Supplementary Materials

Synthesis and Evaluation of Sulfonamide Derivatives of Quinoxaline 1,4-dioxides as Carbonic Anhydrase Inhibitors

Galina I. Buravchenko [a], Alexander M. Scherbakov [b], Diana I. Salnikova [b], Stepan K. Krymov [a], George V. Zatonsky [a], Dominique Schols [c], Daniela Vullo,[d] Claudiu T. Supuran [d], Andrey E. Shchekotikhin [a*]

[a] Gause Institute of New Antibiotics, 11 B. Pirogovskaya Street, Moscow, 119021, Russia; buravchenkogi@gmail.com; krymov.s.k@gmail.com; gzatonsk@gmail.com; shchekotikhin@mail.ru

[b] Department of Experimental Tumor Biology, Institute of Carcinogenesis, Blokhin N.N. National Medical Research Center of Oncology, Kashirskoe sh. 24, 115522 Moscow, Russia; dianasalnikova08@yandex.ru; alex.scherbakov@gmail.com.

[c] Rega Institute for Medical Research, KU Leuven, 3000 Leuven, Belgium, dominique.schols@kuleuven.be.

[d] Department of NEUROFARBA, Section of Pharmaceutical and Nutraceutical Sciences, University of Florence, Florence, Italy, daniela.vullo@unifi.it ; claudiu.supuran@unifi.it.

*Corresponding authors e-mail address: Andrey E. Shchekotikhin shchekotikhin@gause-inst.ru.

Legends to Figures and Tables

Figure S1-S36. ^{1}H and ^{13}C NMR spectra of the compounds **7a-h**; **8a-c**; **8g**; **11-12**; **14-16**. **S2**

Figure S37-S53. Copies of HRMS ESI spectra of the compounds **7a-h**; **8a-c**; **8g**; **11-12**; **14-16**. **S20**

Figure S55-S67. Copies of HPLC spectra of the compounds **7a-h**; **8a-c**; **8g**. **S38**

Figure S68-S70. Copies of 2D NMR spectra of **7a**. **S51**

Copies of NMR Spectra

Figure S1. Copy of ^{1}H NMR spectrum of the derivative **7a**.

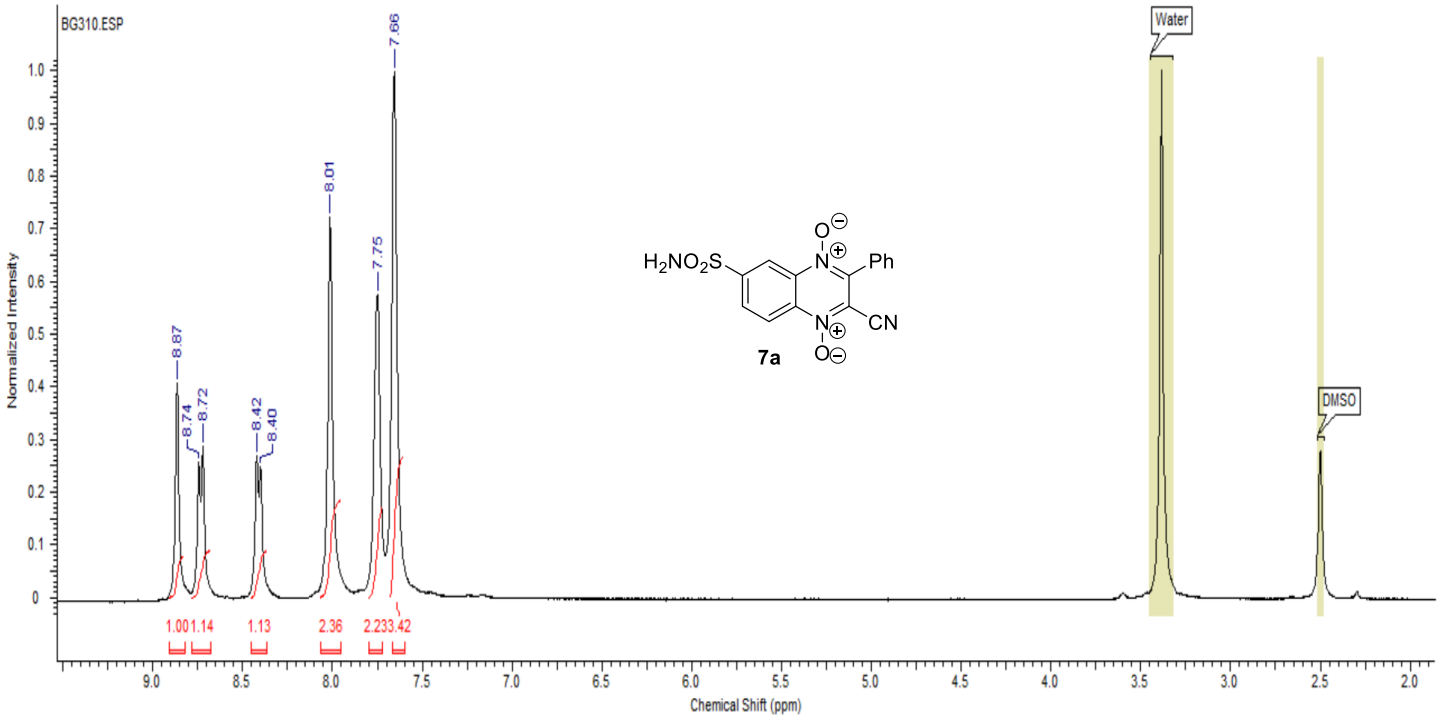


Figure S2. Copy of ^{13}C NMR spectrum of the derivative **7a**.

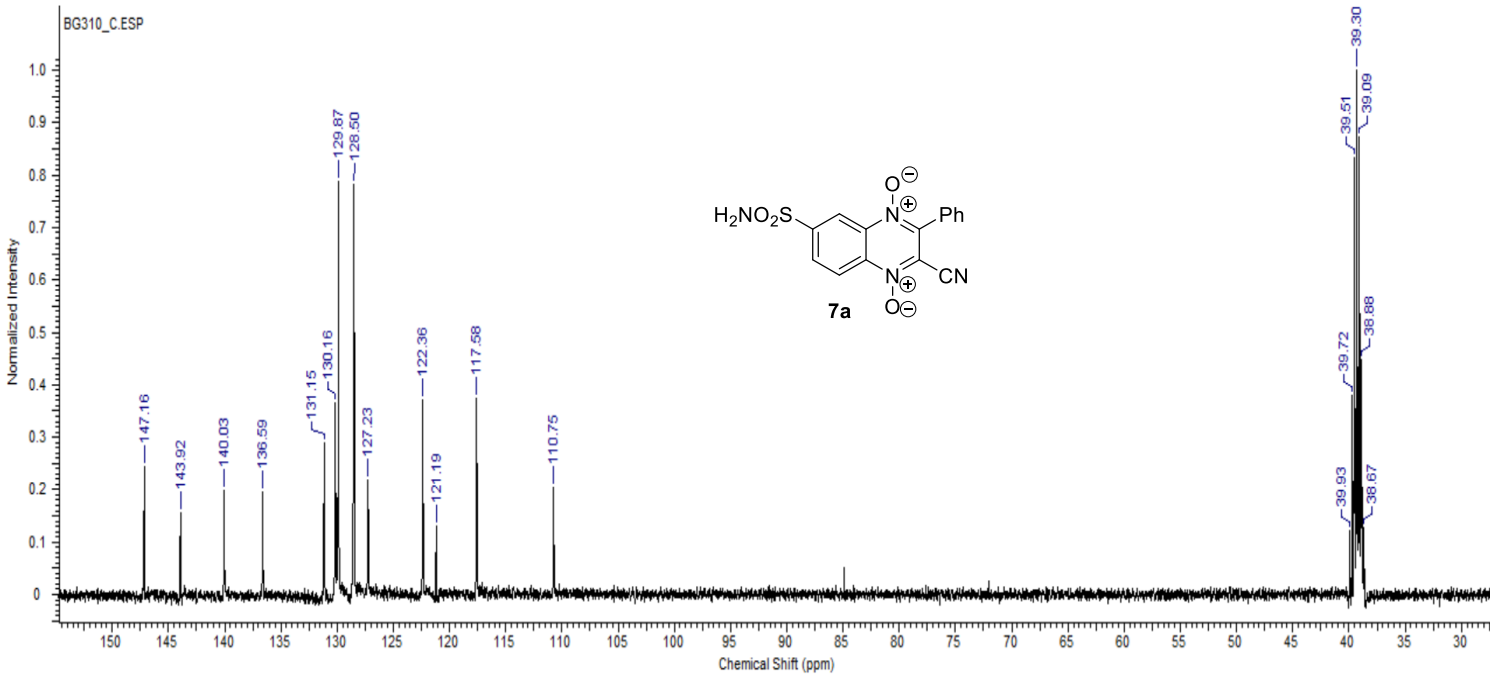


Figure S3. Copy of ^{1}H NMR spectrum of the derivative **7b**.

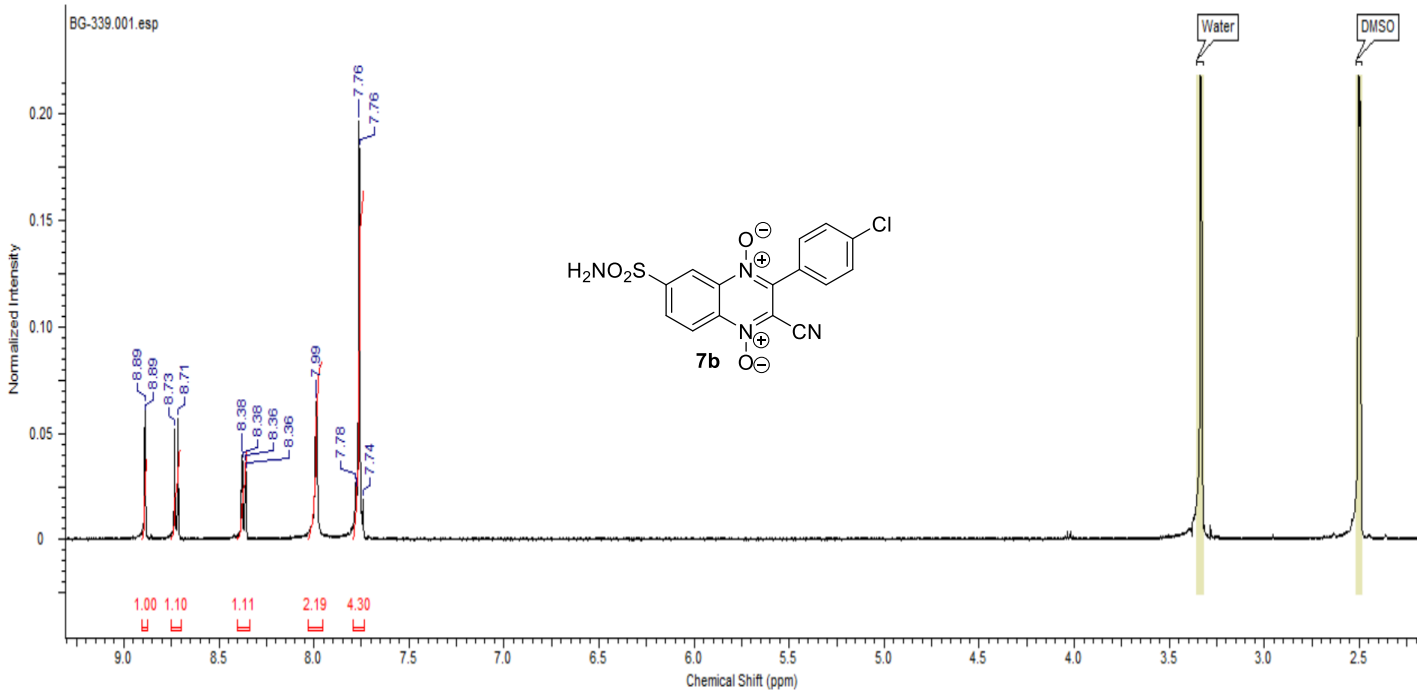


Figure S4. Copy of ^{13}C NMR spectrum of the derivative **7b**.

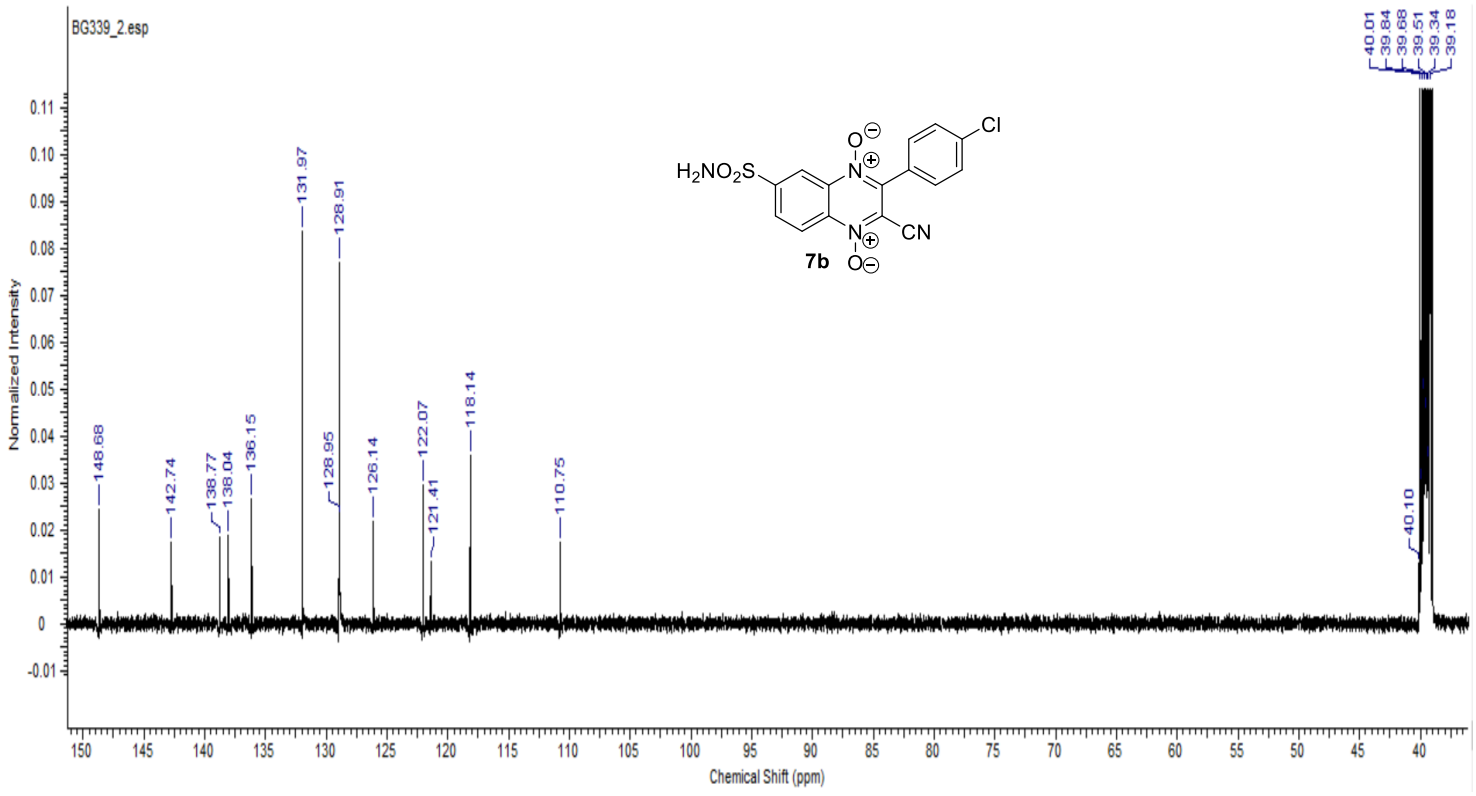


Figure S5. Copy of ^{1}H NMR spectrum of the derivative **7c**.

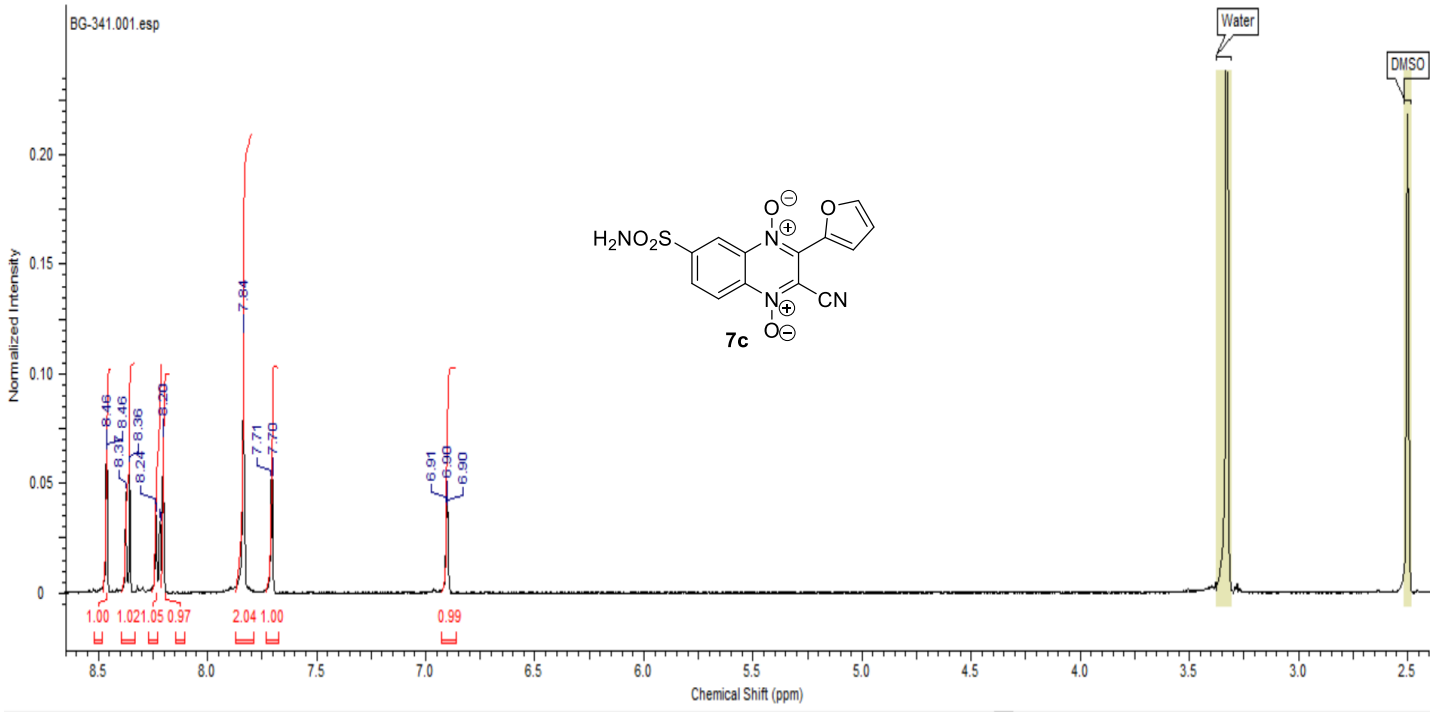


Figure S6. Copy of ^{13}C NMR spectrum of the derivative **7c**.

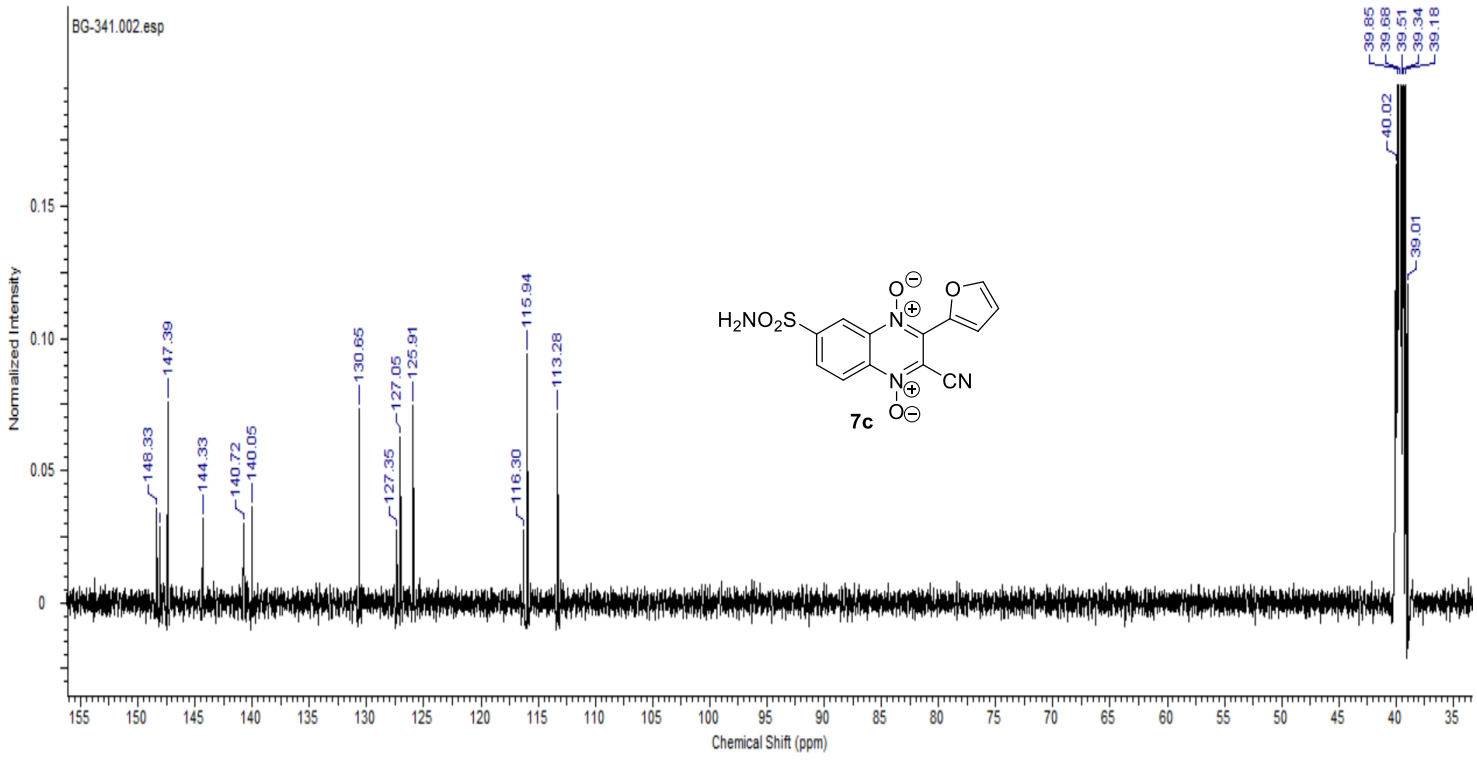


Figure S7. Copy of ^{1}H NMR spectrum of the derivative **7d**.

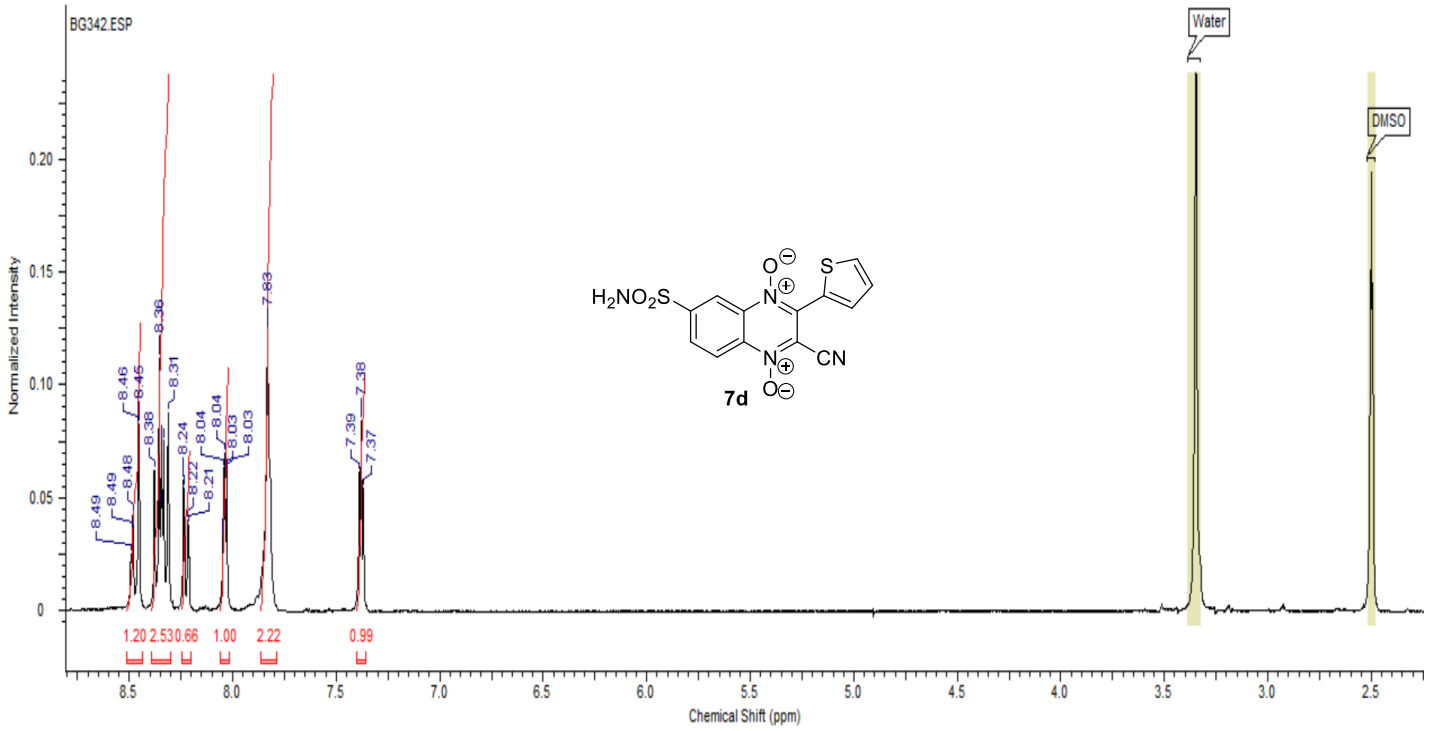


Figure S8. Copy of ^{13}C NMR spectrum of the derivative **7d**.

