
Modulating Intramolecular Chalcogen Bonds in Aromatic (thio)(seleno)phene-Based derivatives

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Supporting Information

- **Figure S1.** Representation of the interacting (**a**) and non-interacting (**b**) conformations considered in the present study.
- **Table S1.** Molecular graphs (AIM) and optimized geometries (Cartesian Coordinates in Å) for all the complexes under study. Green dots indicate bond critical (BCP).
- **Table S2.** Summary of the different parameters regarding family **S**.
- **Table S3.** Summary of the different parameters regarding family **Se**.
- **Table S4.** Molecular electrostatic potential on the 0.001 a.u. electron density isosurface
- **Figure S2.** Superimposition of **S^I** compound (yellow) and crystal structure (PDB ID: 4PX5) ligand (magenta) in the Glucokinase–Glucokinase Regulatory Protein (GK–GKRP) crystal structure.
- **Figure S3.** Relationships distance vs density for the three different interactions, N $\cdots$ S and N $\cdots$ Se

Family Z= S, Se

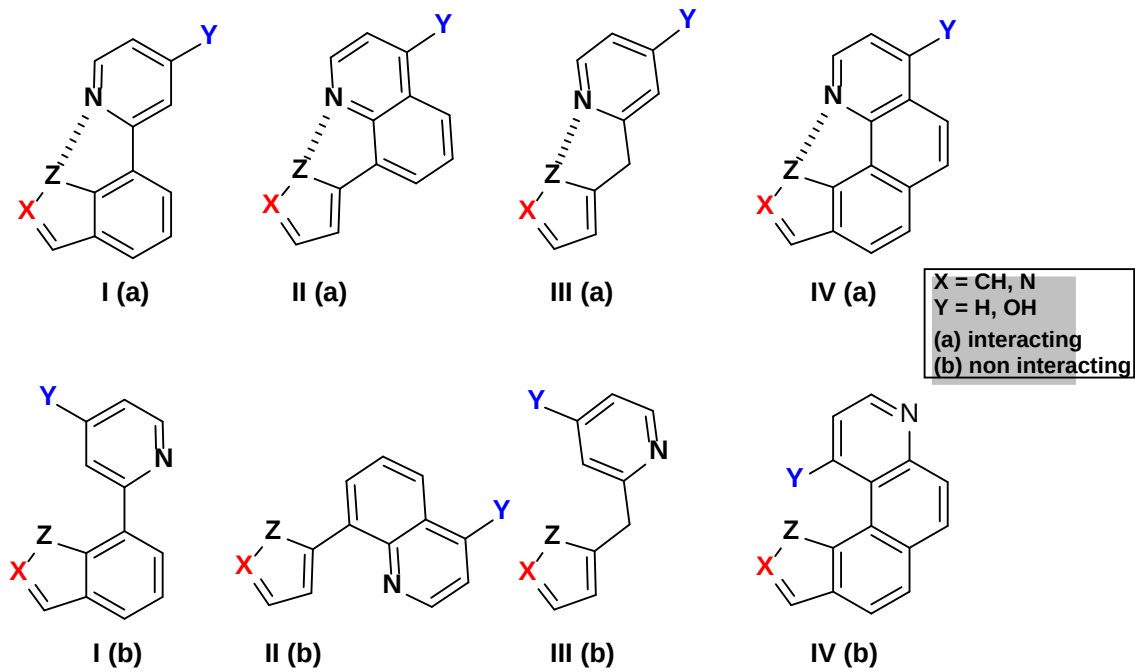
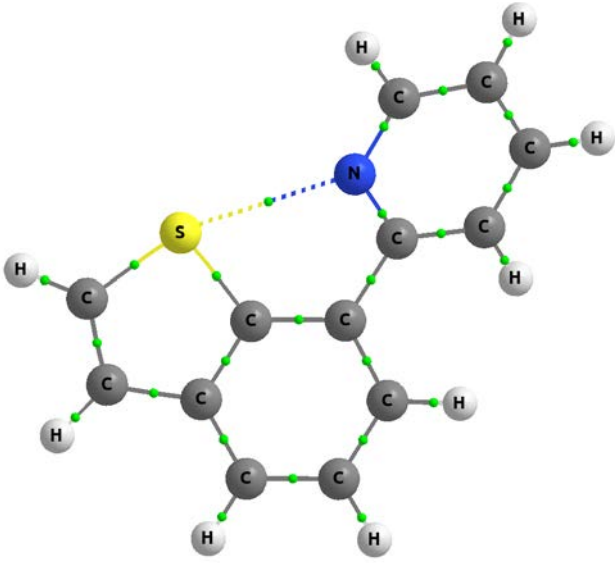
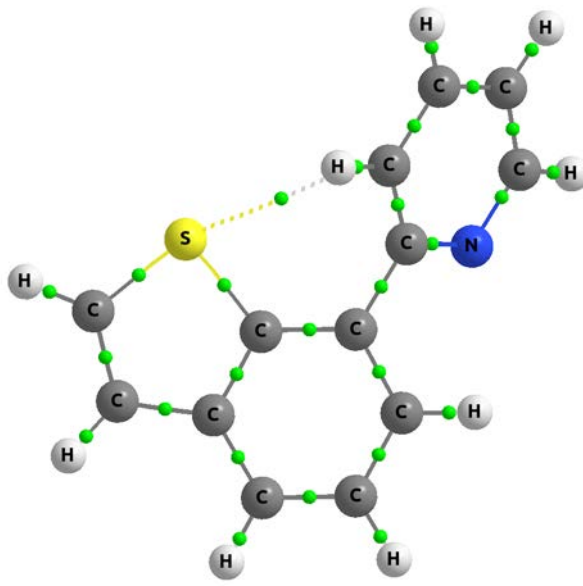
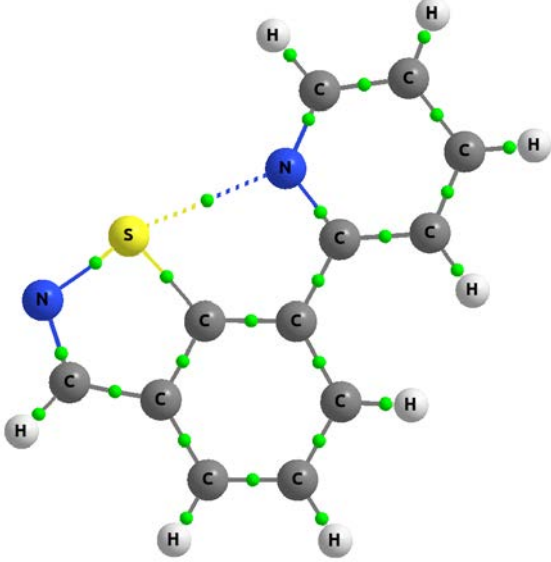
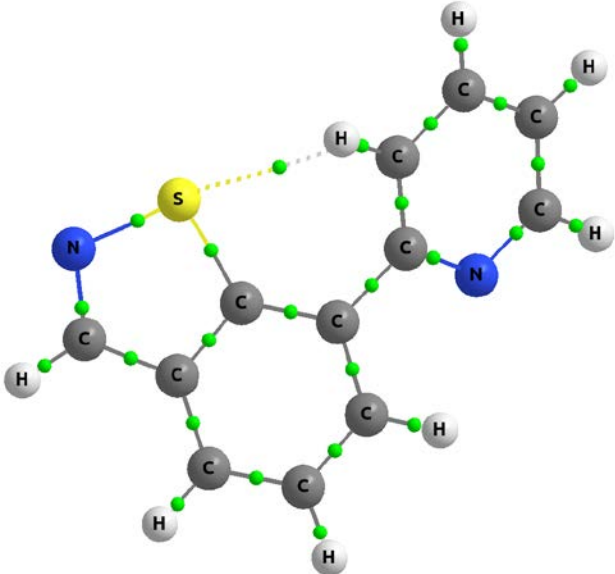
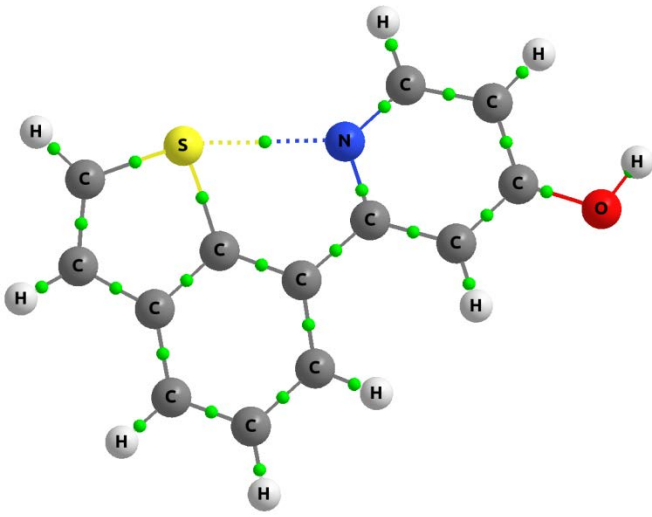
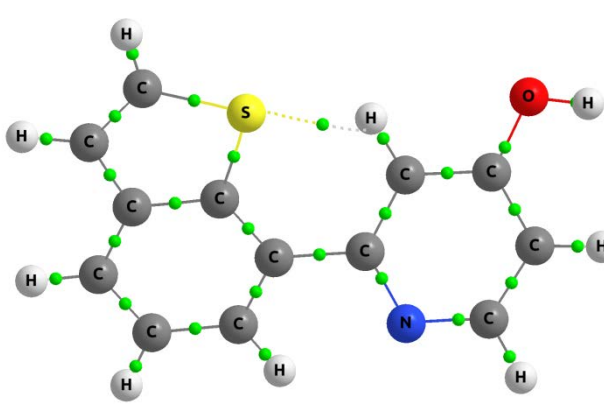


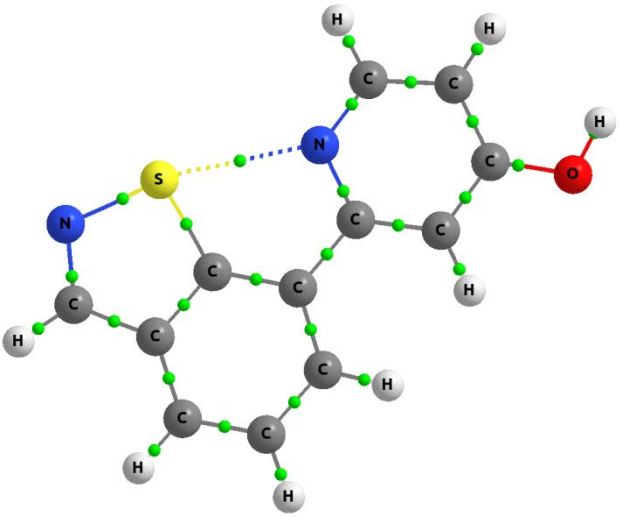
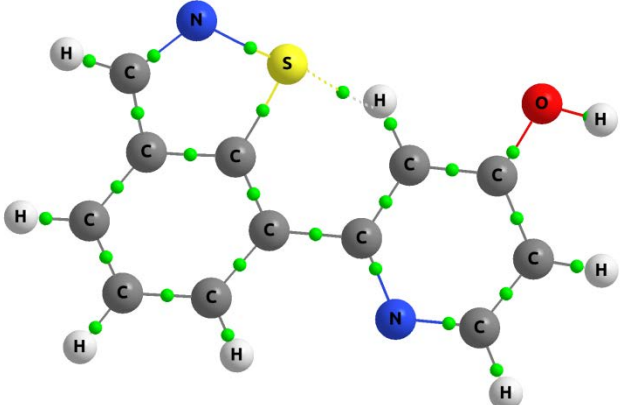
Figure S1. Representation of the interacting (a) and non-interacting (b) conformations considered in the present study.

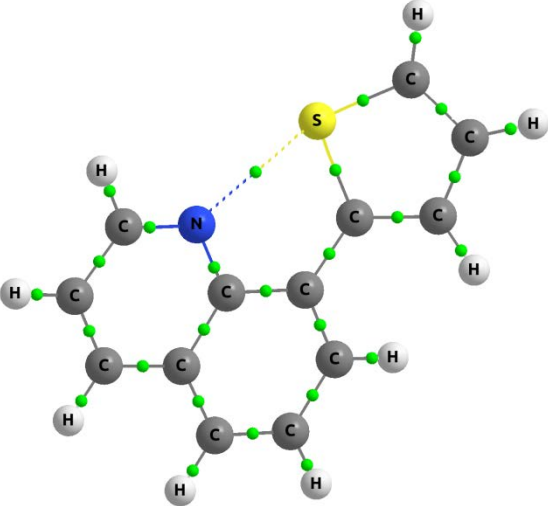
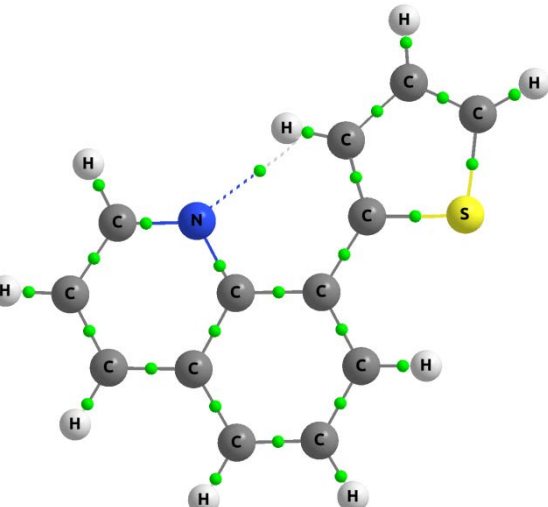
Table S1. Molecular graphs (AIM) and optimized geometries (Cartesian Coordinates in Å) for all the complexes under study. Green dots indicate bond critical (BCP).

