Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Synthesis of novel dispiropyrrolothiazoles by three-component 1,3-dipolar cycloaddition and evaluation of their antimycobacterial activity

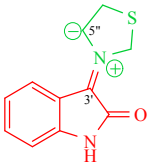
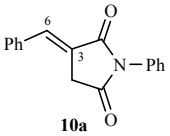
Contents

❖ DFT Data

Table S1. HOMO/LUMO energies, global electrophilicity, electronic chemical potential, chemical hardness of the species and index of reactants (in eV) calculated at the B3LYP/6-31G(d,p) level.

Structure	E_{HOMO} (eV)	E_{LUMO} (eV)	ω (eV)	μ (eV)	η (eV)
anti-**12a**	-5.862	-1.691	1.710	-3.776	4.170
10a	-6.640	-2.045	2.052	-4.343	4.596

Table S2. MO coefficients (in eV) and local electrophilicity indexes (according to the ESP scheme) for the reactive centers of the species involved in the 1,3-dipolar cycloaddition.

Structure	 *anti*-**12a**		 **10a**	
Site	**C-5"**	**C-3'**	**C-3**	**C-6**
f_k^+	0.255	0.171	0.055	0.154
f_k^-	0.253	0.192	0.110	0.030

- **Cartesian coordinates and energies of TSs at the B3LYP/6-31G(d,p) level**

***endo*-TS1**

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.898936	2.592458	-0.156479
C	-0.354245	1.975435	-0.440739
C	-0.986914	2.269684	-1.658288
C	-0.387494	3.166772	-2.546076
C	0.840684	3.760553	-2.241527
C	1.501727	3.475699	-1.041499
C	0.457613	1.255667	1.666953
H	-1.939165	1.821526	-1.918686
H	-0.880945	3.399563	-3.484007
H	1.293655	4.451475	-2.945486
H	2.457116	3.93438	-0.80689
N	1.345989	2.156406	1.082009
H	2.215083	2.410922	1.525735
O	0.562087	0.78913	2.793251
C	-0.833548	-2.114931	0.493483
C	-1.72163	-0.744301	1.708684
C	-0.617774	1.070549	0.65392
C	0.564402	-1.135152	-1.533312

C	0.272566	-1.460646	-0.09761
H	-0.906613	-0.763344	2.425201
N	-1.766864	0.411841	0.969562
C	-3.080825	-1.177551	2.195069
C	-3.036287	0.668712	0.274752
S	-4.328281	-0.196119	1.249442
H	-3.010352	0.279712	-0.745698
H	-3.224995	1.743429	0.256048
H	-3.252006	-2.24436	2.031931
H	-3.198608	-0.961091	3.260608
C	-1.90079	-2.787889	-0.295223
C	-2.449653	-3.982751	0.206518
C	-2.390747	-2.313382	-1.525866
C	-3.444185	-4.672517	-0.485418
H	-2.072607	-4.384505	1.14369
C	-3.38554	-3.00163	-2.218485
H	-1.992761	-1.400056	-1.953323
C	-3.918748	-4.18382	-1.702716
H	-3.843063	-5.595424	-0.074661
H	-3.743844	-2.612236	-3.167064
H	-4.692851	-4.718168	-2.244789
H	-0.531779	-2.690447	1.368362
C	1.530775	-1.410618	0.645689
O	1.72252	-1.723203	1.811013
H	0.396296	-1.985684	-2.207415
H	0.017801	-0.28453	-1.958188
C	3.899758	-0.700777	0.130333
C	4.53323	-1.530139	1.064618
C	4.593756	0.379751	-0.431545
C	5.851602	-1.26933	1.435209
H	3.989316	-2.353331	1.506894
C	5.915131	0.620432	-0.058975
H	4.107357	1.005592	-1.168253
C	6.549339	-0.198308	0.876396
H	6.334198	-1.913528	2.164253
H	6.449567	1.454368	-0.504873
H	7.577993	-0.00441	1.16541
N	2.547101	-0.949124	-0.25022
O	2.6864	-0.422346	-2.518041
C	2.049451	-0.781826	-1.549116

Zero-point energy = 0.45402 Hartree

ZPE is included in the following quantities:

Electronic energy = -1868.505821 Hartree

Internal energy = -1868.477346 Hartree

Enthalpy = -1868.476402 Hartree

Gibbs energy = -1868.566985 Hartree

<u>*exo*-TS1</u>

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.610336	2.053946	-1.214199
C	-1.064292	1.854443	0.0836
C	-1.895663	2.06531	1.193532
C	-3.2124	2.484906	0.994879
C	-3.718891	2.684329	-0.292117
C	-2.918924	2.46576	-1.418497
C	0.554652	1.35934	-1.57288
H	-1.544339	1.89618	2.202134
H	-3.852757	2.645756	1.85588
H	-4.746816	3.007173	-0.423651
H	-3.308683	2.610833	-2.421302
N	-0.634539	1.759614	-2.161227
H	-0.747568	1.791291	-3.162735
O	1.571751	1.052079	-2.203985
C	1.805021	-1.405911	0.442319
C	2.436934	0.557176	0.508756
C	0.294124	1.38609	-0.115798
C	-0.681909	-1.366974	0.512866
C	0.273081	-1.856273	-1.637545
C	0.573953	-1.437134	-0.231934
H	2.733622	0.596948	-0.532785
N	1.297531	1.250426	0.795751
H	0.726107	-2.818837	-1.908577
H	0.594737	-1.137879	-2.402177
O	-0.853287	-1.095763	1.697473
C	-1.244682	-1.990841	-1.672707
N	-1.733202	-1.712784	-0.38487
O	-1.919147	-2.285084	-2.637931
C	-3.110356	-1.790376	-0.015151
C	-4.100153	-1.345335	-0.899632
C	-3.470581	-2.328481	1.226707
C	-5.442924	-1.445439	-0.539274

H	-3.818436	-0.94207	-1.862717
C	-4.81655	-2.411128	1.578419
H	-2.701674	-2.661699	1.910961
C	-5.808035	-1.974709	0.698781
H	-6.205732	-1.104662	-1.233272
H	-5.088506	-2.826241	2.544487
H	-6.855712	-2.04809	0.975138
H	1.694292	-1.482128	1.524138
C	3.02675	-2.072799	-0.08847
C	3.768355	-2.907937	0.764823
C	3.480586	-1.893296	-1.407262
C	4.912046	-3.564002	0.31023
H	3.432162	-3.055678	1.78786
C	4.624982	-2.549612	-1.858885
H	2.951983	-1.216011	-2.07093
C	5.343125	-3.389609	-1.005445
H	5.464562	-4.211677	0.984769
H	4.960511	-2.397024	-2.880587
H	6.234403	-3.897982	-1.360887
C	3.499124	0.705211	1.560006
C	1.041858	1.48347	2.232792
S	2.619691	1.151604	3.116093
H	0.276973	0.785707	2.575347
H	0.723273	2.518227	2.373376
H	4.05451	-0.224609	1.702778
H	4.211449	1.492269	1.290656

Zero-point energy = 0.454337 Hartree

ZPE is included in the following quantities:

Electronic energy = -1868.520831 Hartree

Internal energy = -1868.492438 Hartree

Enthalpy = -1868.491494 Hartree

Gibbs energy = -1868.580675 Hartree.

***endo*-TS2**

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.0587	-1.309645	-0.337783
N	-0.98629	1.267966	0.379188
C	0.353367	1.441966	0.182521
C	1.064994	-0.537436	0.301611

C	2.292281	-0.29252	-0.527744
C	3.042771	-0.433389	1.686709
C	0.97069	2.398064	1.166629
C	-1.479939	1.520408	1.739819
S	-0.173943	2.473093	2.612982
C	1.555997	-0.755742	1.723802
H	0.174979	-1.359486	-1.416657
C	-0.771542	-2.359454	0.237357
C	-1.27903	-3.35085	-0.633011
C	-1.109934	-2.467933	1.605086
C	-2.05035	-4.407005	-0.161546
H	-1.042251	-3.287463	-1.691413
C	-1.880098	-3.529183	2.075198
H	-0.779803	-1.712943	2.309451
C	-2.350928	-4.508109	1.199005
H	-2.415998	-5.156765	-0.857244
H	-2.118369	-3.587635	3.133549
H	-2.949914	-5.334228	1.569703
H	1.44786	-1.798899	2.042704
H	1.084698	-0.135458	2.492363
O	3.793031	-0.39147	2.638877
O	2.358219	-0.165517	-1.733151
C	-1.707717	0.502205	-0.506722
C	-1.462195	0.627346	-1.969834
C	-3.487036	-0.419547	-1.639807
C	-3.031598	-0.072371	-0.337241
C	-3.848202	-0.393954	0.755148
C	-5.080109	-1.017854	0.53987
C	-5.503273	-1.342833	-0.750727
C	-4.703427	-1.049749	-1.860261
O	-0.552048	1.184109	-2.573749
N	-2.533795	-0.025235	-2.571477
H	-2.633388	-0.061883	-3.574123
N	3.402837	-0.198372	0.350038
C	4.737534	0.081368	-0.084967
C	4.959158	1.02993	-1.090052
C	5.816851	-0.591338	0.499062
C	6.261509	1.298213	-1.507776
H	4.120483	1.533463	-1.552779
C	7.114534	-0.305589	0.078267
H	5.641387	-1.314958	1.284154
C	7.342933	0.636206	-0.925524

H	6.427504	2.030538	-2.292136
H	7.948928	-0.826449	0.538215
H	8.355753	0.851848	-1.252282
H	0.638254	1.532199	-0.861451
H	-1.658445	0.582209	2.269146
H	-2.411523	2.0882	1.685922
H	1.958827	2.074839	1.502491
H	1.075048	3.395603	0.727796
H	-3.550076	-0.164106	1.770211
H	-5.711049	-1.255296	1.390374
H	-6.462906	-1.82837	-0.899015
H	-5.026253	-1.301218	-2.865953

Zero-point energy = 0.453549 Hartree

ZPE is included in the following quantities:

Electronic energy = -1868.502627 Hartree

Internal energy = -1868.473928 Hartree

Enthalpy = -1868.472984 Hartree

Gibbs energy = -1868.564115 Hartree

<u>*exo*-TS2</u>

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-3.882123	0.007333	-0.458999
C	-2.706806	-0.662579	-0.887275
C	-2.654164	-1.156589	-2.19518
C	-3.763683	-1.00269	-3.032155
C	-4.91335	-0.346596	-2.584036
C	-4.983574	0.174328	-1.287483
C	-2.455968	0.091469	1.347511
H	-1.764401	-1.646561	-2.573295
H	-3.725269	-1.392537	-4.044308
H	-5.763863	-0.233372	-3.249211
H	-5.872492	0.690443	-0.938188
N	-3.70896	0.421416	0.859382
H	-4.357998	0.975888	1.39624
O	-2.062203	0.320192	2.489774
C	0.293131	-0.948648	1.318094
C	-1.750654	-0.558762	0.210225
C	-0.368031	1.327315	-0.260006

H	-0.073437	-0.391165	2.17257
N	-0.67423	-1.376746	0.463038
C	1.394749	-1.959769	1.532671
C	-0.264562	-2.44396	-0.468339
S	1.021309	-3.391778	0.42844
H	0.140368	-2.009925	-1.38399
H	-1.117125	-3.089757	-0.681205
H	2.383615	-1.552332	1.305819
H	1.404204	-2.312814	2.56756
C	0.833115	0.898182	0.371197
C	1.865603	0.350613	-0.551793
C	3.052178	1.365641	1.190216
C	1.581365	1.660039	1.449068
O	1.685337	-0.243809	-1.602482
O	3.98993	1.703244	1.879452
N	3.141155	0.626267	-0.004508
C	4.376283	0.219682	-0.604558
C	4.54707	0.32422	-1.989253
C	5.409628	-0.275638	0.19858
C	5.751318	-0.076971	-2.565056
H	3.740338	0.699463	-2.605017
C	6.61238	-0.663614	-0.389787
H	5.278905	-0.335236	1.271367
C	6.787424	-0.569386	-1.770678
H	5.878224	0.000953	-3.640644
H	7.413358	-1.042753	0.237654
H	7.724858	-0.876453	-2.224494
H	1.339461	1.37887	2.47932
H	1.433828	2.743767	1.377997
H	-0.448765	1.015513	-1.29707
C	-1.158733	2.513129	0.070515
C	-1.881917	3.136995	-0.9699
C	-1.248945	3.078082	1.361678
C	-2.63373	4.284932	-0.741345
H	-1.835567	2.713321	-1.969192
C	-2.006545	4.225712	1.586332
H	-0.765823	2.594137	2.20006
C	-2.695808	4.84022	0.539219
H	-3.170193	4.748931	-1.564073
H	-2.06133	4.639024	2.589394
H	-3.278432	5.738772	0.719568

Zero-point energy = 0.45429 Hartree

ZPE is included in the following quantities:

Electronic energy = -1868.51064 Hartree

Internal energy = -1868.48227 Hartree

Enthalpy = -1868.481325 Hartree

Gibbs energy = -1868.571118 Hartree

❖ **Spectroscopic data of synthesized compounds 14-17**

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-phenyltetrahydro-*1H*-pyrrolo-[1,2-c][1,3]thiazole (14a)

White solid (43 mg, 89%); mp 216-217 °C; ^{1}H NMR δ = 2.67 (d, 1H, *J* = 18.3 Hz, H-4"), 2.98 (dd, 1H, *J* = 10.5 Hz, 4.8 Hz, H-1), 3.15 (dd, 1H, *J* = 10.5 Hz, 6 Hz, H-1), 3.61 (d, 1H, *J* = 18.3 Hz, H-4"), 3.74 (d, 1H, *J* = 8.2 Hz, H-3), 3.88 (d, 1H, *J* = 8.2 Hz, H-3), 4.25 (d, 1H, *J* = 9.9 Hz, H-7), 4.79-4.86 (m, 1H, H-7a), 6.74-7.83 (m, 14H, Ar-H), 8.11 (bs, 1H, NH); ^{13}C NMR δ = 34.5, 34.8, 50.7, 53.1, 65.0, 70.4, 75.9, 110.3, 122.7, 123.9, 126.1, 128.4, 128.5, 128.9, 129.2, 129.3, 129.5, 130.5, 131.4, 135.0, 140.3, 173.1, 175.5, 177.6. IR: ν =1712, 1774, 3166 cm^{-1}; Anal. Calcd. For $C_{28}H_{23}N_3O_3S$: C, 69.83; H, 4.81; N, 8.73; found: C, 69.94; H, 4.73; N, 8.8.

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (14b)

White solid (41 mg, 83%); mp 178-179 °C; ^{1}H NMR δ = 2.37 (s, 3H, CH_3), 2.71 (d, 1H, *J* = 18.3 Hz, H-4"), 2.99 (dd, 1H, *J* = 11.1 Hz, 4.2 Hz, H-1), 3.22 (dd, 1H, *J* = 11.1 Hz, 6.6 Hz, H-1), 3.56 (d, 1H, *J* = 18.3 Hz, H-4"), 3.98 (s, 2H, H-3), 4.25 (d, 1H, *J* = 9.9 Hz, H-7), 4.96-4.99 (m, 1H, H-7a), 6.78-7.83 (m, 13H, Ar-H), 8.72 (bs, 1H, NH); ^{13}C NMR δ = 20.5, 33.9, 34.3, 50.6, 52.6, 63.6, 69.7, 75.6, 110.2, 122.2, 125.7, 128.0, 128.4, 128.6, 128.8, 129.6, 130.3, 130.8, 137.9, 140.3, 172.6, 175.2, 177.1; IR: ν =1705, 1781, 3227 cm^{-1}; Anal. Calcd. For $C_{29}H_{25}N_3O_3S$: C, 70.28; H, 5.08; N, 8.48. Found: C, 70.47; H, 5.14; N, 8.57.

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methoxyphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (14c)

White solid, yield (44 mg, 86%); mp 230-231 °C; ^{1}H NMR δ = 2.61 (d, 1H, *J* = 18.4 Hz, H-4"), 2.89 (dd, 1H, *J* = 10.2 Hz, 4.2 Hz, H-1), 3.06 (dd, 1H, *J* = 10.2 Hz, 6 Hz, H-1), 3.56 (d, 1H, *J* = 18.4 Hz, H-4"), 3.63 (d, 1H, *J* = 8.7 Hz, H-3), 3.74 (s, 3H, OCH_3), 3.80 (d, 1H, *J* = 8.7 Hz, H-3), 4.11 (d, 1H, *J* = 10.2 Hz, H-7), 4.66-4.67 (m, 1H, H-7a), 6.65-7.77 (m, 13H, Ar-H), 8.36 (bs, 1H, NH); ^{13}C NMR δ = 34.0, 34.2, 50.6, 52.0, 54.8, 64.2, 70.0, 75.6, 109.8, 114.2, 122.1, 123.4, 125.6, 126.1, 127.9, 128.4, 128.8, 130.0, 130.0, 130.9, 139.9, 159.0, 172.8, 175.0, 177.5; IR: ν =1705, 1772, 3144 cm^{-1}; Anal. Calcd. For $C_{29}H_{25}N_3O_4S$: C, 68.08; H, 4.93; N, 8.21. Found: C, 68.20; H, 5.02; N, 7.96.

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-chlorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (14d)

White solid, yield (47 mg, 91%); mp 200-201 °C; ^{1}H NMR δ = 2.59 (d, 1H, *J* = 18.3 Hz, H-4"), 2.95 (dd, 1H, *J* = 10.5 Hz, 5.1 Hz, H-1), 3.06 (dd, 1H, *J* = 10.5 Hz, 6 Hz, H-1), 3.53 (d, 1H, *J* = 18.3 Hz, H-4"), 3.73 (d, 1H, *J* = 7.7 Hz, H-3), 3.84 (d, 1H, *J* = 7.9 Hz, H-3), 4.21 (d, 1H, *J* = 9.9 Hz, H-7), 4.74-4.77 (m, 1H, H-7a), 6.73-7.78 (m, 13H, Ar-H), 7.94 (bs, 1H, NH); ^{13}C NMR δ = 33.8, 34.5, 49.7, 51.8, 64.5, 70.1, 75.2, 109.8, 122.4, 123.2, 125.6, 128.1, 128.4, 129.0, 130.1, 130.4, 130.7, 133.2, 133.9, 139.8,

172.3, 175.1, 177.1; IR: ν =1714, 1775, 3220 cm^{-1}; Anal. Calcd. For $C_{28}H_{22}ClN_3O_3S$: C, 65.17; H, 4.30; N, 8.14. Found: C, 65.29; H, 4.39; N, 8.10.

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-fluorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (14e)

White solid, yield (40 mg, 80%); mp 208-209 °C; ^{1}H NMR δ = 2.57 (d, 1H, *J* = 18.3 Hz, H-4"), 2.92 (dd, 1H, *J* = 10.6 Hz, 5.1 Hz, H-1), 3.09 (dd, 1H, *J* = 10.6 Hz, 6 Hz, H-1), 3.51 (d, 1H, *J* = 18.3 Hz, H-4"), 3.69 (d, 1H, *J* = 8.1 Hz, H-3), 3.81 (d, 1H, *J* = 8.1 Hz, H-3), 4.18 (d, 1H, *J* = 9.9 Hz, H-7), 4.68-4.75 (m, 1H, H-7a), 6.68-7.76 (m, 13H, Ar-H), 8.00 (bs, 1H, NH); ^{13}C δ = 33.8, 34.5, 49.8, 51.7, 64.5, 70.2, 75.2, 109.8, 115.6, 115.9, 122.3, 123.2, 125.6, 128.0, 128.4, 128.5, 130.1, 130.4, 130.7, 130.8, 139.8, 163.7, 172.4, 175.1, 177.0 IR: ν =1717, 1784, 3183 cm^{-1}; Anal. Calcd. For $C_{28}H_{22}FN_3O_3S$: C, 67.32; H, 4.44; N, 8.41. Found: C, 67.19; H, 4.48; N, 8.46.