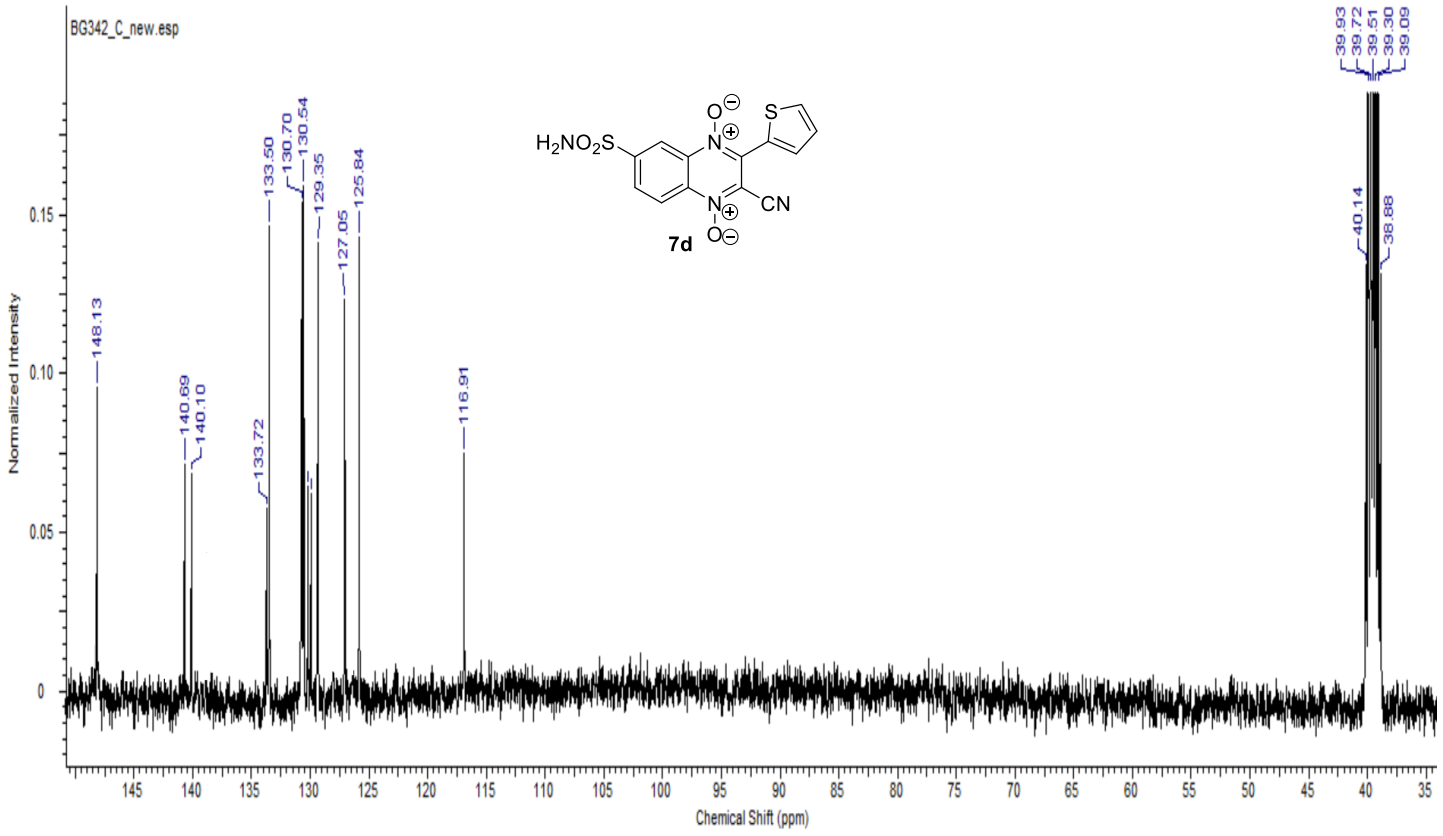


Figure S9. Copy of ^{1}H NMR spectrum of the derivative **7e**.

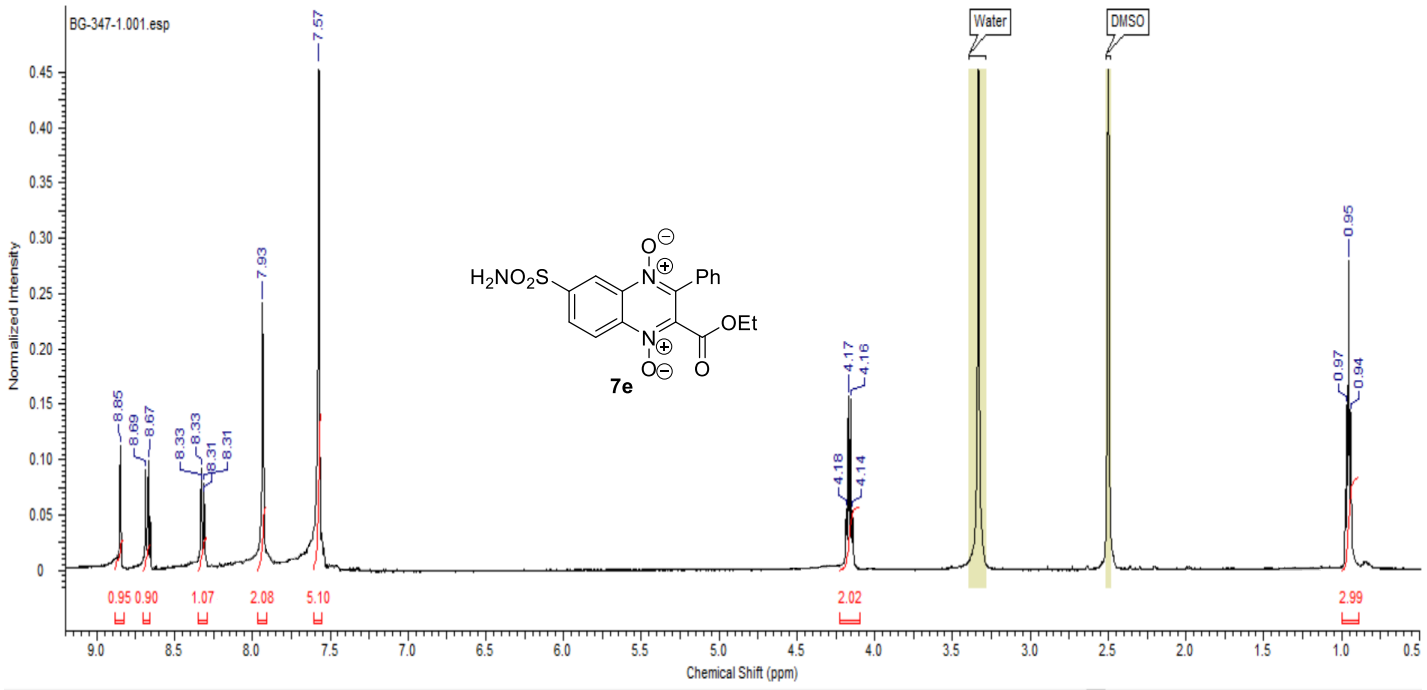


Figure S10. Copy of ^{13}C NMR spectrum of the derivative **7e**.

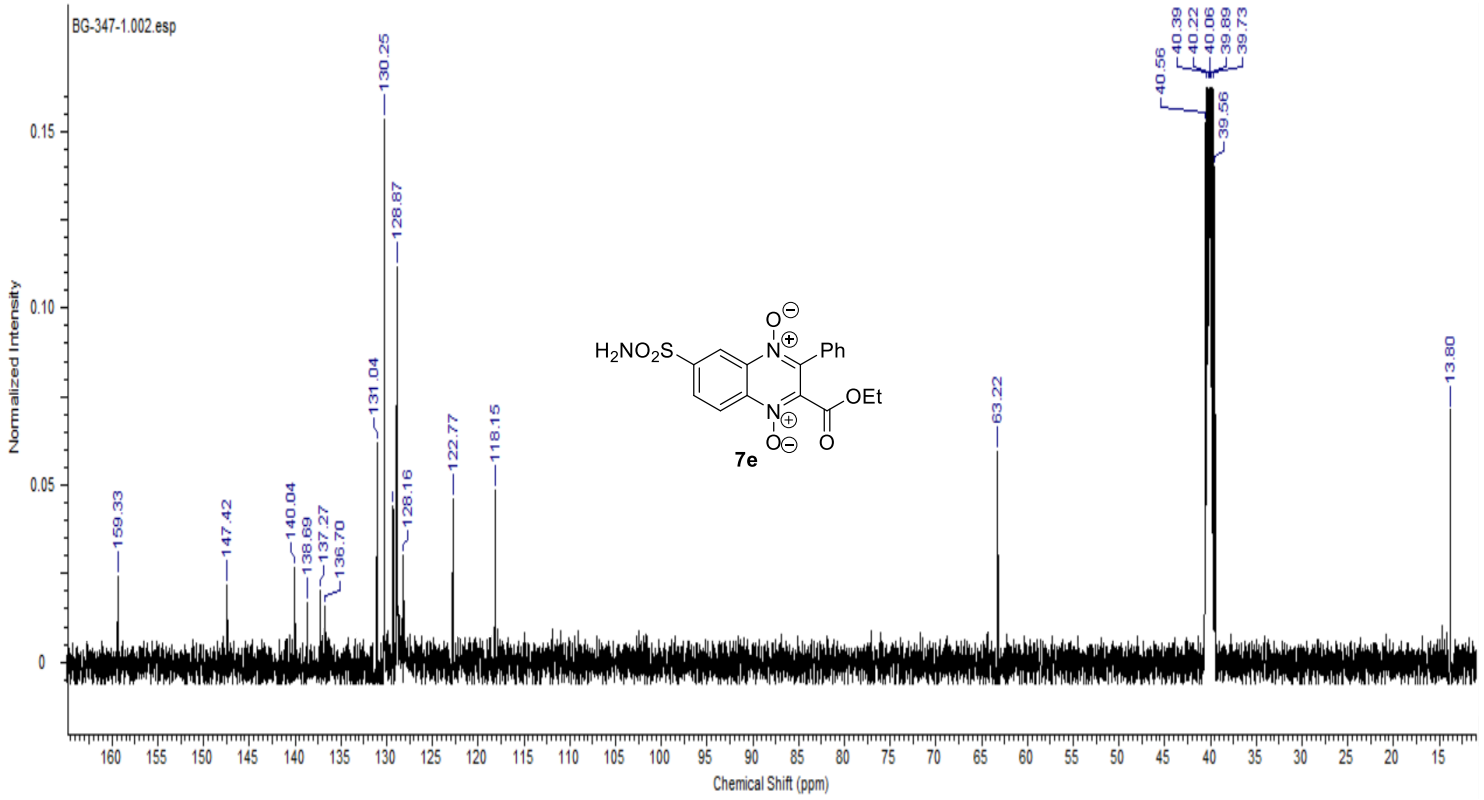


Figure S11. Copy of ^{1}H NMR spectrum of the derivative **7f**.

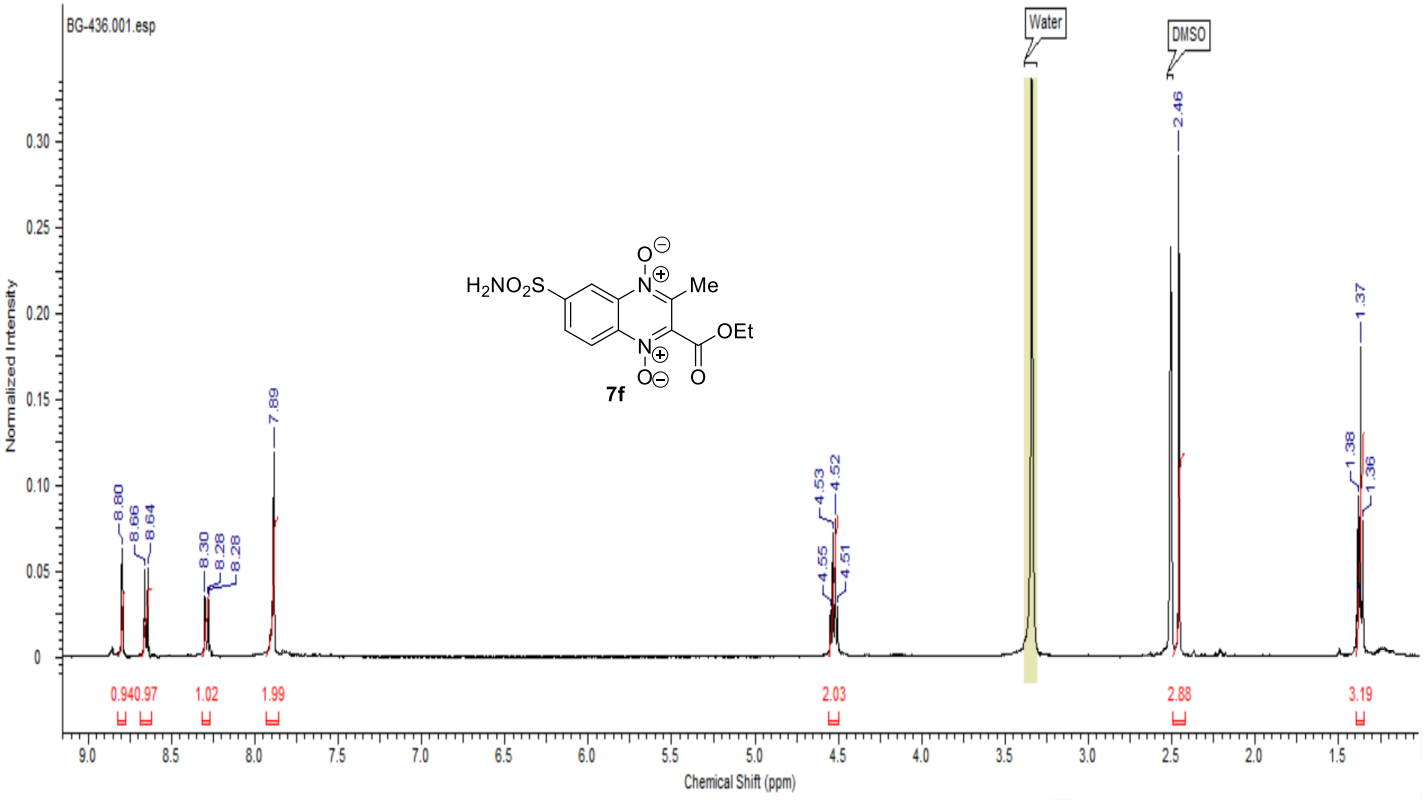


Figure S12. Copy of ^{13}C NMR spectrum of the derivative **7f**.

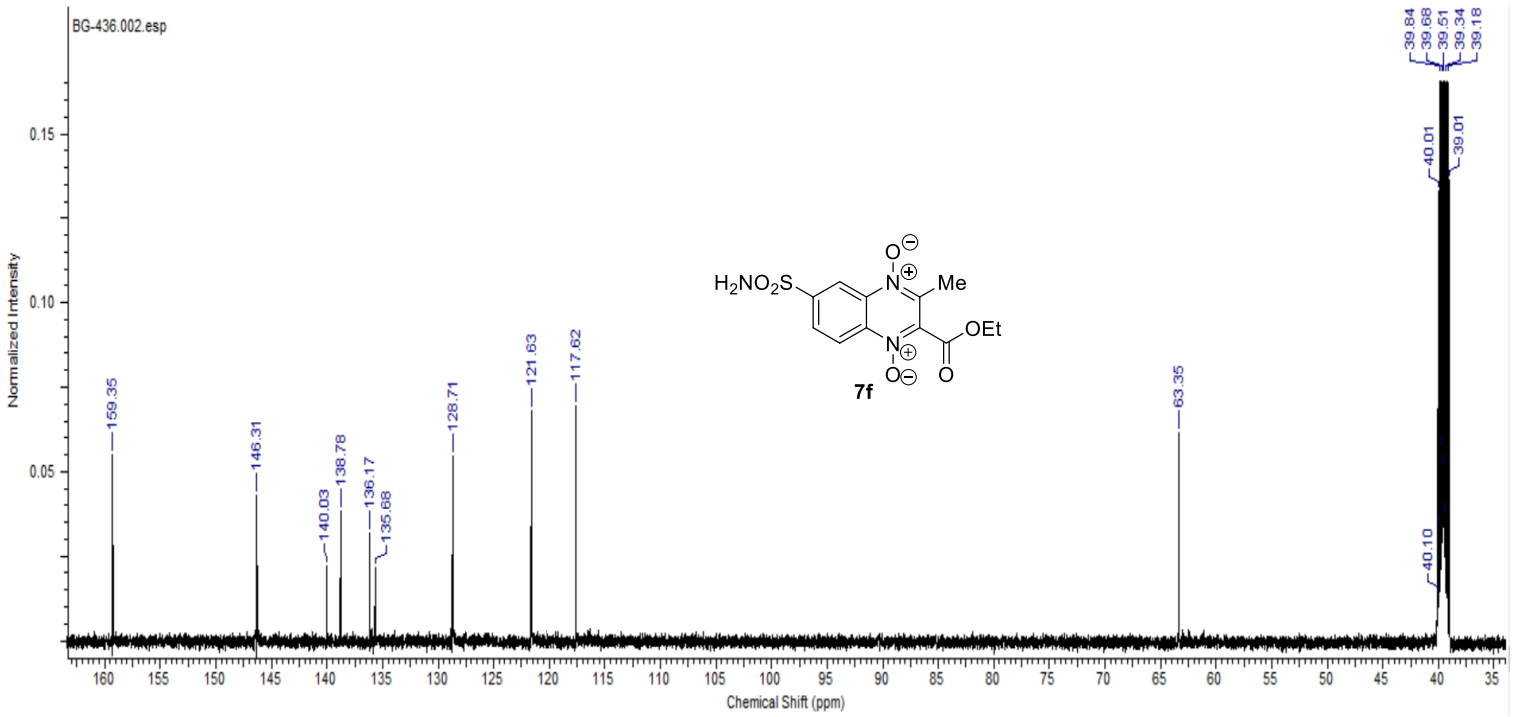


Figure S13. Copy of ^{1}H NMR spectrum of the derivative **7g**.

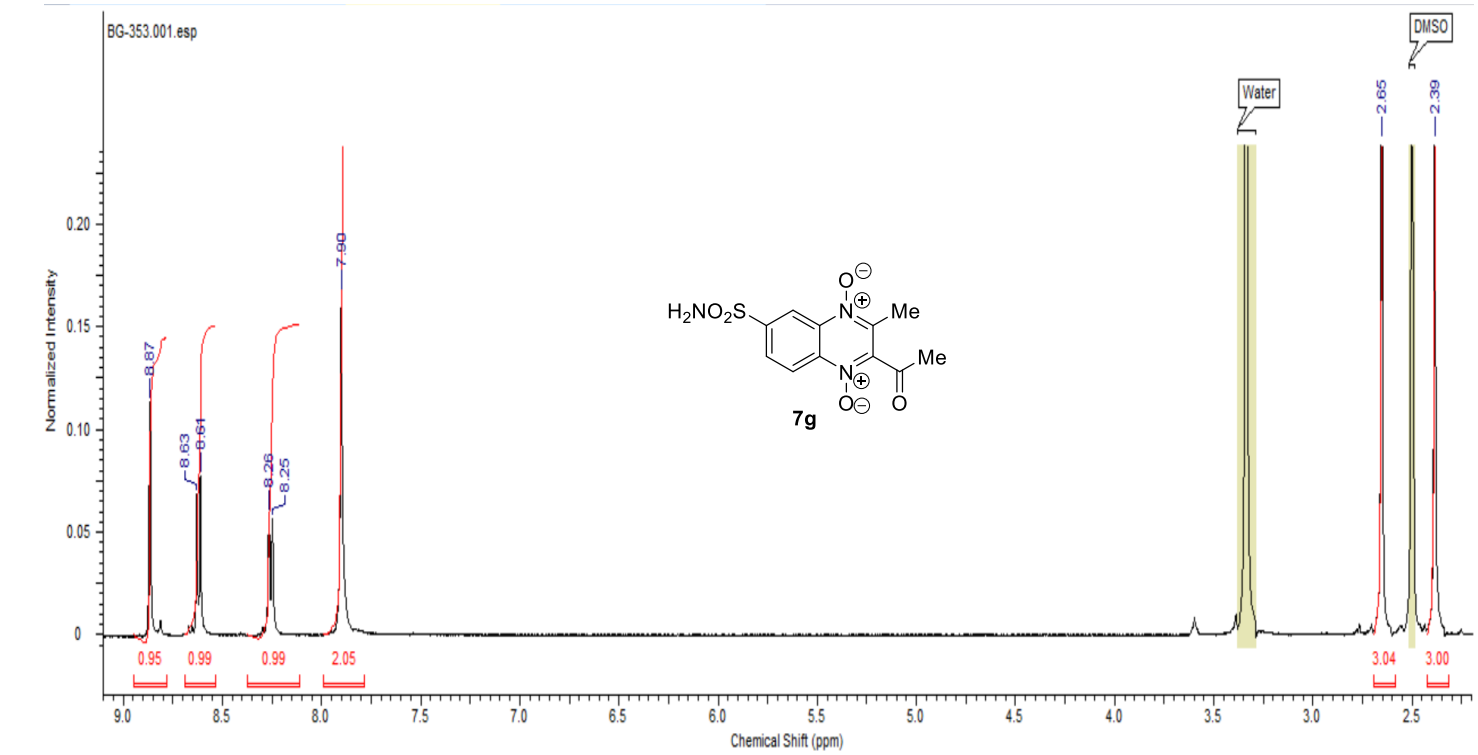


Figure S14. Copy of ^{13}C NMR spectrum of the derivative **7g**.

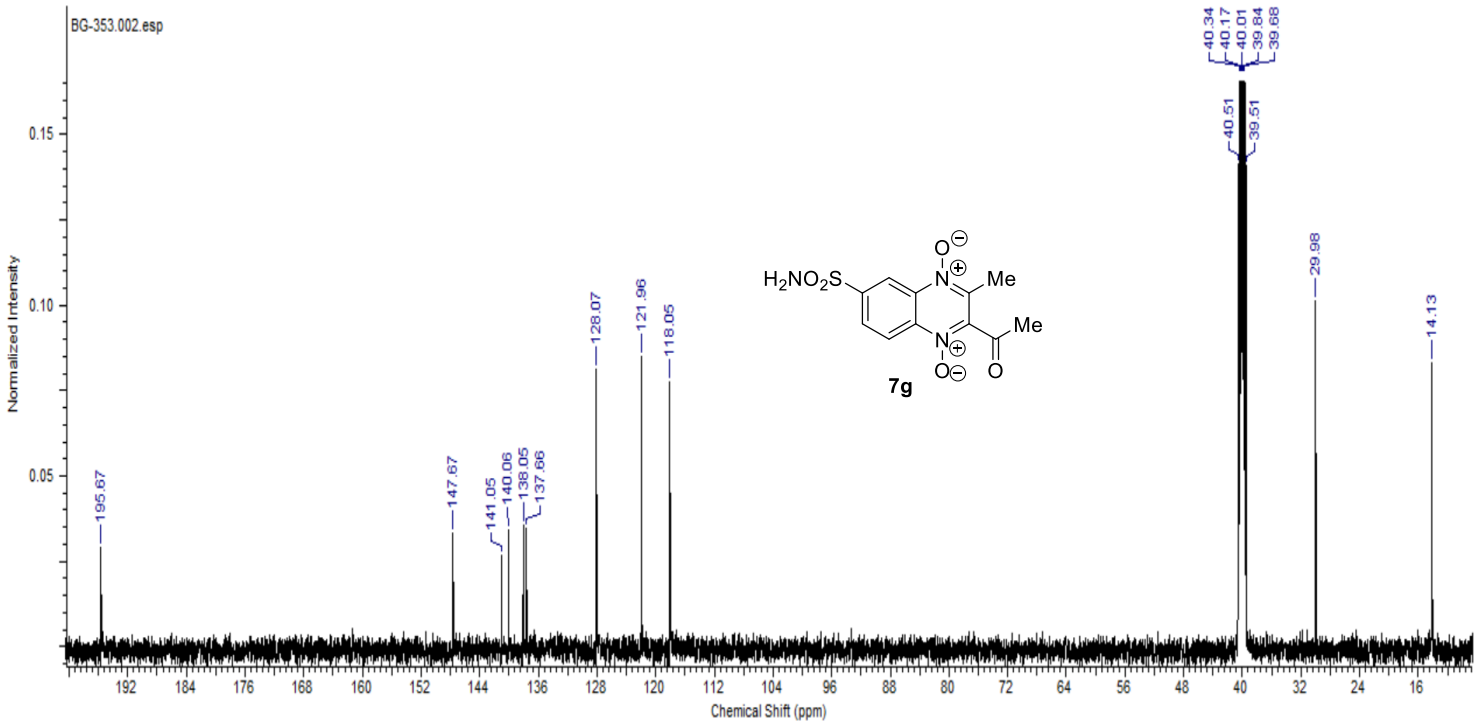


Figure S15. Copy of ^{1}H NMR spectrum of the derivative **7h**.