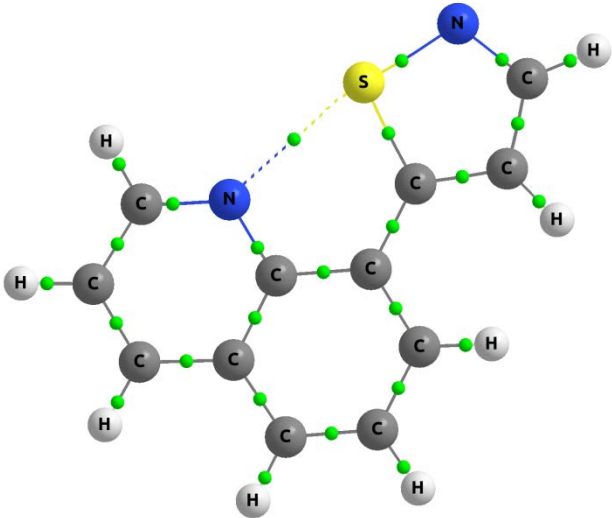
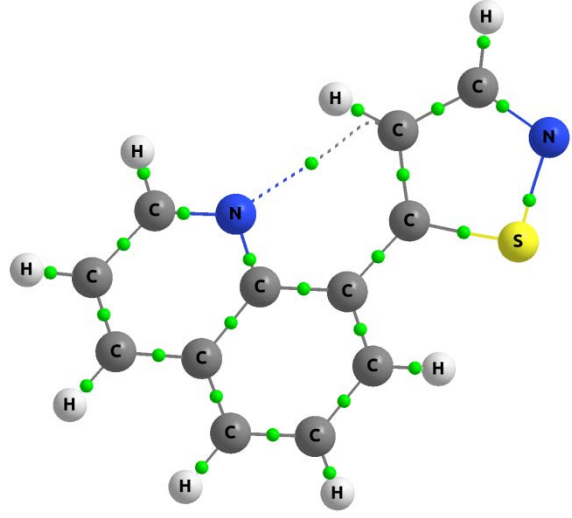
Family S	
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S' (b)	
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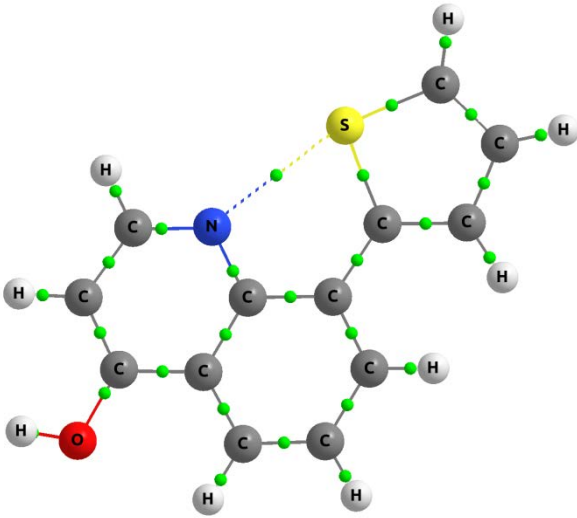
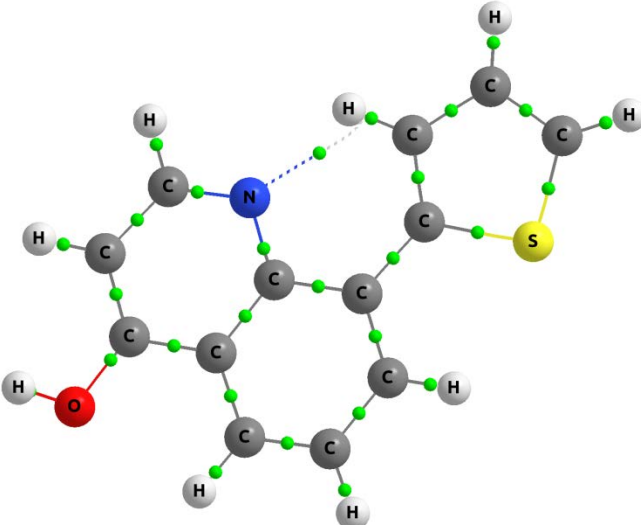
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S'_N (b)	
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S'_{OH} (a)	

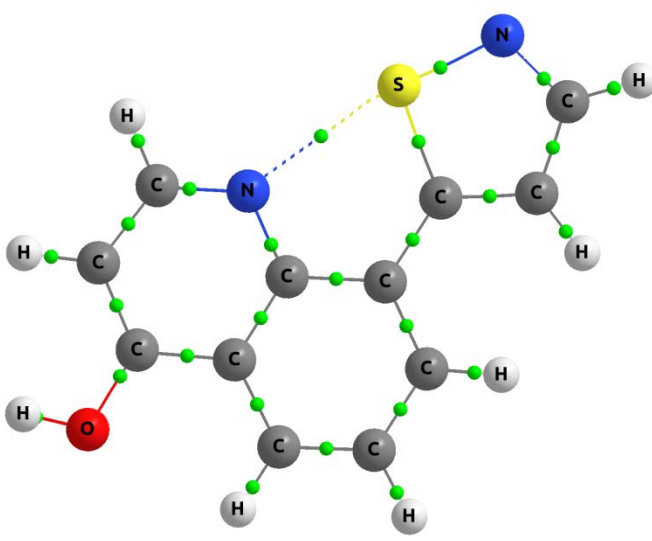
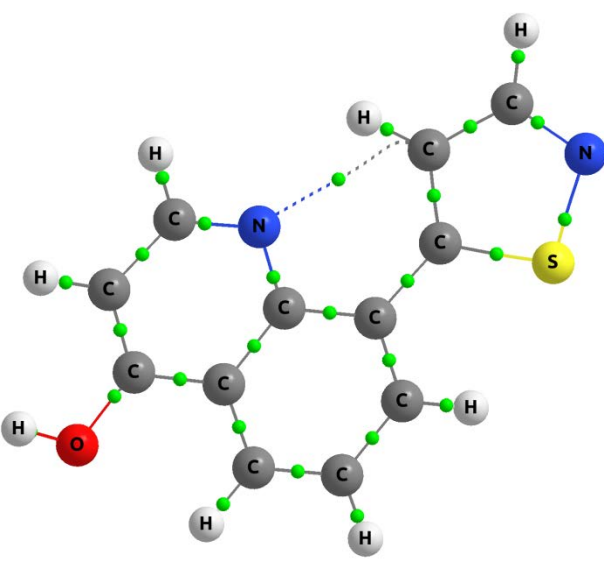
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S^I_{OH} (b)	
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S^I_{NOH} (a)	

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S'_{NOH} (b)	
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S'' (a)	

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S'' (b)	
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S''_N (a)	

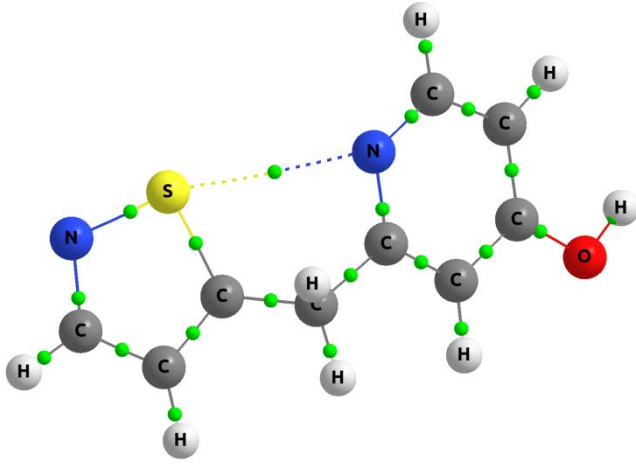
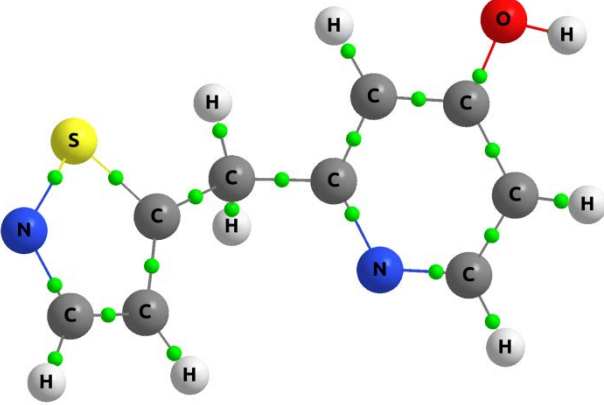
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S^{II}_{OH} (a)	

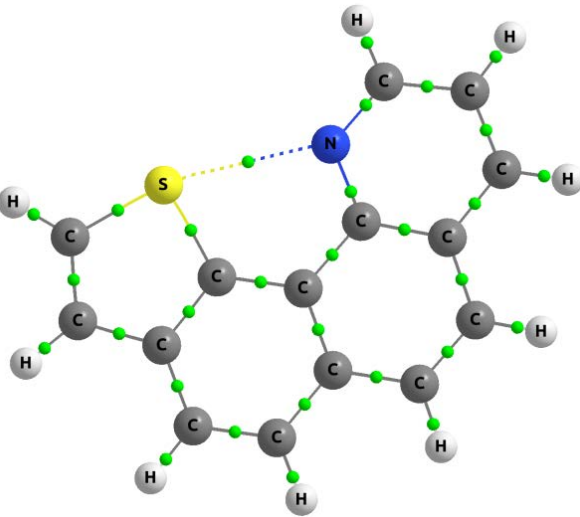
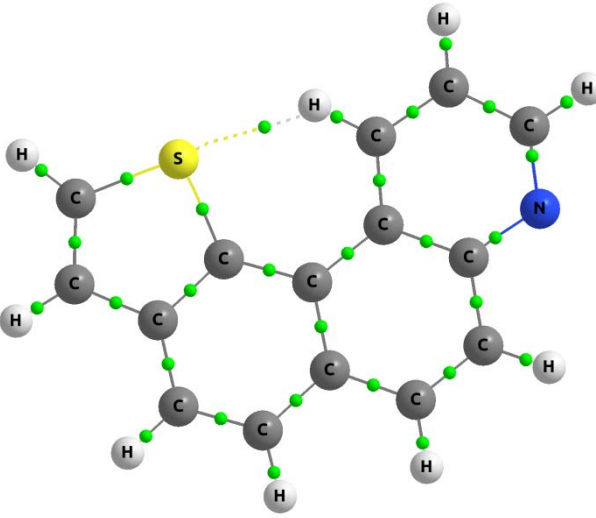
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S^{II}_{OH} (b)	
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S^{II}_{NOH} (a)	

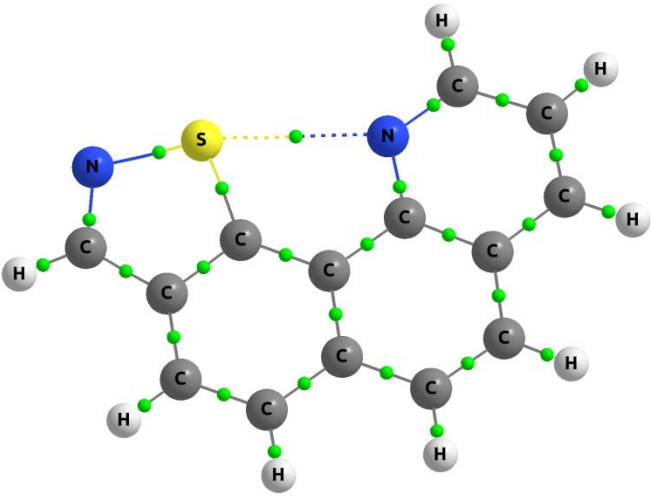
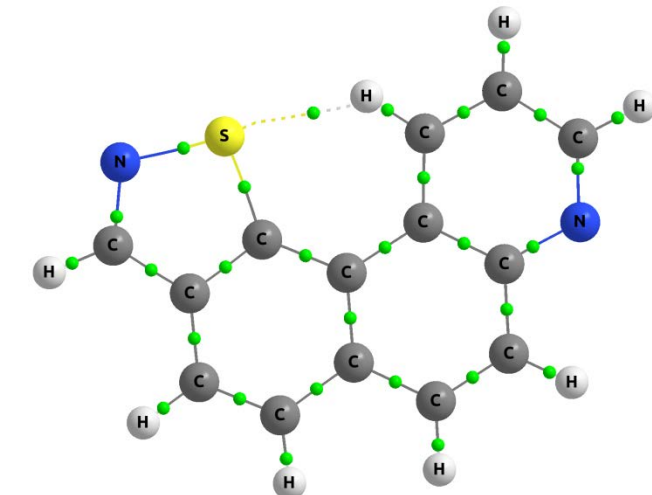
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S^{II}_{NOH} (b)	
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S^{III} (b)	

