843100

6S-b

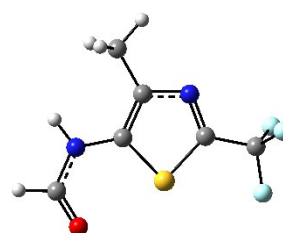


Electronic Energy: -1112.468801 a.u.

C	1.30065600	-0.32931300	-0.40764900
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C	-1.95245500	0.10664200	-0.13296600
S	-0.98756500	-1.33487900	0.11988300
N	-1.27824200	1.21236700	-0.04485600
N	1.67503000	-0.84663300	0.64864600
H	1.79468000	-1.45206800	1.44883800
C	2.77052700	-0.67400200	-0.17123800
H	3.64884500	-1.21887700	0.22460900
O	2.79815000	-0.01301400	-1.17934900
C	0.97499400	2.17716300	0.37443000
C	-3.42231400	0.03576600	-0.40857500
H	1.43042200	2.40677000	-0.59312900
H	0.41773200	3.05051800	0.71533700
H	1.78606500	1.96990400	1.07544500
H	-3.79350700	1.05204700	-0.54069700
H	-3.63481400	-0.53780300	-1.31474900
H	-3.96354900	-0.43260200	0.41828800

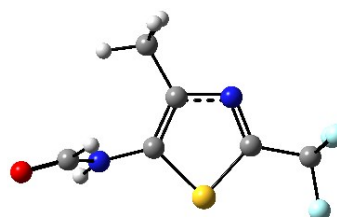
6S-a



Electronic Energy: -1112.472434 a.u.

C	1.41254600	0.33772400	-0.00001700
C	0.75406700	1.54354600	0.00004200
C	-0.97373700	0.18812100	-0.00007900
S	0.30141800	-0.99154400	-0.00006300
N	-0.61189800	1.43150400	0.00000500
N	2.79659000	0.18848400	-0.00005800
H	3.34677600	1.03720000	0.00007000
C	3.45083300	-1.01457200	-0.00007300
H	4.54938200	-0.90408200	0.00006100
O	2.88353100	-2.08421600	-0.00000200
C	1.41959400	2.88647500	0.00009500
C	-2.41459100	-0.24489300	-0.00000300
H	0.65008200	3.66305200	0.00098200
H	2.04814600	3.02519900	0.89090500
H	2.04686000	3.02593000	-0.89150500
F	-3.24054900	0.79874900	-0.00087900
F	-2.69717500	-1.00166400	-1.07876800
F	-2.69753200	-1.00010600	1.07976700

6S-c

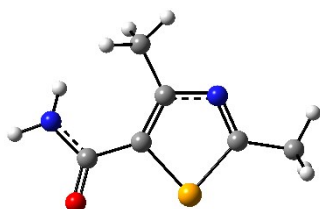


Electronic Energy: -1112.46768 a.u.

C	-1.27611200	-0.04600300	-0.31334500
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C	0.95223600	0.99735100	-0.30188500
C	-1.04463900	0.09262700	-0.02109100
S	-0.09743300	-1.34890200	-0.19744400
N	-0.38500100	1.20611100	-0.08259900
N	2.57758900	-0.87846400	-0.59007400
H	2.71965500	-1.53574300	-1.34431900
C	3.64615700	-0.65423600	0.25793500
H	4.53920000	-1.21474600	-0.07489800
O	3.62978600	0.06124300	1.22697400
C	1.88845500	2.16008400	-0.39734400
C	-2.54021800	0.04052900	0.13935600
H	2.67585500	1.97168400	-1.13058500
H	1.33325500	3.05224800	-0.68646400
H	2.37534500	2.33740800	0.56523100
F	-2.95421600	-1.24028300	0.27667800
F	-3.17510100	0.55606200	-0.92879100
F	-2.94698000	0.72264900	1.21957000

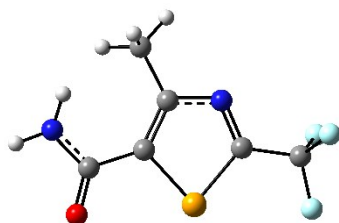
1Se-a



Electronic Energy: -2817.5213201 a.u.

