

Fig S1. 4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5a**)

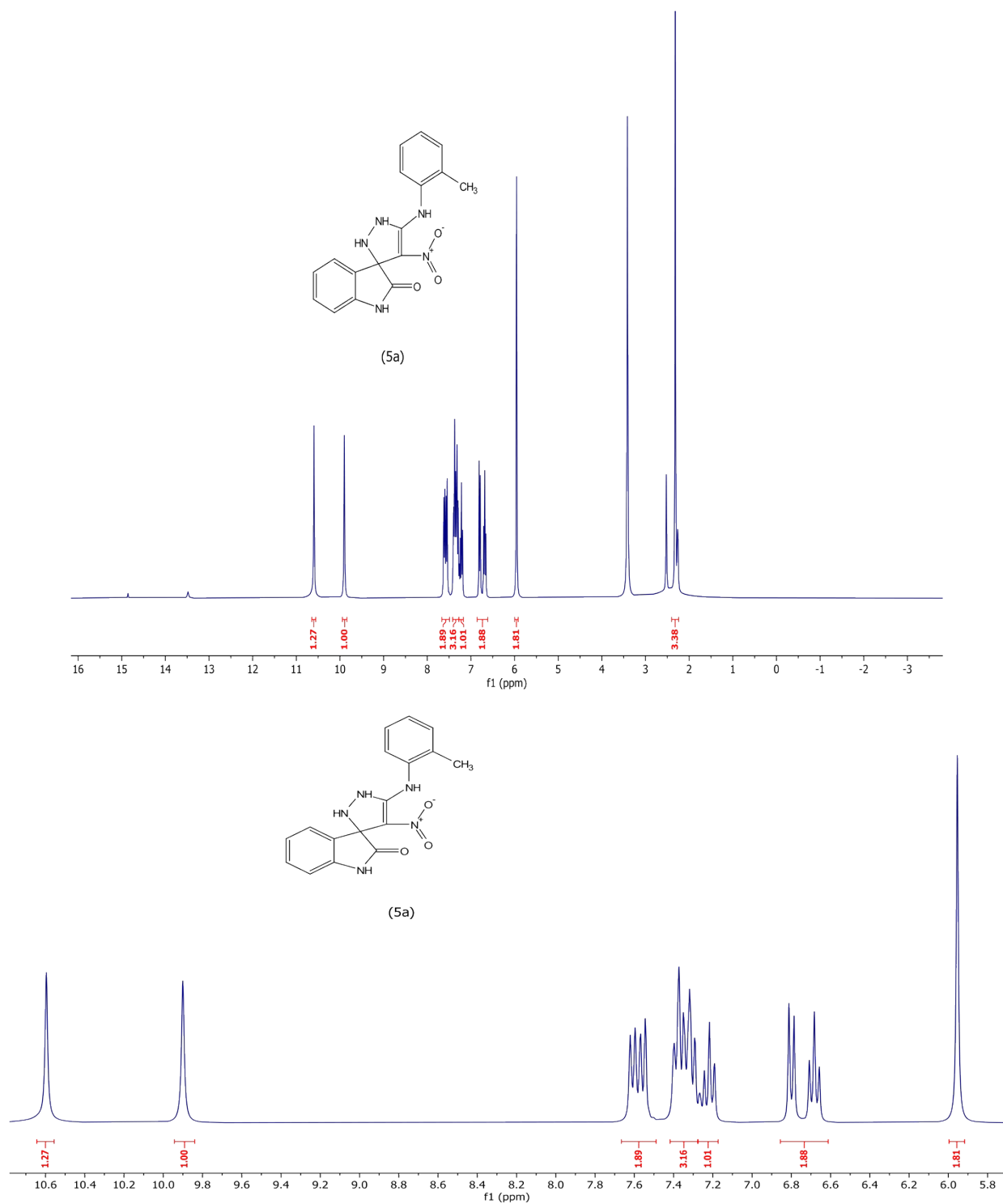


Fig S2. 4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5a**)

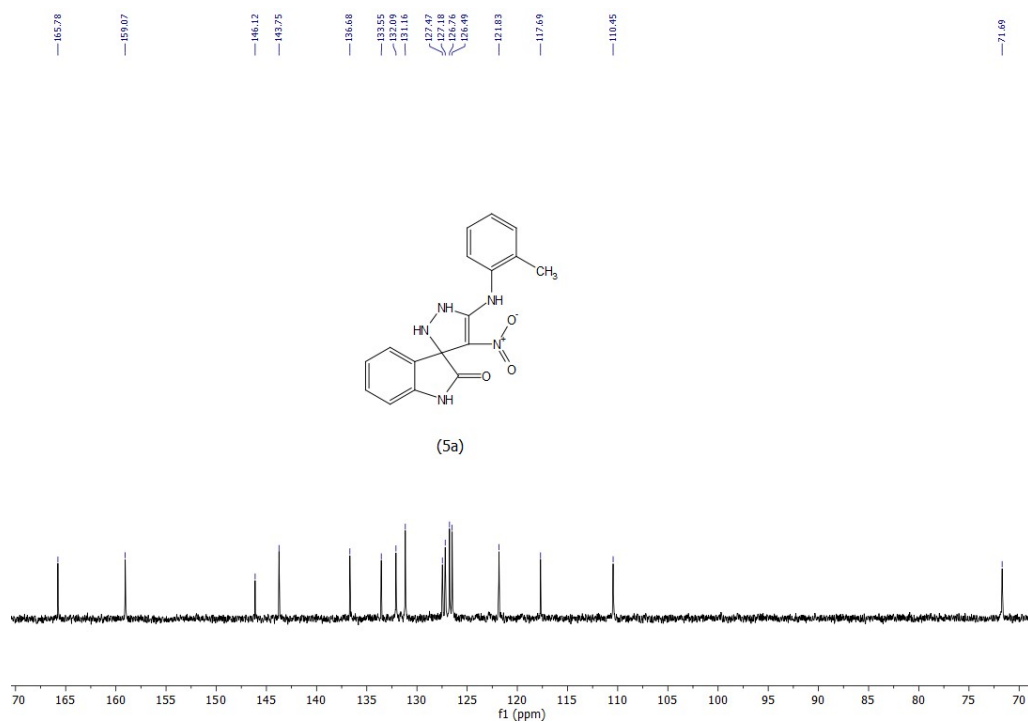
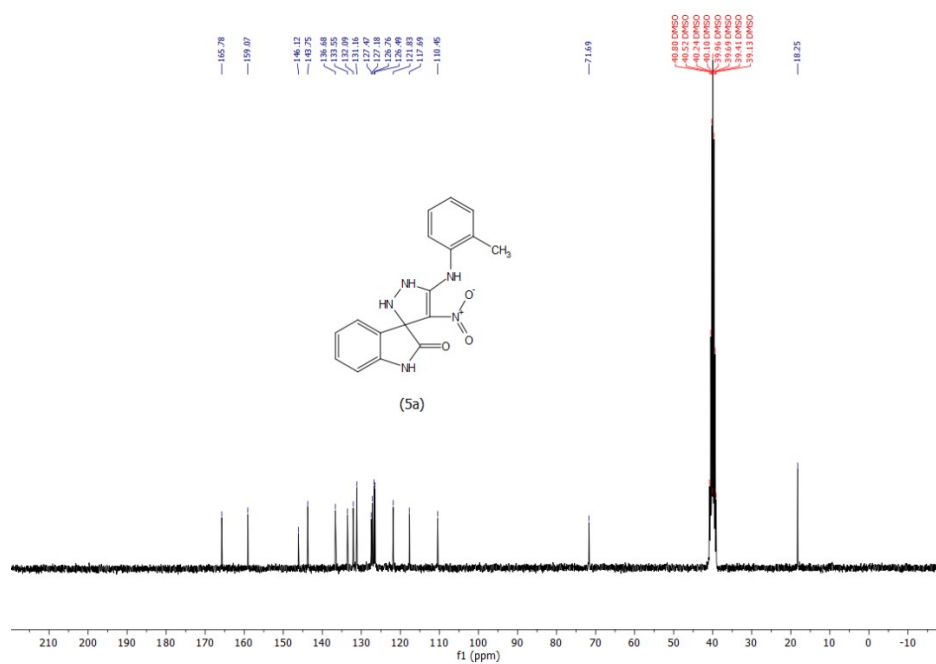
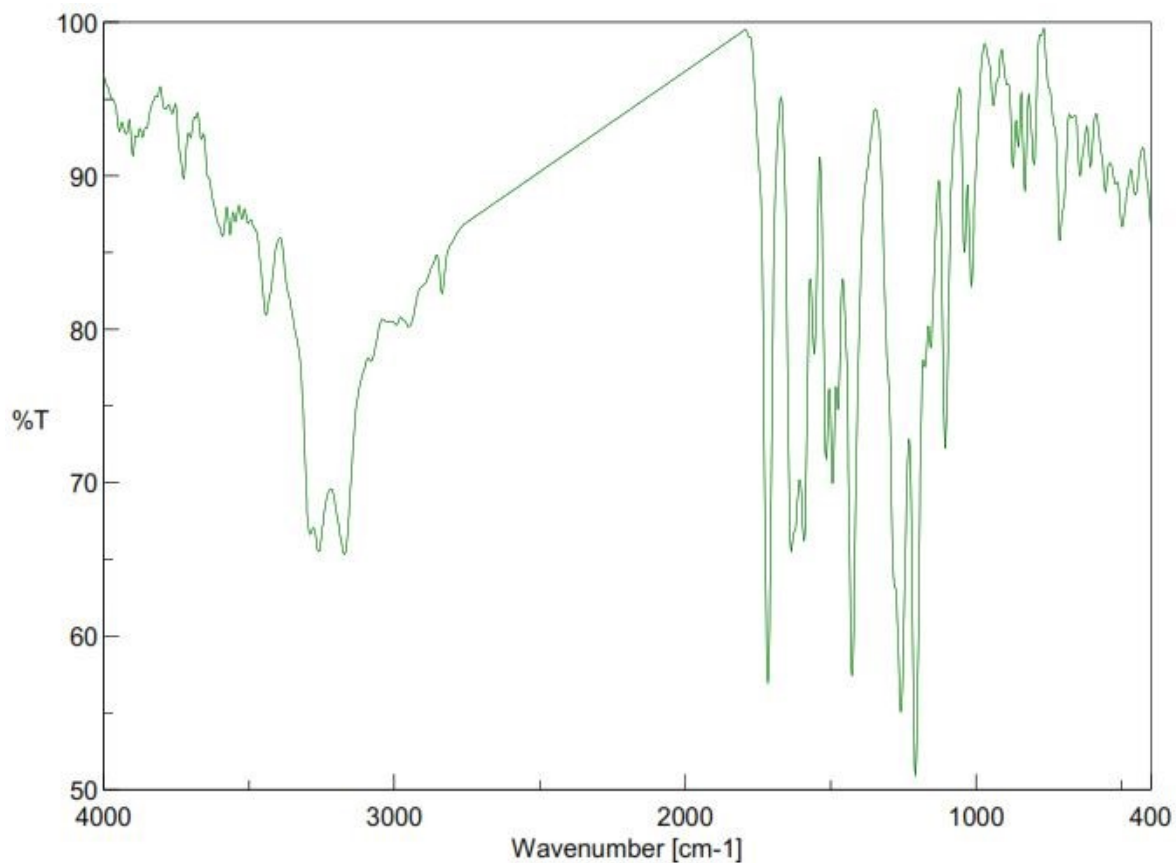


Fig S3. 4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5a**)



Chromatogram C:\EAS Clarity\WORK1\Data\2c 1402.5.14_1_2_2002 5_47_28 AM_052.PRM

Result Table (ESTD – 2c 1402.5.14_1_2_2002 5_47_28 AM_052 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.320	1252.808	0.632	20.93	Refer	Nitrogen	0.137
3	2.457	9168.202	1.922	60.88	Refer	Carbon	1.000
4	9.797	2310.472	0.146	4.64	Refer	Hydrogen	0.252
Total			3.008	86.45			

CHN for C₁₇H₁₅N₅O₃ (**5a**)

Fig S4. 4'-nitro-5'-(p-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5b**)

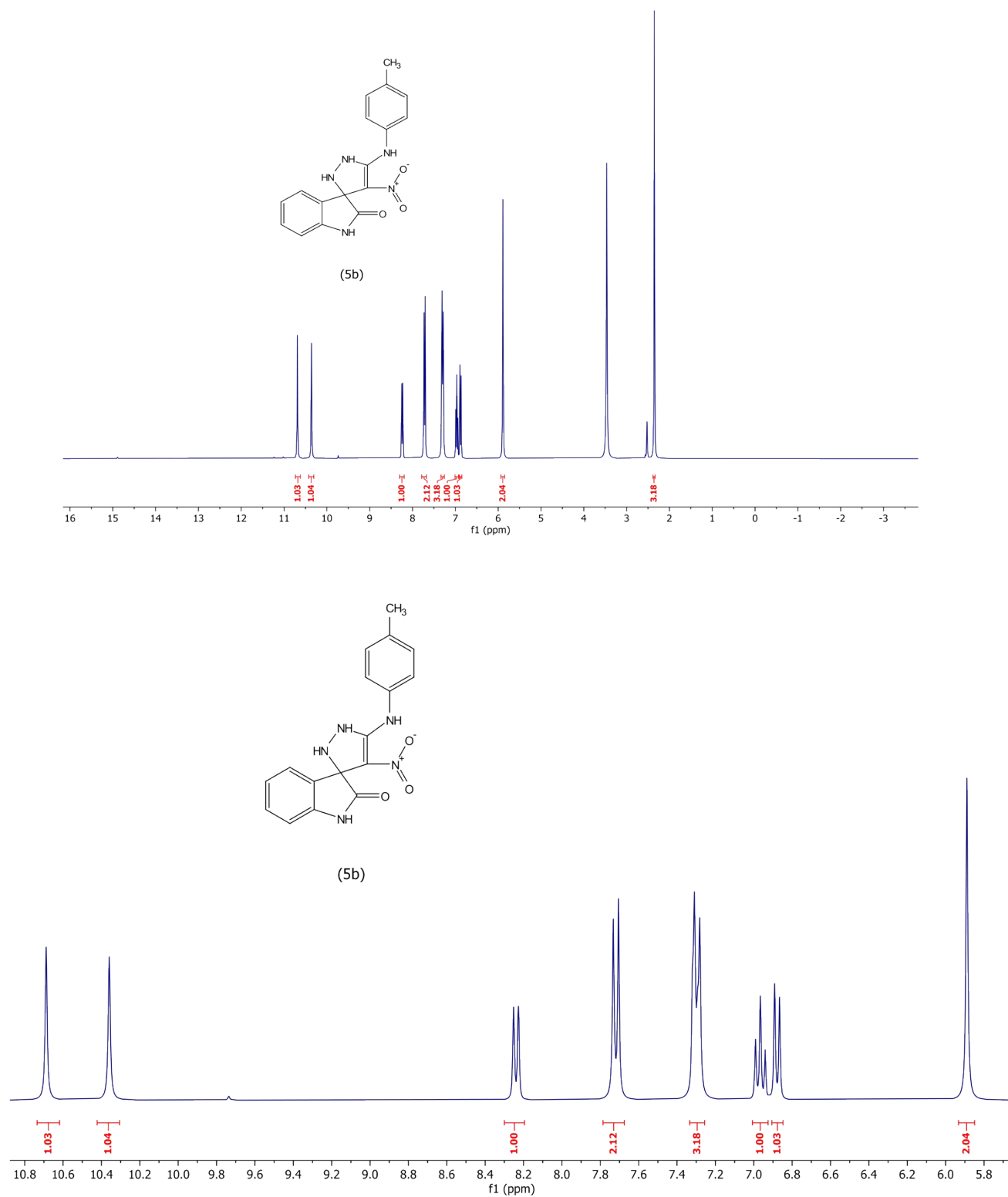


Fig S5. 4'-nitro-5'-(p-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5b**)

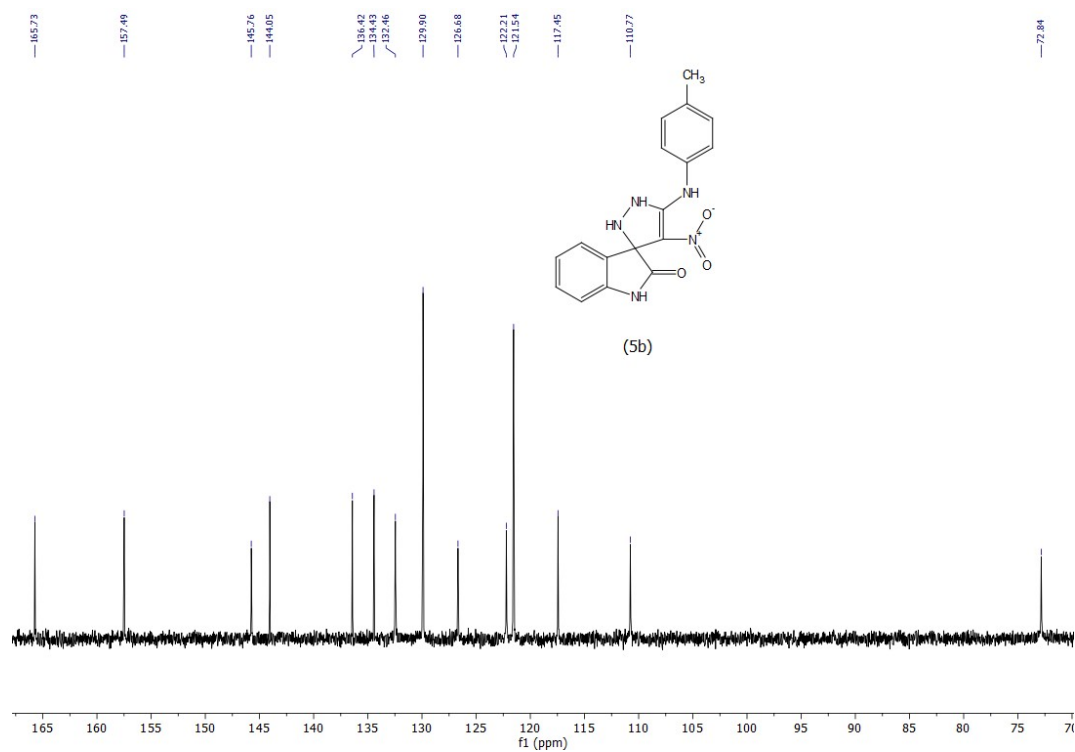
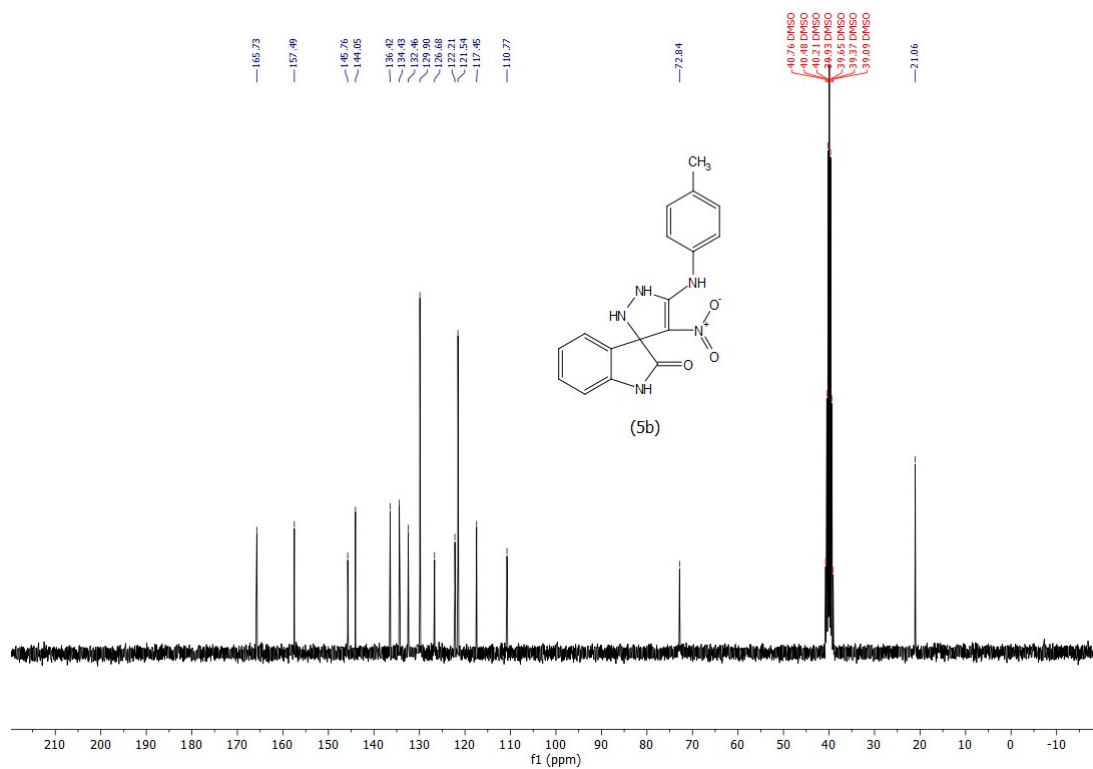


Fig S6. 4'-nitro-5'-(p-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5b**)

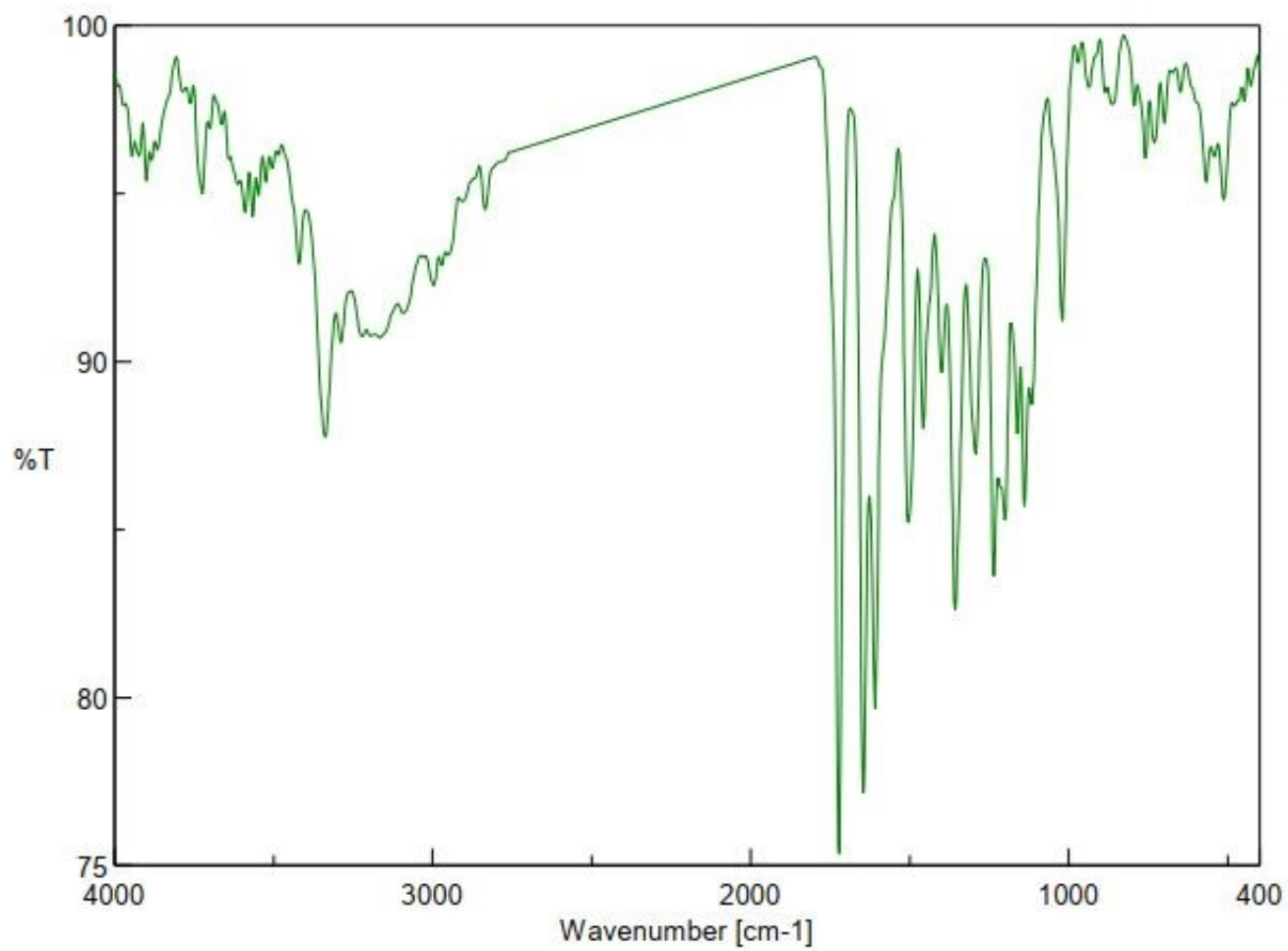


Fig S7. 5'-((4-hydroxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5c**)

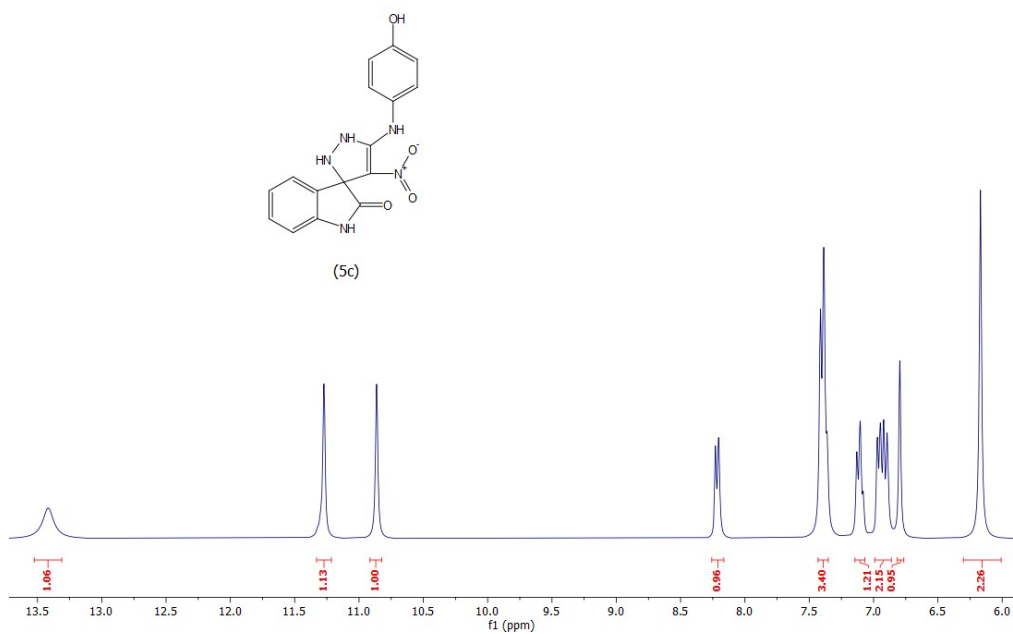
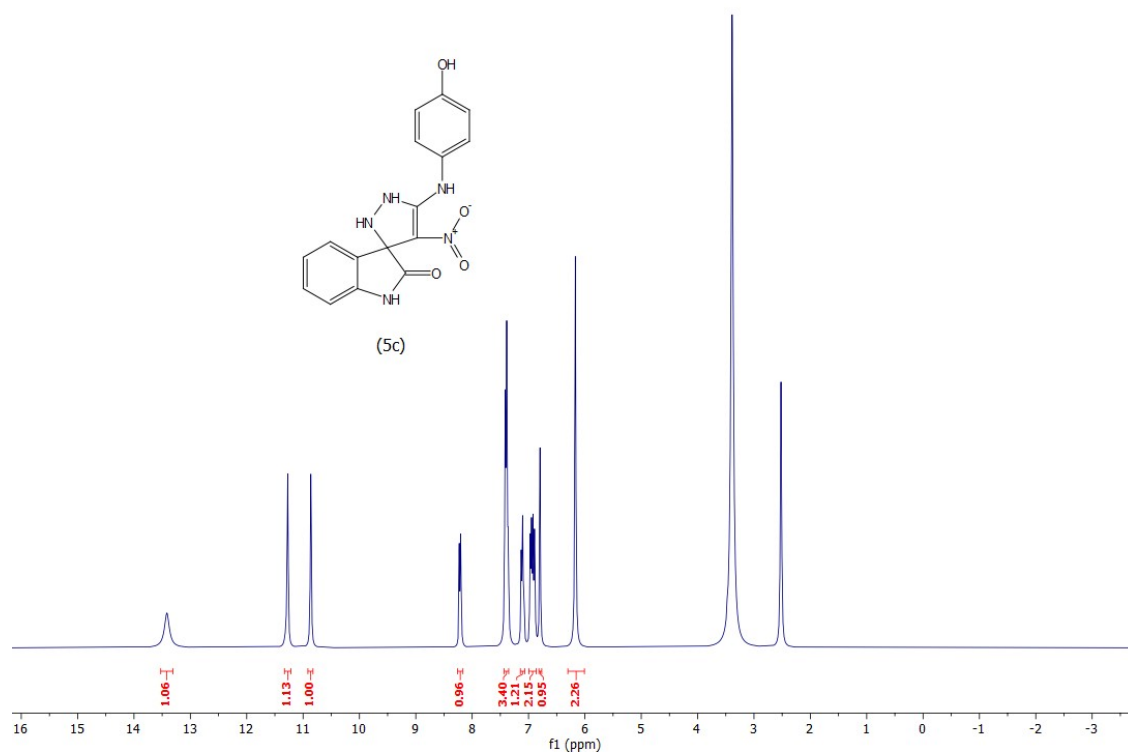