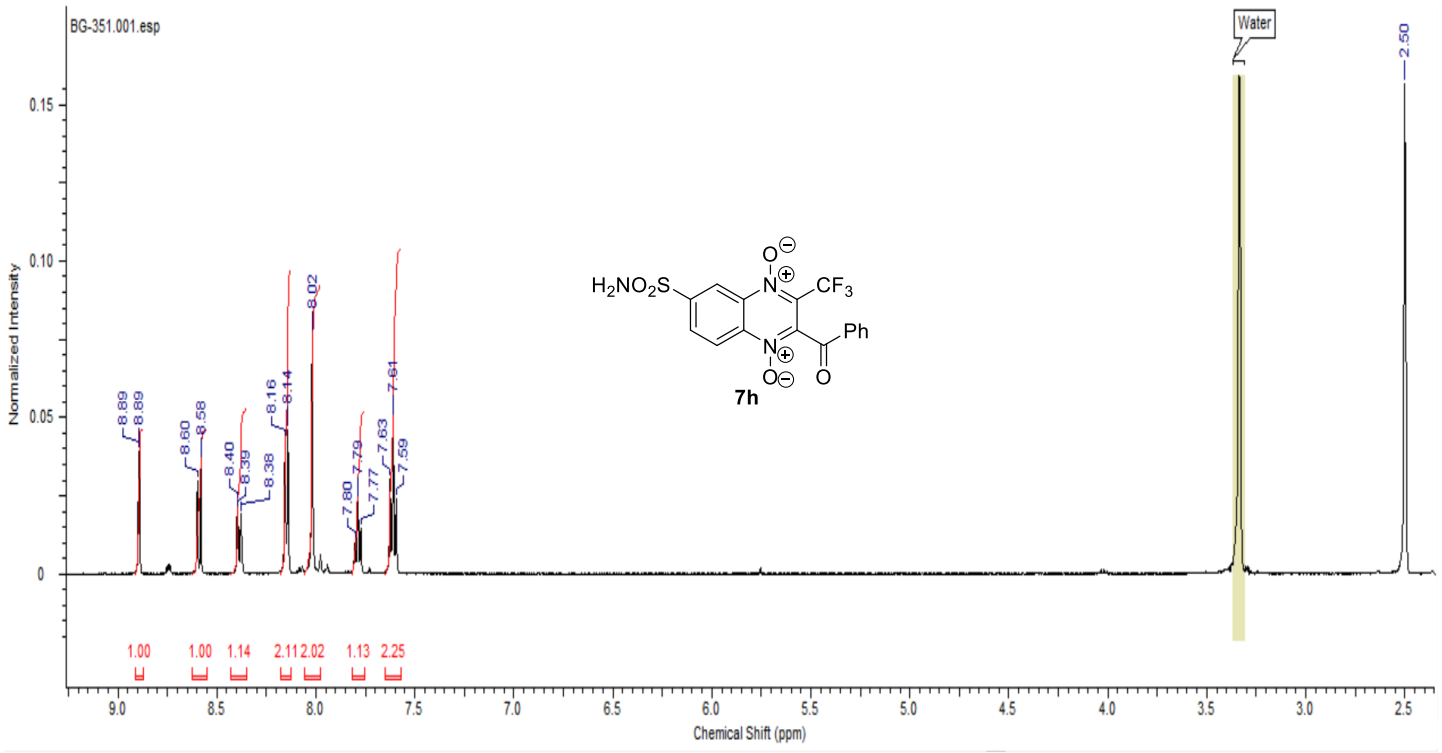


Figure S16. Copy of ^{13}C NMR spectrum of the derivative **7h**.

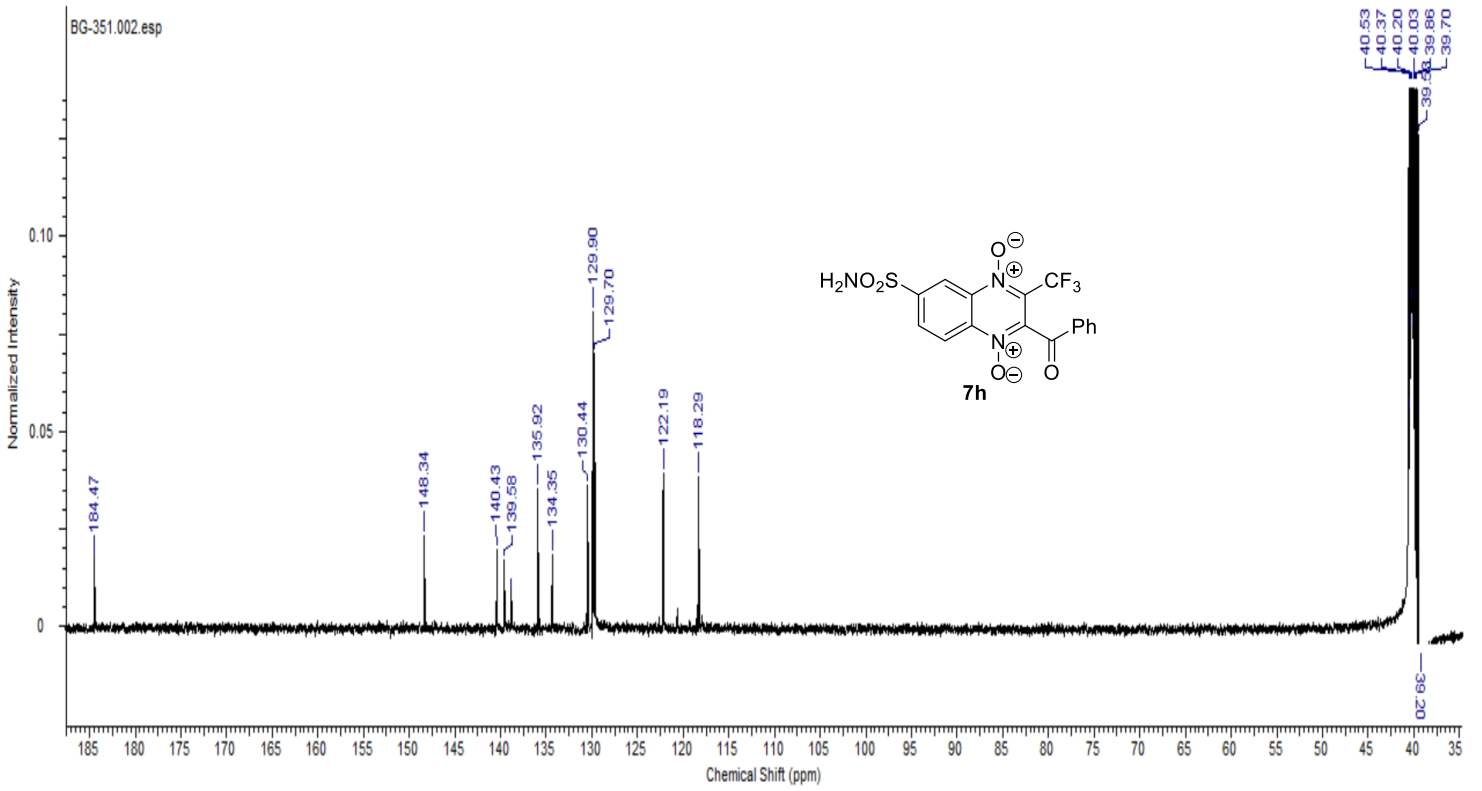


Figure S17. Copy of ^{1}H NMR spectrum of the derivative **8a**.

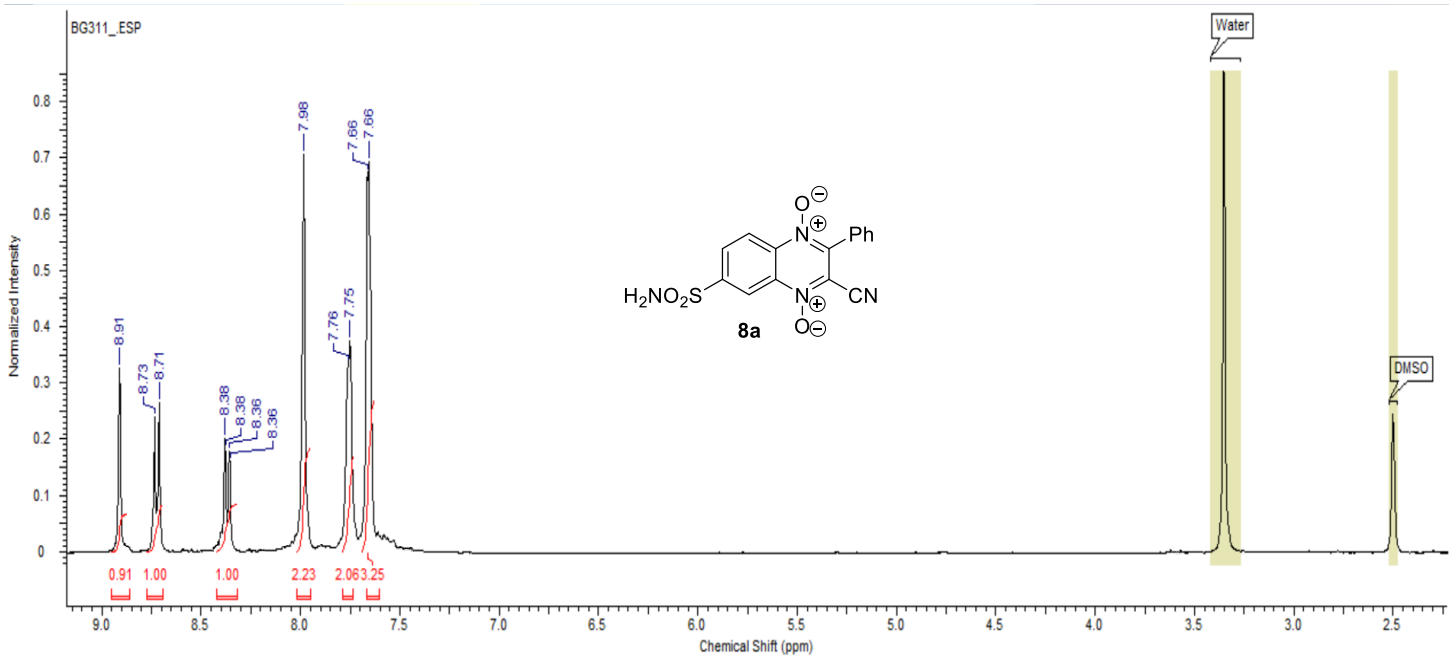


Figure S18. Copy of ^{13}C NMR spectrum of the derivative **8a**.

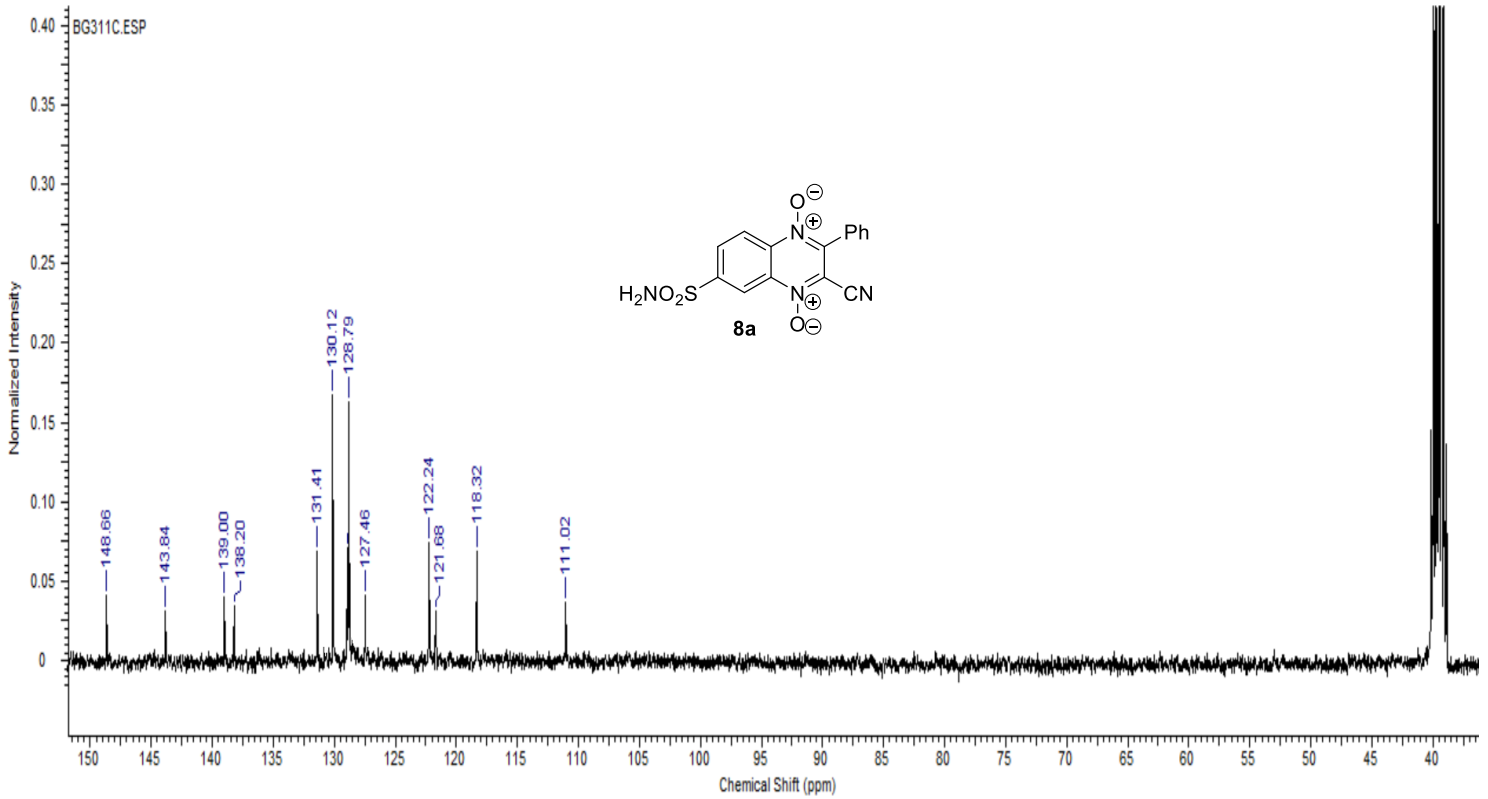


Figure S19. Copy of ^{1}H NMR spectrum of the derivative **8b**.

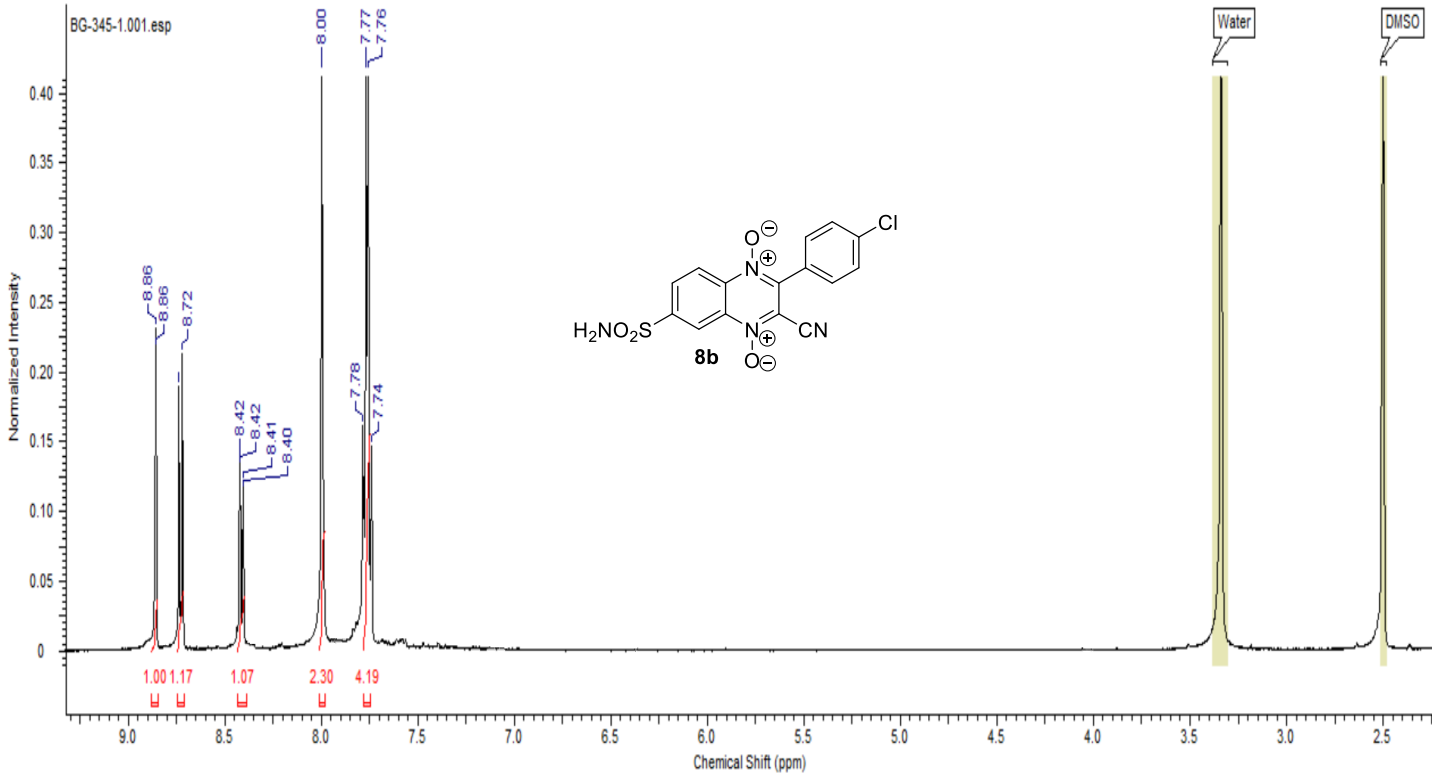


Figure S20. Copy of ^{13}C NMR spectrum of the derivative **8b**.

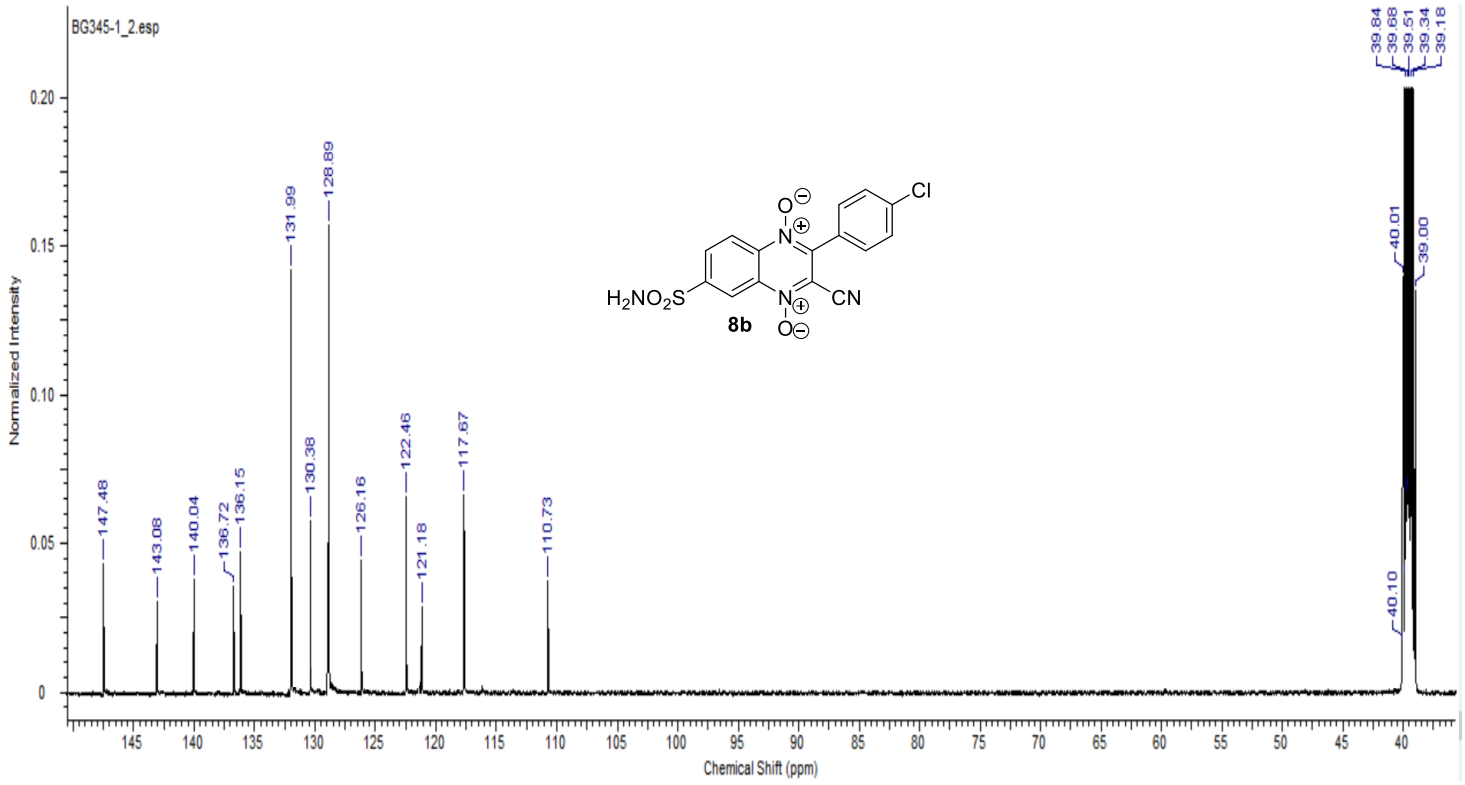


Figure S21. Copy of ^{1}H NMR spectrum of the derivative **8c**.

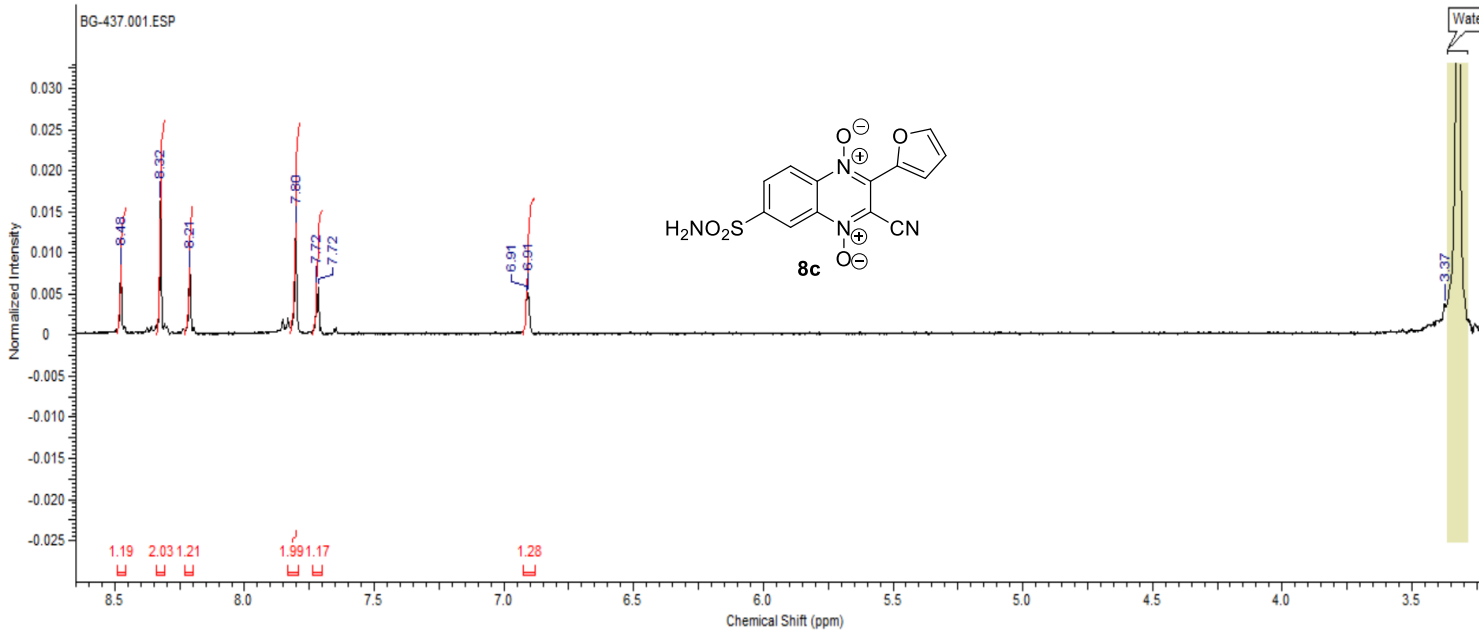


Figure S22. Copy of ^{13}C NMR spectrum of the derivative **8c**.