Spiro[5,2']-oxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylthiophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (14f)

White solid, yield (44 mg, 83%); mp 220-221 °C; ^{1}H NMR δ = 2.48 (s, 3H, SCH_3), 2.64 (d, 1H, *J* = 18.3 Hz, H-4"), 2.94 (dd, 1H, *J* = 10.8 Hz, 4.8 Hz, H-1), 3.12 (dd, 1H, *J* = 10.8 Hz, 6.3 Hz, H-1), 3.59 (d, 1H, *J* = 18.3 Hz, H-4"), 3.70 (d, 1H, *J* = 8.4 Hz, H-3), 3.84 (d, 1H, *J* = 8.4 Hz, H-3), 4.18 (d, 1H, *J* = 9.9 Hz, H-7), 4.72-4.75 (m, 1H, H-7a), 6.71-7.80 (m, 13H, Ar-H), 8.30 (bs, 1H, NH); ^{13}C NMR δ = 15.5, 34.6, 34.8, 50.8, 52.6, 64.0, 70.4, 76.0, 110.4, 122.7, 123.8, 126.1, 127.0, 128.5, 128.9, 129.1, 129.9, 130.5, 131.4, 131.5, 139.1, 140.4, 173.1, 175.5, 177.8; IR: ν =1706, 1775, 3179 cm^{-1}; Anal. Calcd. For $C_{29}H_{25}N_3O_3S_2$: C, 66.01; H, 4.78; N, 7.96. Found: C, 66.16; H, 4.86; N, 7.84.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-phenyltetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15a)

White solid (49 mg, 87%); mp 196-197 °C; ^{1}H NMR δ = 2.59 (d, 1H, *J* = 18.6 Hz, H-4"), 2.89 (dd, 1H, *J* = 10.8 Hz, 4.5 Hz, H-1), 3.07 (dd, 1H, *J* = 10.8 Hz, 6.3 Hz, H-1), 3.53 (d, 1H, *J* = 18.6 Hz, H-4"), 3.58 (d, 1H, *J* = 8.8 Hz, H-3), 3.78 (d, 1H, *J* = 8.8 Hz, H-3), 4.10 (d, 1H, *J* = 10.2 Hz, H-7), 4.65-4.72 (m, 1H, H-7a), 6.64-7.92 (m, 13H, Ar-H), 8.33 (bs, 1H, NH); ^{13}C NMR δ = 33.9, 34.1, 50.4, 52.5, 64.2, 69.7, 75.5, 111.2, 115.1, 125.3, 125.5, 128.0, 128.1, 128.6, 128.8, 128.9, 130.7, 131.7, 132.9, 134.1, 138.8, 172.6, 174.6, 176.8; IR: ν =1706, 1788, 3220 cm^{-1}; Anal. Calcd. For $C_{28}H_{22}BrN_3O_3S$: C, 60.00; H, 3.96; N, 7.50. Found: C, 60.22; H, 3.93; N, 7.65.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15b)

White solid (52 mg, 91%); mp 184-185 °C; ^{1}H NMR δ = 2.28 (s, 3H, CH_3), 2.61 (d, 1H, *J* = 18.4 Hz, H-4"), 2.88 (dd, 1H, *J* = 10.8 Hz, 4.8 Hz, H-1), 3.06 (dd, 1H, *J* = 10.8 Hz, 6.6 Hz, H-1), 3.52 (d, 1H, *J* = 18.4 Hz, H-4"), 3.58 (d, 1H, *J* = 8.4 Hz, H-3), 3.78 (d, 1H, *J* = 8.4 Hz, H-3), 4.06 (d, 1H, *J* = 10.2 Hz, H-7), 4.62-4.69 (m, 1H, H-7a), 6.67-7.92 (m, 12H, Ar-H), 8.75 (bs, 1H, NH); ^{13}C NMR δ = 26.9, 34.4, 34.6, 51.0, 52.9, 64.7, 70.2, 75.9, 111.6, 115.6, 125.9, 126.1, 128.6, 129.0, 129.2, 130.0, 131.3,

131.4, 132.3, 133.4, 138.4, 139.2, 173.1, 175.2, 177.1; IR: ν =1710, 1787, 3236 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}BrN_3O_3S$: C, 60.63; H, 4.21; N, 7.31. Found: C, 60.75; H, 4.15; N, 7.35.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methoxyphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15c)

White solid (49 mg, 83%); mp 178-179 °C; ^{1}H NMR δ = 2.67 (d, 1H, *J* = 18.3 Hz, H-4"), 2.94 (dd, 1H, *J* = 10.8 Hz, 4.5 Hz, H-1), 3.12 (dd, 1H, *J* = 10.8 Hz, 6.3 Hz, H-1), 3.56-3.64 (m, 2H, H-4" and H-3), 3.80 (s, 3H, OCH_3), 3.84 (d, 1H, *J* = 8.7 Hz, H-3) , 4.10 (d, 1H, *J* = 10.2 Hz, H-7), 4.65-4.69 (m, 1H, H-7a), 6.67-7.92 (m, 12H, Ar-H), 8.83 (bs, 1H, NH); ^{13}C NMR δ = 33.7, 34.2, 52.0, 54.8, 64.1, 69.9, 111.2, 114.2, 115.0, 125.4, 125.5, 125.7, 128.1, 128.4, 128.5, 130.0, 130.7, 131.8, 132.9, 138.7, 159.1, 172.7, 174.7, 176.8; IR: ν =1705, 1775, 3236 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}BrN_3O_4S$: C, 58.99; H, 4.10; N, 7.12. Found: C, 59.15; H, 4.15; N, 6.78.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-chlorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15d)

White solid (50 mg, 84%); mp 190-191 °C; ^{1}H NMR δ = 2.60 (d, 1H, *J* = 18.6 Hz, H-4"), 2.95 (dd, 1H, *J* = 10.6 Hz, 5.1 Hz, H-1), 3.13 (dd, 1H, *J* = 10.6 Hz, 6 Hz, H-1), 3.55 (d, 1H, *J* = 18.6 Hz, H-4"), 3.67 (d, 1H, *J* = 8.4 Hz, H-3), 3.84 (d, 1H, *J* = 8.4 Hz, H-3) , 4.15 (d, 1H, *J* = 10.2 Hz, H-7), 4.68-4.75 (m, 1H, H-7a), 6.77-7.95 (m, 12H, Ar-H), 8.28 (bs, 1H, NH); ^{13}C NMR δ = 34.3, 34.7, 50.5, 52.2, 64.8, 70.5, 75.7, 111.8, 115.8, 125.7, 126.0, 128.7, 129.0, 129.1, 129.6, 130.9, 131.1, 131.9, 133.3, 133.6, 139.3, 172.8, 175.2, 177.0; IR: ν =1705, 1781, 3236 cm^{-1}; Anal. Calcd. For $C_{28}H_{21}BrClN_3O_3S$: C, 56.53; H, 3.56; N, 7.06 Found: C, 56.64; H, 3.50; N, 7.13.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-fluorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15e)

White solid (52 mg, 90%); mp 194-195 °C; ^{1}H NMR δ = 2.58 (d, 1H, *J* = 18.6 Hz, H-4"), 2.92 (dd, 1H, *J* = 10.5 Hz, 5.1 Hz, H-1), 3.08 (dd, 1H, *J* = 10.5 Hz, 6 Hz, H-1), 3.47 (d, 1H, *J* = 18.6 Hz, H-4"), 3.64 (d, 1H, *J* = 8.1 Hz, H-3), 3.80 (d, 1H, *J* = 8.1 Hz, H-3) , 4.12 (d, 1H, *J* = 10.2 Hz, H-7), 4.67-4.70 (m, 1H, H-7a), 6.74-7.46 (m, 12H, Ar-H), 7.91 (bs, 1H, NH); ^{13}C NMR δ = 34.2, 34.7, 50.2, 52.2, 64.9, 70.7, 75.5, 111.6, 115.8, 116.2, 116.5, 125.7, 126.0, 128.7, 129.1, 130.6, 131.2, 131.3, 132.0, 133.5, 133.6, 139.3, 164.3, 172.8, 175.4, 176.7; IR: ν =1710, 1793, 3215 cm^{-1}; Anal. Calcd. For $C_{28}H_{21}BrFN_3O_3S$: C, 58.14; H, 3.66; N, 7.26. Found: C, 58.18; H, 3.72; N, 7.13.

Spiro[5,2']-5'-bromooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylthiophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (15f)

White solid (50 mg, 82%); mp 226-227 °C; ^{1}H NMR δ = 2.5 (s, 3H, SCH_3), 2.68 (d, 1H, *J* = 18.3 Hz, H-4"), 2.96 (dd, 1H, *J* = 11.2 Hz, 5.7 Hz, H-1), 3.14 (dd, 1H, *J* = 11.2 Hz, 6 Hz, H-1), 3.63 (d, 1H, *J* = 18.3 Hz, H-4"), 3.66 (d, 1H, *J* = 8.5 Hz, H-3), 3.84 (d, 1H, *J* = 8.5 Hz, H-3) , 4.14 (d, 1H, *J* = 10.2 Hz, H-7), 4.67-4.75 (m, 1H, H-7a), 6.77-8.01 (m, 12H, Ar-H), 8.57 (bs, 1H, NH); ^{13}C NMR δ = 14.9, 33.9, 34.1, 50.7, 52.0, 64.1, 69.8, 75.6, 111.3, 122.2, 115.1, 125.5, 126.4, 128.2, 128.6, 128.6, 129.3, 130.5,

131.4, 131.6, 133.1, 138.8, 172.6, 174.6, 176.7; IR: ν =1705, 1786, 3294 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}BrN_3O_3S_2$: C, 57.42; H, 3.99; N, 6.93. Found: 57.30; H, 4.03; N, 6.88.

Spiro[5,2']-5'-nitrooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-phenyltetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (16a)

White solid (42 mg, 80%); mp 204-205 °C; ^{1}H NMR δ = 2.72 (d, 1H, *J* = 18.4 Hz, H-4"), 3.01 (dd, 1H, *J* = 11.7 Hz, 3 Hz, H-1), 3.18 (dd, 1H, *J* = 11.7 Hz, 6.9 Hz, H-1), 3.49 (d, 1H, *J* = 10.2 Hz, H-3) 3.83 (d, 1H, *J* = 18.4 Hz, H-4"),), 3.91 (d, 1H, *J* = 10.5 Hz, H-3), 4.2 (d, 1H, *J* = 10.5 Hz, H-7), 4.64-4.70 (m, 1H, H-7a), 6.69-8.24 (m, 13H, Ar-H), 8.88 (bs, 1H, NH); ^{13}C NMR δ = 32.5, 35.1, 52.5, 53.2, 63.2, 69.0, 75.5, 109.4, 115.1, 125.3, 125.5, 126.6, 128.2, 128.3, 128.6, 128.6, 129.0, 131.7, 132.9, 138.8, 142.7, 172.6, 174.6, 176.9; IR: ν =1705, 1784, 3237 cm^{-1}; Anal. Calcd. For $C_{28}H_{22}N_4O_5S$: C, 63.87; H, 4.21; N, 10.64. Found: C, 63.98; H, 4.13; N, 10.71.

Spiro[5,2']-5'-nitrooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (16b)

White solid (46 mg, 85%); mp 188-189 °C; ^{1}H NMR δ = 2.29 (s, 3H, CH_3), 2.74 (d, 1H, *J* = 18.3 Hz, H-4"), 3.00 (dd, 1H, *J* = 11.5 Hz, 2.7 Hz, H-1), 3.18 (dd, 1H, *J* = 11.5 Hz, 6.9 Hz, H-1), 3.48 (d, 1H, *J* = 10.2 Hz, H-3), 3.83 (d, 1H, *J* = 18.3 Hz, H-4"), , 3.90 (d, 1H, *J* = 10.2 Hz, H-3), 4.17 (d, 1H, *J* = 10.5 Hz, H-7), 4.60-4.65 (m, 1H, H-7a), 6.69-8.22 (m, 12H, Ar-H), 8.43 (bs, 1H, NH); ^{13}C NMR δ = 21.1, 32.9, 35.7, 53.2, 53.5, 63.6, 69.5, 110.0, 124.6, 125.8, 126.1, 127.1, 128.7, 129.0, 129.1, 130.1, 131.1, 138.8, 143.1, 145.4, 173.0, 174.1, 177.7; IR: ν =1714, 1784, 3253 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}N_4O_5S$: C, 64.43; H, 4.47; N, 10.36. Found: C, 64.49; H, 4.51; N, 10.43.

Spiro[5,2']-5'-nitrooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methoxyphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (16c)

White solid (49 mg, 88%); mp 198-199 °C; ^{1}H NMR δ = 2.79 (d, 1H, *J* = 18.3 Hz, H-4"), 3.05 (dd, 1H, *J* = 11.4 Hz, 2.7 Hz, H-1), 3.22 (dd, 1H, *J* = 11.4 Hz, 6.6 Hz, H-1), 3.53 (d, 1H, *J* = 10.3 Hz, H-3), 3.80 (s, 3H, OCH_3), 3.89 (d, 1H, *J* = 18.3 Hz, H-4"), 3.95 (d, 1H, *J* = 10.3 Hz, H-3), 4.20 (d, 1H, *J* = 10.5 Hz, H-7), 4.68-4.61 (m, 1H, H-7a), 6.75-8.94 (m, 13H, Ar-H and NH); ^{13}C NMR δ = 32.4, 35.2, 52.7, 54.8, 63.1, 69.1, 109.6, 114.3, 124.1, 124.5, 125.3, 125.5, 126.6, 128.2, 128.6, 129.7, 130.6, 142.6, 145.0, 159.3, 172.6, 173.6, 177.4; IR: ν =1717, 1784, 3248 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}N_4O_6S$: C, 62.58; H, 4.35; N, 10.07. Found: C, 62.52; H, 4.42; N, 10.16.

Spiro[5,2']-5'-nitrooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-fluorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (16e)

White solid (47 mg, 86%); mp 222-223 °C; ^{1}H NMR δ = 2.71 (d, 1H, *J* = 18.3 Hz, H-4"), 3.04 (dd, 1H, *J* = 11.5 Hz, 3.3 Hz, H-1), 3.21 (dd, 1H, *J* = 11.5 Hz, 6.6 Hz, H-1), 3.55 (d, 1H, *J* = 9.9 Hz, H-3), 3.85 (d, 1H, *J* = 18.3 Hz, H-4"), 3.94 (d, 1H, *J* = 9.9 Hz, H-3), 4.23 (d, 1H, *J* = 10.5 Hz, H-7), 4.62-4.68 (m, 1H, H-7a), 6.75-8.91 (m, 13H, Ar-H and NH); ^{13}C NMR δ = 33.1, 35.4, 52.8, 63.7, 69.8, 110.0, 116.4, 116.7, 125.7, 125.9, 127.2, 128.8, 129.1, 130.9, 131.0, 143.3, 145.3, 172.6, 174.2, 177.3; IR: ν

=1710, 1777, 3232 cm^{-1}; Anal. Calcd. For $C_{28}H_{21}FN_4O_5S$: C, 61.76; H, 3.89; N, 10.29. Found: C, 61.82; H, 3.96; N, 10.34.

Spiro[5,2']-5'-nitrooxindole-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-thiomethylphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (16f)

White solid (49 mg, 85%); mp 206-207 °C; ^{1}H NMR δ = 2.5 (s, 3H, SCH_3), 2.78 (d, 1H, *J* = 18.4 Hz, H-4"), 3.07 (dd, 1H, *J* = 11.4 Hz, 3.0 Hz, H-1), 3.25 (dd, 1H, *J* = 11.4 Hz, 6.6 Hz, H-1), 3.61 (d, 1H, *J* = 9.9 Hz, H-3), 3.85 (d, 1H, *J* = 18.4 Hz, H-4"), 3.99 (d, 1H, *J* = 9.9 Hz, H-3), 4.23 (d, 1H, *J* = 10.5 Hz, H-7), 4.70-4.74 (m, 1H, H-7a), 6.79-8.93 (m, 13H, Ar-H and NH); ^{13}C NMR δ = 33.1, 35.4, 52.8, 63.5, 69.6, 109.9, 116.4, 116.7, 125.7, 125.9, 127.0, 127.2 128.7, 129.1, 129.5, 129.7, 143.1, 172.4, 174.2, 177.0 ; IR: ν =1710, 1781, 3216 cm^{-1}; Anal. Calcd. For $C_{29}H_{24}N_4O_5S_2$: C, 60.82; H, 4.22; N, 9.78. Found: C, 60.94; H, 3.92; N, 10.49.

Spiro[5,2']-acenaphthene-1'-one-spiro-[6,3'']-*N*-phenylsuccinimide-7-phenyltetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (17a)

Cream solid (49 mg, 95%); mp 216–217 °C; 1H NMR δ = 2.74 (d, 1H, *J* = 18.3 Hz, H-4"), 3.09-3.37 (m, 2H), 3.58 (d, 1H, *J* = 18.3 H-4"), 3.88 (d, 1H, H-3, *J* = 9.0 Hz), 4.05 (d, 1H, H-3, *J* = 9.0 Hz), 4.42 (d, 1H, H-7, *J* = 10.2 Hz), 4.9 (m, 1H, H-7a), 6.29-8.30 (m, 16H, Ar-H) ; 13C NMR (75 MHz, $CDCl_3$): δ = 33.7, 34.9, 51.9, 53.3, 64.1, 69.8, 80.1, 121.7, 125.3, 125.6, 125.9,127.7, 127.9, 128.3, 128.8, 130.0, 130.2, 130.6, 132.3, 134.1, 141.3, 172.2, 174.8, 202.7; IR: ν = 1709, 1791, cm^{-1}; Anal. Calcd. For $C_{32}H_{24}N_2O_3S$: C, 74.40; H, 4.68; N, 5.42. Found: C, 74.55; H, 4.72; N, 5.50.

Spiro[5,2']-acenaphthene-1'-one-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methylphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (17b)

yellow solid (46 mg, 87%; mp 188-189 °C; 1H NMR δ = 2.3 (s, 3H, OCH_3), 2.72 (d, 1H, *J* = 18.3 Hz, H-4"), 3.05 (dd, 1H, *J* = 11.2, 3.6 Hz, H-1), 3.28 (dd, 1H, *J* = 11.2, 6.9 Hz, H-1), 3.61 (d, 1H, *J* = 18.3 Hz, H-4"), 3.71 (d, 1H, *J* = 9.6 Hz, H-3), 3.97 (d, 1H, *J* = 9.6 Hz, H-3), 4.34 (d, 1H, *J* = 10.2 Hz, H-7), 4.78-4.84 (m, 1H, H-7a), 6.29-8.30 (m, 15H, Ar-H) ; 13C NMR (75 MHz, $CDCl_3$): δ = 21.0, 33.8, 35.7, 52.8, 53.3, 64.6, 70.2, 80.8, 121.9, 125.7, 126.1, 126.1, 128.0, 128.3, 128.4, 128.7, 129.1, 129.9, 130.5, 130.6, 131.0, 131.4, 132.7, 132.9, 138.2, 141.5, 172.9, 175.0, 203.8; IR: ν = 1715, 1780, cm^{-1}; Anal. Calcd. For $C_{33}H_{26}N_2O_3S$: C, 74.69; H, 4.94; N, 5.28. Found: C, 74.83; H, 4.90; N, 5.39.

Spiro[5,2']-acenaphthene-1'-one-spiro-[6,3'']-*N*-phenylsuccinimide-7-(4-methoxyphenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (17c)

Yellow solid (49 mg, 90%); mp 158-159 °C; 1H NMR δ = 2.66 (d, 1H, *J* = 18.3 Hz, H-4"), 2.99 (dd, 1H, *J* = 10.9, 3.6 Hz, H-1), 3.21 (dd, 1H, *J* = 10.9, 6.6 Hz, H-1), 3.54 (d, 1H, *J* = 18,3 Hz, H-4"), 3.66 (d, 1H, *J* = 9.1 Hz, H-3), 3.91 (d, 1H, *J* = 9.1 Hz, H-3), 4.27 (d, 1H, *J* = 10.2 Hz, H-7), 4.69-4.76 (m, 1H, H-7a), 6.16-8.22 (m, 15H, Ar-H) ; 13C NMR (75 MHz, $CDCl_3$): δ = 33.5, 35.1, 52.1, 52.9, 64.3, 70.0, 80.2, 114.2, 121.4, 125.3, 125.6, 125.8, 126.0, 126.3, 127.5, 127.8, 127.9, 128.2, 128.6, 129.9, 130.6, 131.6, 132.1, 132.6, 159.0, 141.1, 172.4, 174.7, 203.2; IR: ν = 1714, 1784, cm^{-1}; Anal.

Calcd. For $C_{33}H_{26}N_2O_4S$: C, 72.51; H, 4.79; N, 5.12. Found: C, 72.43; H, 4.83; N, 5.20.

Spiro[5.2']-acenaphthene-1'-one-spiro-[6.3'']-*N*-phenylsuccinimide-7-(4-chlorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (17d)

Cream solid (44 mg, 80%); mp 208–209 °C; 1H NMR δ = 2.55 (d, 1H, *J* = 18.1 Hz, H-4"), 2.97 (dd, 1H, *J* = 11.1, 3.9 Hz, H-1), 3.19 (dd, 1H, *J* = 11.1, 6.6 Hz, H-1), 3.50 (d, 1H, *J* = 18.1 Hz, H-4"), 3.67 (d, 1H, *J* = 9.0 Hz, H-3), 3.88 (d, 1H, *J* = 9.0 Hz, H-3), 4.27 (d, 1H, *J* = 10.2 Hz, H-7), 4.69-4.76 (m, 1H, H-7a), 6.15-8.17 (m, 15H, Ar-H) ; 13C NMR (75 MHz, $CDCl_3$): δ = 33.6, 34.9, 51.7, 52.5, 64.2, 70.0, 80.0, 110.0, 121.6, 125.2, 125.4, 125.8, 127.6, 127.9, 127.9, 128.3, 128.6, 129.0, 130.0, 130.2, 130.5, 130.8, 132.2, 132.9, 141.4, 172.0, 174.2, 203.6; IR: ν = 1720, 1785, cm^{-1}; Anal. Calcd. For $C_{32}H_{23}ClN_2O_3S$: C, 69.75; H, 4.21; Cl, 6.43; N, 5.08. Found: C, 69.90; H, 4.15; N, 5.18.

Spiro[5.2']-acenaphthene-1'-one-spiro-[6.3'']-*N*-phenylsuccinimide-7-(4-fluorophenyl)tetrahydro-*1H*-pyrrolo[1,2-c][1,3]thiazole (17e)

Yellow solid (44 mg, 82%); mp 240-241 °C; 1H NMR δ = 2.63 (d, 1H, *J* = 18.3 Hz, H-4"), 3.03 (dd, 1H, *J* = 11.4, 3.9 Hz, H-1), 3.25 (dd, 1H, *J* = 11.4, 6.9. Hz, H-1), 3.56 (d, 1H, *J* = 18.3 Hz, H-4"), 3.72 (d, 1H, *J* = 9.1 Hz, H-3), 3.94 (d, 1H, *J* = 9.1 Hz, H-3), 4.34 (d, 1H, *J* = 10.2 Hz, H-7), 4.75-4.82 (m, 1H, H-7a), 6.21-8.24 (m, 15H, Ar-H); 13C NMR δ = 33.6, 34.9, 51.8, 52.4, 64.3, 70.1, 80.0, 115.6, 115.9, 121.5, 125.2, 125.4, 125.8, 125.9, 127.6, 127.9, 127.9, 128.1, 128.2, 128.6, 130.1, 130.2, 130.5, 130.6, 131.6, 132.2, 132.4, 141.2, 172.1, 174.7, 203.2; IR: ν = 1709, 1782, cm^{-1}; Anal. calcd. For $C_{32}H_{23}FN_2O_3S$: C, 71.89; H, 4.34; N, 5.24. Found: C, 71.95; H, 4.38; N, 5.31.