Fig S8. 5'-((4-hydroxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5c**)

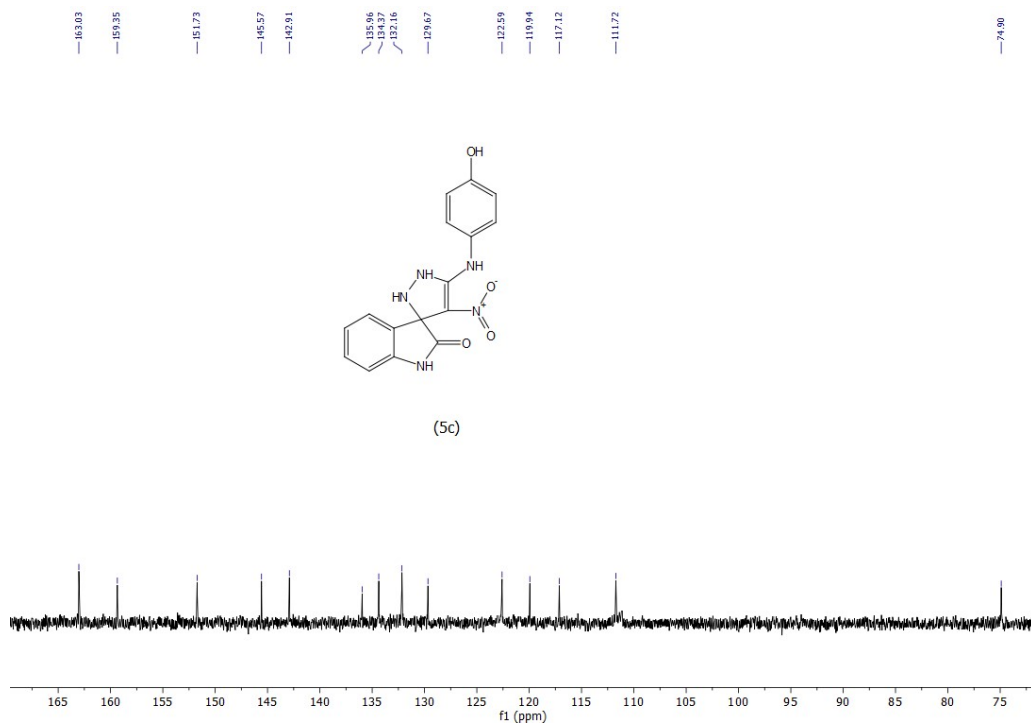
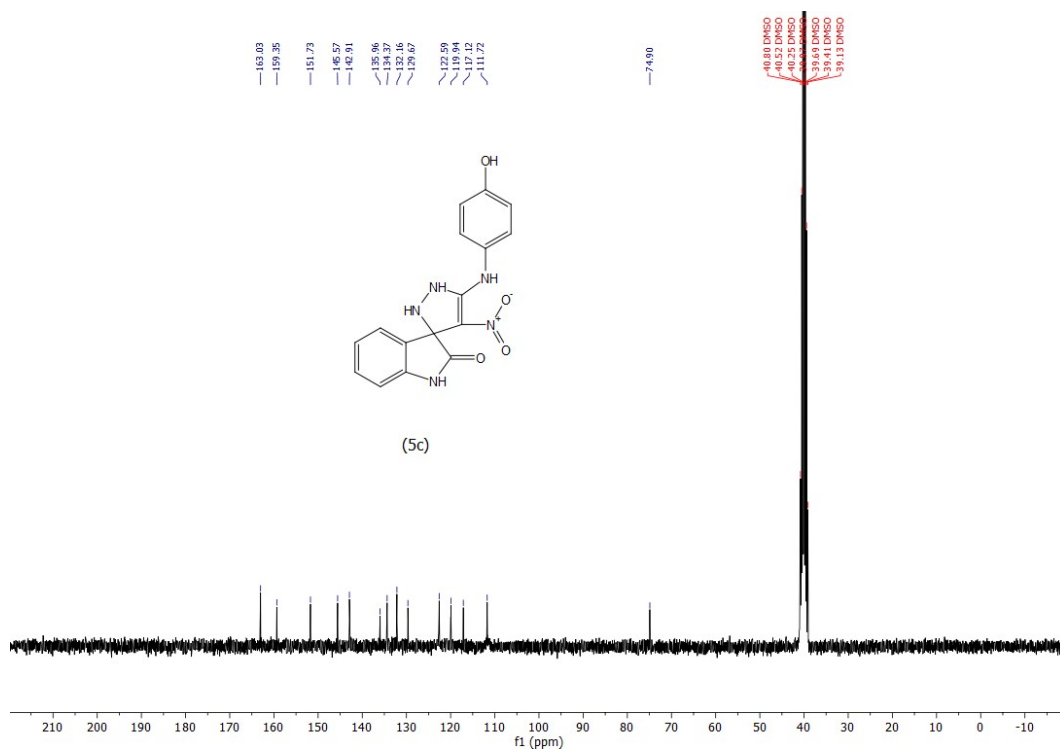
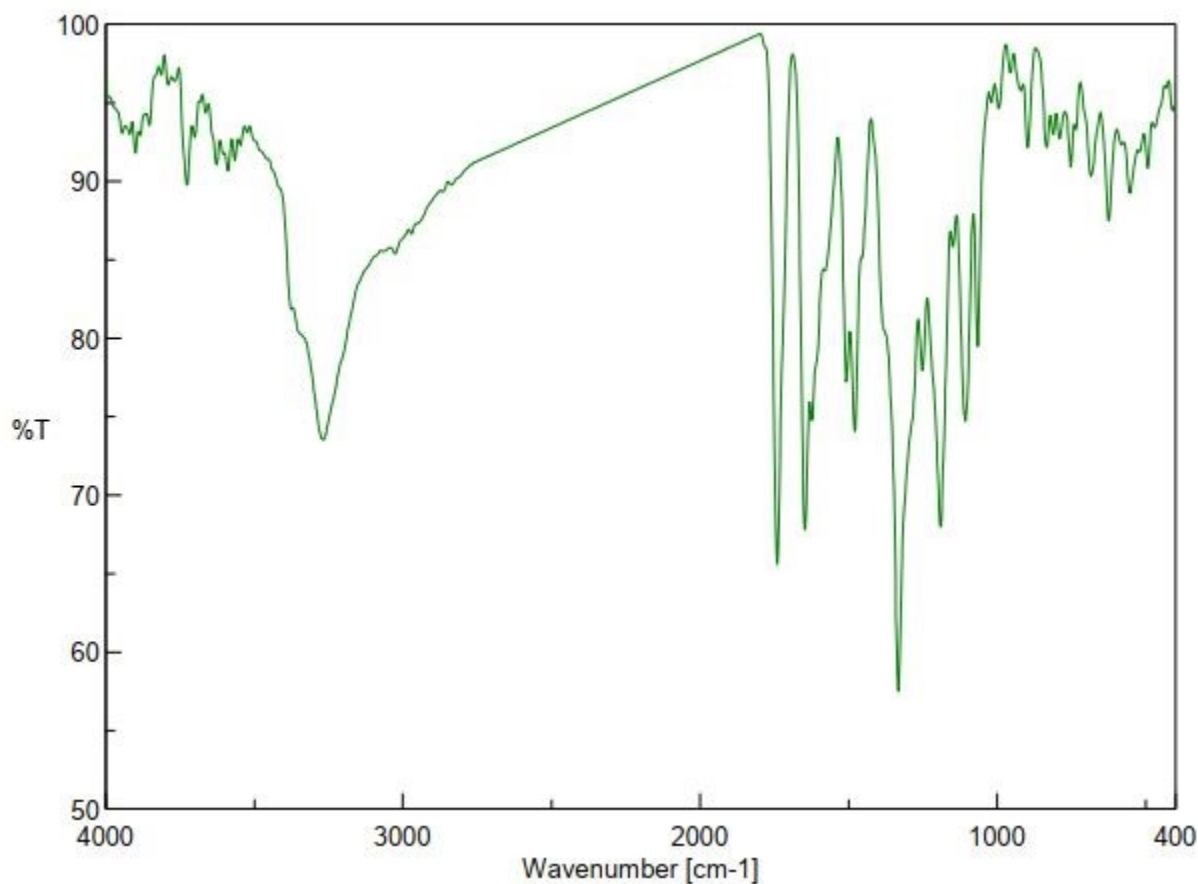


Fig S9. 5'-((4-hydroxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5c**)



Chromatogram C:\EAS Clarity\WORK1\Data\2h 1402.5.15_1_2_2002 3_54_00 AM_061.PRM

Result Table (ESTD - 2h 1402.5.15_1_2_2002 3_54_00 AM_061 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.317	878.660	0.433	20.85	Refer	Nitrogen	0.146
3	2.563	4114.128	0.761	56.21	Refer	Carbon	1.000
4	10.740	1035.756	0.062	3.65	Refer	Hydrogen	0.227
Total			1.858	80.73			

CHN for C₁₆H₁₃N₅O₄ (**5c**)

Fig S10. 5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5d**)

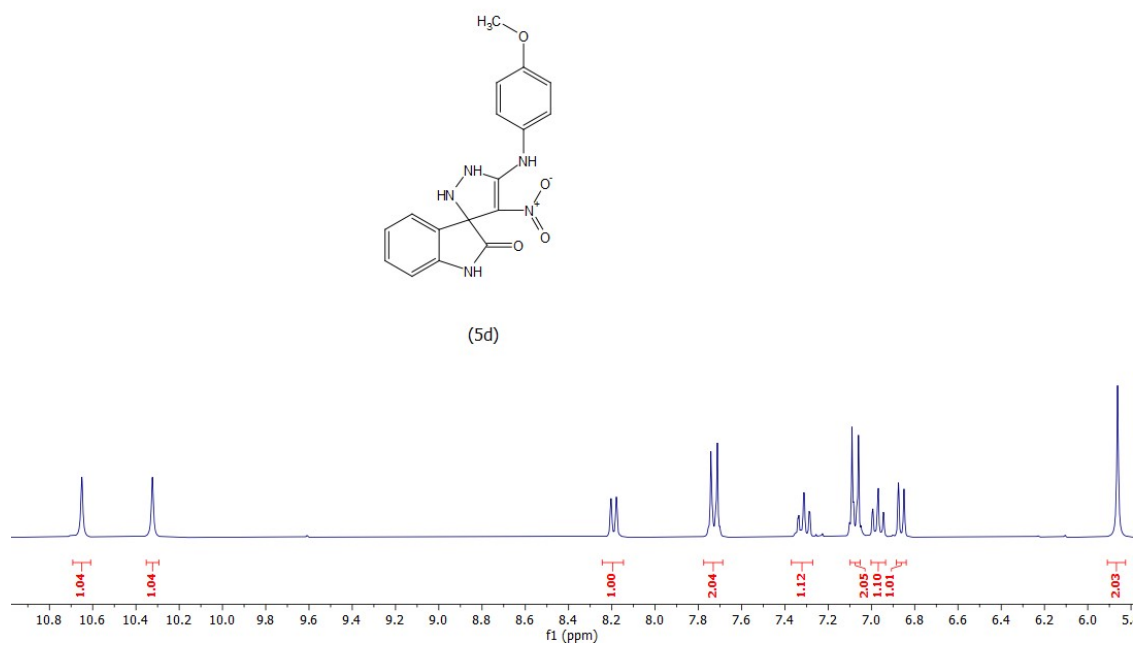
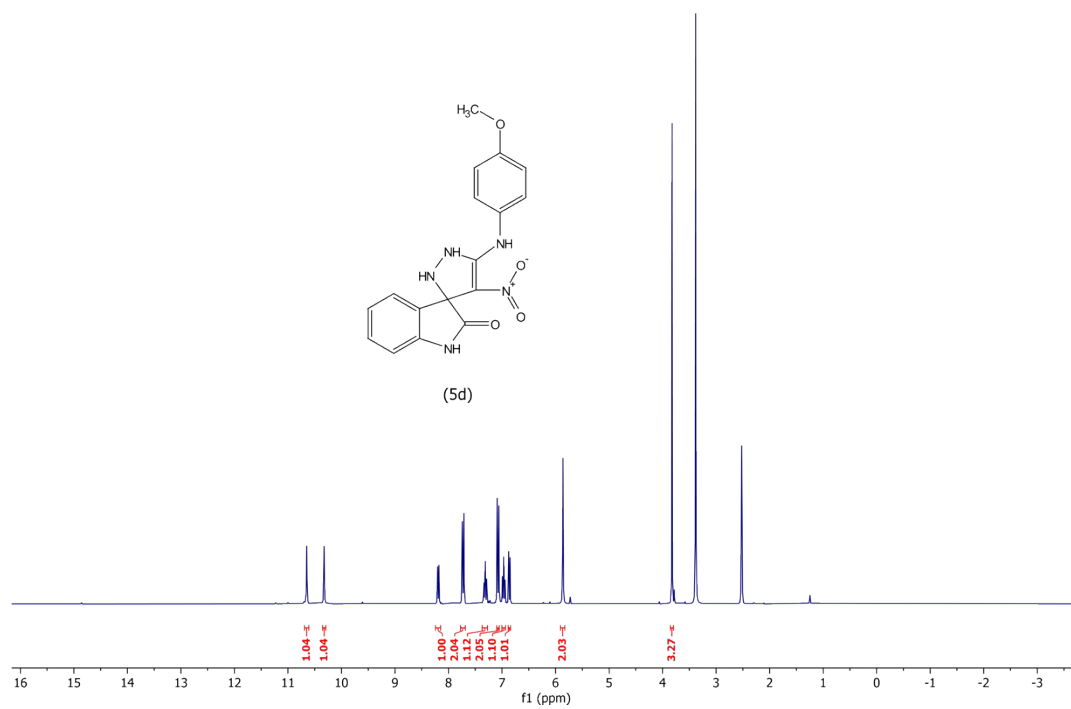


Fig S11. 5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5d**)

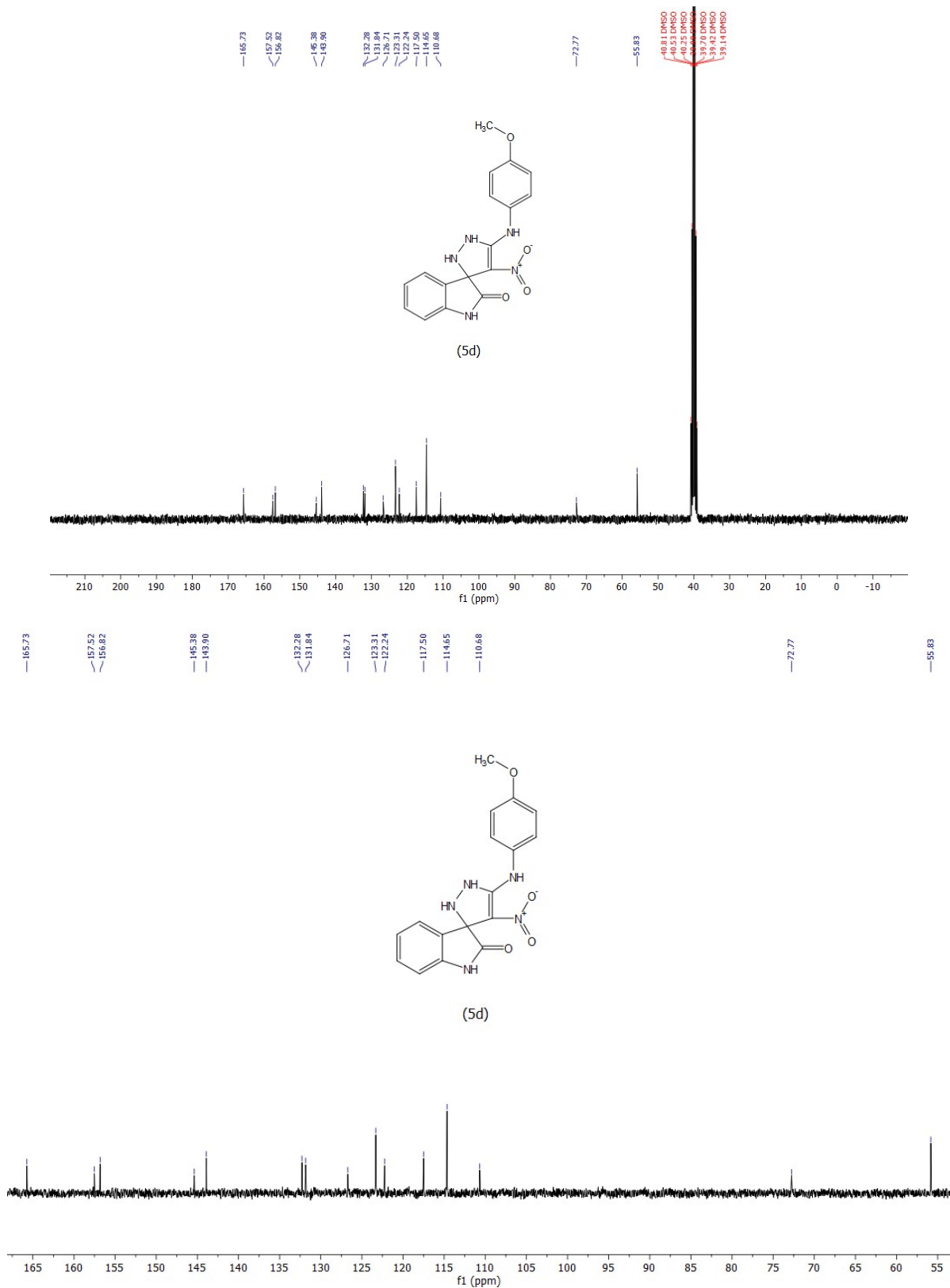
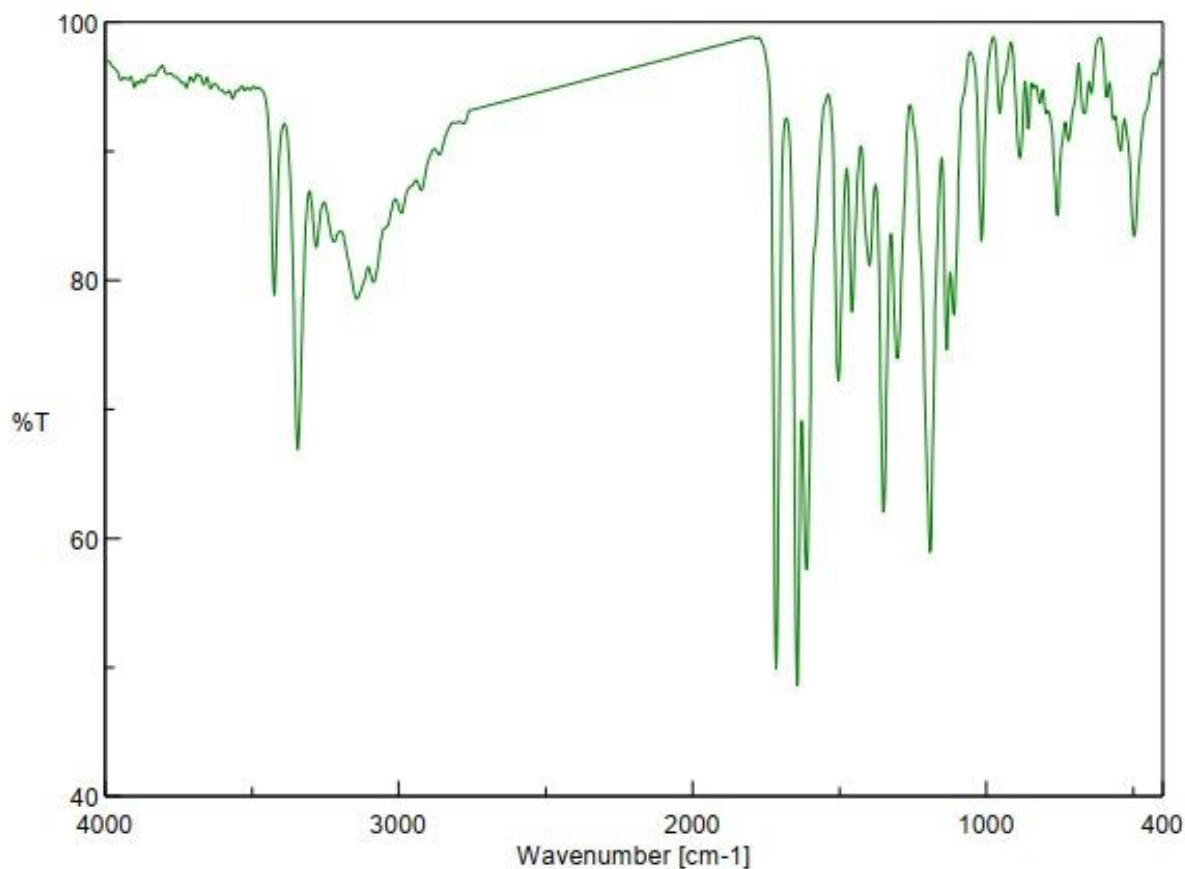


Fig S12. 5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5d**)



Chromatogram C:\EAS Clarity\WORK1\Data\2a 1402.5.14_1_1_2002 3_17_27 AM_047.PRM

Result Table (ESTD - 2a 1402.5.14_1_1_2002 3_17_27 AM_047 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.297	559.797	0.264	19.66	Refer	Nitrogen	0.130
3	2.533	3814.657	0.699	57.53	Refer	Carbon	1.000
4	10.810	907.988	0.054	4.10	Refer	Hydrogen	0.238
Total			1.370	81.29			

CHN for C₁₇H₁₅N₅O₄ (**5d**)

Fig S13. 5'-((3,4-dimethylphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5e**)

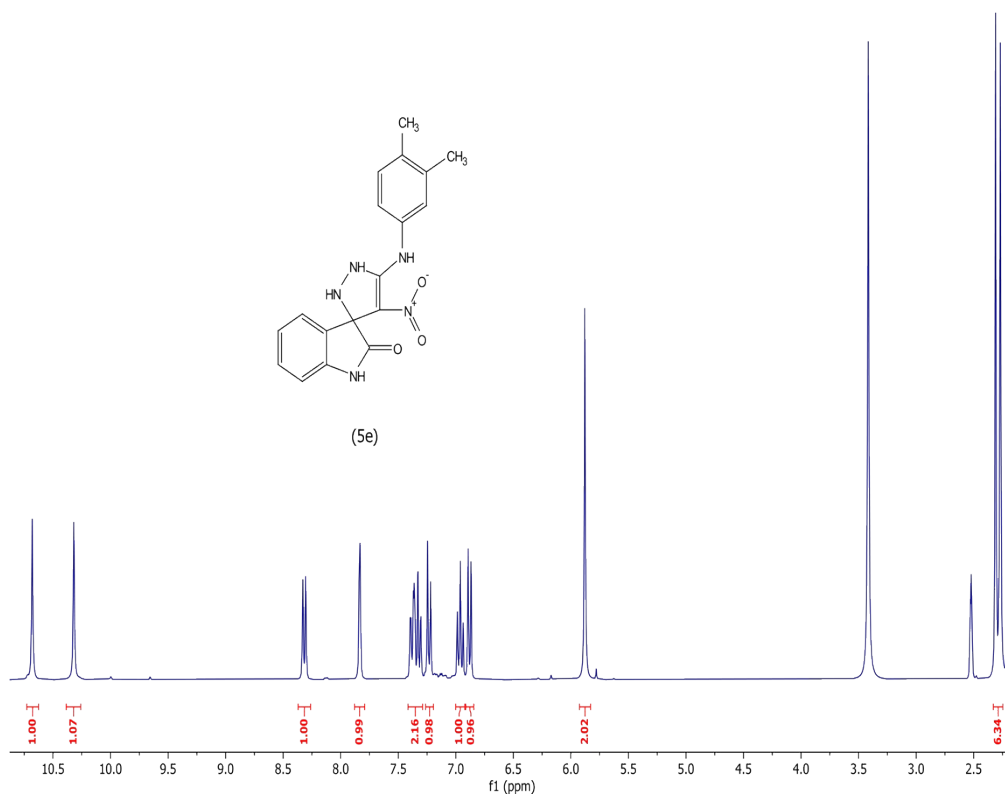
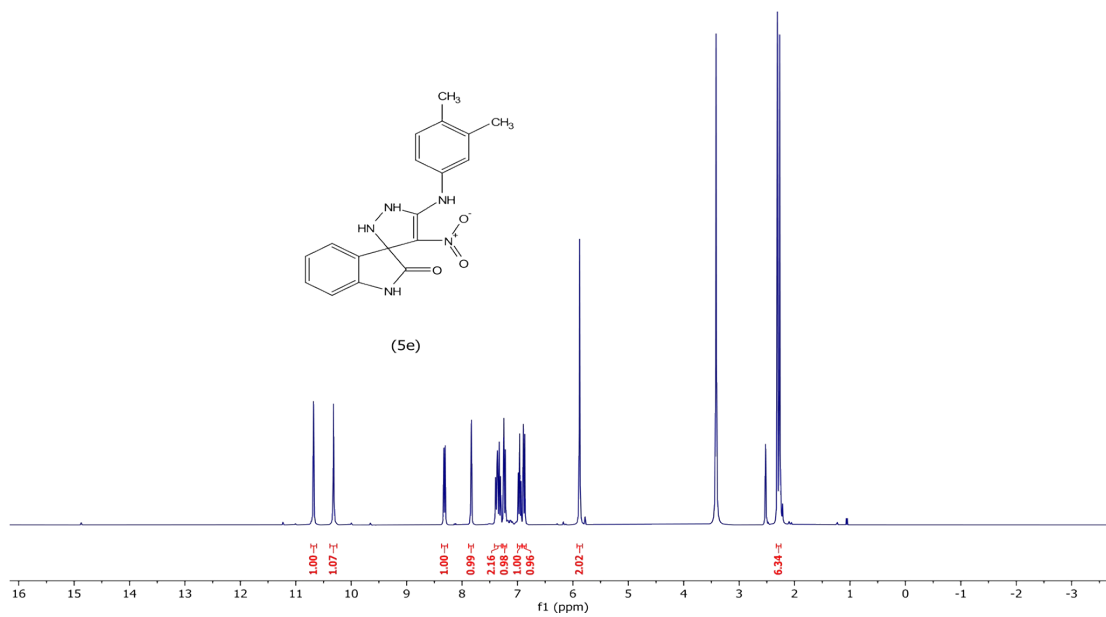


Fig S14. 5'-((3,4-dimethylphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5e**)