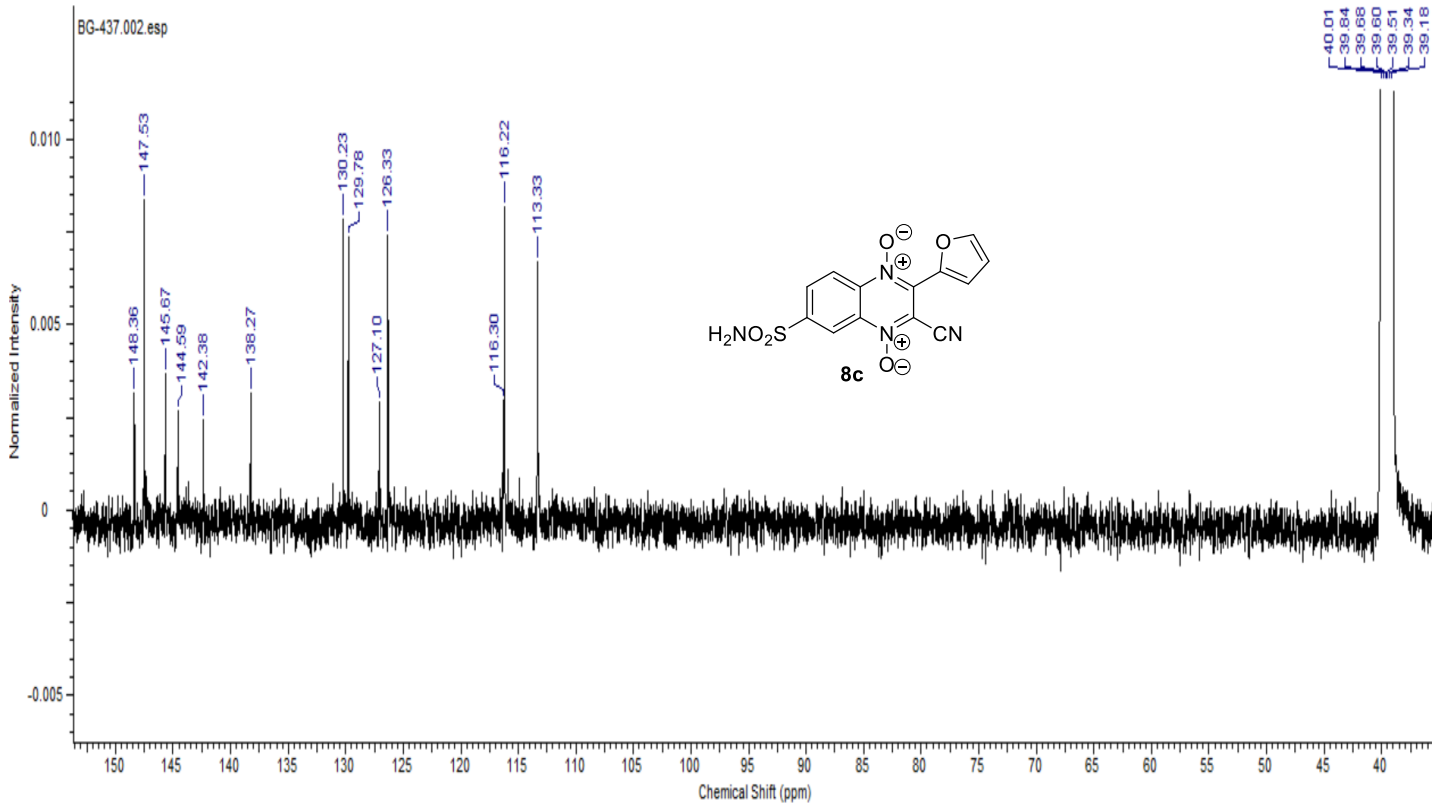


Figure S23. Copy of ^{1}H NMR spectrum of the derivative **8g**.

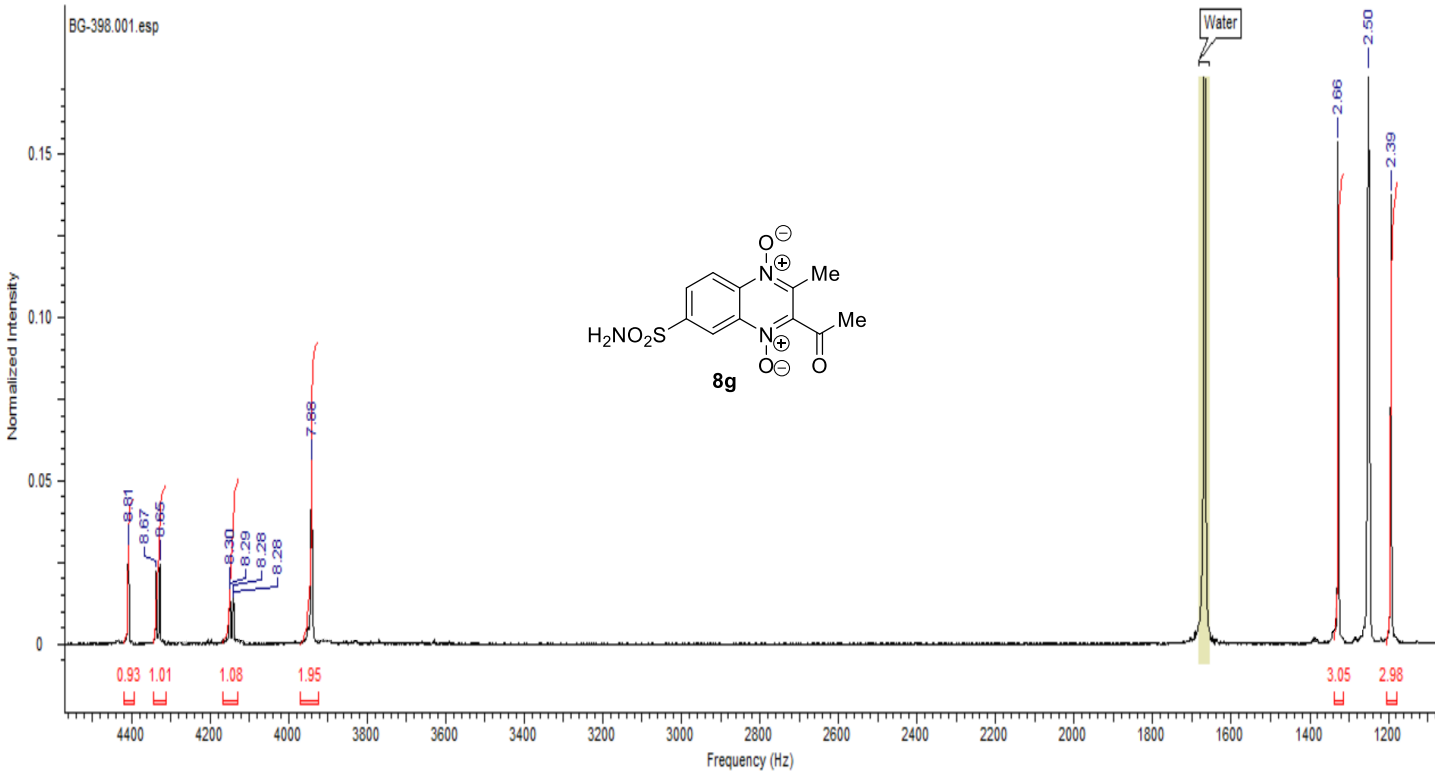


Figure S24. Copy of ^{13}C NMR spectrum of the derivative **8g**.

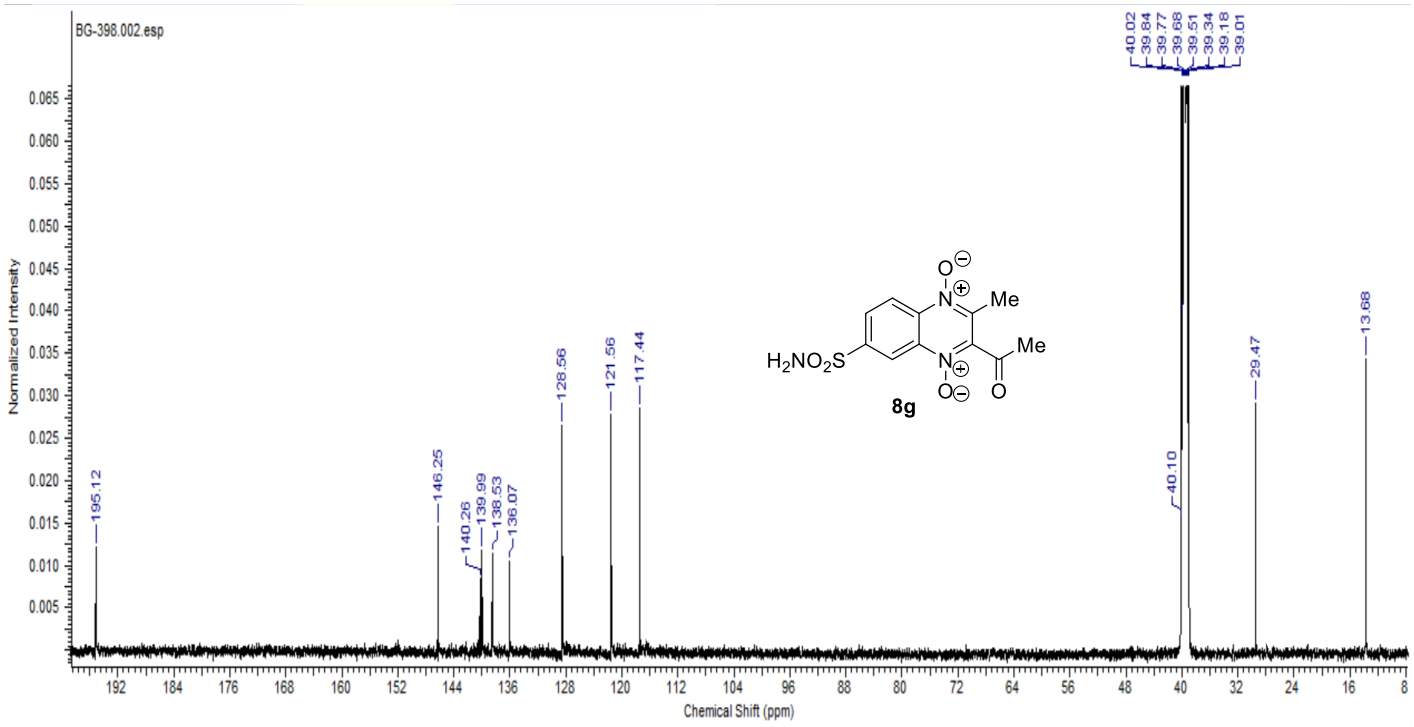


Figure S25. Copy of ^{1}H NMR spectrum of the derivative **11**.

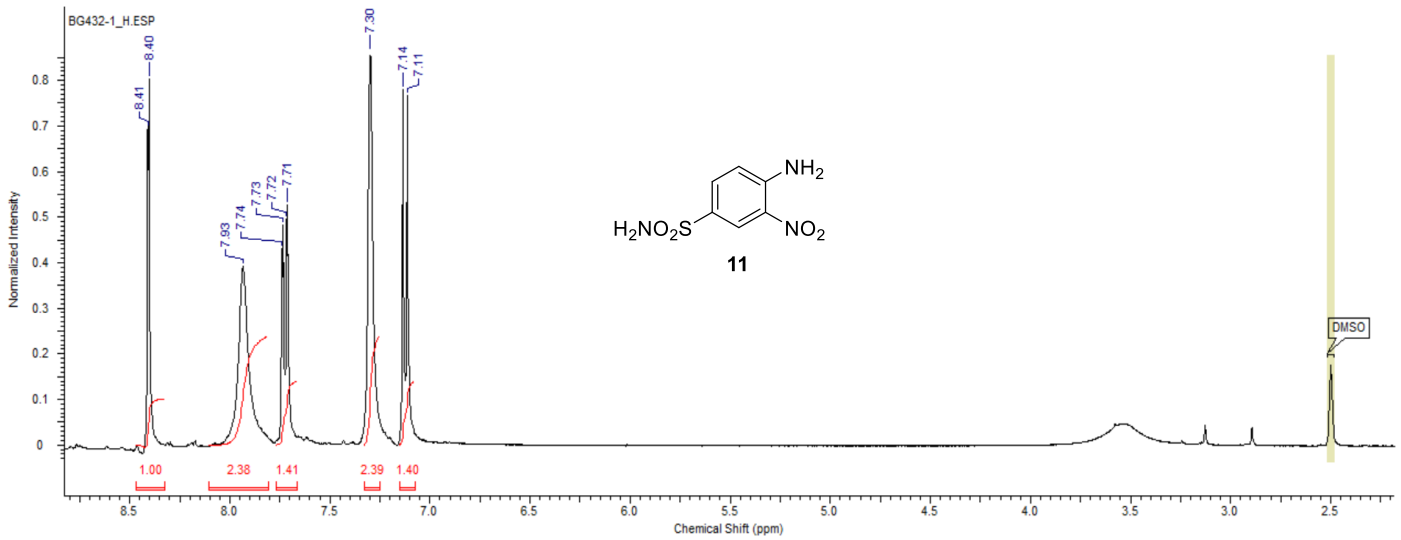


Figure S26. Copy of ^{13}C NMR spectrum of the derivative **11**.

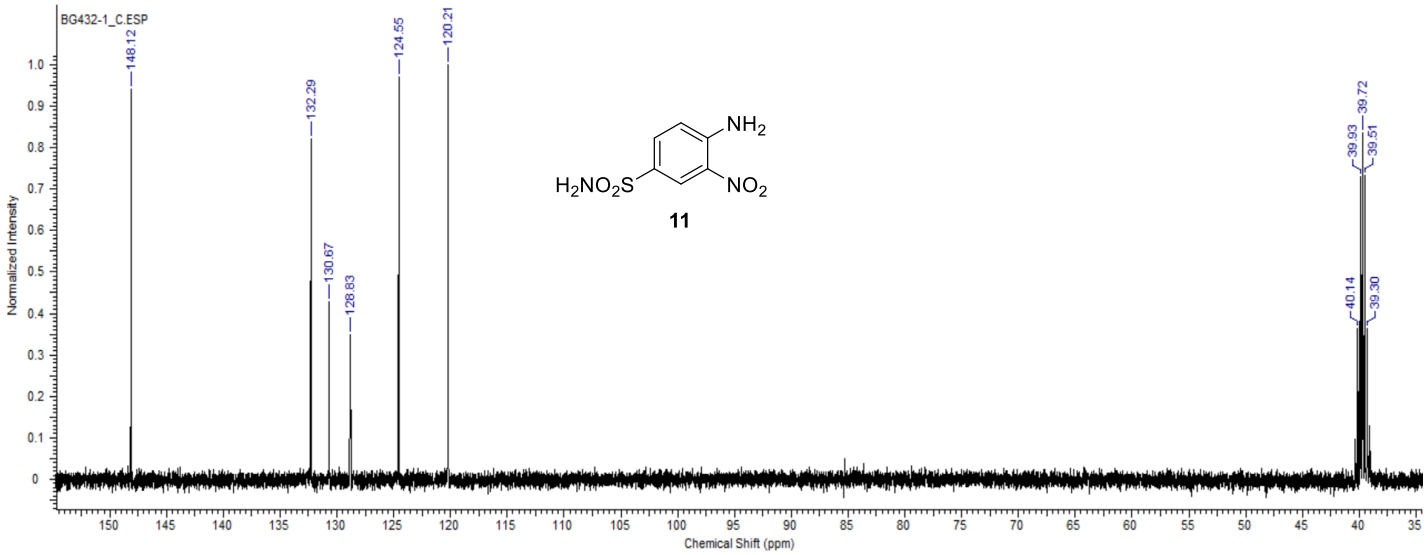


Figure S27. Copy of ^{1}H NMR spectrum of the derivative **12**.

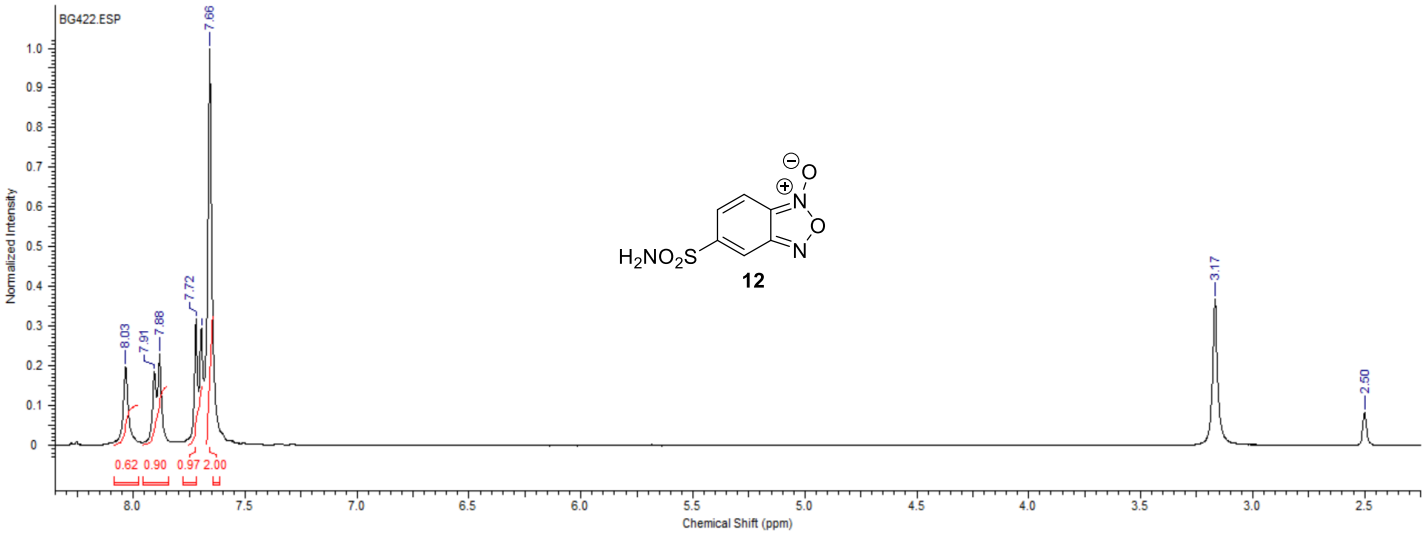


Figure S28. Copy of ^{13}C NMR spectrum of the derivative **12**.

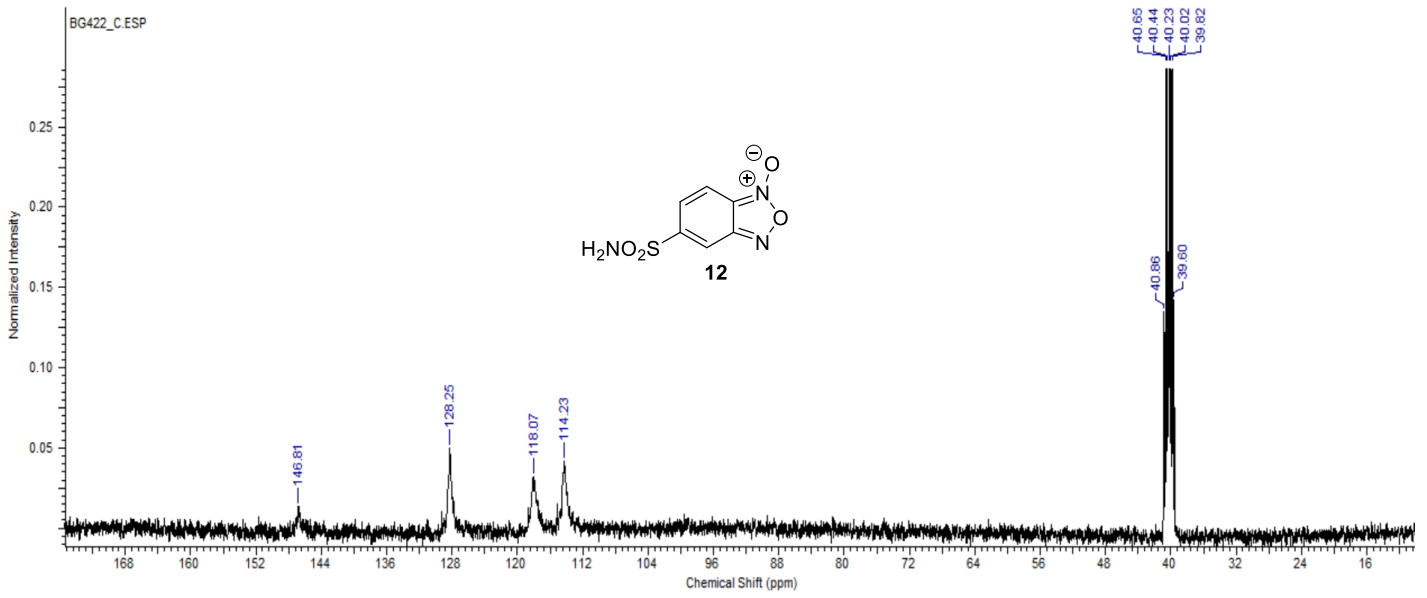


Figure S29. Copy of ^{1}H NMR spectrum of the derivative **14**.

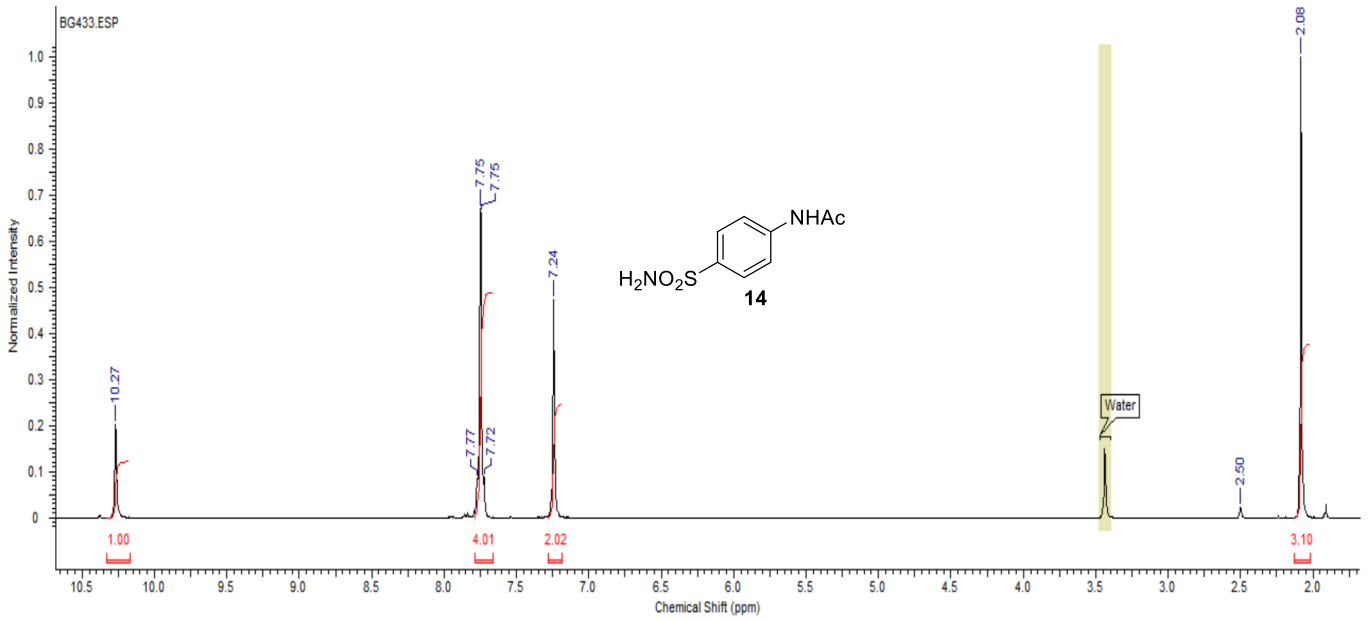


Figure S30. Copy of ^{13}C NMR spectrum of the derivative **14**.

