

Synthesis, structure and antiradical activity of functionally substituted hydrazides of isonicotinic acid

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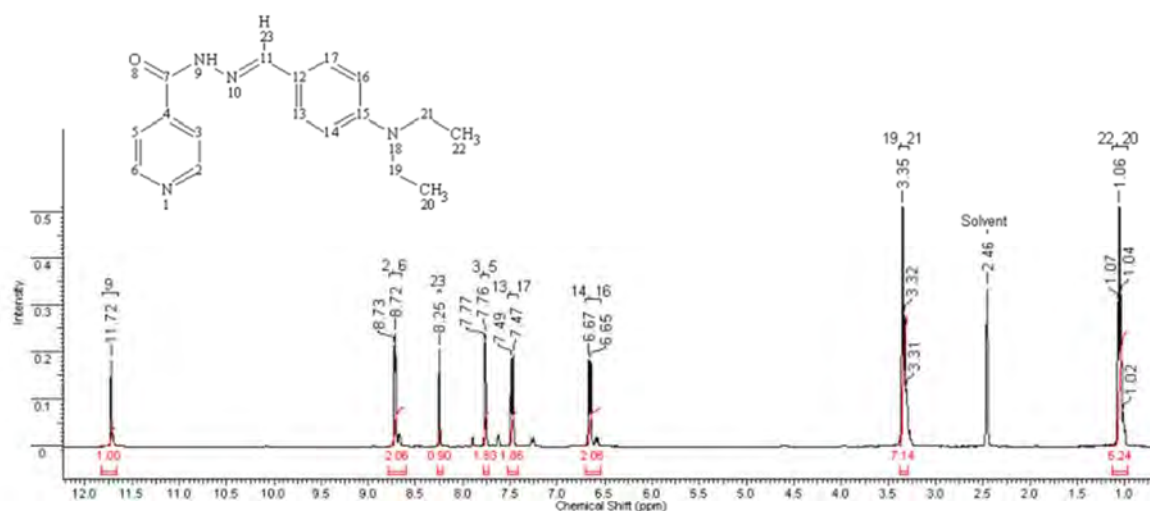
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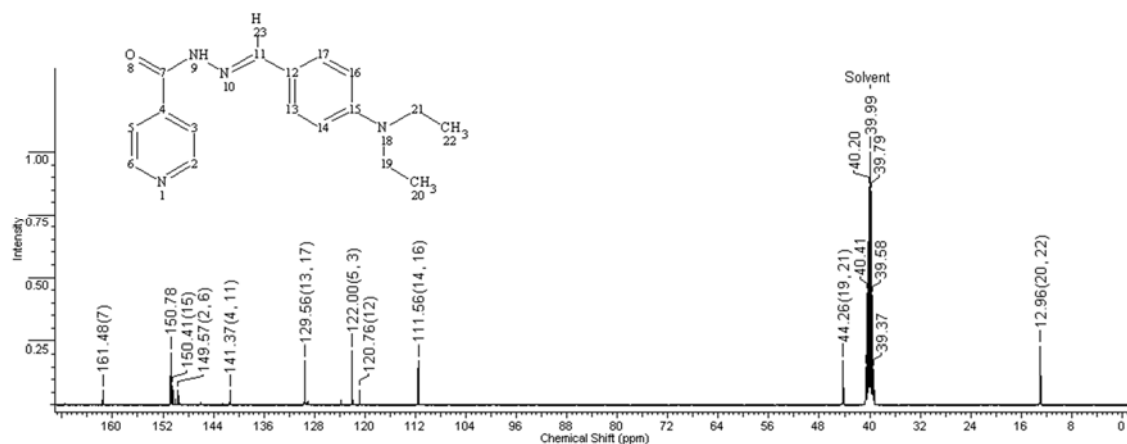
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No.	Atom	Exp. Shift (ppm)	No.	Atom	Exp. Shift (ppm)	No.	(ppm)	Value	Absolute Value
1	22	[0.97 .. 1.13]	8	17	[7.42 .. 7.53]	1	[0.96 .. 1.13]	6.238	1.05685e+2
2	20	[0.97 .. 1.13]	9	3	[7.73 .. 7.81]	2	[3.30 .. 3.36]	7.143	1.21017e+2
3	19	[3.29 .. 3.39]	10	5	[7.73 .. 7.81]	3	[6.55 .. 6.71]	2.059	3.48830e+1
4	21	[3.29 .. 3.39]	11	23	[8.23 .. 8.27]	4	[7.42 .. 7.53]	1.859	3.14910e+1
5	14	[6.55 .. 6.71]	12	2	[8.65 .. 8.78]	5	[7.73 .. 7.79]	1.833	3.10488e+1
6	16	[6.55 .. 6.71]	13	6	[8.65 .. 8.78]	6	[8.21 .. 8.27]	0.904	1.53092e+1
7	13	[7.42 .. 7.53]	14	9	[11.65 .. 11.81]	7	[8.60 .. 8.79]	2.064	3.49590e+1
						8	[11.67 .. 11.82]	0.996	1.66748e+1

Fig. S-1. ^1H -NMR-spectrum of **1** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	2	149.57	148.690	0.880	10	14	111.56	111.460	0.096
2	3	122.00	126.050	-4.054	11	15	150.41	147.880	2.529
3	4	141.37	138.210	3.161	12	16	111.56	111.460	0.096
4	5	122.00	126.050	-4.054	13	17	129.56	127.850	1.707
5	6	149.57	148.690	0.880	14	19	44.26	44.850	-0.589
6	7	161.48	162.470	-0.991	15	20	12.96	12.860	0.099
7	11	141.37	144.550	-3.179	16	21	44.26	44.850	-0.589
8	12	120.76	121.800	-1.043	17	22	12.96	12.860	0.099
9	13	129.56	127.850	1.707					

Fig. S-2. ^{13}C -NMR-spectrum of **1** (100.53 MHz, DMSO- d_6)

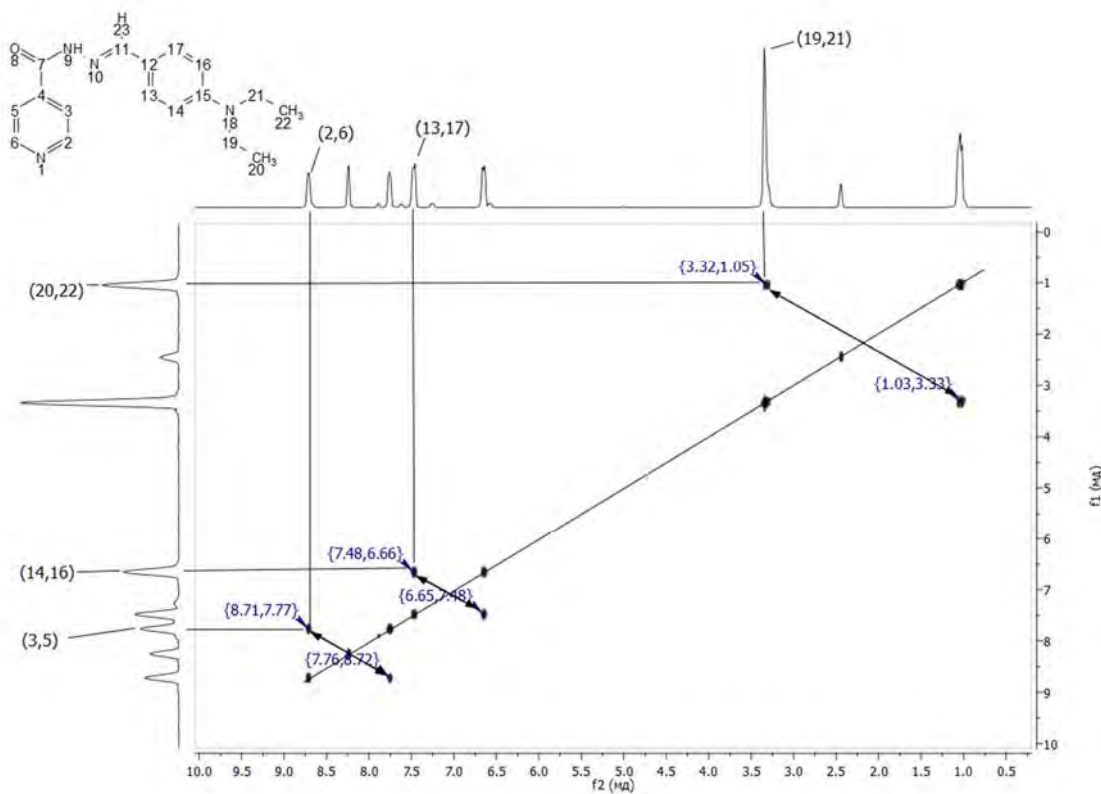


Fig. S-3. COSY ^1H - ^1H -NMR-spectrum of **1** (399.78 MHz, DMSO- d_6)

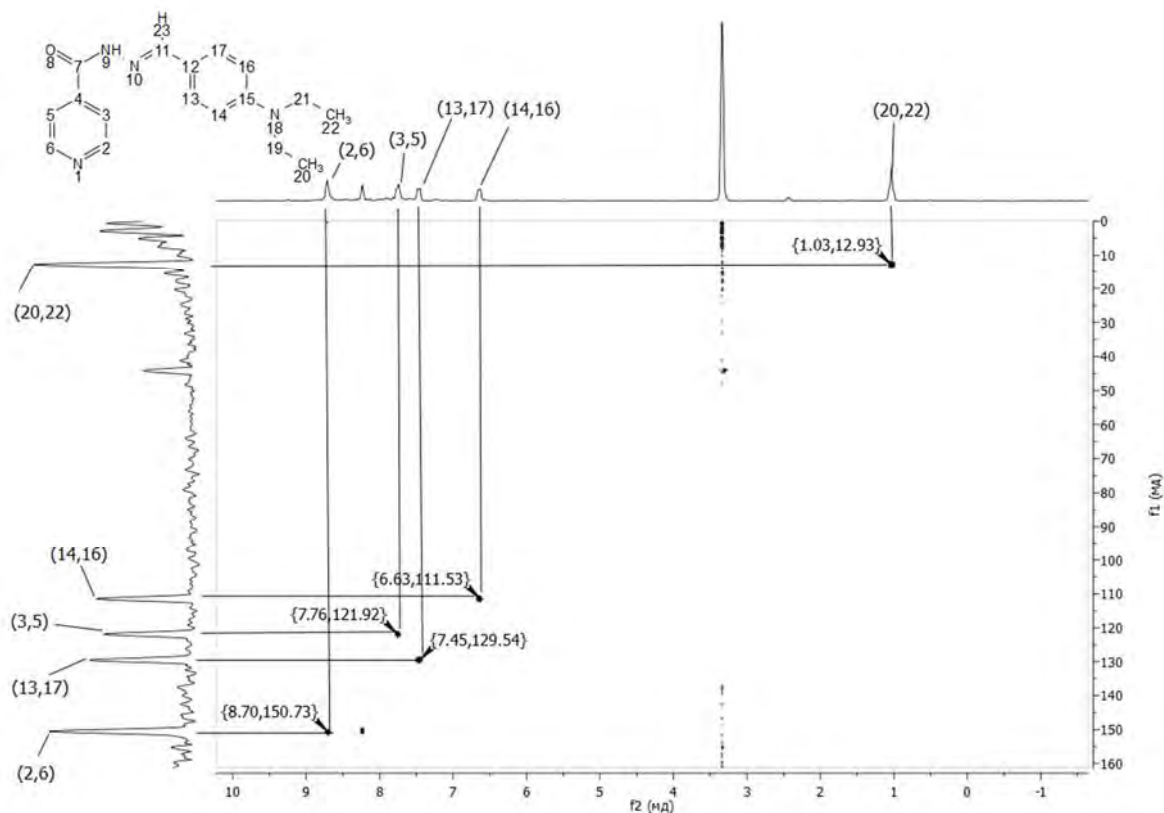


Fig. S-4. HMQC ^1H - ^{13}C -NMR-spectrum of **1** (399.78 MHz, 100.53 MHz, DMSO- d_6)