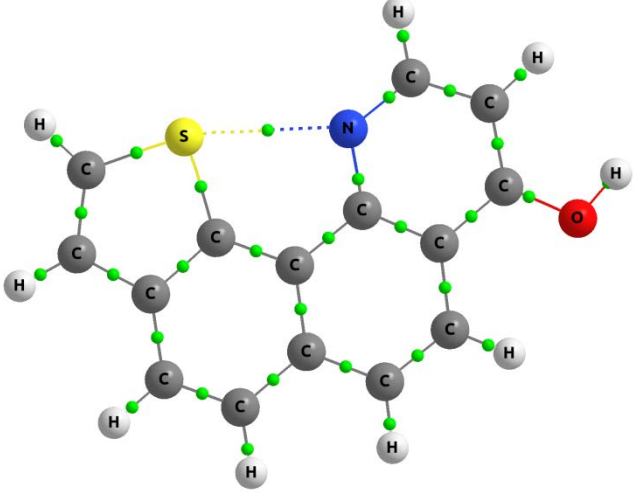
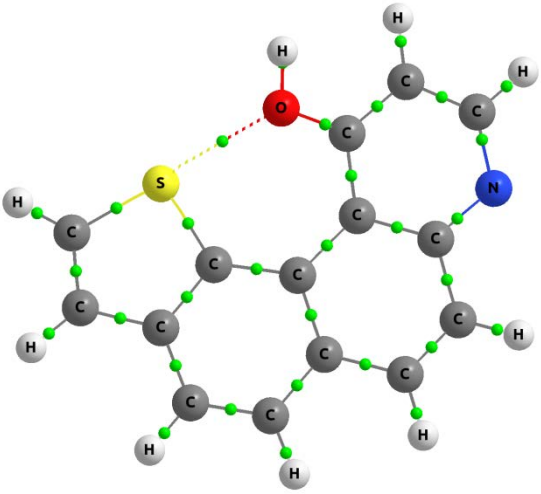
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	<table><tr><td>C</td><td>-1.18438100</td><td>0.54804700</td><td>0.4993690</td></tr><tr><td>C</td><td>-2.05049200</td><td>1.3249720</td><td>-0.2921440</td></tr><tr><td>C</td><td>-3.19005000</td><td>0.7214370</td><td>-0.8502350</td></tr><tr><td>C</td><td>-3.4171100</td><td>-0.6414180</td><td>-0.5972370</td></tr><tr><td>C</td><td>-2.4963130</td><td>-1.33824300</td><td>0.2061770</td></tr><tr><td>N</td><td>-1.4003360</td><td>-0.76647700</td><td>0.7499540</td></tr><tr><td>H</td><td>-3.88158500</td><td>1.3009950</td><td>-1.4701930</td></tr><tr><td>H</td><td>-1.83202000</td><td>2.3835010</td><td>-0.4675750</td></tr><tr><td>H</td><td>-4.2883160</td><td>-1.1583610</td><td>-1.0104690</td></tr><tr><td>H</td><td>-2.6406730</td><td>-2.40189300</td><td>0.4260610</td></tr><tr><td>C</td><td>0.08653100</td><td>1.11182800</td><td>1.0990290</td></tr><tr><td>H</td><td>0.09912800</td><td>2.21121200</td><td>1.0143910</td></tr><tr><td>H</td><td>0.11499600</td><td>0.85074000</td><td>2.1710430</td></tr><tr><td>C</td><td>1.30520900</td><td>0.56183900</td><td>0.3989000</td></tr><tr><td>C</td><td>2.38199900</td><td>1.2685680</td><td>-0.1395420</td></tr><tr><td>S</td><td>1.5856040</td><td>-1.12706500</td><td>0.1394160</td></tr><tr><td>C</td><td>3.33913400</td><td>0.3881990</td><td>-0.7104840</td></tr><tr><td>H</td><td>2.46511900</td><td>2.3585440</td><td>-0.1170590</td></tr><tr><td>H</td><td>4.26877600</td><td>0.6931730</td><td>-1.2001320</td></tr><tr><td>N</td><td>3.0685850</td><td>-0.9301290</td><td>-0.6442020</td></tr></table>	C	-1.18438100	0.54804700	0.4993690	C	-2.05049200	1.3249720	-0.2921440	C	-3.19005000	0.7214370	-0.8502350	C	-3.4171100	-0.6414180	-0.5972370	C	-2.4963130	-1.33824300	0.2061770	N	-1.4003360	-0.76647700	0.7499540	H	-3.88158500	1.3009950	-1.4701930	H	-1.83202000	2.3835010	-0.4675750	H	-4.2883160	-1.1583610	-1.0104690	H	-2.6406730	-2.40189300	0.4260610	C	0.08653100	1.11182800	1.0990290	H	0.09912800	2.21121200	1.0143910	H	0.11499600	0.85074000	2.1710430	C	1.30520900	0.56183900	0.3989000	C	2.38199900	1.2685680	-0.1395420	S	1.5856040	-1.12706500	0.1394160	C	3.33913400	0.3881990	-0.7104840	H	2.46511900	2.3585440	-0.1170590	H	4.26877600	0.6931730	-1.2001320	N	3.0685850	-0.9301290	-0.6442020
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	<table><tr><td>C</td><td>1.2183220</td><td>-0.22056800</td><td>0.6720380</td></tr><tr><td>C</td><td>1.7723290</td><td>-1.2847700</td><td>-0.0664630</td></tr><tr><td>C</td><td>2.9269630</td><td>-1.0570890</td><td>-0.8320810</td></tr><tr><td>C</td><td>3.48454300</td><td>0.2325280</td><td>-0.8315370</td></tr><tr><td>C</td><td>2.86371200</td><td>1.2318600</td><td>-0.0611230</td></tr><tr><td>N</td><td>1.75248700</td><td>1.02454000</td><td>0.6799840</td></tr><tr><td>H</td><td>3.3795630</td><td>-1.8658480</td><td>-1.4147230</td></tr><tr><td>H</td><td>1.3016100</td><td>-2.2734270</td><td>-0.0396960</td></tr><tr><td>H</td><td>4.38308500</td><td>0.4634170</td><td>-1.4114920</td></tr><tr><td>H</td><td>3.27478900</td><td>2.2471690</td><td>-0.0320410</td></tr><tr><td>C</td><td>-0.0658190</td><td>-0.39129100</td><td>1.4598140</td></tr><tr><td>H</td><td>-0.1897560</td><td>-1.44244200</td><td>1.7693930</td></tr><tr><td>H</td><td>-0.01225700</td><td>0.23353600</td><td>2.3659420</td></tr><tr><td>C</td><td>-1.23249000</td><td>0.04740900</td><td>0.6081030</td></tr><tr><td>C</td><td>-1.55075700</td><td>1.33279400</td><td>0.1645280</td></tr><tr><td>S</td><td>-2.3684640</td><td>-1.0539920</td><td>-0.0829930</td></tr><tr><td>C</td><td>-2.68617900</td><td>1.3069180</td><td>-0.6869610</td></tr><tr><td>H</td><td>-0.98182500</td><td>2.22423800</td><td>0.4394970</td></tr><tr><td>H</td><td>-3.14104100</td><td>2.1807570</td><td>-1.1626130</td></tr></table>	C	1.2183220	-0.22056800	0.6720380	C	1.7723290	-1.2847700	-0.0664630	C	2.9269630	-1.0570890	-0.8320810	C	3.48454300	0.2325280	-0.8315370	C	2.86371200	1.2318600	-0.0611230	N	1.75248700	1.02454000	0.6799840	H	3.3795630	-1.8658480	-1.4147230	H	1.3016100	-2.2734270	-0.0396960	H	4.38308500	0.4634170	-1.4114920	H	3.27478900	2.2471690	-0.0320410	C	-0.0658190	-0.39129100	1.4598140	H	-0.1897560	-1.44244200	1.7693930	H	-0.01225700	0.23353600	2.3659420	C	-1.23249000	0.04740900	0.6081030	C	-1.55075700	1.33279400	0.1645280	S	-2.3684640	-1.0539920	-0.0829930	C	-2.68617900	1.3069180	-0.6869610	H	-0.98182500	2.22423800	0.4394970	H	-3.14104100	2.1807570	-1.1626130				
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H	-0.1897560	-1.44244200	1.7693930																																																																														
H	-0.01225700	0.23353600	2.3659420																																																																														
C	-1.23249000	0.04740900	0.6081030																																																																														
C	-1.55075700	1.33279400	0.1645280																																																																														
S	-2.3684640	-1.0539920	-0.0829930																																																																														
C	-2.68617900	1.3069180	-0.6869610																																																																														
H	-0.98182500	2.22423800	0.4394970																																																																														
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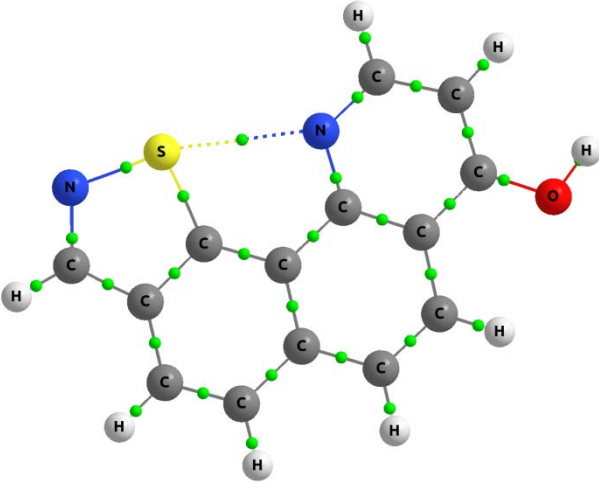
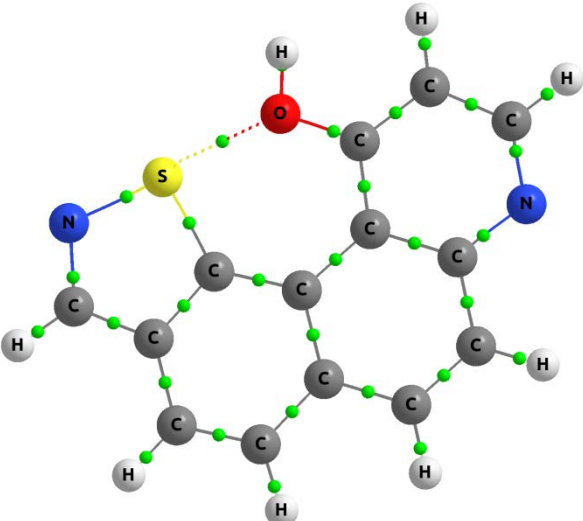
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	C O 1.5967300766 0.947875792 -0.1148595061			
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	C O 3.0424242494 -0.9325608325 0.3410525744			
	C O 2.1864710383 -1.7065744792 -0.4592502815			
	N O 1.0858421833 -1.2255459051 -1.0763652757			
	H O 1.3337566711 2.0026804133 0.01343862			
	H O 3.9222003578 -1.385739296 0.8117096693			
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	H O -0.3947575908 1.6449146483 -1.8026296285			
	H O -0.6660433723 -0.005157263 -2.4416012489			
	C O -1.6256778494 0.4447088227 -0.5525935982			
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	S O -2.0533382228 -1.1023050438 0.1241821867			
	C O -3.4119501465 0.9674735856 0.8912800583			
	H O -2.3356697381 2.498012303 -0.3356541457			
	H O -4.1455759709 1.5942286671 1.4051507274			
	O O 3.5001660307 1.2895815992 1.2641730717			
	H O 4.2471976799 0.8010018354 1.6410956145			
C O -3.3215937464 -0.4078495933 1.0800455749				
H O -3.9275474918 -1.0434362575 1.7271142763				
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	C O -1.5976972093 -0.8283869191 -0.4957499803			
	C O -2.7734955545 -0.7161951049 0.2619261289			
	C O -3.1807907228 0.5584128604 0.6886501767			
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	H O -1.2611746568 -1.8127154963 -0.8366060564			
	H O -4.0910179173 0.6995679854 1.2822654609			
	H O -2.686920401 2.669038079 0.6387467615			
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	H O 0.4650012047 -0.6253658012 -2.1999582868			
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	H O 2.0088404772 2.3413730932 -0.2288497942			
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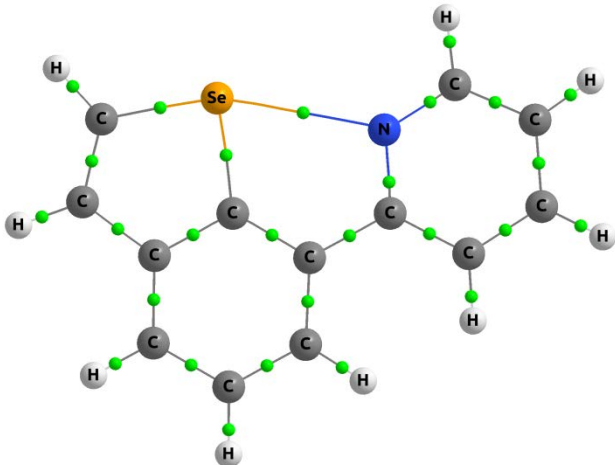
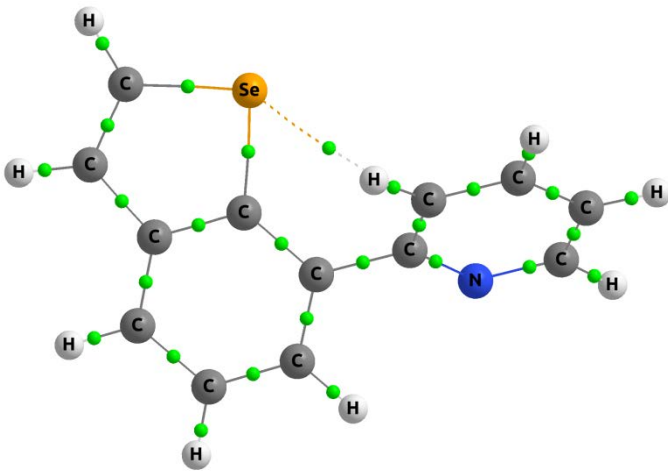
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S^{III}_{NOH} (b)	
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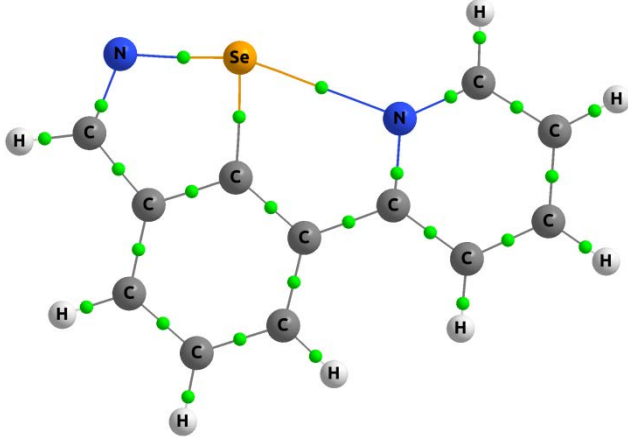
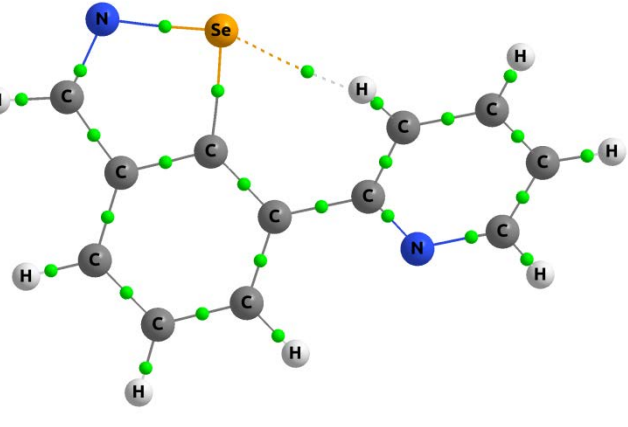
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S^{IV}(b)	
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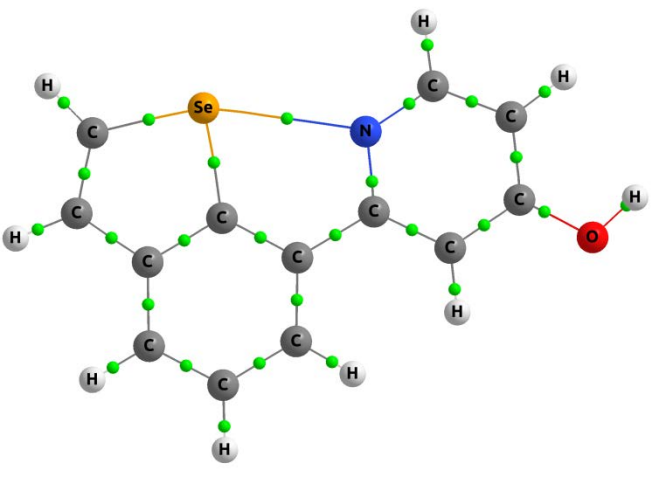
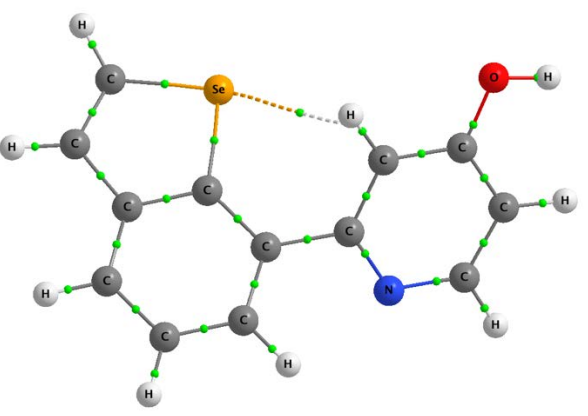
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S^{IV}_N (b)	
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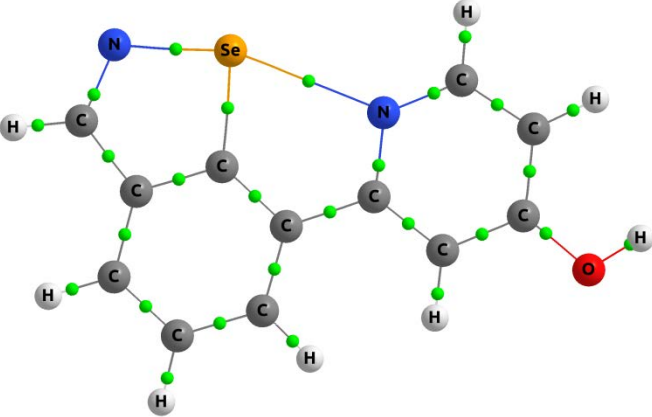
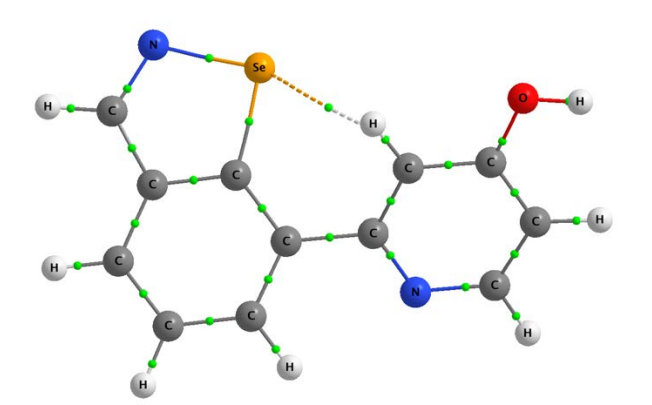
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S^{IV}_{OH} (b)	
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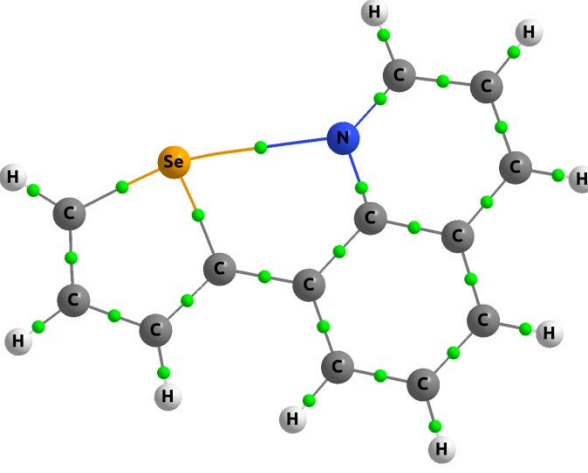
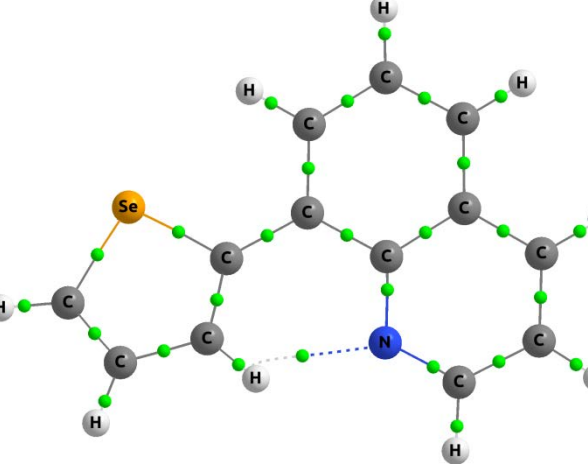
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S^{IV}_{NOH} (b)	
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Family Se	
Se^I (a)	