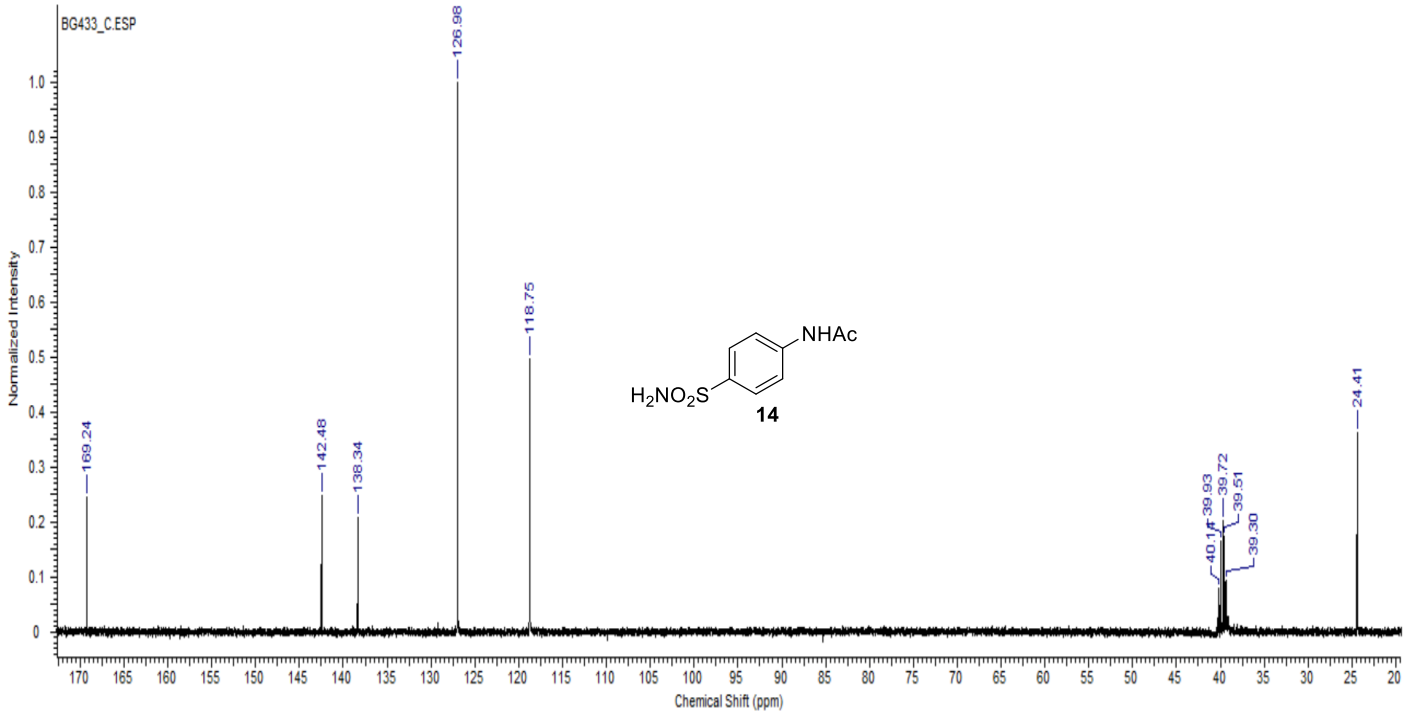


Figure S31. Copy of ^{1}H NMR spectrum of the derivative **15**.

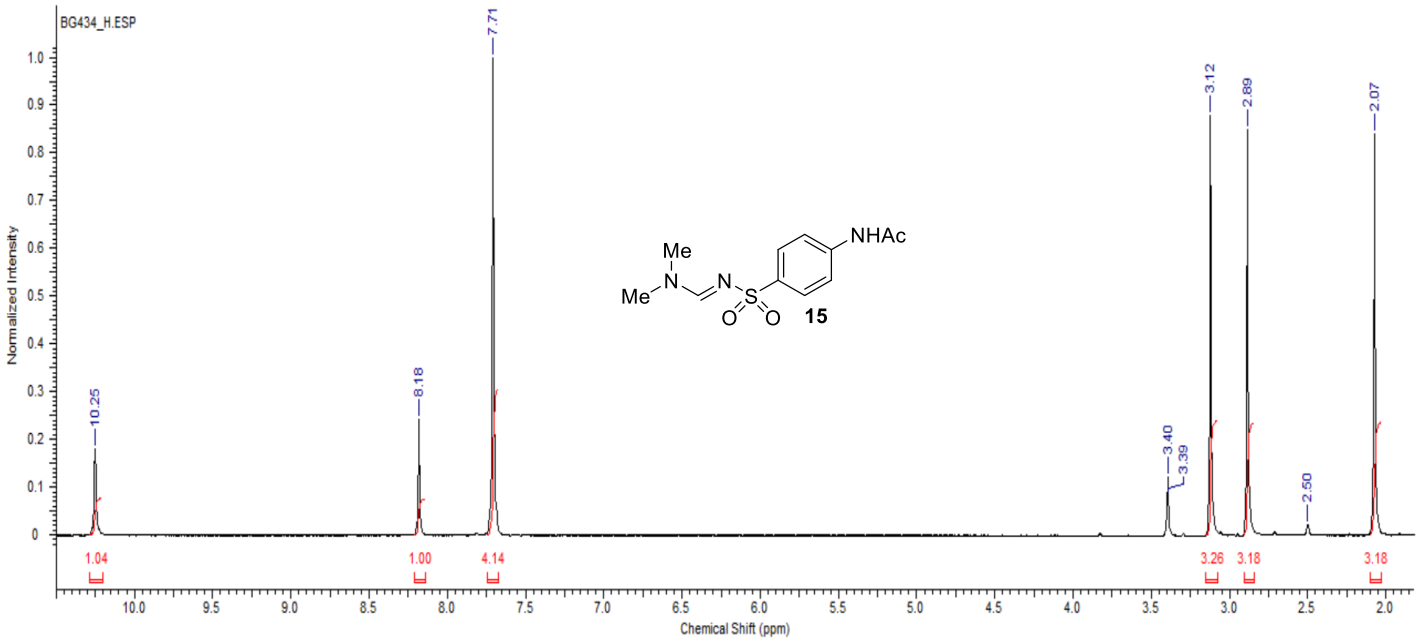


Figure S32. Copy of ^{13}C NMR spectrum of the derivative **15**.

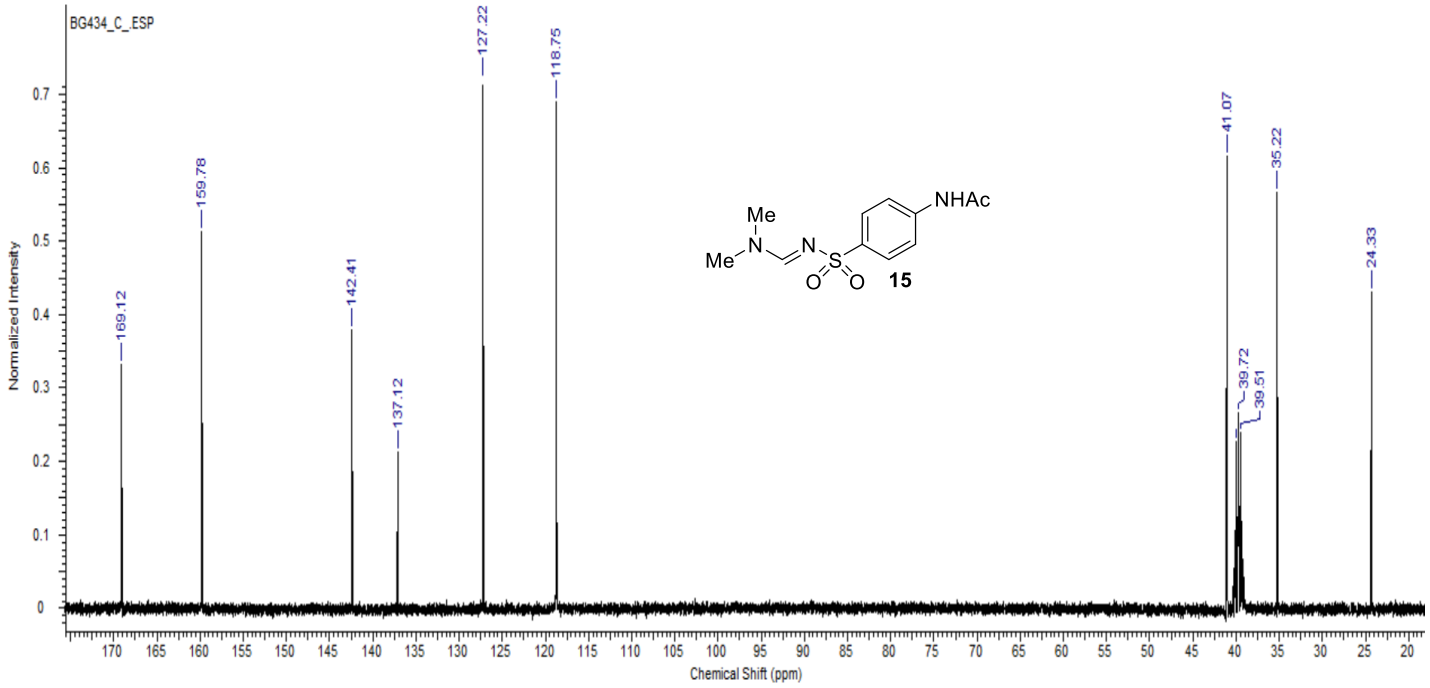


Figure S33. Copy of ^{1}H NMR spectrum of the derivative **16**.

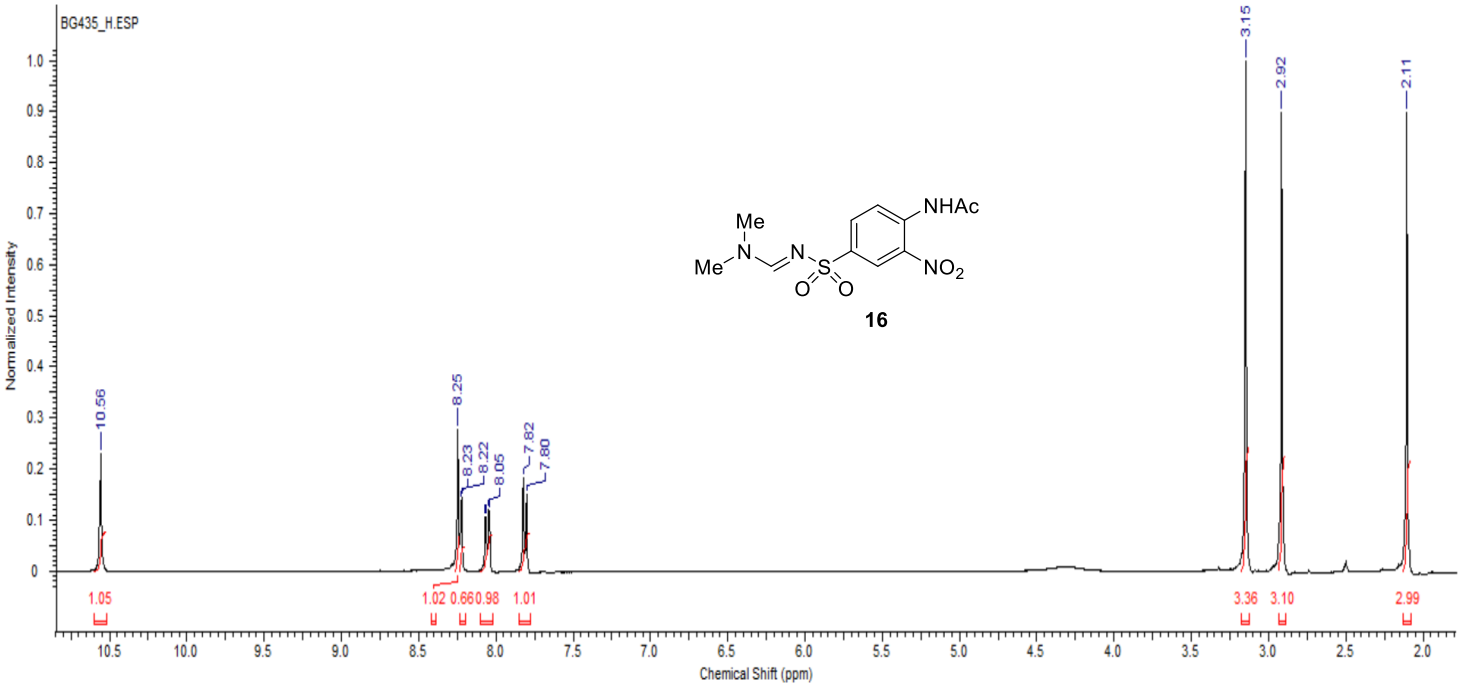


Figure S34. Copy of ^{13}C NMR spectrum of the derivative **16**.

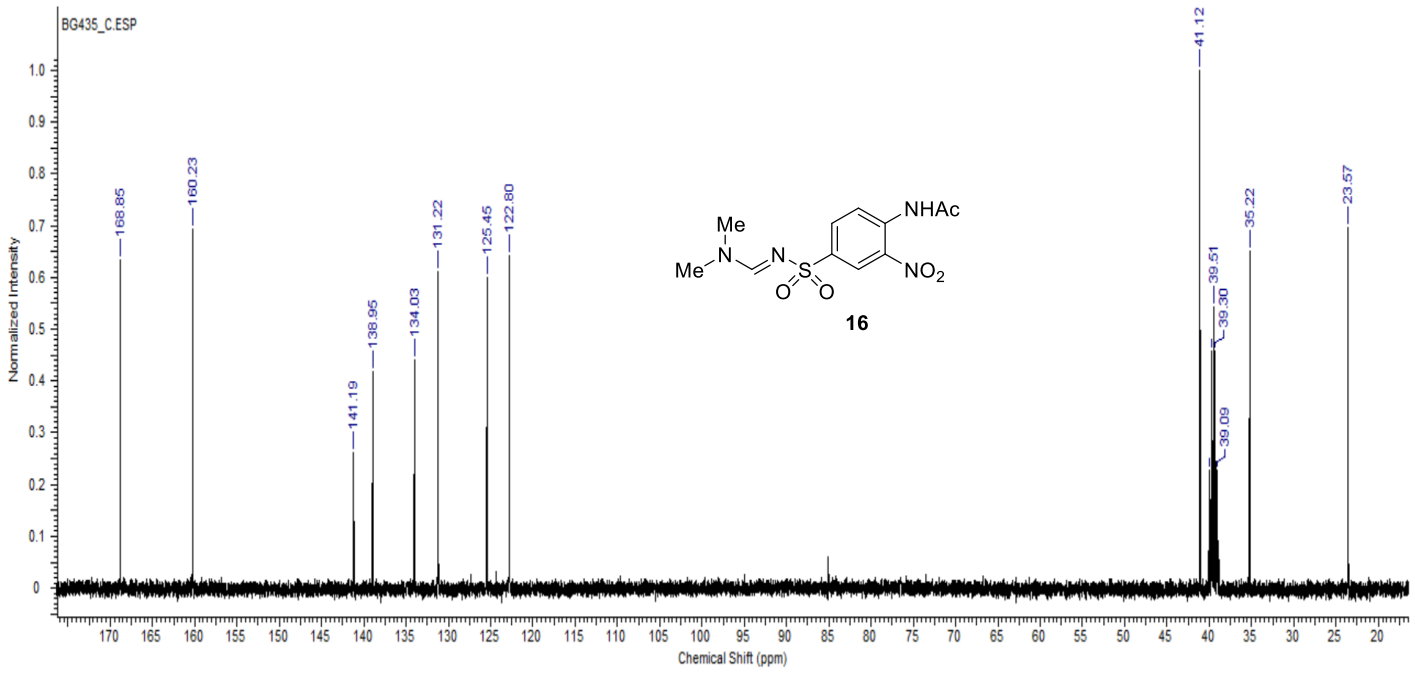


Figure S35. Copy of ^{1}H NMR spectrum of the derivative **18**.

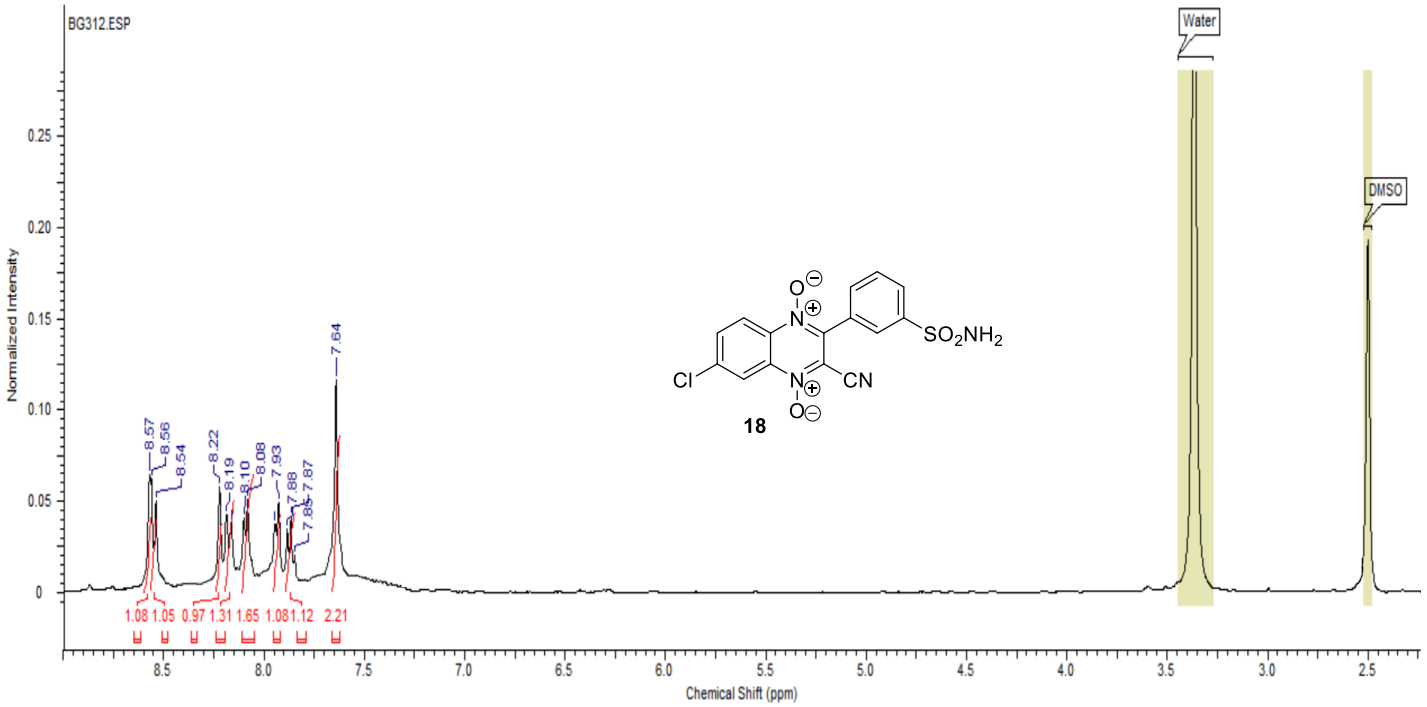
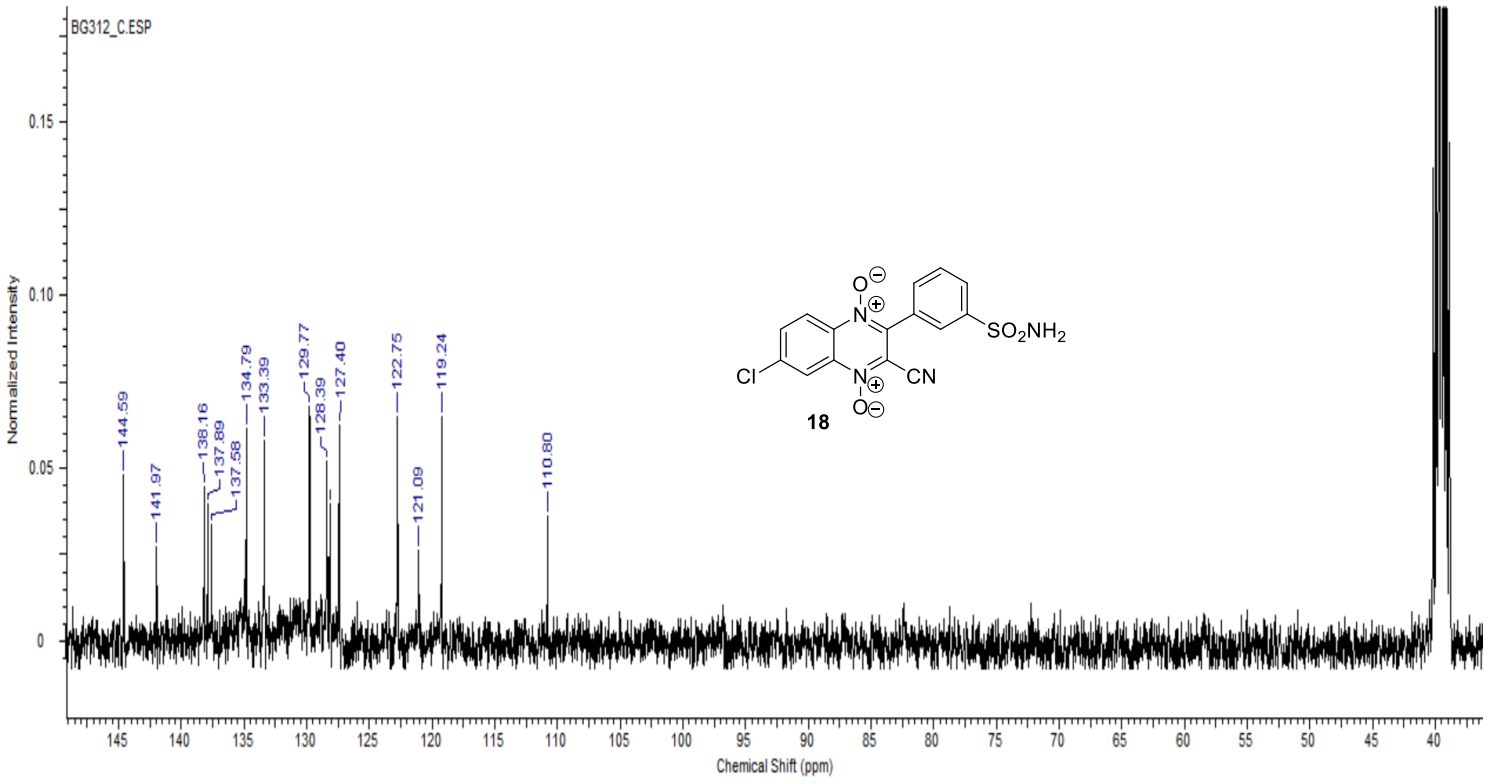


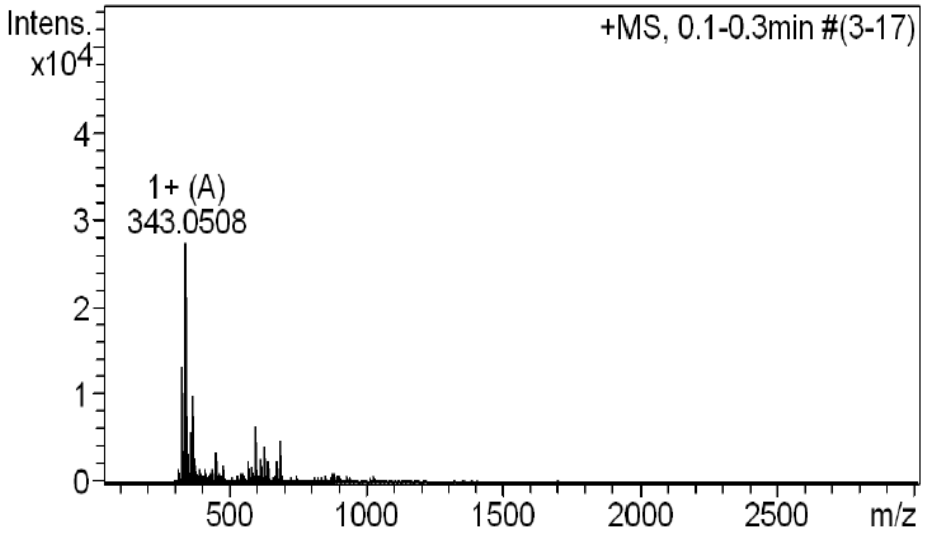
Figure S36. Copy of ^{13}C NMR spectrum of the derivative **18**.



Copies of HRMS ESI Analysis

Figure S37. Copy of HRMS ESI analysis of the derivatives **7a**.

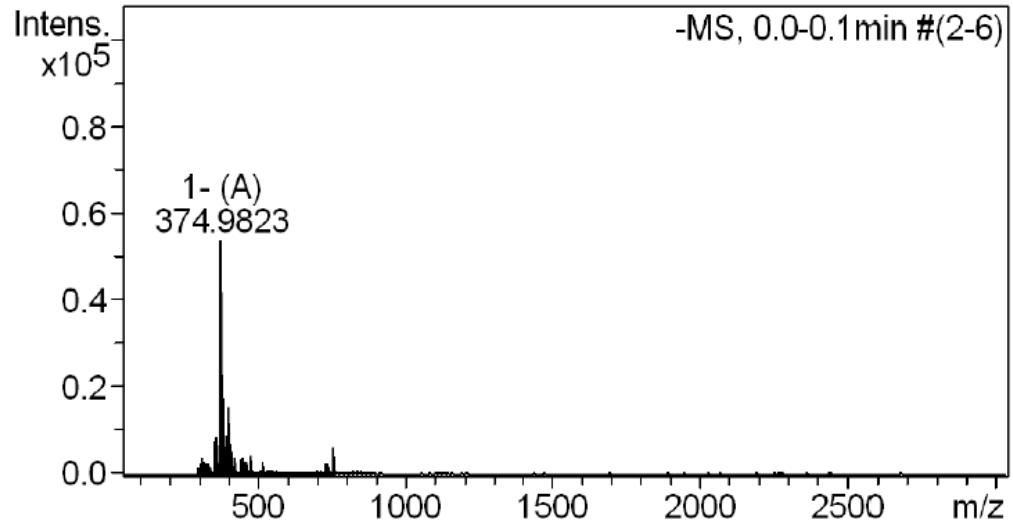
+MS, 0.1-0.3min #(3-17)



#	m/z	Res.	S/N	I	I %
1	329.0705	12592	477.0	13290	48.5
2	330.0732	13818	94.6	2654	9.7
3	343.0508	14238	920.7	27377	100.0
4	344.0516	11589	140.8	4212	15.4
5	358.3690	10931	178.5	5723	20.9
6	369.3820	12142	297.6	10027	36.6
7	451.2188	13411	70.8	3272	12.0
8	596.5999	14650	105.7	6469	23.6
9	624.6326	14744	64.9	4051	14.8
10	685.0901	13506	73.5	4731	17.3

Figure S38. Copy of HRMS ESI analysis of the derivatives **7b**.