C	0.70488800	0.08674900	-0.00524100
C	0.25953100	1.38568100	-0.04499700
C	-1.80040100	0.47703000	0.01313300
N	-1.10738500	1.57340100	-0.02888600
C	2.05029700	-0.53263500	-0.02100400
O	2.19310400	-1.72539600	-0.24523400
N	3.12545100	0.29063900	0.20982800
H	3.01106700	1.16455100	0.69493300
H	4.01116800	-0.18144100	0.31420900
C	-3.29749200	0.45719700	0.04211800
C	1.10112400	2.63107600	-0.12867900
H	0.49919300	3.43026400	-0.56047000
H	1.41709600	2.96770800	0.86641400
H	1.99085200	2.48533000	-0.74283800
H	-3.70494400	-0.10338900	-0.80355800
H	-3.67005700	-0.00887700	0.95864000
H	-3.66086100	1.48398900	-0.00493100
Se	-0.75507300	-1.10334800	0.02473200

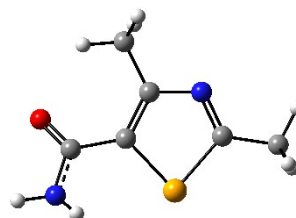
2Se-a



Electronic Energy: -3114.9143790 a.u.

C	-0.77358300	1.22020100	-0.12140500
C	1.11875100	0.08935200	-0.01130400
S	0.02017200	-1.22212900	-0.26602700
N	0.58627600	1.26997900	0.05048000
N	-2.61084700	-0.43315400	-0.48982000
H	-2.93265300	-0.73732900	-1.40106800
C	-3.54263600	-0.50880600	0.52945100
H	-3.11341000	-0.20722500	1.50176700
O	-4.68476300	-0.85688900	0.37037300
C	-1.56537500	2.49012100	-0.09943700
C	2.60545000	-0.13011400	0.10981100
H	-1.13053000	3.20968900	-0.79692000
H	-2.60576900	2.31488600	-0.37299700
H	-1.53662100	2.94297400	0.89552000
F	3.27675100	0.47247500	-0.88528500
F	3.08008800	0.34840600	1.26972900
F	2.89287000	-1.44978100	0.05776700

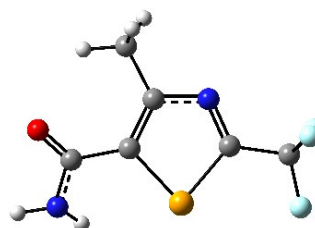
1Se-b



Electronic Energy: -2817.5210352 a.u.

C	0.71395300	0.13472200	0.00385000
C	0.20946300	1.40929200	-0.06348500
C	-1.82310900	0.42630700	-0.02840800
N	-1.16735800	1.53552500	-0.08529500
C	2.14372800	-0.26968700	0.03621900
O	3.03657900	0.48128600	0.39209100
N	2.40022200	-1.57216500	-0.32842900
H	1.76311600	-2.06871800	-0.93087600
H	3.37709200	-1.81580100	-0.39796300
C	-3.31681900	0.33393900	-0.02116900
C	1.00265600	2.68009000	-0.12394500
H	2.06720700	2.48520300	-0.21515500
H	0.64816900	3.29121000	-0.95822000
H	0.83465900	3.25593500	0.79174600
H	-3.72658800	1.34252900	-0.07847700
H	-3.68362300	-0.24813300	-0.87092200
H	-3.67994800	-0.14529200	0.89212300
Se	-0.70888200	-1.11702100	0.07966800

2Se-b

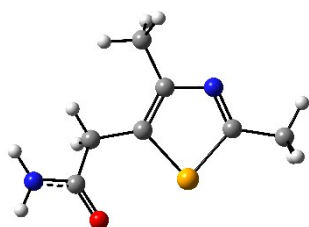


Electronic Energy: -3114.9130323 a.u.

C	1.42104700	0.12269400	0.00602500
C	0.87839800	1.38886400	0.04320500
C	-1.06741800	0.29946700	0.00332400
N	-0.49474100	1.45993800	0.03711700
C	2.81179700	-0.40047400	0.01109400
O	3.02376500	-1.58957300	0.19454700
N	3.82482800	0.49792100	-0.18086800
H	3.65938800	1.40589600	-0.57970500
H	4.74940100	0.10499200	-0.27283300
C	-2.56884100	0.16700000	-0.01333700
C	1.62385200	2.69459500	0.10786300
H	0.94084400	3.46986900	0.45252500
H	2.47442100	2.64597700	0.79030000
H	1.98720200	2.99800700	-0.88120000
Se	0.07552600	-1.18628100	-0.01385000
F	-3.13049300	0.73662200	1.06530300
F	-2.92838400	-1.13690400	-0.02246200
F	-3.10477600	0.74333800	-1.10254400