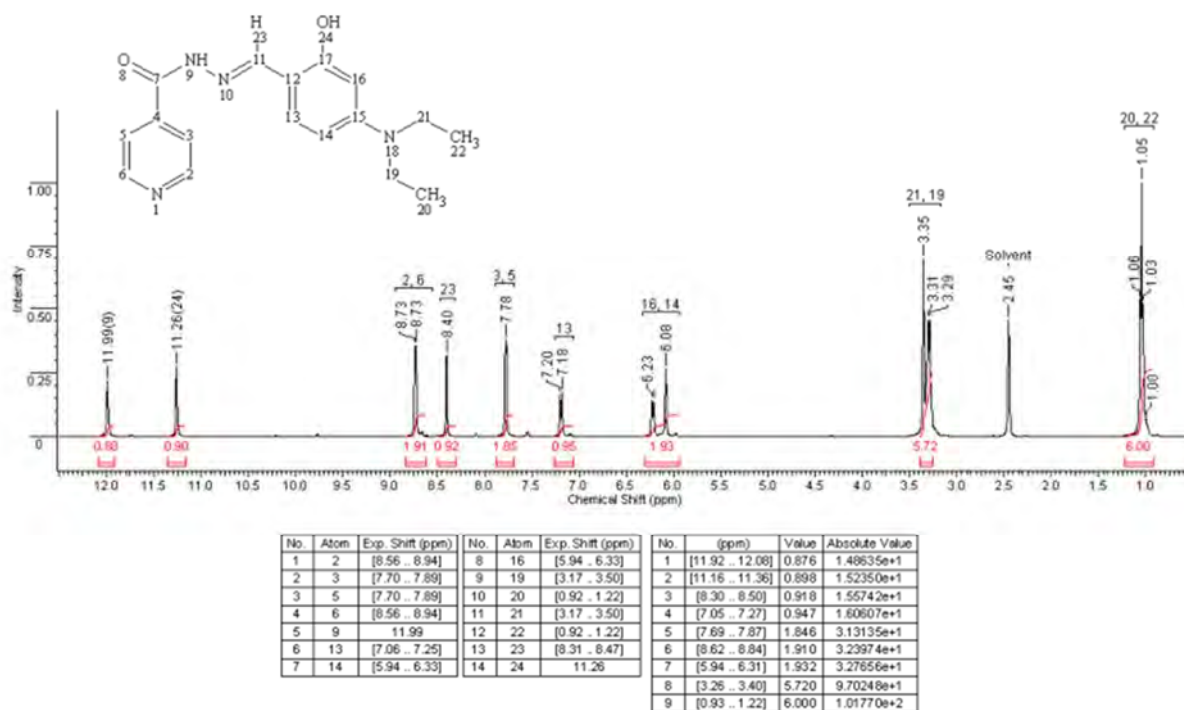
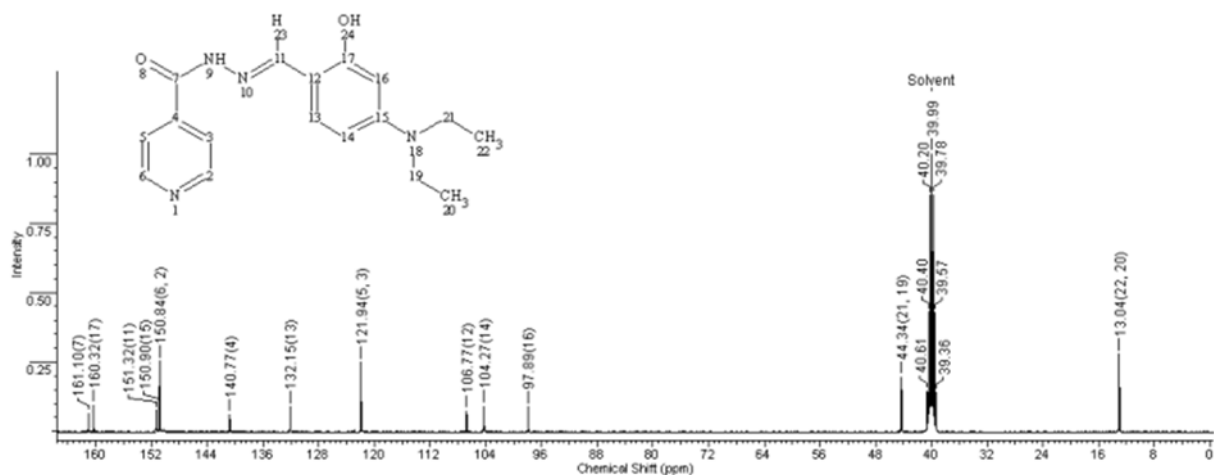


Fig. S-5. ^1H -NMR-spectrum of **2** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	2	150.84	148.690	2.148	10	14	104.27	102.210	2.061
2	3	121.94	126.050	-4.111	11	15	150.90	147.470	3.426
3	4	140.77	138.210	2.560	12	16	97.89	96.310	1.583
4	5	121.94	126.050	-4.111	13	17	160.32	163.590	-3.274
5	6	150.84	148.690	2.148	14	19	44.34	44.600	-0.263
6	7	161.10	162.470	-1.372	15	20	13.04	12.300	0.745
7	11	151.32	143.750	7.565	16	21	44.34	44.600	-0.263
8	12	106.77	112.170	-5.400	17	22	13.04	12.300	0.745
9	13	132.15	132.890	-0.739					

Fig. S-6. ^{13}C -NMR-spectrum of **2** (100.53 MHz, DMSO-d_6)

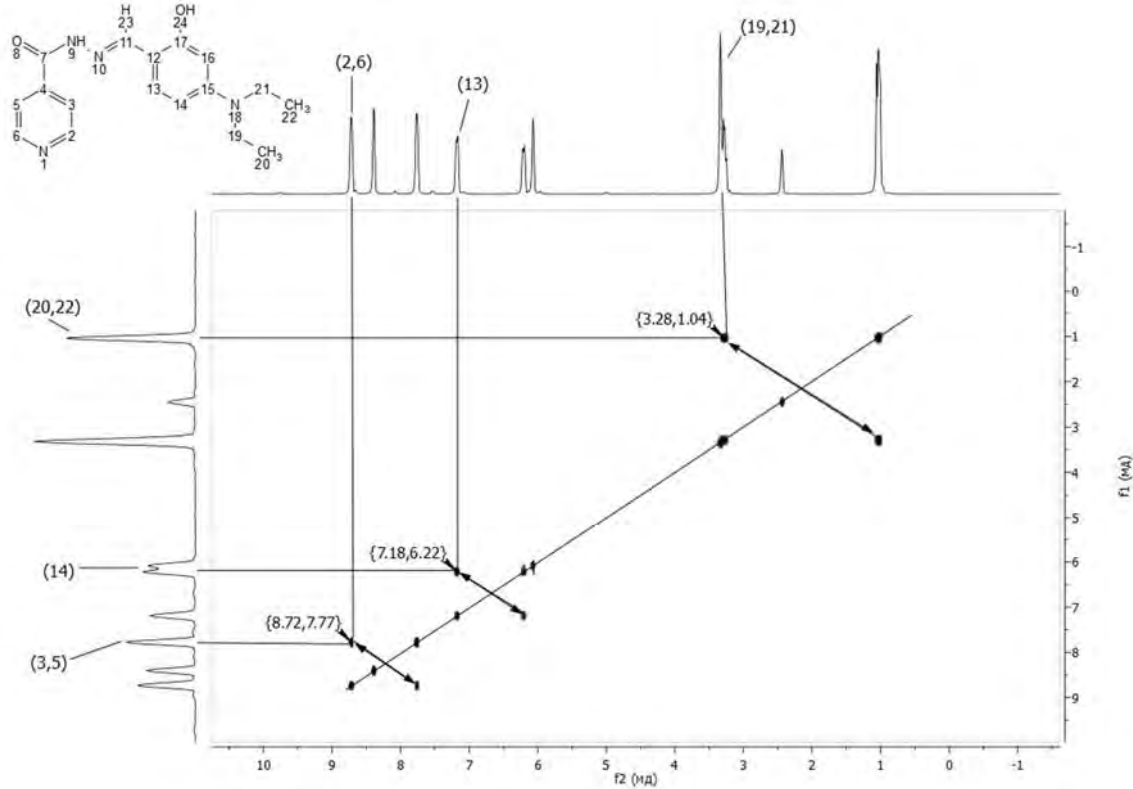


Fig. S-7. COSY ^1H - ^1H -NMR-spectrum of **2** (399.78 MHz, DMSO-d_6)

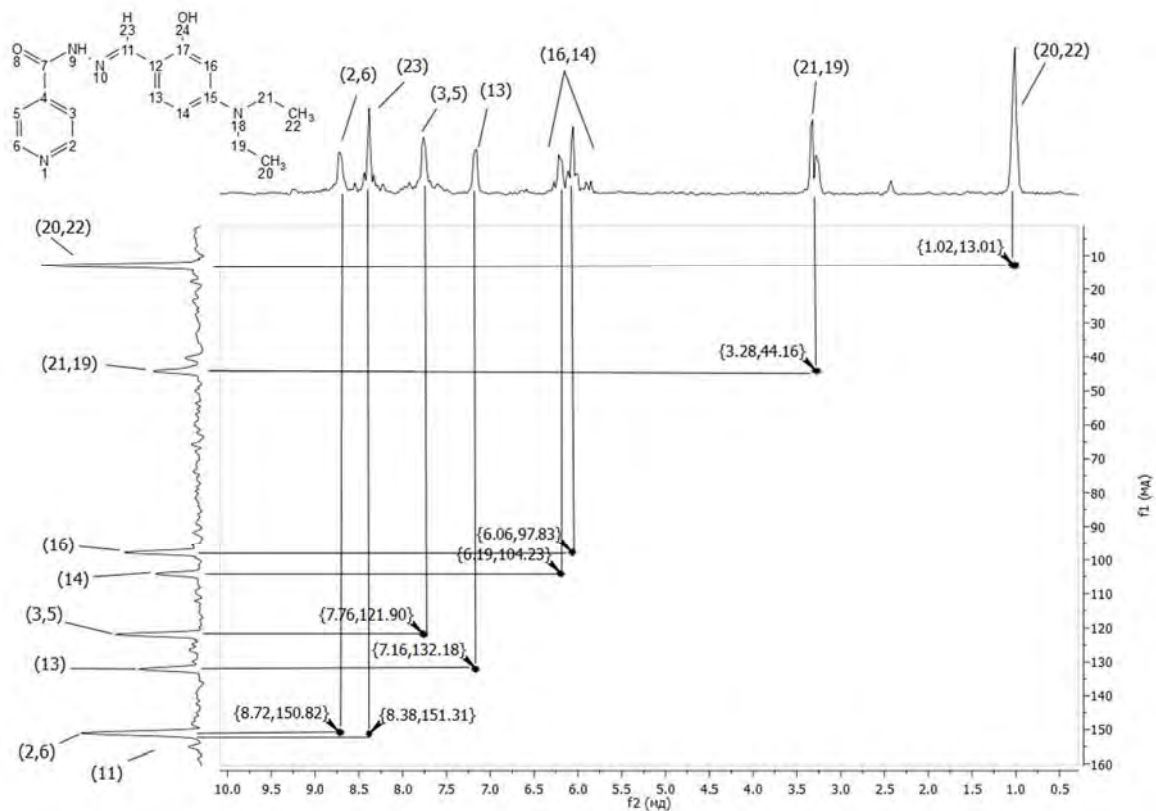


Fig. S-8. HMQC ^1H - ^{13}C -NMR-spectrum of **2** (399.78 MHz, 100.53 MHz, DMSO- d_6)