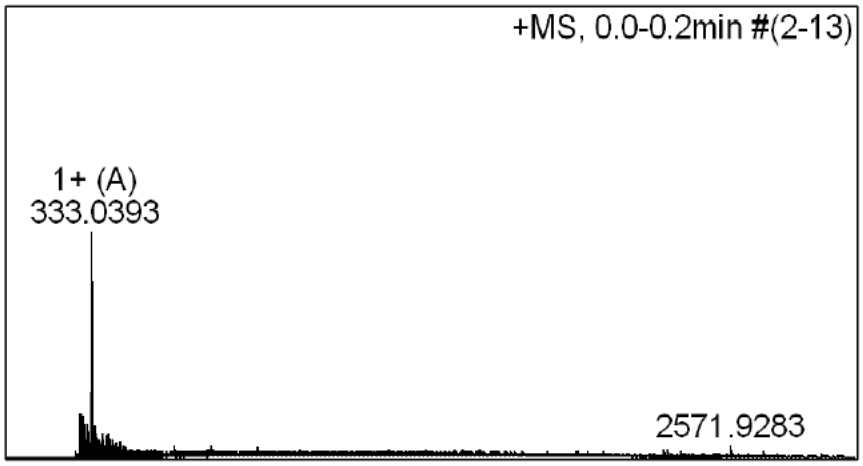
-MS, 0.0-0.1min #(2-6)



#	m/z	Res.	S/N	I	I %
1	349.9889			7572	14.1
2	358.9898			8557	16.0
3	374.9822			53590	100.0
4	376.9794			22863	42.7
5	382.0024			5517	10.3
6	392.9910			8656	16.2
7	401.9959			15125	28.2
8	403.9858			7196	13.4
9	750.9739			5951	11.1

Figure S39. Copy of HRMS ESI analysis of the derivatives **7c**.

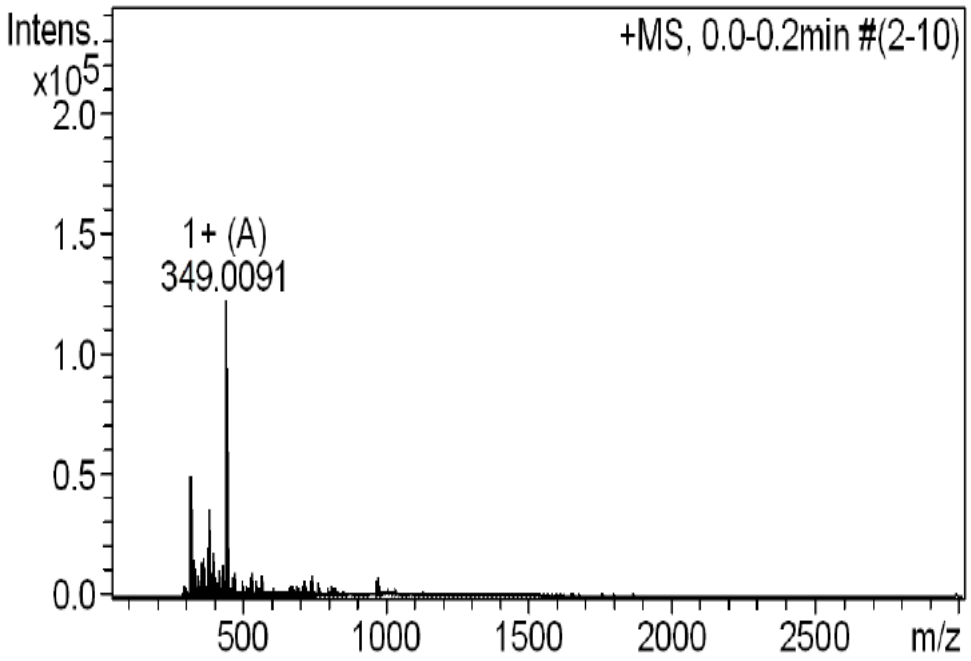
+MS, 0.0-0.2min #(2-13)



#	m/z	Res.	S/N	I	I %
1	301.0405			2756	14.3
2	317.0633			3477	18.1
3	333.0393			19225	100.0
4	342.0657			3007	15.6
5	344.0780			6008	31.3
6	360.0810			2626	13.7
7	384.1094			2028	10.5
8	403.1100			1976	10.3

Figure S40. Copy of HRMS ESI analysis of the derivatives **7d**.

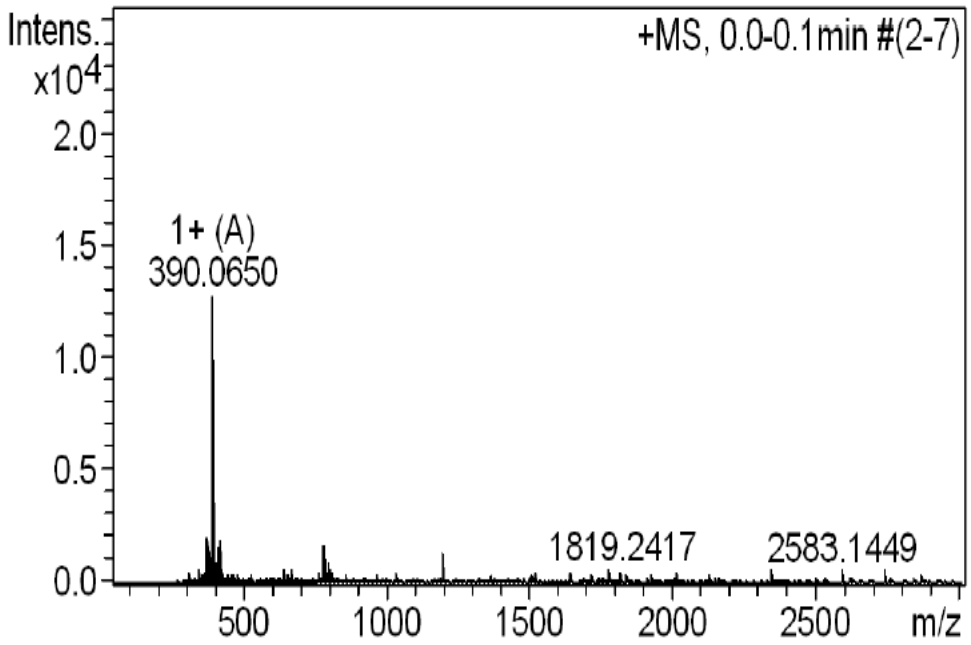
+MS, 0.0-0.2min #(2-10)



#	m/z	Res.	S/N	I	I %
1	317.0152	6204	125.6	16002	13.2
2	318.0231	6084	323.2	35582	29.3
3	319.0204	5818	160.4	17803	14.7
4	333.0476	6045	120.9	14461	11.9
5	349.0091	5952	1111.6	121459	100.0
6	380.1998	5980	153.0	19904	16.4
7	383.2063	6162	275.5	35777	29.5
8	399.1810	6139	133.2	17756	14.6
9	445.1771	6289	575.8	79637	65.6
10	446.1793	6453	126.1	17786	14.6

Figure S41. Copy of HRMS ESI analysis of the derivatives **7e**.

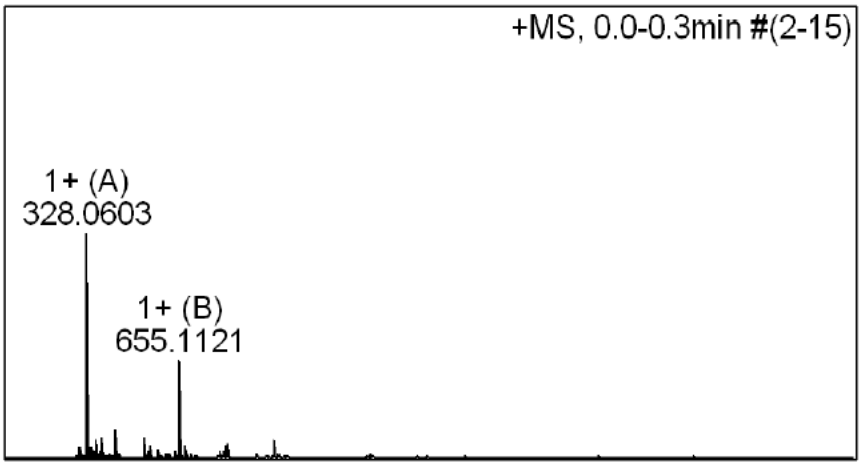
+MS, 0.0-0.1min #(2-7)



#	m/z	Res.	S/N	I	I %
1	374.0714			1939	15.2
2	390.0649			12731	100.0
3	392.0737			4024	31.6
4	409.1039			1579	12.4
5	412.0477			1372	10.8
6	779.1266			1620	12.7
7	781.1349			1610	12.6

Figure S42. Copy of HRMS ESI analysis of the derivatives **7f**.

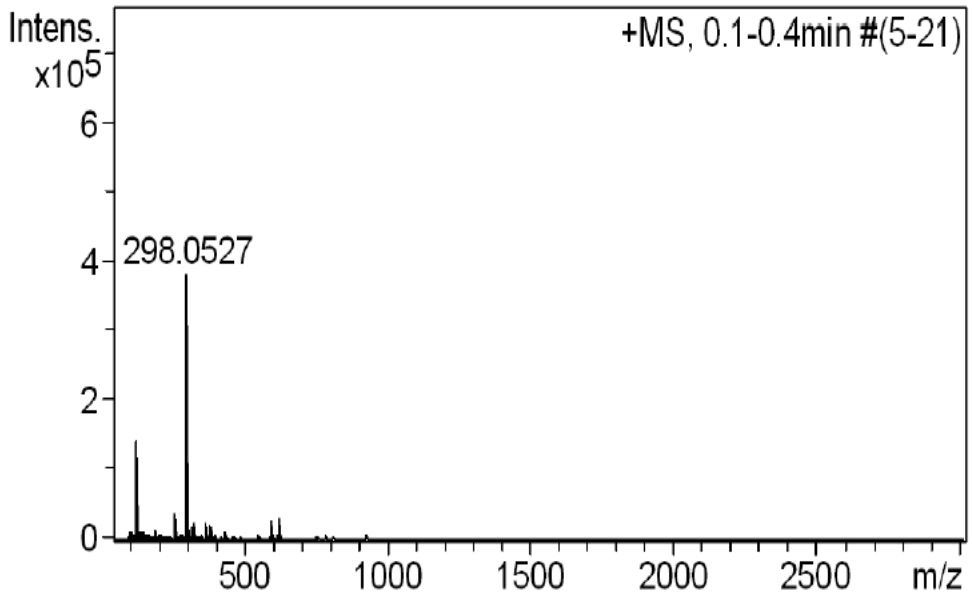
+MS, 0.0-0.3min #(2-15)



#	m/z	Res.	S/N	I	I %
1	328.0603	5814	3401.6	741290	100.0
2	329.0631	6243	514.2	112606	15.2
3	361.2220	6018	244.8	56907	7.7
4	381.2971	6615	251.0	58908	7.9
5	383.2010	6507	262.9	61743	8.3
6	431.1621	6652	363.4	87290	11.8
7	531.2155	6832	250.4	63087	8.5
8	655.1121	7233	1196.8	322891	43.6
9	656.1158	7503	354.4	95995	12.9
10	982.1678	7493	289.5	60284	8.1

Figure S43. Copy of HRMS ESI analysis of the derivatives **7g**.

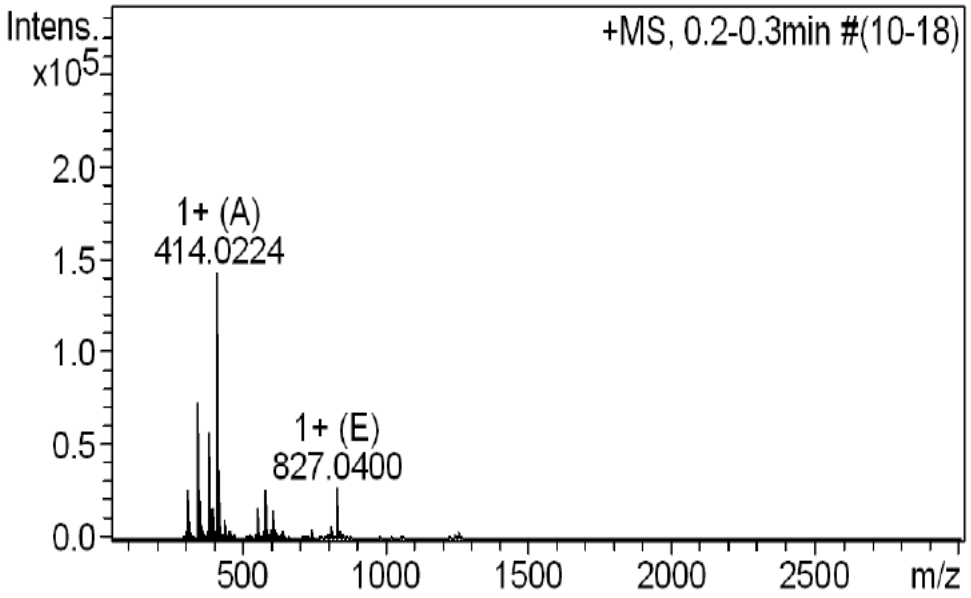
+MS, 0.1-0.4min #(5-21)



#	m/z	I	I %
1	118.0914	140718	36.9
2	258.1751	36295	9.5
3	259.1601	22030	5.8
4	298.0527	381462	100.0
5	299.0533	50586	13.3
6	322.0487	22802	6.0
7	361.2221	23378	6.1
8	375.2048	21375	5.6
9	595.0901	25279	6.6
10	622.0265	30286	7.9

Figure S44. Copy of HRMS ESI analysis of the derivatives **7h**.

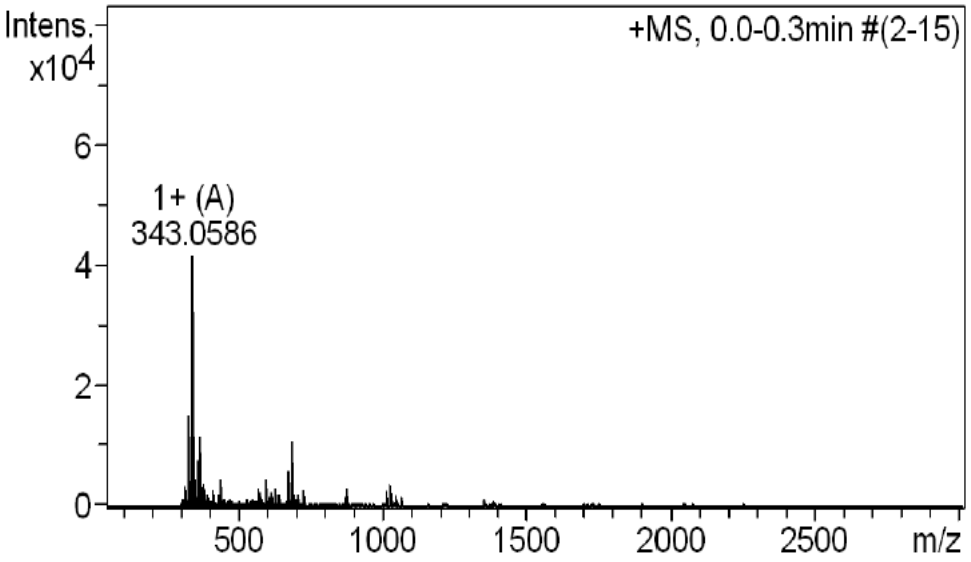
+MS, 0.2-0.3min #(10-18)



#	m/z	Res.	S/N	I	I %
1	313.2609	9994	463.0	25806	18.1
2	341.2925	10413	1136.6	73271	51.3
3	353.2514	9670	386.2	26281	18.4
4	381.2827	10062	503.9	38484	27.0
5	383.1890	11025	737.3	56707	39.7
6	414.0224	11537	1658.9	142744	100.0
7	415.0226	9690	298.7	25820	18.1
8	551.4819	11483	127.2	15718	11.0
9	579.5142	9492	213.5	26375	18.5
10	827.0400	10153	246.7	26917	18.9

Figure S45. Copy of HRMS ESI analysis of the derivatives **8a**.

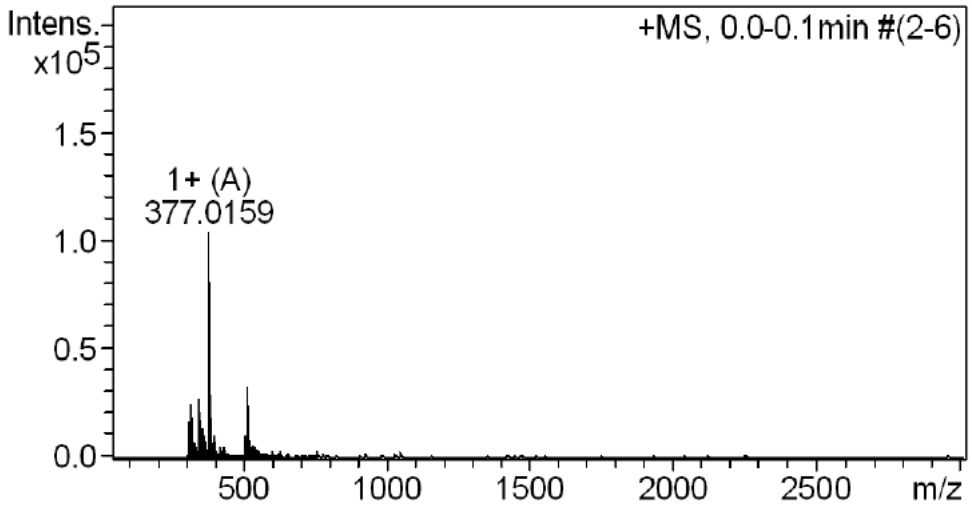
+MS, 0.0-0.3min #(2-15)



#	m/z	Res.	S/N	I	I %
1	329.0791	12056	372.0	14917	35.9
2	343.0586	16289	979.2	41543	100.0
3	344.0603	11036	133.4	5687	13.7
4	358.3774	11949	168.5	7461	18.0
5	369.3900	12943	250.4	11403	27.4
6	440.0421	14433	78.0	4209	10.1
7	596.6007	14172	63.4	4264	10.3
8	671.1166	14659	84.0	5794	13.9
9	685.0957	12447	155.8	10762	25.9
10	686.0957	13567	66.9	4648	11.2

Figure S46. Copy of HRMS ESI analysis of the derivatives **8b**.

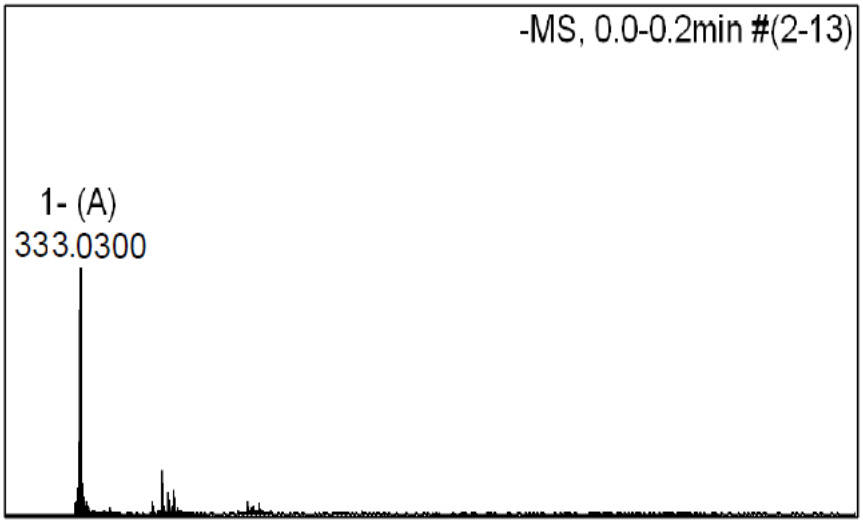
+MS, 0.0-0.1min #(2-6)



#	m/z	Res.	S/N	I	I %
1	313.2783	5924	187.6	15879	15.3
2	318.1647	5824	279.1	24132	23.2
3	341.3097	6173	278.0	26516	25.5
4	353.2705	5946	176.0	17107	16.4
5	377.0159	5922	1037.7	104014	100.0
6	378.0187	6047	195.5	19689	18.9
7	379.0139	6084	393.5	39609	38.1
8	381.3026	6374	226.9	22942	22.1
9	513.7862	6418	272.2	32629	31.4
10	514.2872	6759	175.4	21100	20.3

Figure S47. Copy of HRMS ESI analysis of the derivatives **8c**.

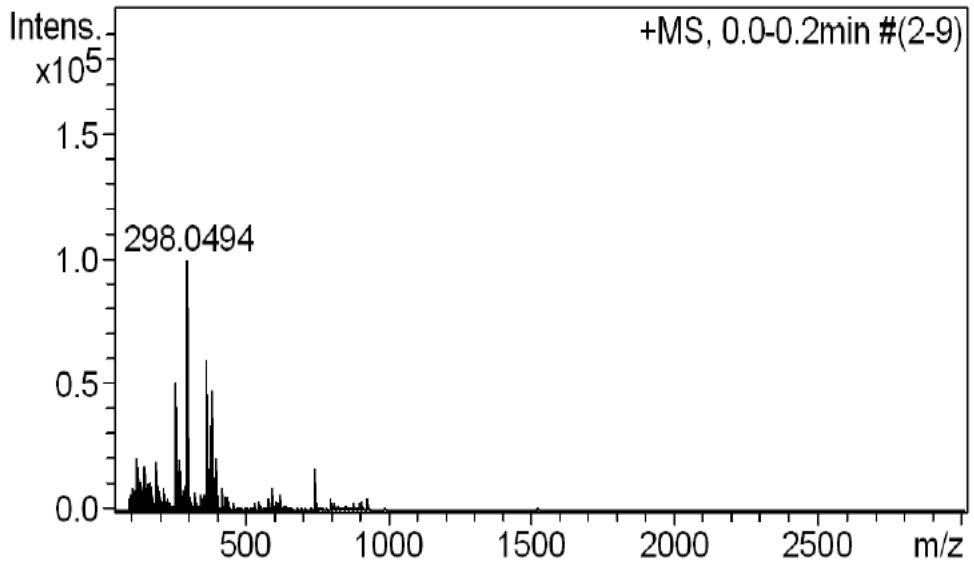
-MS, 0.0-0.2min #(2-13)



#	m/z	Res.	S/N	I	I %
1	299.0126	5155	55.1	4632	5.7
2	300.0150	5279	226.7	15650	19.1
3	301.0118	5276	95.7	6663	8.2
4	315.0055	5579	484.4	36424	44.6
5	316.0097	5350	96.9	7351	9.0
6	333.0300	5153	1193.0	81747	100.0
7	599.9871	6032	189.8	14429	17.7
8	600.0330	6136	63.3	4854	5.9
9	615.0251	6076	90.7	6959	8.5
10	635.0059	6196	99.4	7670	9.4

Figure S48. Copy of HRMS ESI analysis of the derivatives **8g**.

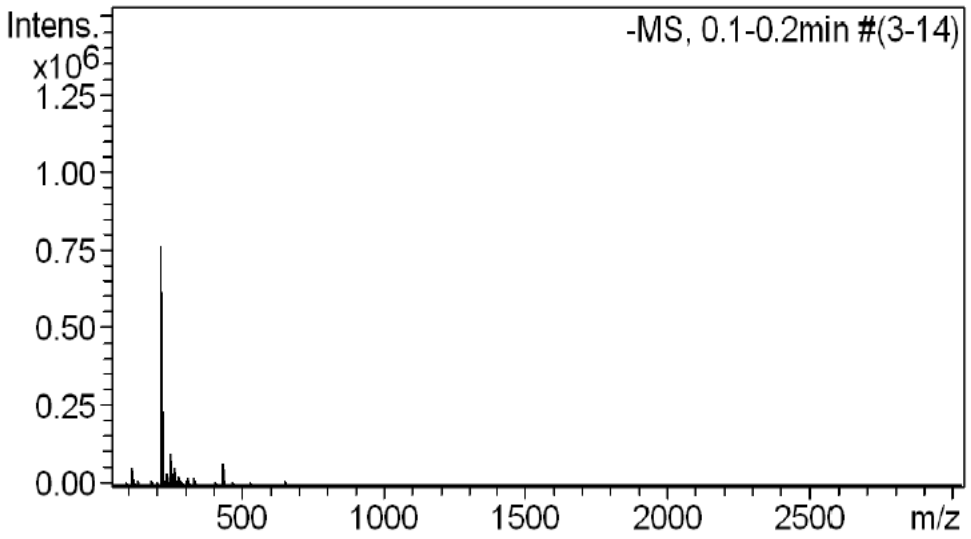
+MS, 0.0-0.2min #(2-9)



#	m/z	I	I %
1	124.0860	20819	20.9
2	151.0983	17013	17.1
3	185.0809	18874	18.9
4	259.1549	50464	50.6
5	271.0741	19744	19.8
6	298.0494	99759	100.0
7	361.2218	59597	59.7
8	378.2452	33863	33.9
9	383.2010	47091	47.2
10	399.1773	20477	20.5

Figure S49. Copy of HRMS ESI analysis of the derivatives **11**.