C	1.43074300	0.15819600	0.00258900
C	0.86268700	1.41034800	0.07495400
C	-1.07717600	0.29845200	0.02286300
N	-0.51475300	1.45435500	0.09171200
C	2.88481200	-0.16901500	-0.03905500
O	3.71754800	0.61302600	-0.46018100
N	3.21762100	-1.43145300	0.39116900
H	2.62706700	-1.92283400	1.04341100
H	4.20683700	-1.62768100	0.43684900
C	-2.57600000	0.13345600	0.00952100
C	1.58982700	2.71899700	0.14336800
H	1.19393100	3.31300400	0.97065600
H	2.66157000	2.57851000	0.25046800
H	1.40917700	3.28233600	-0.77723100
Se	0.09242300	-1.17219900	-0.08989100
F	-2.90507200	-1.17630600	-0.07747700
F	-3.13597200	0.61973000	1.12858700
F	-3.13570900	0.76372100	-1.03466700

3Se-a

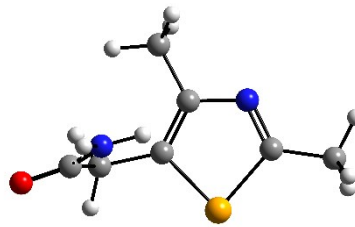


Electronic Energy: -2856.73836 a.u.

C	-2.16027900	-0.09273300	-0.13121700
C	-0.66313600	1.58207000	-0.00431500
C	0.27066300	0.60396000	0.18858200
N	-1.97789100	1.18482400	-0.18847500
C	1.72989400	0.78220100	0.48841600
H	1.89641700	0.77248700	1.57520100
H	2.05732500	1.76335200	0.13617300
C	2.64389300	-0.31220000	-0.06916900
N	3.87977600	0.11045300	-0.45322100
O	2.31160800	-1.48229800	-0.11598300
C	-0.41731000	3.06557900	-0.01898100
C	-3.49591800	-0.74501200	-0.32335900
H	-0.88975300	3.53859300	0.84792700
H	0.64291400	3.32148600	-0.00526600
H	-0.86940300	3.50720200	-0.91066800
H	-3.49962500	-1.39379700	-1.20408700
H	-3.76988600	-1.35829900	0.53972100
H	-4.24781100	0.03350400	-0.45765300
H	4.53919100	-0.57815900	-0.78021300
H	4.14962600	1.07858900	-0.44316100
Se	-0.56652700	-1.09402100	0.15711800

4Se-a

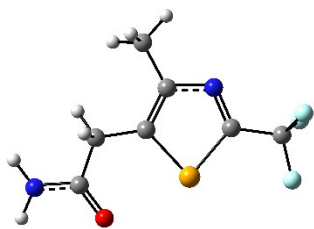
3Se-b



Electronic Energy: -2856.741616 a.u.

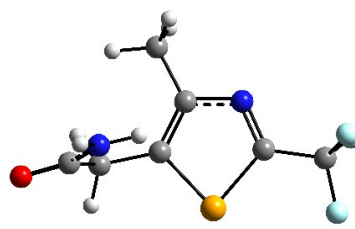
C	-2.16027900	-0.09273300	-0.13121700
C	-0.66313600	1.58207000	-0.00431500
C	0.27066300	0.60396000	0.18858200
N	-1.97789100	1.18482400	-0.18847500
C	1.72989400	0.78220100	0.48841600
H	1.89641700	0.77248700	1.57520100
H	2.05732500	1.76335200	0.13617300
C	2.64389300	-0.31220000	-0.06916900
N	3.87977600	0.11045300	-0.45322100
O	2.31160800	-1.48229800	-0.11598300
C	-0.41731000	3.06557900	-0.01898100
C	-3.49591800	-0.74501200	-0.32335900
H	-0.88975300	3.53859300	0.84792700
H	0.64291400	3.32148600	-0.00526600
H	-0.86940300	3.50720200	-0.91066800
H	-3.49962500	-1.39379700	-1.20408700
H	-3.76988600	-1.35829900	0.53972100
H	-4.24781100	0.03350400	-0.45765300
H	4.53919100	-0.57815900	-0.78021300
H	4.14962600	1.07858900	-0.44316100
Se	-0.56652700	-1.09402100	0.15711800

4Se-b



Electronic Energy: -3154.134136 a.u.