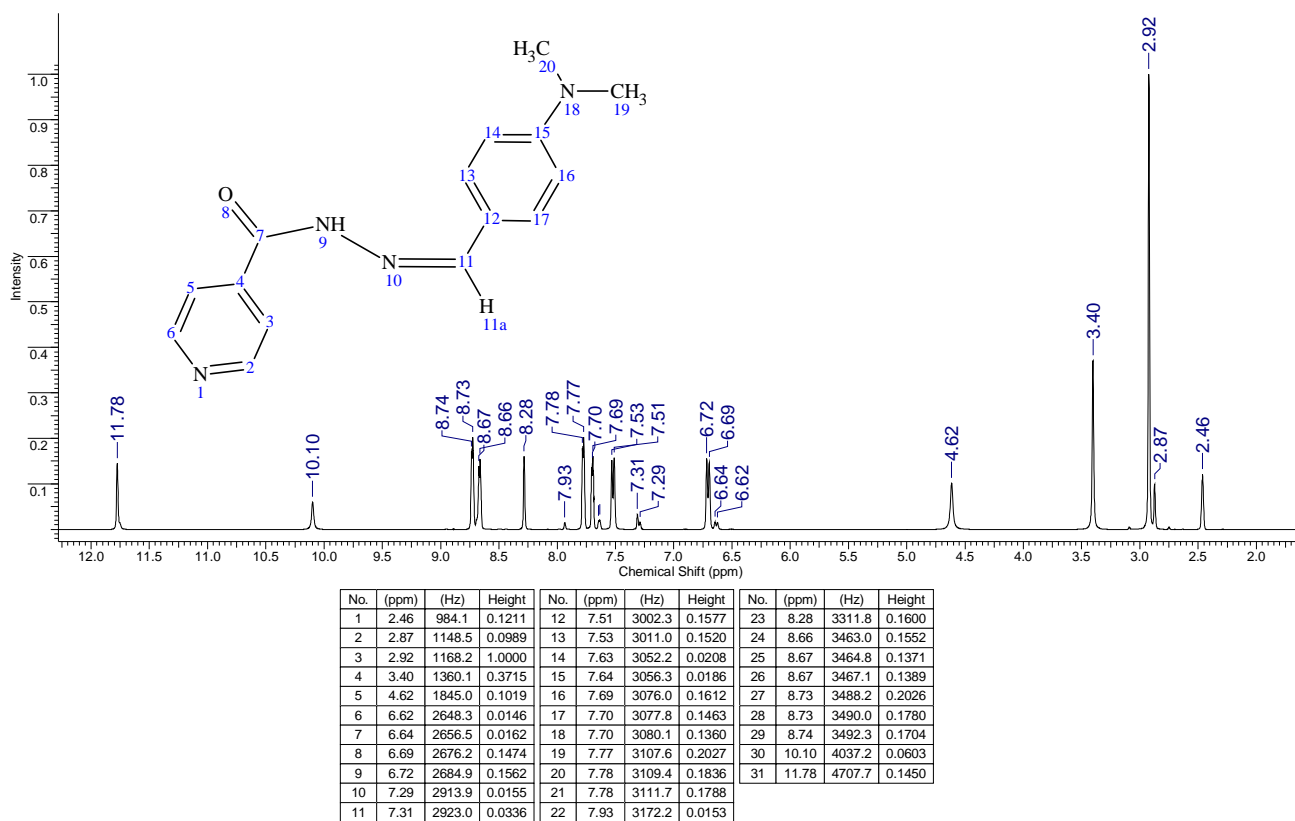


Fig. S-9. ^1H -NMR-spectrum of **3** (399.78 MHz, DMSO- d_6)

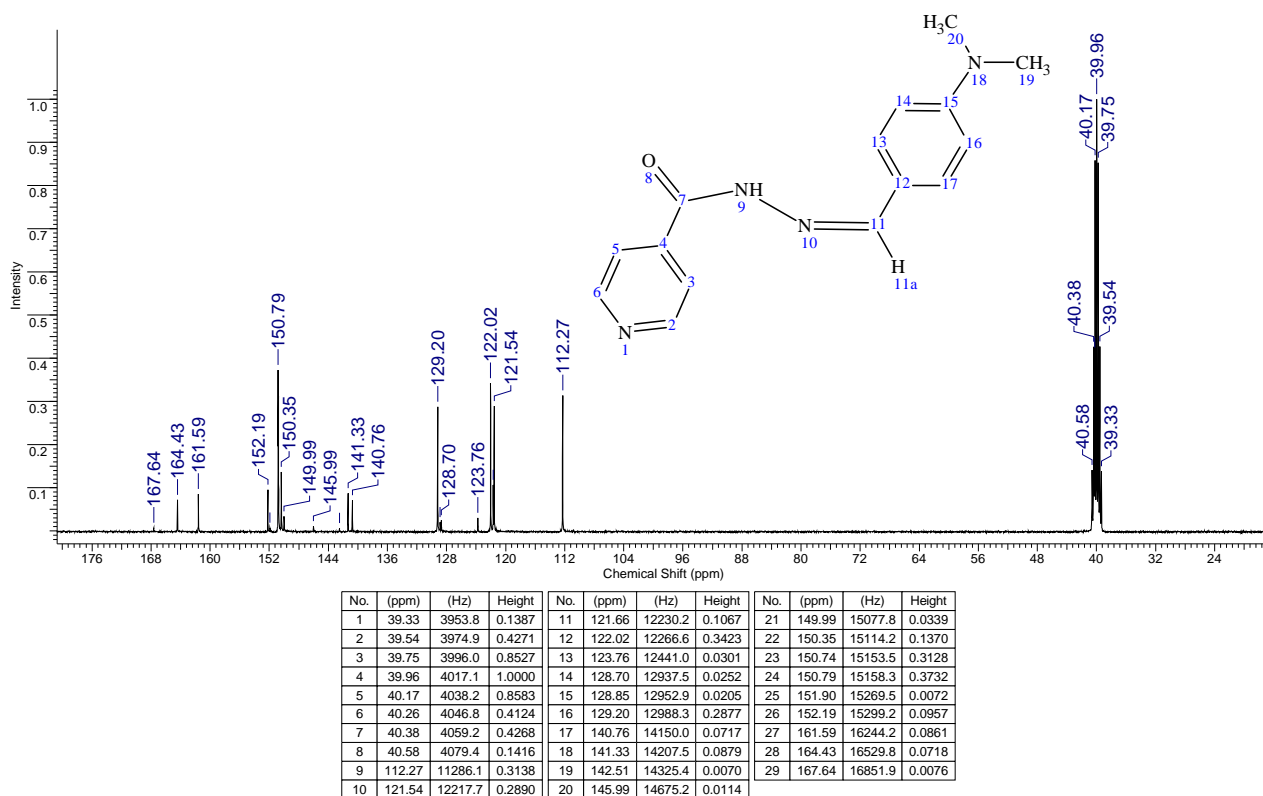


Fig. S-10. ^{13}C -NMR-spectrum of **3** (100.53 MHz, DMSO-d_6)

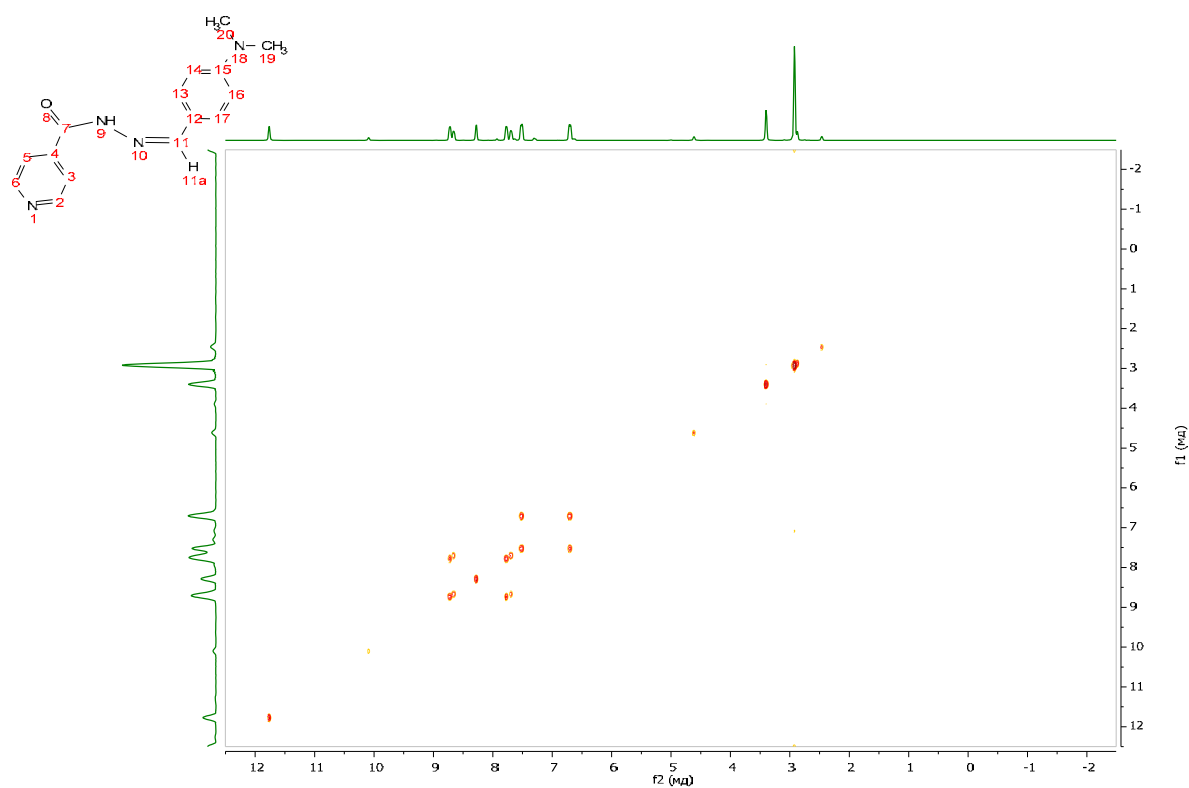


Fig. S-11. COSY ^1H - ^1H -NMR-spectrum of **3** (399.78 MHz, DMSO-d_6)