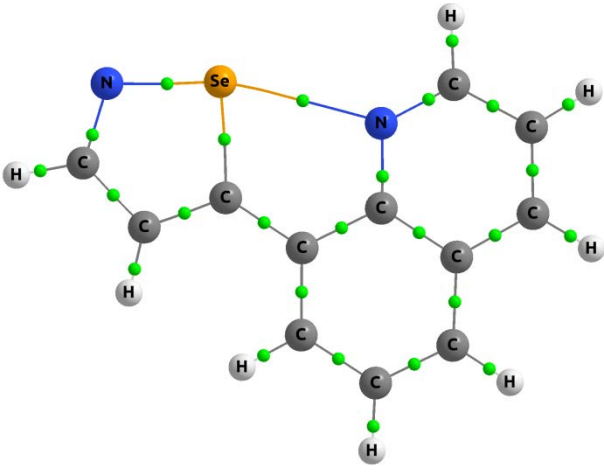
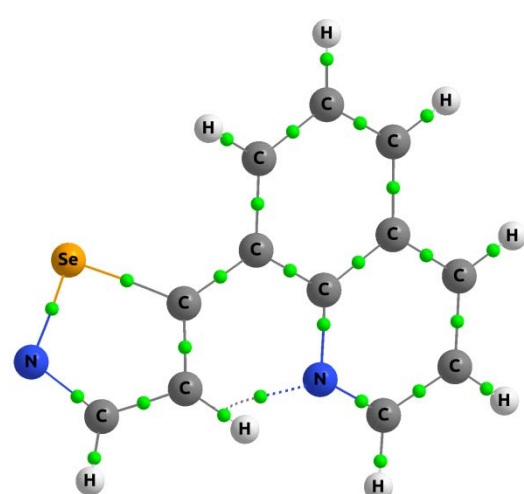
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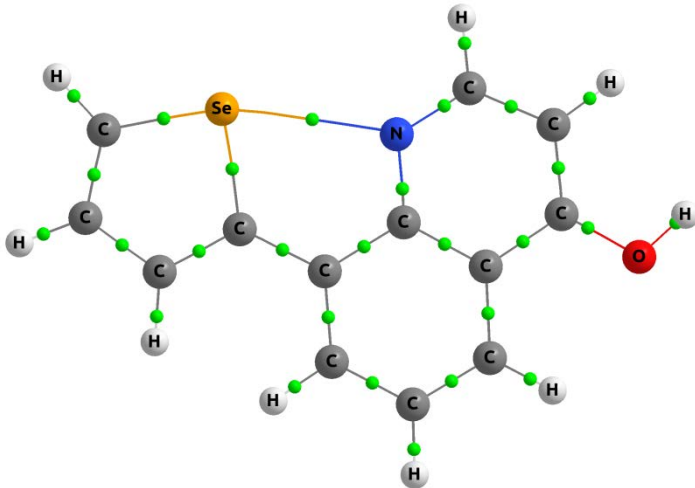
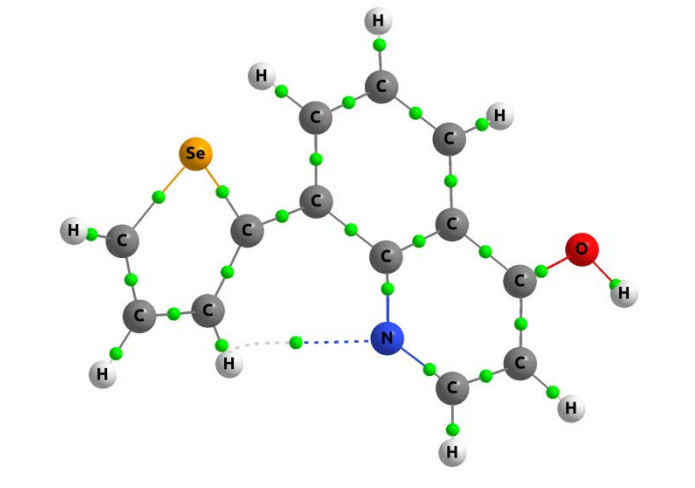
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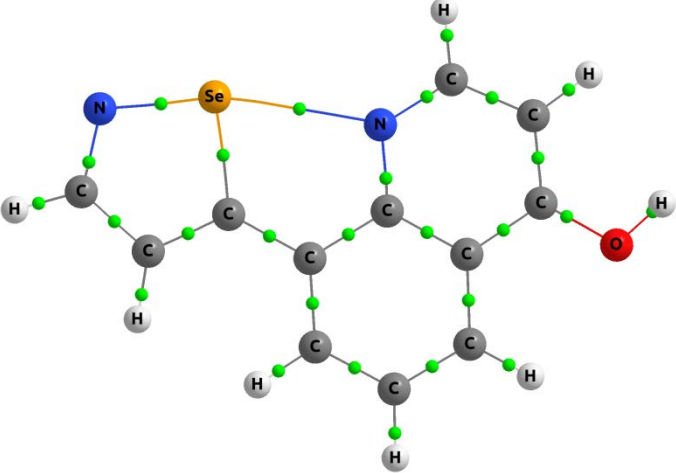
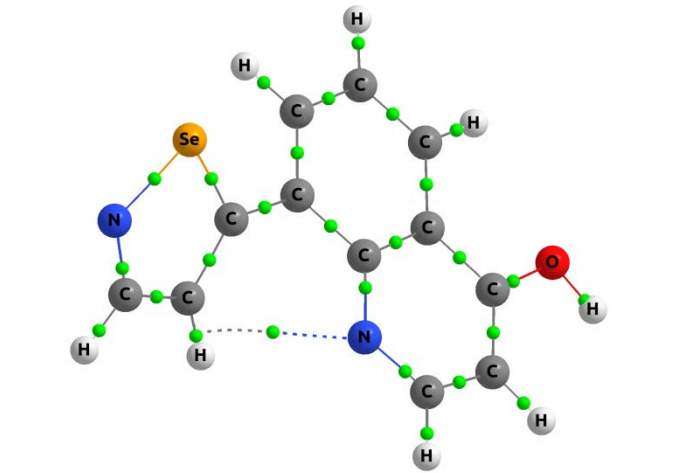
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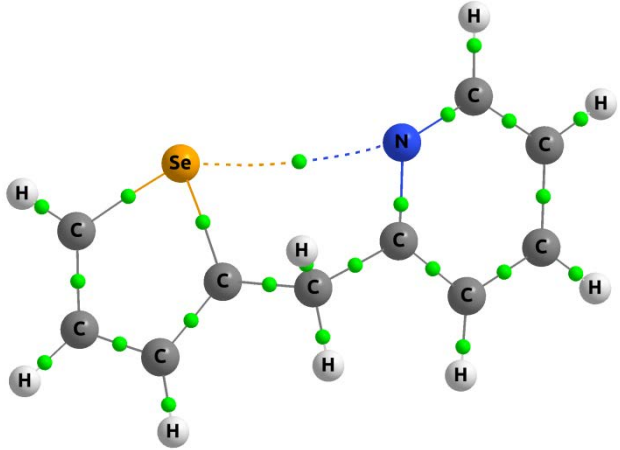
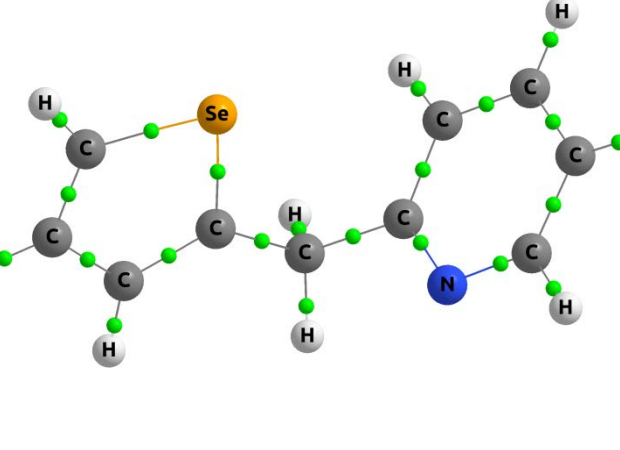
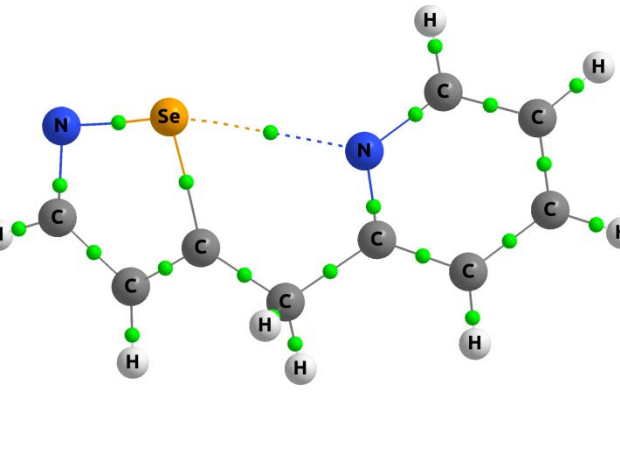
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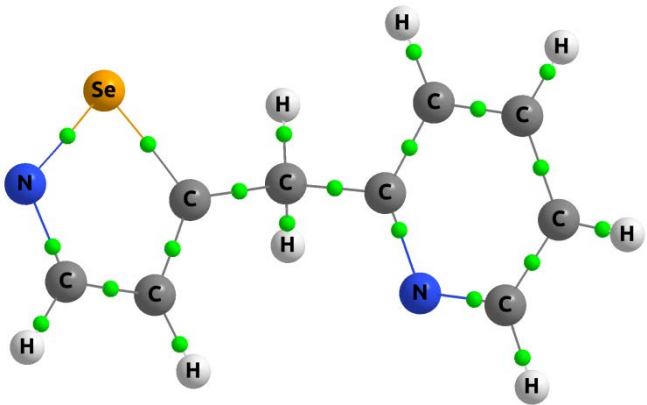
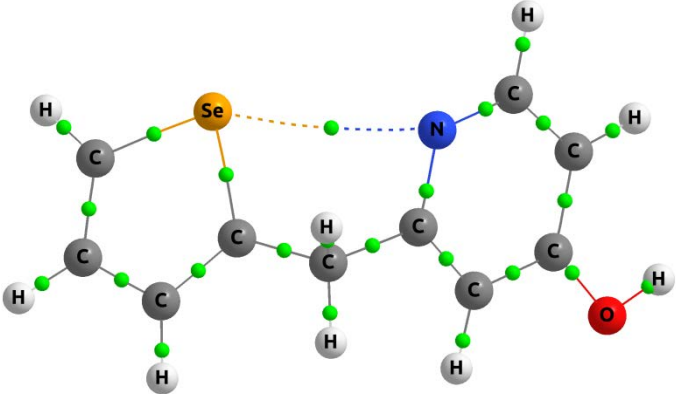
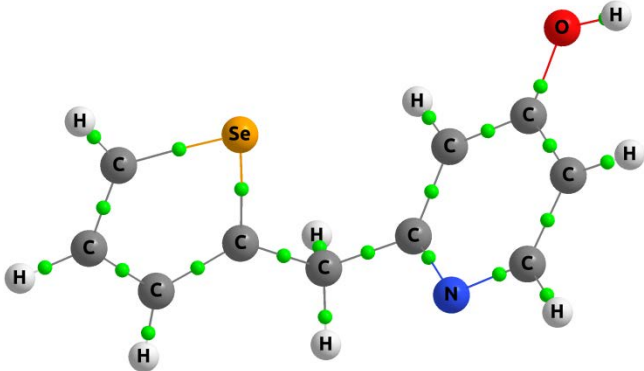
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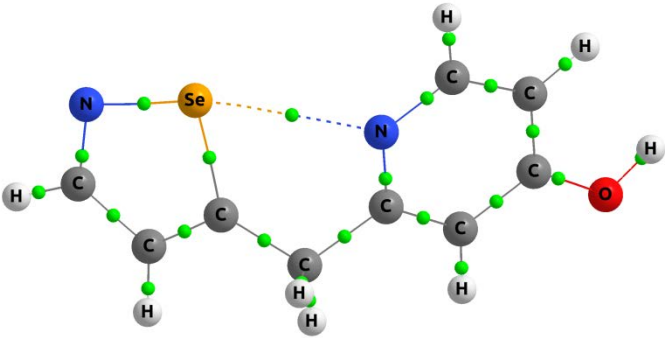
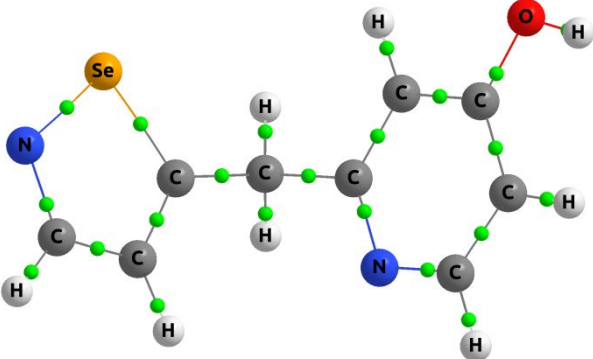
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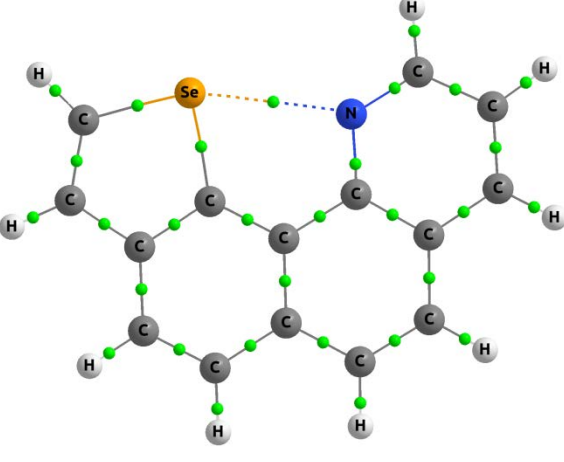
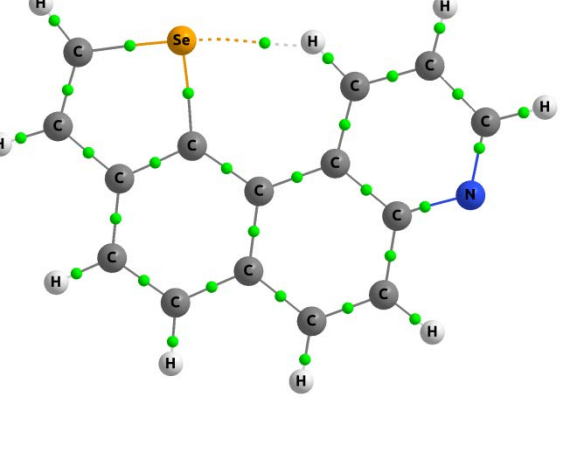
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Se^{II}_{OH} (b)	
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Se^{II}_{NOH} (a)	