❖ **^{1}H- and ^{13}C-NMR Spectra of compounds 14-17** (Fig. S1 to S42)

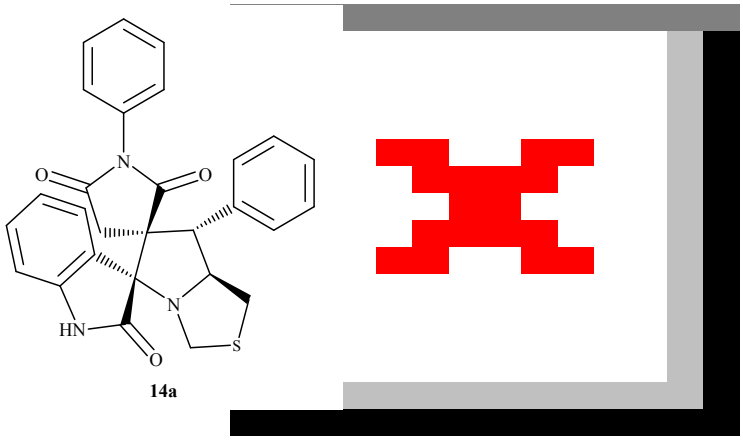


Fig. S1. ^{1}H NMR spectrum of **14a** in $CDCl_3$

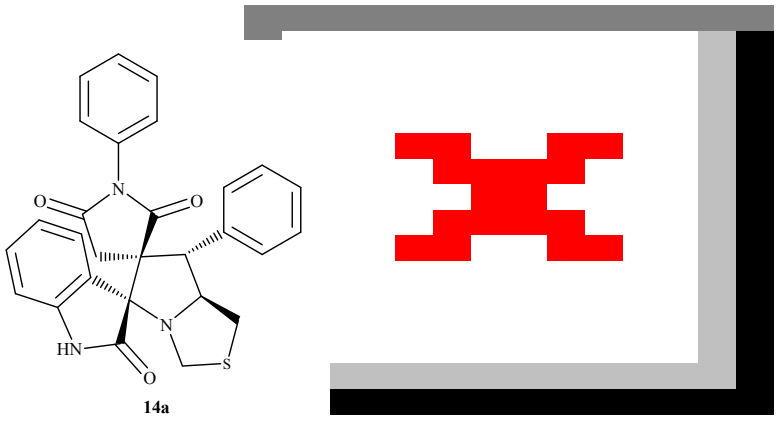


Fig. S2. ^{13}C NMR spectrum of **14a** in $CDCl_3$

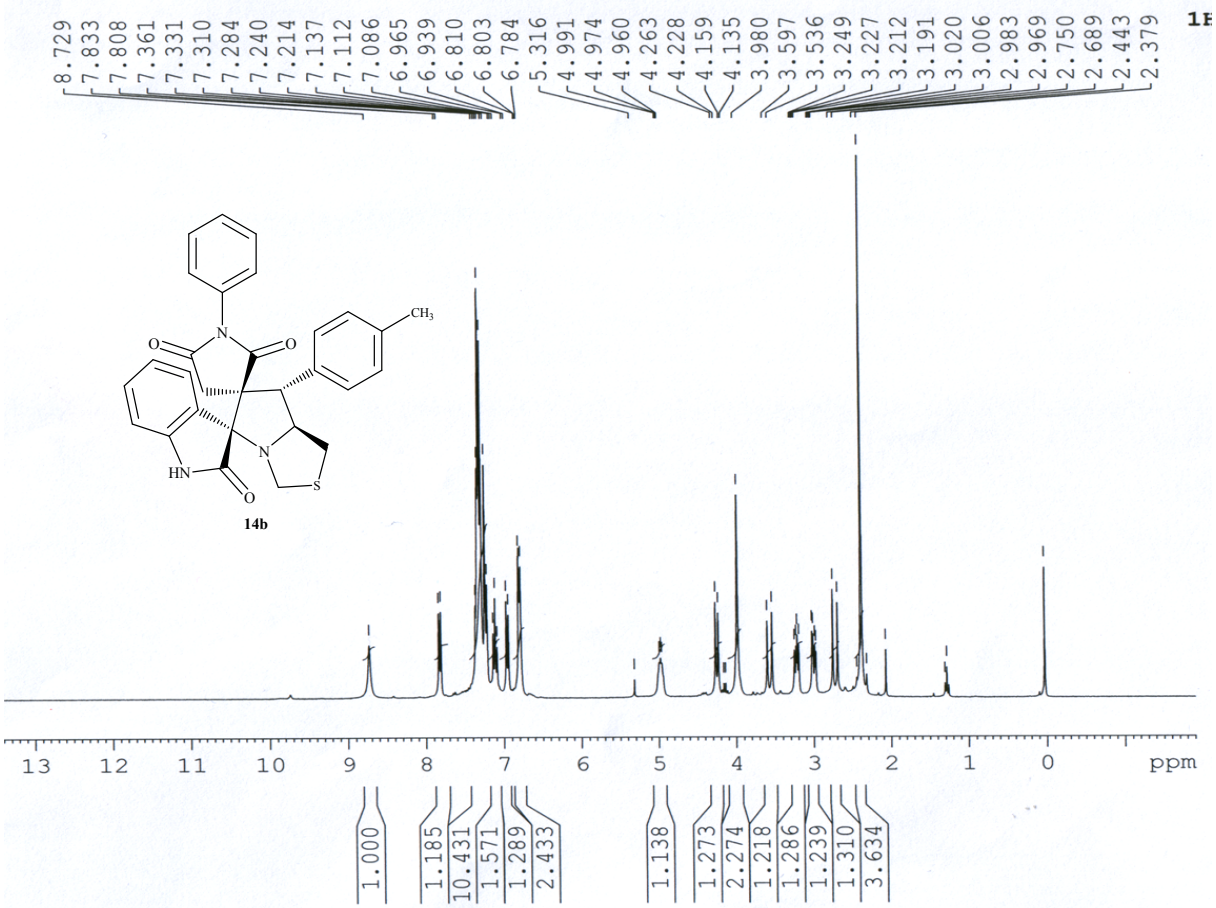


Fig. S3. ^{1}H NMR spectrum of **14b** in $CDCl_3$

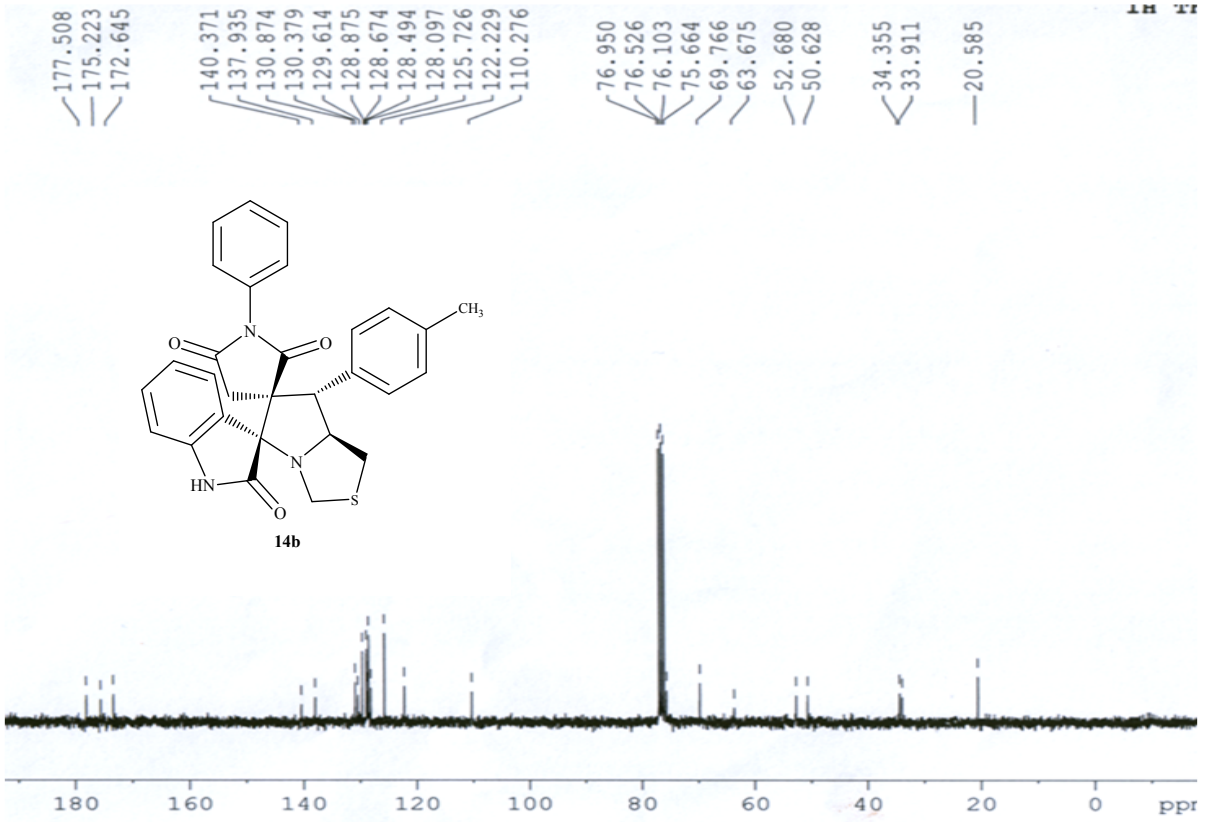


Fig. S4. ^{13}C NMR spectrum of **14b** in $CDCl_3$

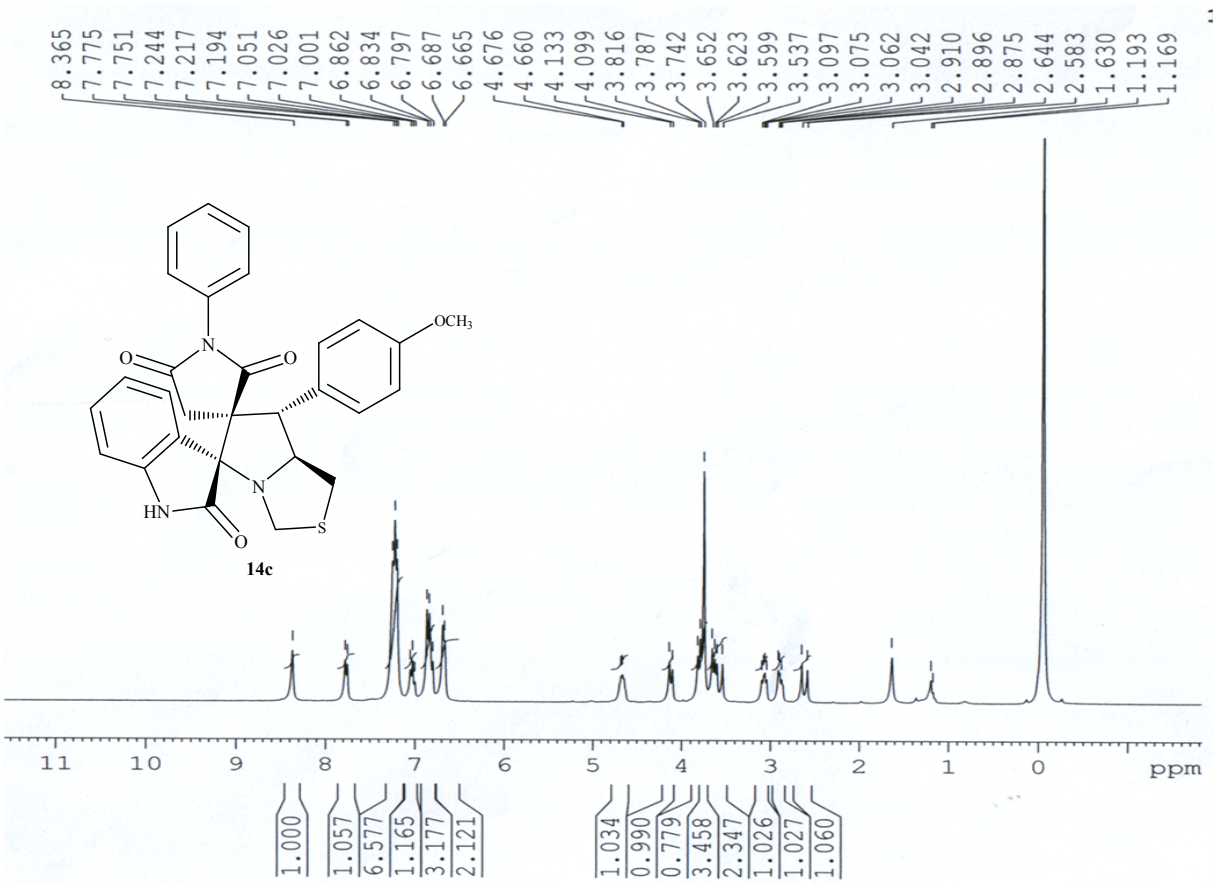


Fig. S5. ^{1}H NMR spectrum of **14c** in $CDCl_3$

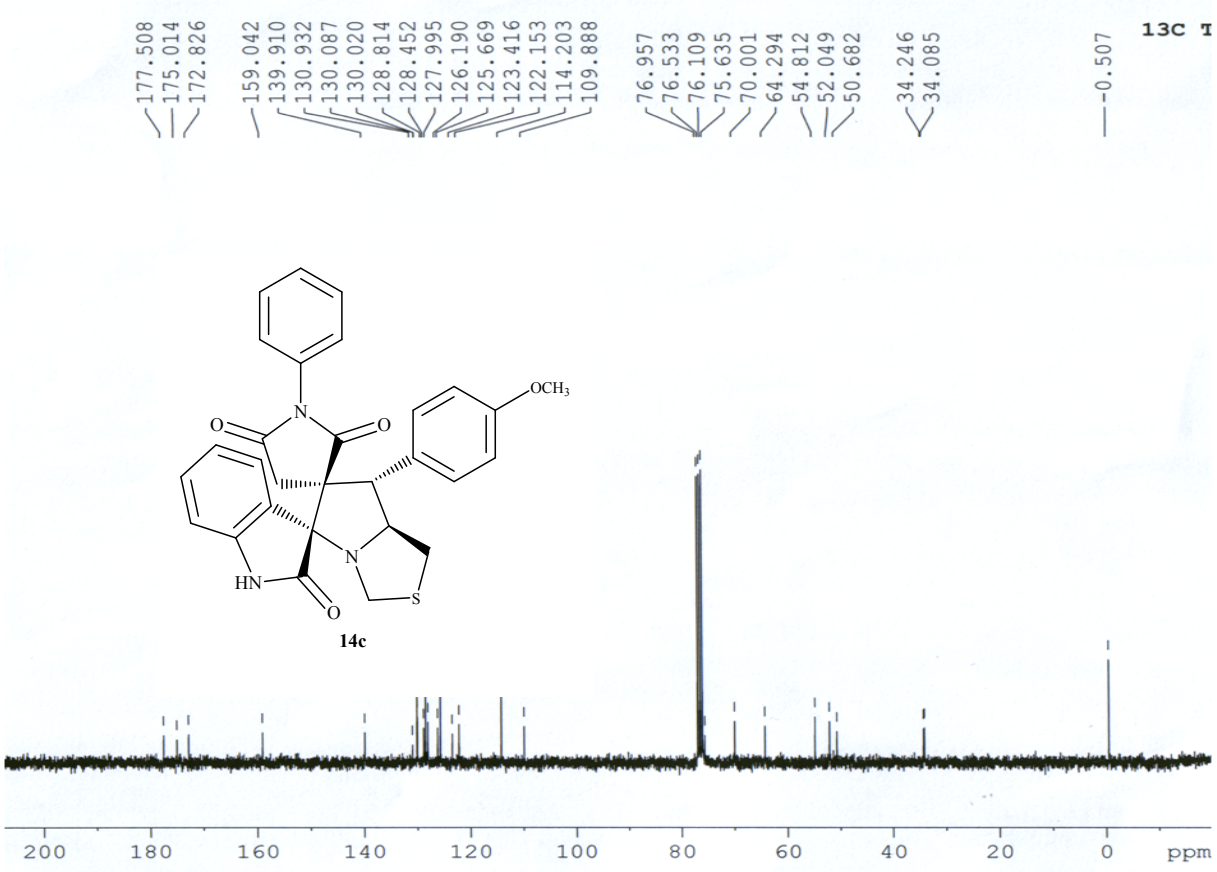


Fig. S6. ^{13}C NMR spectrum of **14c** in $CDCl_3$

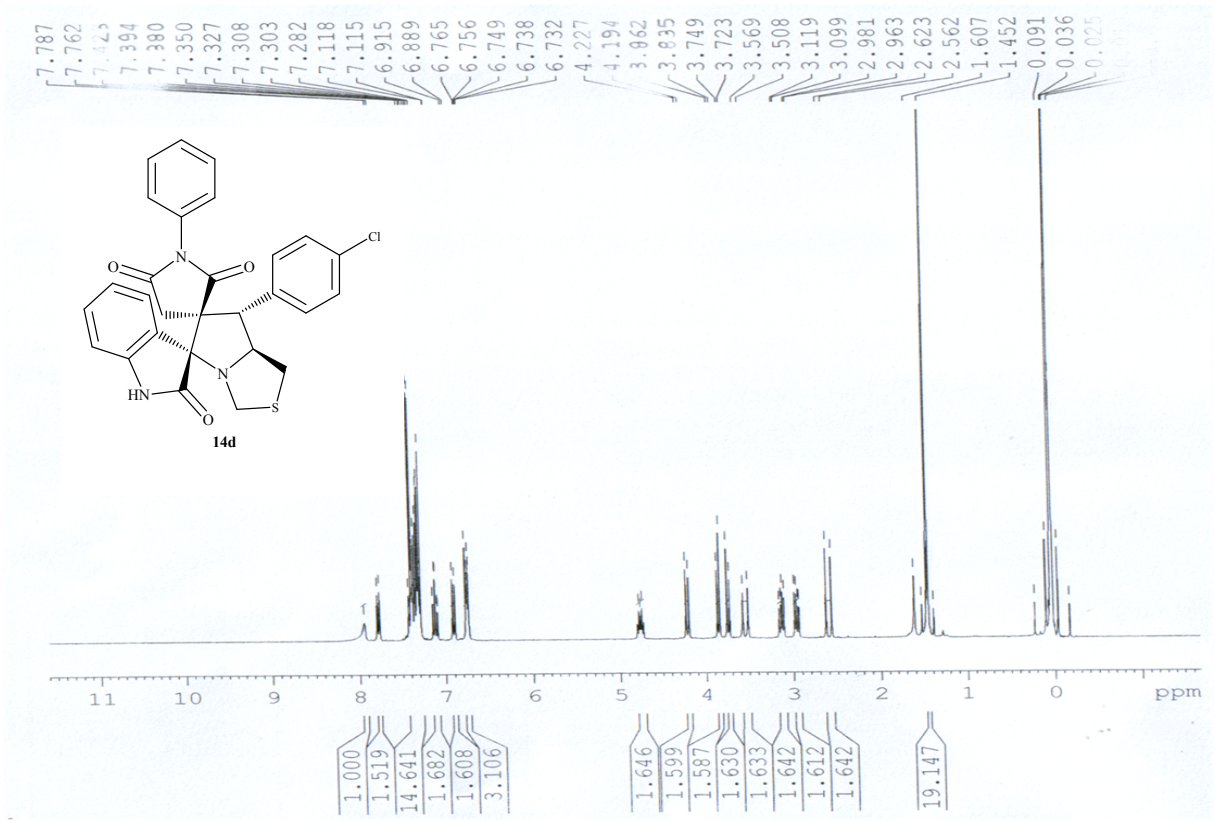