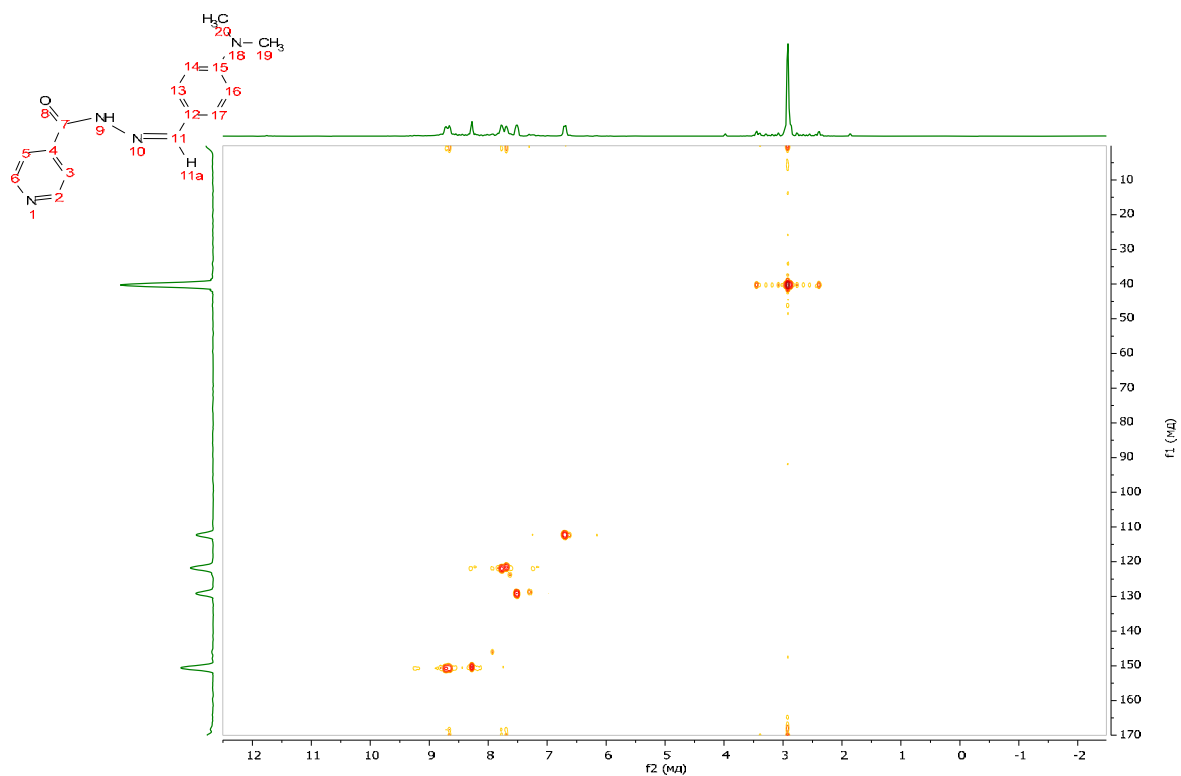


Fig. S-12. HMQC ^1H - ^{13}C -NMR-spectrum of **3** (399.78 MHz, 100.53 MHz, DMSO- d_6)

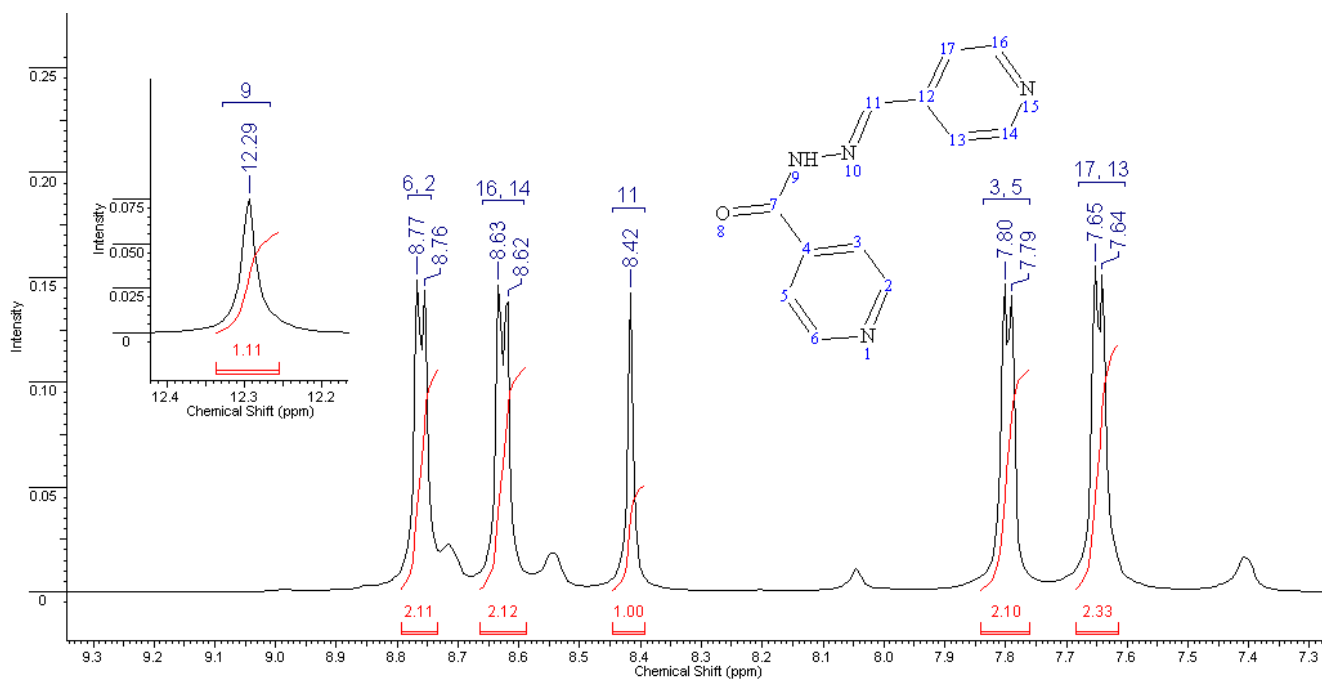


Fig. S-13. ^1H -NMR-spectrum of **4** (399.78 MHz, DMSO- d_6)

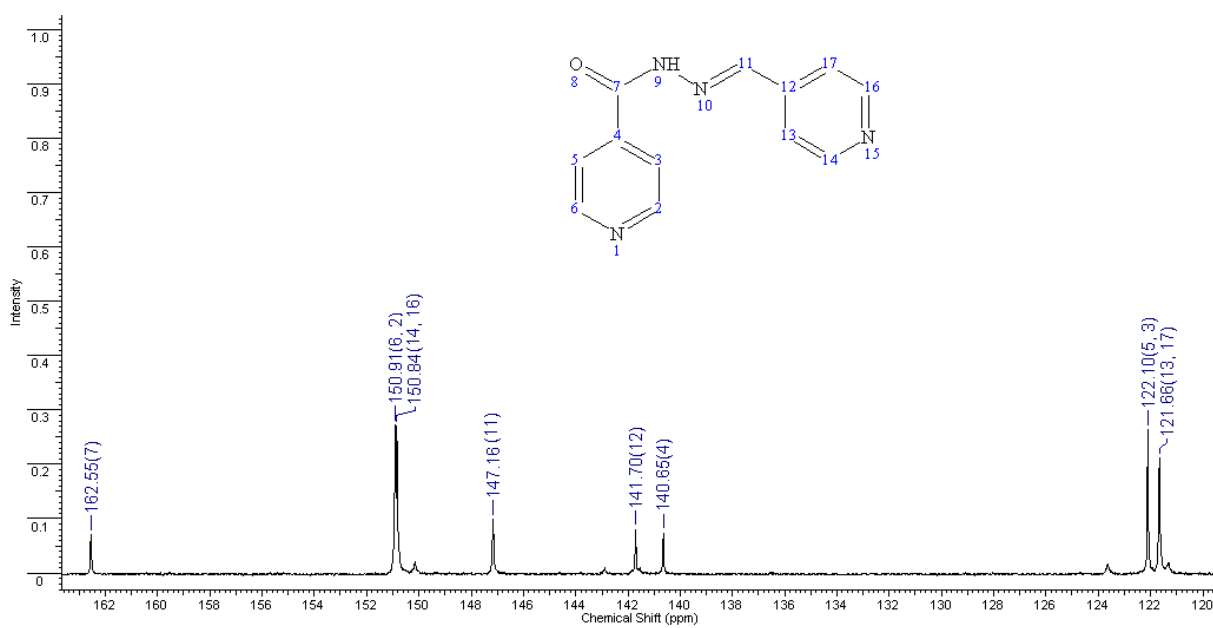


Fig. S-14. $^{13}\text{C-NMR}$ -spectrum of **4** (100.53 MHz, DMSO-d_6)

