

## Helicity discrimination in *N,N'*-dibenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthrolines and their thiono- and selenocarbonyl analogues by inclusion complexation with chiral diols

### Supporting information

Teresa Olszewska,<sup>a\*</sup> Artur Sikorski,<sup>b</sup> Aleksander Herman,<sup>a</sup> and Tadeusz Połowski<sup>a</sup>

<sup>a</sup>Department of Chemistry, Technical University, 80-233 Gdańsk, Poland

<sup>b</sup>Faculty of Chemistry, University of Gdańsk, 80-952 Gdańsk, Poland

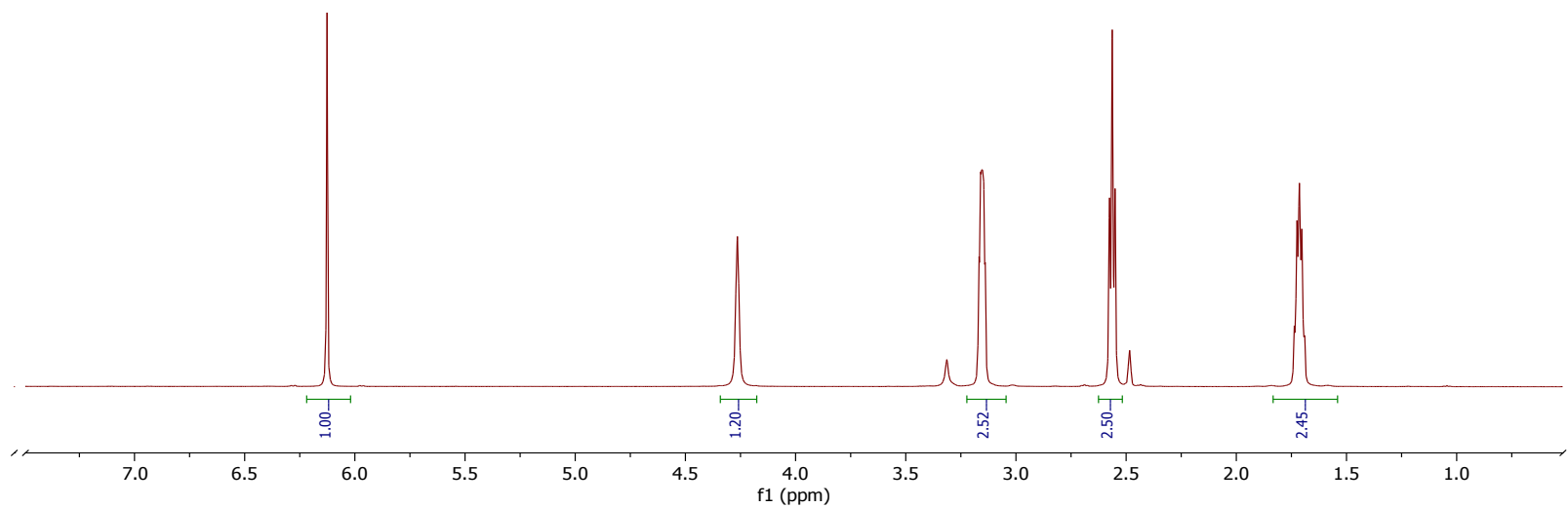
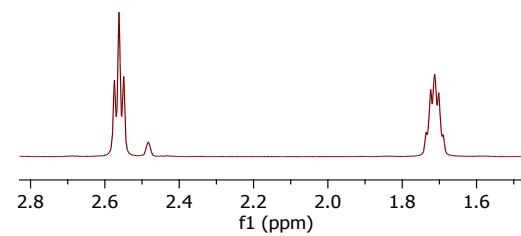
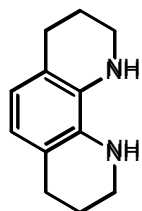
\* Corresponding author. Tel.; +48 58 3471425; fax: +48 58 3472694.

E-mail address: [terolsze@pg.gda.pl](mailto:terolsze@pg.gda.pl) (T. Olszewska).

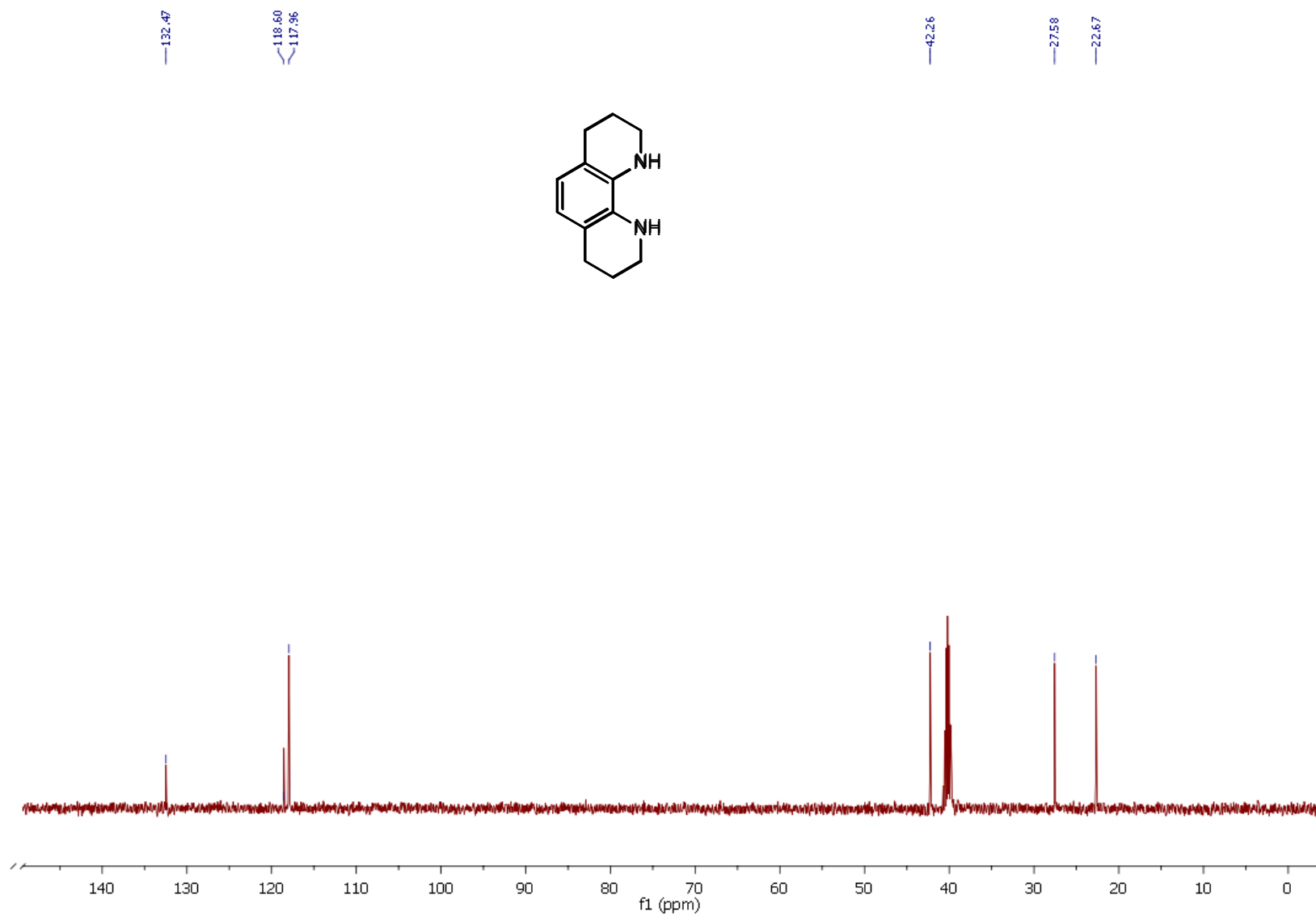
### Table of Contents

1) 1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>4</b> ) – <sup>1</sup> H NMR.....	1
2) 1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>4</b> ) – <sup>13</sup> C NMR.....	2
3) <i>N,N'</i> -dibenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5a</b> ) – <sup>1</sup> H NMR.....	3
4) <i>N,N'</i> -dibenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5a</b> ) – <sup>13</sup> C NMR.....	4
5) <i>N,N'</i> -dithionobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5b</b> ) – <sup>1</sup> H NMR.....	5
6) <i>N,N'</i> -dithionobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5b</b> ) – <sup>13</sup> C NMR.....	6
7) <i>N,N'</i> -diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5c</b> ) – <sup>1</sup> H NMR.....	7
8) <i>N,N'</i> -diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5c</b> ) – <sup>13</sup> C NMR.....	8
9) <i>N,N'</i> -diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5c</b> ) – <sup>77</sup> Se NMR.....	9
10) <i>N</i> -benzoyl- <i>N'</i> -selenidobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5d</b> ) – <sup>1</sup> H NMR.....	10
11) <i>N</i> -benzoyl- <i>N'</i> -selenidobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5d</b> ) – <sup>1</sup> H NMR.....	11
12) <i>N</i> -benzoyl- <i>N'</i> -selenidobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline ( <b>5d</b> ) – <sup>77</sup> Se NMR.....	12
13) <i>N,N'</i> -Terephthaloyl-bis(1-benzoyl-1,2,3,4,7,8,9,10-octahydro-[1,10]phenanthroline) ( <b>7</b> ) – <sup>1</sup> H NMR.....	13
14) <b>Fig. 1S</b> Molecular structures of the compounds ( <b>5a-5d</b> ).....	14
15) <b>Fig. 2S</b> Crystal packing of compounds ( <b>5a-5d</b> ).....	15
16) <b>Fig. 3S</b> Molecular structure and crystal packing of the complex ( <b>5c·6a</b> ).....	16
17) <b>Fig. 6S</b> Molecular structure of the bisamide ( <b>7</b> ).....	17
18) <b>Table 1</b> DFT TZ2P LDA ZORA calculated structures and energies - compounds ( <b>5a-5c</b> ).....	18