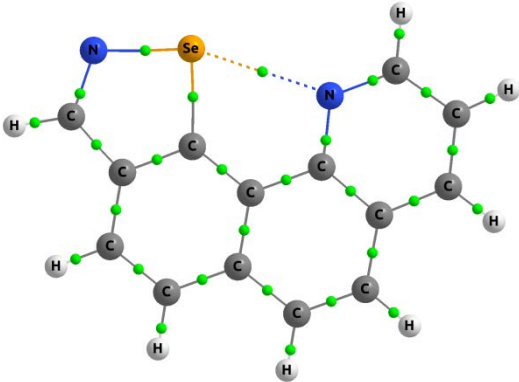
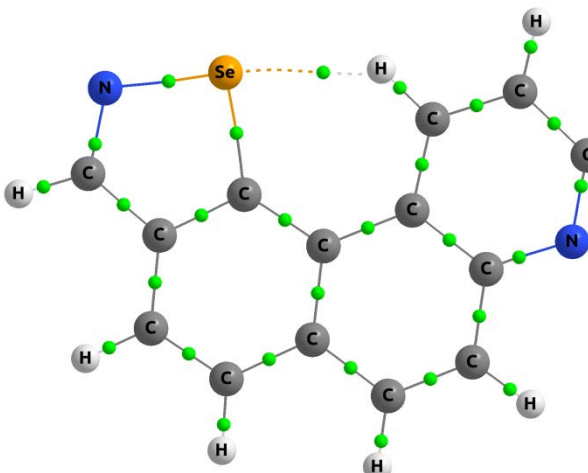
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Se ^{IV} _{NOH} (b)	
	C 1.3173138571 3.176244646 -0.9387474546 C 2.2811455312 2.2370538151 -0.5971775266 C 1.8769822141 0.904277808 -0.2793481849 C 0.4665473292 0.613091611 -0.3280883901 C -0.0445270621 2.7730481309 -0.9651605643 H 3.8853365941 0.1437256008 0.1003707302 H 1.5904693004 4.2063651424 -1.1902298937 C 2.8220589839 -0.1035932088 0.06747819 C 0.0265508004 -0.7211586164 -0.0091981029 H -0.8116728569 3.5037830612 -1.2449853048 C 0.9840043141 -1.6894360581 0.3298270388 C 2.3677489213 -1.3853231772 0.3634838376 H 0.6455065062 -2.6950677644 0.600677485 H 3.0825474524 -2.1669568611 0.6379650553 N -0.479671372 1.5468359604 -0.6753364514 C -1.3961499529 -1.0830881802 -0.0536414126 C -2.5252385066 -0.3520266761 0.3264822883 Se -1.9754940261 -2.7574811375 -0.6488214085 C -3.7408447301 -1.0741989501 0.1776104001 H -2.4625092104 0.6699470781 0.7013574689 H -4.7239597226 -0.6664215371 0.4357155988 N -3.7178571383 -2.3299320345 -0.3097408709 O 3.6259939097 2.5000485005 -0.5435094651 H 3.770216774 3.428336907 -0.7820258325
Se ^{III} (a)	

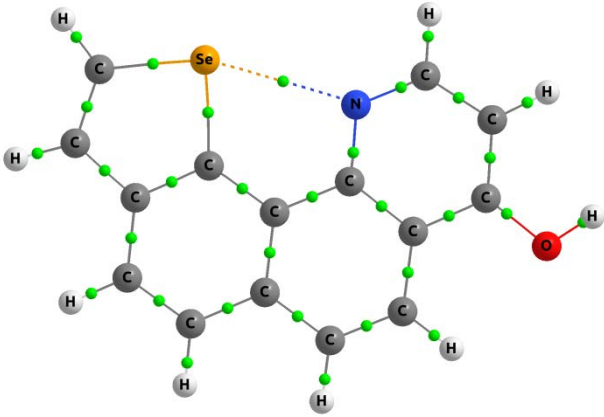
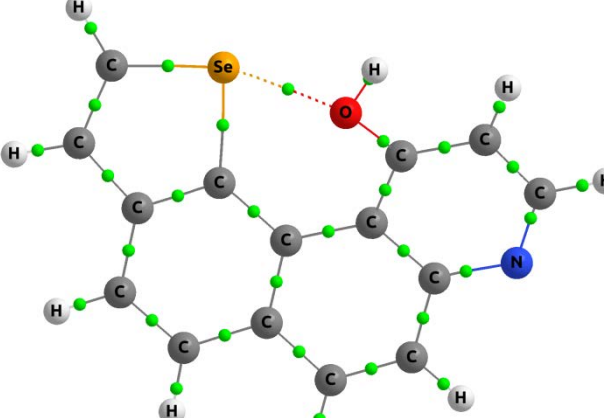
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Se ^{III} (b)	
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	N -3.5987943685 -0.6648170591 0.8879727491 H 4.0481887011 0.9446259838 0.4266807729
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Se^{III}_{OH} (b)	
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Se^{III}_{NOH} (a)	
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Se^{III}_{NOH} (b)	
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Se^{IV} (a)	