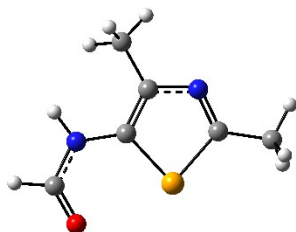
C	1.40375200	0.25321200	0.00640000
C	-0.23103300	1.76367500	0.01057200
C	-1.06421600	0.67838900	0.11865900
Se	-0.06521600	-0.91866000	0.15330100
C	-2.55432400	0.73736400	0.26993300
H	-2.94944700	1.56218700	-0.33167200
H	-2.81587200	0.97106300	1.31193400
C	-3.29819700	-0.55362000	-0.07400800
O	-2.76171900	-1.64722200	-0.05265500
N	-4.61661300	-0.39417700	-0.36188500
C	2.82187700	-0.23674400	-0.08746000
F	3.37313000	0.03463800	-1.28645200
F	3.61056500	0.31999400	0.84917000
F	2.87472000	-1.57942100	0.08288300
C	-0.67676800	3.20084600	-0.01687300
H	-0.92845900	3.56260000	0.98613100
H	0.13420800	3.81893900	-0.40106800
H	-1.55572400	3.34809900	-0.65060500
N	1.12032300	1.51193600	-0.06005100
H	-5.06192000	0.50703400	-0.38631900
H	-5.16994100	-1.21766200	-0.53959400



Electronic Energy: -3154.134275 a.u.

C	-1.37198800	0.27252300	-0.03180700
C	0.50945600	1.44218800	-0.32145800
C	1.10107200	0.21990500	-0.53080000
Se	-0.18613300	-1.15270500	-0.37613700
C	2.53826700	-0.08307300	-0.83251500
H	2.97368800	0.72588300	-1.42525300
H	2.63536900	-0.97941600	-1.44842900
C	3.50592100	-0.29462500	0.35315900
O	4.65505700	-0.62630200	0.14557100
N	2.99977200	-0.06963800	1.59399900
C	-2.83347400	0.05217500	0.25791800
F	-3.14954000	-1.25671100	0.12625600
F	-3.15241100	0.41925000	1.51232800
F	-3.61747000	0.74813400	-0.57948600
C	1.20287400	2.77367600	-0.36814300
H	0.75646100	3.40222300	-1.14332000
H	1.07817600	3.29689900	0.58364300
H	2.26952100	2.67766500	-0.56812400
N	-0.84298500	1.44522800	-0.05028300
H	2.03404000	0.16958500	1.74294700
H	3.60533100	-0.21225300	2.38658800

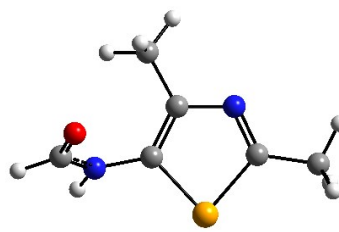
5Se-a



Electronic Energy: -2817.505572 a.u.

C	0.58406800	0.60473100	-0.00096300
C	-0.36340100	1.59068600	0.00678900
C	-1.84299600	-0.10825500	-0.00103500
N	-1.67943000	1.17309700	0.00536500
N	1.96598700	0.80684000	-0.01427000
H	2.28943500	1.76315100	-0.04762400
C	2.91121100	-0.18132200	-0.00071600
H	3.93649000	0.22485700	-0.01686800
O	2.66628800	-1.36924000	0.02374800
C	-0.07567300	3.06707400	0.00516900
C	-3.18346500	-0.77654000	0.00275200
H	-0.96905700	3.60191300	0.32707600
H	0.73821200	3.33273100	0.68852400
H	0.18913400	3.43415400	-0.99334500
H	-3.95470000	-0.00535100	0.00891200
H	-3.32173100	-1.40540100	-0.88162100
H	-3.31363000	-1.41140100	0.88408400

5Se-b

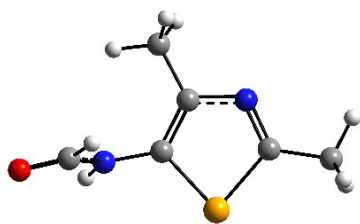


Electronic Energy: -2817.501555 a.u.