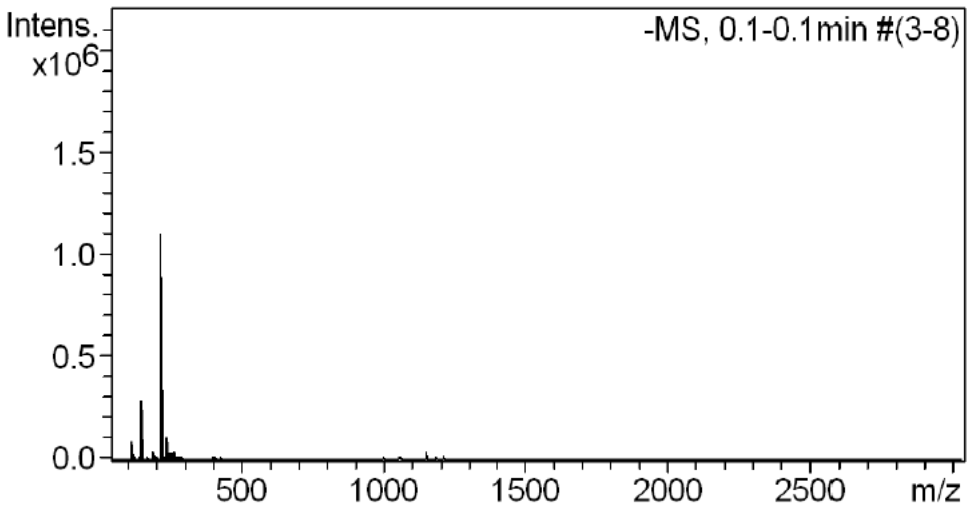
-MS, 0.1-0.2min #(3-14)



#	m/z	I	I %
1	112.9850	55290	7.3
2	216.0066	759951	100.0
3	217.0043	66918	8.8
4	218.0030	36987	4.9
5	234.9553	36526	4.8
6	251.9816	96791	12.7
7	253.9783	38981	5.1
8	260.9904	50465	6.6
9	279.9405	29199	3.8
10	433.0156	66905	8.8

Figure S50. Copy of HRMS ESI analysis of the derivatives **12**.

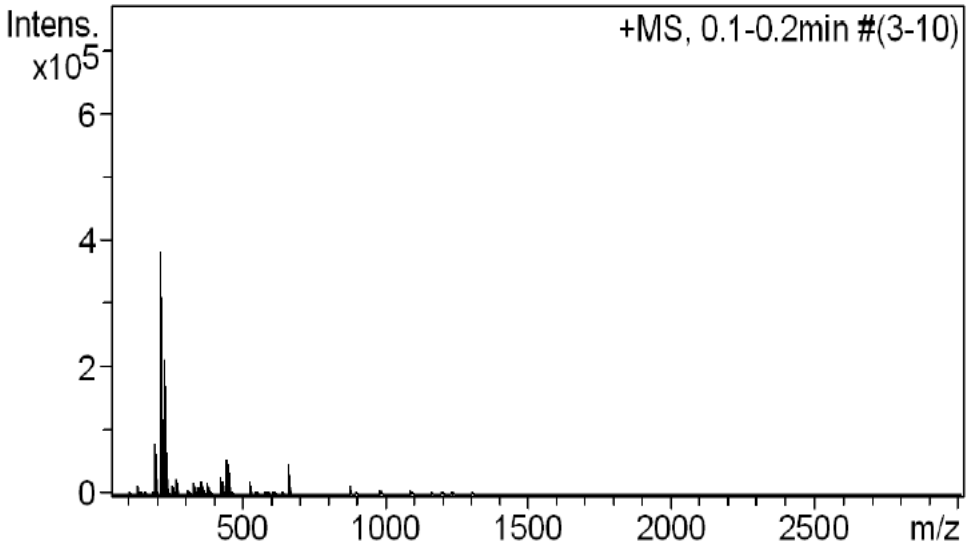
-MS, 0.1-0.1min #(3-8)



#	m/z	I	I %
1	112.9716	88404	8.0
2	150.0154	286559	26.1
3	189.9551	42609	3.9
4	213.9739	85688	7.8
5	214.9763	150360	13.7
6	216.0085	1099596	100.0
7	234.9394	106563	9.7
8	236.9359	38786	3.5
9	255.2107	31617	2.9
10	265.1259	41238	3.8

Figure S51. Copy of HRMS ESI analysis of the derivatives **14**.

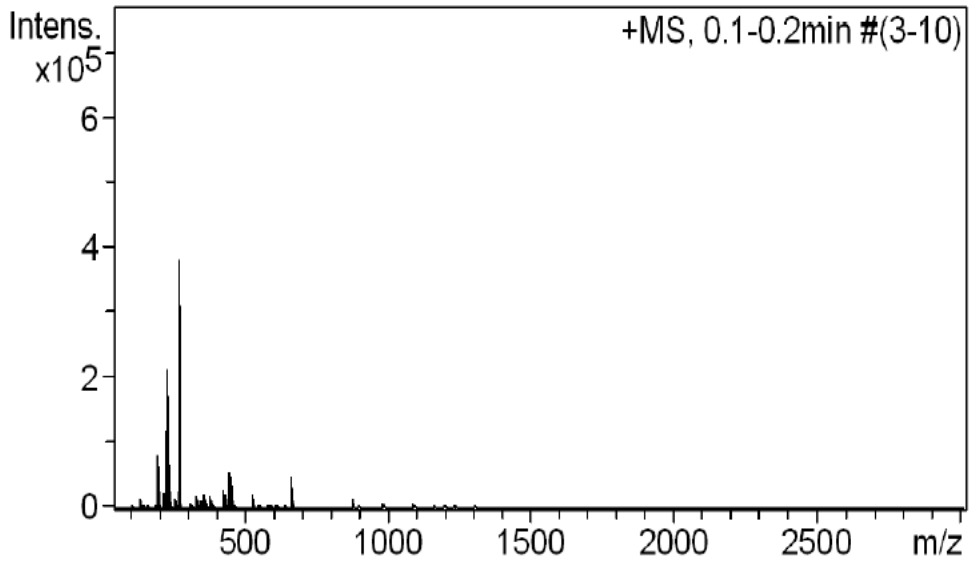
+MS, 0.1-0.2min #(3-10)



#	m/z	I	I %
1	198.0200	79113	20.6
2	215.0470	384009	100.0
3	216.0486	40115	10.4
4	232.0725	210297	54.8
5	237.0266	28890	7.5
6	270.0862	24697	6.4
7	423.2511	27108	7.1
8	446.1064	54545	14.2
9	451.0617	46407	12.1
10	660.1441	46528	12.1

Figure S52. Copy of HRMS ESI analysis of the derivatives **15**.

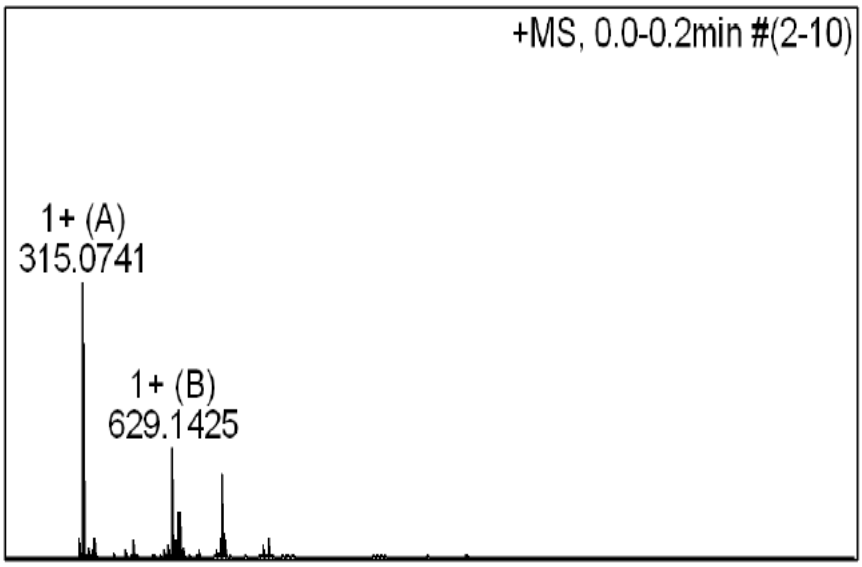
+MS, 0.1-0.2min #(3-10)



#	m/z	I	I %
1	198.0200	79113	20.6
2	215.0470	24697	6.4
3	216.0486	40115	10.4
4	232.0725	210297	54.8
5	237.0266	28890	7.5
6	270.0862	384009	100.0
7	423.2511	27108	7.1
8	446.1064	54545	14.2
9	451.0617	46407	12.1
10	660.1441	46528	12.1

Figure S53. Copy of HRMS ESI analysis of the derivatives **16**.

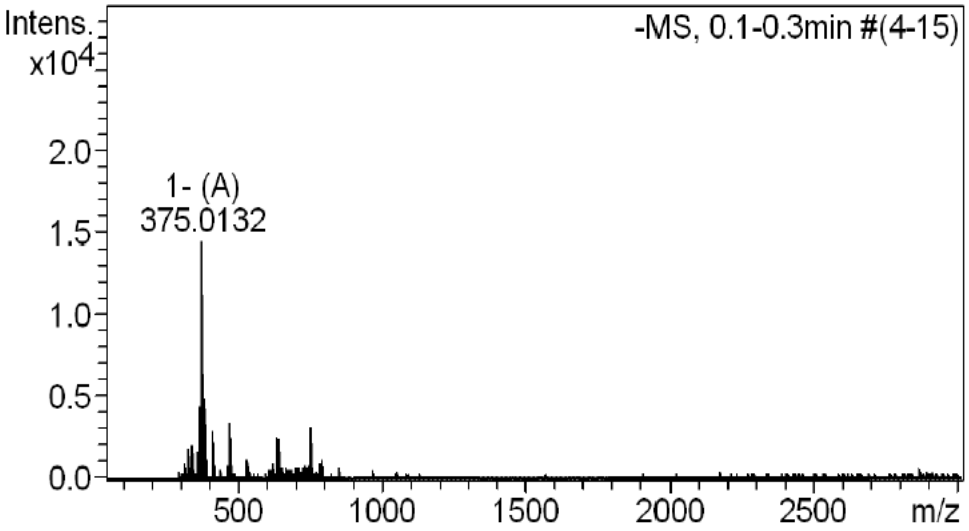
+MS, 0.0-0.2min #(2-10)



#	m/z	Res.	S/N	I	I %
1	315.0731			75307	100.0
2	629.1402			30153	40.0
3	651.1200			12670	16.8
4	1295.2211			12511	16.6
5	1609.2884			23044	30.6

Figure S54. Copy of HRMS ESI analysis of the derivatives **18**.

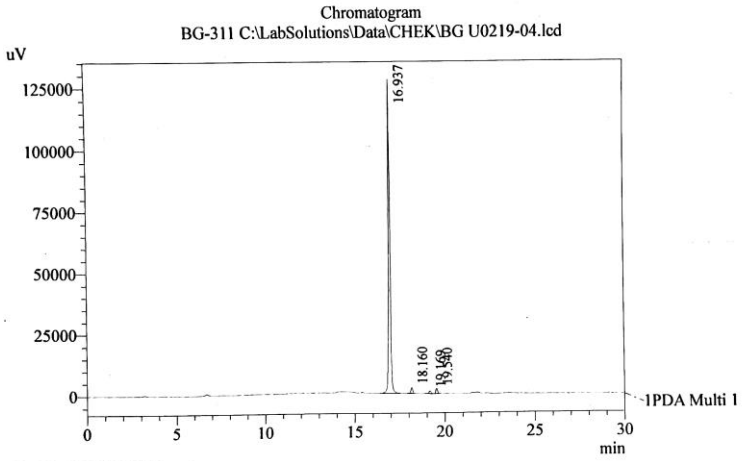
-MS, 0.1-0.3min #(4-15)



#	m/z	Res.	S/N	I	I %
1	367.9853	13464	151.5	4345	30.0
2	369.9795	12819	92.7	2667	18.4
3	375.0132	12785	501.7	14472	100.0
4	376.0169	12132	106.2	3073	21.2
5	377.0124	13331	217.7	6298	43.5
6	383.9793	13036	144.0	4198	29.0
7	385.9771	12983	104.2	3046	21.1
8	410.9877	13927	95.2	2855	19.7
9	470.9989	15840	105.9	3361	23.2
10	751.0112	16648	58.5	3092	21.4

Copies of HPLC Analysis

Figure S55. Copy HPLC analysis of the derivative **7a**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

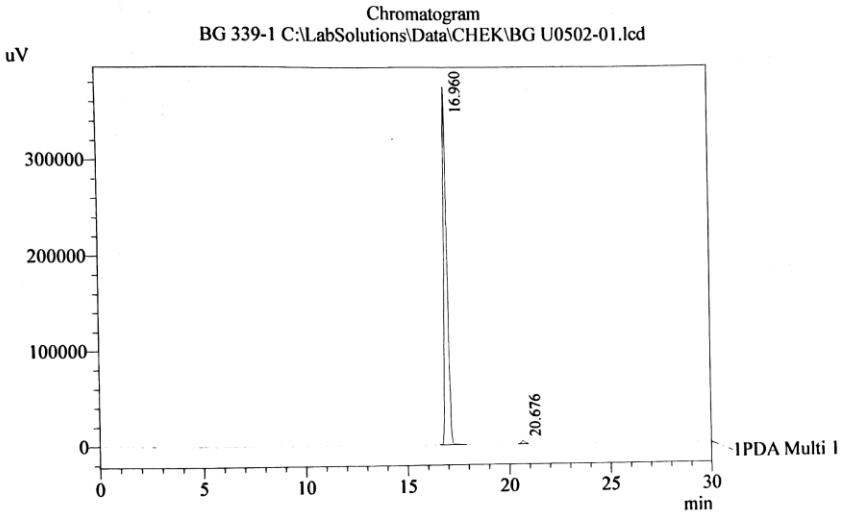
Peak#	Ret. Time	Area	Height	Area %
1	16.937	1069823	127742	96.467
2	18.160	16684	2427	1.504
3	19.169	7836	1157	0.707
4	19.540	14665	2153	1.322
Total		1109008	133479	100.000

Method Filename : FOS Cv.lcm 19.02.2024 13:19:56

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	20
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	20
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S56. Copy HPLC analysis of the derivative **7b**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

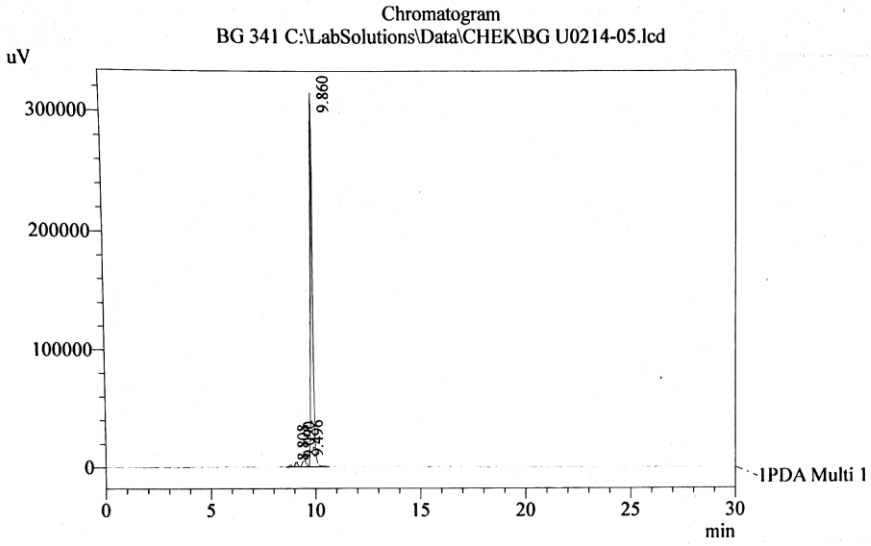
Peak#	Ret. Time	Area	Height	Area %
1	16.960	4423944	376008	99.040
2	20.676	42884	3472	0.960
Total		4466828	379480	100.000

Method Filename : FOS Cv.lcm 02.05.2024 12:48:55

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S57. Copy HPLC analysis of the derivative **7c**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

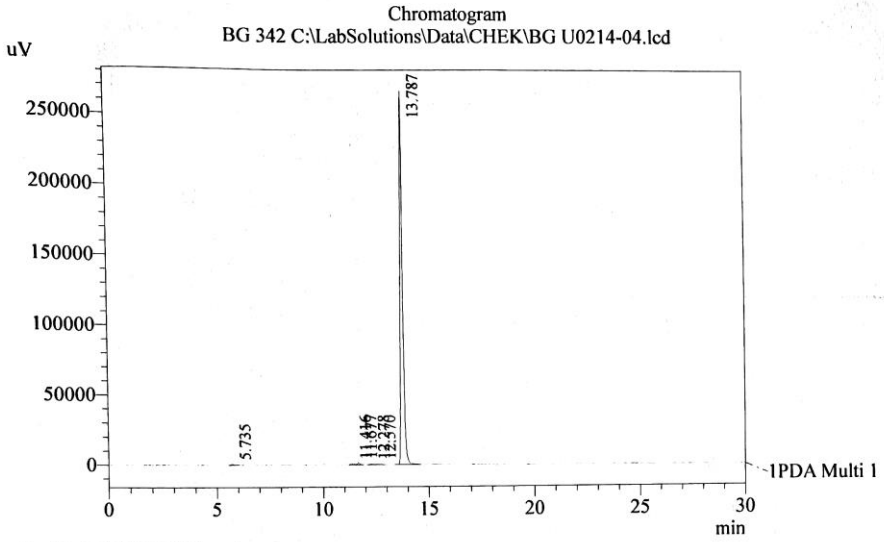
Peak#	Ret. Time	Area	Height	Area %
1	8.808	13042	1743	0.496
2	9.090	31396	4134	1.193
3	9.496	68893	5568	2.618
4	9.860	2517785	314791	95.693
Total		2631116	326235	100.000

Method Filename : FOS Cv.lcm 15.02.2024 12:30:13

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S58. Copy HPLC analysis of the derivative **7d**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

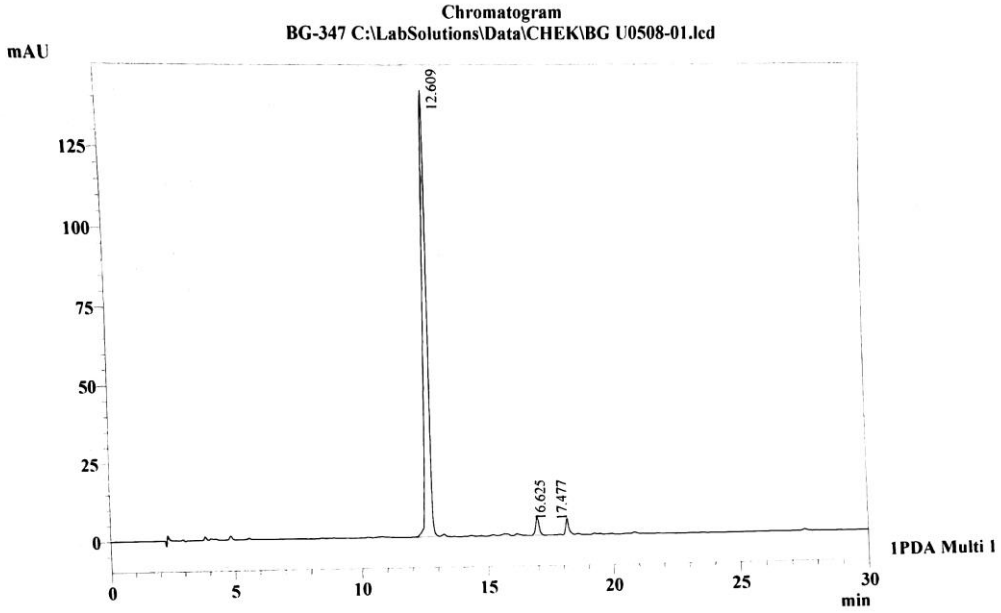
Peak#	Ret. Time	Area	Height	Area %
1	5.735	2963	484	0.127
2	11.416	6428	798	0.275
3	11.677	8524	1066	0.364
4	12.278	3950	521	0.169
5	12.570	4358	605	0.186
6	13.787	2313360	267031	98.879
Total		2339583	270505	100.000

Method Filename : FOS Cv.lcm 15.02.2024 11:49:35

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S59. Copy HPLC analysis of the derivative **7e**.



1 PDA Multi 1 / 270nm 4nm

PeakTable

PDA Ch1 270nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	12.609	1682637	141823	96.739
2	16.625	27938	3566	1.606
3	17.477	28776	3568	1.654
Total		1739350	148958	100.000

Method

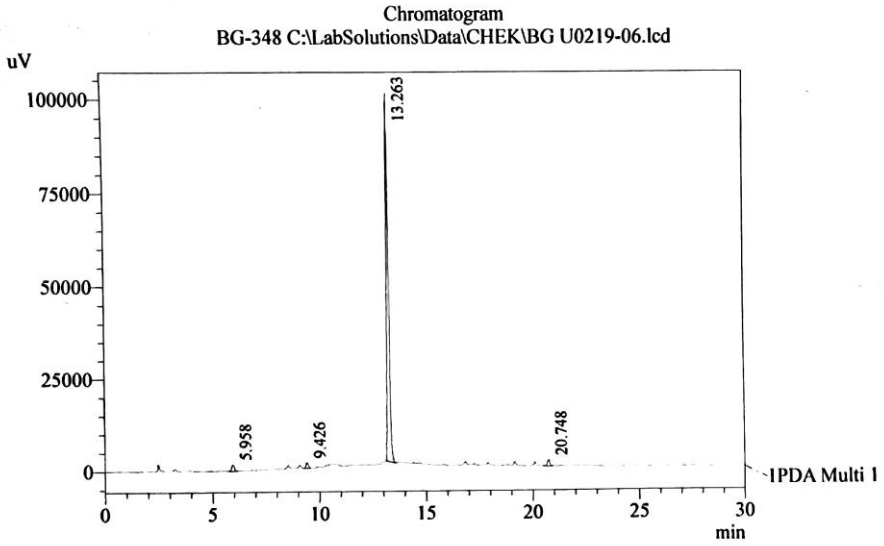
<<LC Program>>

Time	Unit	Command	Value
0.10	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Method Filename : FOS Bv.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18,.size 5mkm, 4,6*250mm, N 86912
Elution: A - H3PO4 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20mkl.

Figure S60. Copy HPLC analysis of the derivative **7f**.



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

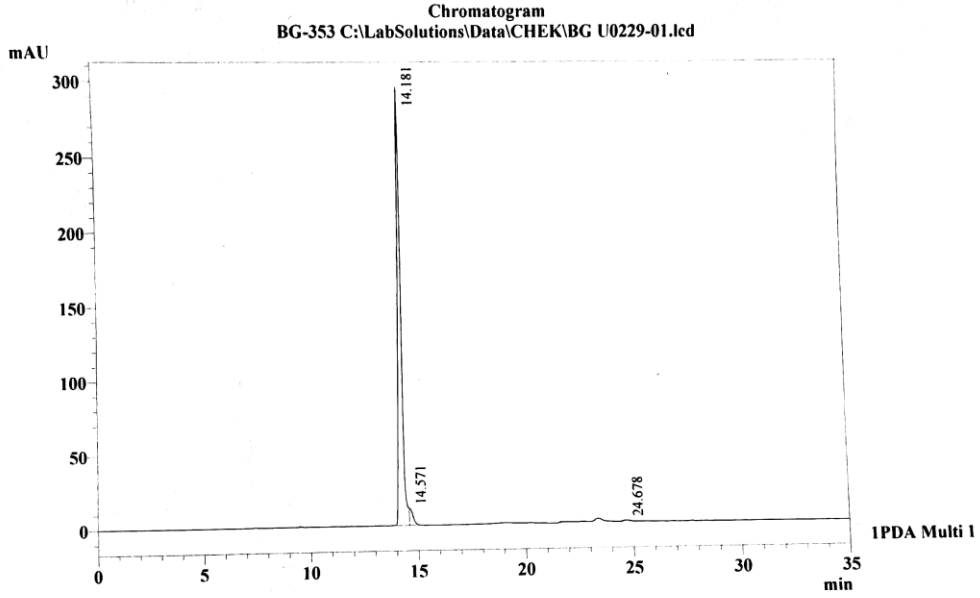
Peak#	Ret. Time	Area	Height	Area %
1	5.958	14245	1718	1.923
2	9.426	11247	1529	1.519
3	13.263	701459	98971	94.717
4	20.748	13632	1738	1.841
Total		740583	103956	100.000

Method Filename : FOS Cv.lcm 19.02.2024 14:59:05

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	20
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	20
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S61. Copy HPLC analysis of the derivative **7g**.