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Se^{IV} (a)	

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Se^{IV}_N (b)	
	C -2.5895682847 0.4069771053 0.0220598213 C -1.3480535303 -0.2956438927 0.019807914 C -0.0954197976 0.4096624075 0.0122353 C -0.1667098668 1.8463467197 0.0071336699 C -1.428179008 2.5274211581 0.0095423145 C -2.6232388532 1.8322547783 0.0168489626 C -3.7356126276 -0.4618027941 0.0298297607 H -1.4237677713 3.6220851642 0.0054235682 H -3.5846605817 2.3549749134 0.0186722911 H -4.7653655592 -0.0855028883 0.0324702763 Se -1.7583414544 -2.133509484 0.0283196979 C 1.2126978949 -0.2209641604 0.0094515338 C 2.3953690876 0.6039566486 0.001712905 C 2.7251458368 -2.1321110422 0.010649918 C 3.8157198961 -1.2287531328 0.0029847761 H 2.9027506556 -3.2108763516 0.0139831243 H 4.8453540498 -1.6022515626 0.0003337501 C 2.2803146533 2.0317124482 -0.0031813248 C 1.0381947445 2.6275158678 -0.0005282896 H 0.9486097806 3.7189385331 -0.0042648499 H 3.2050302018 2.6152606662 -0.0090022129 N -3.5658367071 -1.7800590378 0.0341081384 N 3.6708613393 0.100688203 -0.0014182003 C 1.4271053569 -1.6263996337 0.0138629502 H 0.5993494249 -2.3359779934 0.0197647749
Se^{IV}_{OH} (a)	

	C -2.5124786884 0.4598051456 -0.0000604992 C -1.2671392492 -0.2337373177 0.0000324828 C -0.0299203443 0.4730974103 0.0000659867 C -0.0653495755 1.9054358334 0.0000522713 C -1.323574944 2.5899336622 -0.00002852 C -2.5206626279 1.8888677342 -0.0000932354 C -3.6656007951 -0.3990764996 -0.00012684 H -1.3243515139 3.6849821549 -0.0000492634 H -3.4773116092 2.4215582317 -0.000163178 H -4.690236817 -0.0158652178 -0.0002115112 Se -1.5161912615 -2.0970815955 0.0001312556 C 1.2453631141 -0.2015713332 0.0001170311 C 2.451389724 0.5708095767 0.0001714886 C 3.6795190762 -0.1473740423 0.0002082542 C 2.4058613088 -2.2012865638 0.0000933014 C 3.6576699825 -1.5416254103 0.0001759107 H 2.3706603923 -3.2961255559 0.0000676881 H 4.5853605186 -2.1234393308 0.0002033113 C 2.3963210702 2.0041894557 0.0001788536 C 1.1682568367 2.6401500404 0.0001172393 H 1.1218212641 3.7347186186 0.0001091582 H 3.3270953318 2.5759689868 0.0002158432 N 1.2270918862 -1.5689439445 0.0000610737 O 4.8324236395 0.5968836736 0.0002702799 H 5.5910113292 -0.0061860773 0.0002920621 C -3.3640533075 -1.747280977 -0.0000722346 H -4.0883890008 -2.5653119083 -0.0001006
Se^{IV}_{OH} (b)	
	C,-2.6016786362,0.5141261247,-0.0702713407 C,-1.3506143644,-0.180289156,-0.0117508739 C,-0.0986310484,0.5260067462,-0.1218521205 C,-0.1813603933,1.9628464085,-0.1863493507 C,-1.4412858948,2.6258176927,-0.3371319902 C,-2.6295477236,1.9197878258,-0.3054343051 C,-3.7615843964,-0.2854868405,0.2126041826 H,-1.443871317,3.7161042923,-0.4357291242 H,-3.5925056301,2.4332841004,-0.3923943085 H,-4.7777428157,0.117428567,0.1746977939 Se,-1.6580191299,-1.9760831582,0.4913865741 C,1.2345474956,-0.0575814726,-0.0681404575 C,2.3670792826,0.7752109343,0.2576211659 C,2.8532232453,-1.889666511,-0.1535905539 C,3.8396750721,-1.0047340143,0.3318765137 H,3.1070694272,-2.930172978,-0.3841583561 H,4.8479649301,-1.3723824379,0.5491173252 C,2.2128203154,2.1999829328,0.2783367865 C,0.9948082198,2.7694785875,-0.0151013631 H,0.8865373567,3.8581790747,-0.060390013 H,3.1017961045,2.7995234708,0.4921846789 N,3.633497274,0.3062330601,0.4880821923 C,1.5680099949,-1.4053147163,-0.3977911813 O,0.6219254063,-2.165212019,-1.0377107736 H,0.992099075,-3.0466740971,-1.204146216 C,-3.4839811051,-1.5876710661,0.5682488576 H,-4.2043580645,-2.365939161,0.8278491378
Se^{IV}_{NOH} (a)	

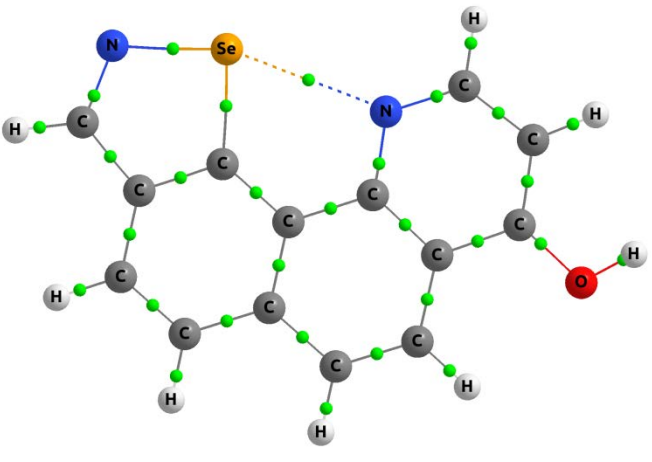
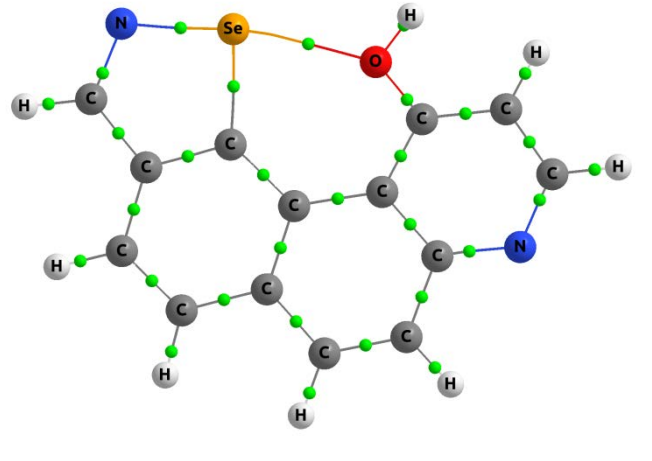
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Se^{IV}_{NOH} (b) 	C -2.5875810091 0.5193304565 -0.0671201198 C -1.3456940977 -0.1900925962 -0.0589288584 C -0.0904484229 0.5234703905 -0.1362473664 C -0.1824020953 1.9633079196 -0.1669699058 C -1.444895486 2.6344268772 -0.266710614 C -2.6334791936 1.9337317002 -0.2303098652 C -3.733132282 -0.3115175254 0.1782740327 H -1.4429957342 3.7270467532 -0.3322956779 H -3.59946548 2.446397068 -0.274582155 H -4.7571628504 0.0811615342 0.18620232 Se -1.7689720404 -1.9953022404 0.2976184166 C 1.2461046151 -0.0554329671 -0.0814802797 C 2.384066909 0.7903152037 0.1967750668 C 2.8695766642 -1.8898310102 -0.1086974837 C 3.8694368465 -0.9789162597 0.2941003936 H 3.1155651308 -2.942657033 -0.2845879659 H 4.8873208001 -1.3320602665 0.4892040287 C 2.2255874763 2.2125060142 0.2136464927 C 0.9925752099 2.7746784375 -0.024706677 H 0.8759389554 3.8629073972 -0.0546241404 H 3.1188393163 2.816532803 0.3933888778 N -3.5589271371 -1.6051186249 0.4282445735 N 3.6598331158 0.334877498 0.4067194981 C 1.5763902475 -1.4204059653 -0.3319142611 O 0.6056230728 -2.228006751 -0.868211298 H 0.9664044692 -3.1219438135 -0.9819160323

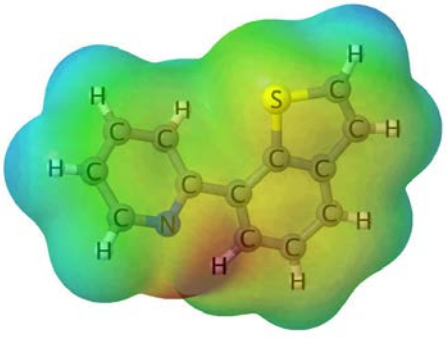
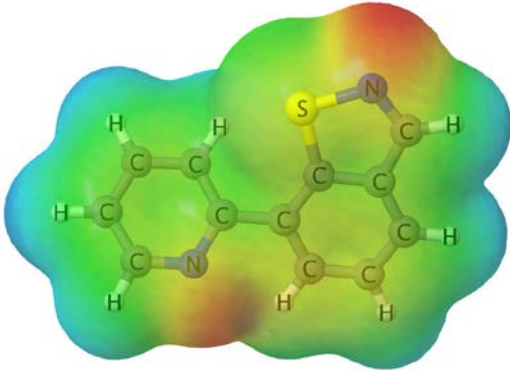
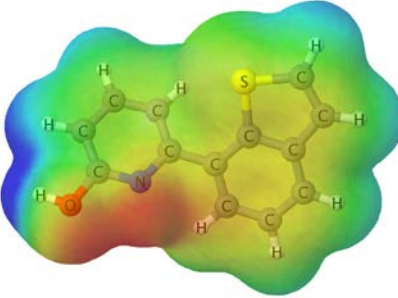
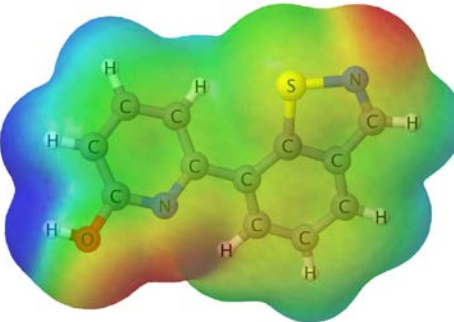
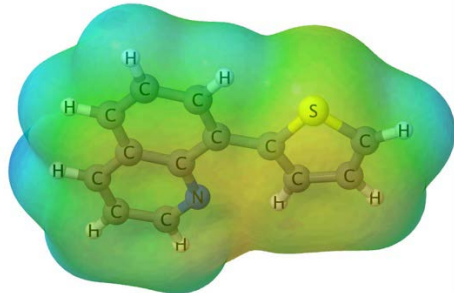
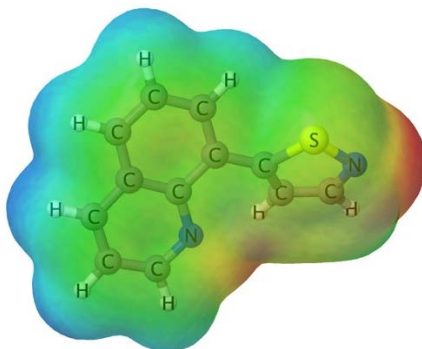
Table S2. Interaction energies (ΔE), kJ/mol, $N\cdots S$ intramolecular distances, Å, and electron density and Laplacian at the bond critical point (ρ , $\nabla^2\rho$), a.u., for family S at the MP2/jul-cc-pVTZ//MP2/jul-cc-pVDZ computational level.