C	-0.61549800	-0.13941000	0.38479900
C	-0.39043900	1.20192900	0.27674300
C	1.75142300	0.62691000	-0.15113500
N	0.90424500	1.58804800	-0.01617300
N	-1.84309600	-0.77854300	0.61635900
H	-1.90996200	-1.42946700	1.38644400
C	-2.94693800	-0.67785300	-0.20553200
H	-3.77471300	-1.31040600	0.16840400
O	-3.02996800	0.00879700	-1.19322700
C	-1.43586200	2.26317800	0.44058700
C	3.20880700	0.82187800	-0.43093100
H	-2.21681700	1.94462700	1.13370100
H	-0.97322800	3.17799900	0.81272400
H	-1.91696100	2.47665300	-0.51818500
H	3.40381200	1.89203500	-0.50761500
H	3.82707900	0.40501300	0.36906100
H	3.50457700	0.34027500	-1.36687500

Se -0.20908300 -1.10642700 -0.00496400

5Se-c

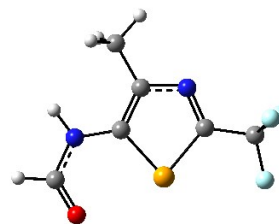


Electronic Energy: -2817.501414 a.u.

C	0.58271900	0.14051800	-0.26555800
C	0.06314600	1.39337100	-0.10612900
C	-1.92379500	0.35440400	0.14678200
N	-1.29721200	1.48224000	0.11913700
N	1.92526700	-0.20428100	-0.47855700
H	2.22825900	-0.50397200	-1.39788900
C	2.87242200	-0.30987600	0.51881900
H	2.46206600	-0.02729200	1.50501100
O	4.01276800	-0.65905000	0.33431300
C	0.84713000	2.66991600	-0.16906000
C	-3.40007900	0.22554100	0.35827800
H	0.81997500	3.18223100	0.79706600
H	1.88681000	2.48860900	-0.44019500
H	0.39936400	3.34369400	-0.90411700
H	-3.82061200	1.22432700	0.47921200
H	-3.88166800	-0.26259900	-0.49340000
H	-3.62439300	-0.36493300	1.25070300
Se	-0.80051700	-1.16460600	-0.11334500

Se 0.98349800 -1.11216000 0.05822600

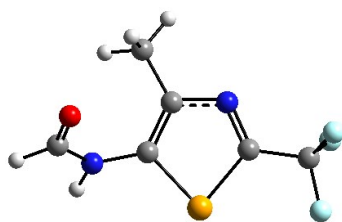
6Se-a



Electronic Energy: -3114.900821 a.u.

C	-1.39905200	0.55488000	0.00003700
C	-0.64470300	1.70437000	-0.00003400
C	1.07750900	0.28599700	-0.00002700
N	0.71440800	1.52529100	-0.00006300
N	-2.79044300	0.50831400	0.00010800
H	-3.28473400	1.38956300	0.00018800
C	-3.52892000	-0.64526600	0.00010700
H	-4.61343400	-0.45301200	-0.00001200
O	-3.04602100	-1.75760800	-0.00018800
C	-1.20600700	3.09952300	-0.00005000
C	2.52323700	-0.11922100	-0.00004800
H	-0.38132900	3.81092900	-0.00110300
H	-1.82031000	3.29588800	-0.88600600
H	-1.81862800	3.29656900	0.88692300
Se	-0.32396900	-0.98931000	0.00007800
F	2.63237000	-1.47023900	-0.00019200
F	3.17835800	0.33749400	-1.08313100
F	3.17831600	0.33724900	1.08317000

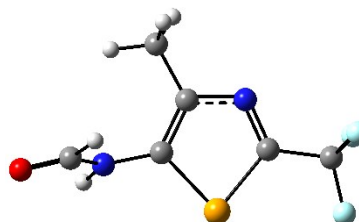
6Se-b



Electronic Energy: -3114.894329 a.u.

C	1.37328000	-0.15617000	-0.38457400
C	0.97924900	1.15711200	-0.34223900
C	-1.06241900	0.30204400	-0.01321800
N	-0.36338100	1.37528700	-0.13689700
N	2.67900300	-0.64285200	-0.53032400
H	2.85961800	-1.33307300	-1.24594000
C	3.72758200	-0.33612300	0.31812200
H	4.64728600	-0.87134800	0.01734500
O	3.67043100	0.41788700	1.25573900
C	1.89121100	2.33513900	-0.49981400
C	-2.55886700	0.32907700	0.15543900
H	2.70608700	2.11210700	-1.19168000
H	1.32358400	3.18723000	-0.87370300
H	2.34165500	2.59962000	0.46052600
Se	-0.09769100	-1.31661400	-0.10570200

6Se-c

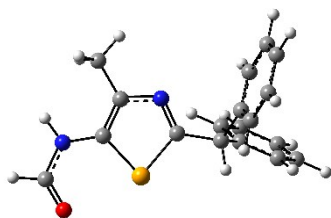


Electronic Energy: -3114.893307 a.u.