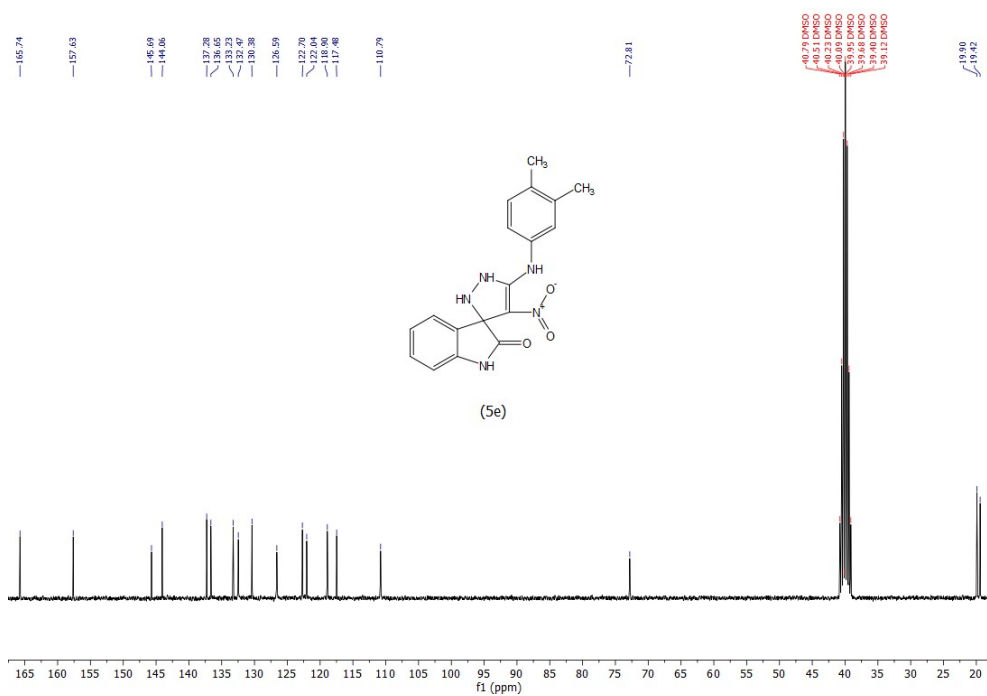
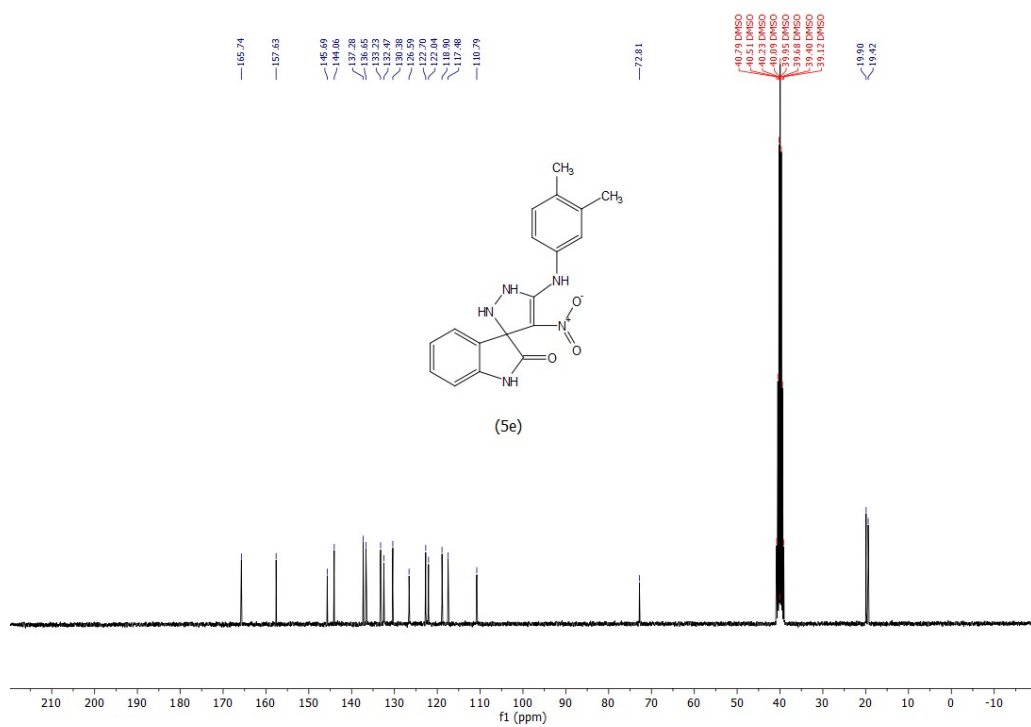
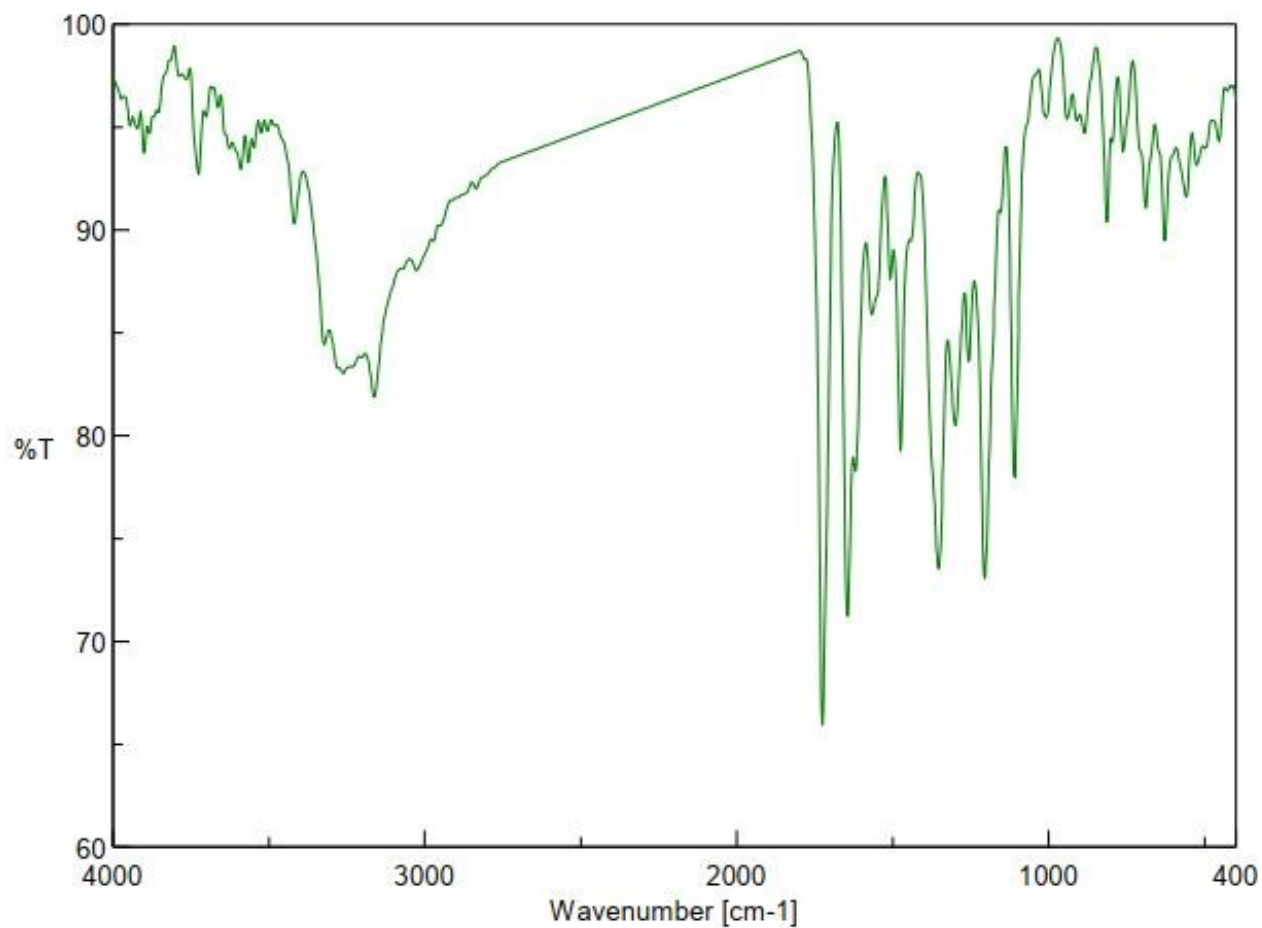


Fig S15. 5'-((3,4-dimethylphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5e**)



Chromatogram C:\EAS Clarity\WORK1\Data\2y 1402.5.15_1_1_2002 2_24_00 AM_051.PRM

Result Table (ESTD – 2y 1402.5.15_1_1_2002 2_24_00 AM_051 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.265	763.257	0.378	20.21	Refer	Nitrogen	0.132
3	2.236	4470.097	0.862	61.04	Refer	Carbon	1.000
4	10.113	1045.445	0.061	4.56	Refer	Hydrogen	0.249
Total			1.301	85.81			

CHN for C₁₈H₁₇N₅O₃ (**5e**)

Fig S16. 5'-((3-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5f**)

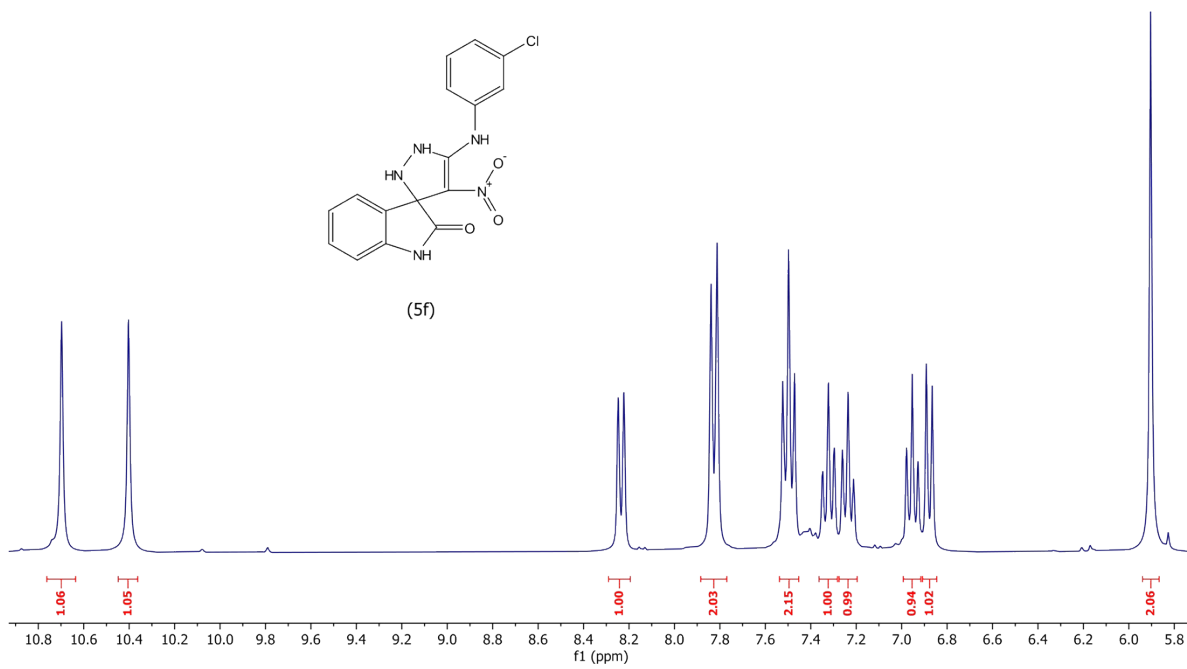
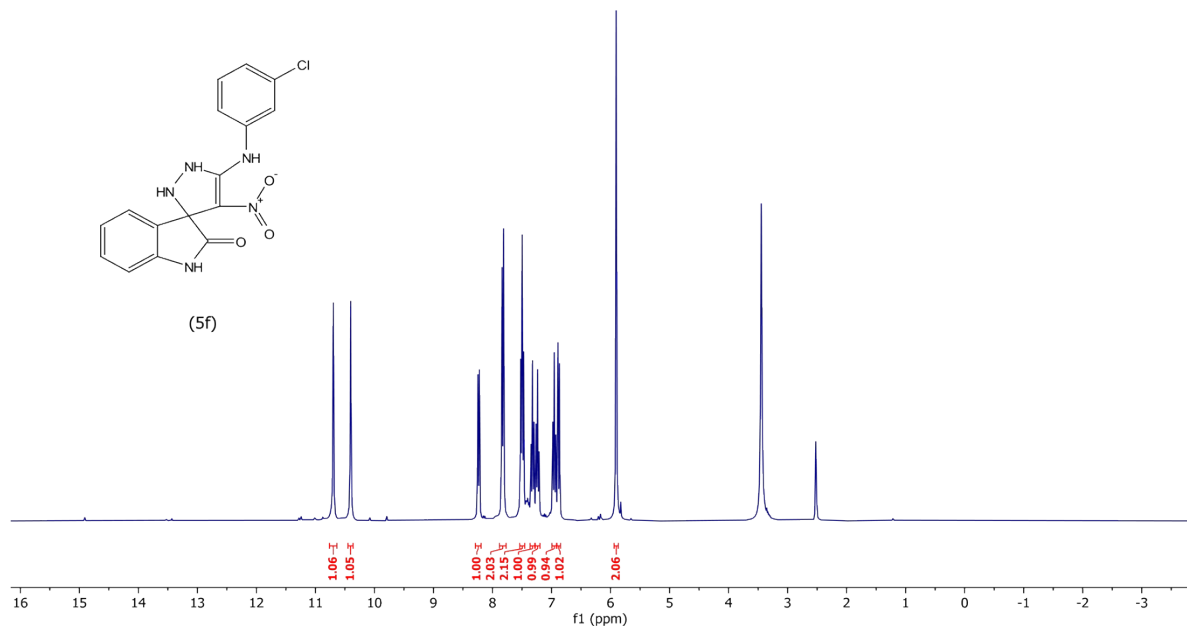


Fig S17. 5'-((3-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5f**)

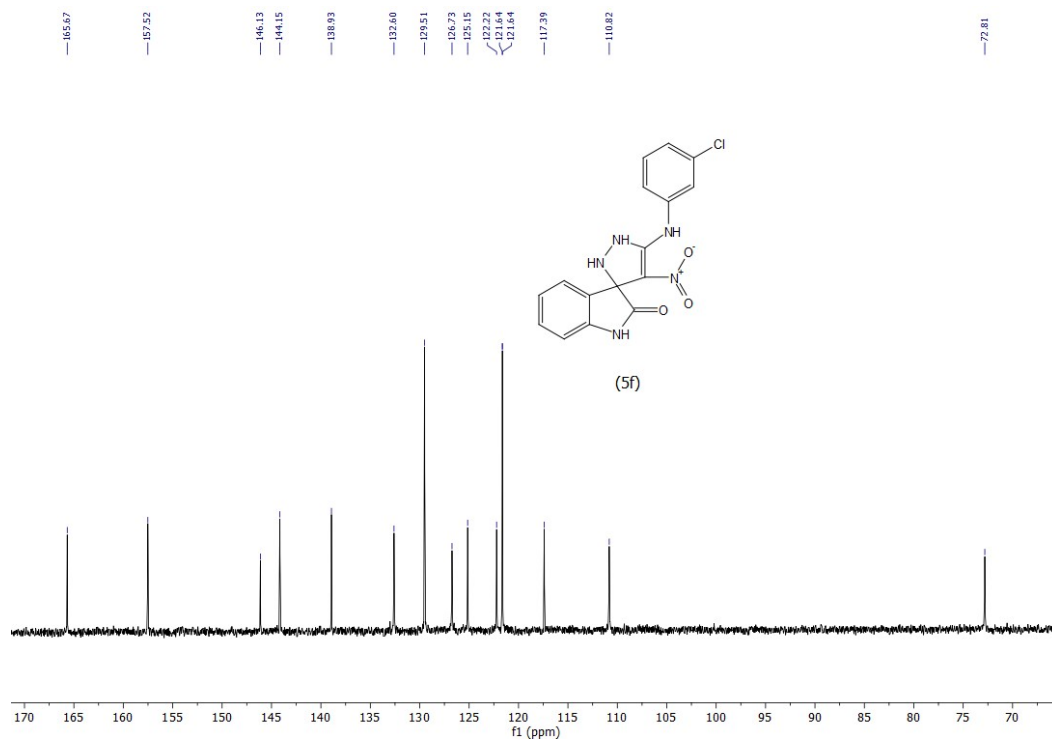
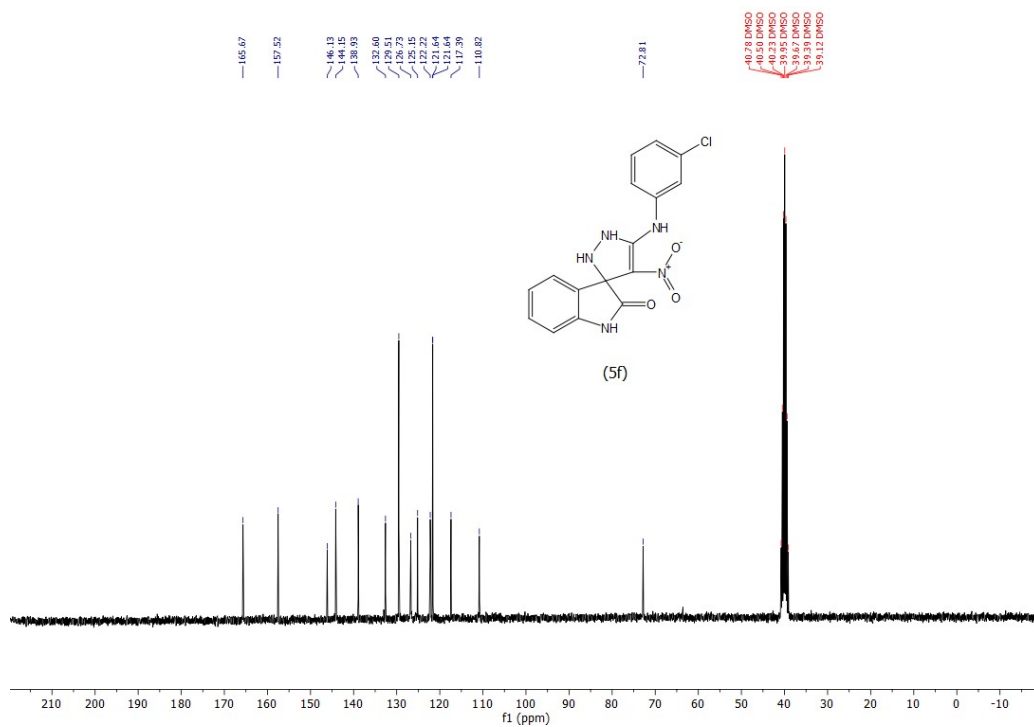
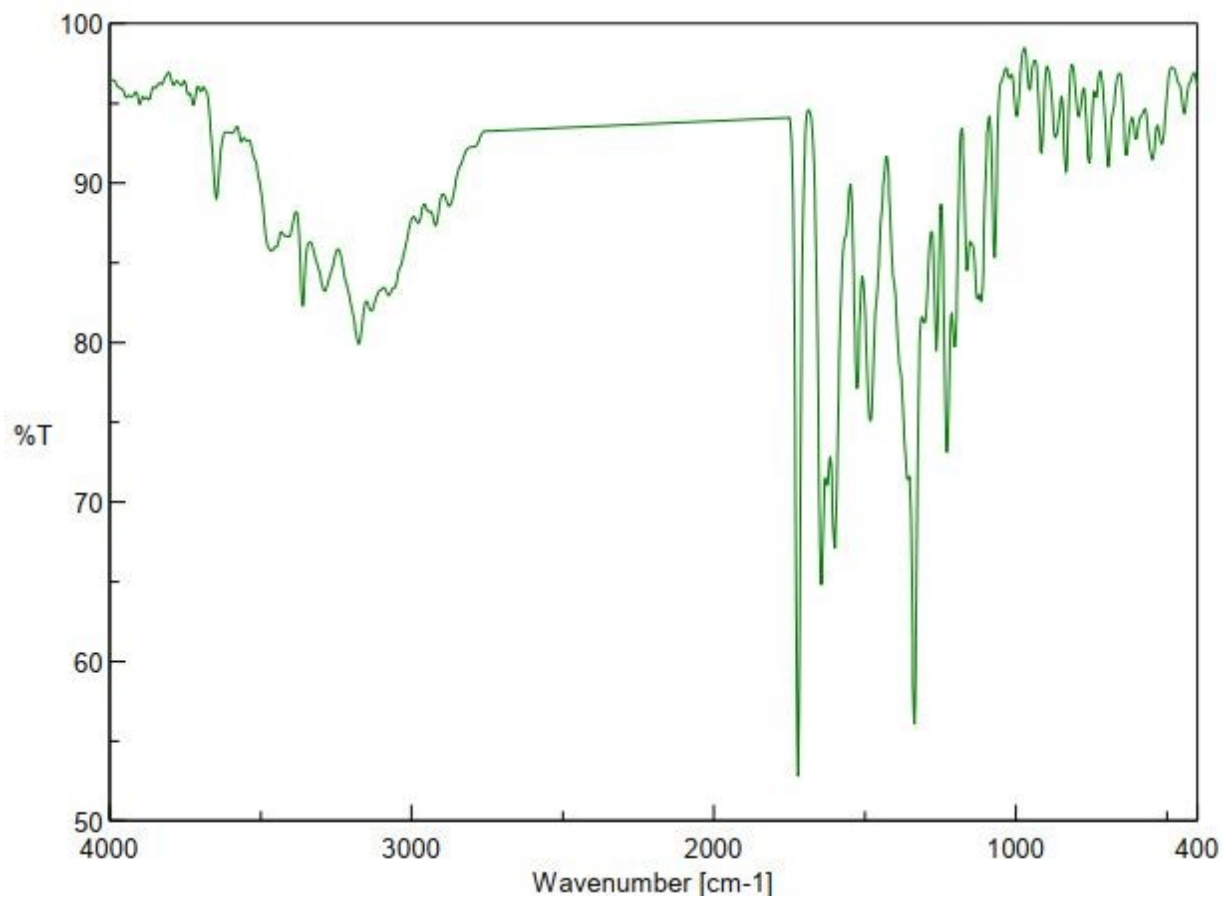


Fig S18. 5'-((3-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5f**)



Chromatogram C:\EAS Clarity\WORK1\Data\2s 1402.5.14_1_1_2002 4_17_27 AM_049.PRM

Result Table (ESTD - 2s 1402.5.14_1_1_2002 4_17_27 AM_049 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.327	1113.369	0.558	19.25	Refer	Nitrogen	0.138
3	2.483	7590.153	1.532	53.49	Refer	Carbon	1.000
4	10.037	1720.601	0.107	3.45	Refer	Hydrogen	0.215
	Total		2.543	76.19			

CHN for C₁₆H₁₂ClN₃O₃ (**5f**)

Fig S19. 5'-((4-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5g**)

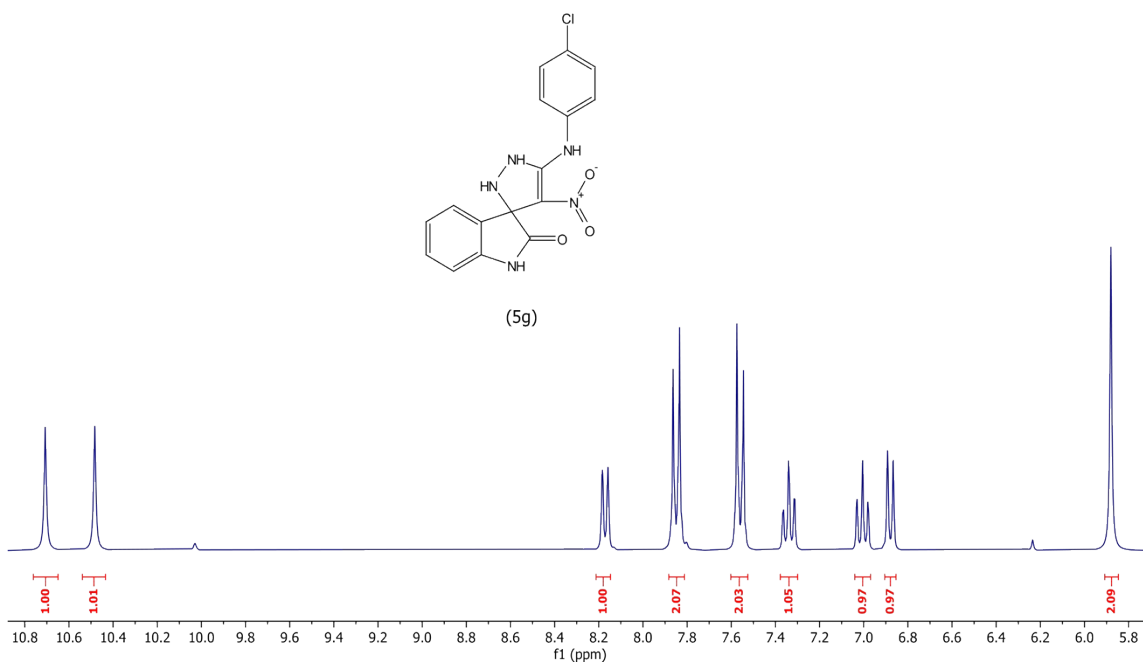
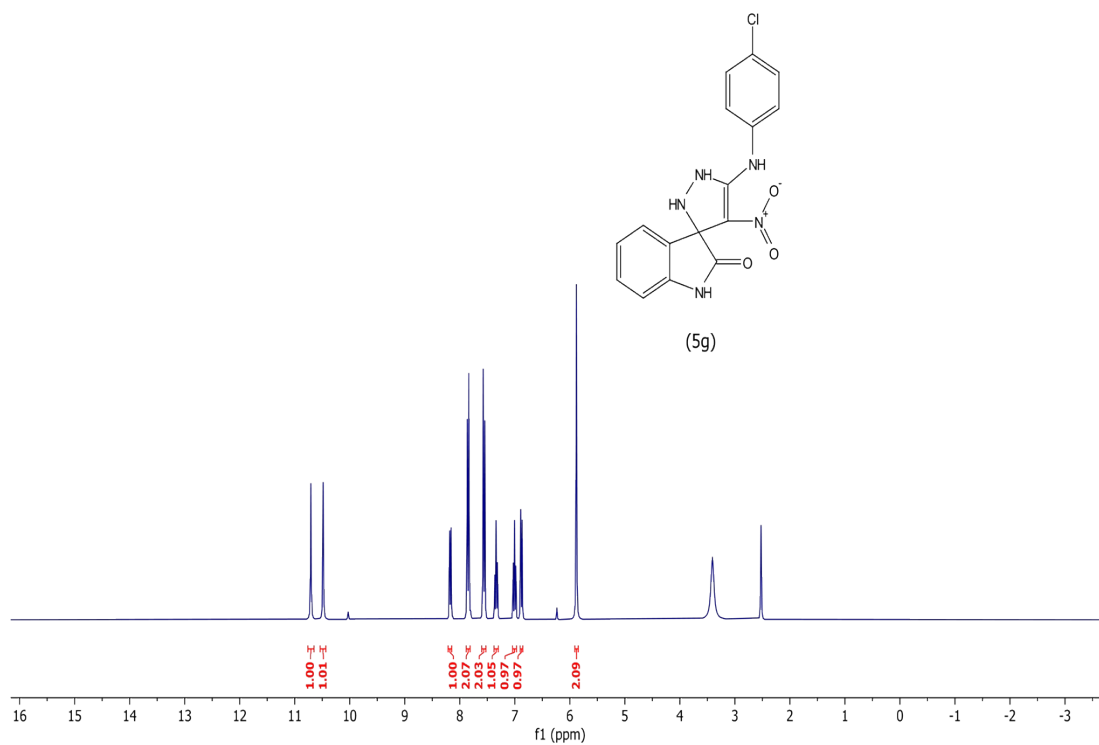


Fig S20. 5'-((4-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5g**)