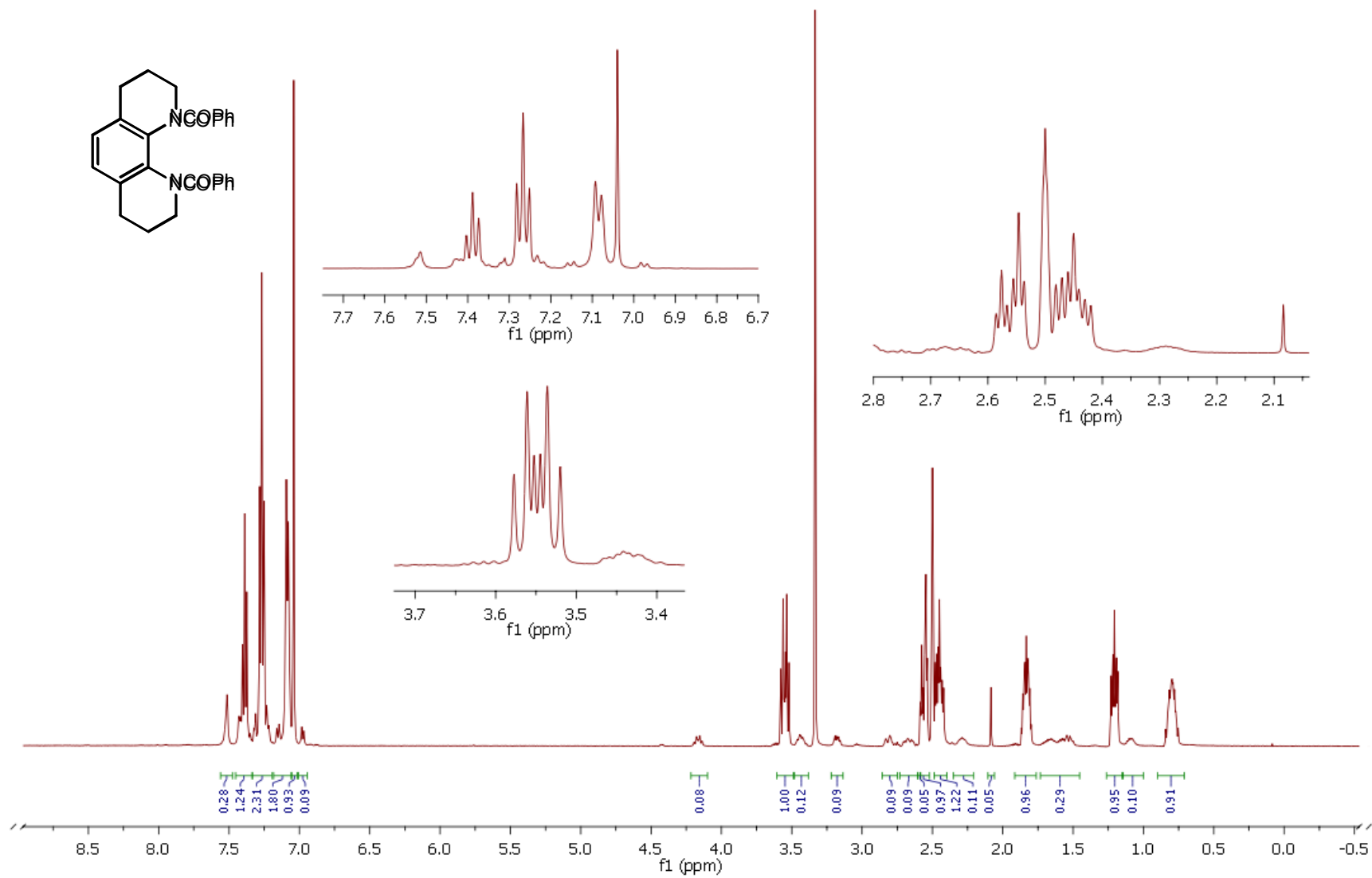
1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**4**) –  $^1\text{H}$  NMR



1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**4**) –  $^{13}\text{C}$  NMR

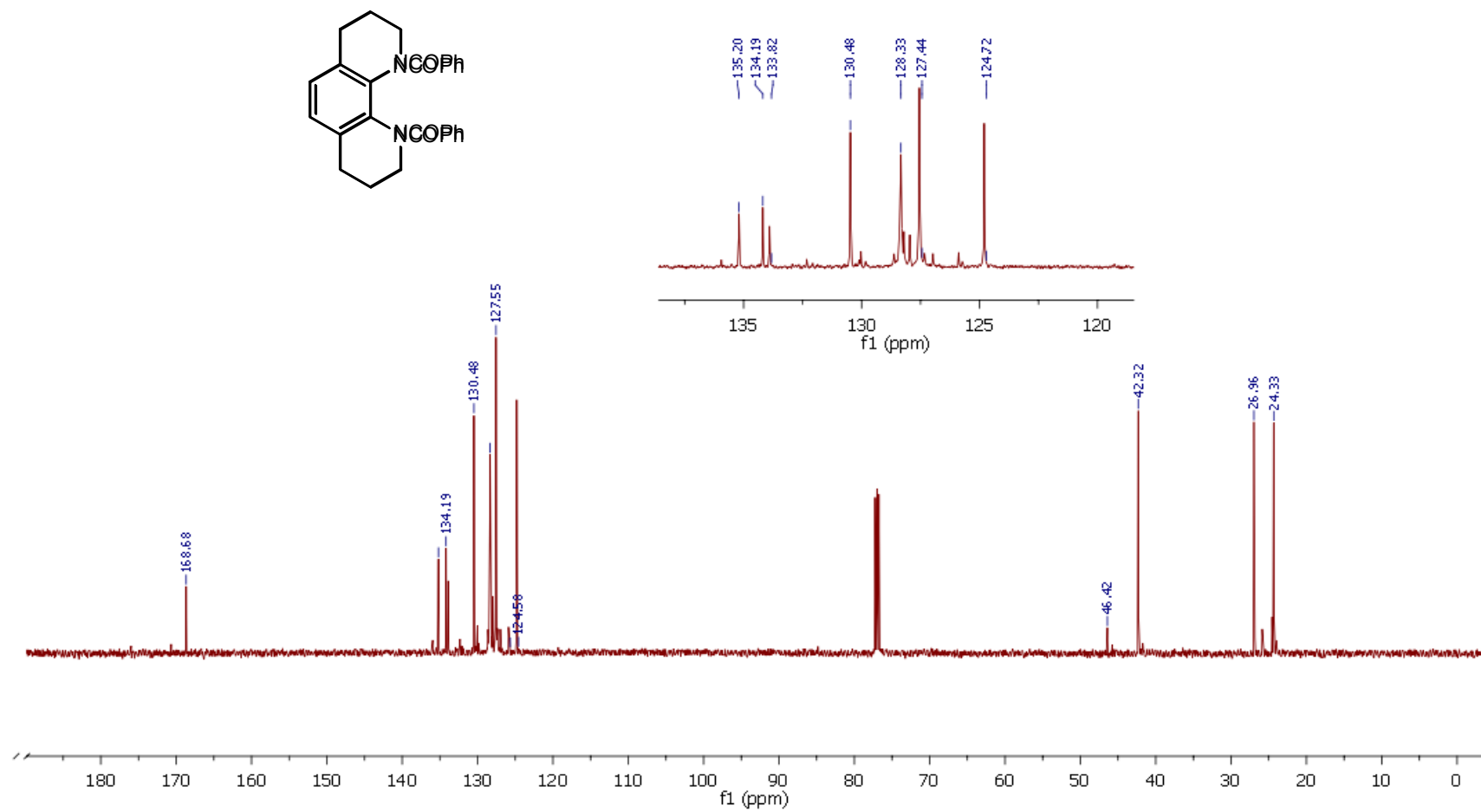


*N,N'*-dibenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5a**) – <sup>1</sup>H NMR