Fig. S7. ^{1}H NMR spectrum of **14d** in $CDCl_3$

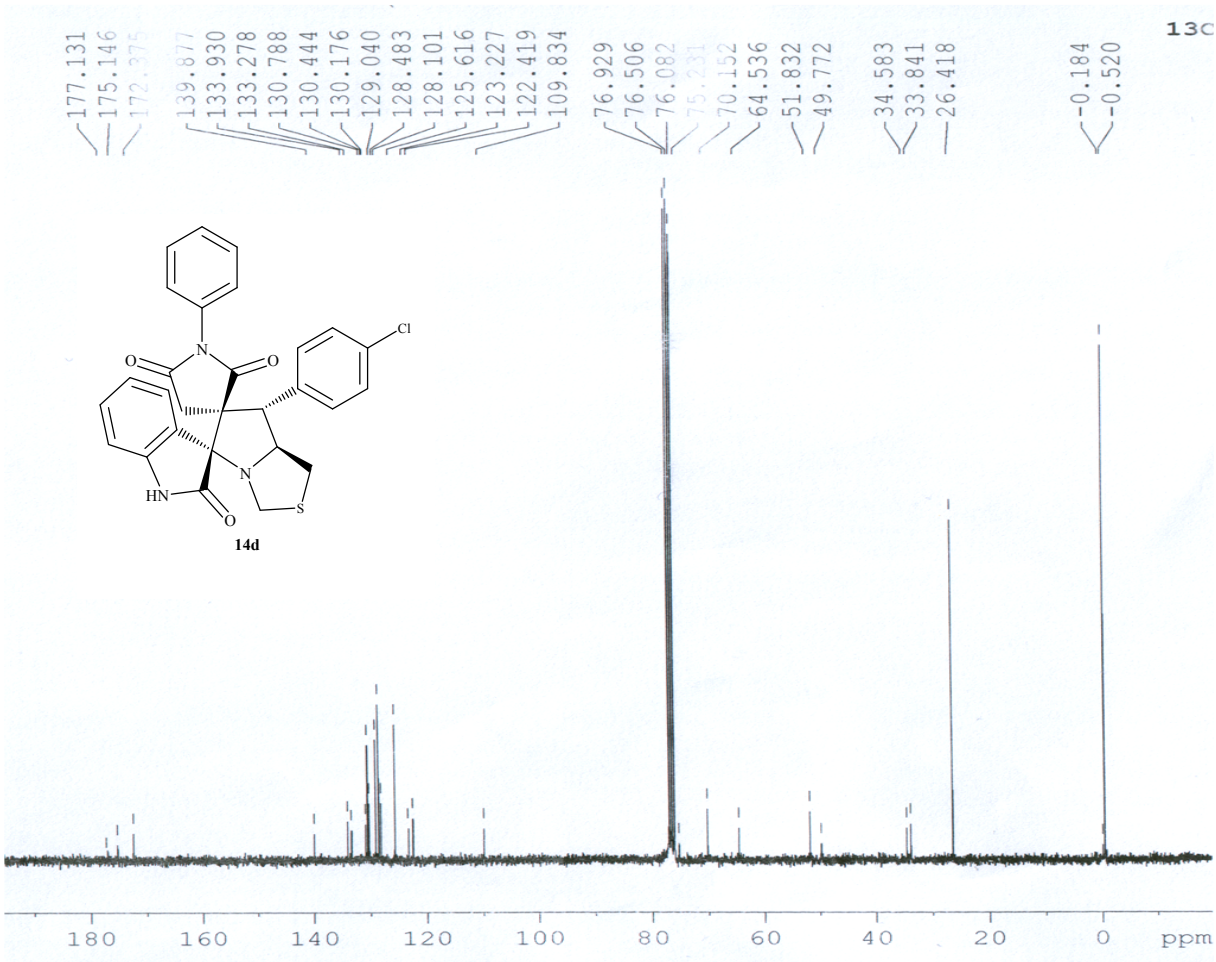


Fig. S8. ^{13}C NMR spectrum of **14d** in $CDCl_3$

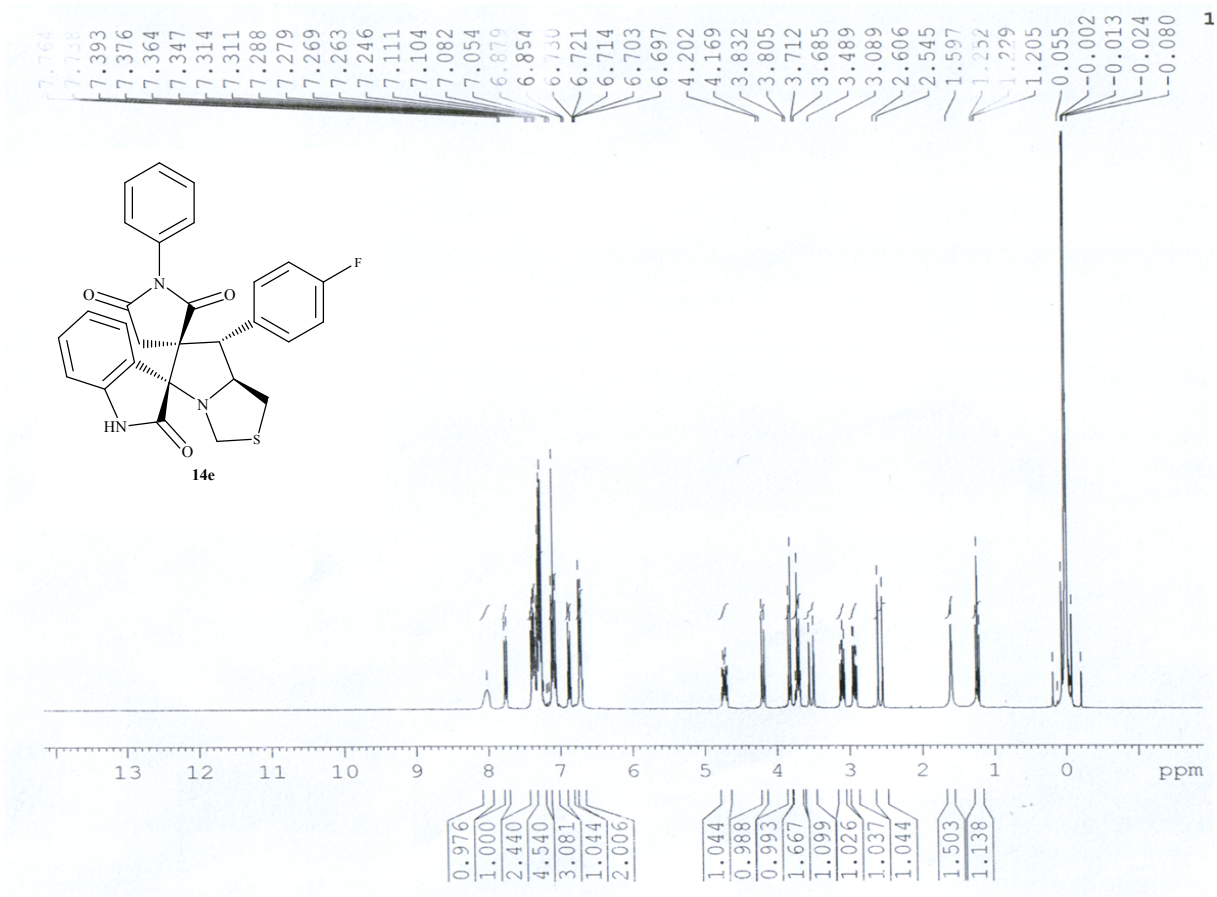


Fig. S9. ^{1}H NMR spectrum of **14e** in $CDCl_3$

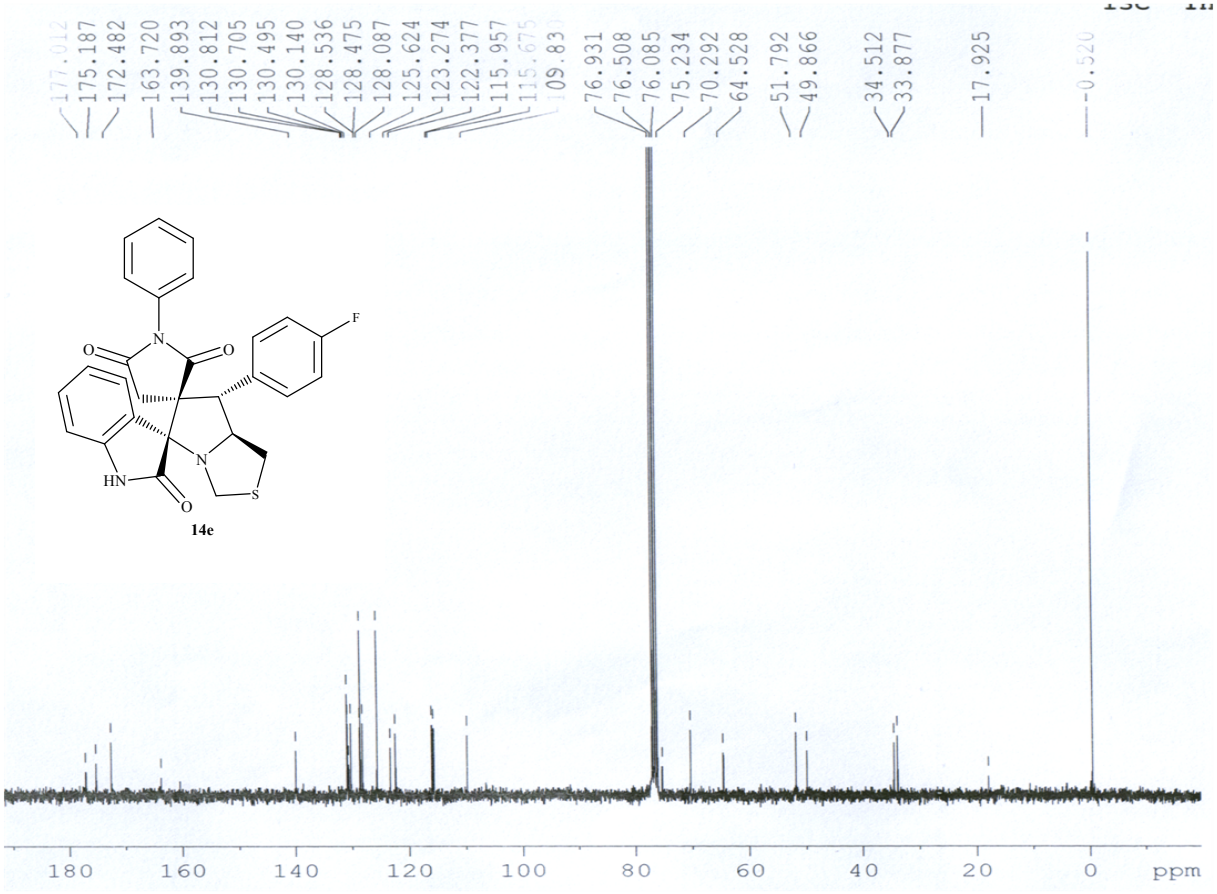


Fig. S10. ^{13}C NMR spectrum of **14e** in $CDCl_3$

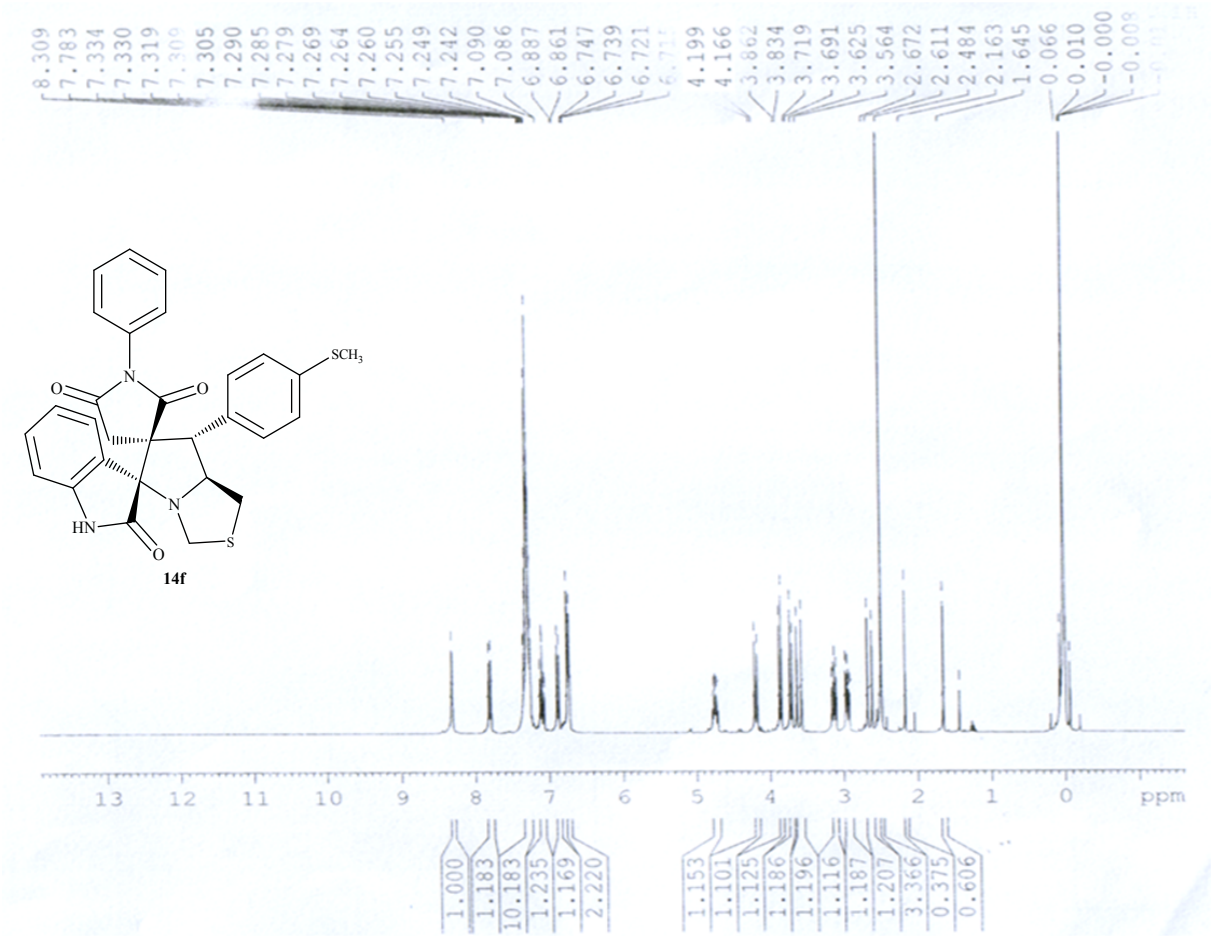


Fig. S11. ^{1}H NMR spectrum of **14f** in $CDCl_3$

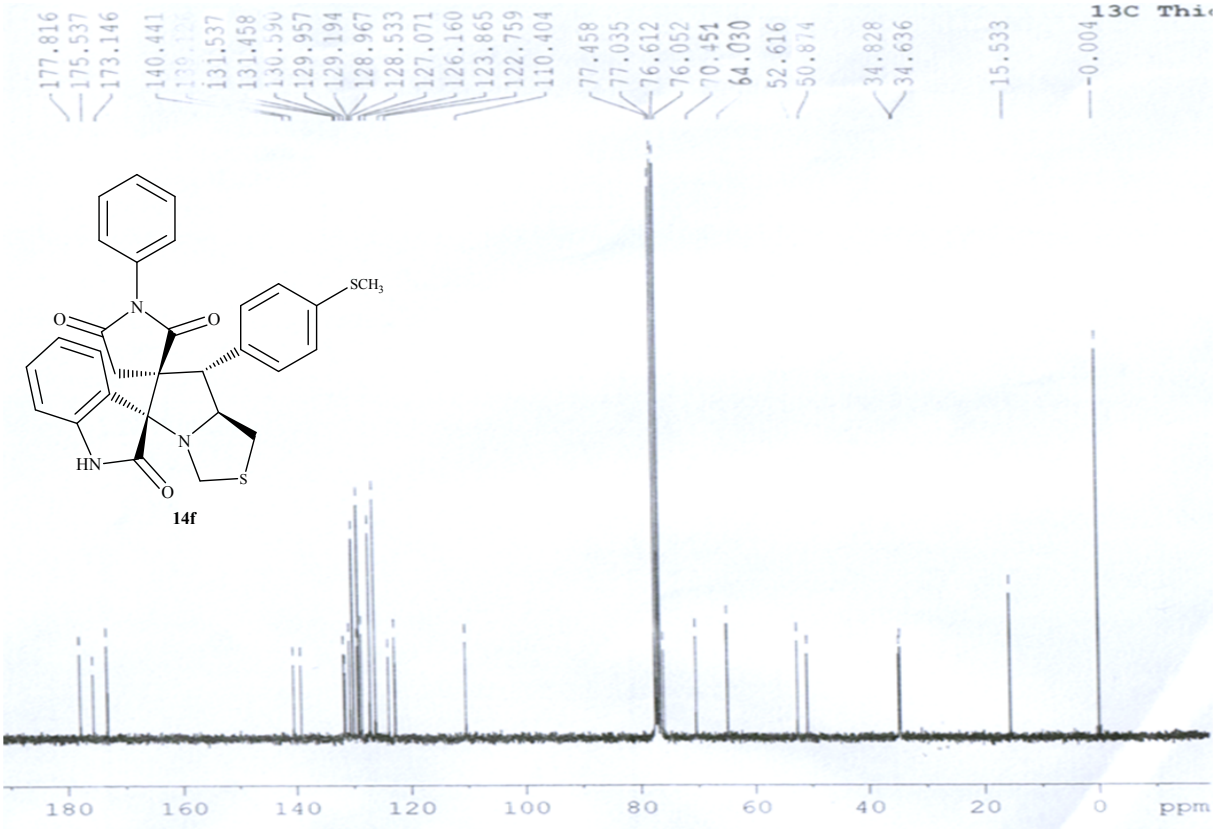


Fig. S12. ^{1}H NMR spectrum of **14f** in $CDCl_3$

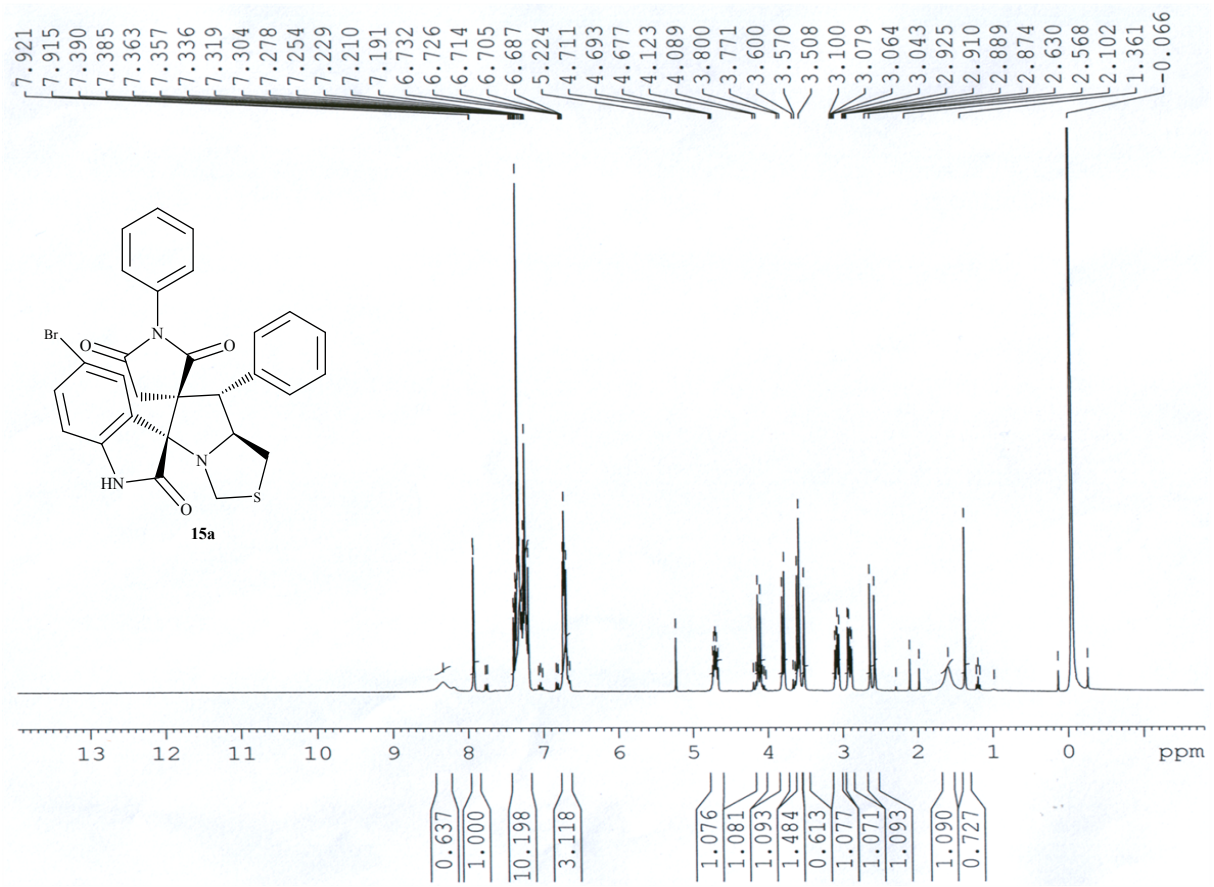


Fig. S13. ^{1}H NMR spectrum of **15a** in $CDCl_3$

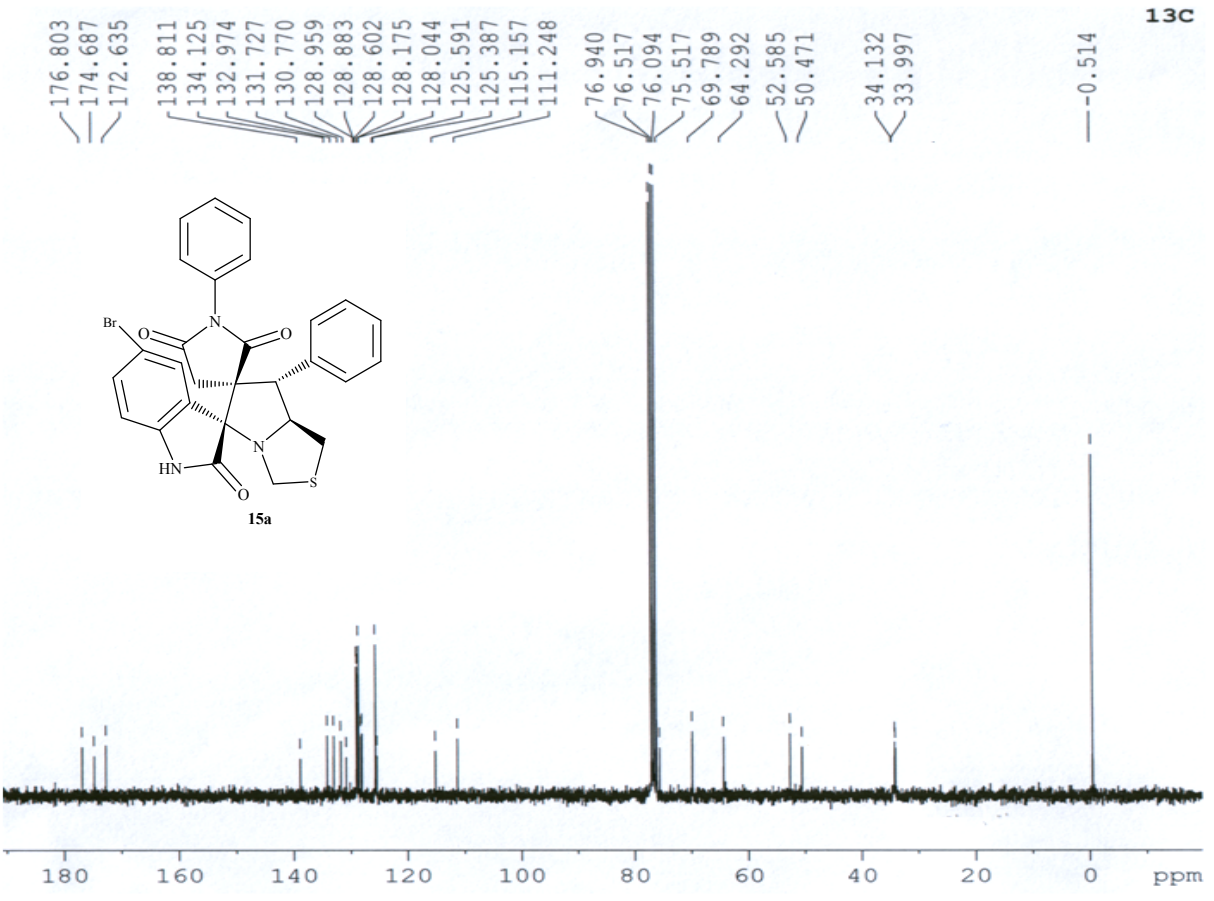