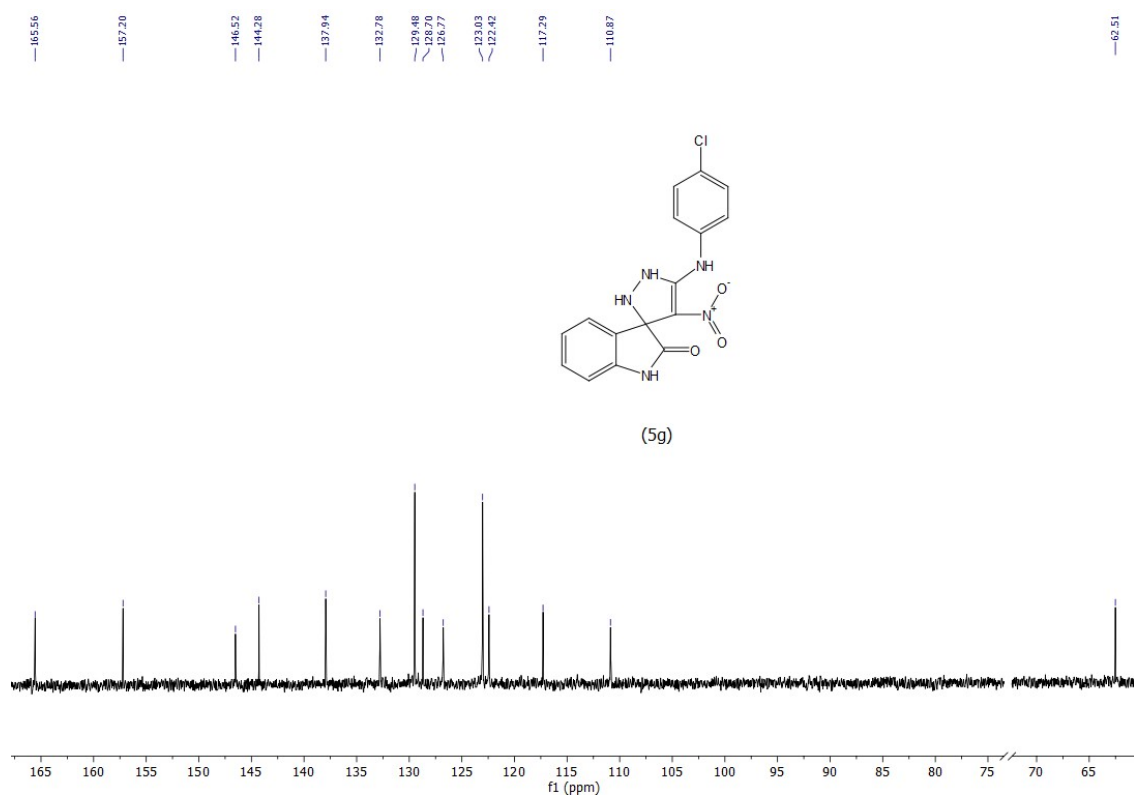
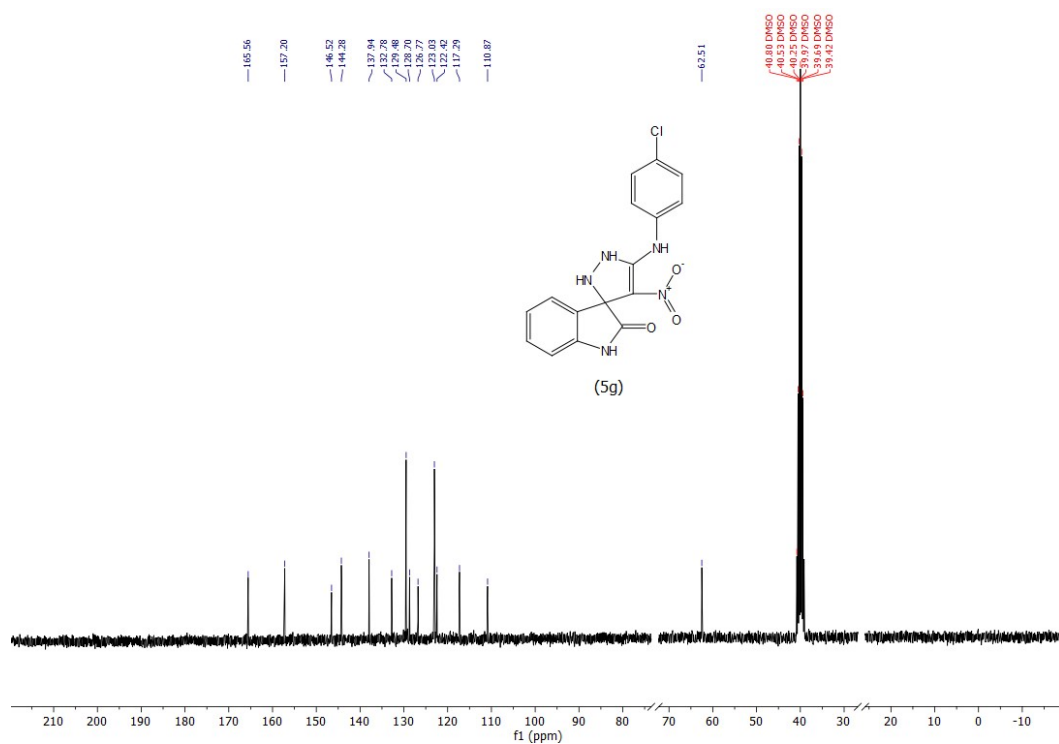


Fig S21. 5'-((4-chlorophenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5g**)

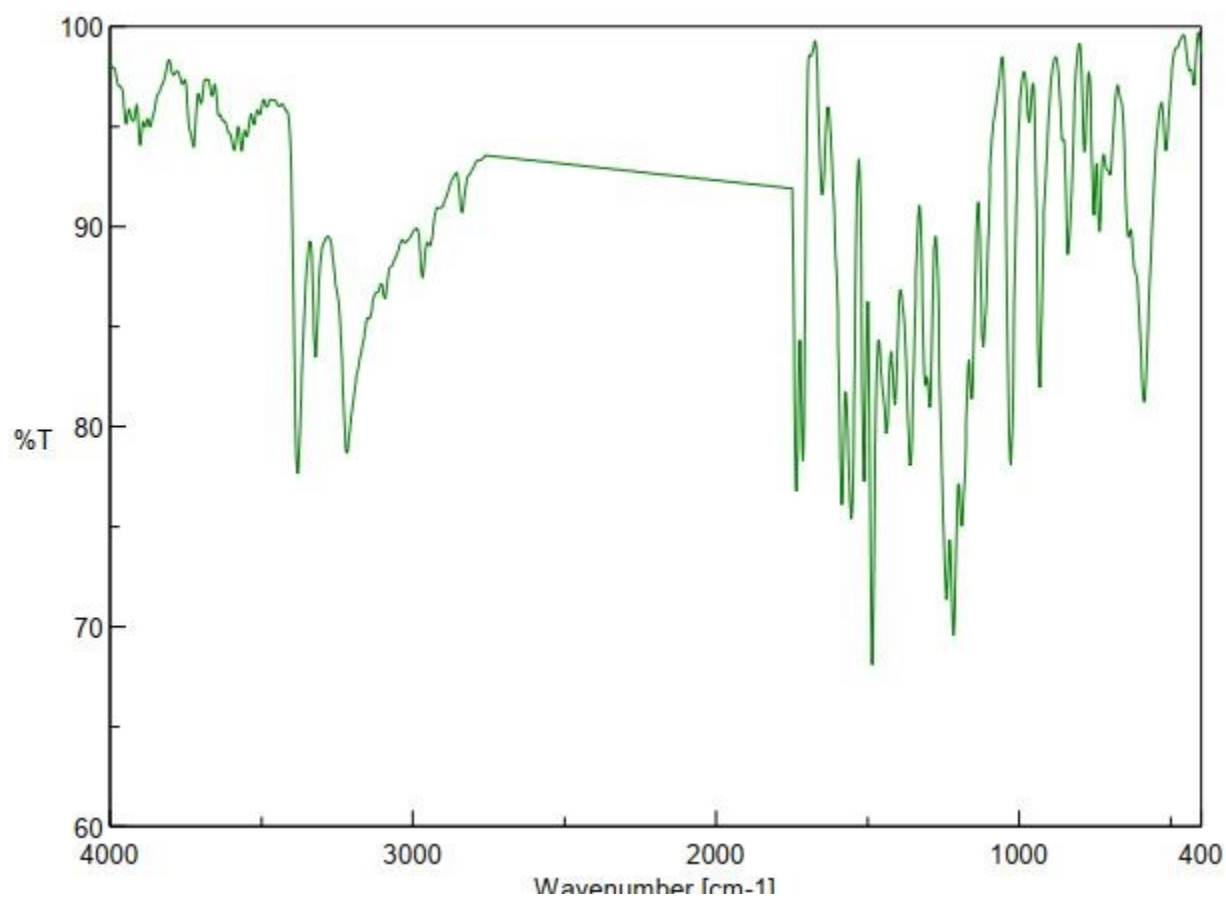


Fig S22. 5-methoxy-5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5h**)

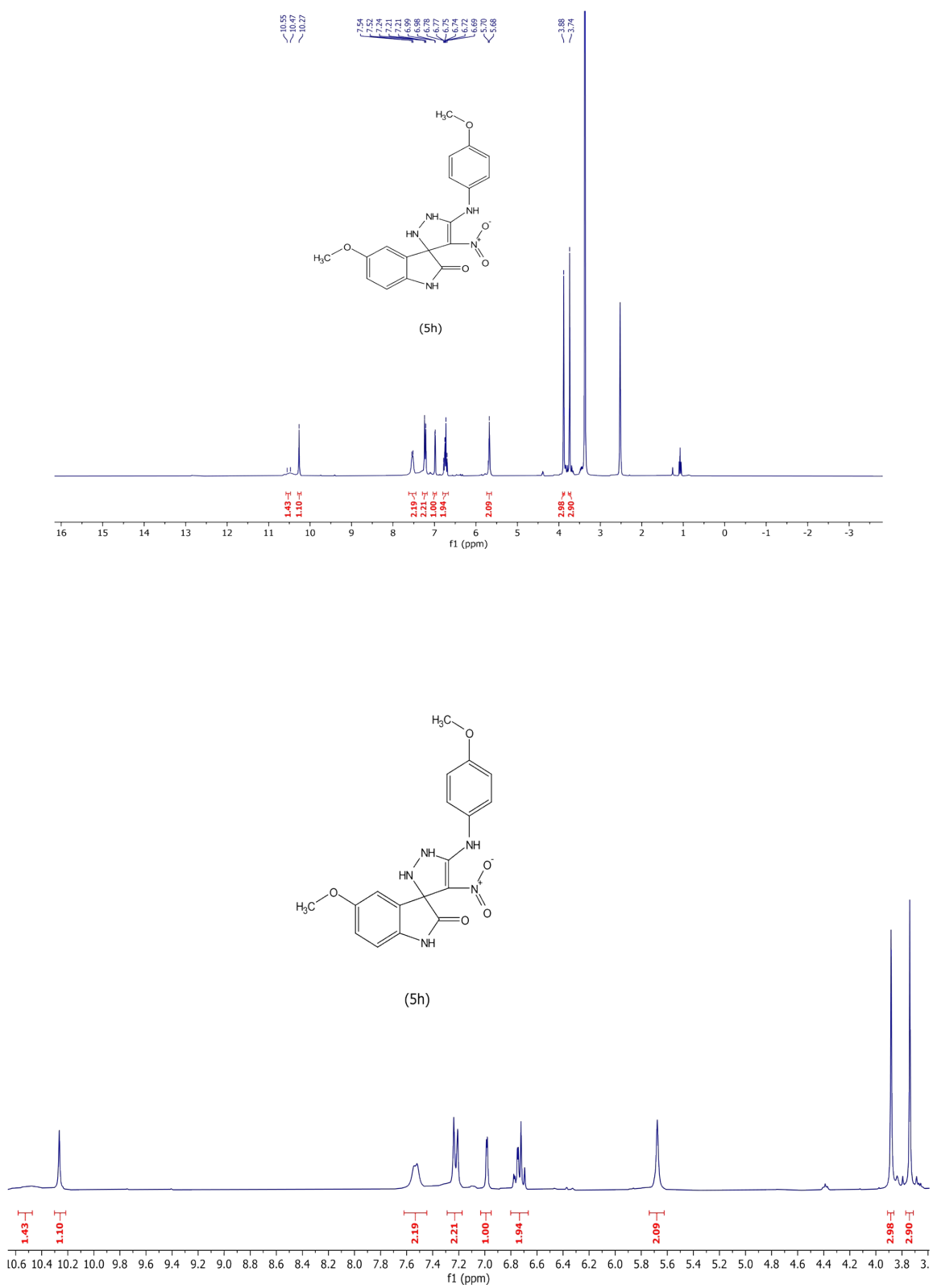


Fig S23. 5-methoxy-5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5h**)

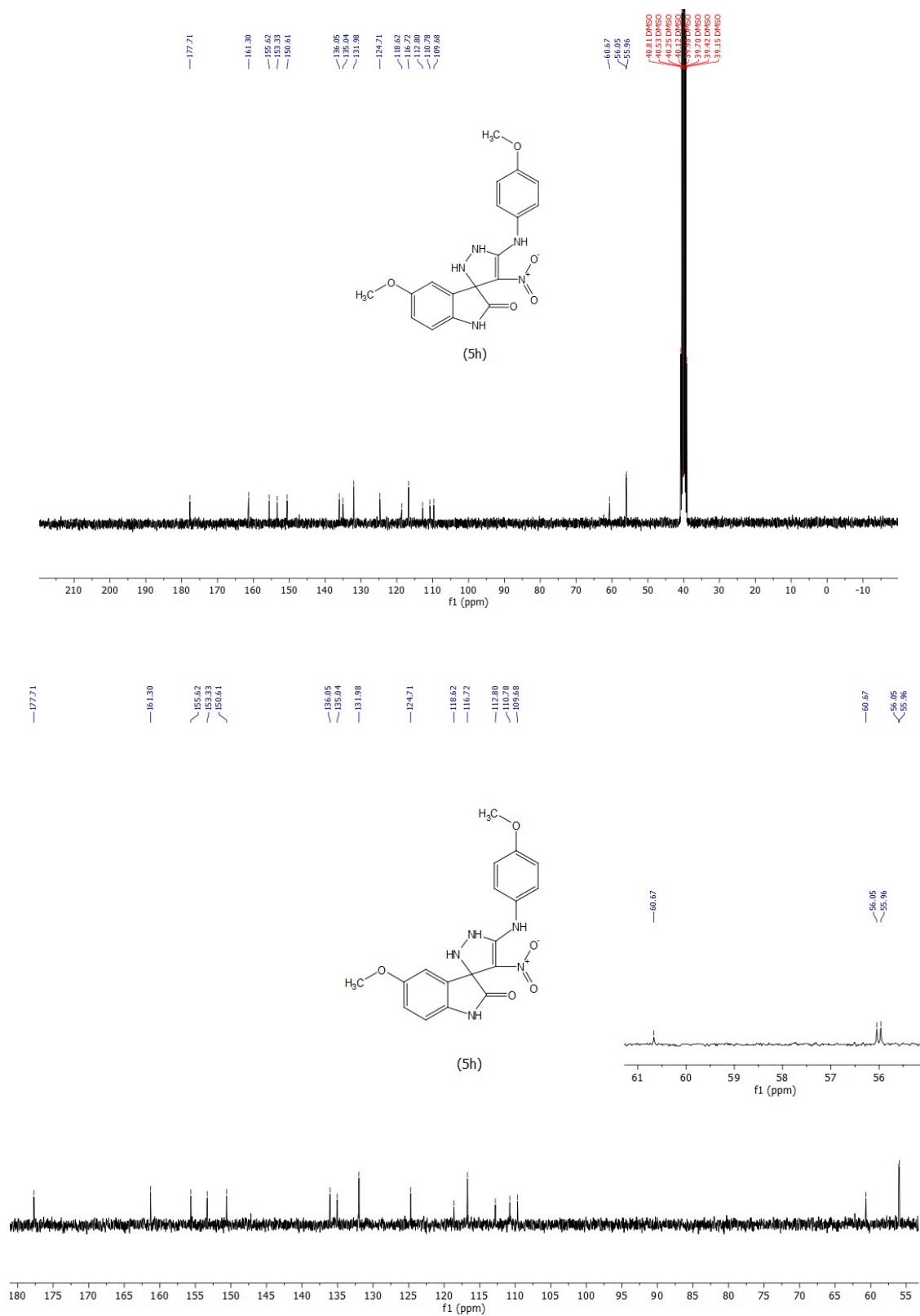
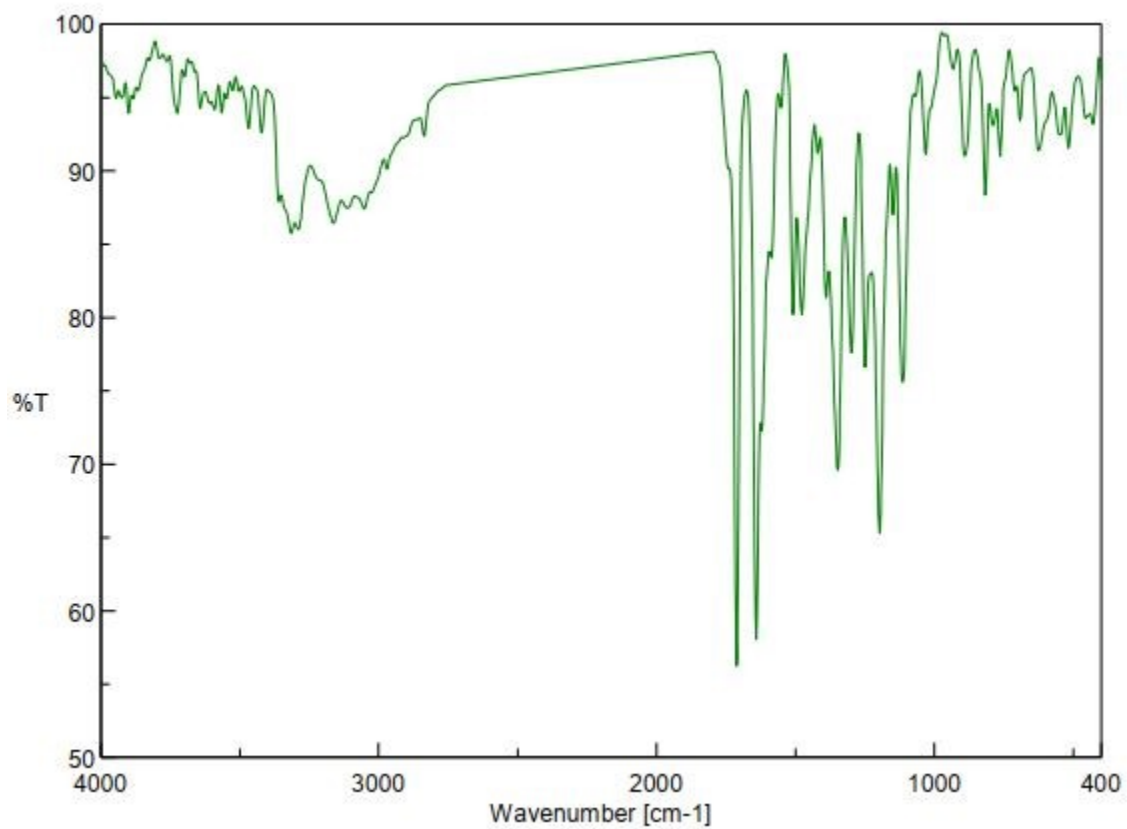


Fig S24. 5-methoxy-5'-((4-methoxyphenyl)amino)-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5h**)



Chromatogram C:\EAS Clarity\WORK1\Data\p3 1402.5.15_1_1_2002 2_54_01 AM_061.PRM

Result Table (ESTD – p3 1402.5.15_1_1_2002 2_54_01 AM_061 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.320	763.257	0.372	18.63	Refer	Nitrogen	0.127
3	2.547	4470.097	0.865	56.69	Refer	Carbon	1.000
4	10.613	1095.688	0.066	4.41	Refer	Hydrogen	0.228
Total			1.774	79.73			

CHN for C₁₈H₁₇N₅O₅ (**5h**)

Fig S25. 5'-((3,4-dimethylphenyl)amino)-5-methoxy-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5i**)

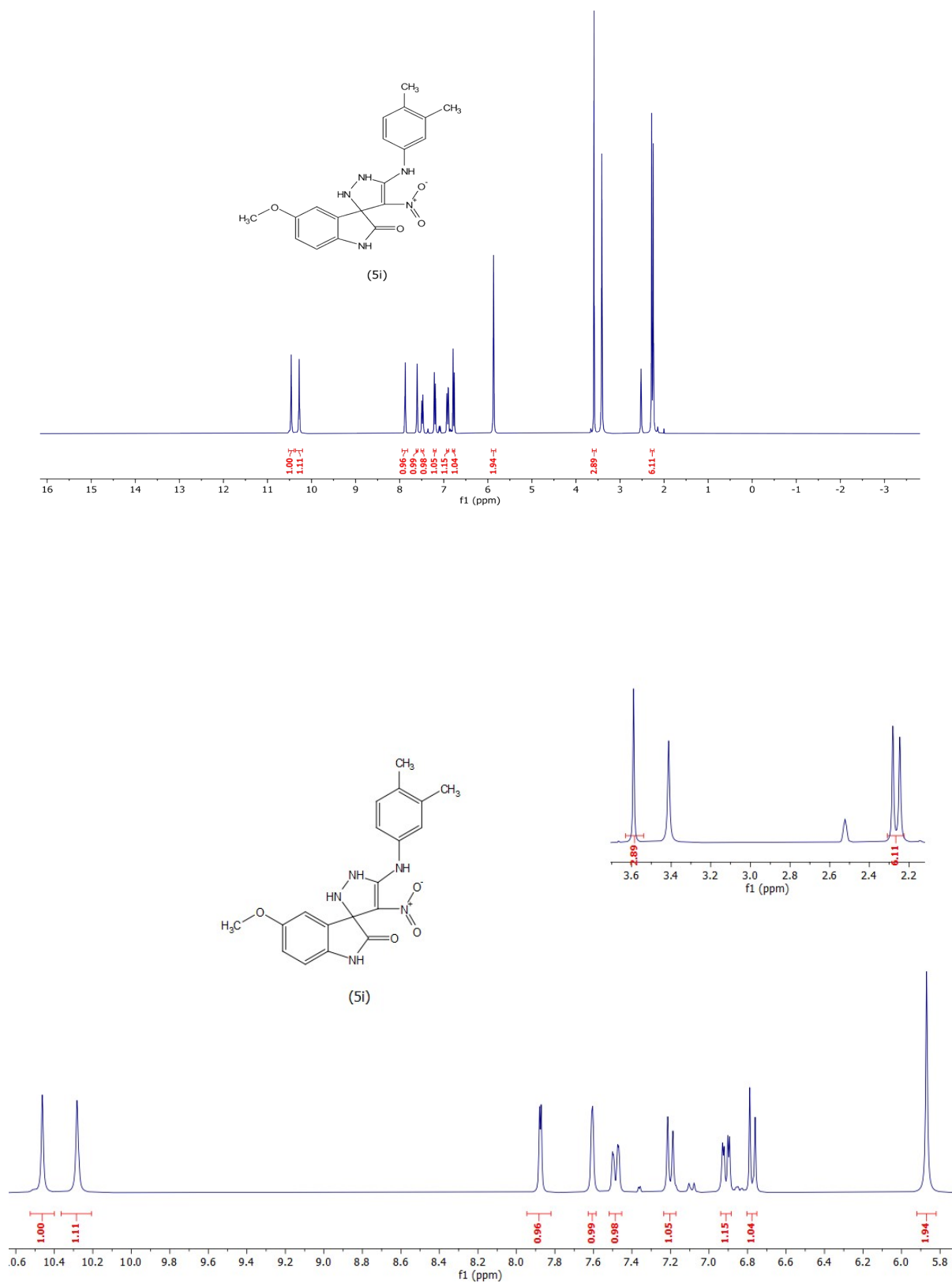


Fig S26. 5'-((3,4-dimethylphenyl)amino)-5-methoxy-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5i**)

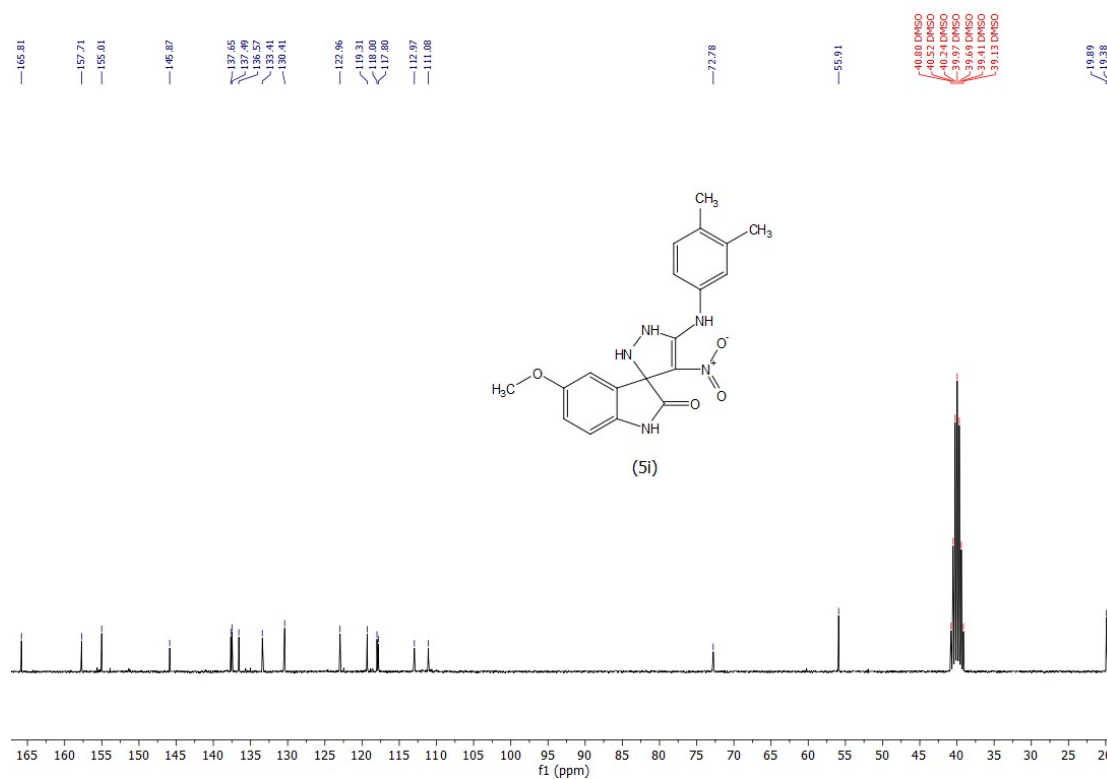
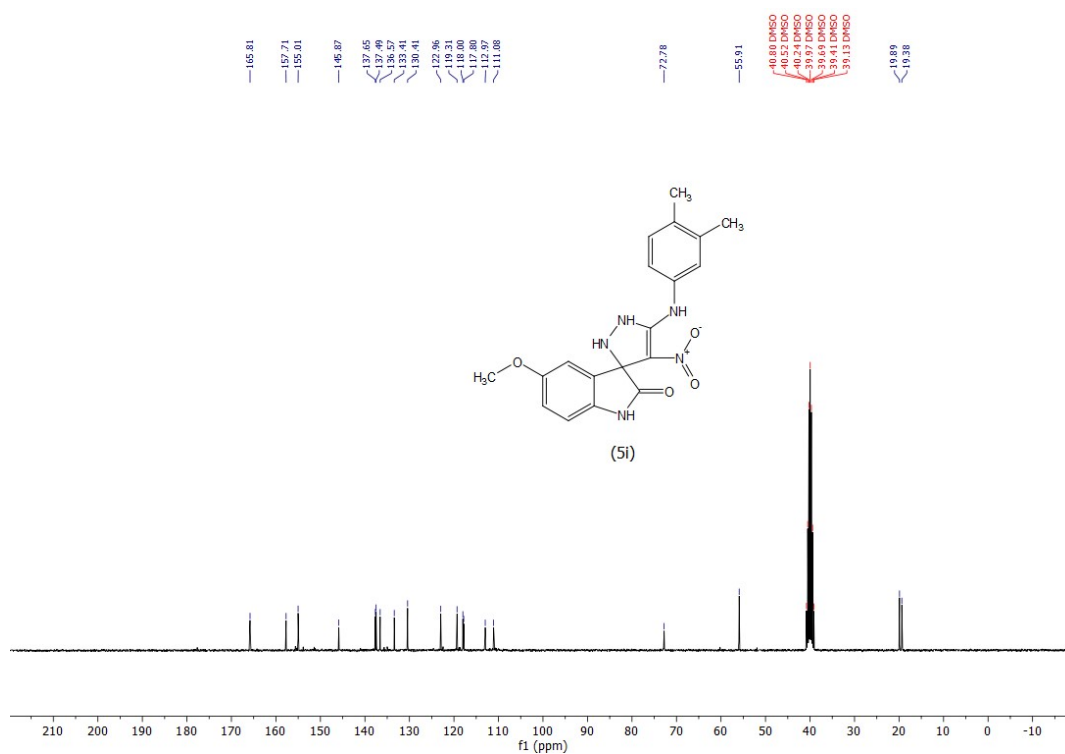
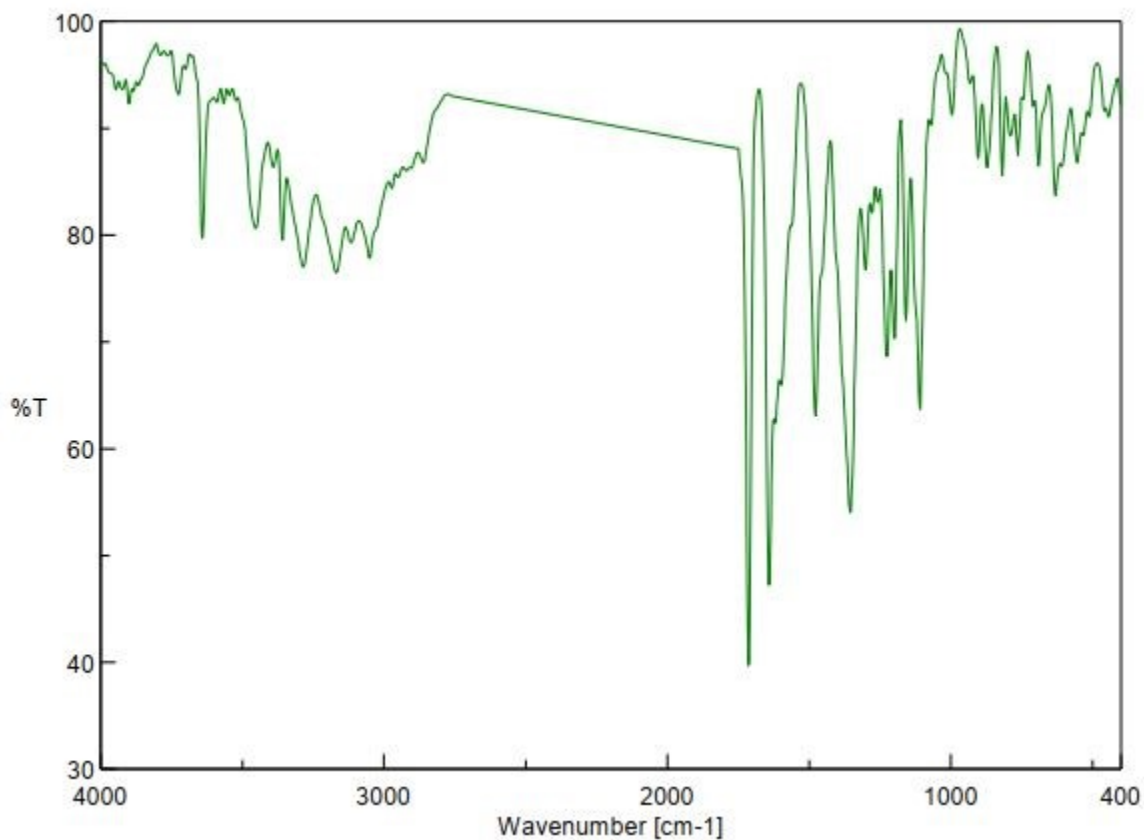