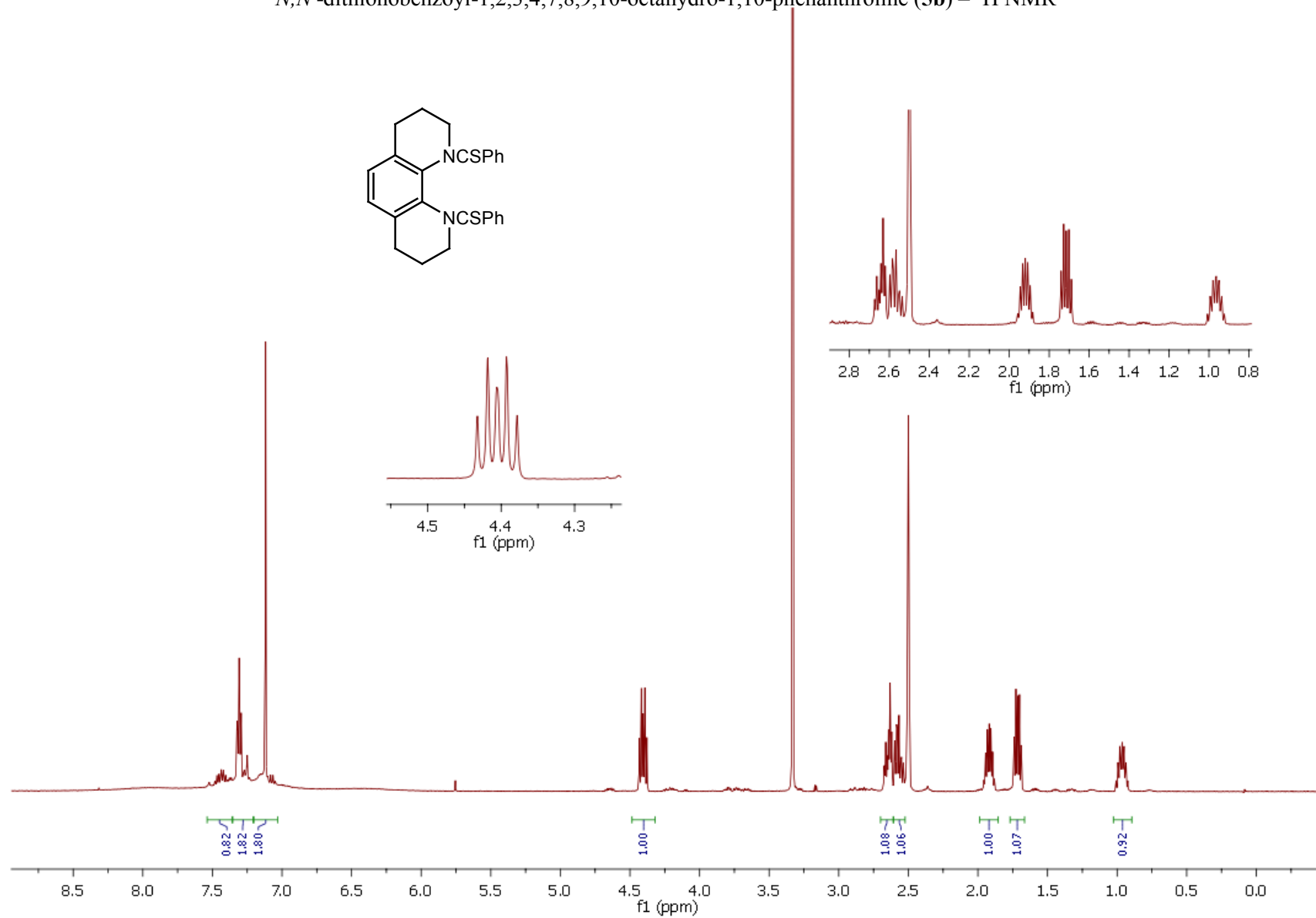




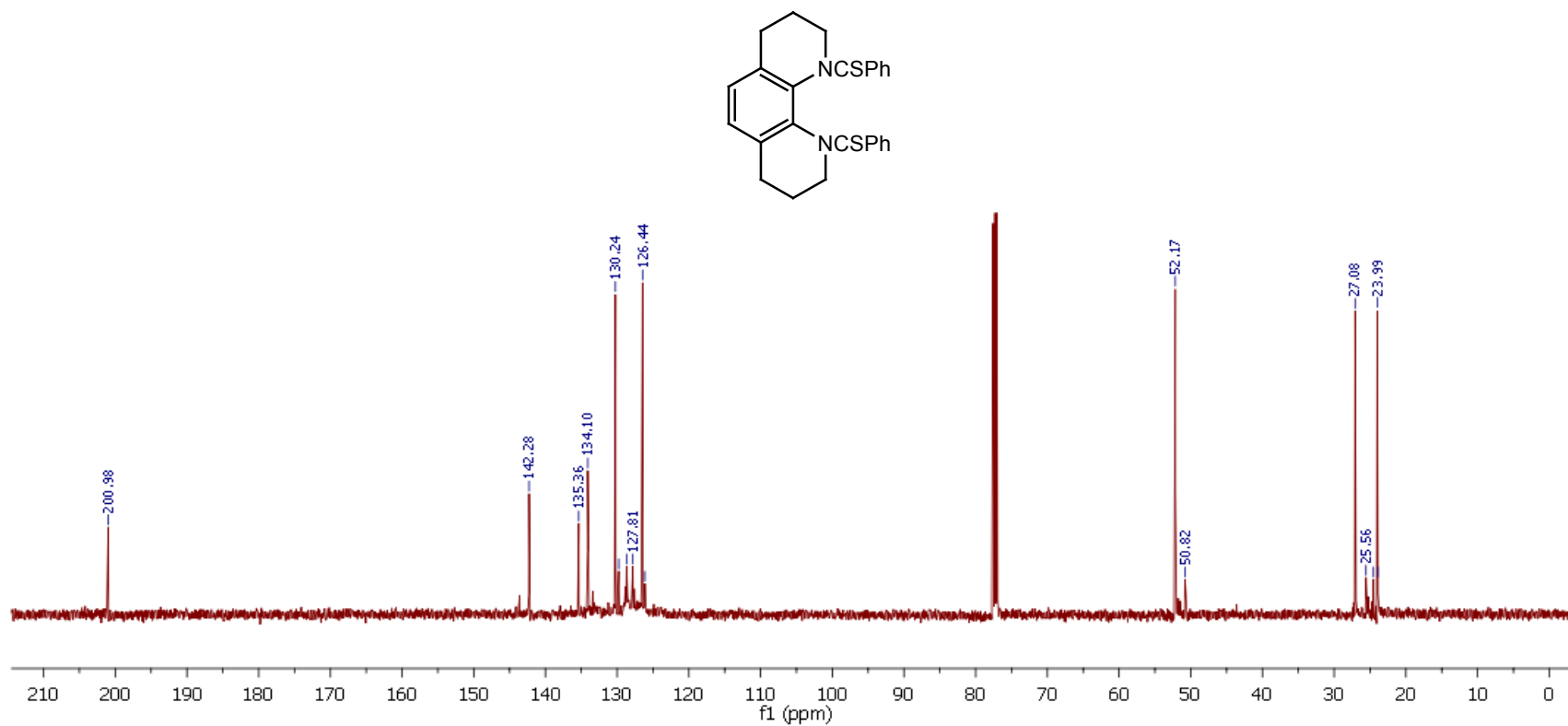
*N,N'*-dibenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5a**) –  $^{13}\text{C}$  NMR



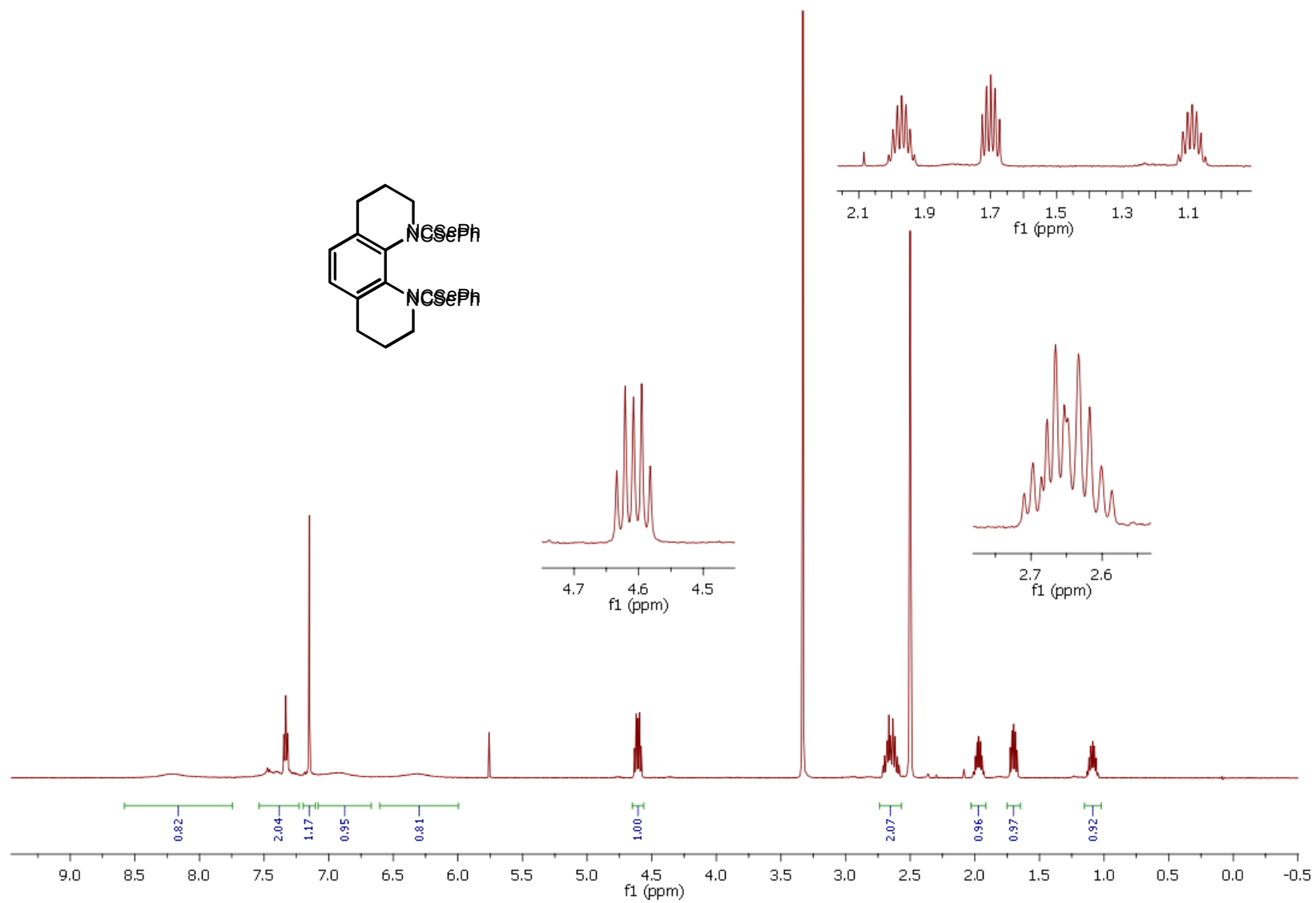
*N,N'*-dithionobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5b**) – <sup>1</sup>H NMR



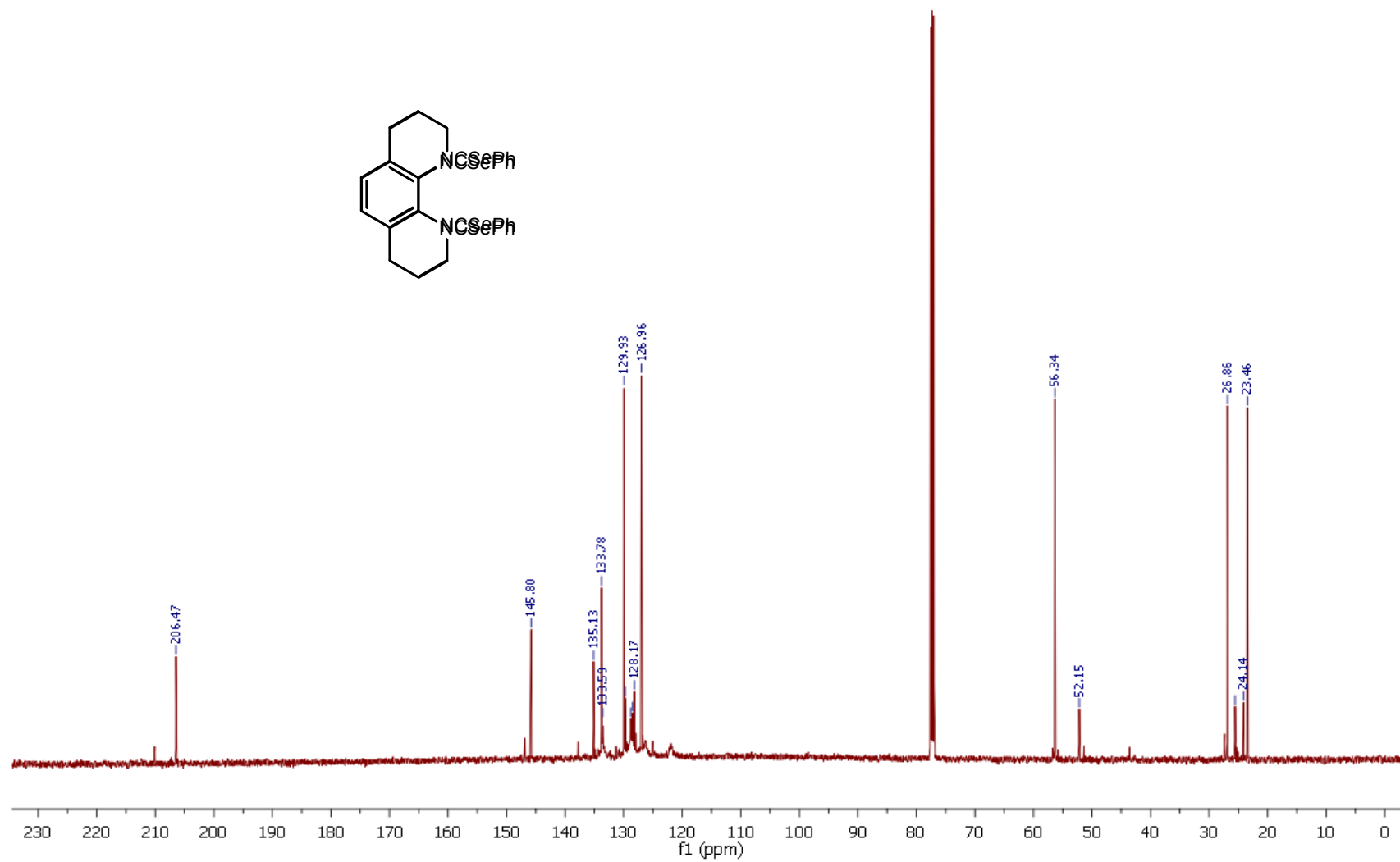
*N,N'*-dithionobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5b**) –  $^{13}\text{C}$  NMR