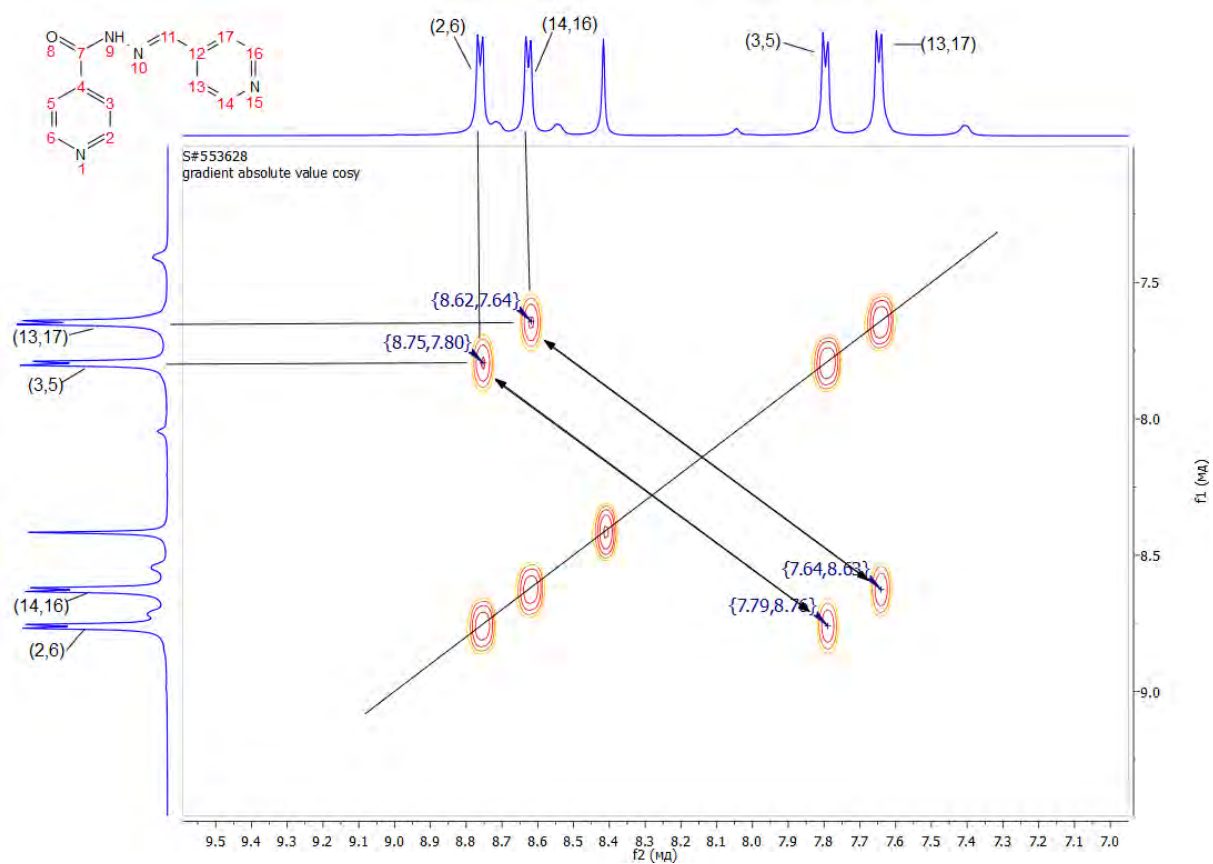


Fig. S-15. COSY $^1\text{H-NMR}$ -spectrum of **4** (399.78 MHz, DMSO-d_6)

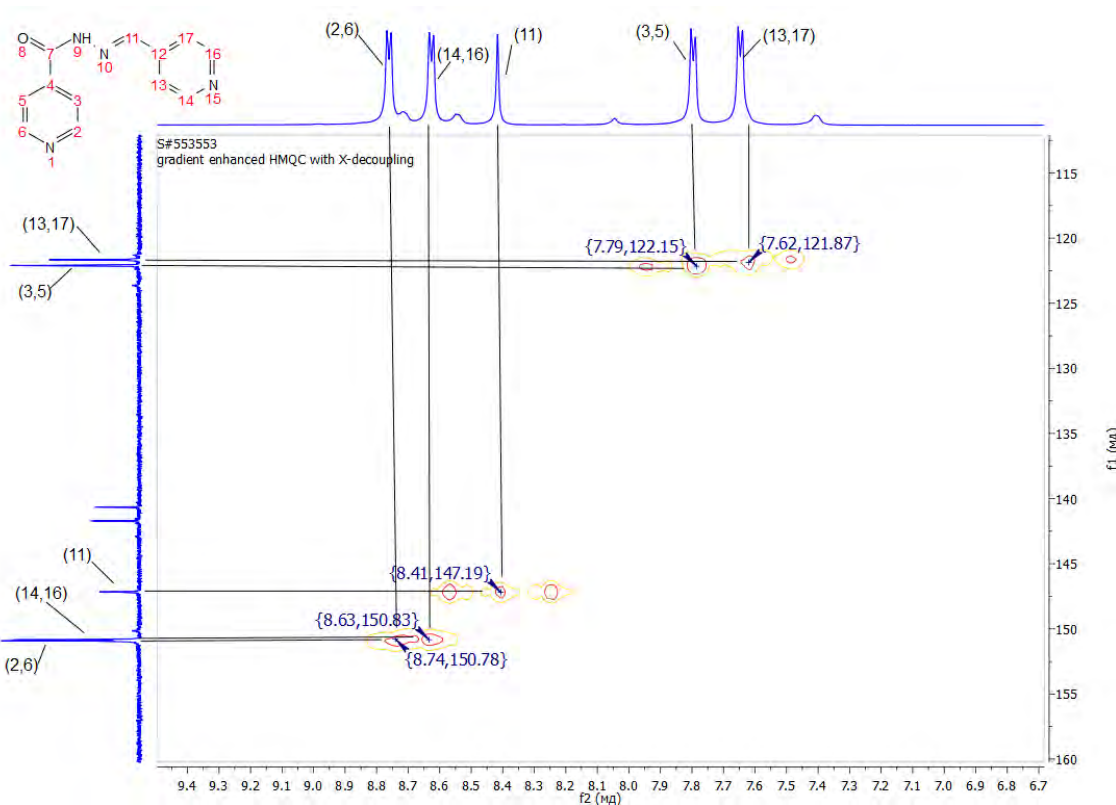


Fig. S-16. HMQC ^1H - ^{13}C -NMR-spectrum of **4** (399.78 MHz, 100.53 MHz, DMSO- d_6)

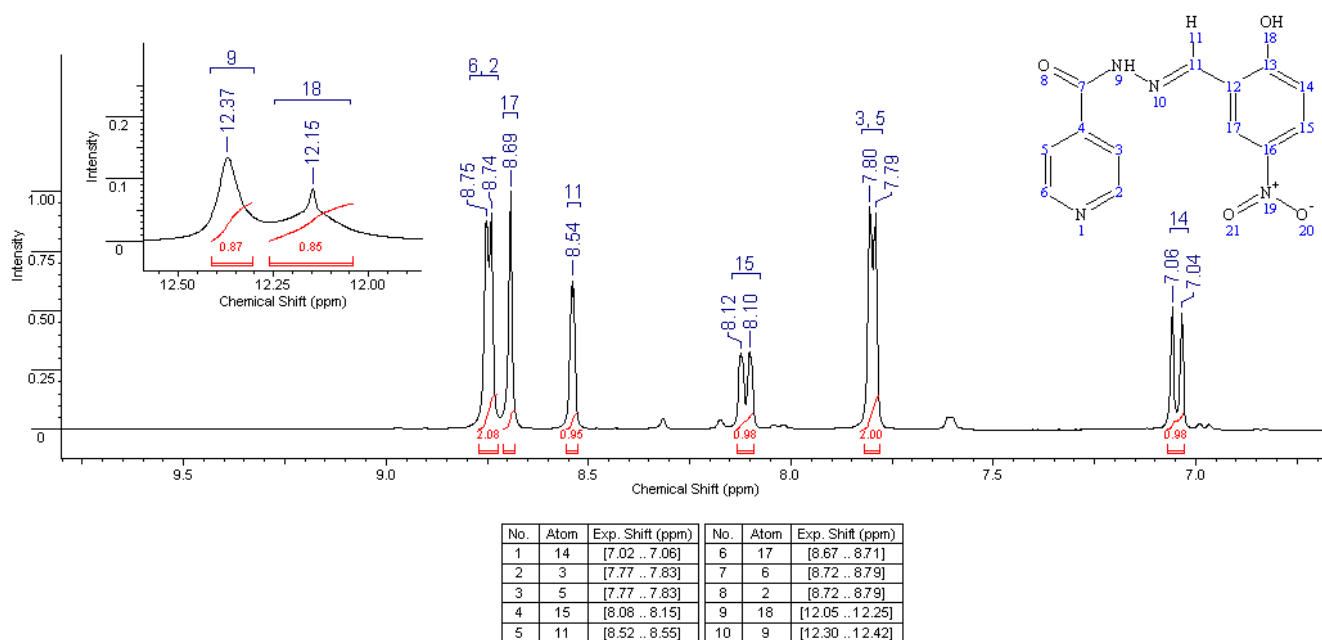
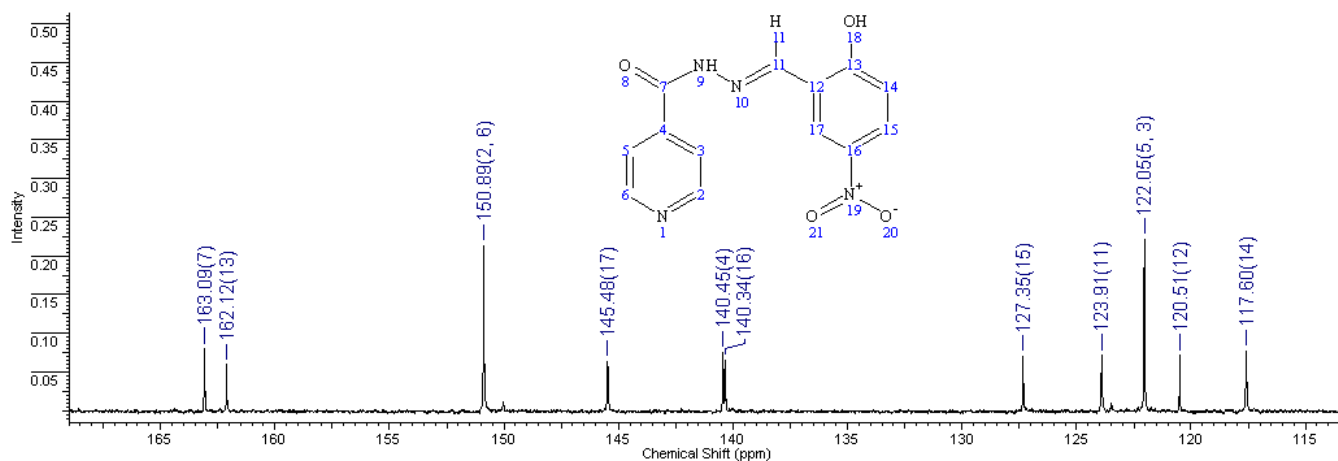


Fig. S-17. ^1H -NMR-spectrum of **5** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	14	117.60	114.750	2.851	8	4	140.45	138.210	2.236
2	12	120.51	119.320	1.189	9	6	150.89	148.690	2.196
3	17	145.48	122.150	23.330	10	2	150.89	148.690	2.196
4	15	127.35	124.420	2.925	11	11	123.91	149.200	-25.287
5	3	122.05	126.050	-3.997	12	13	162.12	159.910	2.208
6	5	122.05	126.050	-3.997	13	7	163.09	162.470	0.620
7	16	140.34	138.030	2.311					

Fig. S-18. ^{13}C -NMR-spectrum of **5** (100.53 MHz, DMSO-d_6)