Fig S27. 5'-((3,4-dimethylphenyl)amino)-5-methoxy-4'-nitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5i**)



Chromatogram C:\EAS Clarity\WORK1\Data\p1 1402.5.15_1_2_2002 1_24_00 AM_056.PRM

Result Table (ESTD - p1 1402.5.15_1_2_2002 1_24_00 AM_056 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.303	1001.297	0.498	18.66	Refer	Nitrogen	0.124
3	2.457	8102.185	1.655	59.21	Refer	Carbon	1.000
4	9.827	2181.694	0.137	4.97	Refer	Hydrogen	0.269
Total			2.814	82.84			

CHN for C₁₉H₁₉N₅O₄ (**5i**)

Fig S28. 4',5-dinitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5j**)

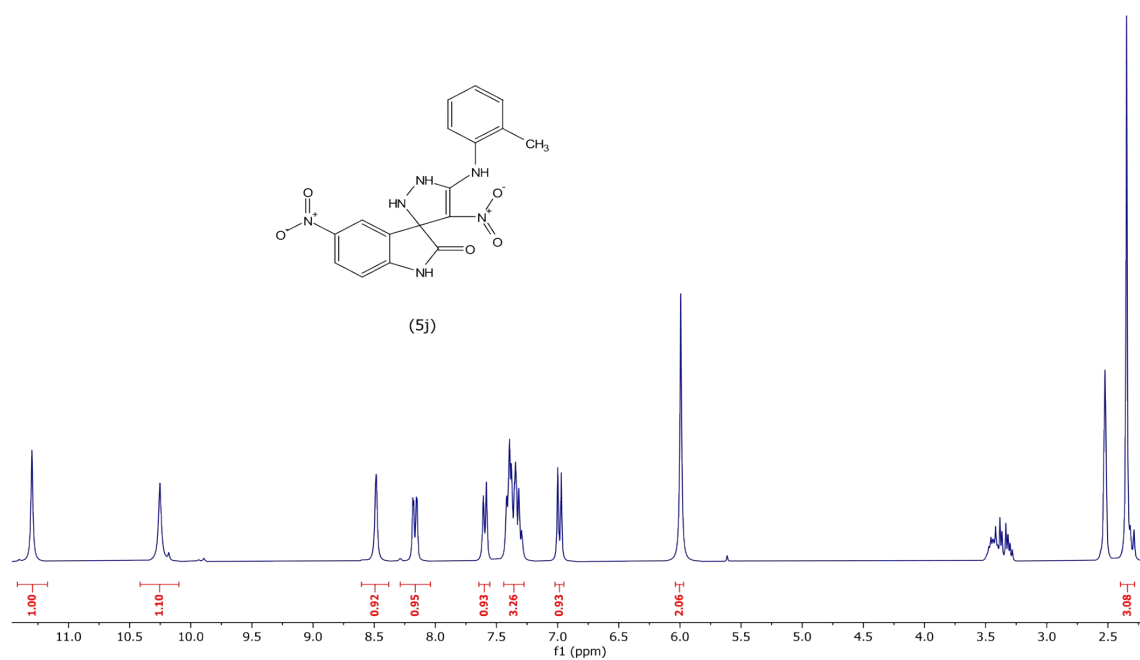
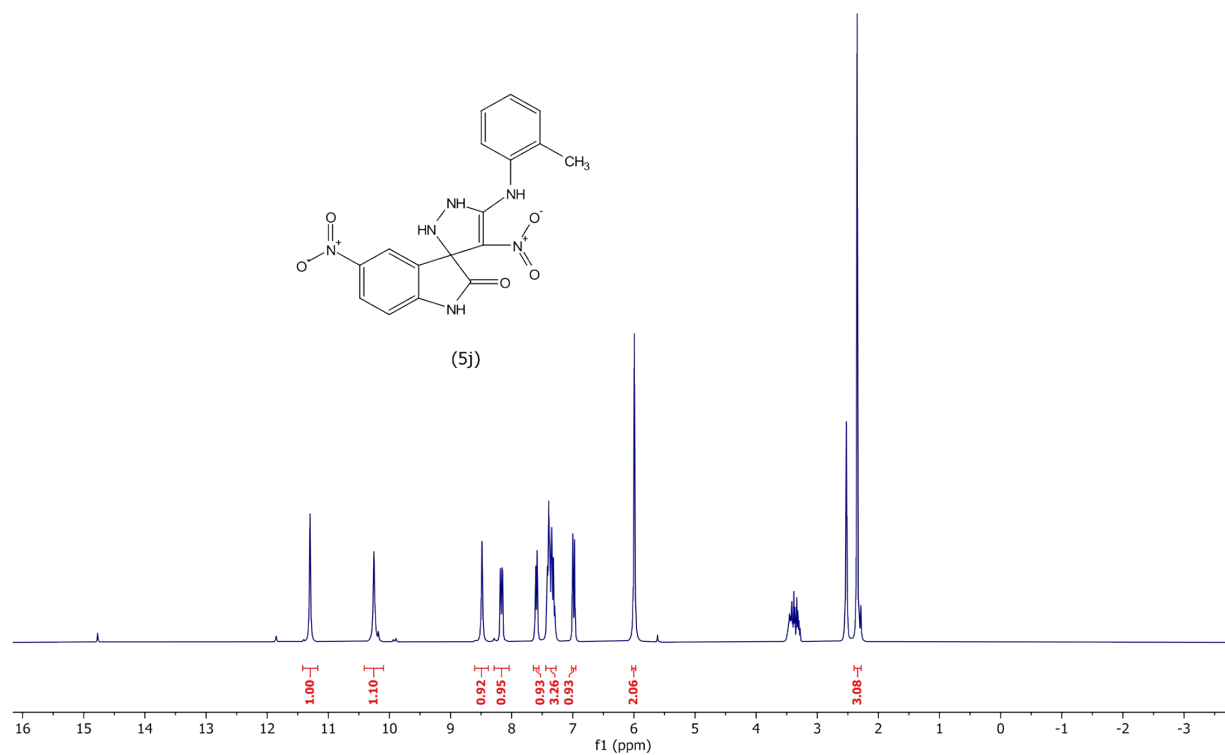


Fig S29. 4',5-dinitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5j**)

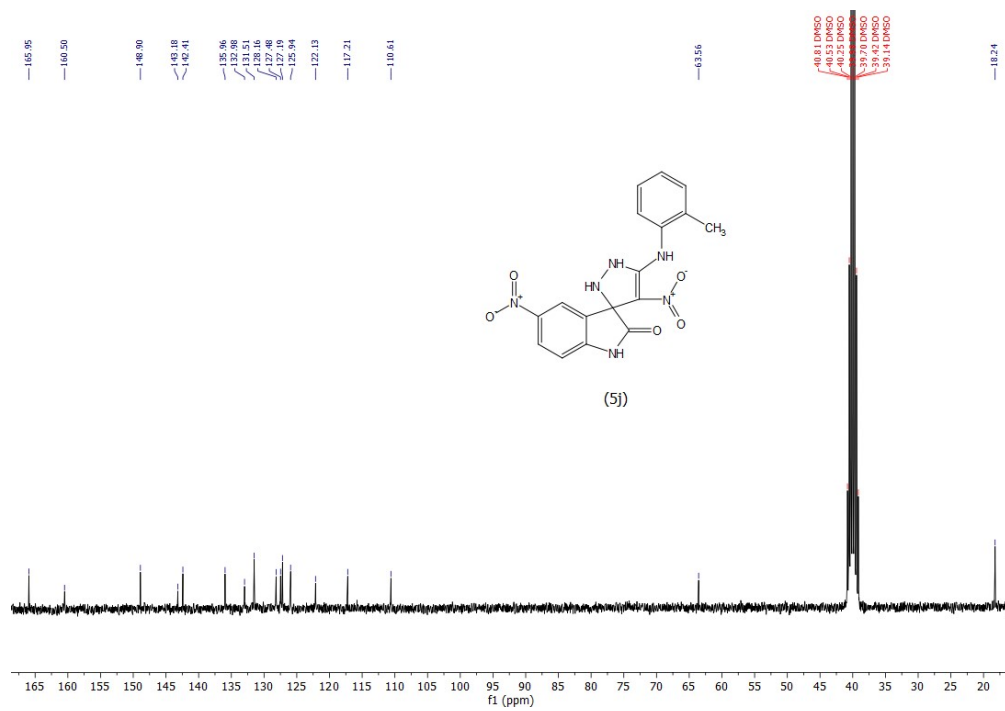
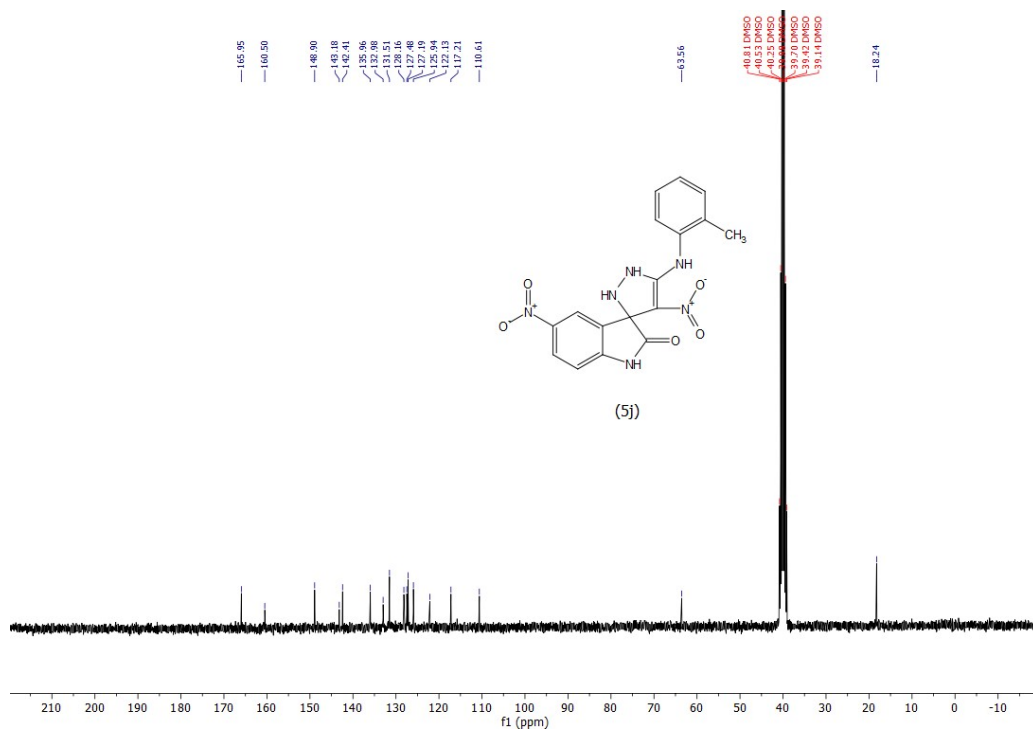


Fig S30. 4',5-dinitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5j**)

Chromatogram C:\EAS Clarity\WORK1\Data\2u 1402.5.14_1_1_2002 4_47_28 AM_050.PRM

Result Table (ESTD – 2u 1402.5.14_1_1_2002 4_47_28 AM_050 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.320	787.064	0.385	22.28	Refer	Nitrogen	0.155
3	2.560	4126.818	0.763	54.11	Refer	Carbon	1.000
4	10.560	1098.419	0.066	3.77	Refer	Hydrogen	0.232
	Total		1.879	80.42			

CHN for C₁₇H₁₄N₆O₅ (**5j**)

Fig S31. 5'-((2,5-dimethoxyphenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5k**)

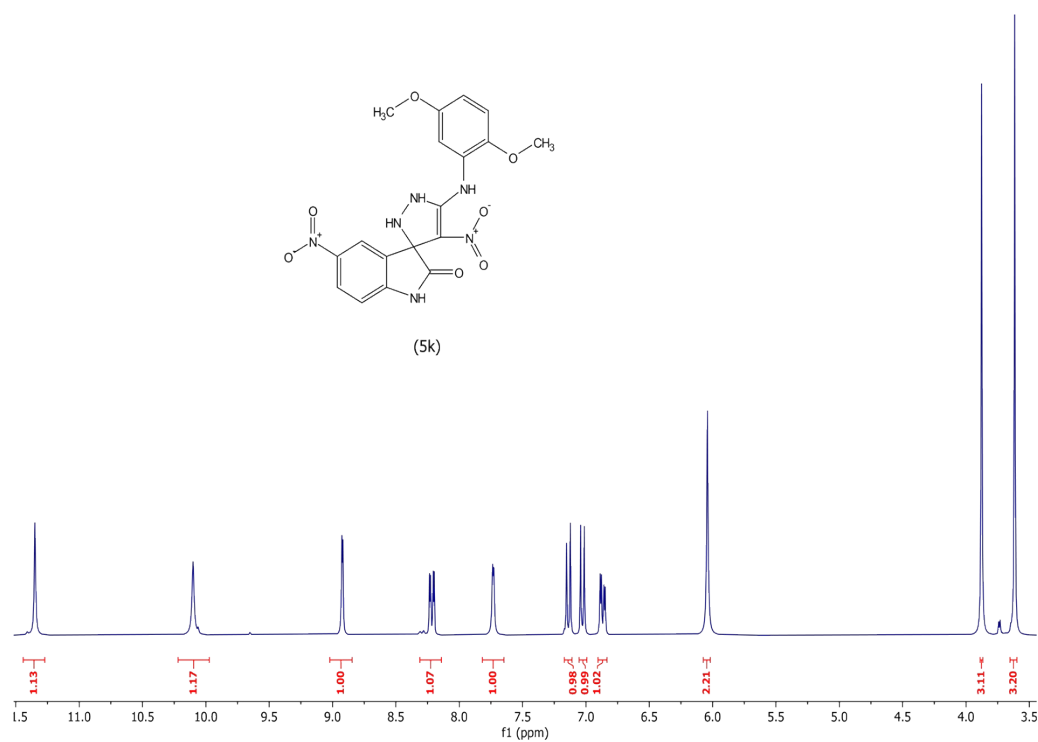
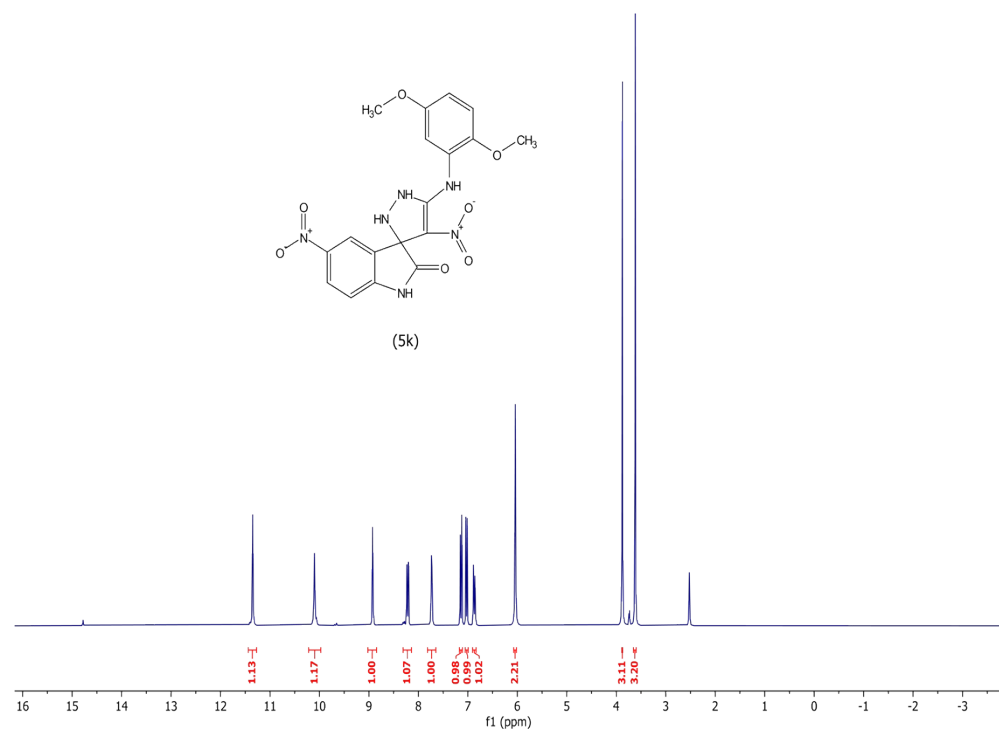


Fig S32. 5'-((2,5-dimethoxyphenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5k**)

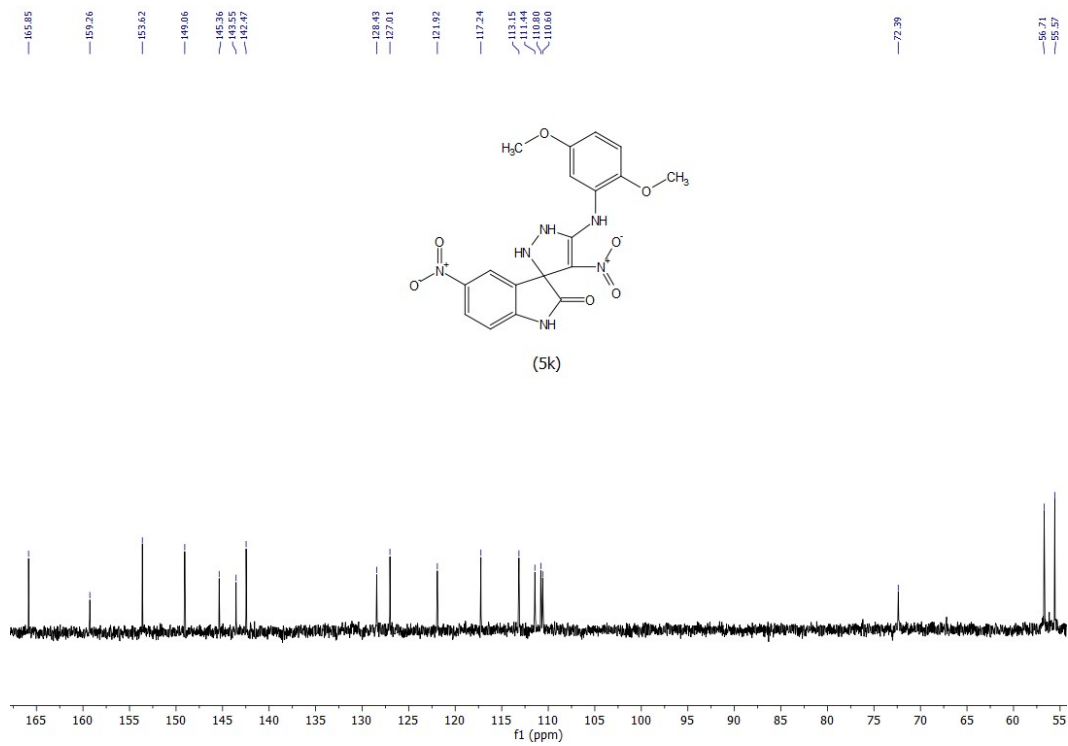
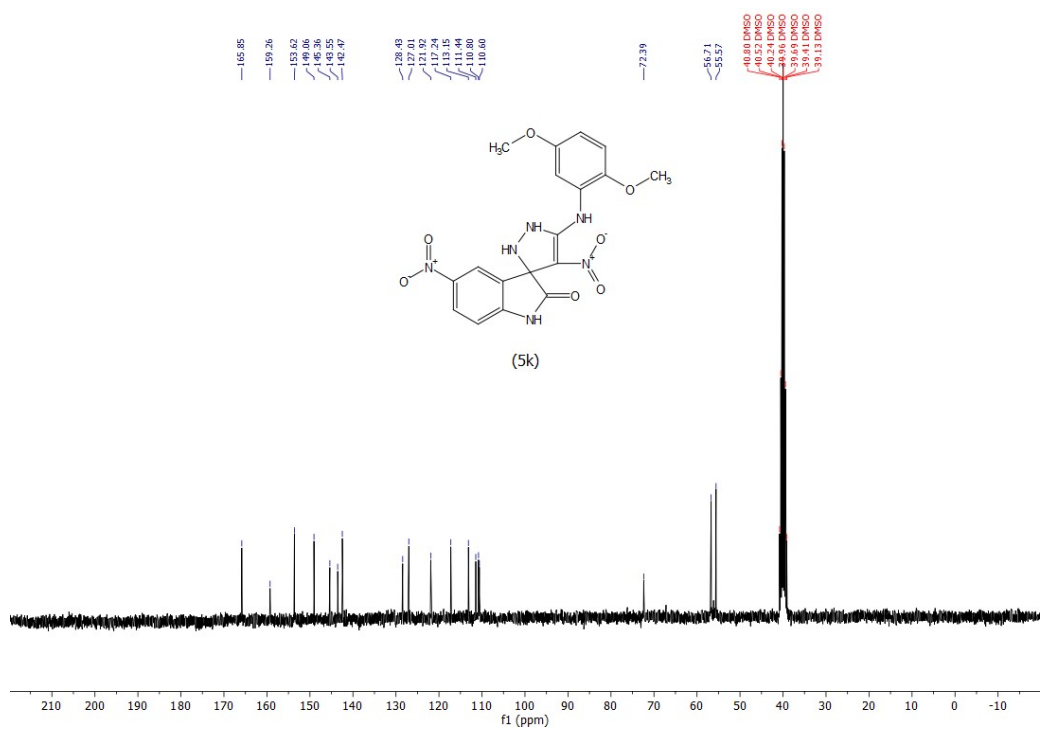
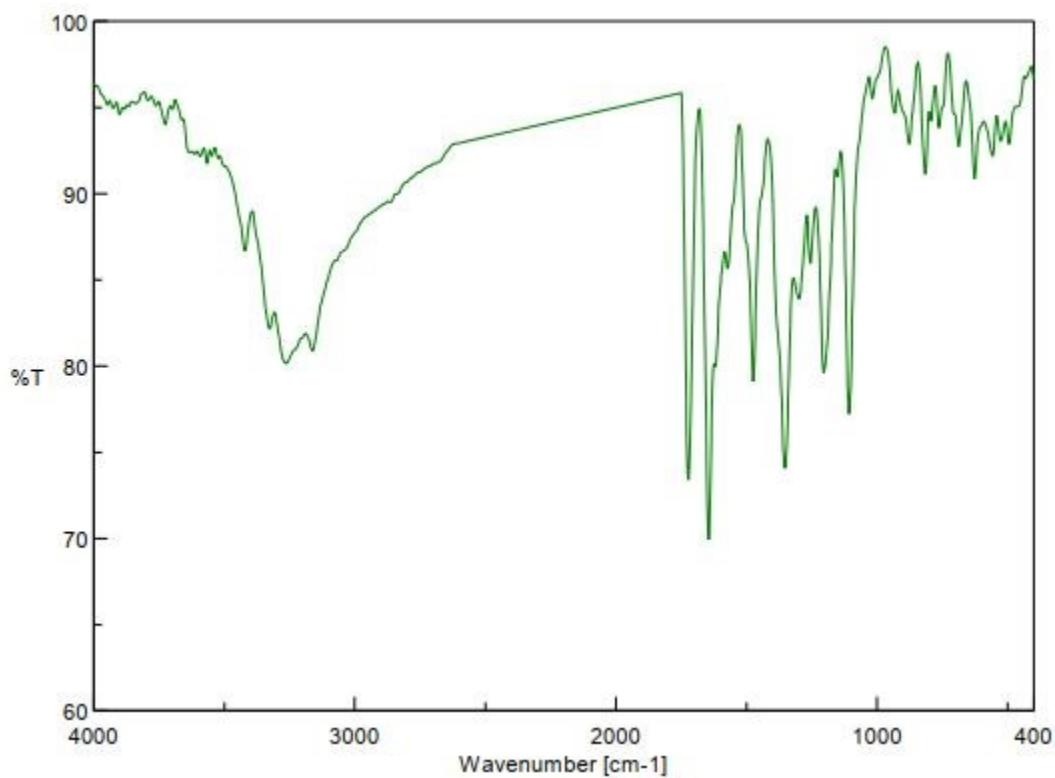


Fig S33. 5'-((2,5-dimethoxyphenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5k**)



Chromatogram C:\EAS Clarity\WORK1\Data\2p 1402.5.14-2_1_1_2002 5_17_28 AM_051.PRM

Result Table (ESTD - 2p 1402.5.14-2_1_1_2002 5_17_28 AM_051 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.320	798.922	0.391	19.21	Refer	Nitrogen	0.138
3	2.567	3968.702	0.730	50.68	Refer	Carbon	1.000
4	10.470	1283.489	0.078	3.97	Refer	Hydrogen	0.230
	Total		2.035	73.86			

CHN for C₁₈H₁₆N₆O₇ (**5k**)

Fig S34. 5'-((4-chlorophenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5I**)