Fig. S14. ^{13}C NMR spectrum of **15a** in $CDCl_3$

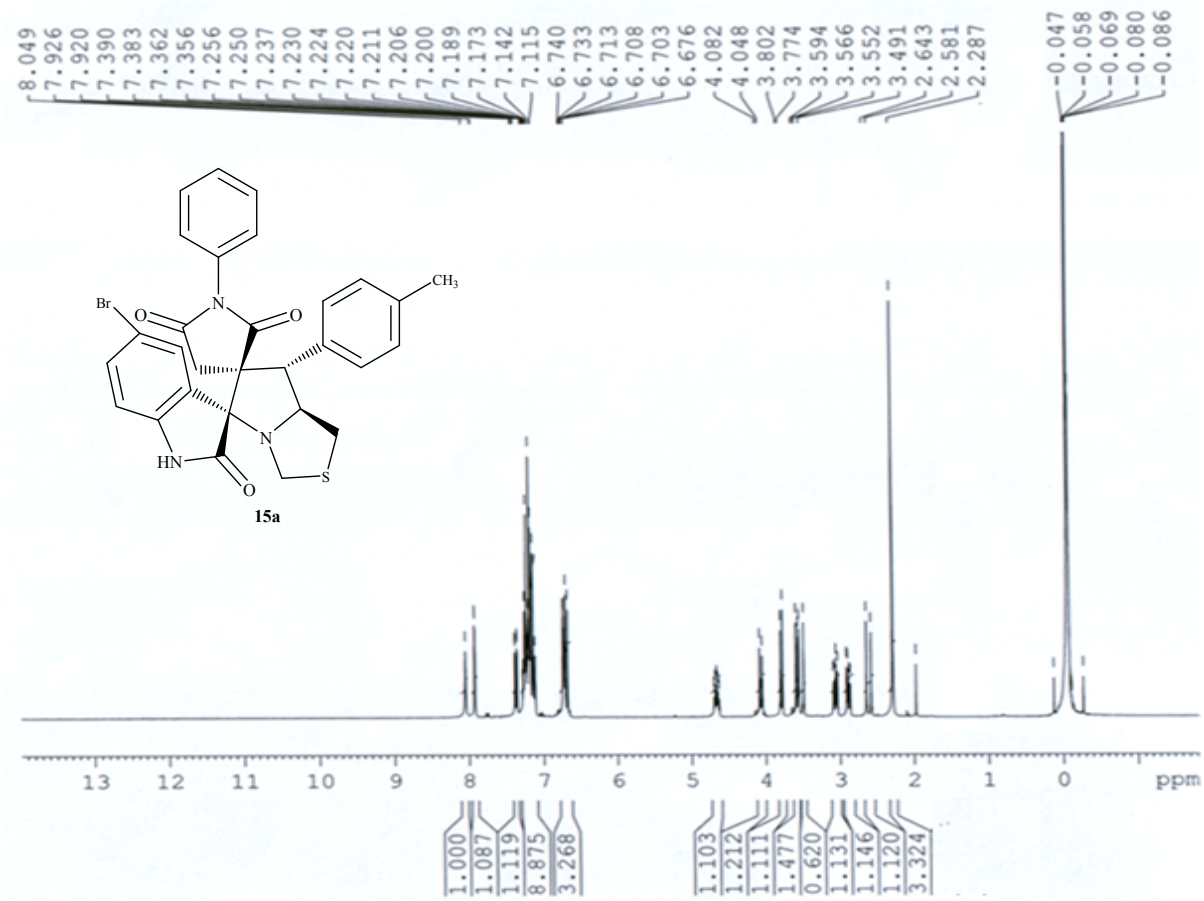


Fig. S15. ^{1}H NMR spectrum of **15b** in $CDCl_3$

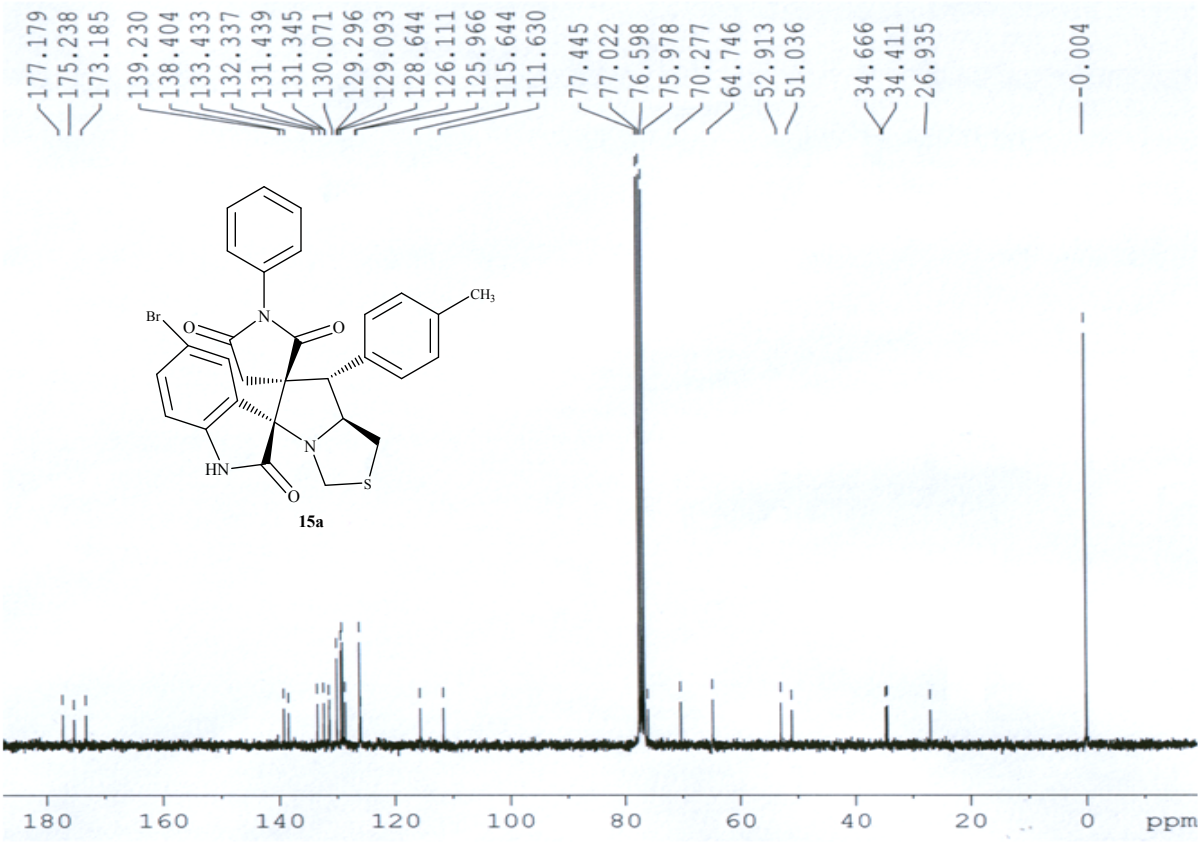


Fig. S16. ^{1}H NMR spectrum of **15b** in $CDCl_3$

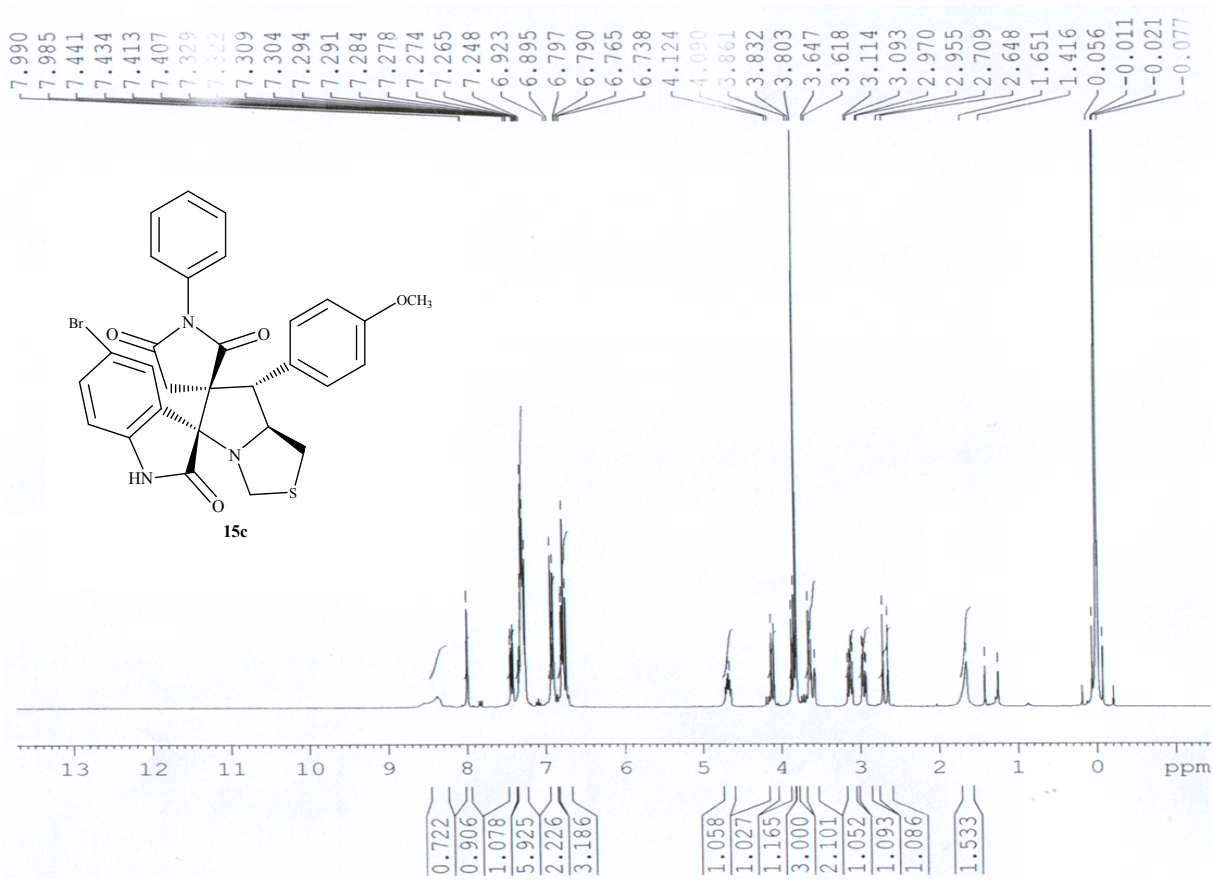


Fig. S17. ^{1}H NMR spectrum of **15c** in $CDCl_3$

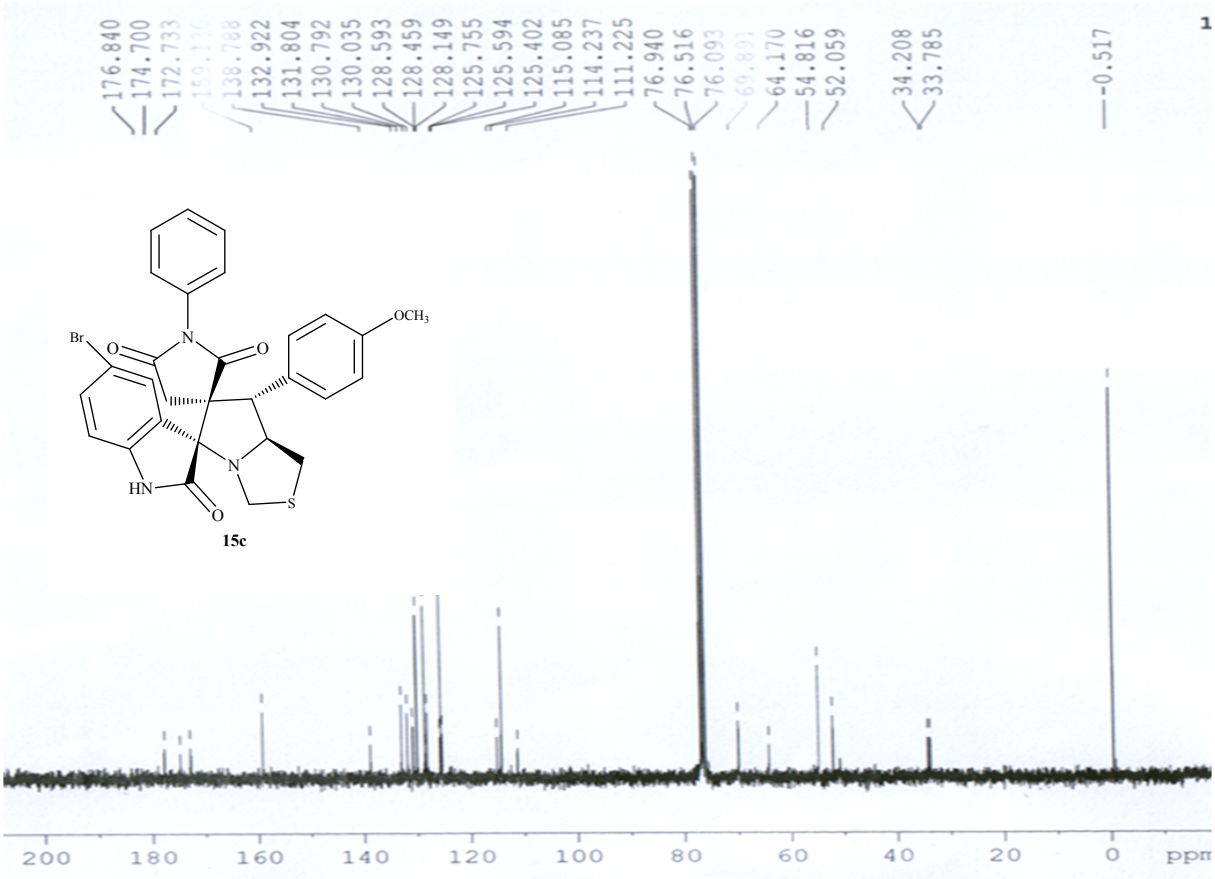


Fig. S18. ^{1}H NMR spectrum of **15c** in $CDCl_3$

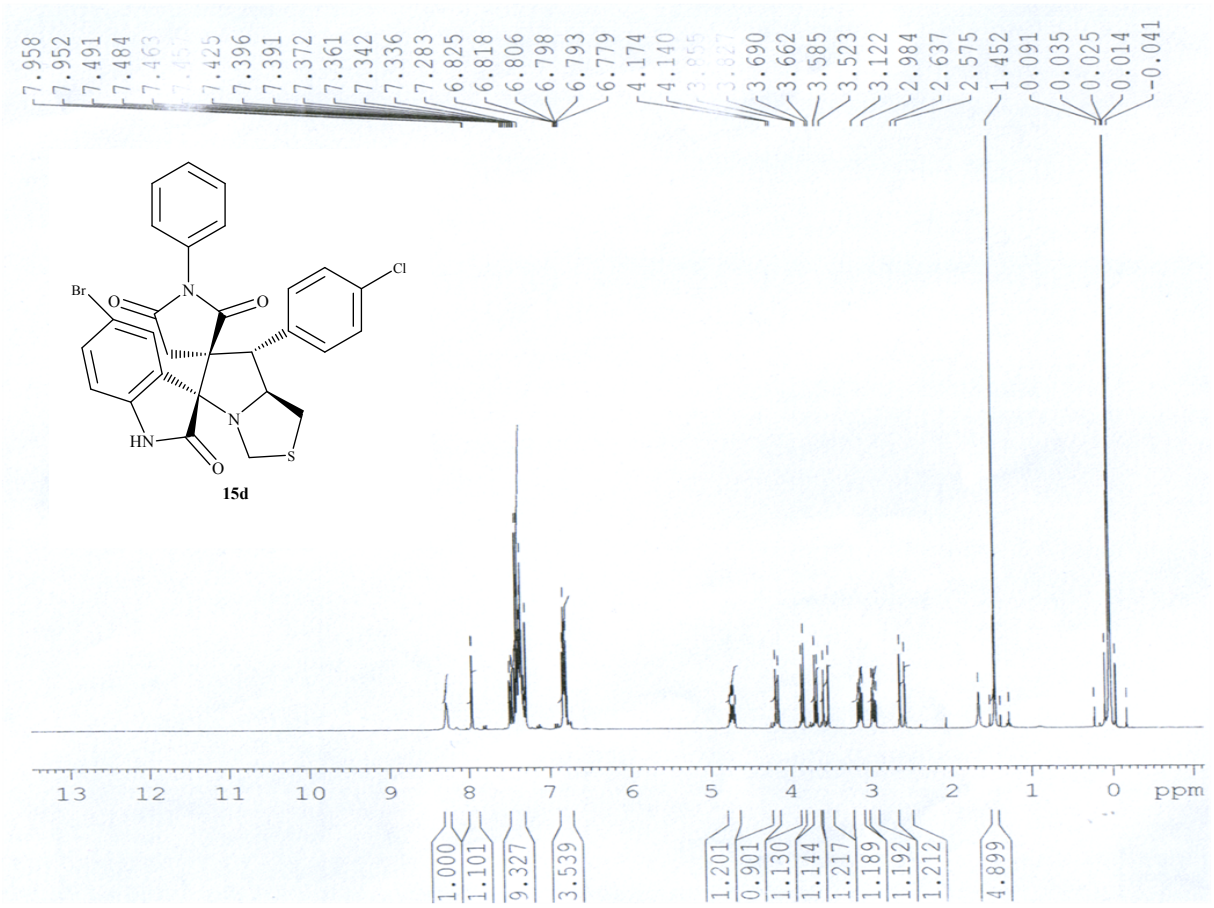


Fig. S19. ^{1}H NMR spectrum of **15d** in $CDCl_3$

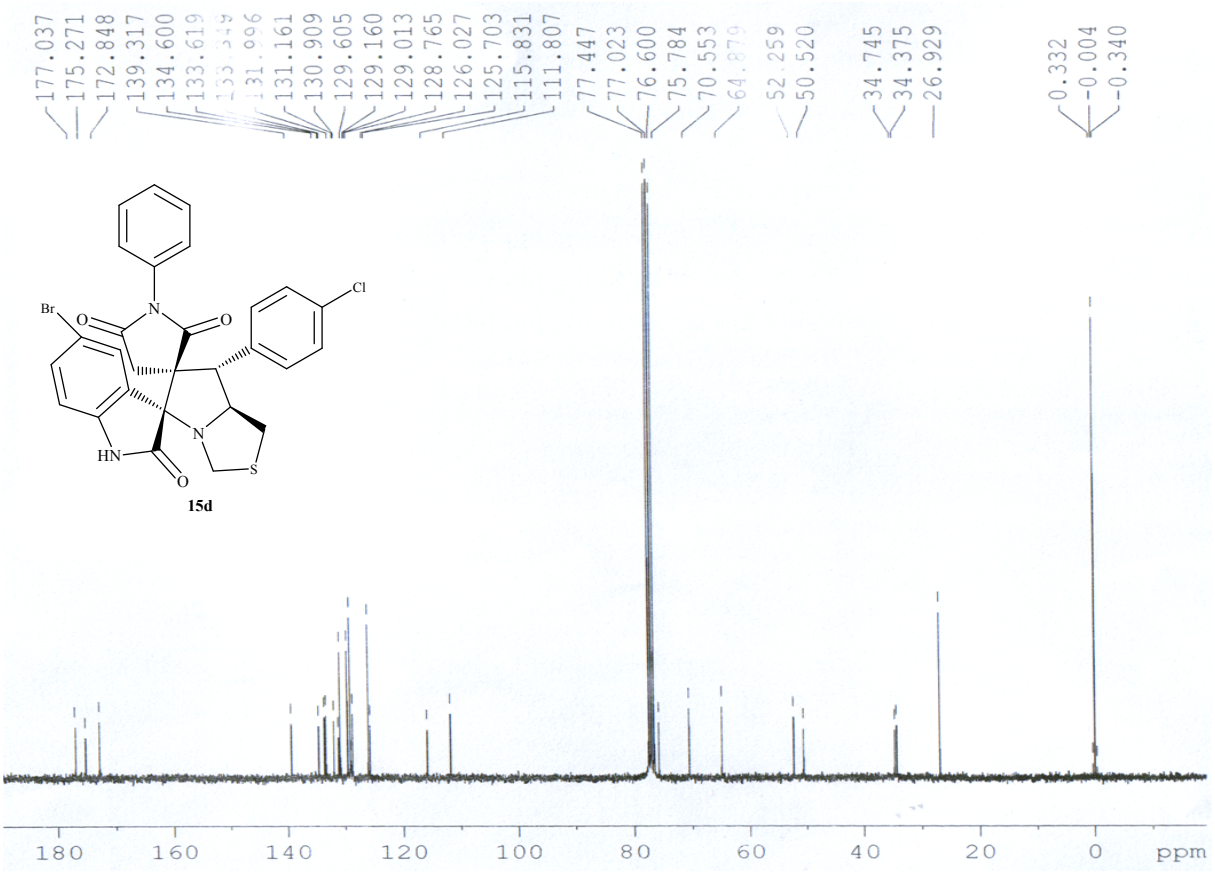


Fig. S20. ^{13}C NMR spectrum of **15d** in $CDCl_3$

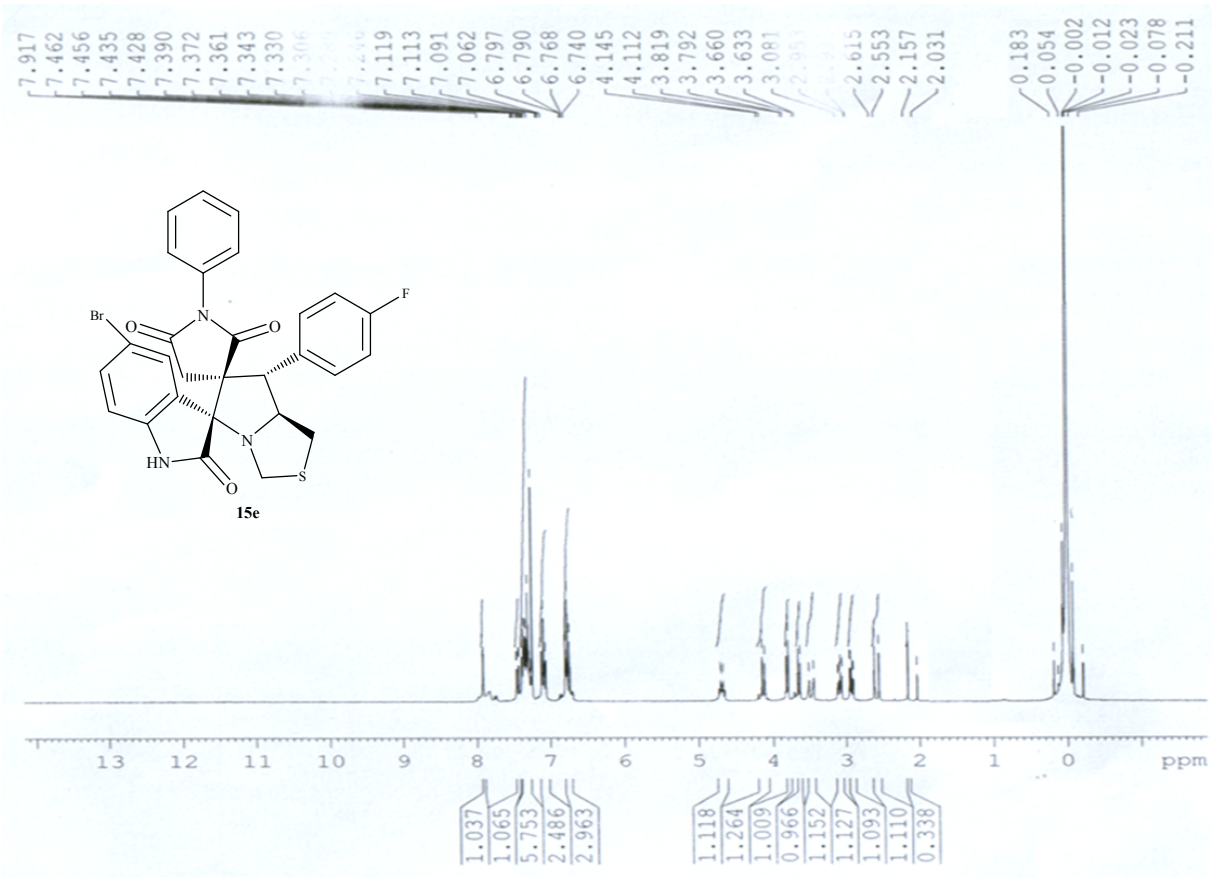