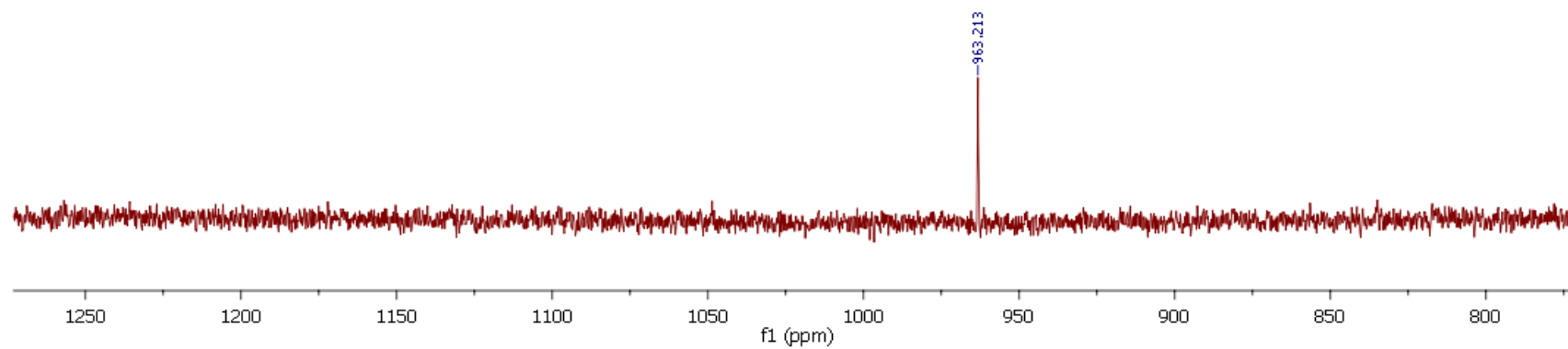
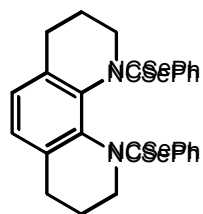
*N,N'*-diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5c**) – <sup>1</sup>H NMR



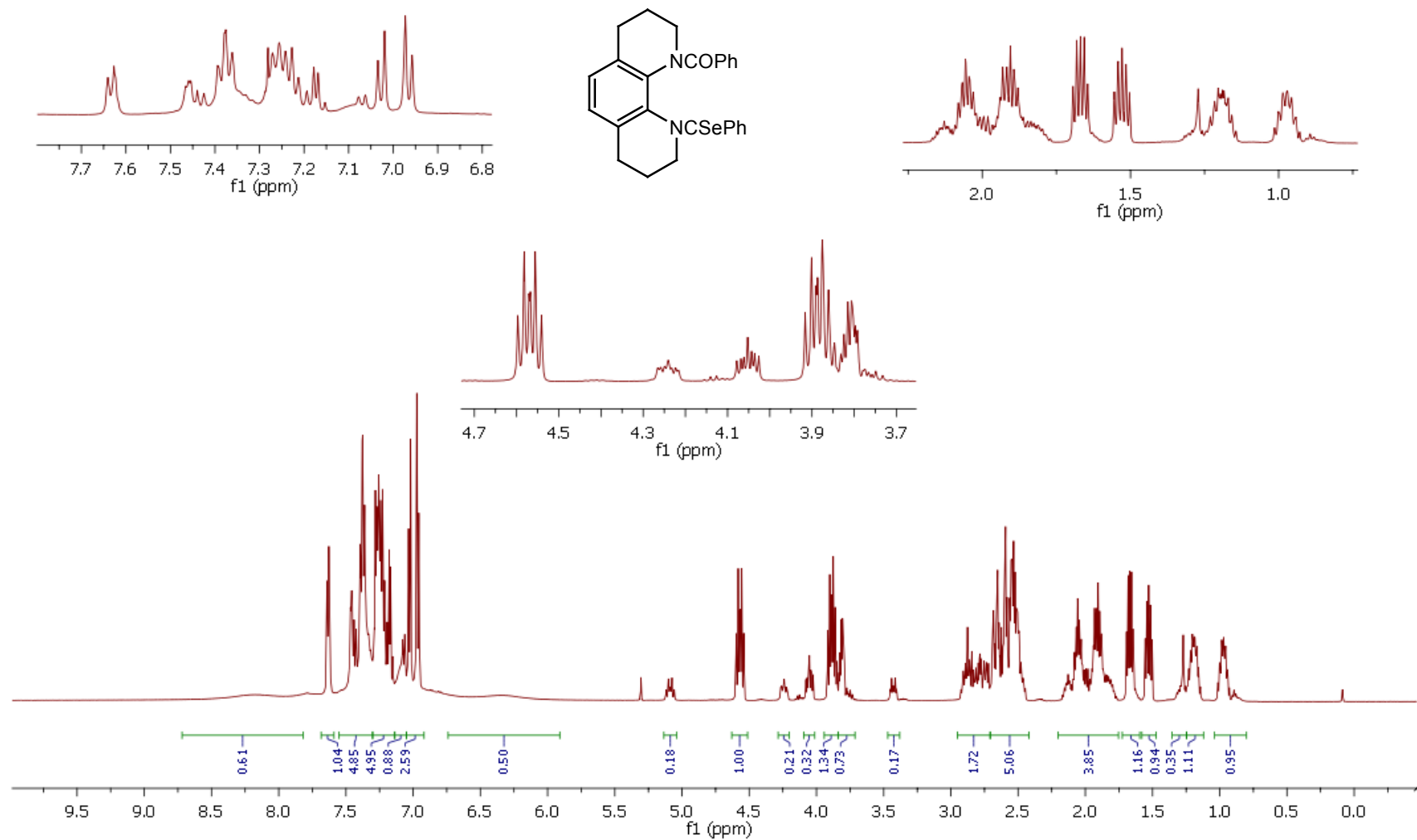
*N,N'*-diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5c**) –  $^{13}\text{C}$  NMR



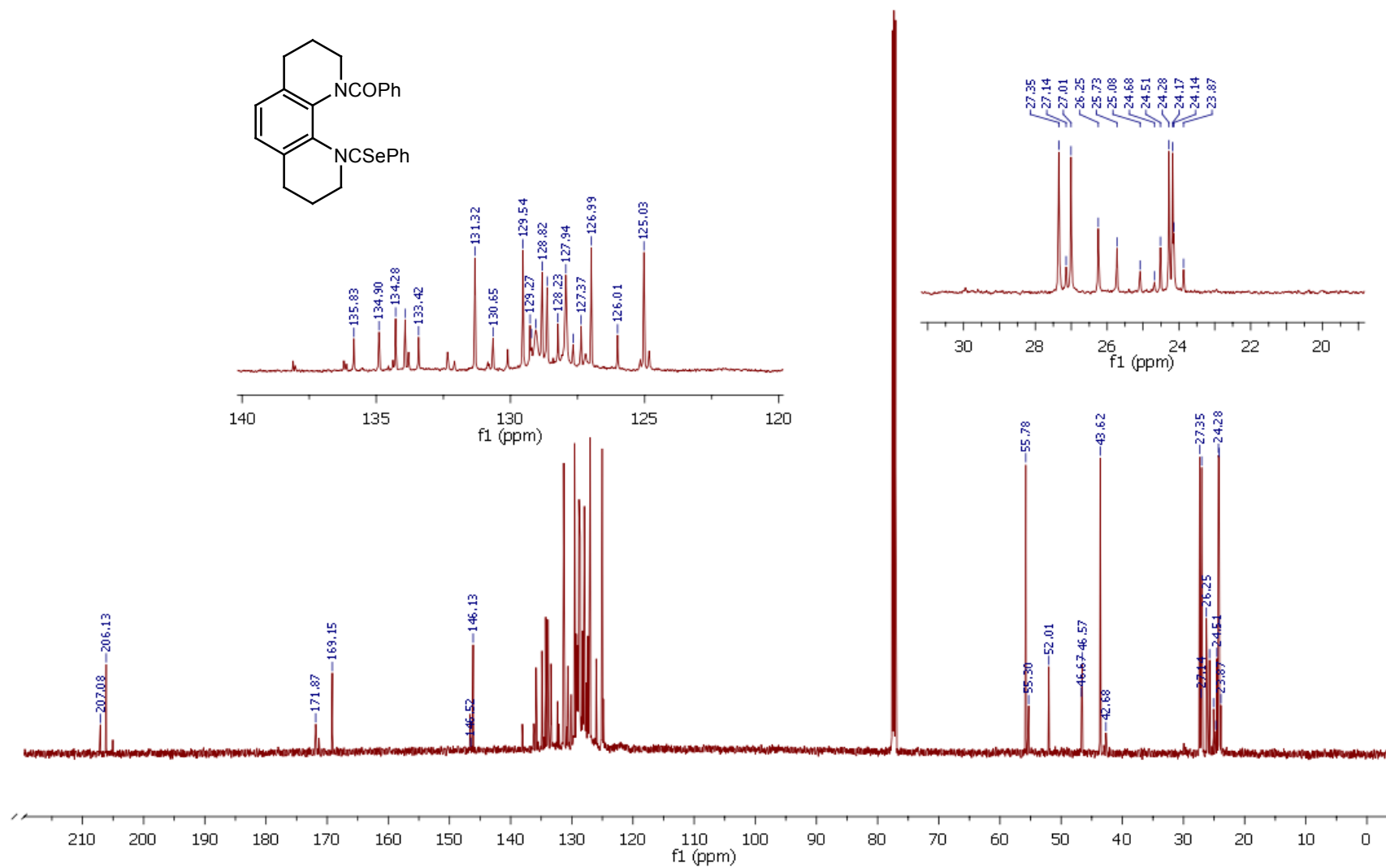
*N,N'*-diselenobenzoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5c**) –  $^{77}\text{Se}$  NMR