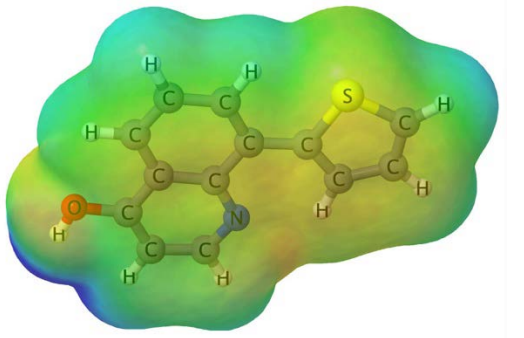
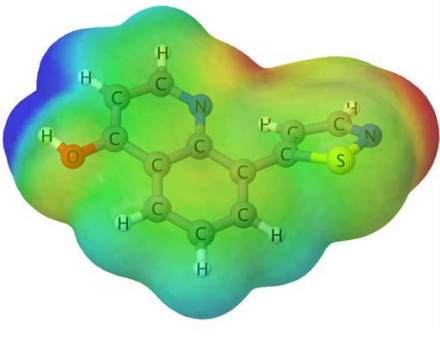
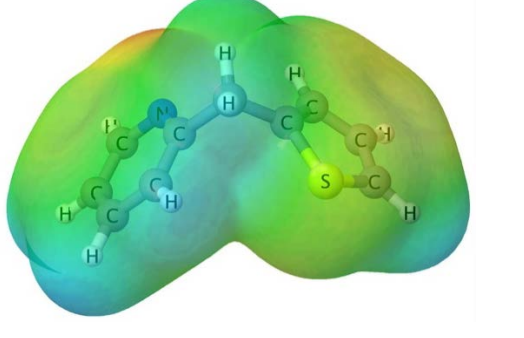
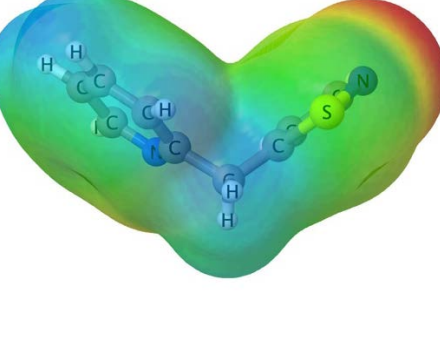
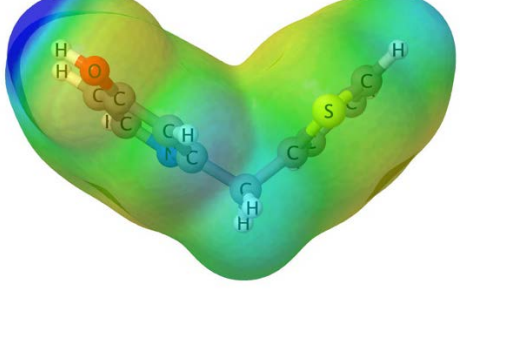
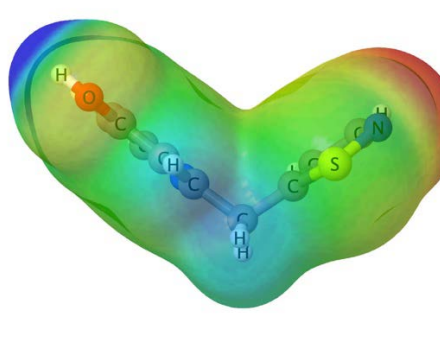
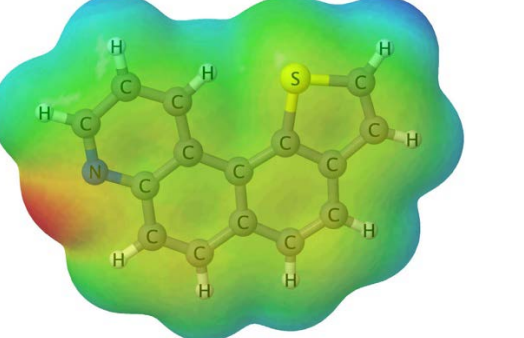
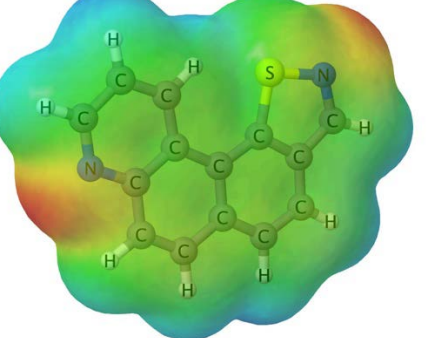
Family S	ΔE kJ/mol	Dist. $N\cdots S$ (Å)	ρ	$\nabla^2\rho$
S^I (a)	-5.6	2.81	0.0198	0.0623
S^I (b)	0.0	2.62 (S $\cdots$ H)	0.0113	0.0394
S^I_N (a)	-12.6	2.70	0.0245	0.0743
S^I_N (b)	0.0	2.64 (S $\cdots$ H)	0.0122	0.0412
S^I_{OH} (a)	-5.4	2.82	0.0195	0.0615
S^I_{OH} (b)	0.0	2.71 (S $\cdots$ H)	0.0115	0.0403
S^I_{NOH} (a)	-11.8	2.70	0.0244	0.0742
S^I_{NOH} (b)	0.0	2.64 (S $\cdots$ H)	0.0122	0.0415
S^{II} (a)	-3.2	2.84	0.0189	0.0593
S^{II} (b)	0.0	2.54 (N $\cdots$ H)	0.0126	0.0454
S^{II}_N (a)	-10.1	2.71	0.0243	0.0735
S^{II}_N (b)	0.0	2.60 (N $\cdots$ H)	-	-
S^{II}_{OH} (a)	-3.5	2.83	0.0193	0.0605
S^{II}_{OH} (b)	0.0	2.53 (N $\cdots$ H)	0.0128	0.0461
S^{II}_{NOH} (a)	-10.5	2.70	0.0247	0.0748
S^{II}_{NOH} (b)	0.0	2.59 (N $\cdots$ H)	-	-
S^{III} (a)	-	-	-	-
S^{III} (b)	0.0	2.32 (N $\cdots$ H)	-	-
S^{III}_N (a)	-1.1	3.07	0.0117	0.0374
S^{III}_N (b)	0.0	-	-	-
S^{III}_{OH} (a)	-1.2	3.36	-	-
S^{III}_{OH} (b)	0.0	-	-	-
S^{III}_{NOH} (a)	-1.5	3.06	0.0119	0.0378
S^{III}_{NOH} (b)	0.0	-	-	-
S^{IV} (a)	-20.3	2.81	0.0202	0.0625
S^{IV} (b)	0.0	2.32 (S $\cdots$ H)	0.0208	0.0609
S^{IV}_N (a)	-21.0	2.80	0.0200	0.0609
S^{IV}_N (b)	0.0	2.33 (S $\cdots$ H)	0.0193	0.0573
S^{IV}_{OH} (a)	-50.6	2.80	0.0205	0.0637
S^{IV}_{OH} (b)	0.0	2.73 (O $\cdots$ S)	0.0212	0.0749
S^{IV}_{NOH} (a)	-47.2	2.80	0.0203	0.0618
S^{IV}_{NOH} (b)	0.0	2.65 (O $\cdots$ S)	0.0237	0.0845

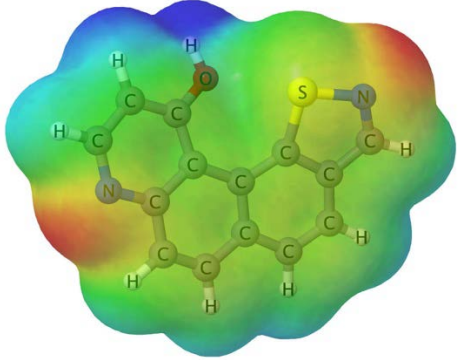
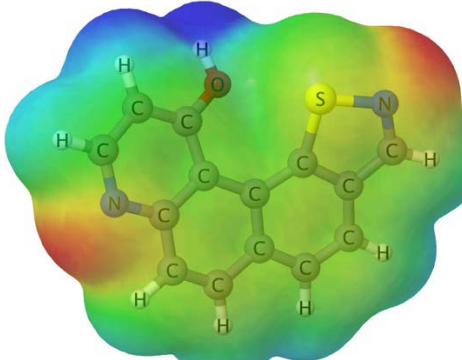
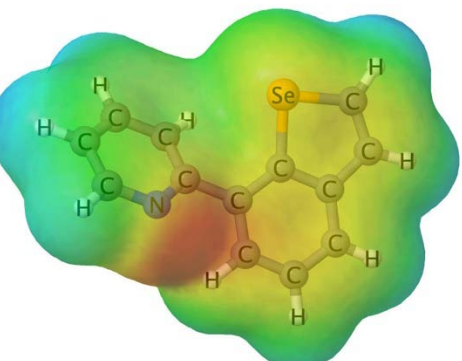
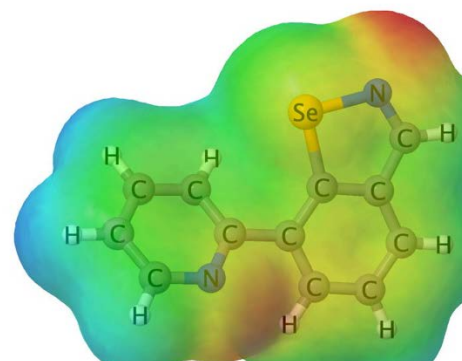
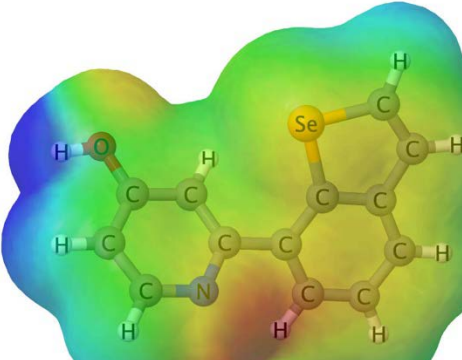
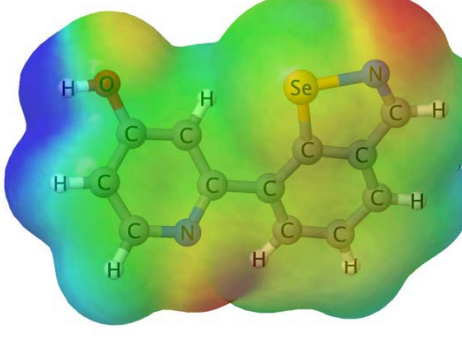
Table S3. Interaction energies (ΔE), kJ/mol, N $\cdots$ S intramolecular distances, Å, and electron density and Laplacian at the bond critical point (ρ , $\nabla^2\rho$), a.u., for family **Se** at the MP2/jul-cc-pVTZ//MP2/jul-cc-pVDZ computational level.

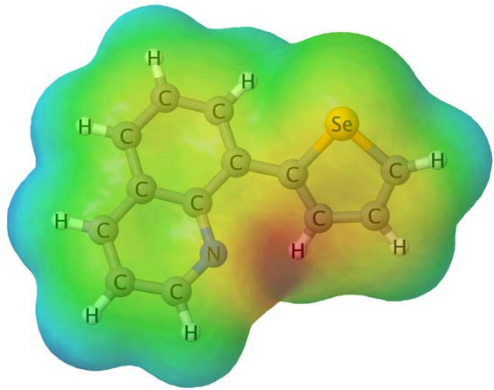
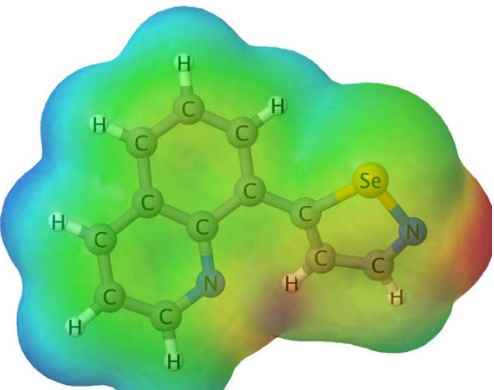
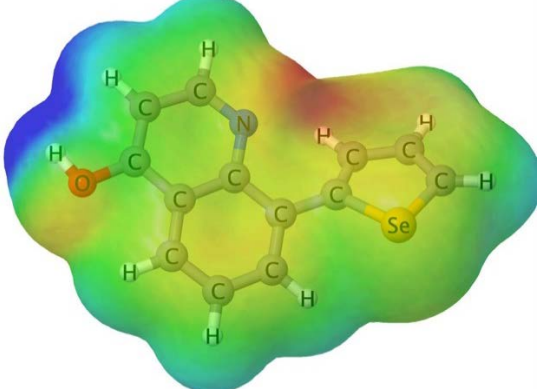
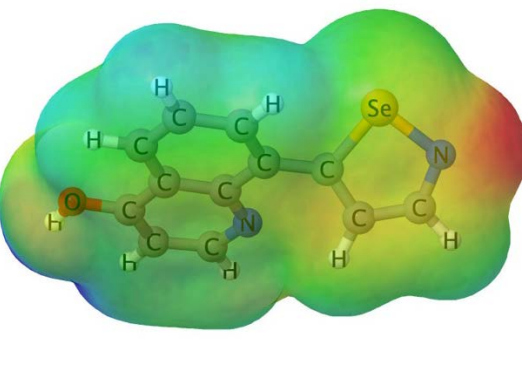
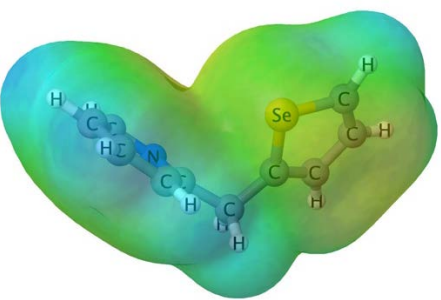
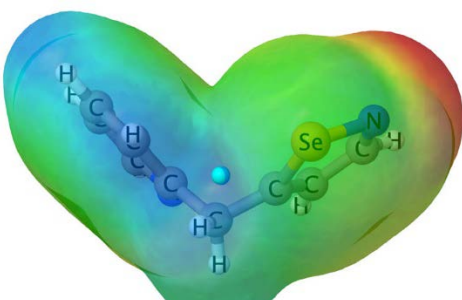
Family Se	ΔE kJ/mol	Dist. N $\cdots$ Se (Å)	ρ	$\nabla^2\rho$
Se ^I (a)	-11.7	2.73	0.0267	0.0744
Se ^I (b)	0.0	2.77(S $\cdots$ H)	0.0120	0.0387
Se ^I _N (a)	-21.2	2.66	0.0300	0.0792
Se ^I _N (b)	0.0	2.70(S $\cdots$ H)	0.0127	0.0398
Se ^I _{OH} (a)	-11.1	2.73	0.0267	0.0743
Se ^I _{OH} (b)	0.0	2.76(S $\cdots$ H)	0.0121	0.0395
Se ^I _{NOH} (a)	-20.8	2.66	0.0298	0.0791
Se ^I _{NOH} (b)	0.0	2.69(S $\cdots$ H)	0.0128	0.0585
Se ^{II} (a)	-11.2	2.74	0.0259	0.0724
Se ^{II} (b)	0.0	2.52(N $\cdots$ H)	0.0128	0.0455
Se ^{II} _N (a)	-21.4	2.68	0.0292	0.0778
Se ^{II} _N (b)	0.0	2.97(N $\cdots$ C)	0.0122	4.4473
Se ^{II} _{OH} (a)	-11.6	2.73	0.0263	0.0736
Se ^{II} _{OH} (b)	0.0	2.52(N $\cdots$ H)	0.0130	0.0462
Se ^{II} _{NOH} (a)	-21.9	2.66	0.0297	0.0791
Se ^{II} _{NOH} (b)	0.0	2.97(N $\cdots$ C)	0.0123	0.0450
Se ^{III} (a)	-4.4	3.19	0.0107	0.0339
Se ^{III} (b)	0.0	-	-	-
Se ^{III} _N (a)	-8.0	2.88	0.0193	0.0549
Se ^{III} _N (b)	0.0	-	-	-
Se ^{III} _{OH} (a)	-4.3	3.18	0.0111	0.0342
Se ^{III} _{OH} (b)	0.0	-	-	-
Se ^{III} _{NOH} (a)	-8.3	2.89	0.0190	0.0541
Se ^{III} _{NOH} (b)	0.0	-	-	-
Se ^{IV} (a)	-28.0	2.80	0.0230	0.0645
Se ^{IV} (b)	0.0	2.35(S $\cdots$ H)	0.0215	0.0583
Se ^{IV} _N (a)	-29.4	2.79	0.0235	0.0638
Se ^{IV} _N (b)	0.0	2.37(S $\cdots$ H)	0.0201	0.0550
Se ^{IV} _{OH} (a)	-57.0	2.79	0.0234	0.0655
Se ^{IV} _{OH} (b)	0.0	2.75(S $\cdots$ O)	0.0227	0.0736
Se ^{IV} _{NOH} (a)	-53.7	2.77	0.0240	0.0652
Se ^{IV} _{NOH} (b)	0.0	2.66(S $\cdots$ O)	0.0259	0.0847