1 PDA Multi 1 / 385nm 4nm

PeakTable

PDA Ch1 385nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	14.181	3243431	295737	95.697
2	14.571	125395	11383	3.700
3	24.678	20460	960	0.604
Total		3389286	308080	100.000

Method

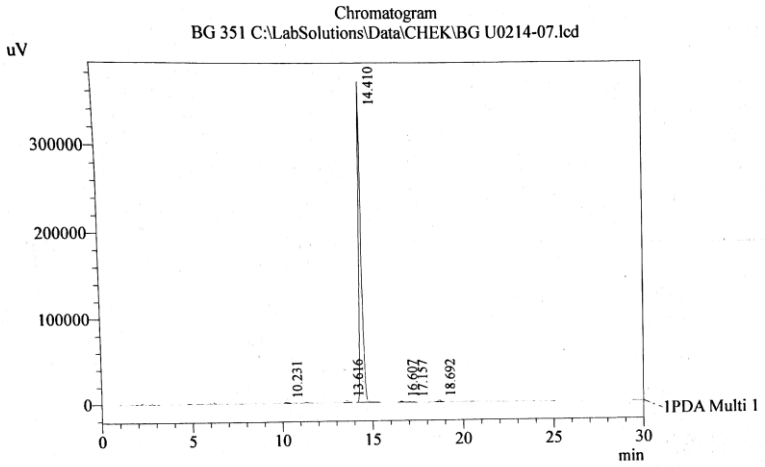
<<LC Program>>

Time	Unit	Command	Value
0.10	Pumps	B.Conc	10
30.00	Pumps	B.Conc	50
33.00	Pumps	B.Conc	10
45.00	Controller	Stop	

Method Filename : FOS A.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18,.size 5mkm, 4,6*250mm, N 86912
Elution: A - H3PO4 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20mkl.

Figure S62. Copy HPLC analysis of the derivative **7h**.



1 PDA Multi 1 / 275nm 4nm

PDA Ch1 275nm 4nm

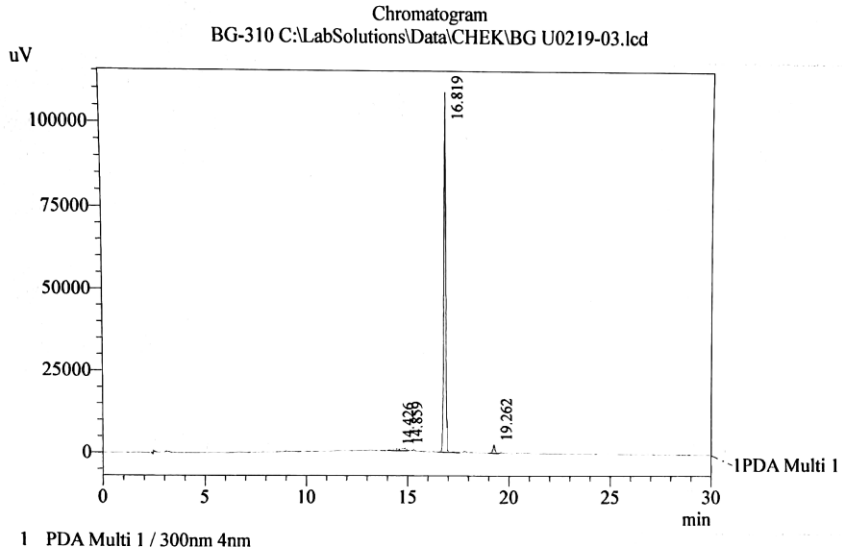
Peak#	Ret. Time	Area	Height	Area %
1	10.231	12383	1592	0.327
2	13.616	18386	2216	0.486
3	14.410	3707036	370558	97.986
4	16.607	11907	1361	0.315
5	17.157	14927	1345	0.395
6	18.692	18594	1954	0.491
Total		3783233	379024	100.000

Method Filename : FOS Cv.lcm 15.02.2024 14:02:12

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S63. Copy HPLC analysis of the derivative **8a**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

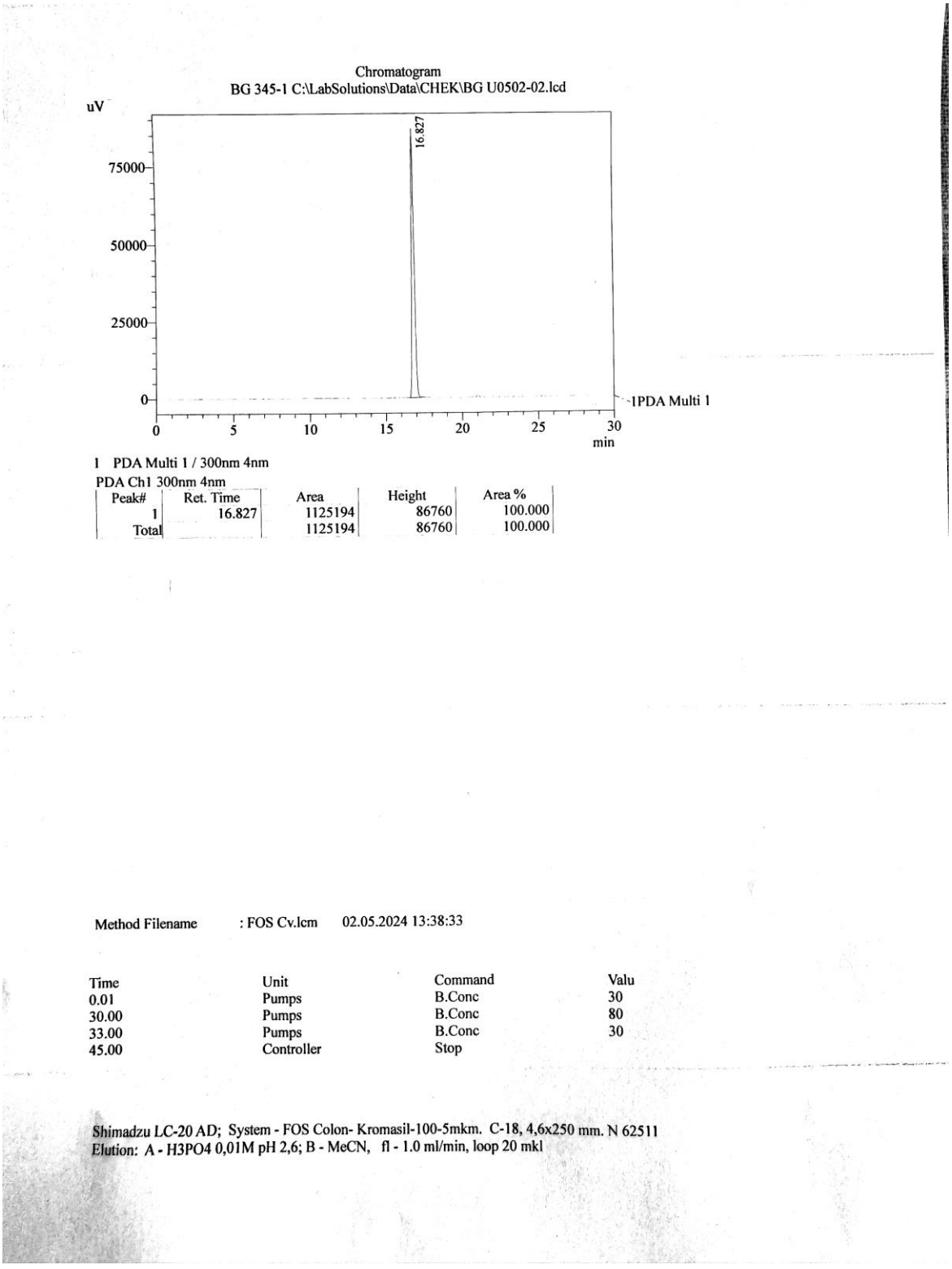
Peak#	Ret. Time	Area	Height	Area %
1	14.426	12250	475	1.342
2	14.859	12616	778	1.382
3	16.819	867961	108888	95.107
4	19.262	19788	2551	2.168
Total		912614	112692	100.000

Method Filename : FOS Cv.lcm 19.02.2024 12:32:34

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	20
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	20
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S64. Copy HPLC analysis of the derivative **8b**.



1 PDA Multi 1 / 300nm 4nm
PDA Ch1 300nm 4nm

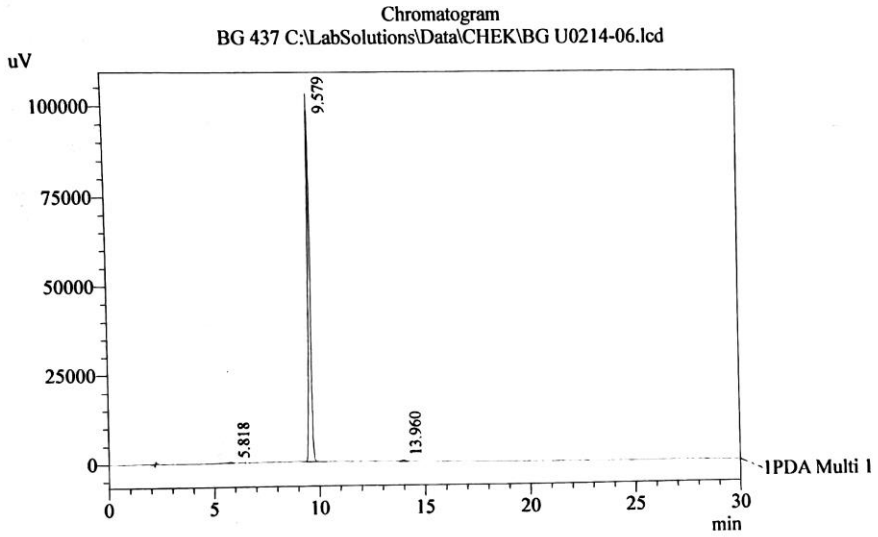
Peak#	Ret. Time	Area	Height	Area %
1	16.827	1125194	86760	100.000
Total		1125194	86760	100.000

Method Filename : FOS Cv.lcm 02.05.2024 13:38:33

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S65. Copy HPLC analysis of the derivative **8c**.



1 PDA Multi 1 / 300nm 4nm

PDA Ch1 300nm 4nm

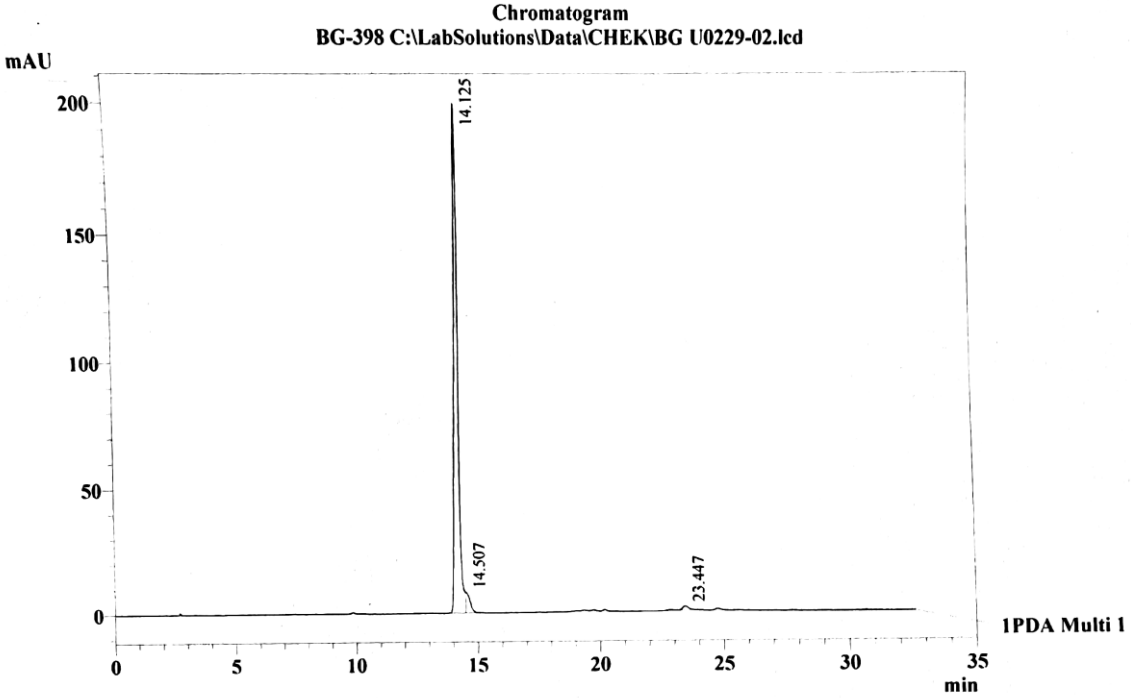
Peak#	Ret. Time	Area	Height	Area %
1	5.818	1098	114	0.118
2	9.579	926621	103070	99.463
3	13.960	3901	436	0.419
Total		931619	103621	100.000

Method Filename : FOS Cv.lcm 15.02.2024 13:17:11

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	40
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	40
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S66. Copy HPLC analysis of the derivative **8g**.



1 PDA Multi 1 / 385nm 4nm

PeakTable

PDA Ch1 385nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	14.125	2219217	199749	95.026
2	14.507	93594	7983	4.008
3	23.447	22573	1492	0.967
Total		2335384	209223	100.000

Method

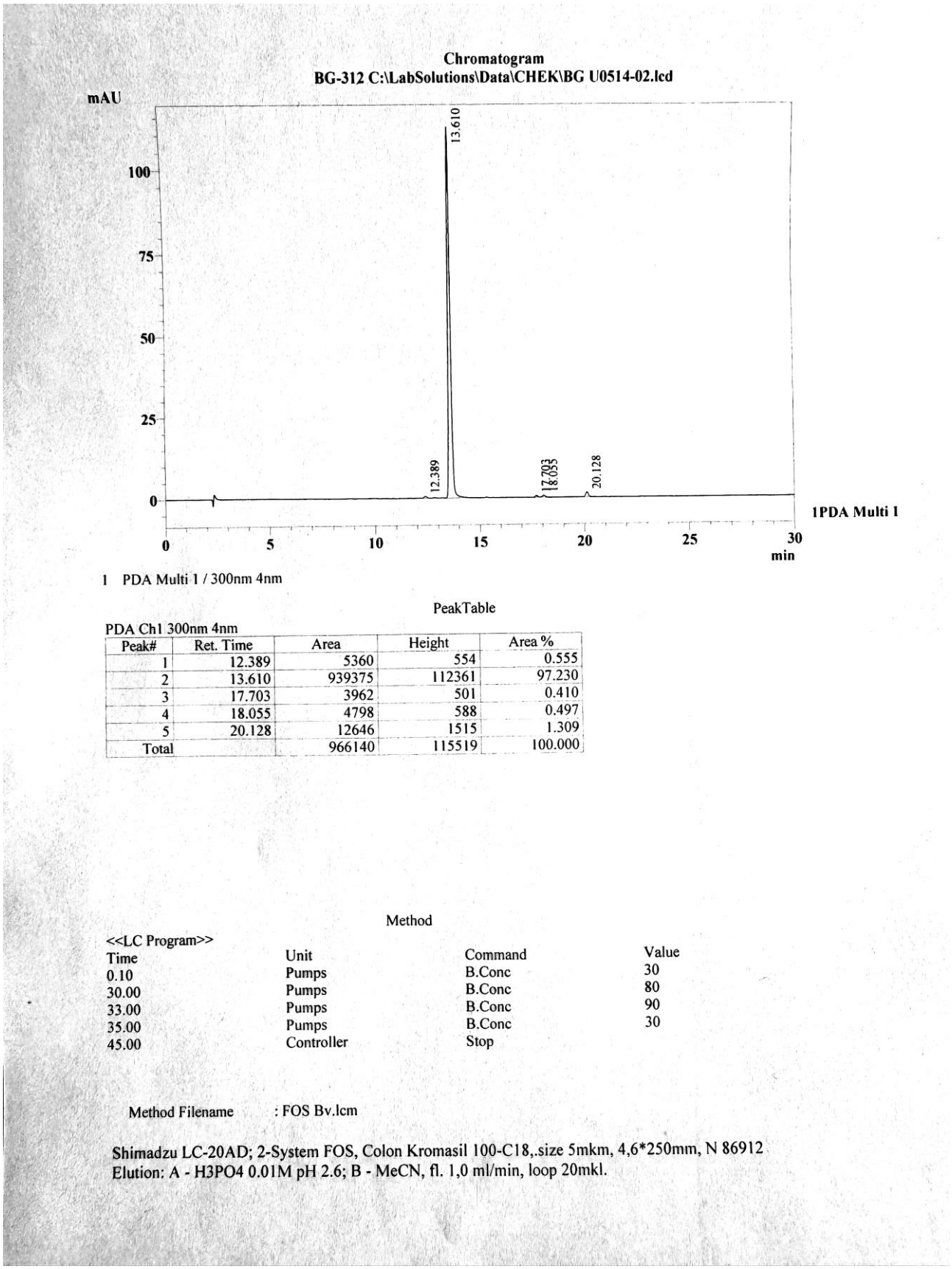
<<LC Program>>

Time	Unit	Command	Value
0.10	Pumps	B.Conc	10
30.00	Pumps	B.Conc	50
33.00	Pumps	B.Conc	10
45.00	Controller	Stop	

Method Filename : FOS A.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18,.size 5mkm, 4,6*250mm, N 86912
Elution: A - H3PO4 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20mkl.

Figure S67. Copy HPLC analysis of the derivative **18**.



1 PDA Multi 1 / 300nm 4nm

PeakTable

PDA Ch1 300nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	12.389	5360	554	0.555
2	13.610	939375	112361	97.230
3	17.703	3962	501	0.410
4	18.055	4798	588	0.497
5	20.128	12646	1515	1.309
Total		966140	115519	100.000

Method

<<LC Program>>

Time	Unit	Command	Value
0.10	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
33.00	Pumps	B.Conc	90
35.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Method Filename : FOS Bv.lcm

Shimadzu LC-20AD; 2-System FOS, Colon Kromasil 100-C18,.size 5mkm, 4,6*250mm, N 86912
Elution: A - H3PO4 0.01M pH 2.6; B - MeCN, fl. 1,0 ml/min, loop 20mkl.

Copies of 2D NMR Spectra of 7a.

Figure S68. ^{1}H-^{13}C HSQC spectrum for compound **7a**.

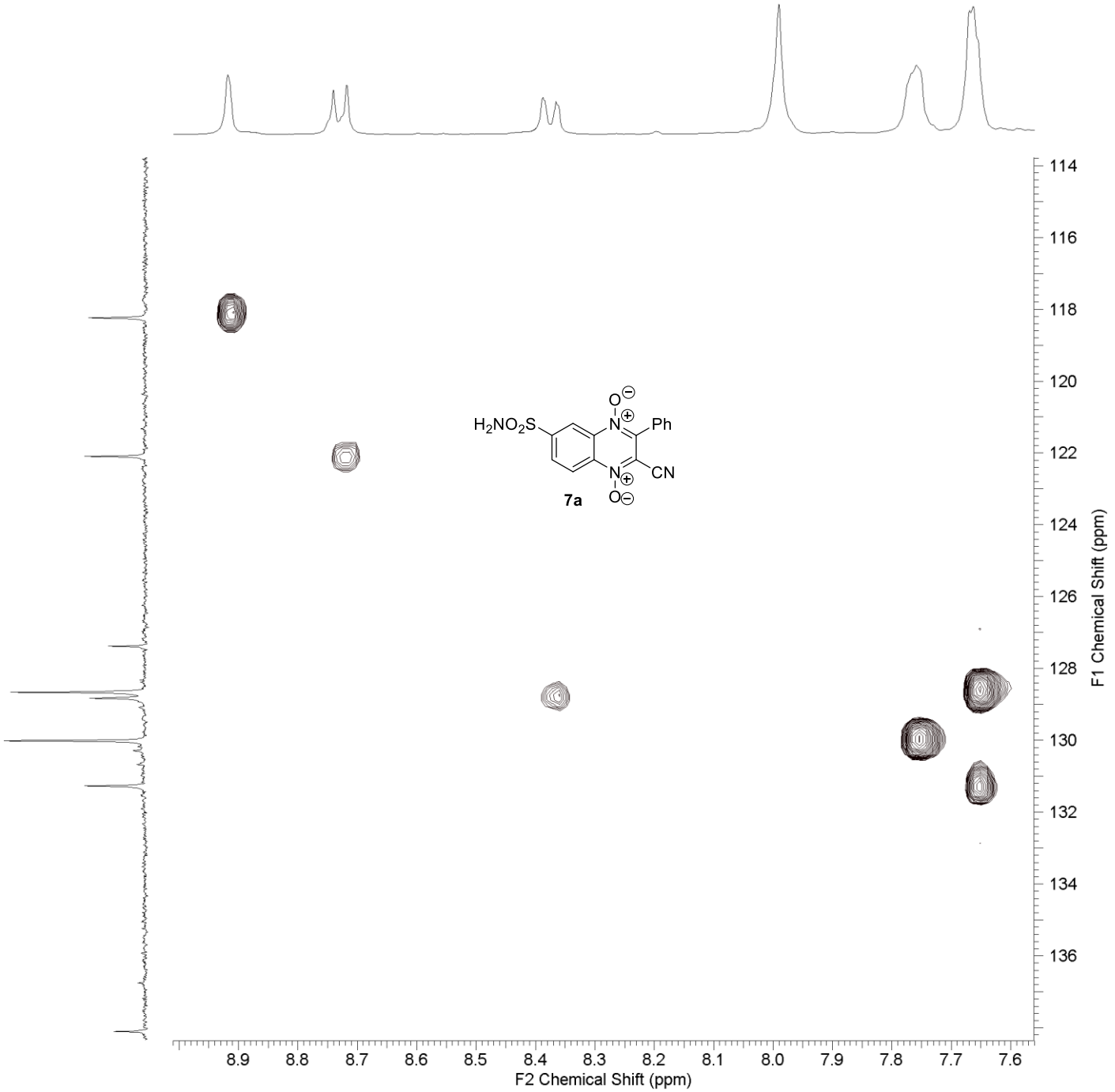


Figure S69. HMBC spectrum for compound **7a**.

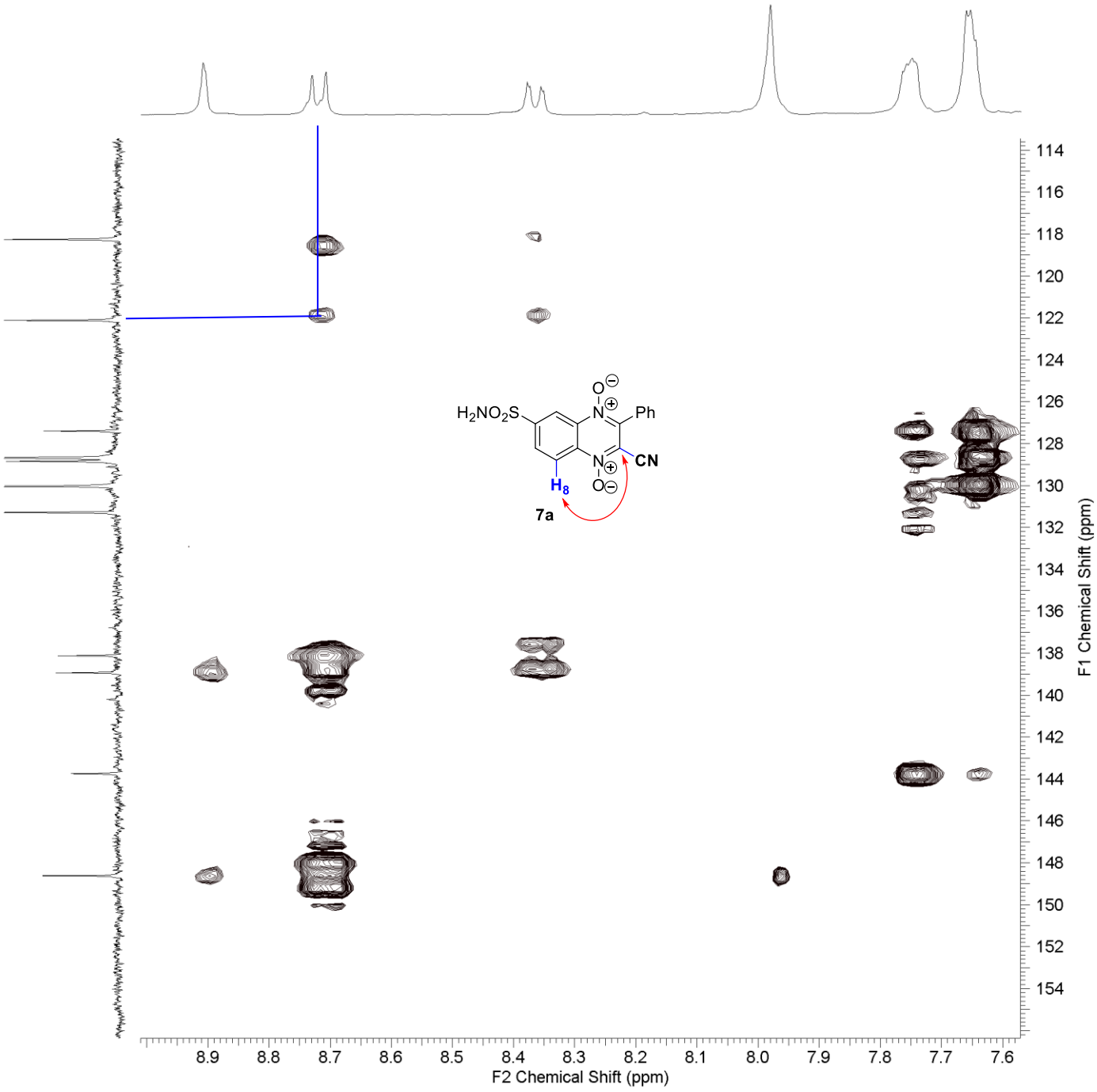


Figure S70. Selective NOE spectrum at H-5 at 7.75 ppm for compound **7a**.