*N*-benzoyl-*N'*-selenidobezoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5d**) – <sup>1</sup>H NMR

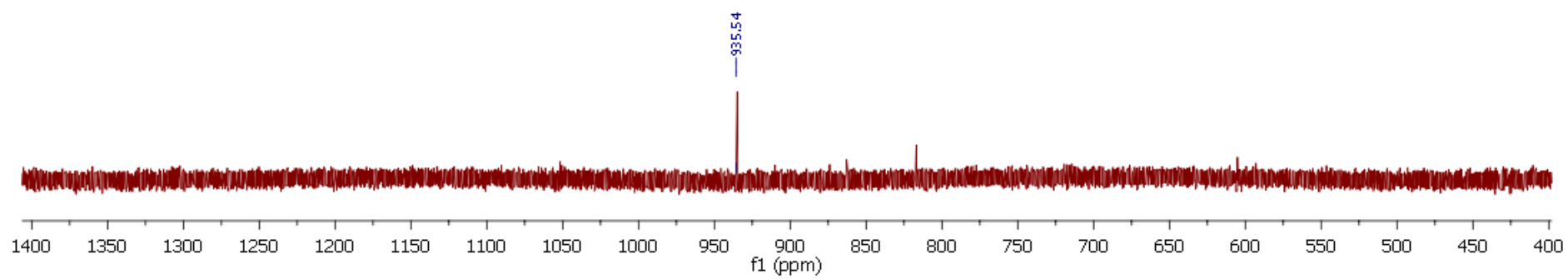
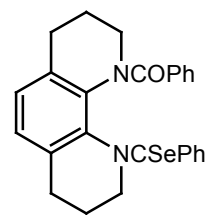


*N*-benzoyl-*N'*-selenidobezoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5d**) – <sup>13</sup>C NMR

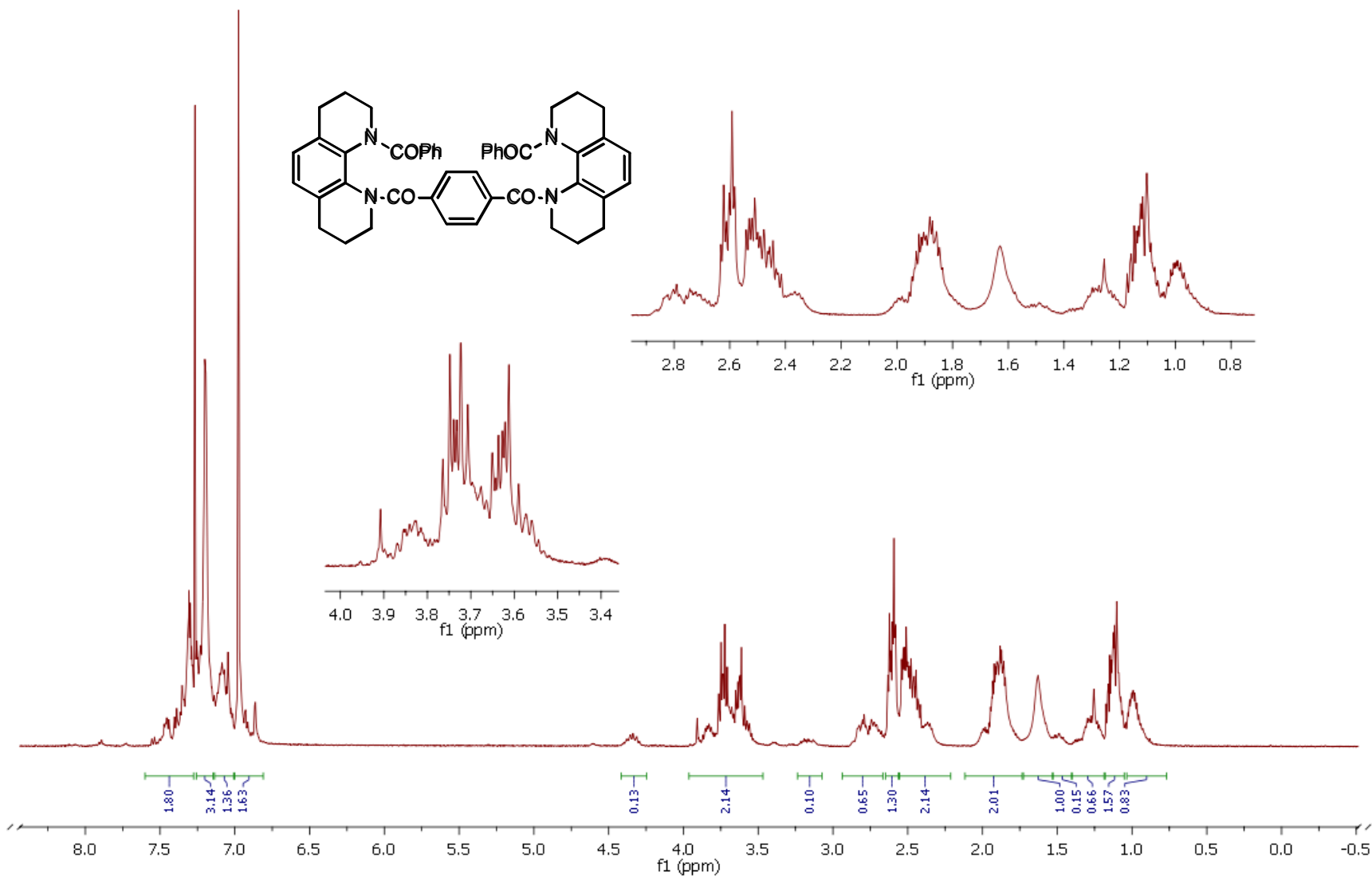


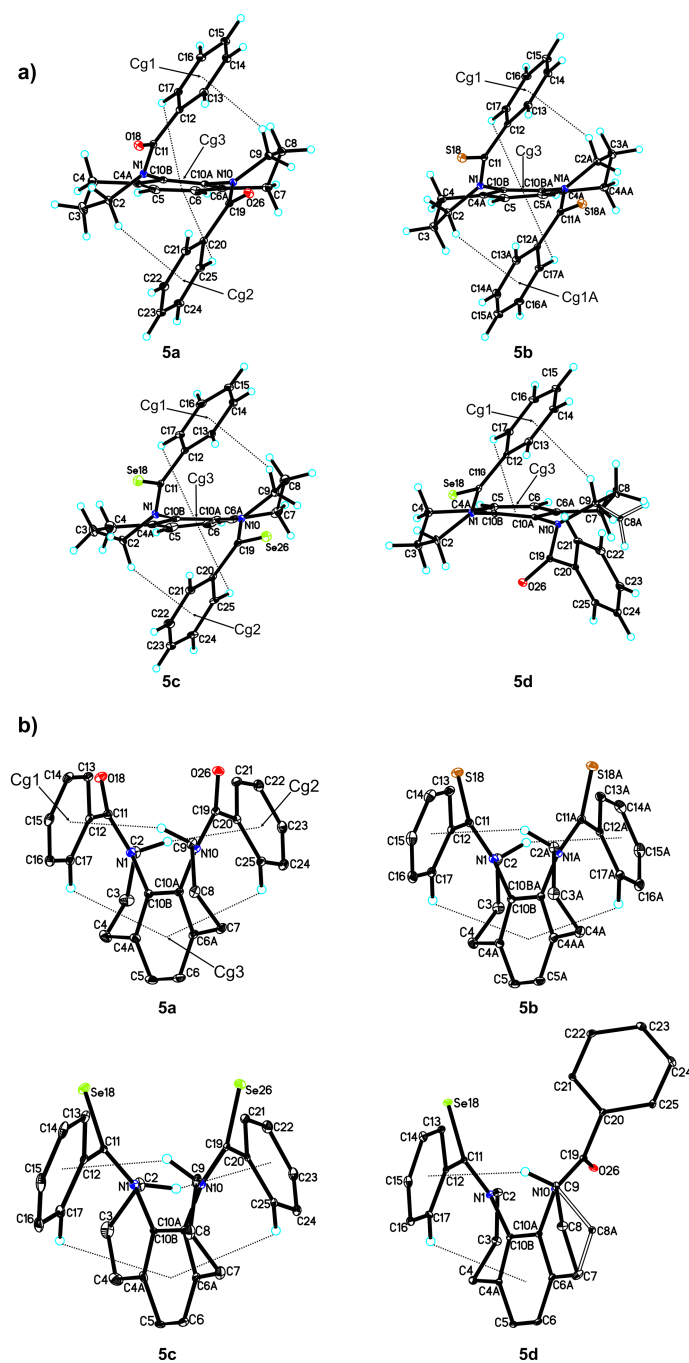


*N*-benzoyl-*N'*-selenidobezoyl-1,2,3,4,7,8,9,10-octahydro-1,10-phenanthroline (**5d**) –  $^{77}\text{Se}$  NMR