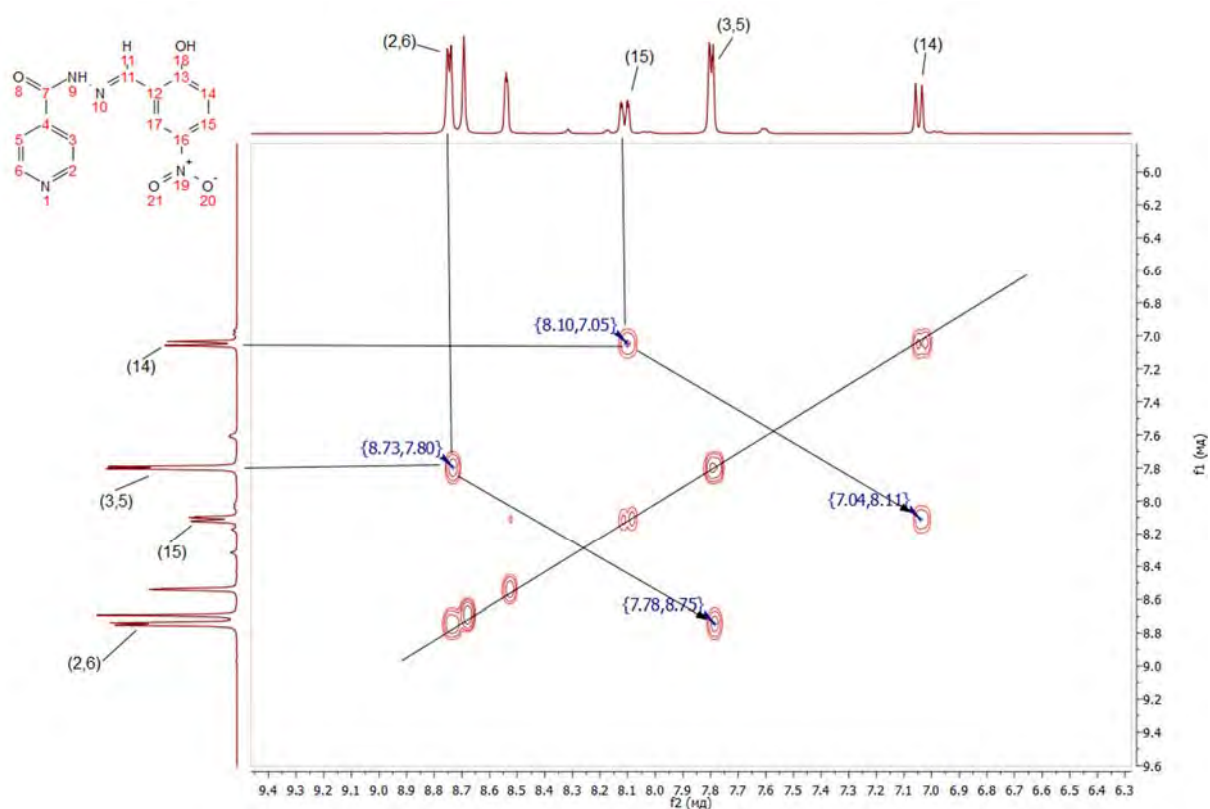


Fig. S-19. COSY ^1H - ^1H -NMR-spectrum of **5** (399.78 MHz, DMSO-d_6)

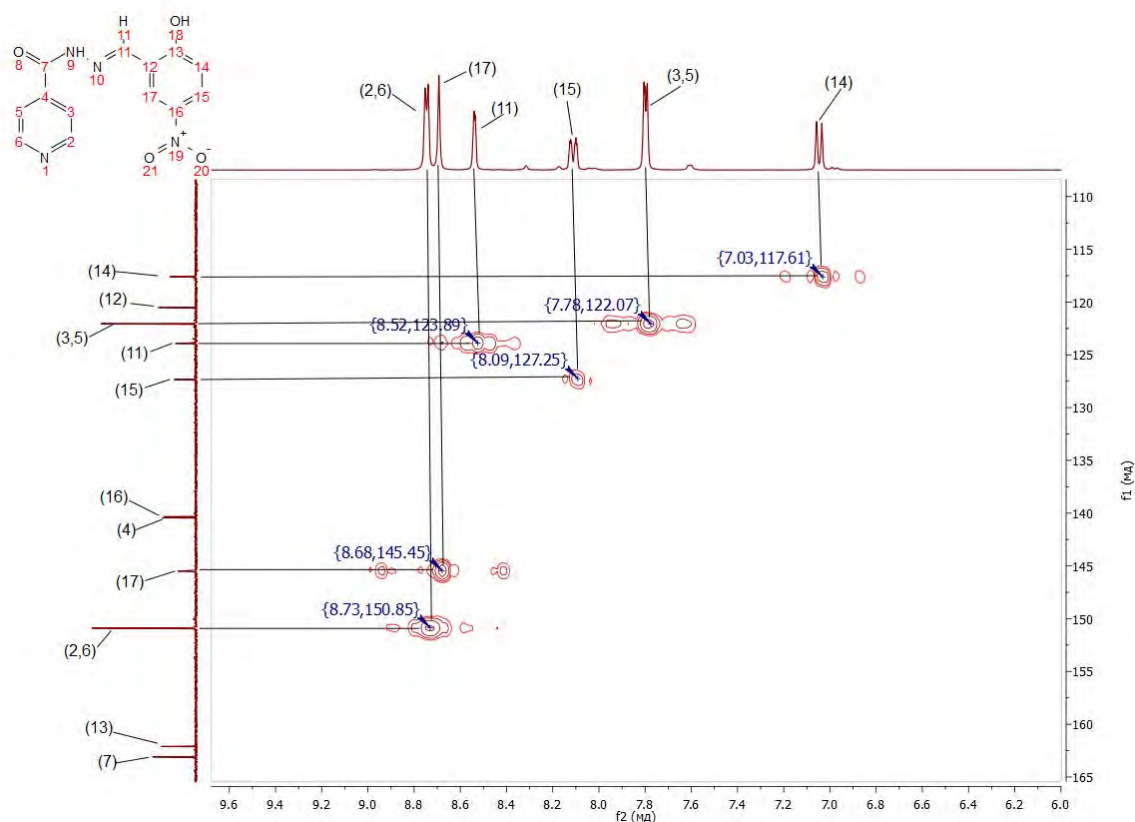


Fig. S-20. HMQC ^1H - ^{13}C -NMR-spectrum of **5** (399.78 MHz, 100.53 MHz, DMSO- d_6)

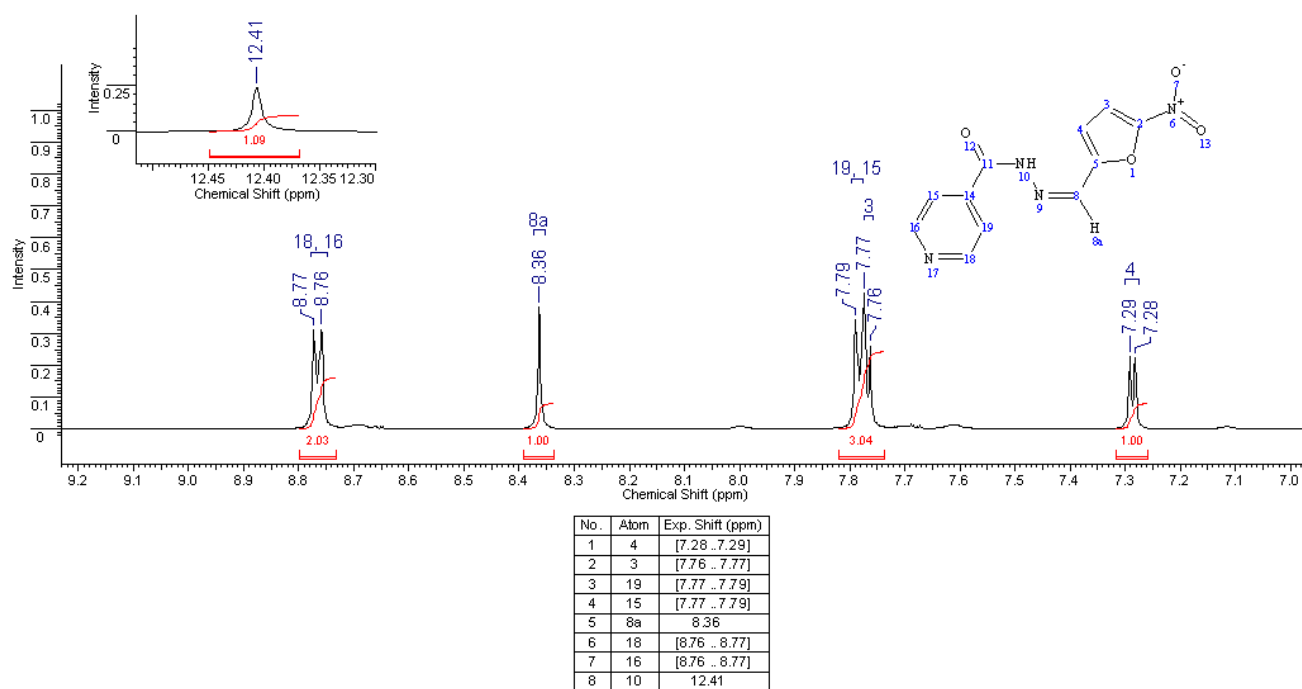
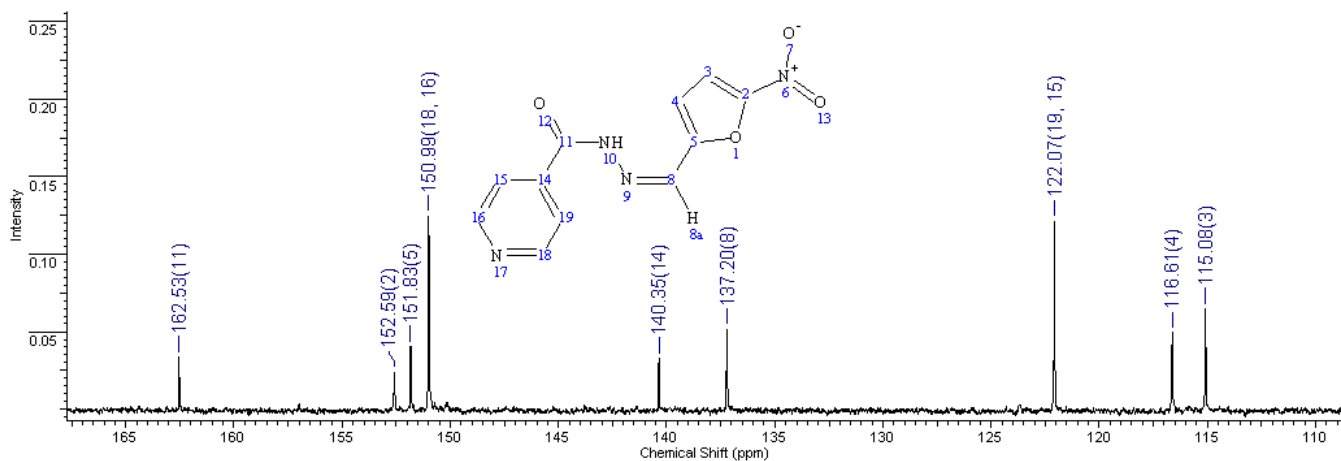


Fig. S-21. ^1H -NMR-spectrum of **6** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	4	116.61	111.060	5.549	7	5	151.83	149.550	2.280
2	3	115.08	114.950	0.134	8	16	150.99	150.950	0.041
3	19	122.07	122.830	-0.757	9	18	150.99	150.950	0.041
4	15	122.07	122.830	-0.757	10	2	152.59	152.800	-0.207
5	14	140.35	142.810	-2.460	11	11	162.53	162.240	0.288
6	8	137.20	148.840	-11.636					

Fig. S-22. ^{13}C -NMR-spectrum of **6** (100.53 MHz, DMSO-d_6)