C	-1.33270200	0.09247500	-0.29105200
C	-0.80022100	1.35148500	-0.17268700
C	1.15212300	0.27849100	0.01423800
N	0.56367700	1.42380200	-0.00336300
N	-2.68332700	-0.24665200	-0.42986200
H	-3.01227400	-0.66159900	-1.29363300
C	-3.62139500	-0.16175800	0.58322700
H	-3.18604900	0.24255000	1.51428000
O	-4.77505100	-0.48606800	0.45783500
C	-1.57675500	2.63270000	-0.22974900
C	2.64943800	0.15245300	0.14757100
H	-1.57251600	3.12853100	0.74521100
H	-1.10812300	3.31456800	-0.94278200
H	-2.61055600	2.46082800	-0.52828800
Se	0.03337200	-1.22537300	-0.16367000

F	-2.92591600	1.05220500	1.22422000
F	-3.17364000	0.85332200	-0.91958400
F	-3.03708200	-0.92622500	0.32310500

7Se-a



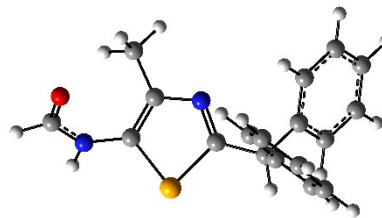
Electronic Energy: - a.u.

C	-2.69131200	-0.46341700	0.46760500
C	-1.78111700	-0.98283200	1.34786900
C	-0.26422700	-0.25936400	-0.13440000
N	-0.45397200	-0.85449700	0.99758900
N	-4.07442000	-0.50519300	0.63795600
H	-4.42078500	-0.97214000	1.46842500
C	-4.98089300	0.03679700	-0.23081500
H	-6.02686500	-0.10875400	0.10799500
O	-4.68216900	0.61030200	-1.25346600
C	-2.14526600	-1.66909600	2.63290200
C	1.10059000	0.07854000	-0.69234300
H	-1.22557000	-1.90549600	3.18008700
H	-2.77176200	-1.03048000	3.27598300
H	-2.68548300	-2.61304200	2.45521300
H	0.99247500	0.18579200	-1.78311900
Se	-1.84239200	0.29377400	-1.01545600
C	1.62567400	1.41208800	-0.16320700
C	2.68970900	2.02559200	-0.83558200
C	1.10438600	2.02765700	0.97589500
C	3.21917900	3.22945400	-0.38116200
H	3.11046000	1.54456000	-1.72215200
C	1.63614700	3.23479700	1.43341400
H	0.27920500	1.56085000	1.51456300
C	2.69184400	3.83979500	0.75805700
H	4.04635800	3.69561300	-0.91843800
H	1.21664600	3.70314100	2.32487800
H	3.10383500	4.78436300	1.11547500
C	2.08008500	-1.06064300	-0.44899800
C	2.35766500	-1.97164400	-1.46951800
C	2.68992800	-1.22966100	0.79774000
C	3.23384500	-3.03543600	-1.25425900
H	1.88160300	-1.84833800	-2.44527200
C	3.56346400	-2.29117300	1.01455300
H	2.47560500	-0.52041800	1.59841100
C	3.83959800	-3.19695800	-0.01061100
H	3.44340700	-3.73760500	-2.06245100
H	4.03411000	-2.41267600	1.99127600
H	4.52840700	-4.02525900	0.16072000

7Se-c

F	3.01215100	-1.14995400	0.18270200
F	3.28971200	0.72397200	-0.88580500
F	3.09479500	0.73167300	1.27316900

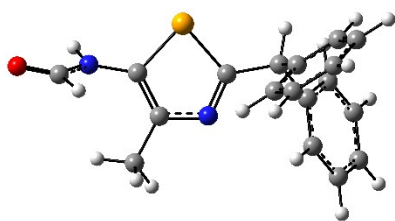
7Se-b



Electronic Energy: - a.u.