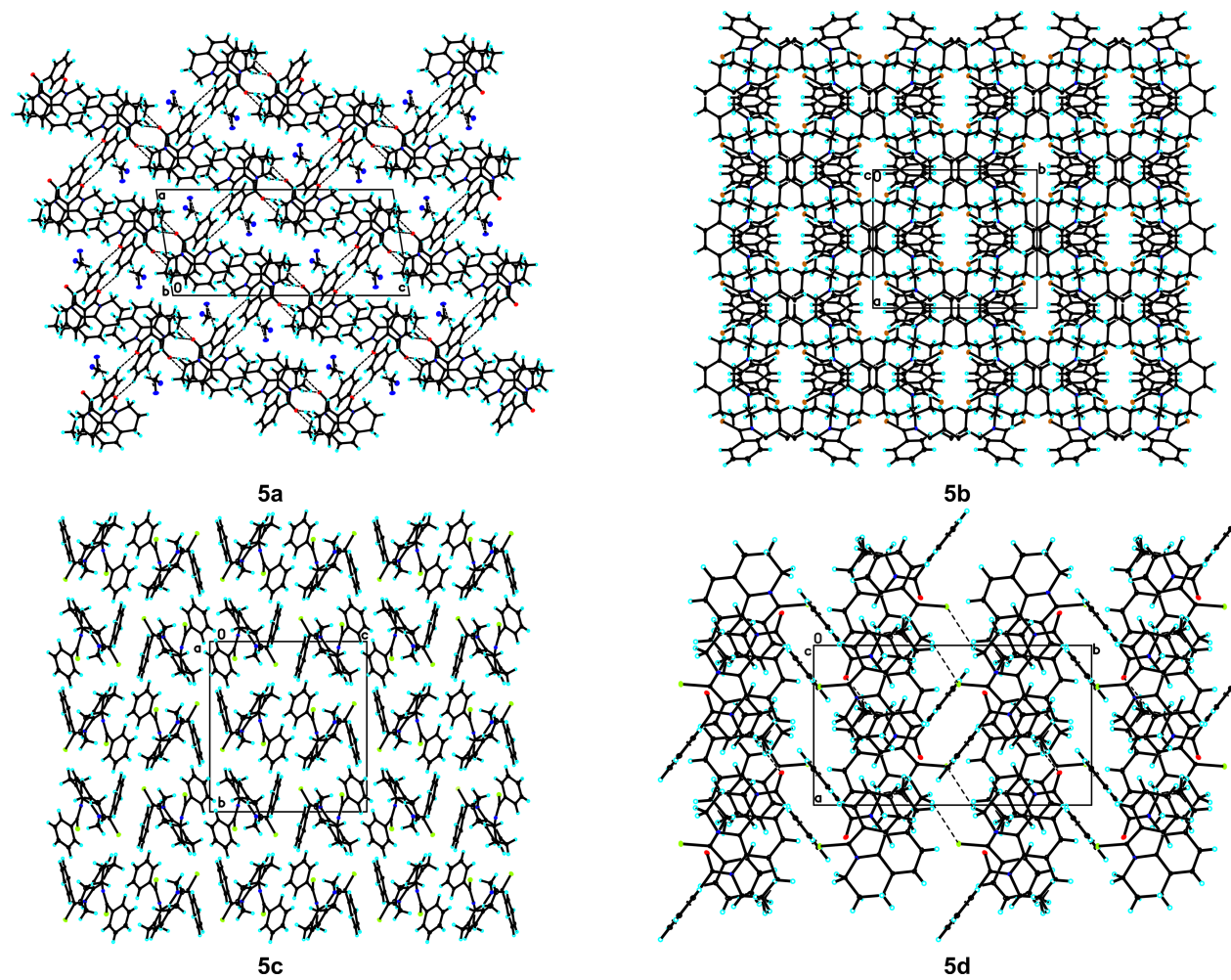


*N,N'*-Terephthaloyl-bis(1-benzoyl-1,2,3,4,7,8,9,10-octahydro-[1,10]phenanthroline) (**7**) – <sup>1</sup>H NMR

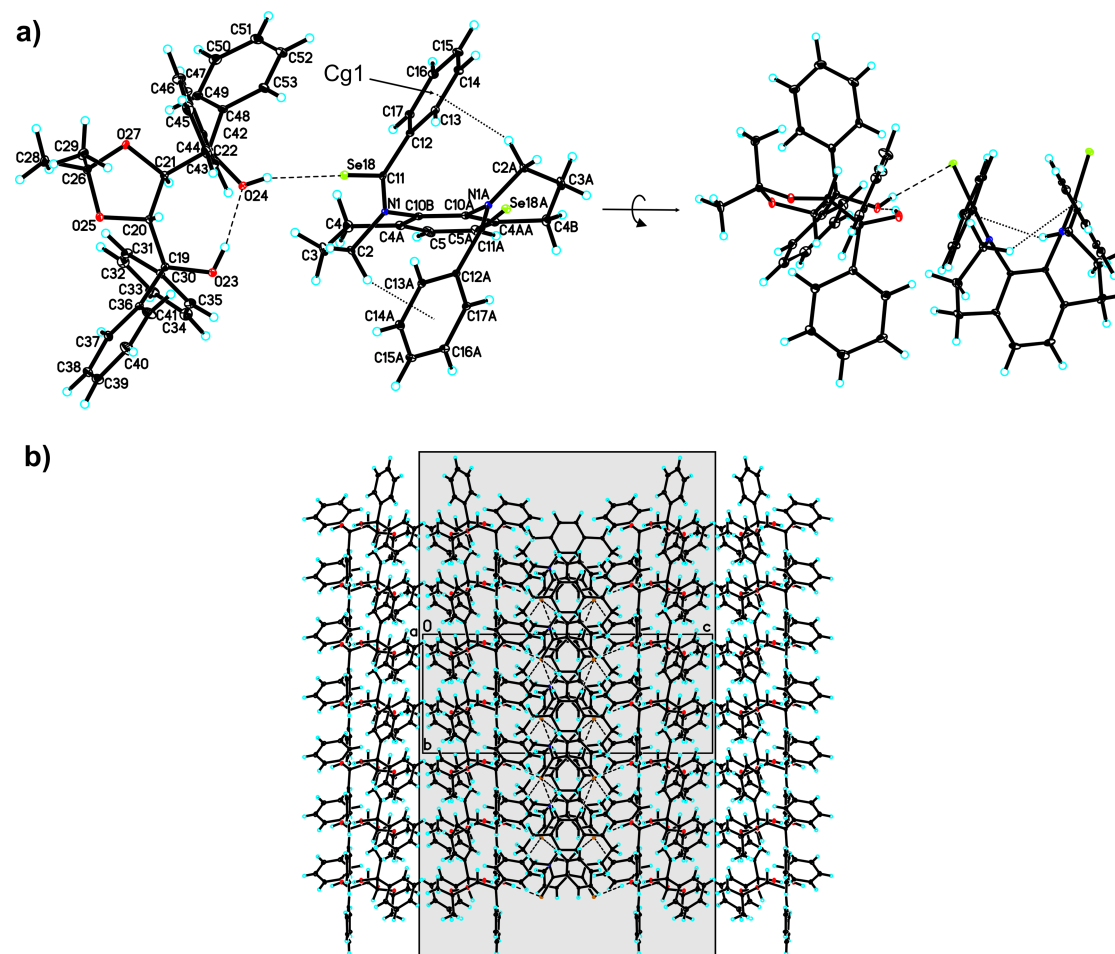




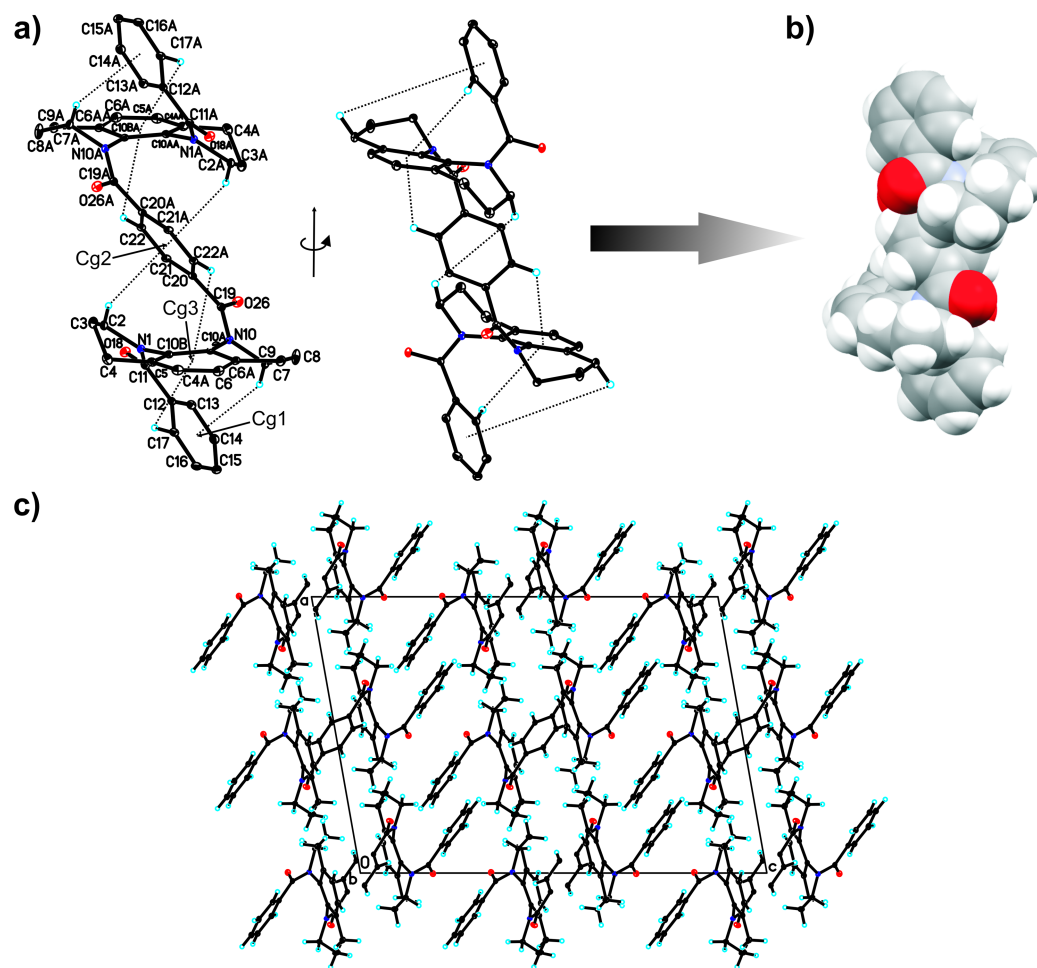
**Fig. 1S** Molecular structures of the compounds **5a-5d** showing the atom labeling scheme and 20% probability displacement ellipsoids viewed approximately parallel in the central phenantroline ring (a) and viewed approximately perpendicular to the central phenantroline ring (b). C–H... $\pi$  hydrogen bonds are represented by dotted lines (H atoms not involved in these interactions have been omitted). Cg1, Cg2 and Cg3 denote the ring centroids. The solvent molecule (CH<sub>2</sub>Cl<sub>2</sub>) for **5a** has been omitted.