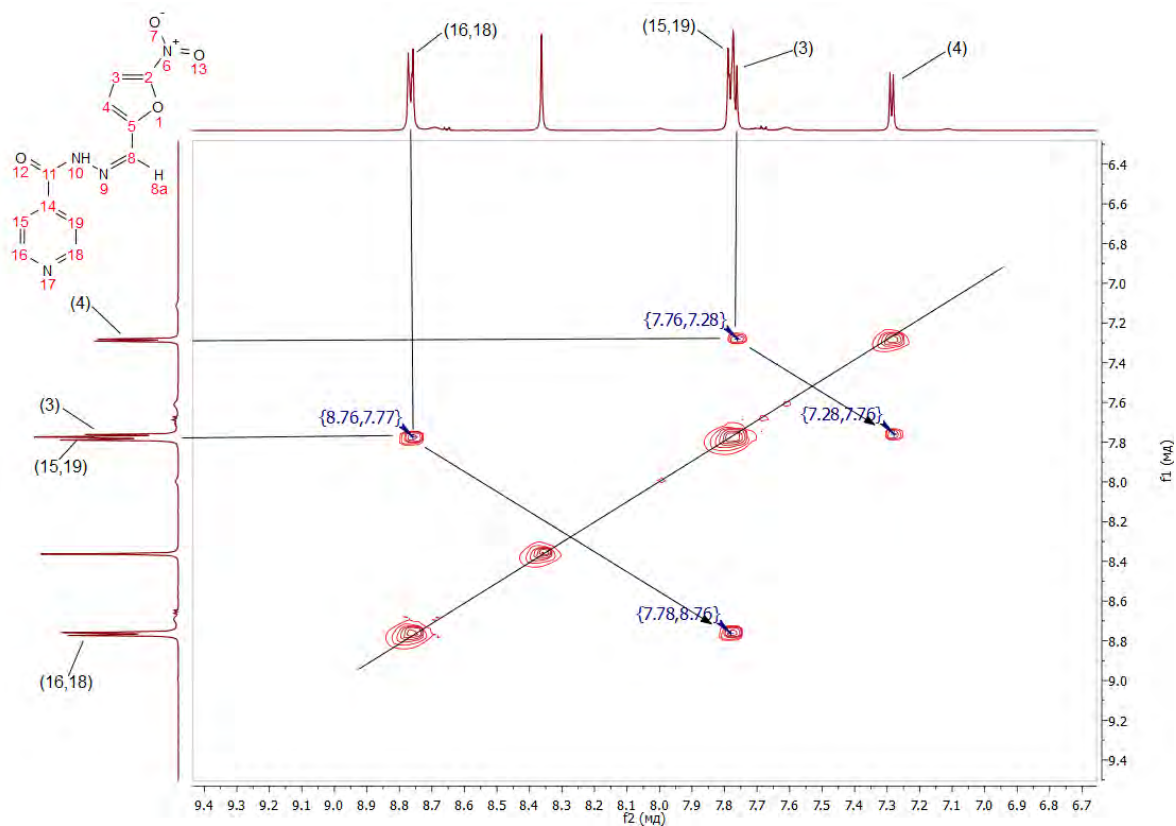


Fig. S-23. COSY ^1H - ^1H -NMR-spectrum of **6** (399.78 MHz, DMSO-d_6)

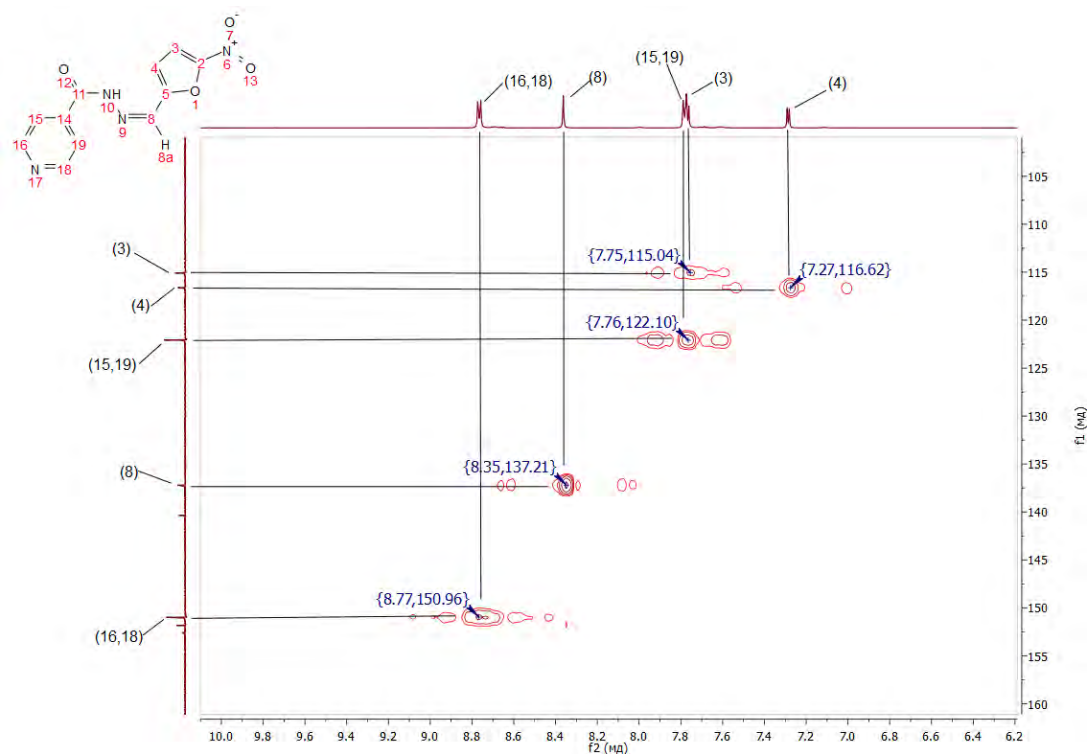
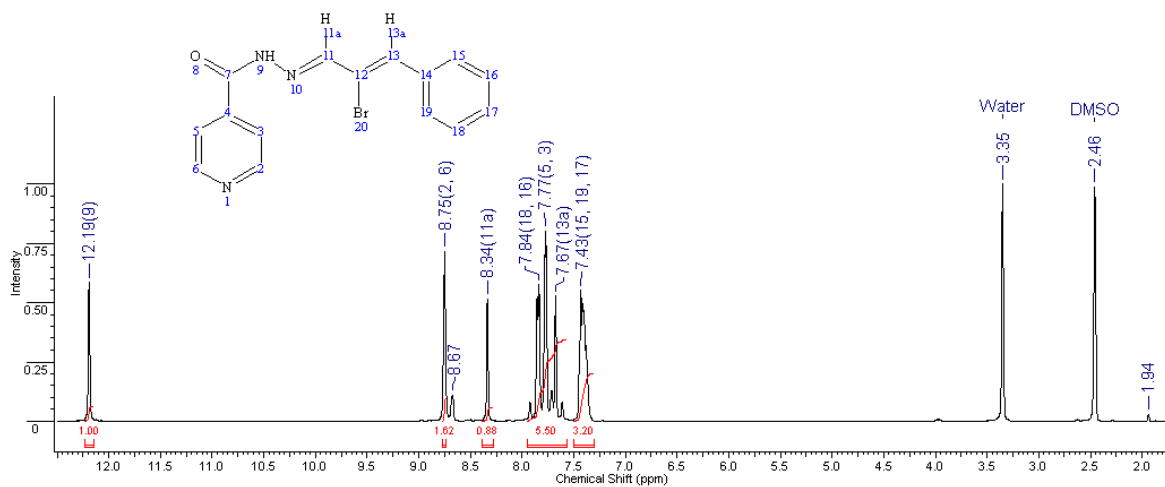
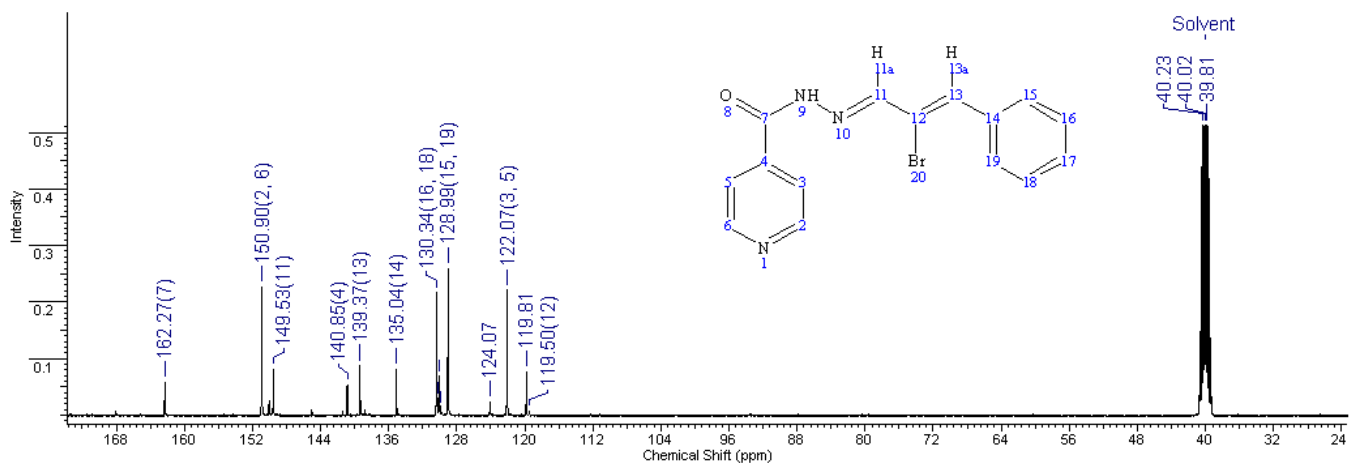


Fig. S-24. HMQC ^1H - ^{13}C -NMR-spectrum of **6** (399.78 MHz, 100.53 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	2	8.75	8.909	-0.161	7	13a	7.67	8.035	-0.360
2	3	7.77	7.862	-0.089	8	15	7.43	7.582	-0.152
3	5	7.77	7.862	-0.089	9	16	7.84	7.367	0.469
4	6	8.75	8.909	-0.161	10	17	7.43	7.659	-0.229
5	9	12.19	-	-	11	18	7.84	7.367	0.469
6	11a	8.34	7.173	1.163	12	19	7.43	7.582	-0.152

Fig. S-25. ^1H -NMR-spectrum of **7** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	2	150.90	150.950	-0.054	9	13	139.37	137.740	1.628
2	3	122.07	122.830	-0.757	10	14	135.04	133.230	1.810
3	4	140.85	143.770	-2.924	11	15	128.99	125.700	3.285
4	5	122.07	122.830	-0.757	12	16	130.34	129.260	1.079
5	6	150.90	150.950	-0.054	13	17	130.01	129.450	0.555
6	7	162.27	162.240	0.030	14	18	130.34	129.260	1.079
7	11	149.53	159.850	-10.318	15	19	128.99	125.700	3.285
8	12	119.50	122.430	-2.932					

Fig. S-26. ^{13}C -NMR-spectrum of **7** (100.53 MHz, DMSO-d_6)