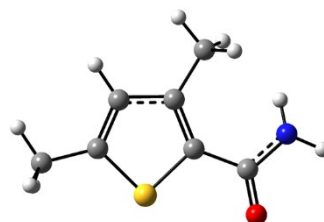
C	-2.75944600	-0.46430700	-0.30248500
C	-2.04514300	-1.00245800	0.73054100
C	-0.24661300	-0.24971800	-0.38939400
N	-0.67200900	-0.86314700	0.66123100
N	-4.15440900	-0.43502800	-0.42292400
H	-4.57342000	-0.70445200	-1.30562200
C	-4.98832300	0.08657600	0.54083400
H	-6.05107200	0.05248100	0.21522000
O	-4.63005000	0.51531800	1.60851900
C	-2.64747900	-1.72084900	1.89564900
C	1.20473400	0.04232100	-0.69644500
H	-3.58036300	-2.22074200	1.60099600
H	-1.93431000	-2.46338500	2.27350900
H	-2.89617100	-1.00970800	2.69641000
H	1.29266000	0.12060000	-1.79072800
Se	-1.61309800	0.35779400	-1.54727000
C	2.11669500	-1.09305300	-0.25518200
C	2.74335600	-1.89351500	-1.21110300
C	2.34887800	-1.34438400	1.10115600
C	3.59321500	-2.93068200	-0.82456800
H	2.56621900	-1.70369200	-2.27243400
C	3.19250000	-2.38067900	1.48781300
H	1.86063800	-0.72227300	1.85183400
C	3.81882400	-3.17659400	0.52677700
H	4.07901600	-3.54512500	-1.58387600
H	3.36562400	-2.56854800	2.54831700
H	4.48279600	-3.98578700	0.83358100
C	1.65966300	1.38047900	-0.11732400
C	2.76462500	2.00983900	-0.70062900
C	1.04931100	1.97225900	0.99026300
C	3.25297400	3.20784100	-0.18876700
H	3.25174300	1.54514300	-1.56138300
C	1.54057100	3.17340000	1.50544100
H	0.18579900	1.49465400	1.45631300
C	2.64054900	3.79416400	0.91949500
H	4.11399100	3.68692000	-0.65672900
H	1.05397100	3.62593500	2.37049500
H	3.02020200	4.73381800	1.32255300

TH-a



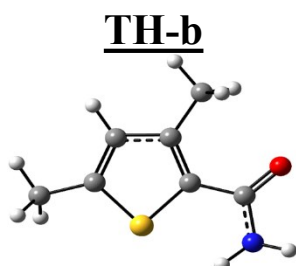
Electronic Energy: - a.u.

C	-2.70071700	-0.47259700	-0.10606900
C	-1.93369200	-0.86391100	0.95687600
C	-0.19312900	-0.22391800	-0.31040100
N	-0.56814100	-0.71059000	0.82541900
N	-4.09681700	-0.48292600	-0.17405500
H	-4.57371700	-1.03694200	-0.88081200
C	-4.90055600	0.32805900	0.59580500
H	-4.30165400	0.95340500	1.29460700
O	-6.10246400	0.34587400	0.52033900
C	-2.46555300	-1.45218300	2.22712400
C	1.24559300	0.05456600	-0.68601100
H	-2.35537100	-0.74247600	3.06063400
H	-3.52549600	-1.71649200	2.12801300
H	-1.88788600	-2.35081900	2.48173000
H	1.28819100	0.11473400	-1.78373900
Se	-1.60400800	0.19706000	-1.48758200
C	2.15886100	-1.08837900	-0.26430800
C	2.47502000	-1.29971100	1.08166200
C	2.68543100	-1.94807300	-1.22950400
C	3.30279500	-2.35567500	1.44994500
H	2.06455900	-0.63139900	1.83915100
C	3.51829000	-3.00542200	-0.86147900
H	2.44197700	-1.78993900	-2.28286300
C	3.82781200	-3.21157200	0.47997200
H	3.54147400	-2.51268400	2.50273800
H	3.92464200	-3.66838500	-1.62646500
H	4.47780600	-4.03743300	0.77172000
C	1.73002900	1.39947600	-0.14747500
C	2.78695000	2.03697400	-0.80696400
C	1.18987800	1.99388000	0.99476600
C	3.29352400	3.24502700	-0.33659600
H	3.22105000	1.57337100	-1.69622200
C	1.69817000	3.20491100	1.46707900
H	0.36910400	1.50747300	1.52297000
C	2.74844700	3.83439800	0.80454300
H	4.11596200	3.73026100	-0.86384500
H	1.26530700	3.65771800	2.36011400
H	3.14182400	4.78209000	1.17403200



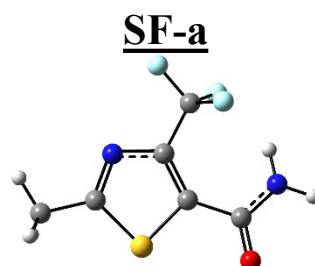
Electronic Energy: -799.05271222 a.u.