**Fig. 2S** Crystal packing of compounds **5a-5d**. C–H···X (where X = Se, S, O) hydrogen bonds are represented by dashed lines.

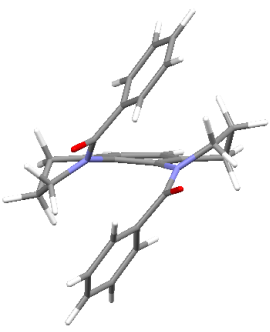
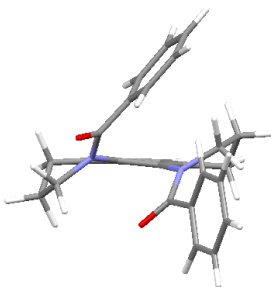


**Fig. 3S** Molecular structure showing the atom labeling scheme and 20% probability displacement ellipsoids (a) and crystal packing of the complex **5c·6a** (b) (the layers are highlighted in grey). O–H···Se, O–H···O and C–H···Se hydrogen bonds are represented by dashed lines. Cg1 denote the ring centroid.

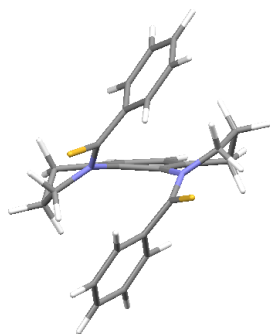


**Fig. 6S** Molecular structure of the bisamide **7** showing the atom labeling scheme and 20% probability displacement ellipsoids (a,) *meso*-helical structure of **7** (b) and crystal packing of bisamide **7** (c). The intramolecular C–H··· $\pi$  interactions are represented by dotted lines and (H atoms not involved in these interactions have been omitted, as well as solvent molecule (CHCl<sub>3</sub>)) and C–H···O hydrogen bonds are represented by dashed lines. Cg1, Cg2 and Cg3 denote the ring centroids.

**Table 1** DFT TZ2P LDA ZORA calculated structures, bonding energies and Cartesian coordinates of atoms of folded and partially unfolded compounds **5a–5c**.

Folded				Partially Unfolded			
							
<b>5a</b>				<b>5a</b>			
54 BE = -36541.59 kJ/mol				54 BE = -36523.68 kJ/mol			
C	-0.34070678	-2.58474579	-0.55791132	C	-0.48489180	-2.44273148	-0.54916684
C	0.77069498	-3.36074875	-0.28677741	C	0.56932405	-3.26938662	-0.21053302
C	1.98644061	-2.76439586	-0.00600510	C	1.79919711	-2.73022704	0.12352631
C	2.07988588	-1.38928142	0.09918248	C	1.96207456	-1.35911809	0.20314494
C	0.95045238	-0.59274599	-0.10475063	C	0.89824919	-0.51475575	-0.10617286
C	-0.24787899	-1.19104185	-0.52291767	C	-0.30617381	-1.05864926	-0.55159722
N	1.11484345	0.78448644	0.07207453	N	1.09461988	0.86624642	0.05731072
N	-1.40343670	-0.47624125	-0.85431103	N	-1.39606967	-0.29628144	-0.97535671
C	3.35304362	-0.66753701	0.34605233	C	3.23952247	-0.69689072	0.56691555
C	2.30890431	1.43149776	-0.46523850	C	2.36296925	1.43417454	-0.38859978
C	-1.69167580	-3.14524753	-0.80977254	C	-1.86574134	-2.91150937	-0.82803517
C	-2.65638845	-2.37975770	0.07512858	C	-2.79498068	-2.05511439	0.01561048
C	-2.69112353	-0.92668076	-0.33182078	C	-2.70201917	-0.60406157	-0.40667550
H	0.67806336	-4.44967047	-0.31719808	H	0.41994743	-4.35251220	-0.21533209
H	2.88065922	-3.37181506	0.15731480	H	2.64449985	-3.38034071	0.36439895
C	0.20930258	1.63703065	0.64968973	C	0.20462719	1.54963997	0.85294755
C	-1.45502336	0.68669287	-1.57937658	C	-1.36144854	0.77117346	-1.82393040
H	4.20565503	-1.35929095	0.27629725	H	4.06329456	-1.42595206	0.57905340
H	3.36495697	-0.22783977	1.36156090	H	3.17074100	-0.26072871	1.58155887
H	2.58440117	2.20925398	0.26490612	H	2.62517807	2.23714342	0.31599228
H	2.05148429	1.96185493	-1.40012343	H	2.24045182	1.89273867	-1.38793936
H	-1.70316932	-4.22543356	-0.60127238	H	-1.96532162	-3.98181918	-0.59421145
H	-1.98380661	-3.00851722	-1.86837741	H	-2.11864737	-2.77928528	-1.89697287
H	-2.32039192	-2.47354941	1.12230880	H	-2.49814878	-2.16479839	1.07157653
H	-3.67715881	-2.78825407	0.02200398	H	-3.84138042	-2.38671584	-0.06655195
H	-2.99360962	-0.27739266	0.50980905	H	-2.88289380	0.07881023	0.44015653
H	-3.42223848	-0.74904280	-1.13676830	H	-3.43480319	-0.35405170	-1.18899483
C	3.43354067	0.44718462	-0.67916194	C	3.47436519	0.40380666	-0.44462282
H	3.36255126	0.00169637	-1.68656969	H	3.50710722	-0.05119127	-1.44919594
H	4.39217830	0.98563083	-0.62761141	H	4.43681258	0.91342196	-0.28507442
O	0.31199157	2.84527253	0.47729677	O	-0.71099059	0.97896365	1.42862266
O	-2.46447657	1.38001127	-1.54966643	O	-2.34704010	1.48643604	-1.95968355
C	-0.83073820	1.09763365	1.55185075	C	0.36946709	3.01732437	1.00702515
C	-0.32679022	1.04981975	-2.46282966	C	-0.15120398	1.03434940	-2.64298345
C	-0.14190270	2.40222273	-2.71954080	C	0.03939808	2.35397518	-3.03506843
C	0.82793286	2.81381980	-3.61293231	C	1.10535886	2.70079909	-3.84311026
C	1.60664961	1.87523623	-4.27222459	C	1.97508348	1.72144827	-4.29800390
C	1.41324070	0.52468385	-4.03284881	C	1.76571694	0.39871681	-3.94606534
C	0.45161261	0.10982079	-3.12861479	C	0.71041843	0.05284185	-3.11914071
C	-2.00911688	1.82516109	1.65665716	C	0.03022631	3.55329905	2.24347320
C	-2.98499080	1.44192319	2.55610563	C	0.07731457	4.91798387	2.45077777
C	-2.78132177	0.34063299	3.37301776	C	0.42854107	5.76607500	1.41240973
C	-1.60087174	-0.37844064	3.28341769	C	0.73381402	5.24151455	0.16872196
C	-0.62724283	-0.00534993	2.37352524	C	0.71602185	3.87303888	-0.03121426
H	-0.78314839	3.11545783	-2.19620674	H	-0.69566027	3.08888365	-2.69511295
H	0.97337547	3.87912837	-3.80489265	H	1.25013566	3.74266554	-4.13858598
H	2.36332036	2.19904618	-4.99109753	H	2.81003277	1.98849581	-4.95029239
H	2.00729816	-0.21816938	-4.56965926	H	2.42702918	-0.38114788	-4.33021497
H	0.28963190	-0.95866790	-2.95207036	H	0.54871756	-0.99683859	-2.85328728
H	-2.13205041	2.69752375	1.01042218	H	-0.29049866	2.86379662	3.02863886
H	-3.91235114	2.01420912	2.62928387	H	-0.17579331	5.32976956	3.43013674
H	-3.54499748	0.04829058	4.09788461	H	0.45259849	6.84698135	1.57120803
H	-1.42761394	-1.23216922	3.94226165	H	0.98550220	5.90698086	-0.66054760
H	0.31166248	-0.56576528	2.31435451	H	0.94370043	3.46590087	-1.02067374

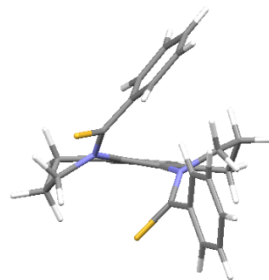




**5b**

54 BE=-35861.78 kJ/mol

C	-0.38272702	-2.54612162	-0.51322588
C	0.72873013	-3.32680029	-0.26135311
C	1.95391049	-2.73744237	-0.02116202
C	2.06027410	-1.36280911	0.06407132
C	0.93362815	-0.55631162	-0.12254208
C	-0.28184063	-1.15158969	-0.50012148
N	1.11650694	0.82787090	0.04468910
N	-1.44548739	-0.43276013	-0.82831065
C	3.35557932	-0.66724325	0.26193024
C	2.32741310	1.43639350	-0.50248182
C	-1.73733157	-3.11796859	-0.71051344
C	-2.66424971	-2.32704574	0.18760665
C	-2.72177475	-0.90133157	-0.29155341
H	0.62498343	-4.41490040	-0.27223574
H	2.84869629	-3.34827963	0.12488560
C	0.24405988	1.65000499	0.68191797
C	-1.47562986	0.67289023	-1.61549668
H	4.18797062	-1.38070736	0.17068877
H	3.41548174	-0.21428154	1.27021179
H	2.64963664	2.17672789	0.25083038
H	2.06223642	2.01853839	-1.40262971
H	-1.73392314	-4.19243092	-0.47431594
H	-2.06877905	-3.00970701	-1.76110208
H	-2.28691077	-2.37411915	1.22406257
H	-3.68770515	-2.73237057	0.19085699
H	-3.05321126	-0.20965604	0.50263438
H	-3.44773029	-0.78417422	-1.11548295
C	3.41209128	0.42938397	-0.77996924
H	3.27989006	-0.01862883	-1.78019687
H	4.37984270	0.95400820	-0.77931781
S	0.36442007	3.29517091	0.55615483
S	-2.81806848	1.63684327	-1.69268400
C	-0.74243420	1.06718611	1.59962153
C	-0.34225310	0.94432157	-2.50729083
C	0.00087448	2.26064996	-2.80034291
C	0.99366318	2.53779992	-3.71957556
C	1.64478369	1.50458815	-4.37633940
C	1.29960361	0.19145016	-4.10277504
C	0.31837525	-0.08940004	-3.16981263
C	-1.98575246	1.67403125	1.74809115
C	-2.88464468	1.20866706	2.68775034
C	-2.54703682	0.14323619	3.50866777
C	-1.30646536	-0.45862985	3.37801048
C	-0.41166885	-0.00679721	2.42541762
H	-0.53817523	3.05893007	-2.28376665
H	1.25747235	3.57609792	-3.93267934
H	2.41672412	1.72509458	-5.11783736
H	1.78899968	-0.62832865	-4.63365665
H	0.03672161	-1.12883394	-2.97234123
H	-2.22251452	2.52437789	1.10332427
H	-3.85961987	1.69100610	2.78724316
H	-3.25022612	-0.21058480	4.26671563
H	-1.02145905	-1.28044423	4.03889836
H	0.57550120	-0.47281560	2.34148653