Fig. S21. ^{1}H NMR spectrum of **15e** in $CDCl_3$

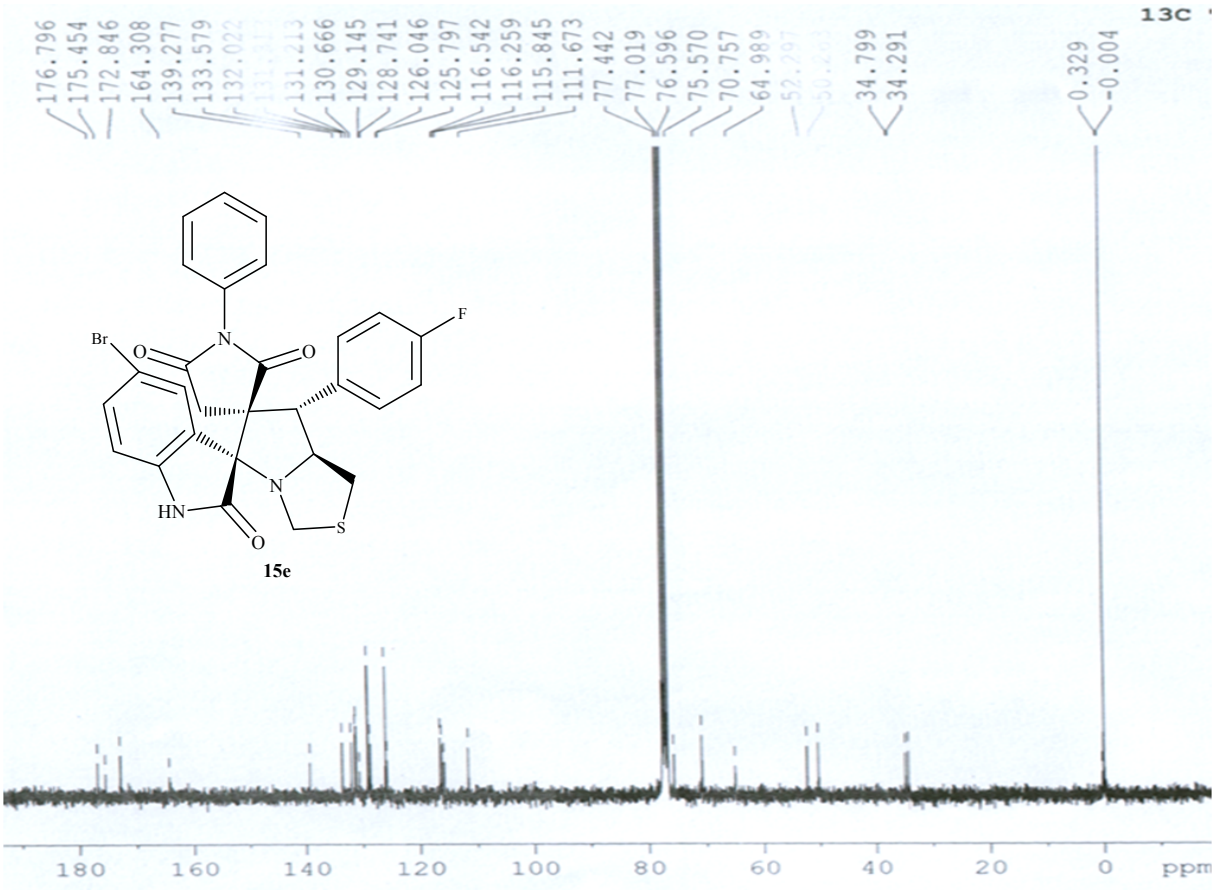


Fig. S22. ^{13}C NMR spectrum of **15e** in $CDCl_3$

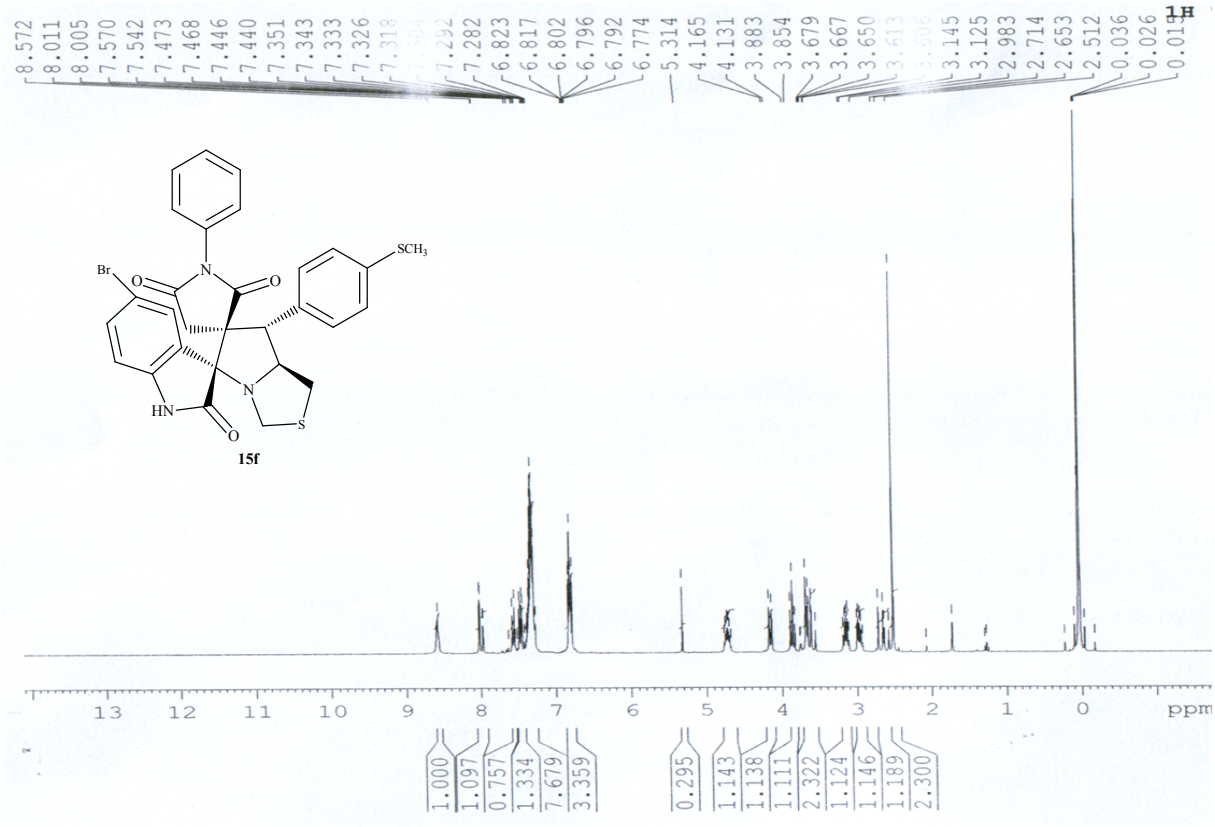


Fig. S23. ^{1}H NMR spectrum of **15f** in $CDCl_3$

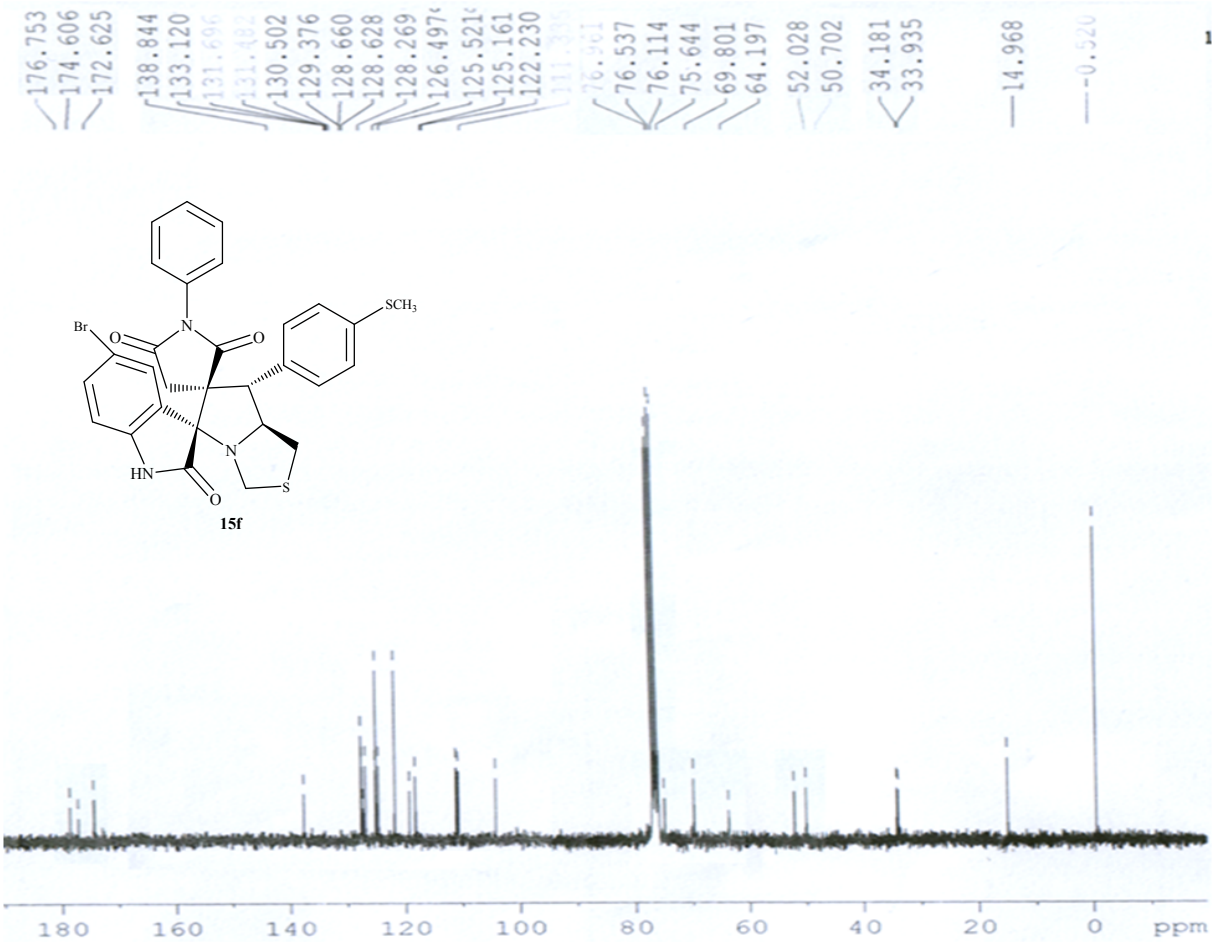


Fig. S24. ^{13}C NMR spectrum of **15f** in $CDCl_3$

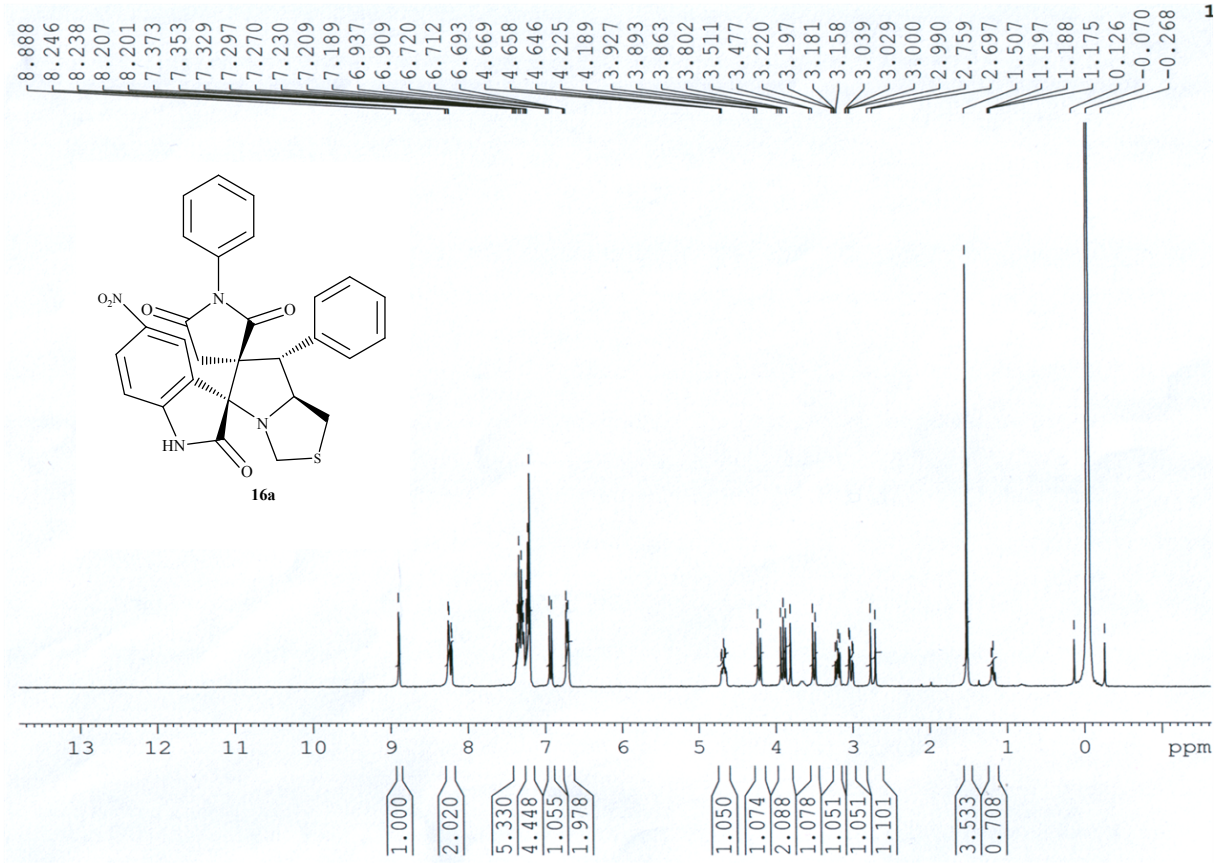


Fig. S25. ^{1}H NMR spectrum of **16a** in $CDCl_3$

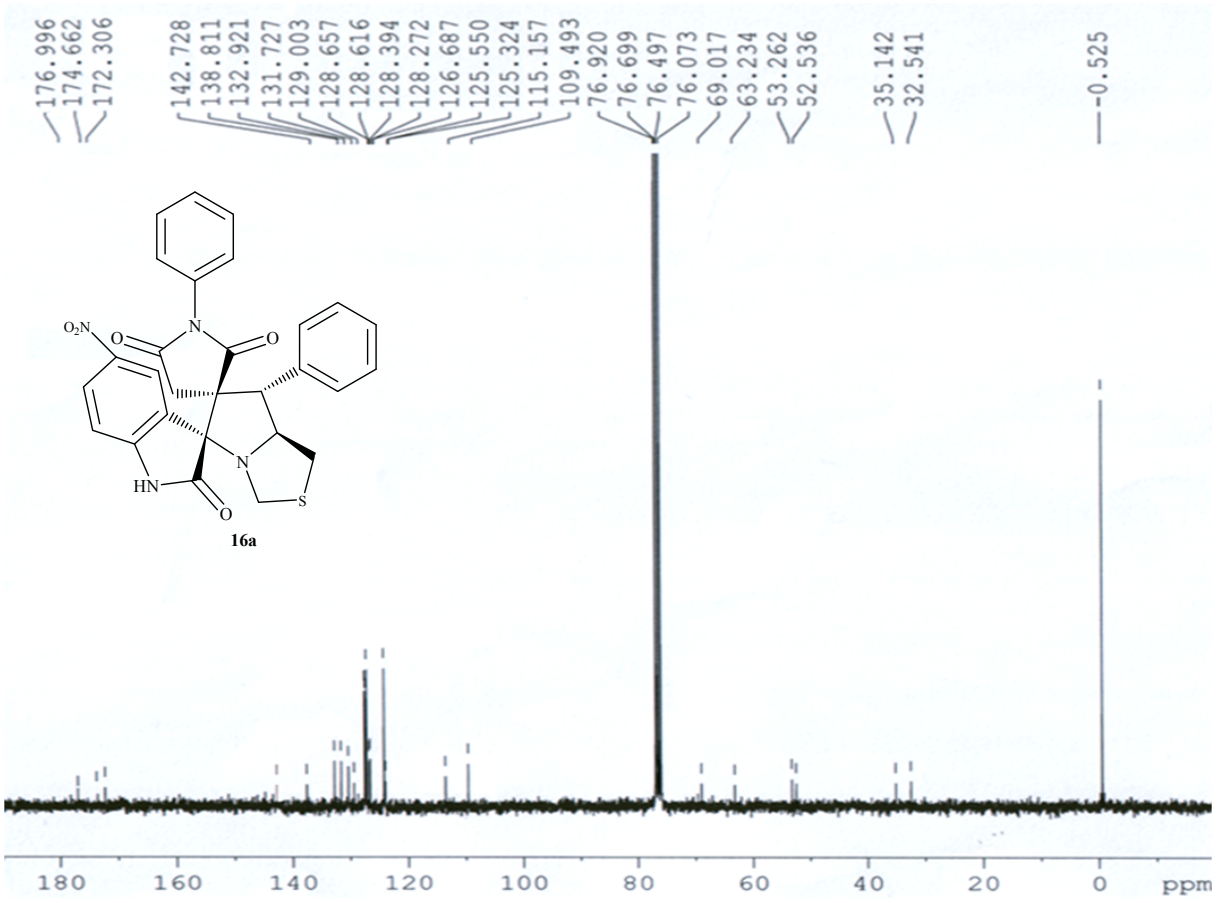


Fig. S26. ^{13}C NMR spectrum of **16a** in $CDCl_3$

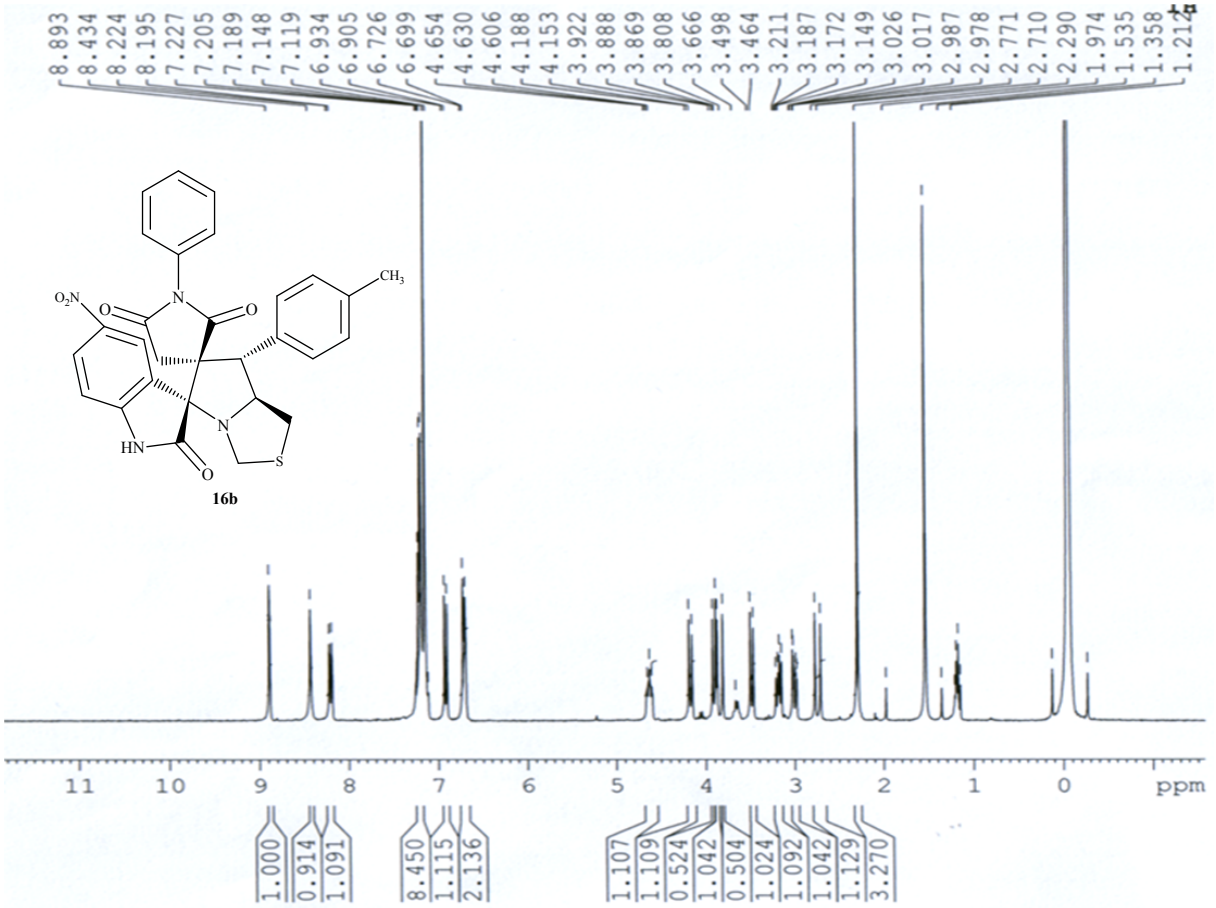


Fig. S27. ^{1}H NMR spectrum of **16b** in $CDCl_3$

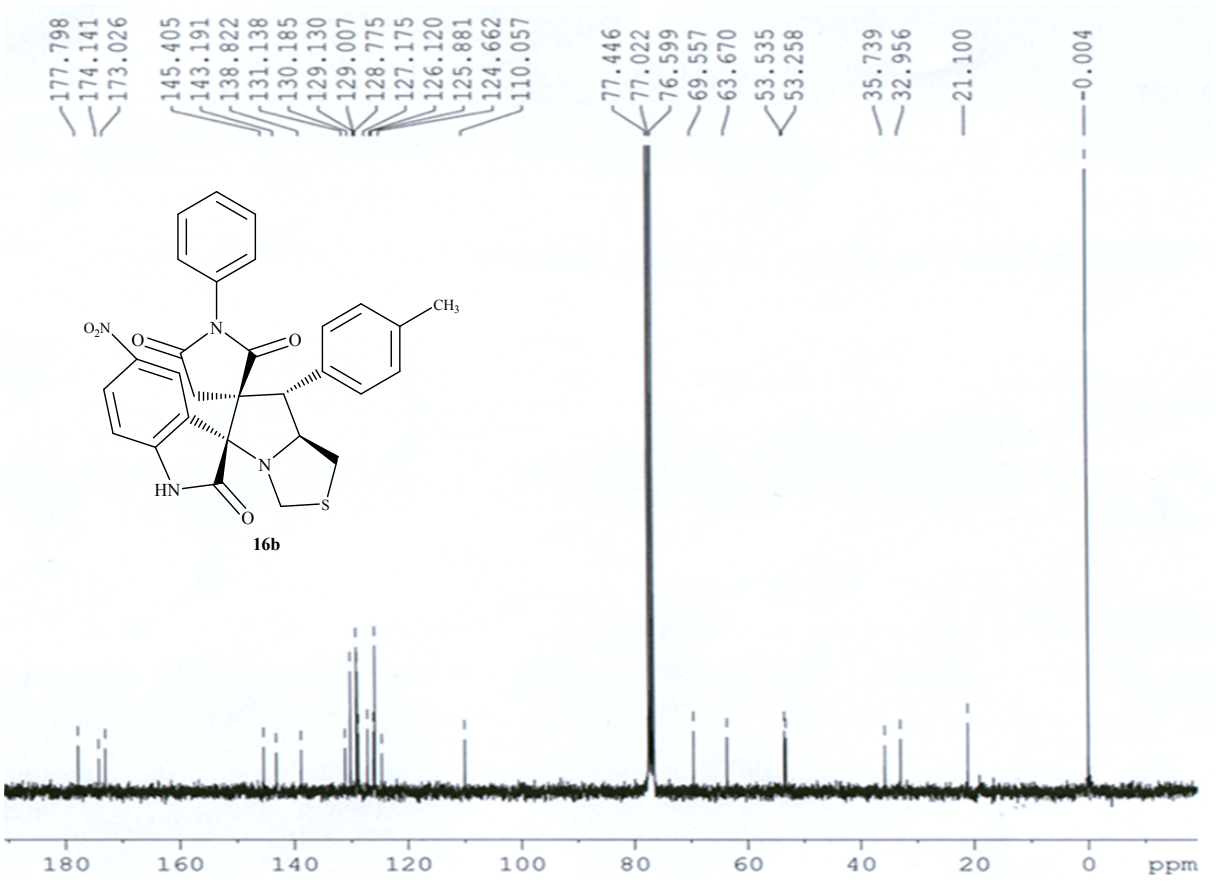