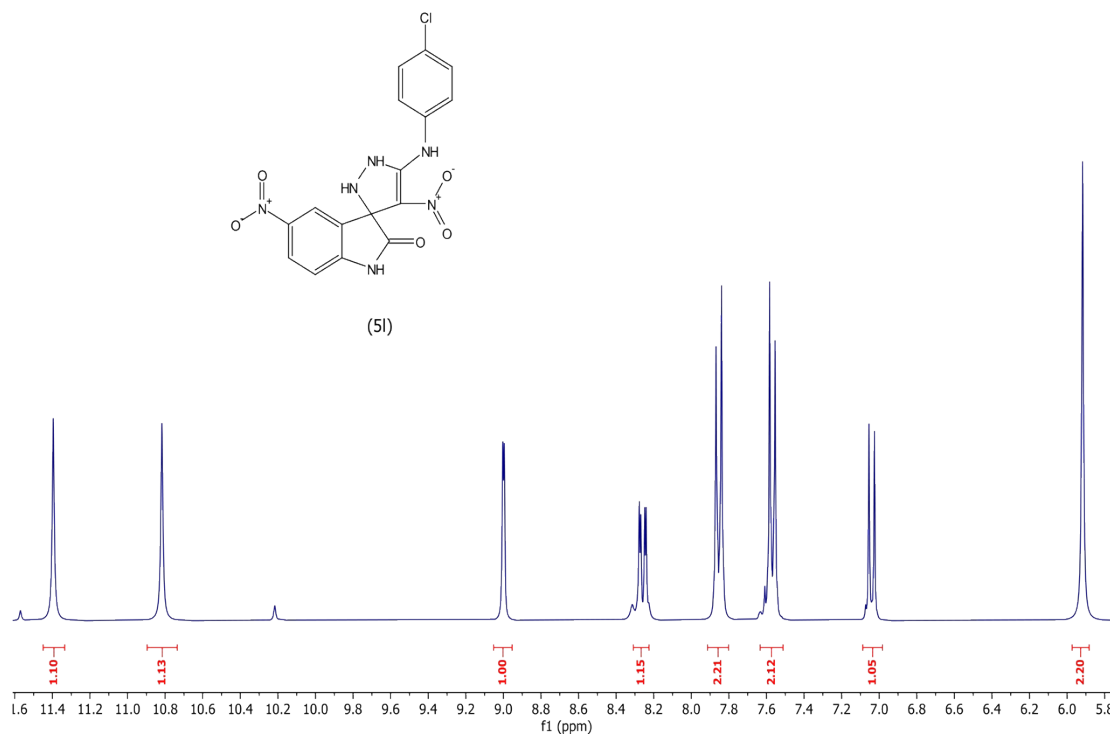
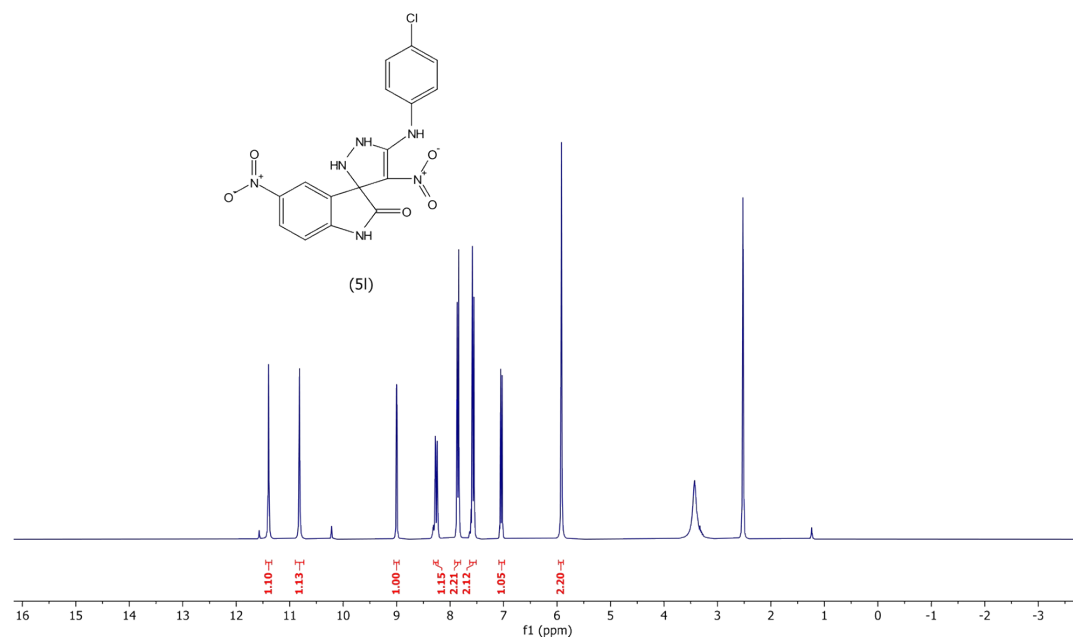


Fig S35. 5'-((4-chlorophenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5I**)

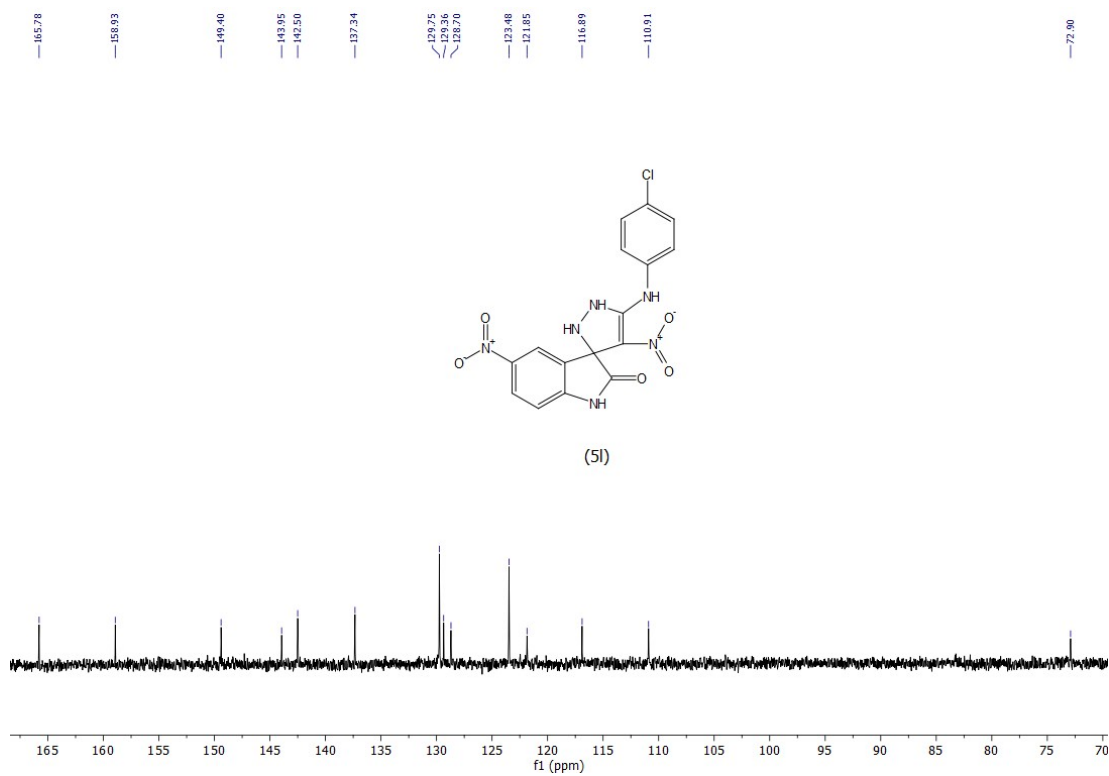
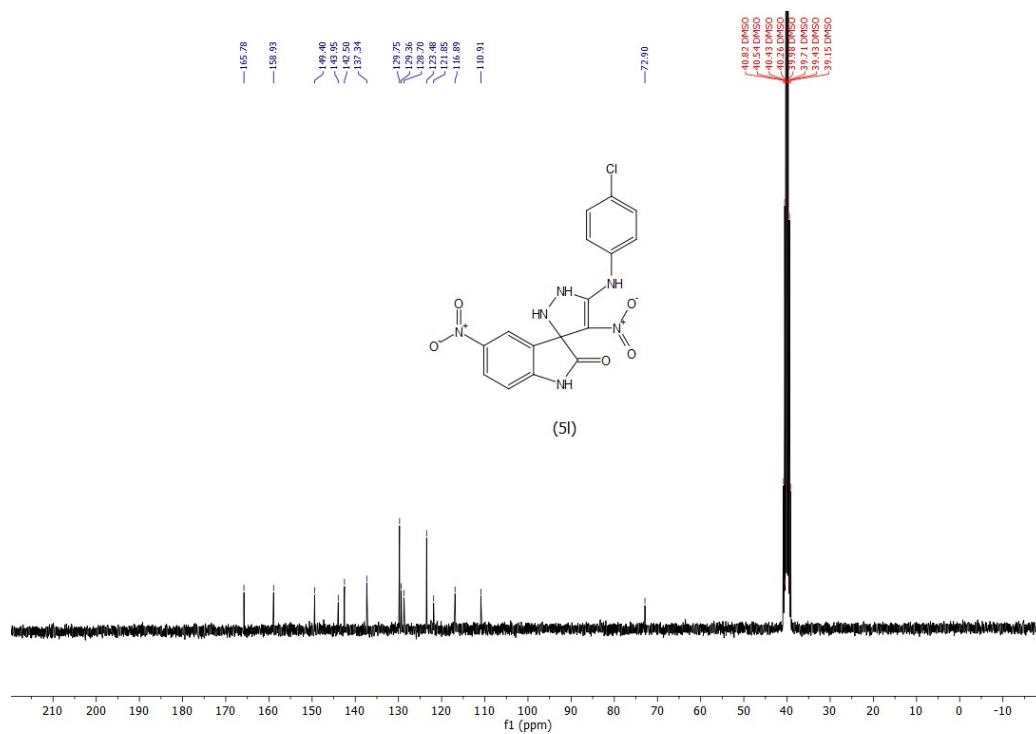
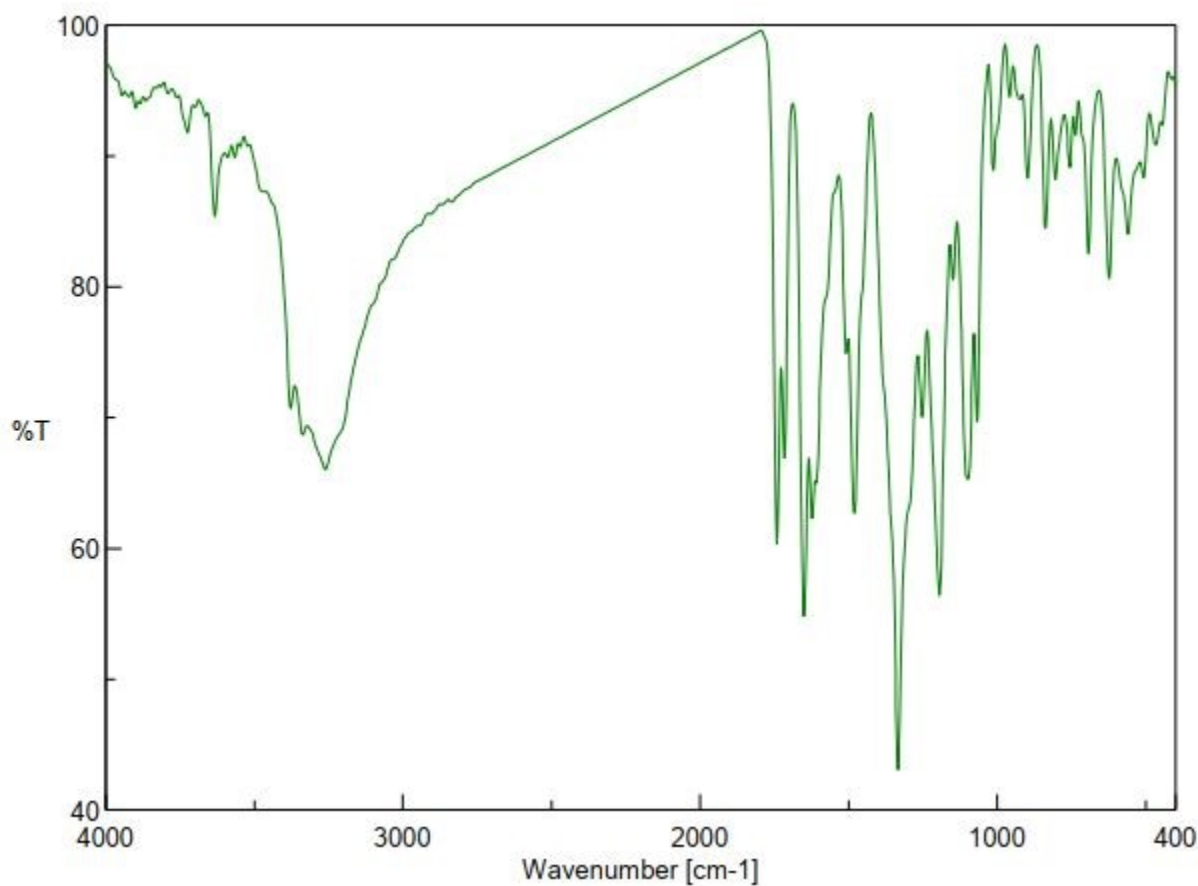


Fig S36. 5'-((4-chlorophenyl)amino)-4',5-dinitro-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5I**)



Chromatogram C:\EAS Clarity\WORK1\Data\2q 1402.5.14_1_1_2002 3_47_27 AM_048.PRM

Result Table (ESTD - 2q 1402.5.14_1_1_2002 3_47_27 AM_048 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.303	902.678	0.446	20.51	Refer	Nitrogen	0.152
3	2.547	3942.636	0.725	48.09	Refer	Carbon	1.000
4	10.733	920.297	0.054	2.62	Refer	Hydrogen	0.196
Total			2.073	71.22			

CHN for C₁₆H₁₁ClN₆O₅ (**5I**)

Fig S37. 4'-nitro-5'-(o-tolylamino)-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5m**)

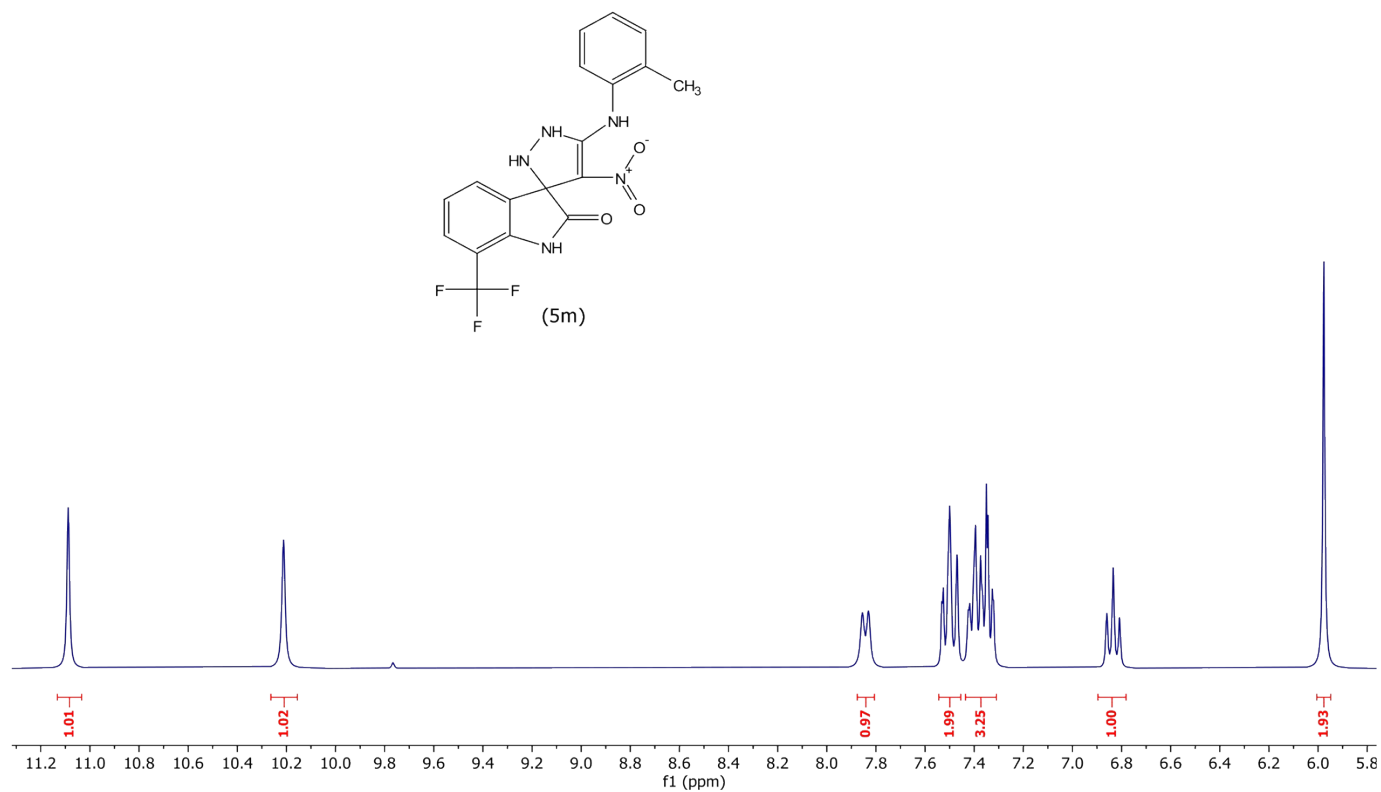
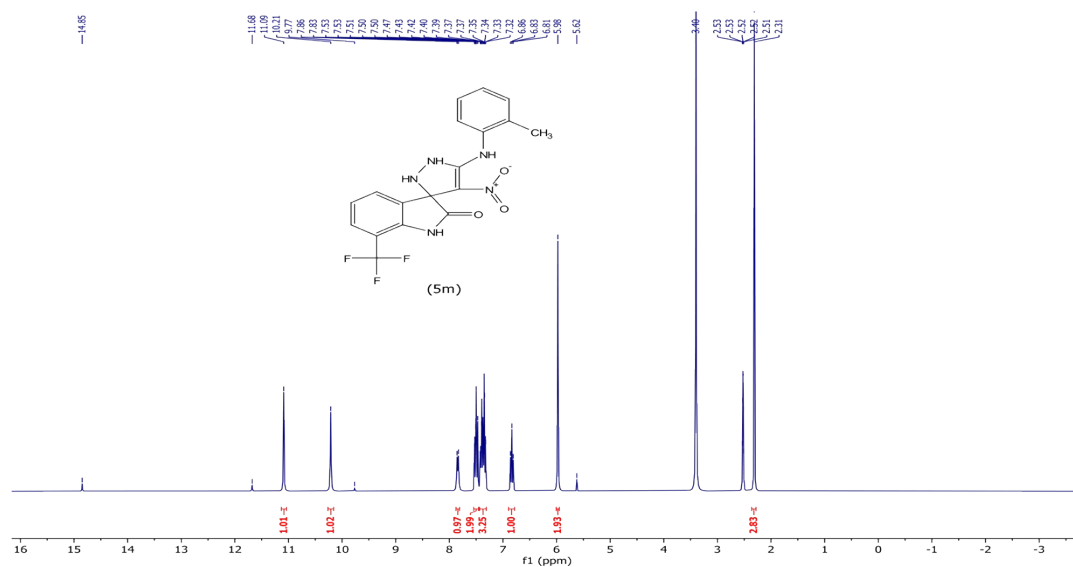


Fig S38. 4'-nitro-5'-(o-tolylamino)-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5m**)

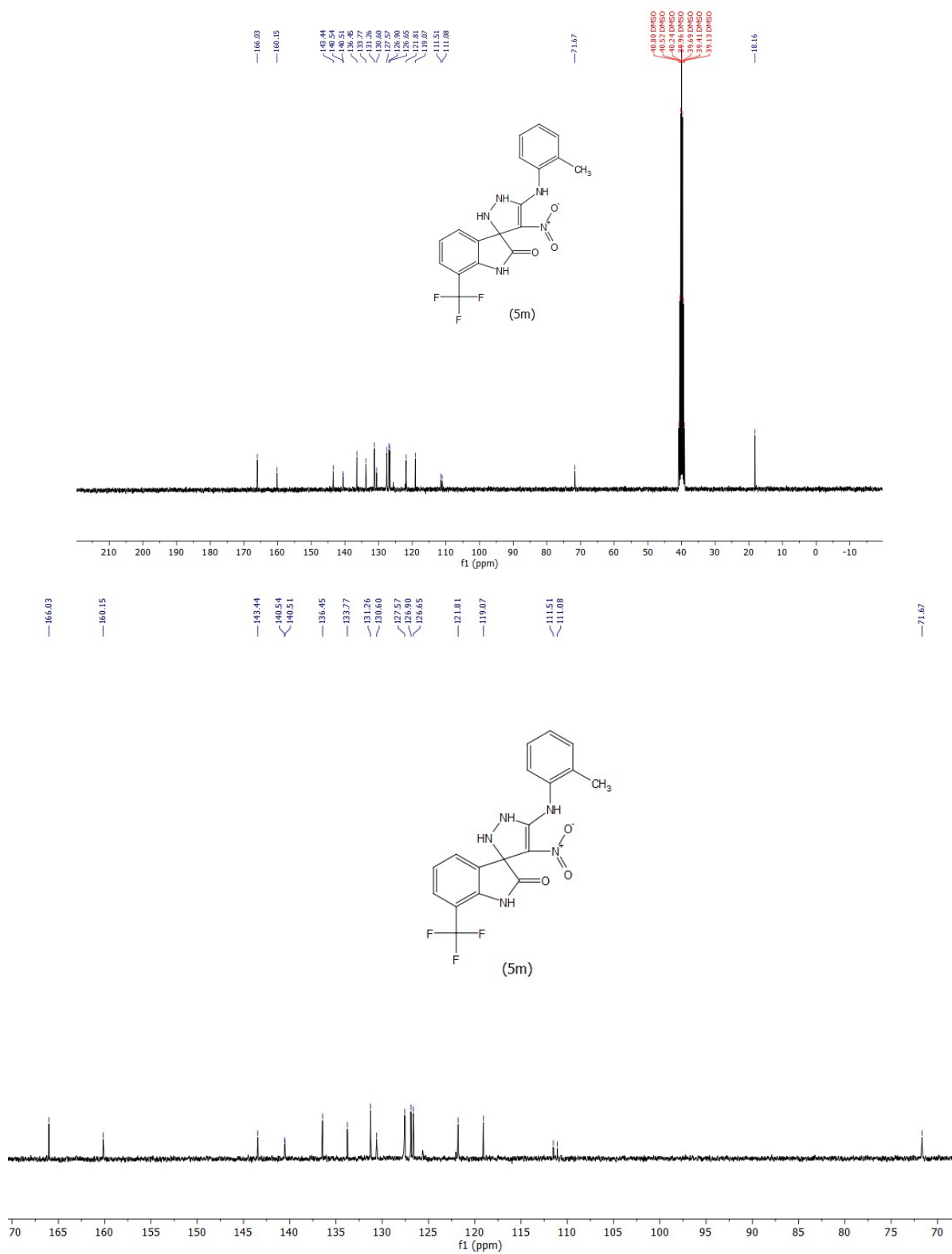
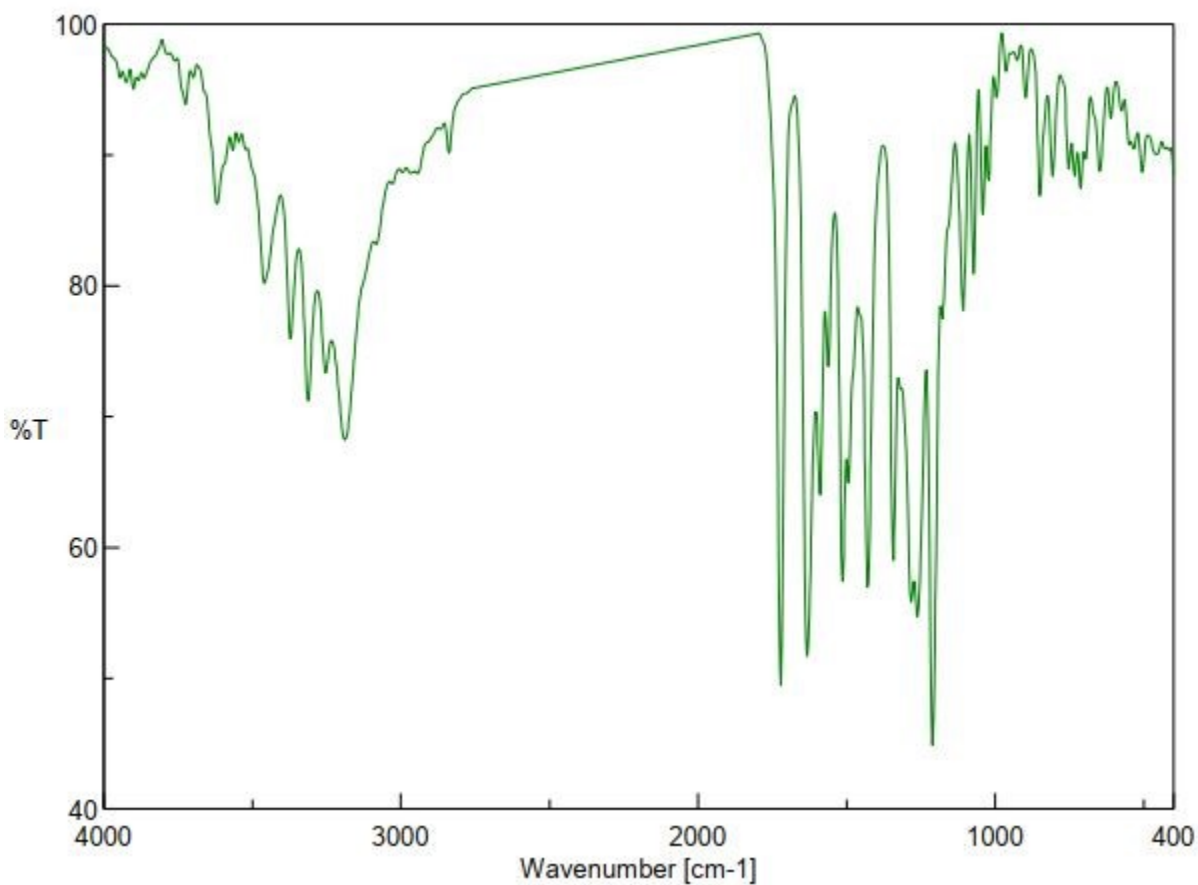


Fig S39. 4'-nitro-5'-(o-tolylamino)-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5m**)



Chromatogram C:\EAS Clarity\Work1\DATA\2g 1402.5.14_1_1_2002 6_17_28 AM_053.PRM

Result Table (ESTD - 2N 1402.5.15_1_2_2002 2_24_00 AM_058 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.297	559.797	0.264	17.13	Refer	Nitrogen	0.147
3	2.533	3814.657	0.699	52.89	Refer	Carbon	1.000
4	10.810	907.988	0.054	3.30	Refer	Hydrogen	0.238
Total			1.370	73.32			

CHN for C₁₈H₁₄F₃N₅O₃ (**5m**)

Fig S40. 5'-((3-chlorophenyl)amino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one(**5n**)