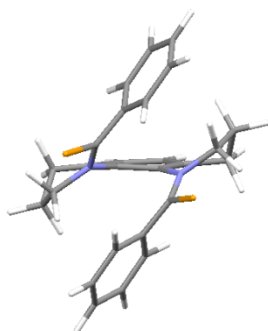


**5b**

54 BE=-35838.97 kJ/mol

C	-0.34954925	-2.43506600	-0.58000701
C	0.72854300	-3.20222852	-0.17883732
C	1.91015342	-2.60168834	0.21171228
C	1.99510597	-1.22285302	0.29021262
C	0.90475330	-0.44038557	-0.07555567
C	-0.24475897	-1.04441099	-0.58505243
N	1.02885040	0.95044784	0.11091191
N	-1.34692724	-0.32324708	-1.06758629
C	3.21751459	-0.48962340	0.70289768
C	2.27863763	1.56797970	-0.34301695
C	-1.69050521	-2.98986380	-0.89140994
C	-2.67929066	-2.15267470	-0.10010915
C	-2.67060706	-0.73414185	-0.60970432
H	0.63170562	-4.29120502	-0.17734054
H	2.77495131	-3.20604858	0.49777100
C	0.18836266	1.58938041	0.96656056
C	-1.27112604	0.74573710	-1.89680648
H	4.07451321	-1.17528125	0.77494591
H	3.07362039	-0.03402137	1.70114174
H	2.47613062	2.41044606	0.33542988
H	2.14460651	1.98210928	-1.35876829
H	-1.73582916	-4.05539048	-0.62125307
H	-1.92207392	-2.91034678	-1.97056583
H	-2.38902732	-2.17901213	0.96416197
H	-3.70540526	-2.54346732	-0.17560659
H	-3.01847480	-0.01551123	0.15149665
H	-3.33812373	-0.61051937	-1.48028017
C	3.44505145	0.59667889	-0.32648151
H	3.55266813	0.12220719	-1.31646060
H	4.36895683	1.16227186	-0.13107962
S	-0.95711132	0.81791805	1.87357067
S	-2.56974570	1.74703295	-2.11845630
C	0.30615454	3.05221102	1.05874834
C	-0.05563970	0.94482273	-2.70543607
C	0.25784308	2.22552423	-3.15277783
C	1.35337856	2.44996423	-3.96211399
C	2.14466090	1.38714960	-4.37003050
C	1.81783007	0.10284044	-3.97161982
C	0.73144218	-0.11944204	-3.14449194
C	0.24127509	3.67892472	2.29897949
C	0.28075327	5.05635903	3.38927693
C	0.35127997	5.82994901	1.24049962
C	0.39761062	5.21406971	0.00174419
C	0.38960092	3.83551981	-0.08772157
H	-0.42378313	3.03384693	-2.87139597
H	1.58481910	3.46500287	-4.29248316
H	3.00509951	1.55829897	-5.02124062
H	2.41051031	-0.74676964	-4.31823229
H	0.47958731	-1.14314948	-2.85211196
H	0.13684628	3.05100943	3.18765082
H	0.24090483	5.53649083	3.36947079
H	0.36271362	6.92032261	1.31141430
H	0.43297877	5.81526498	-0.90998005
H	0.42001269	3.34783712	-1.06637527

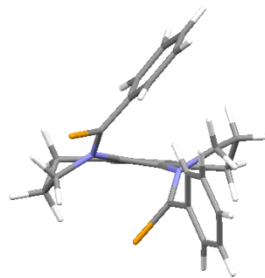




5c

54 BE=-35684.33 kJ/mol

C	-0.36305659	-2.58061162	-0.50497649
C	0.75081677	-3.35890015	-0.25693717
C	1.97537219	-2.76709082	-0.01991268
C	2.08042106	-1.39235562	0.06375652
C	0.95172343	-0.58746239	-0.12052954
C	-0.26462971	-1.18560165	-0.49122790
N	1.13363876	0.79989106	0.04438580
N	-1.43260393	-0.46802476	-0.81746219
C	3.37804380	-0.69799054	0.24990165
C	2.34579044	1.40154771	-0.50996285
C	-1.71648937	-3.15777990	-0.69416154
C	-2.63703548	-2.36873929	0.21104604
C	-2.70313067	-0.94556696	-0.27309490
H	0.64847981	-4.44723298	-0.26712223
H	2.87224743	-3.37572214	0.12238189
C	0.26799409	1.61354230	0.68782787
C	-1.46075932	0.62530533	-1.61077787
H	4.20828074	-1.41335591	0.15394013
H	3.44811854	-0.24036585	1.25529620
H	2.67734330	2.13758118	0.24492399
H	2.07540770	1.98951953	-1.40476817
H	-1.70735819	-4.23213094	-0.45767911
H	-2.05597520	-3.05105172	-1.74226129
H	-2.25054598	-2.41200410	1.24422112
H	-3.65974756	-2.77563533	0.22388158
H	-3.03548358	-0.25136724	0.51879459
H	-3.43346701	-0.83542840	-1.09536321
C	3.42394449	0.39197270	-0.79862253
H	3.27817251	-0.06049583	-1.79485608
H	4.39160428	0.91656187	-0.81245540
Se	0.41448825	3.41091571	0.57522503
Se	-2.93693185	1.66046327	-1.72807429
C	-0.72562307	1.04722998	1.60019867
C	-0.33279643	0.91135600	-2.49742153
C	0.00497016	2.23010524	-2.79153726
C	1.00028513	2.51204127	-3.70609588
C	1.66156345	1.48301933	-4.35903648
C	1.32411756	0.16796014	-4.08500888
C	0.34154636	-0.11844547	-3.15518433
C	-1.96960856	1.65734606	1.74142429
C	-2.87879000	1.19033027	2.66989056
C	-2.55335119	0.12115948	3.49071124
C	-1.31220938	-0.48185070	3.37149984
C	-0.40743063	-0.03008184	2.42858214
H	-0.54059545	3.02649742	-2.27835876
H	1.25840862	3.55199281	-3.91803911
H	2.43508141	1.70797633	-5.09738589
H	1.82146192	-0.64902437	-4.61288182
H	0.06524719	-1.15979414	-2.95920698
H	-2.20030056	2.50874025	1.09539393
H	-3.85414004	1.67378673	2.75945077
H	-3.26652131	-0.23507492	4.23818289
H	-1.03600643	-1.30773102	4.03114211
H	0.57889246	-0.49964709	2.35334314



5c

54 BE=-35662.78 kJ/mol

C	-0.32939185	-2.43776824	-0.57691328
C	0.74915768	-3.20067421	-0.16807017
C	1.93137794	-2.59717896	0.21547555
C	2.01683002	-1.21753394	0.28187939
C	0.92413243	-0.43991984	-0.08484169
C	-0.22518786	-1.04737996	-0.59080066
N	1.04771902	0.95252752	0.09637935
N	-1.32650591	-0.32796332	-1.08431386
C	3.24067098	-0.47776662	0.67828624
C	2.29154598	1.57021267	-0.37987092
C	-1.67064519	-2.99686237	-0.88008571
C	-2.65440869	-2.14975866	-0.09351715
C	-2.65066793	-0.74143742	-0.62683325
H	0.65242072	-4.28960837	-0.15755488
H	2.79667282	-3.19926228	0.50487041
C	0.23498362	1.59324497	0.96628645
C	-1.24144517	0.72845677	-1.92067777
H	4.09931794	-1.16131744	0.75049602
H	3.10317863	-0.01249992	1.67297066
H	2.49392763	2.41816912	0.29092200
H	2.14316616	1.97668608	-1.39658061
H	-1.71492733	-4.05932393	-0.59834255
H	-1.90653847	-2.92868697	-1.95902301
H	-2.35445356	-2.15542413	0.96858541
H	-3.68121700	-2.54098623	-0.15462017
H	-3.00599650	-0.01062861	0.11976720
H	-3.31438148	-0.63643051	-1.50381944
C	3.45771001	0.59810656	-0.36537381
H	3.55502063	0.11308234	-1.35139897
H	4.38358832	1.16562275	-0.18524545
Se	-0.97430183	0.76478636	2.01474301
Se	-2.66183266	1.81512596	-2.17295395
C	0.33391307	3.05330037	1.03952576
C	-0.03091402	0.93212855	-2.72737641
C	0.28386015	2.20795081	-3.19181791
C	1.38581254	2.42638961	-3.99281058
C	2.18948368	1.36393832	-4.37580575
C	1.86593783	0.08426701	-3.96070556
C	0.77149691	-0.13234829	-3.14292246
C	0.35801834	3.70343451	2.26968542
C	0.38659499	5.08247778	2.33063986
C	0.35729960	5.83501791	1.16598522
C	0.31641083	5.19632215	-0.06150794
C	0.32287194	3.81655315	-0.12478260
H	-0.40376251	3.01912864	-2.93297750
H	1.61306599	3.43808893	-4.33603245
H	3.05650368	1.53164355	-5.01899885
H	2.46735080	-0.76728922	-4.28729524
H	0.52275906	-1.15433665	-2.84176506
H	0.33386505	3.09268599	3.17611322
H	0.41805744	5.58081806	3.30209140
H	0.35875166	6.92651340	1.21676015
H	0.27117038	5.78021954	-0.98425391
H	0.28539386	3.30796814	-1.09232204