Fig. S28. ^{13}C NMR spectrum of **16b** in $CDCl_3$

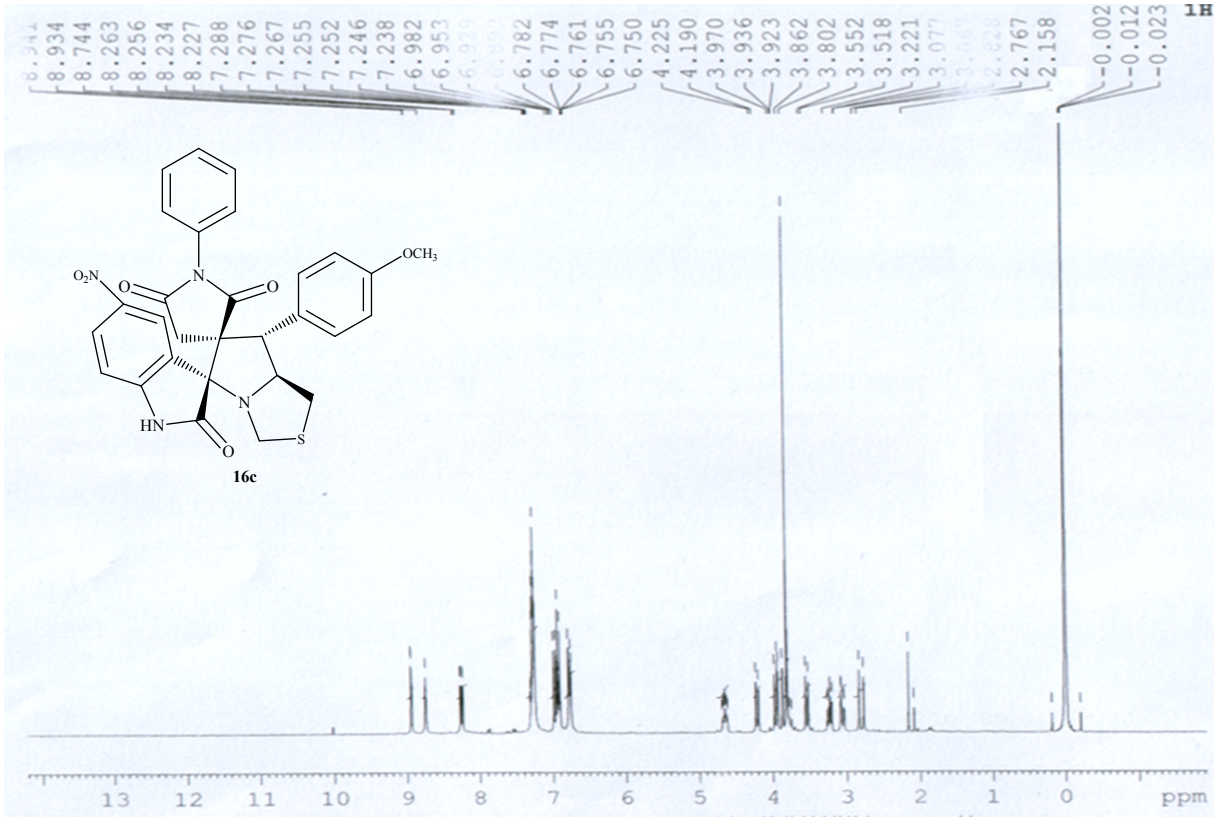


Fig. S29. ^{1}H NMR spectrum of **16c** in $CDCl_3$

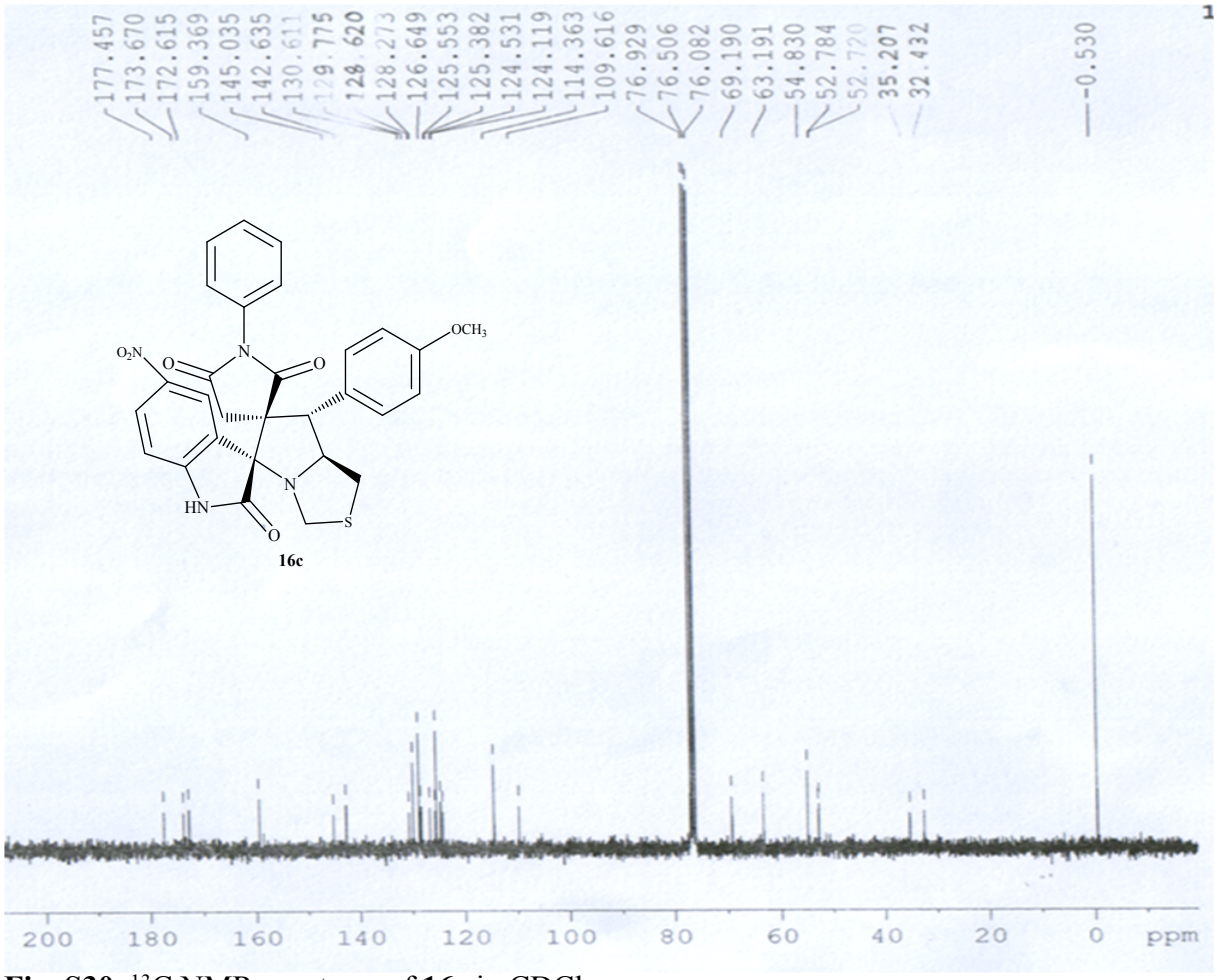


Fig. S30. ^{13}C NMR spectrum of **16c** in $CDCl_3$

Fig. S31. ^{1}H NMR spectrum of **16e** in $CDCl_3$

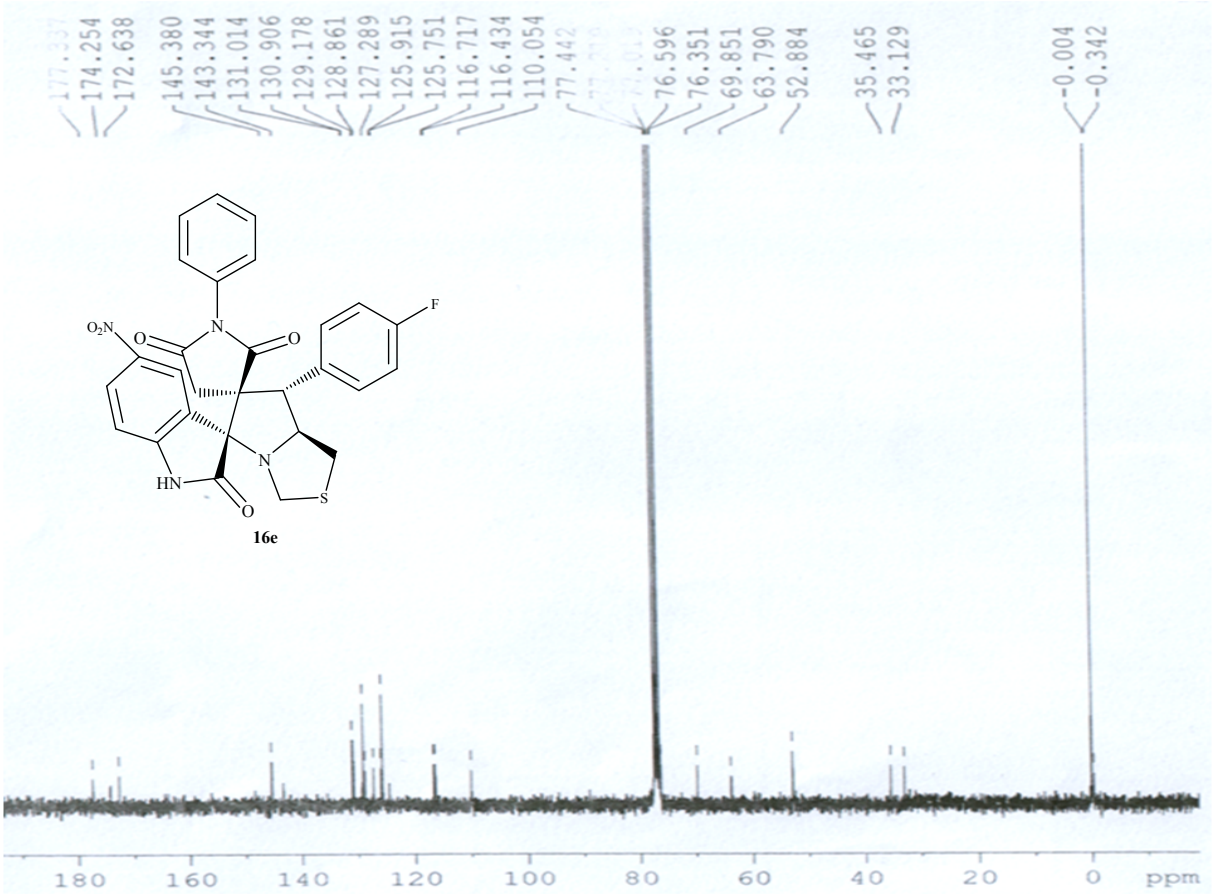


Fig. S32. ^{13}C NMR spectrum of **16e** in $CDCl_3$

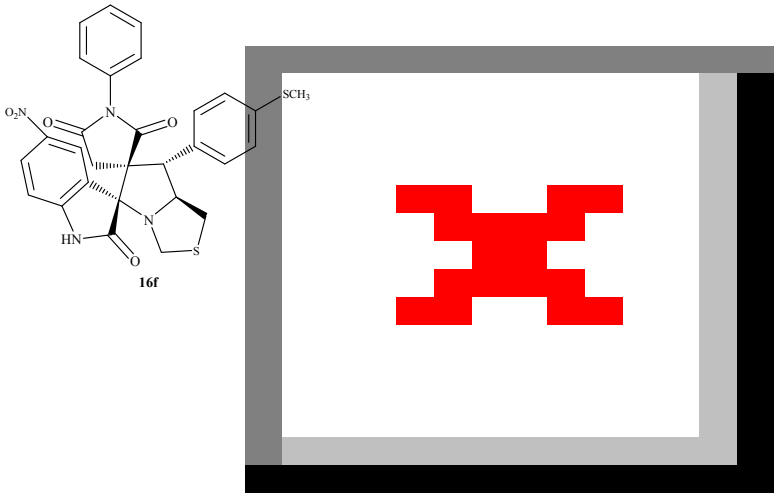


Fig. S33. ^{1}H NMR spectrum of **16f** in $CDCl_3$

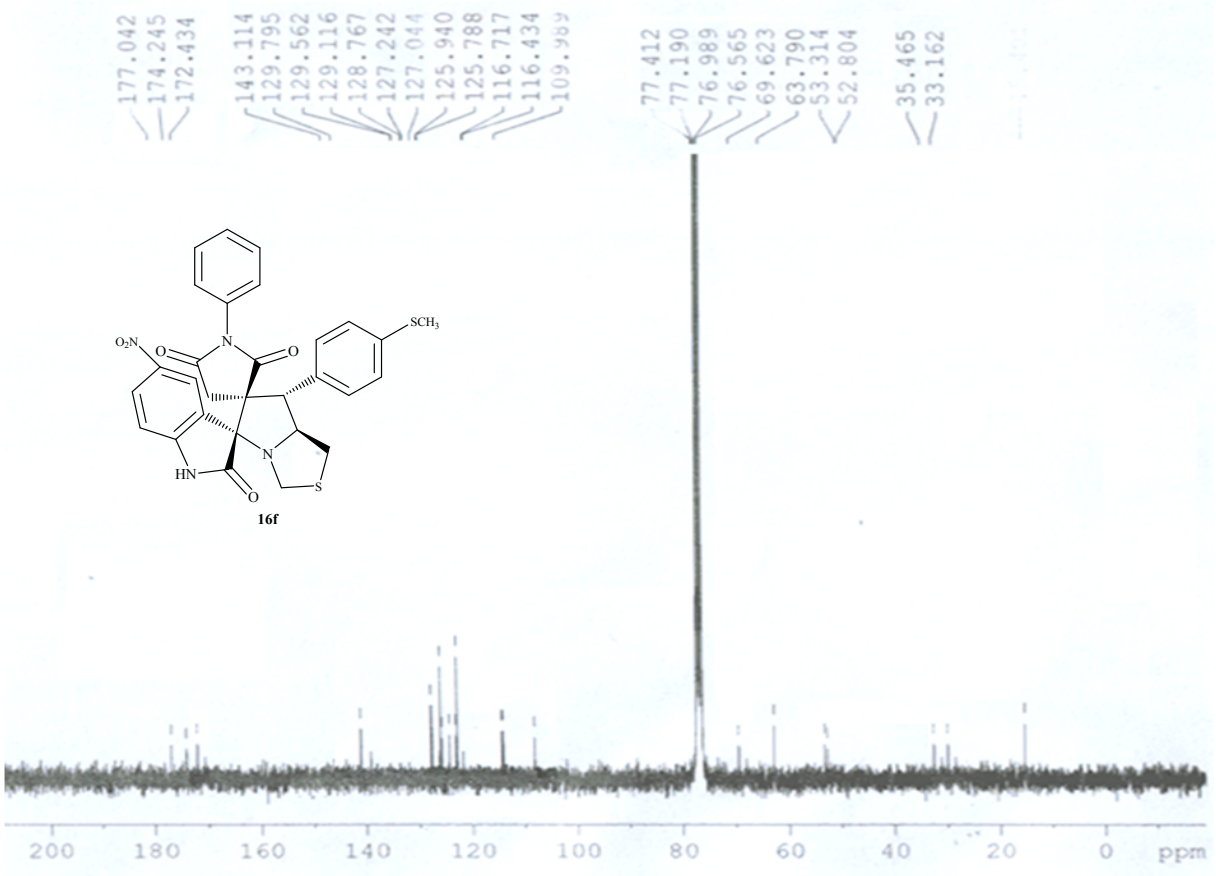


Fig. S34. ^{13}C NMR spectrum of **16f** in $CDCl_3$

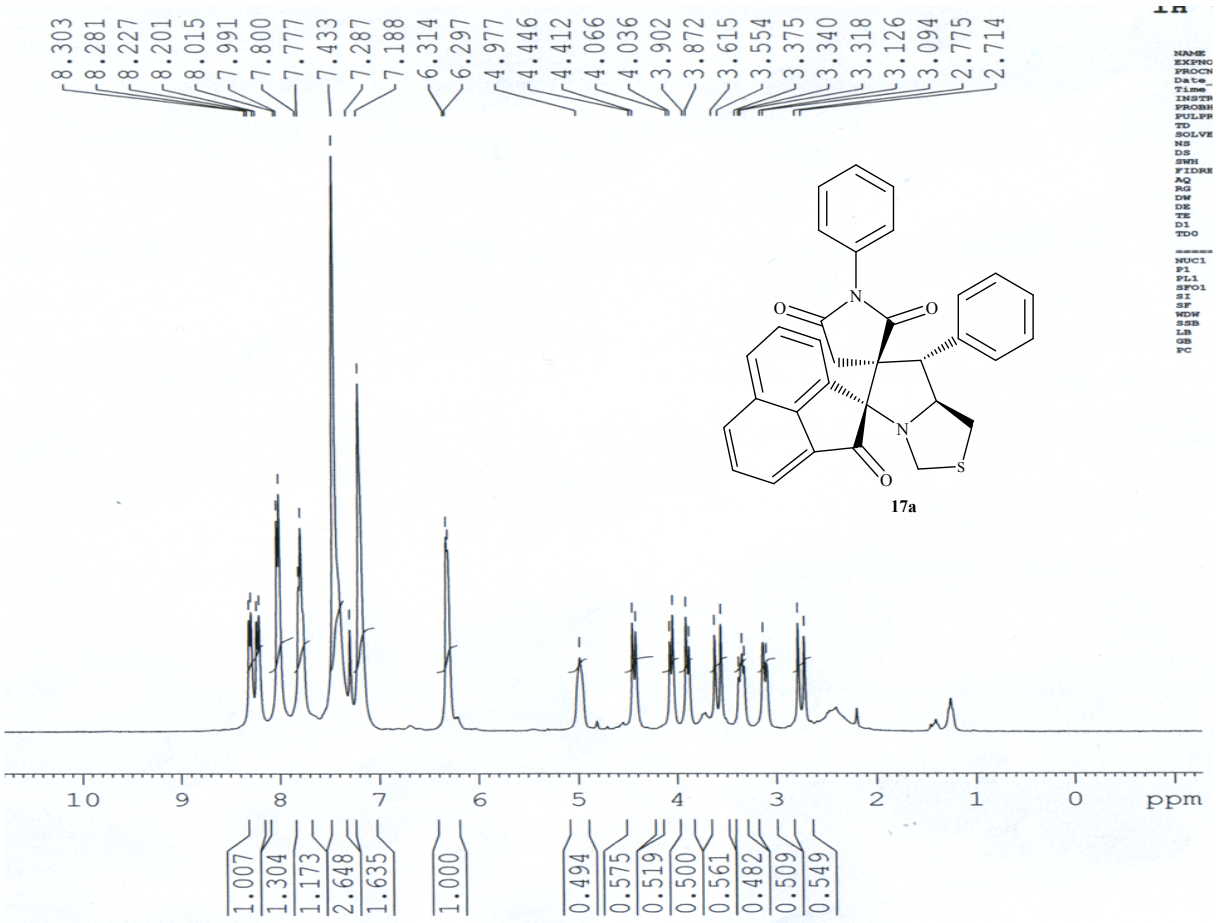


Fig. S35. ^{1}H NMR spectrum of **17a** in $CDCl_3$