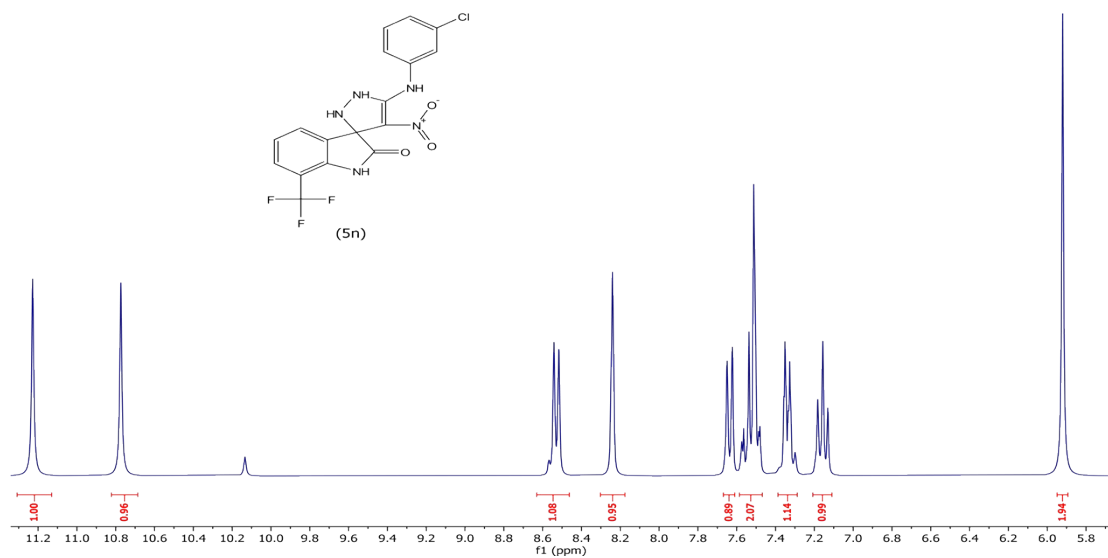
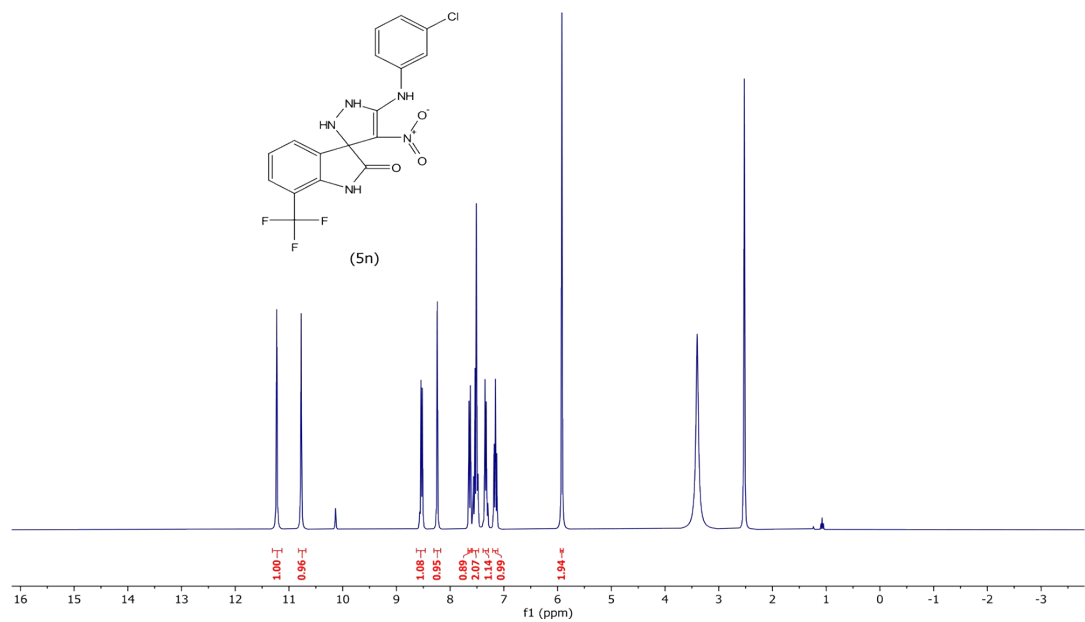


Fig S41. 5'-((3-chlorophenyl)amino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one(**5n**)

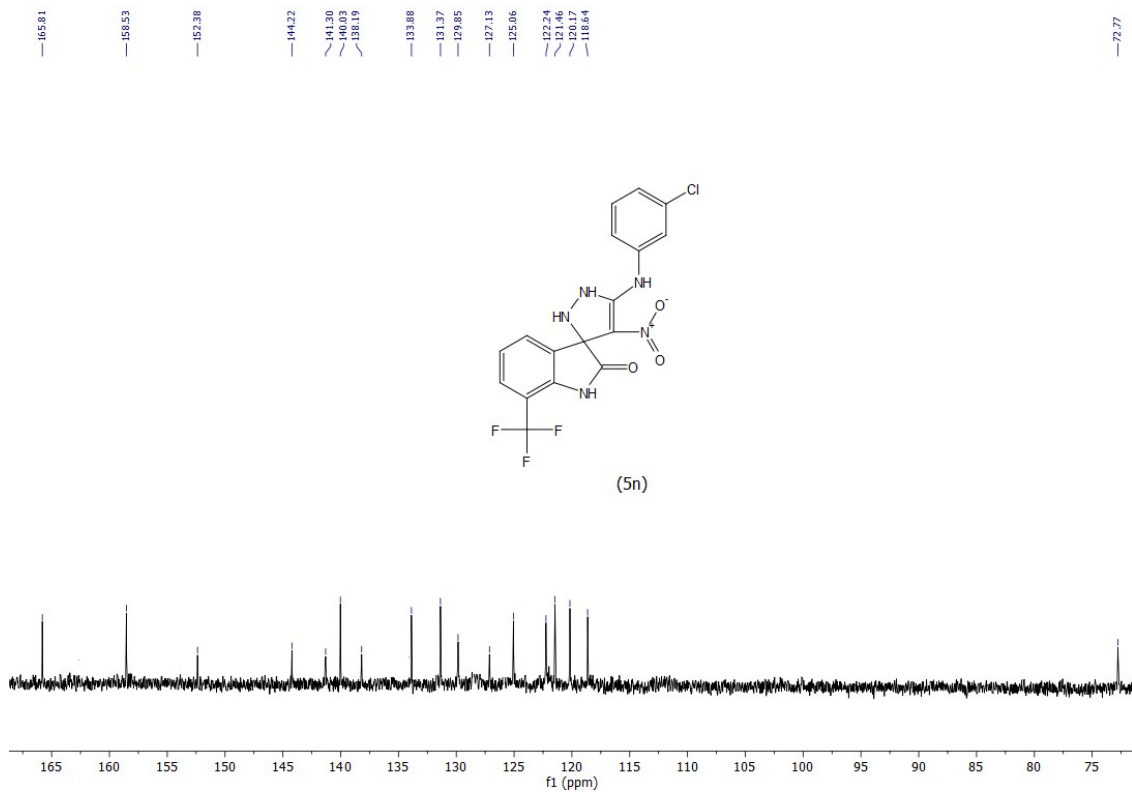
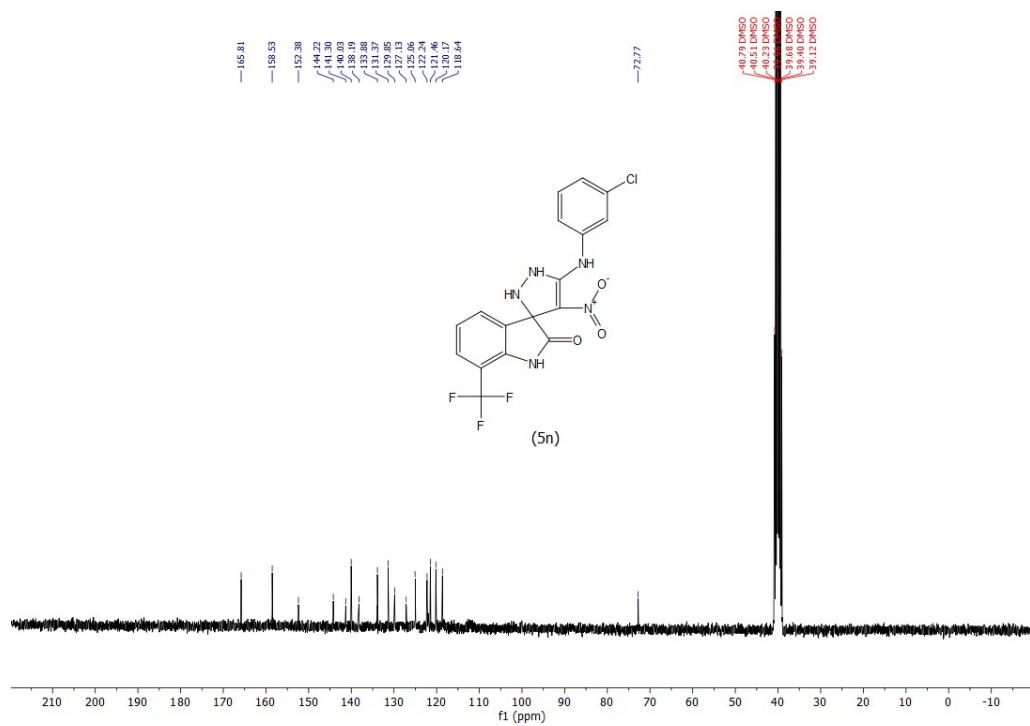
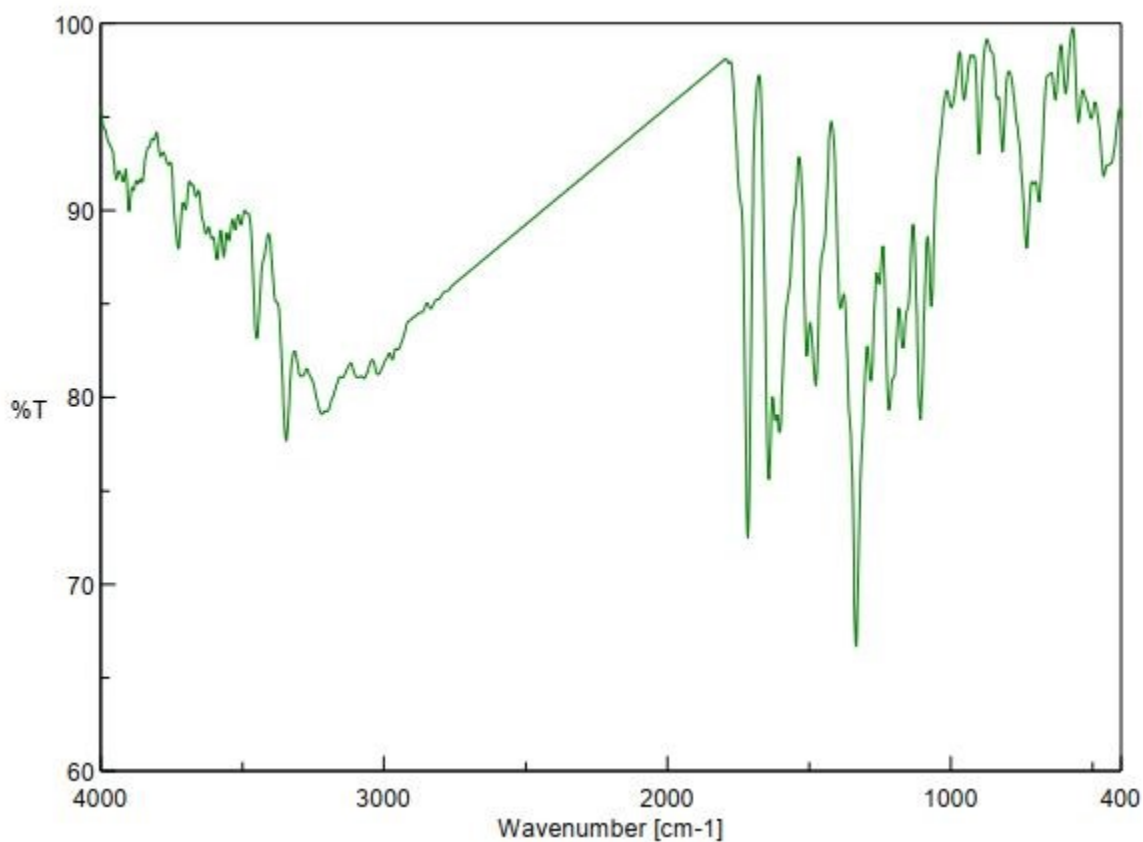


Fig S42. 5'-((3-chlorophenyl)amino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one(**5n**)



Chromatogram C:\EAS Clarity\WORK1\Data\2r 1402.5.15_1_2_2002 2_54_00 AM_059.PRM

Result Table (ESTD – 2r 1402.5.15_1_2_2002 2_54_00 AM_059 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.293	294.808	0.124	16.79	Refer	Nitrogen	0.131
3	2.607	2279.781	0.390	48.55	Refer	Carbon	1.000
4	12.220	291.768	0.013	2.78	Refer	Hydrogen	0.185
Total			0.866	68.12			

CHN for C₁₇H₁₁ClF₃N₅O₃ (**5n**)

Fig S43. 5'-(naphthalen-1-ylamino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5o**)

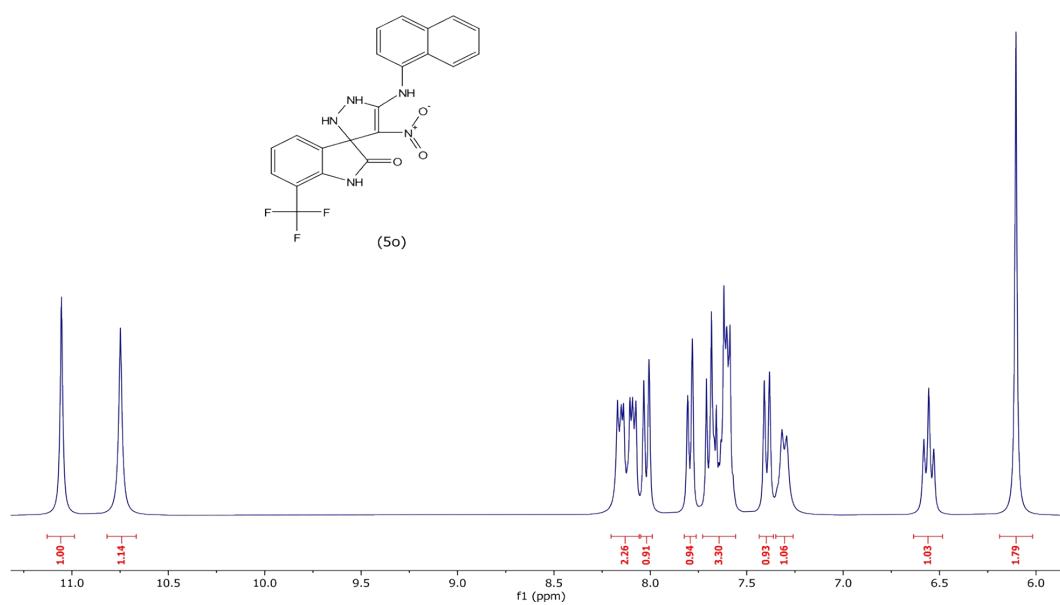
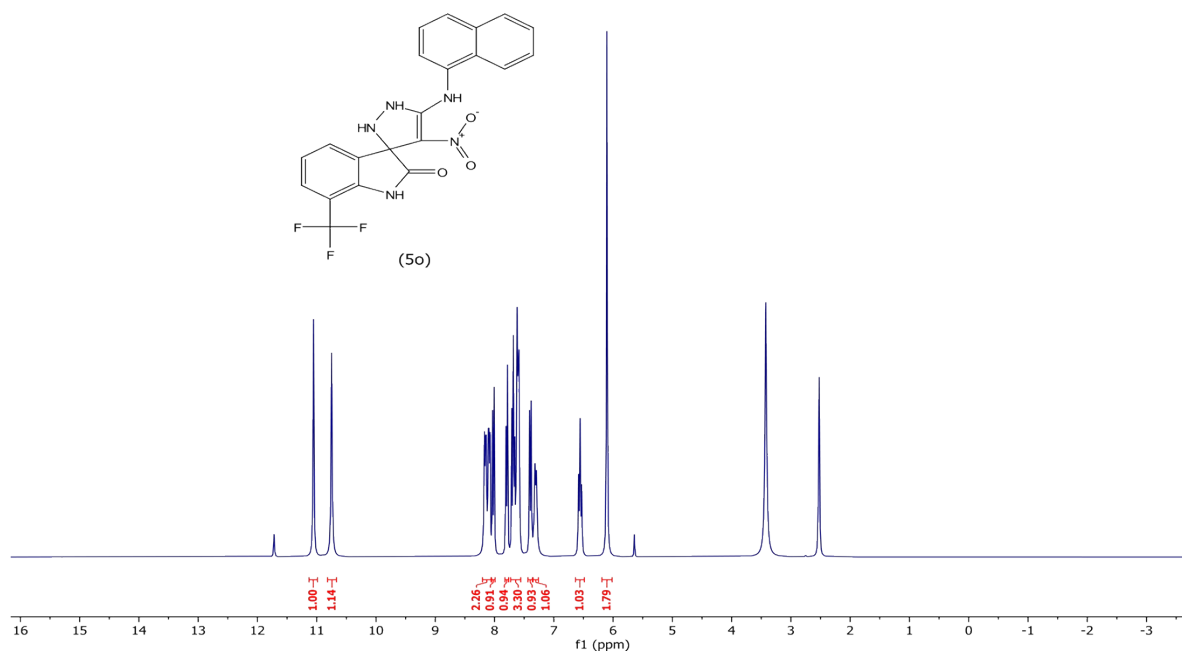


Fig S44. 5'-(naphthalen-1-ylamino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**50**)

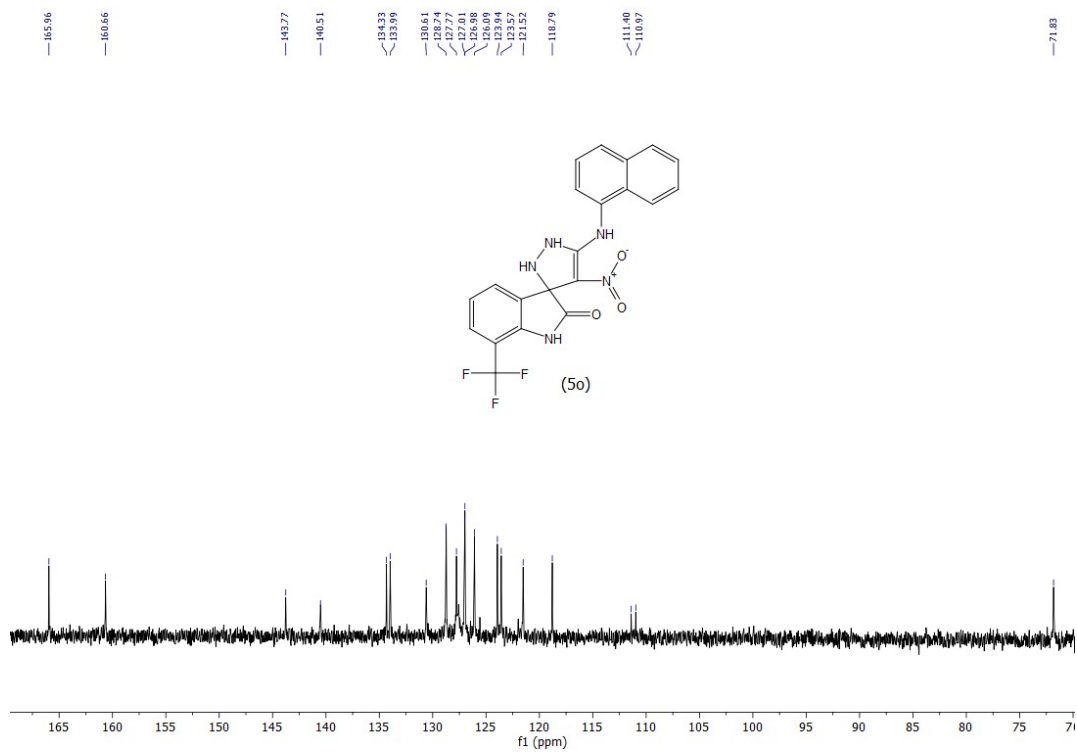
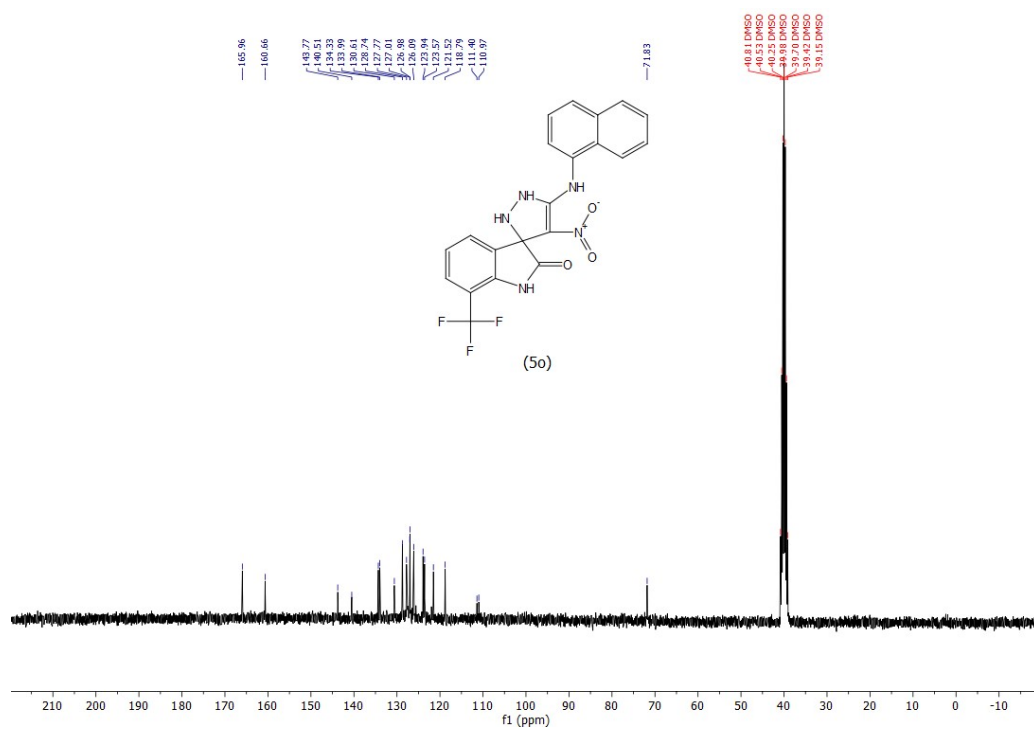


Fig S45. 5'-(naphthalen-1-ylamino)-4'-nitro-7-(trifluoromethyl)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5o**)

Chromatogram C:\EAS Clarity\WORK1 \DATA\2i 1402.5.15_1_2_2002 4_24_00 AM_062.PRM

Result Table (ESTD – 2i 1402.5.15_1_2_2002 4_24_00 AM_062 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.320	322.499	0.138	15.88	Refer	Nitrogen	0.143
3	2.635	2257.372	0.386	57.44	Refer	Carbon	1.000
4	11.985	448.038	0.023	3.63	Refer	Hydrogen	0.232
	Total		1.118	76.95			

CHN for C₂₁H₁₄F₃N₅O₃ (**5o**)

Fig S46. 5-chloro-4'-(o-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5p**)

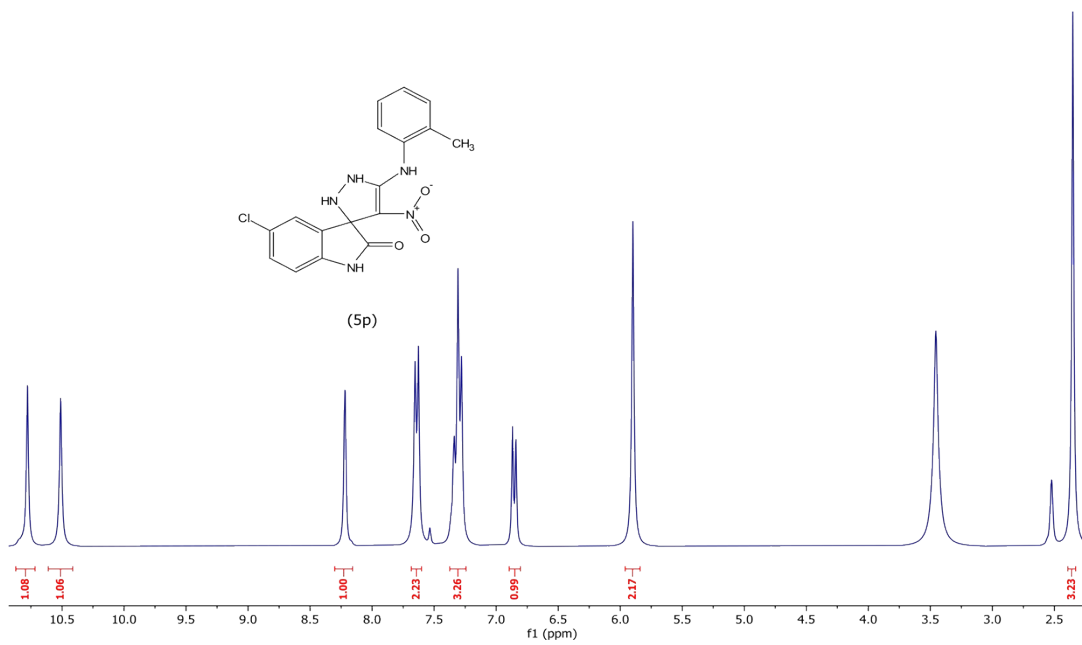
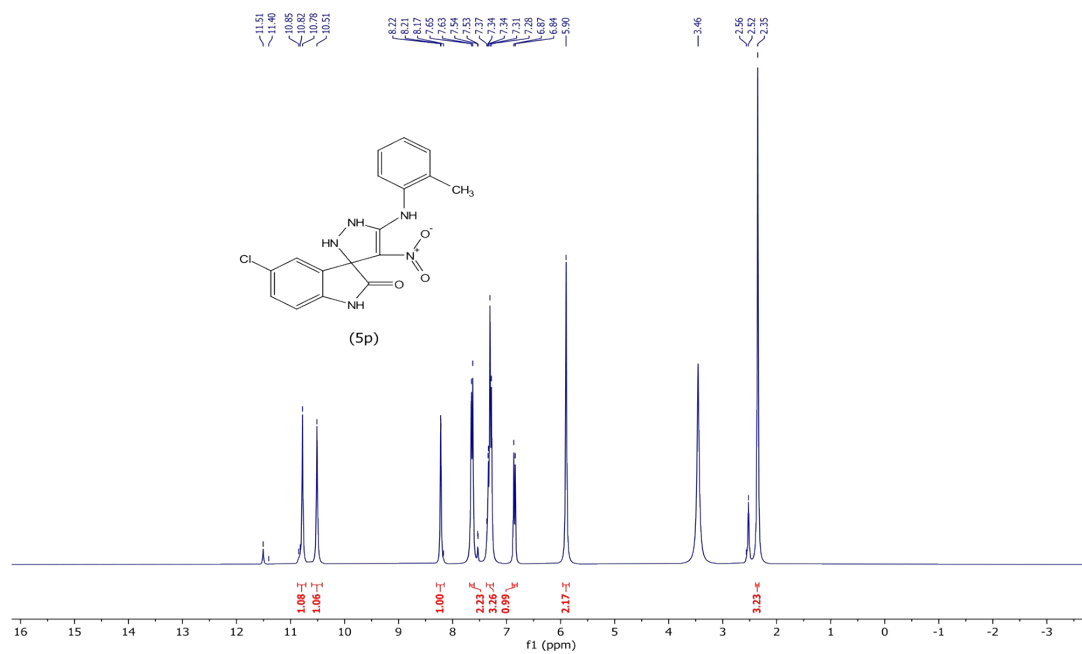


Fig S47. 5-chloro-4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5p**)