C	-0.52047500	-0.08776600	-0.00091300
C	-0.04444600	1.20957700	-0.03946700
C	1.97514600	0.00973400	0.02115000
S	0.78411700	-1.24271900	0.03260900
C	-1.87998700	-0.67334800	-0.01547100
O	-2.05792600	-1.86581500	-0.21180000
N	-2.93638400	0.18879600	0.17691000
H	-2.80226400	1.05769600	0.66637500
H	-3.83129300	-0.26340100	0.29239500
C	3.44182000	-0.30008100	0.04861900
C	-0.86791100	2.47023700	-0.11387700
H	-0.25548300	3.30126700	-0.46777400
H	-1.71560200	2.36360400	-0.79347700
H	-1.25701800	2.76038600	0.87011400
H	4.01892800	0.62644300	0.02957200
H	3.72141000	-0.85247200	0.95045900
H	3.74414200	-0.90322900	-0.81237300
C	1.37961200	1.24353900	-0.02433800
H	1.94685000	2.16680100	-0.05523800



Electronic Energy: -799.05383938 a.u.

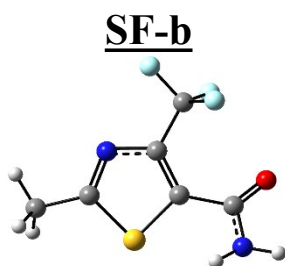
C	-0.53194800	-0.05213300	0.01838900
C	-0.01358900	1.22462500	-0.05214200
C	1.97989300	-0.02995800	-0.00268500
S	0.74732500	-1.24494100	0.08896900



Electronic Energy: -1112.49068651 a.u.

C	-0.14851900	0.79036700	0.02730400
C	0.05809600	-0.57171300	0.01443200
C	-2.14520300	-0.63336600	0.03544200
S	-1.85642000	1.08118400	0.02606200

C	-1.96426000	-0.42540300	0.03656100	N	-1.05804100	-1.35684700	0.01973100
O	-2.84608700	0.38819900	0.26566600	C	0.70898900	2.01842300	-0.00938300
N	-2.24923900	-1.75315200	-0.19107400	O	0.20862700	3.08666400	-0.32508600
H	-1.60351200	-2.33907000	-0.69603000	N	2.01729600	1.88418200	0.32268000
H	-3.22932600	-1.97662400	-0.27378000	H	2.40325600	1.04393600	0.71929200
C	3.43540000	-0.38631200	0.01704100	H	2.57507100	2.72332500	0.31213500
C	-0.81673400	2.49497100	-0.09731500	C	-3.52417400	-1.21465500	0.06041400
H	-0.20394500	3.31940600	-0.46887600	C	1.39165600	-1.27137300	-0.05922400
H	-1.70268200	2.38780700	-0.72219700	H	-3.44418000	-2.29779500	-0.02601300
H	-1.17735600	2.75766900	0.90147700	H	-4.03844800	-0.97372500	0.99488300
H	4.03875400	0.52165000	-0.04035300	H	-4.13405900	-0.83571100	-0.76337400
H	3.71084100	-0.91523100	0.93418800	F	1.27326500	-2.59550900	-0.07822600
H	3.70888000	-1.02611600	-0.82712200	F	2.17763700	-0.95630600	1.02060000
C	1.41278200	1.21366100	-0.06862000	F	2.09489800	-0.89815400	-1.14948600
H	2.00525700	2.11933000	-0.12601200				



Electronic Energy: -1112.48586461 a.u.

C	-0.11041900	0.79297400	0.02658900
C	0.04356900	-0.56885300	-0.02047200
C	-2.16588800	-0.56220600	0.03307500
S	-1.80906200	1.15253500	0.07452200
N	-1.10452000	-1.31064800	-0.01632000
C	0.93456900	1.86421700	0.12935700
O	1.91393500	1.73773400	0.83153000
N	0.65498800	3.00218500	-0.58163600
H	0.01791800	2.97931600	-1.36157700
H	1.36977800	3.71465300	-0.58449400
C	-3.56679100	-1.08615600	0.07130000
C	1.35962100	-1.31008900	-0.08256200
H	-3.52777000	-2.17327500	0.00998400
H	-4.07130500	-0.80347300	0.99910000
H	-4.16107500	-0.70517500	-0.76318800
F	2.27482700	-0.63493900	-0.80631800
F	1.87547000	-1.51496400	1.14301000
F	1.20356100	-2.51393800	-0.65918700