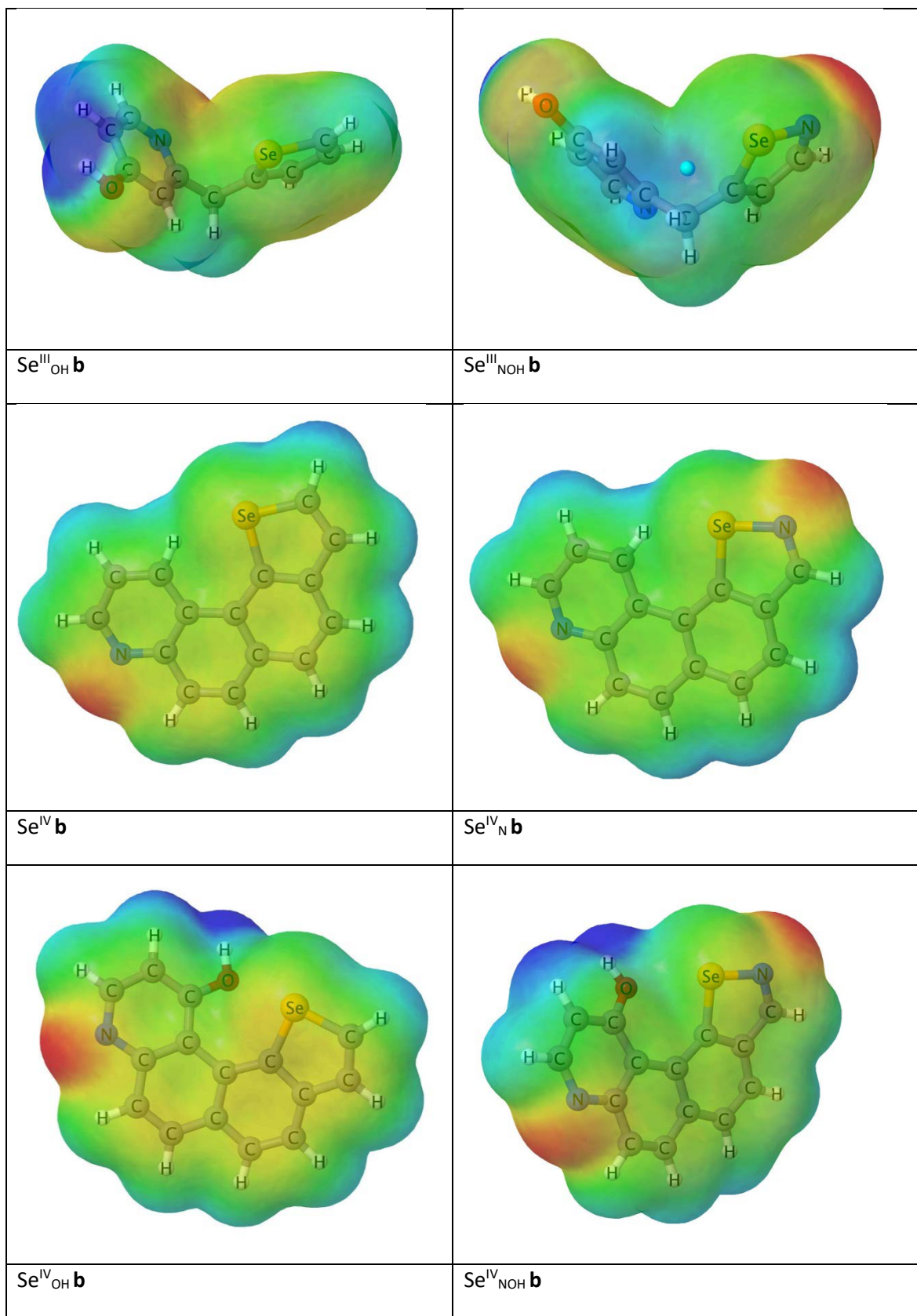
Table S4. Molecular electrostatic potential on the 0.001 au electron density isosurface for selected compounds at the MP2/jul-cc-pVDZ computational level.

	
$S^I \mathbf{b}$	$S^I_N \mathbf{b}$
	
$S^{I_{OH}} \mathbf{b}$	$S^{I_{NOH}} \mathbf{b}$
	
$S^{II} \mathbf{b}$	$S^{II}_N \mathbf{b}$

	
$S^{\text{II}}_{\text{OH}} \mathbf{b}$	$S^{\text{II}}_{\text{NOH}} \mathbf{b}$
	
$S^{\text{III}} \mathbf{b}$	$S^{\text{III}}_{\text{N}} \mathbf{b}$
	
$S^{\text{III}}_{\text{OH}} \mathbf{b}$	$S^{\text{III}}_{\text{NOH}} \mathbf{b}$
	

$S^{IV}b$	S^{IV}_Nb
	
$S^{IV}_{OH}b$	$S^{IV}_{NOH}b$
	
Se^Ib	Se^I_Nb
	
$Se^I_{OH}b$	$Se^I_{NOH}b$

 3D electrostatic potential map of the Se^{II} b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a hydrogen atom (H). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.	 3D electrostatic potential map of the Se^{II}_N b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a nitrogen atom (N). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.
Se ^{II} b	Se ^{II} _N b
 3D electrostatic potential map of the Se^{II}_{OH} b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a hydroxyl group (OH). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.	 3D electrostatic potential map of the Se^{II}_{NOH} b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a nitro group (NOH). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.
Se ^{II} _{OH} b	Se ^{II} _{NOH} b
 3D electrostatic potential map of the Se^{III} b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a hydrogen atom (H). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.	 3D electrostatic potential map of the Se^{III}_N b complex. The molecule consists of a pyridine ring connected to a five-membered ring containing a selenium atom (Se) and a nitrogen atom (N). The electrostatic potential is shown as a green and blue isosurface, with blue indicating electron-rich regions and green indicating electron-poor regions.
Se ^{III} b	Se ^{III} _N b



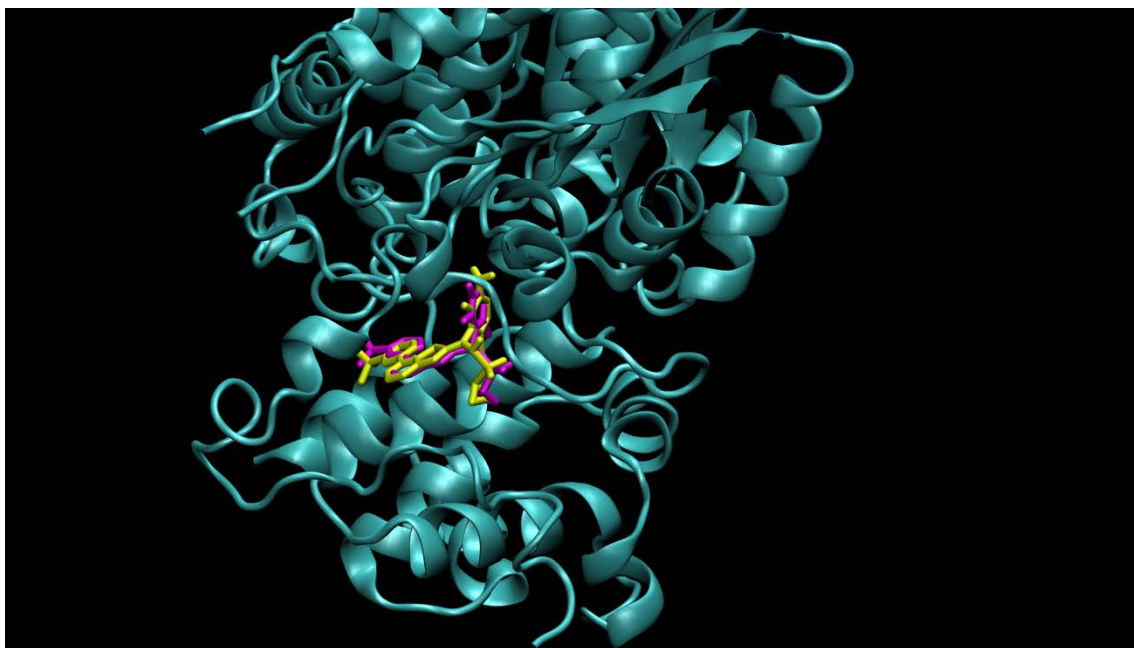


Figure S2. Superimposition of S^I compound (yellow) and crystal structure (PDB ID: 4PX5) ligand (magenta) in the Glucokinase–Glucokinase Regulatory Protein (GK–GKRP) crystal structure.

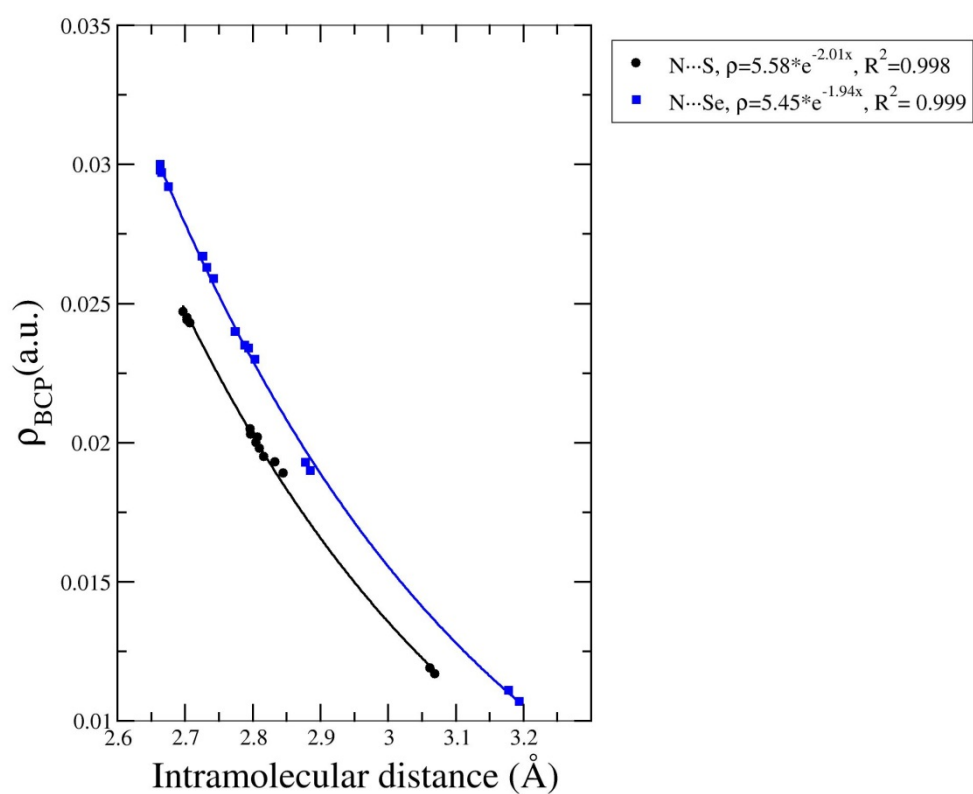


Figure S3. Relationships between distance (Å) and the electron density value at the bond critical point (ρ) for the three different interactions under study, $N\cdots S$ and $N\cdots Se$.