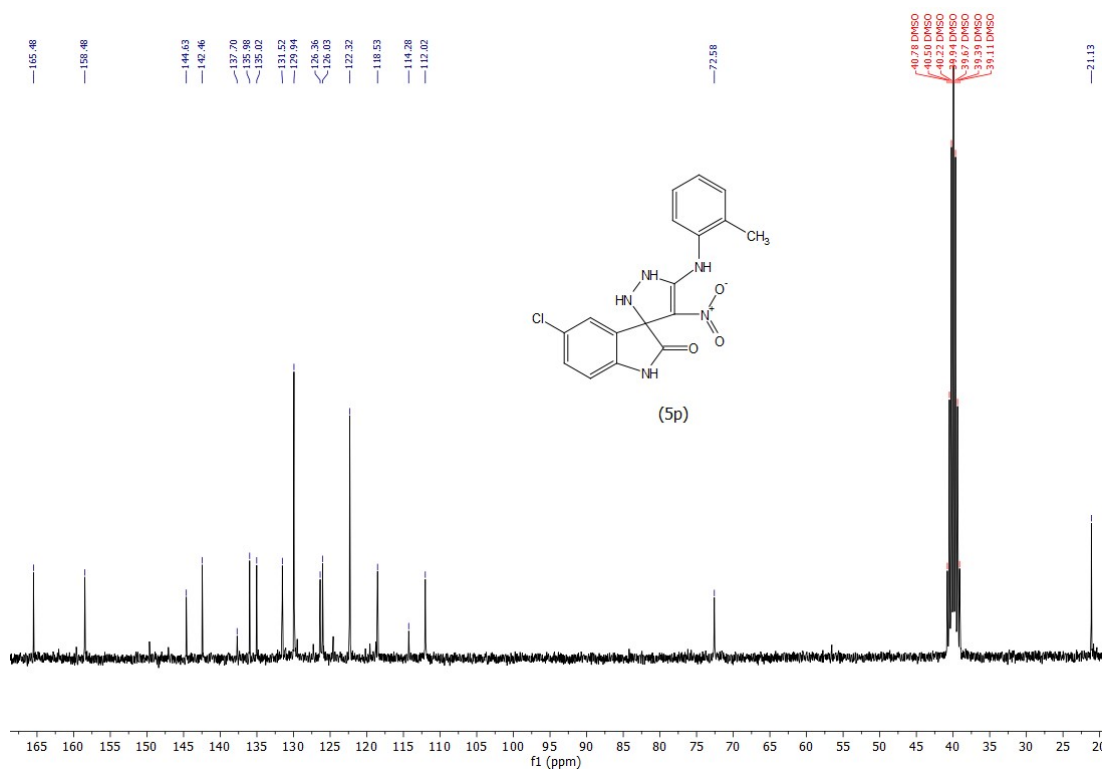
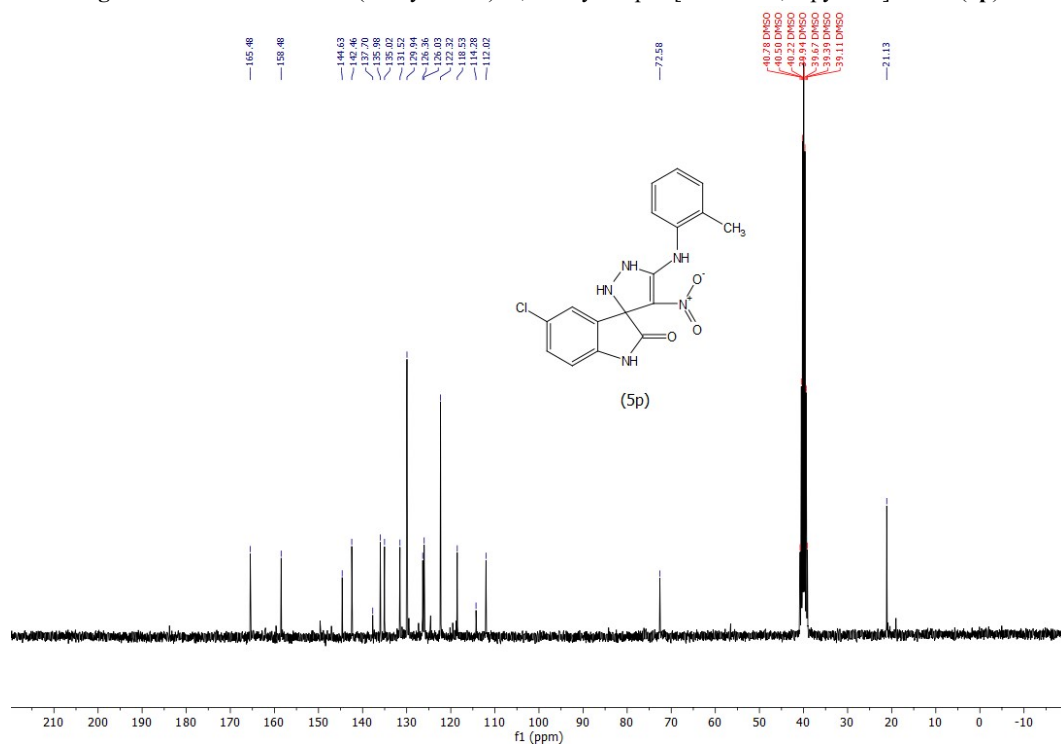
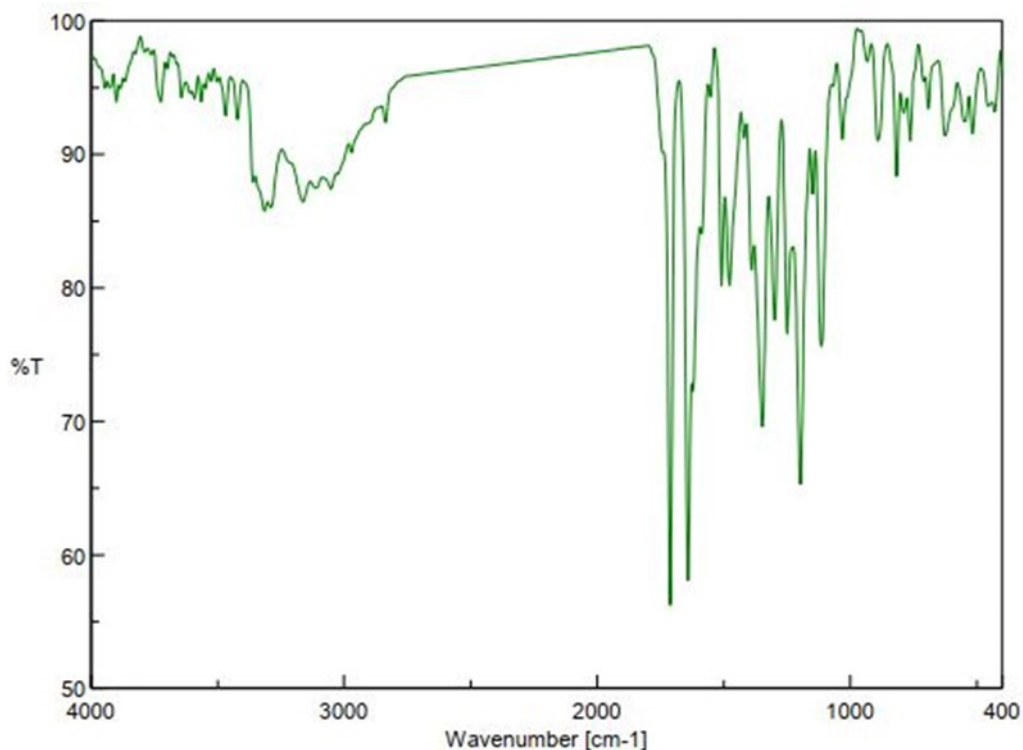


Fig S48. 5-chloro-4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5p**)



Chromatogram C:\EAS Clarity\WORK1\Data\2t 1402.5.15_1_1_2002 2_54_01 AM_060.PRM

Result Table (ESTD – 2t 1402.5.15_1_1_2002 2_54_01 AM_060 - INT7 - 1)

	Reten. Time [min]	Response	Weight [mg]	Weight [%]	Peak Type	Element Name	Carbon Response Ratio
1	1.265	798.808	0.226	19.11	Refer	Nitrogen	0.129
3	2.305	2142.781	0.530	54.49	Refer	Carbon	1.000
4	10.223	980.768	0.045	3.82	Refer	Hydrogen	0.205
	Total		0.801	77.42			

CHN for C₁₇H₁₄ClN₅O₃ (**5p**)

Fig S49. 5-bromo-4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5q**)

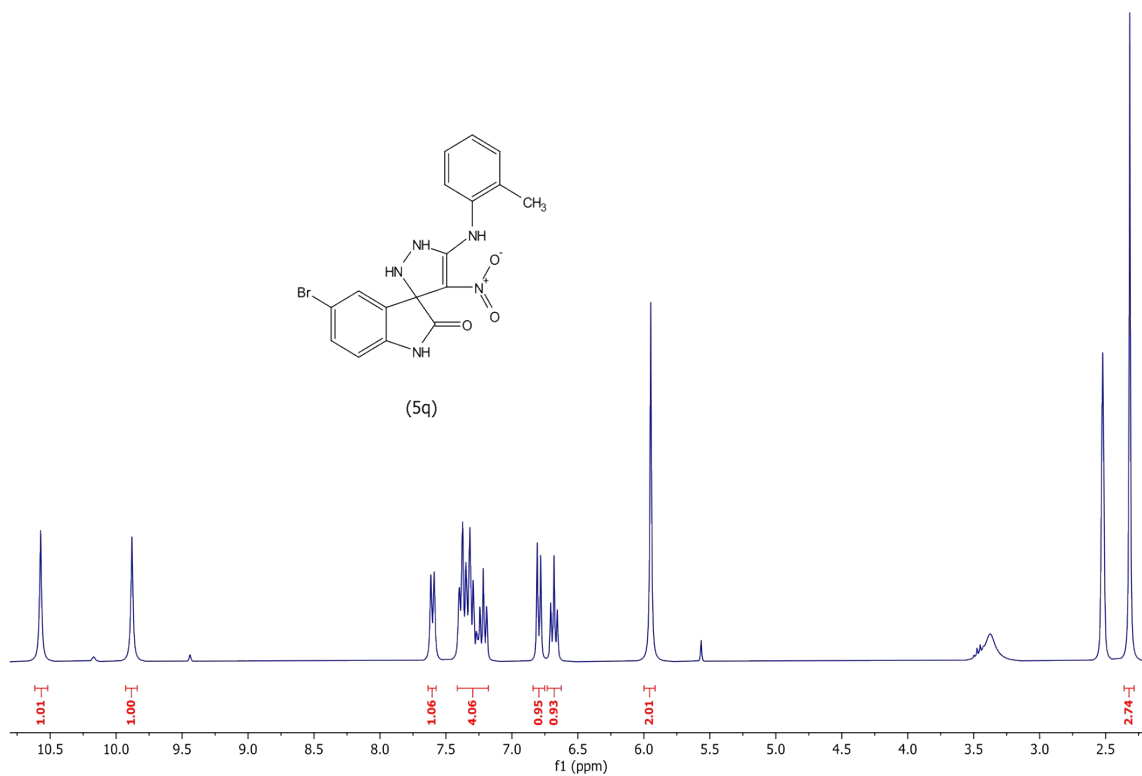
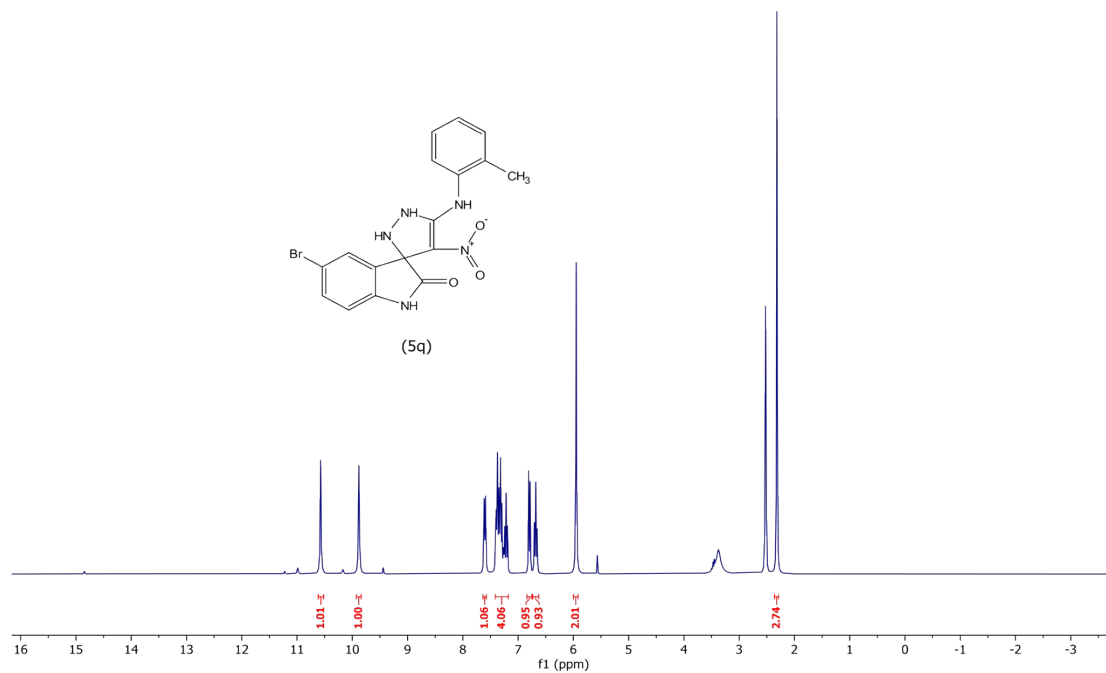


Fig S50. 5-bromo-4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5q**)

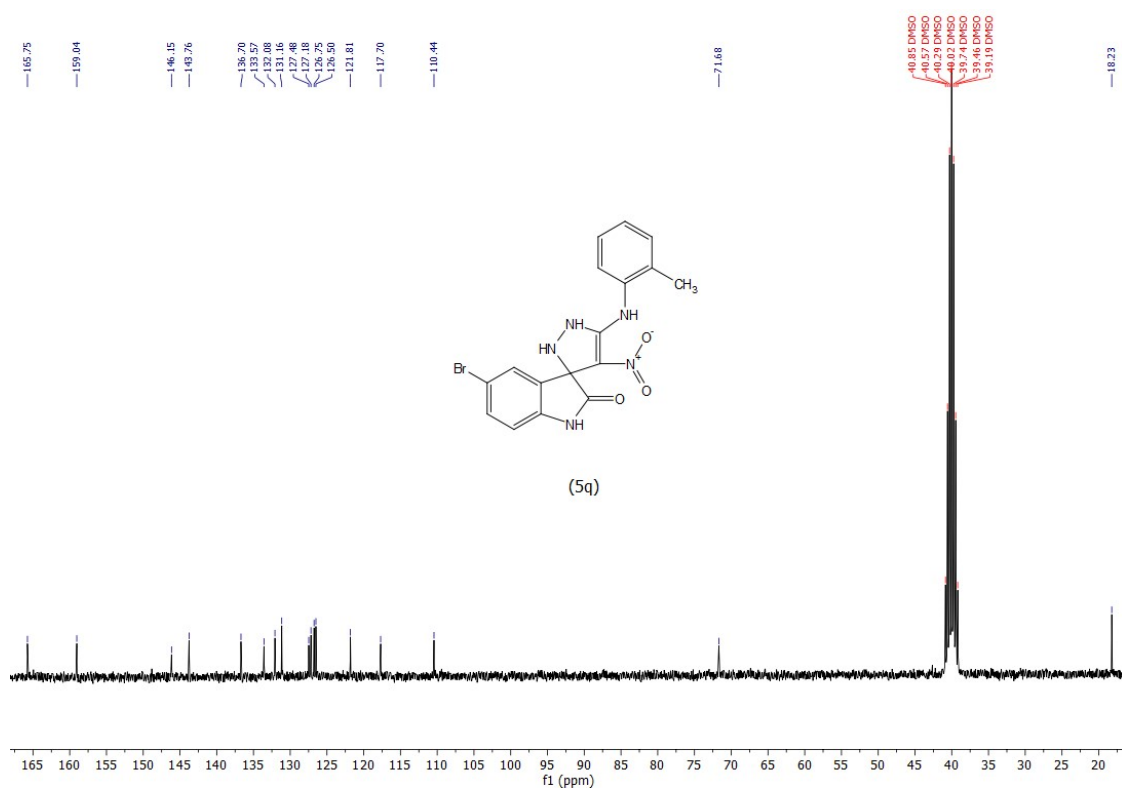
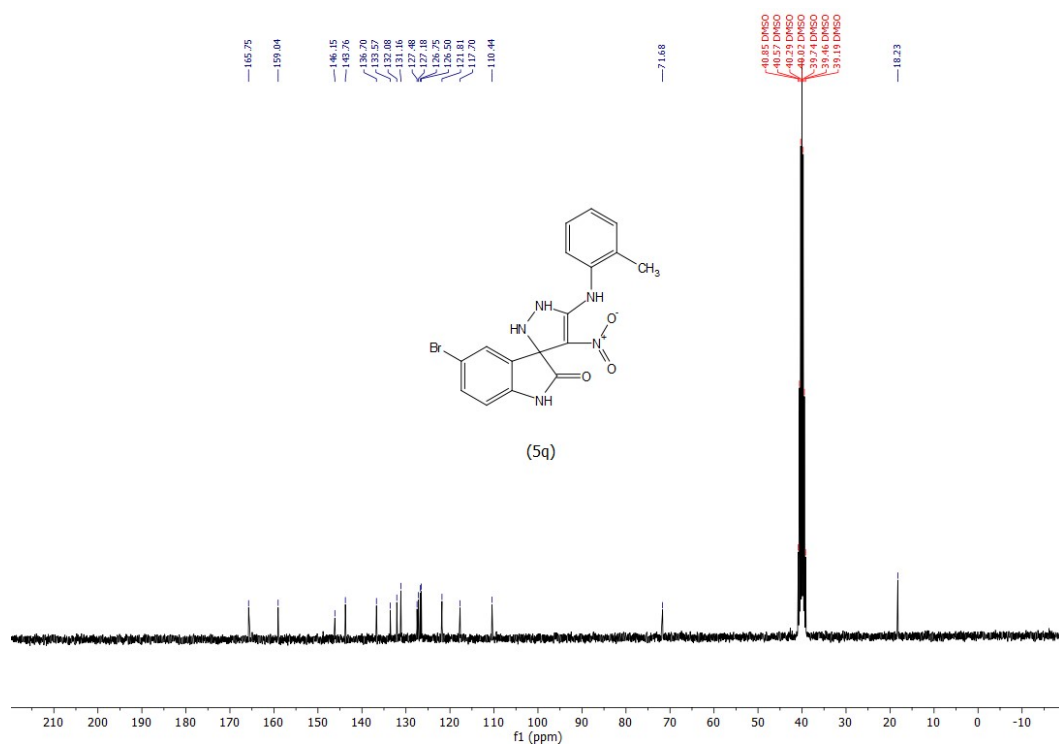


Fig S51. 5-bromo-4'-nitro-5'-(o-tolylamino)-1',2'-dihydrospiro[indoline-3,3'-pyrazol]-2-one (**5q**)

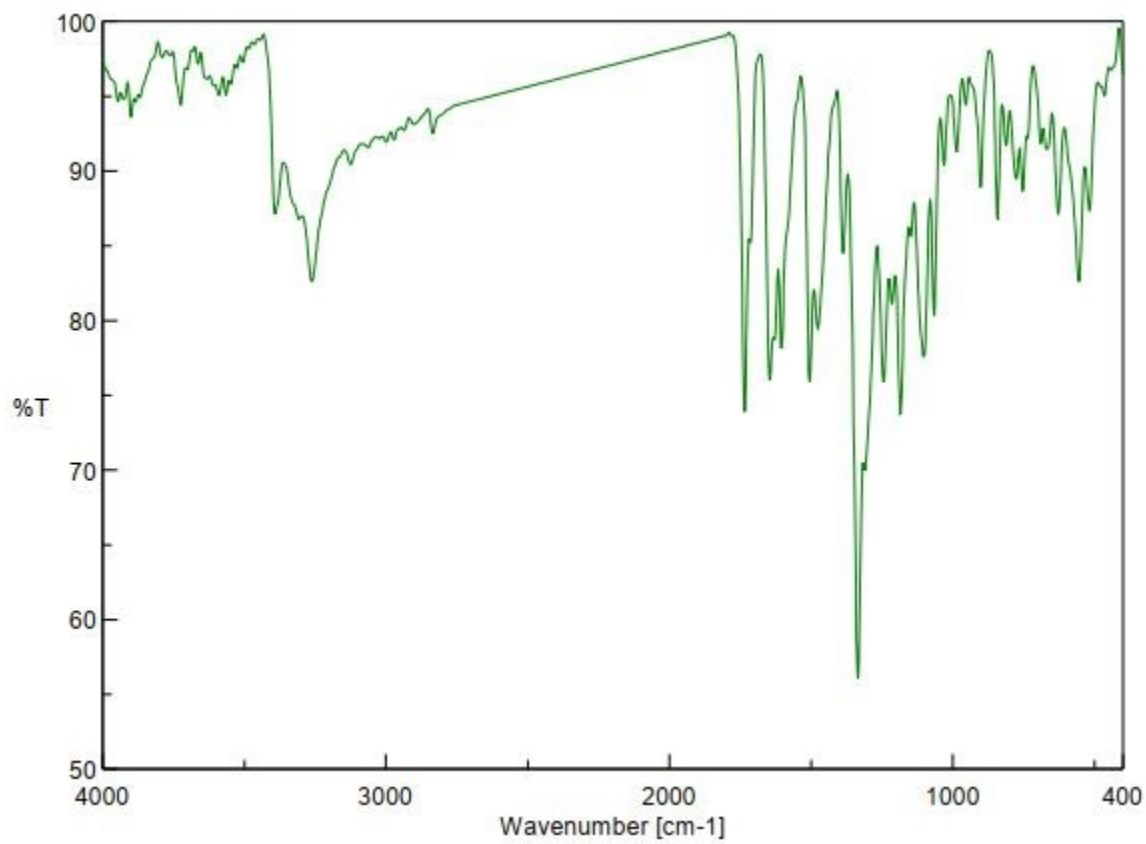


Table S1. Results of molecular docking study of **5a-q** against AChE binding site

Entry	Binding energy	Moiety of compound	Distance	Residue	Type of interactions
5a	-7.297	Spiroindoline Spiroindoline NO ₂ of spiroindoline	4.60 4.05 4.14	Phe297 Tyr341 Trp86	Pi-pi-stack Pi-pi-stack Pi-cation
5b	-7.014	Phenyl Pyrazole NO ₂ of Pyrazole	6.48 4.08 5.20	Tyr341 Tyr337 Phe295	Pi-pi-stack Pi-pi-stack Pi-cation
5c	-8.077	OH of phenyl Phenyl Phenyl NH Pyrazole Spiroindoline	3.09 4.10 3.92 1.89 4.49 4.27	Phe295 Phe297 Tyr341 Tyr124 Tyr337 Trp86	H-bound Pi-pi-stack Pi-pi-stack H-bound Pi-pi-stack Pi-pi-stack
5d	-7.239	Pyrazole Phenyl	5.18 4.36	Tyr337 Tyr341	Pi-pi-stack Pi-pi-stack)2
5e	-7.208	2,3 dimethylphenyl Pyrazole Pyrazole	5.40 5.41 5.16	Tyr124 Trp86 Tyr337	Pi-pi-stack Pi-pi-stack Pi-pi-stack
5g	-7.860	Pyrazole Pyrazole 4-Chlorophenyl	5.43 4.54 4.01	Trp86 Trp86 Tyr341	Pi-pi-stack Pi-pi-stack Pi-pi-stack
5h	-7.714	NO ₂ of Pyrazole Pyrazole Pyrazole Pyrazole Methoxy phenyl	5.91 4.74 5.25 5.14 5.14	Phe295 Tyr341 Phe338 Tyr337 Trp286	Pi-cation Pi-pi-stack Pi-pi-stack Pi-pi-stack Pi-pi-stack
5i	-6.747	Pyrazole 3,4 dimethylphenyl	4.96 5.89	Tyr337 Tyr341	Pi-pi-stack Pi-pi-stack
5j	-8.396	NH of spiroindoline NO ₂ of spiroindoline NO ₂ of Pyrazole Pyrazole Pyrazole	3.22 3.17 6.43 5.10 5.06	His447 Tyr133 Phe295 Tyr341 Phe338	H-bound H-bound Pi-cation Pi-pi-stack Pi-pi-stack
5k	-8.956	NO ₂ of Pyrazole Pyrazole Pyrazole NH of spiroindoline NO ₂ of spiroindoline	6.24 3.89 4.29 3.21 2.59	Phe295 Tyr341 Phe338 His447 Tyr133	Pi-cation Pi-pi-stack Pi-pi-stack H-bound H-bound
5l	-8.606	NO ₂ of Pyrazole Pyrazole NH of Pyrazole NO ₂ of spiroindoline	6.20 4.97 2.75 3.04	His447 Tyr337 Tyr124 Tyr133	Pi-cation Pi-pi-stack H-bound H-bound
5m	-9.010	NH of Pyrazole NH of Pyrazole Pyrazole Phenyl	2.77 2.99 3.82 5.29	Tyr341 Tyr124 Trp86 Tyr341	H-bound H-bound Pi-pi-stack Pi-pi-stack

5n	-7.510	Spiroindoline Pyrazole Pyrazole NO ₂ of Pyrazole	3.98 5.27 4.83 5.90	Trp86 Phe338 Tyr341 Phe291	Pi-pi-stack Pi-pi-stack Pi-pi-stack Pi-cation
5o	-7.472	Pyrazole Pyrazole Naphtyl Naphtyl	4.68 5.25 3.83 4.27	Trp86 Tyr337 Tyr341 Tyr341	Pi-pi-stack Pi-pi-stack Pi-pi-stack Pi-pi-stack
5p	-5.316	Spiroindoline Spiroindoline	3.67 4.20	Trp86	Pi-pi-stack Pi-pi-stack
5q	-7.234	Pyrazole NO ₂ of Pyrazole Spiroindoline Phenyl	Phe329 Trp82 Trp82 Trp231	5.27 6.05 5.34 5.38	Pi-pi-stack Pi-cation Pi-pi-stack Pi-pi-stack

Table S2. Results of molecular docking study of **5a-q** against BChE binding site

Entry	Binding energy	Moiety of compound	Distance	Residue	Type of interactions
5a	-6.593	Nitro 2-methylphenyl Pyrazole Spiroindoline	5.03 4.31 5.73 2.14	Tyr332 Trp231 His438 Asp70	Pi-cation Pi-pi-stack Pi-cation H-bound
5b	-7.010	Pyrazole Pyrazole Pyrazole Spiroindoline	3.97, 3.61 4.33 5.31 2.78	Trp82 His438 His438 Glu197	(Pi-pi-stack) 2 Pi-pi-stack Pi-cation H-bound
5c	-5.615	Nitro 4-OH phenyl Pyrazole Pyrazole spiroindoline	2.25 1.89 5.34 4.16, 4.41 5.51 2.55	Gly116 Ala328 Phe329 Trp82 Glu116 Glu197	H-bound H-bound Pi-pi-stack (Pi-pi-stack) 2 Pi-cation H-bound
5d	6.737	C=O of Spiroindoline Pyrazole Pyrazole Phenyl Phenyl	2.85 4.96 5.33 3.97 5.27	Glu197 His438 Trp82 Tyr332 Phe329	H-bound Pi-cation (Pi-pi-stack)2 Pi-pi-stack Pi-pi-stack
5e	-6.593	C=O of Spiroindoline Nitro	2.90 4.64	Glu197 Trp82	H-bound Pi-cation
5f	-5.530	C=O of Spiroindoline Nitro	2.94 5.85	Glu197 Trp82	H-bound Pi-cation
5g	-5.517	C=O of Spiroindoline Pyrazole Pyrazole	2.92 5.53 4.49	Glu197 His438 Trp82	H-bound Pi-cation Pi-pi-stack)2

5h	-6.145	NH of Spiroindoline Spiroindoline Pyrazole	2.89 4.22 5.16	His438 Trp82 Trp82	H-bound (Pi-pi-stack)2 Pi-pi-stack
5i	-7.095	NH of Spiroindoline Spiroindoline	2.99 4.02	His438 Trp82	H-bound (Pi-pi-stack)2
5j	-6.831	NO ₂ of Pyrazole Pyrazole NO ₂ of Spiroindoline NO ₂ of Spiroindoline NO ₂ of Spiroindoline	3.33 5.28 4.21 4.55 6.26	Gly116 Phe329 His438 Phe329 Trp231	H-bound Pi-pi-stack Pi-cation Pi-cation Pi-cation
5k	-6.146	C=O of Spiroindoline Spiroindoline NO ₂ of Spiroindoline NO ₂ of Spiroindoline NO ₂ of Pyrazole	2.68 3.97 4.16 4.65 3.99	Tyr332 Trp82 Trp82 Glu197 Phe329	H-bound Pi-pi-stack Pi-cation)2 H-bound Pi-cation
5l	-6.278	NH of Spiroindoline Pyrazole Spiroindoline NO ₂ of Pyrazole NO ₂ of Pyrazole	2.97 4.95 3.91 5.24 4.46	His438 Trp82 Trp82 His438 His438	H-bound Pi-pi-stack Pi-pi-stack)2 Pi-cation Salt bridge
5m	-6.592	NO ₂ of Pyrazole NO ₂ of Pyrazole Spiroindoline	3.00 2.85 4.96	His438 Gly116 Trp231	H-bound H-bound Pi-pi-stack)2
5n	-6.307	NO ₂ of Pyrazole Spiroindoline	2.94 5.40	His438 Trp231	H-bound Pi-pi-stack)2
5o	-6.213	NO ₂ of Pyrazole Pyrazole naphtyl	5.36 3.12 4.14	Tyr332 Thr120 Trp82	Pi-cation H-bound Pi-pi-stack
5p	-7.886	NH of Spiroindoline Spiroindoline Pyrazole Phenyl	2.97 3.60 3.91 3.87	His438 Trp82 Tyr332 Tyr332	H-bound Pi-pi-stack)2 H-bound Pi-pi-stack
5q	-6.372	Pyrazole NO ₂ of Pyrazole Spiroindoline Phenyl	Phe329 Trp82 Trp82 Trp231	5.27 6.05 5.34 5.38	Pi-pi-stack Pi-cation Pi-pi-stack Pi-pi-stack