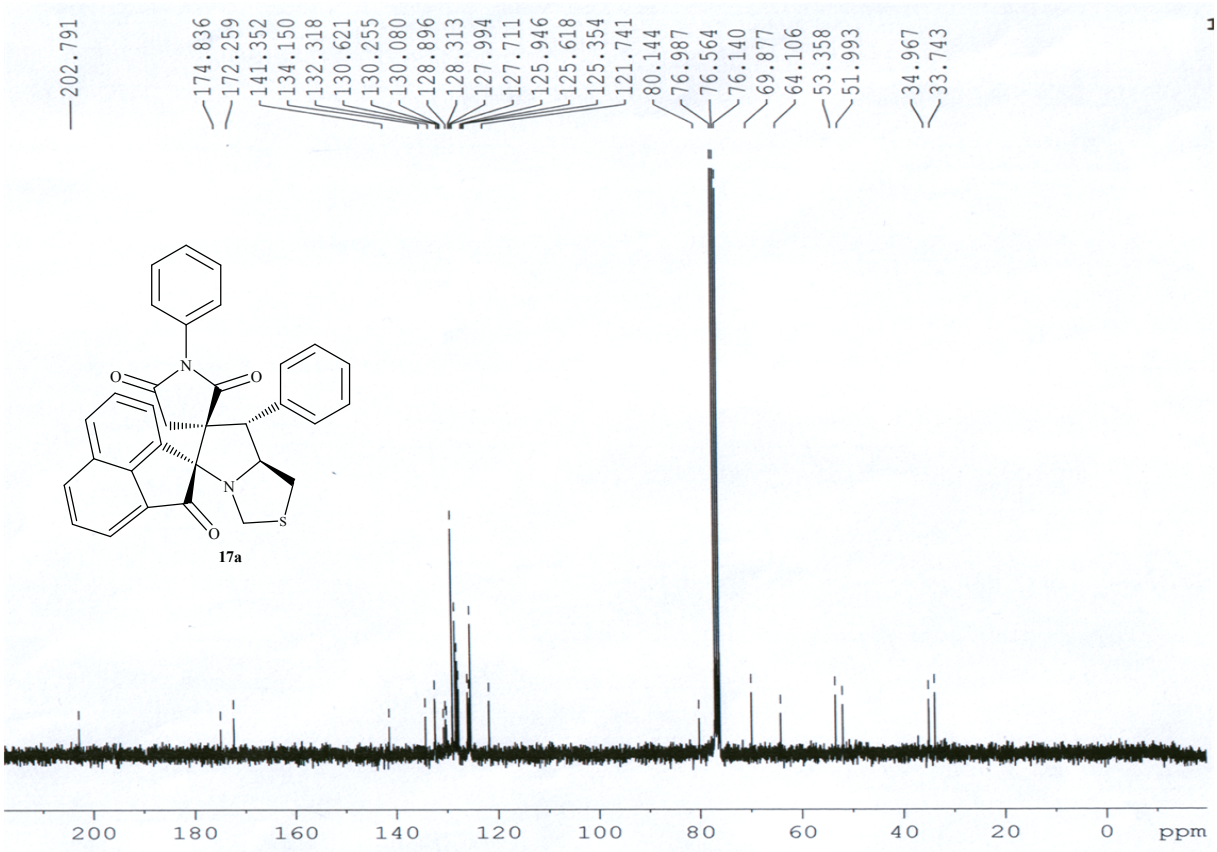


Fig. S36. ^{13}C NMR spectrum of **17a** in $CDCl_3$

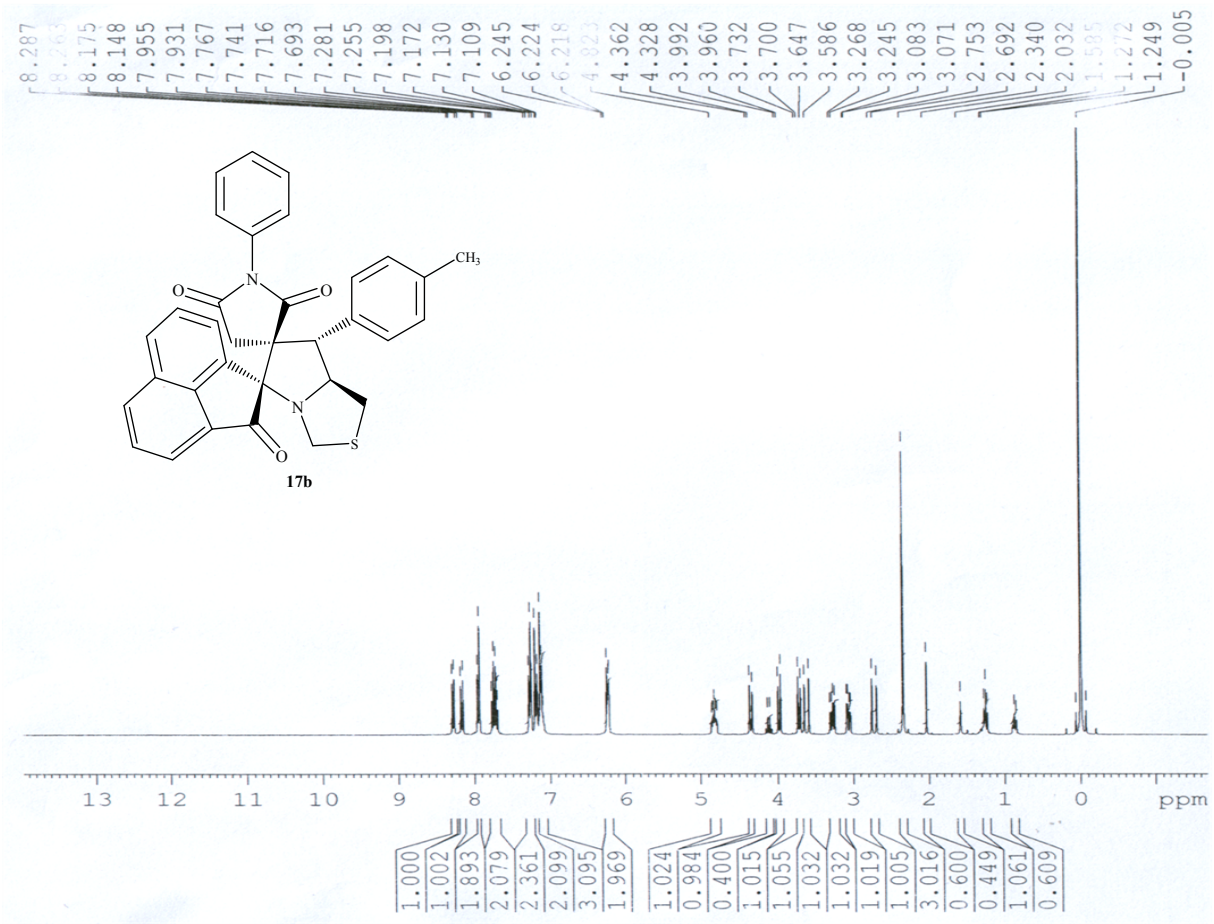


Fig. S37. ^{1}H NMR spectrum of **17b** in $CDCl_3$

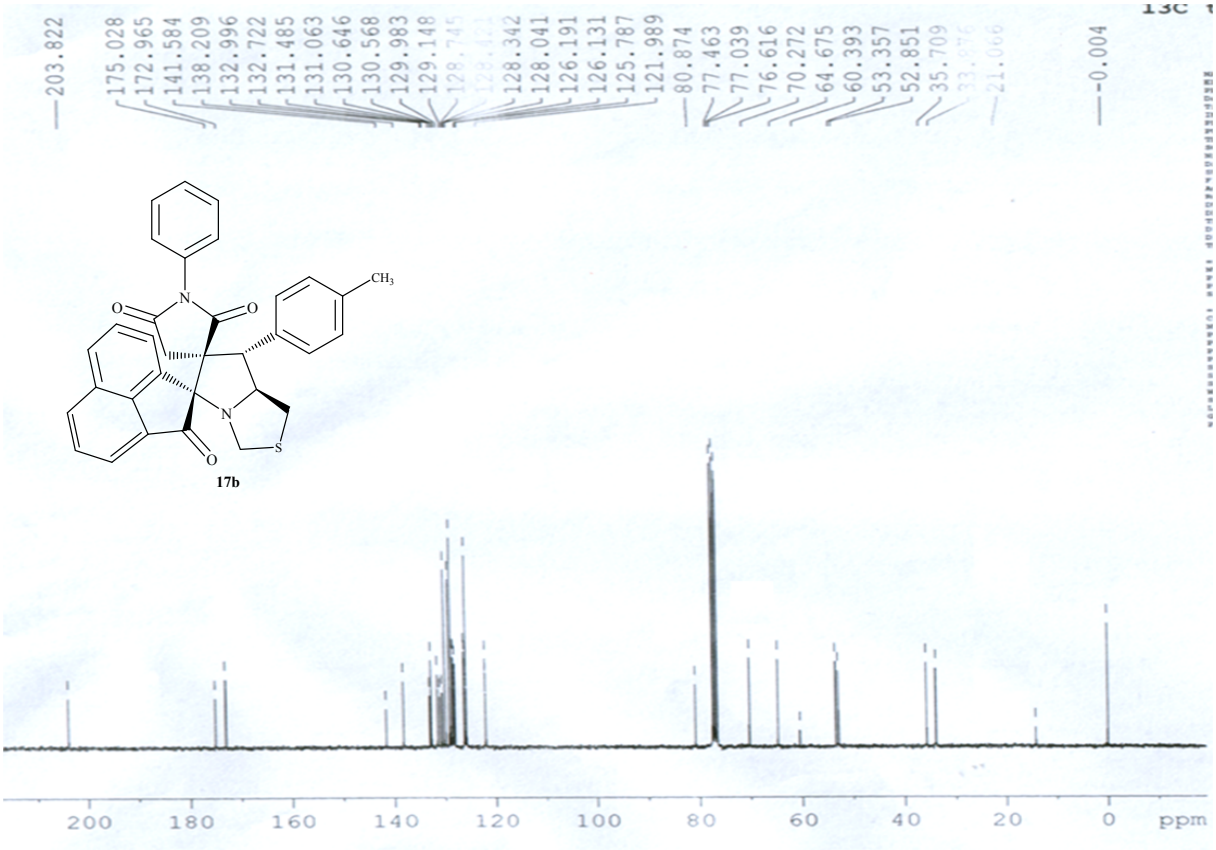


Fig. S38. ^{13}C NMR spectrum of **17b** in $CDCl_3$

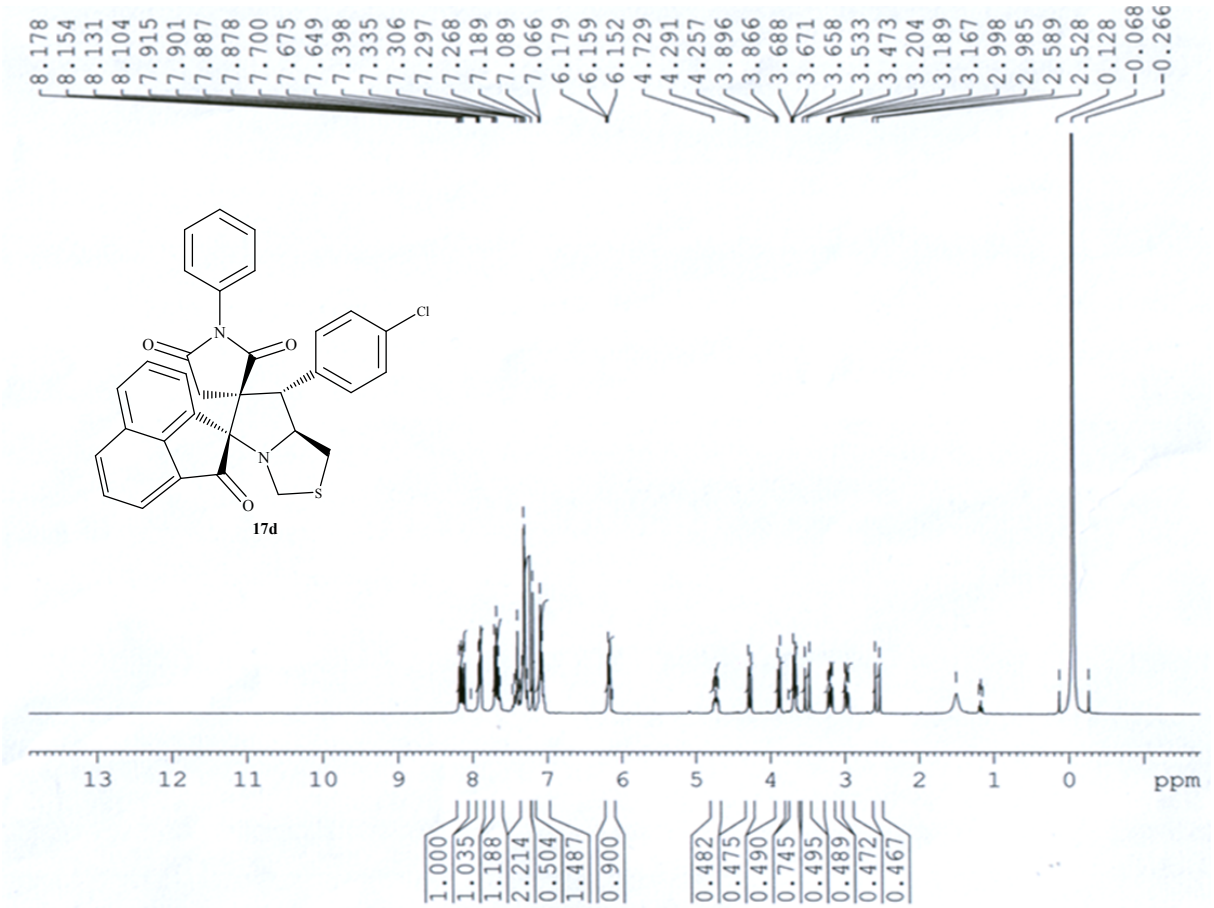


Fig. S39. ^{1}H NMR spectrum of **17d** in $CDCl_3$

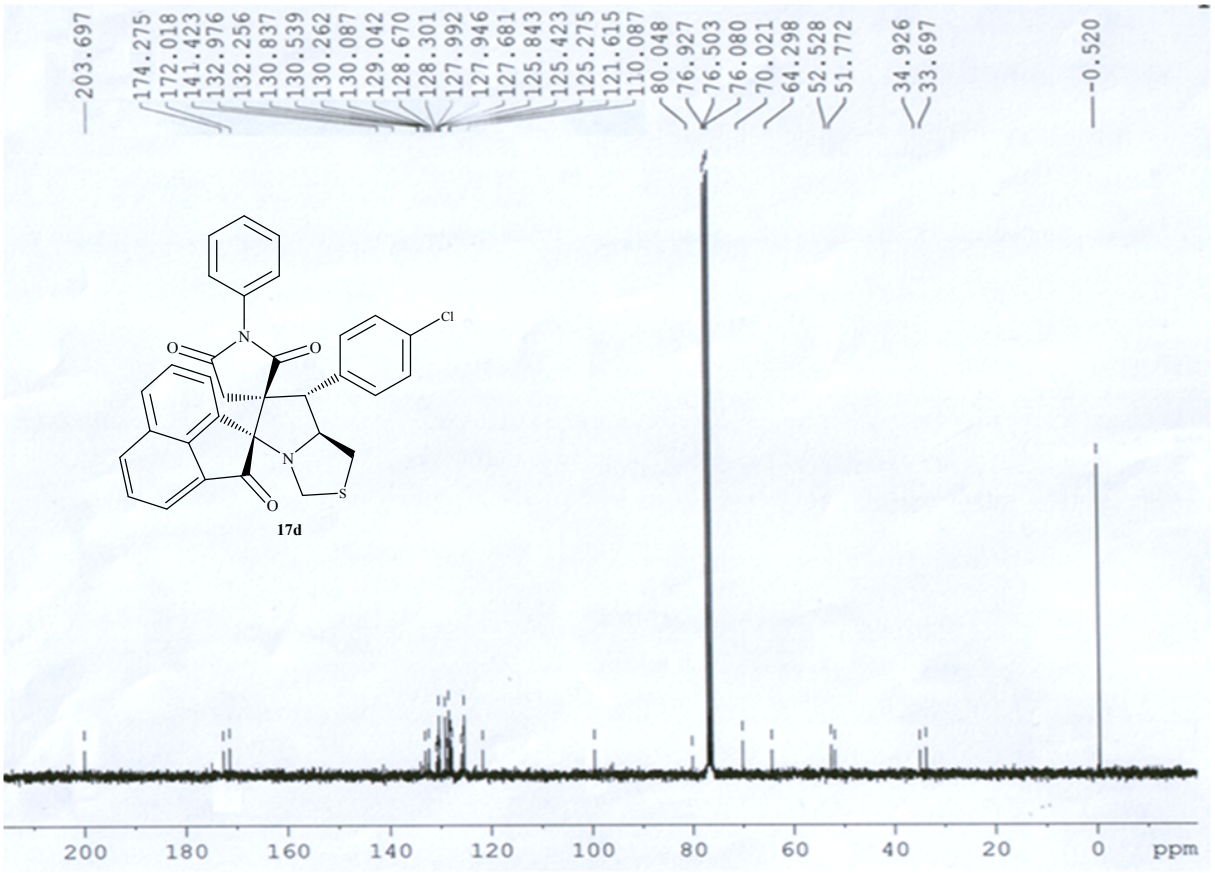


Fig. S40. ^{13}C NMR spectrum of **17d** in $CDCl_3$

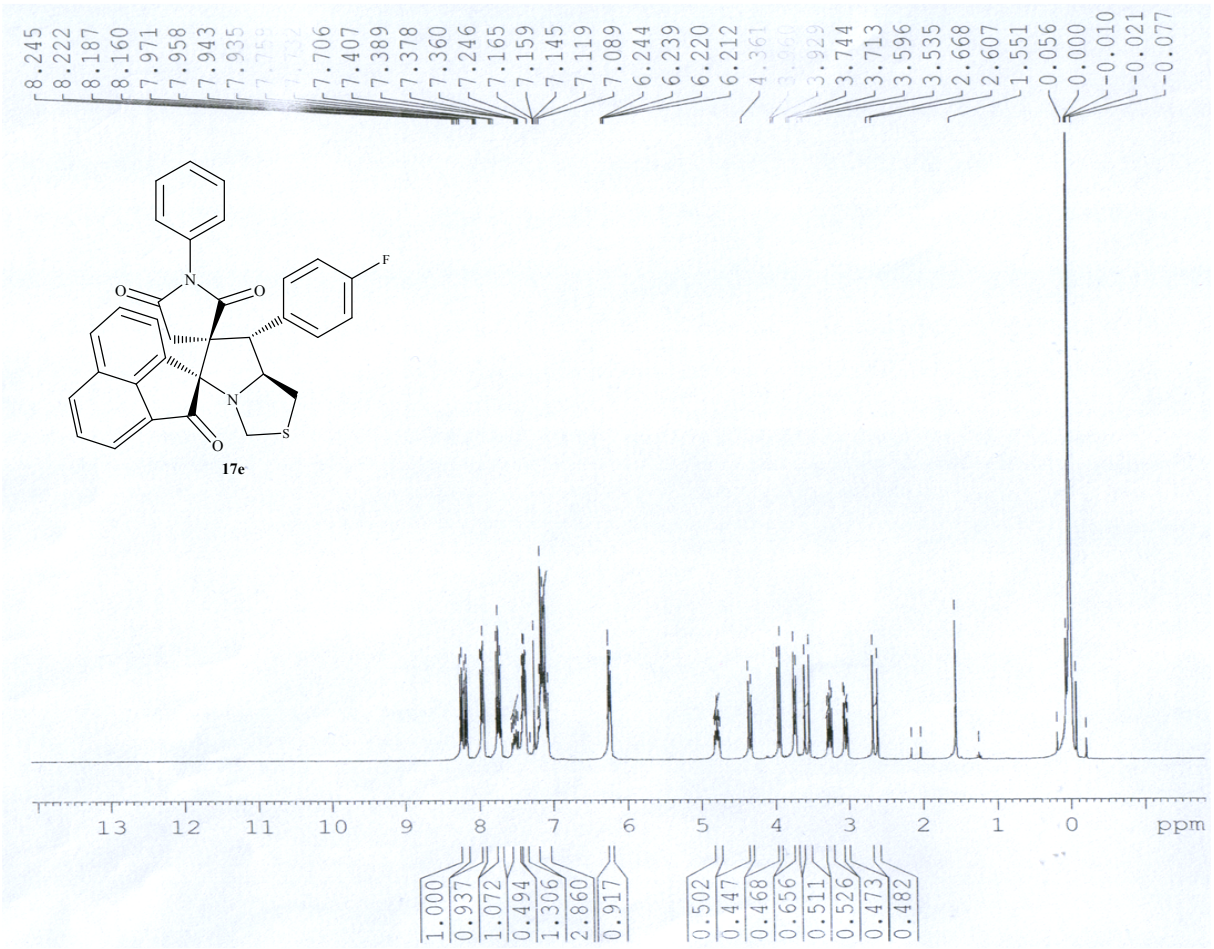


Fig. S41. ^{1}H NMR spectrum of **17e** in $CDCl_3$

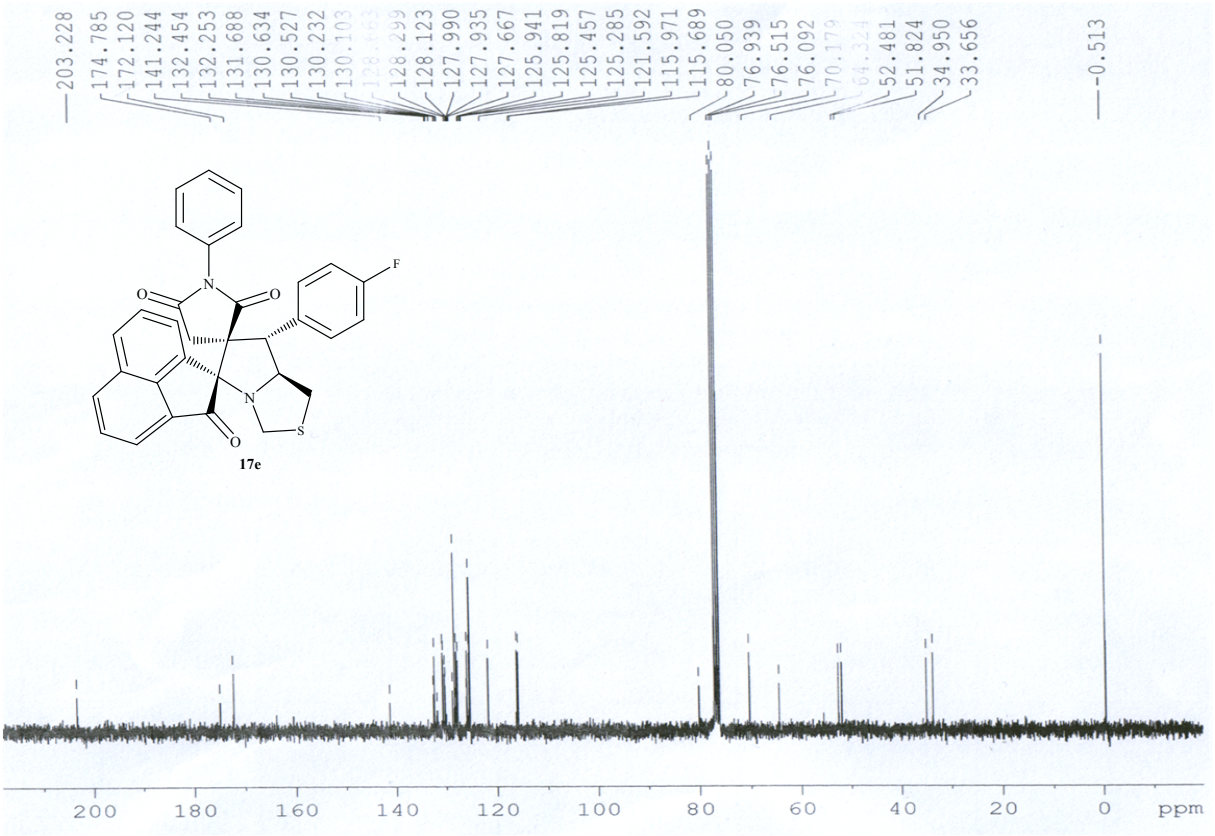


Fig. S42. ^{13}C NMR spectrum of **17e** in $CDCl_3$