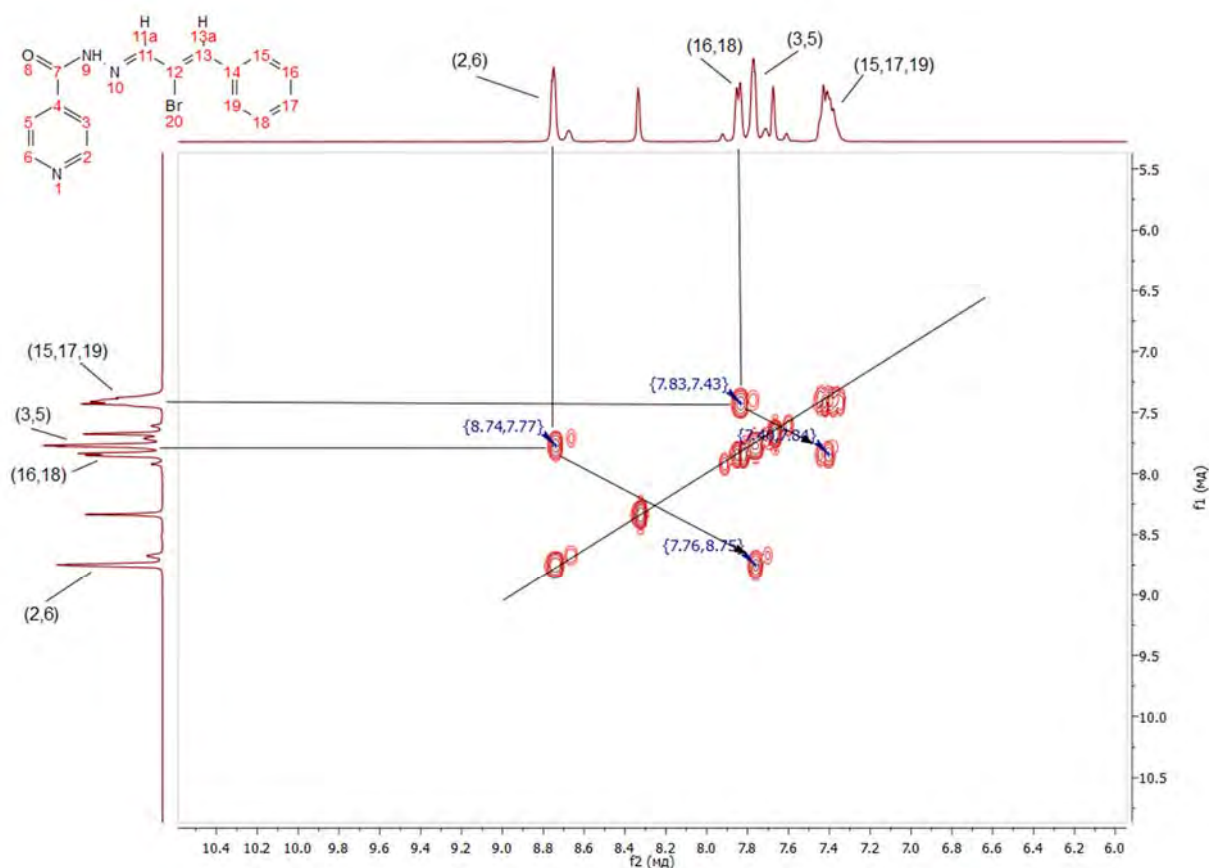


Fig. S-27. COSY ^1H - ^1H -NMR-spectrum of **7** (399.78 MHz, DMSO-d_6)

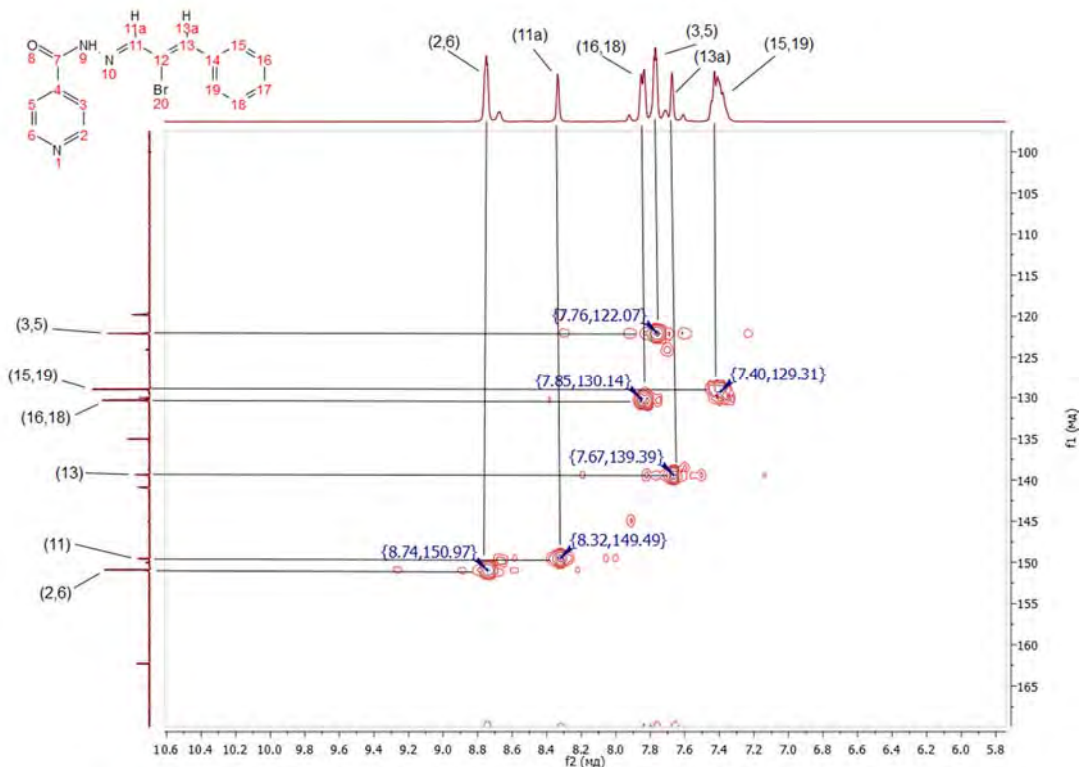


Fig. S-28. HMBC ^1H - ^{13}C -NMR-spectrum of **7** (399.78 MHz, 100.53 MHz, DMSO- d_6)

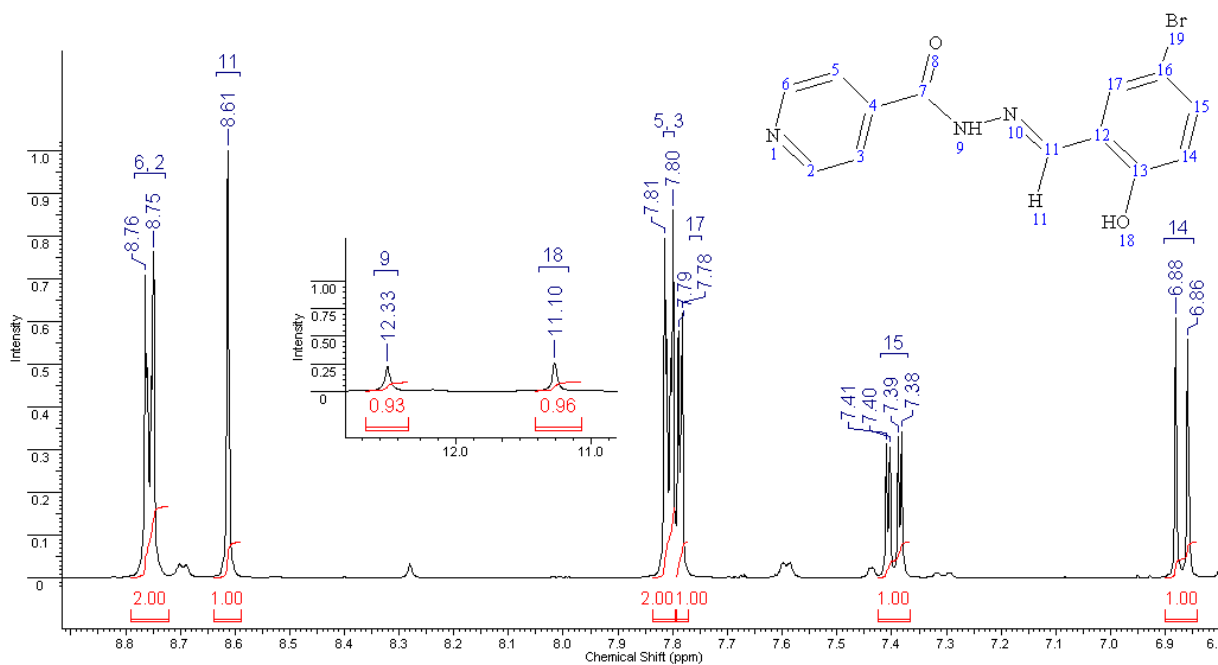


Fig. S-29. ^1H -NMR-spectrum of **8** (399.78 MHz, DMSO- d_6)

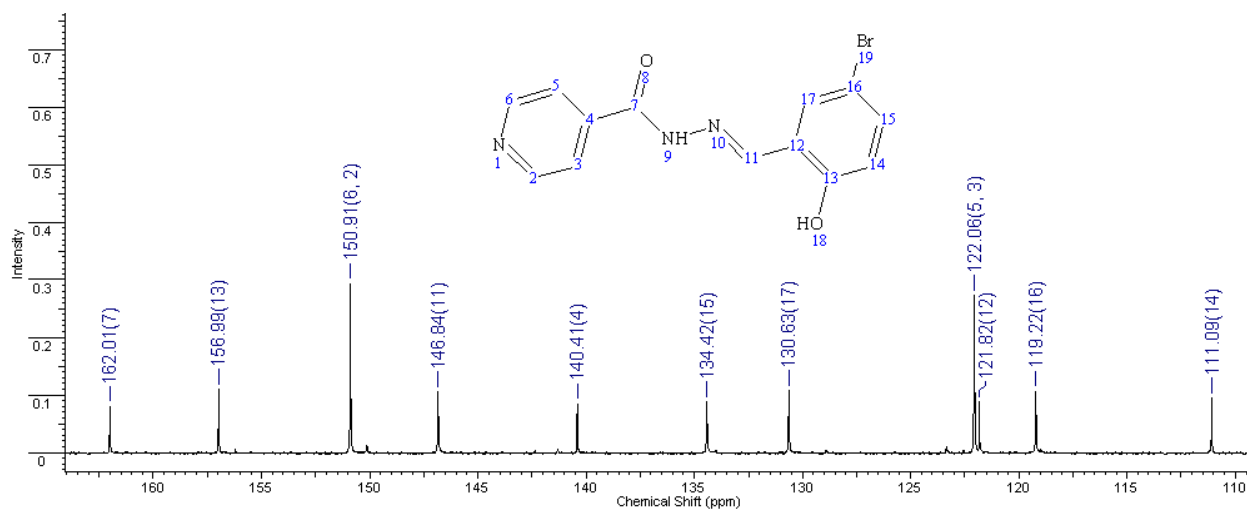


Fig. S-30. ^{13}C -NMR-spectrum of **8** (100.53 MHz, DMSO-d_6)

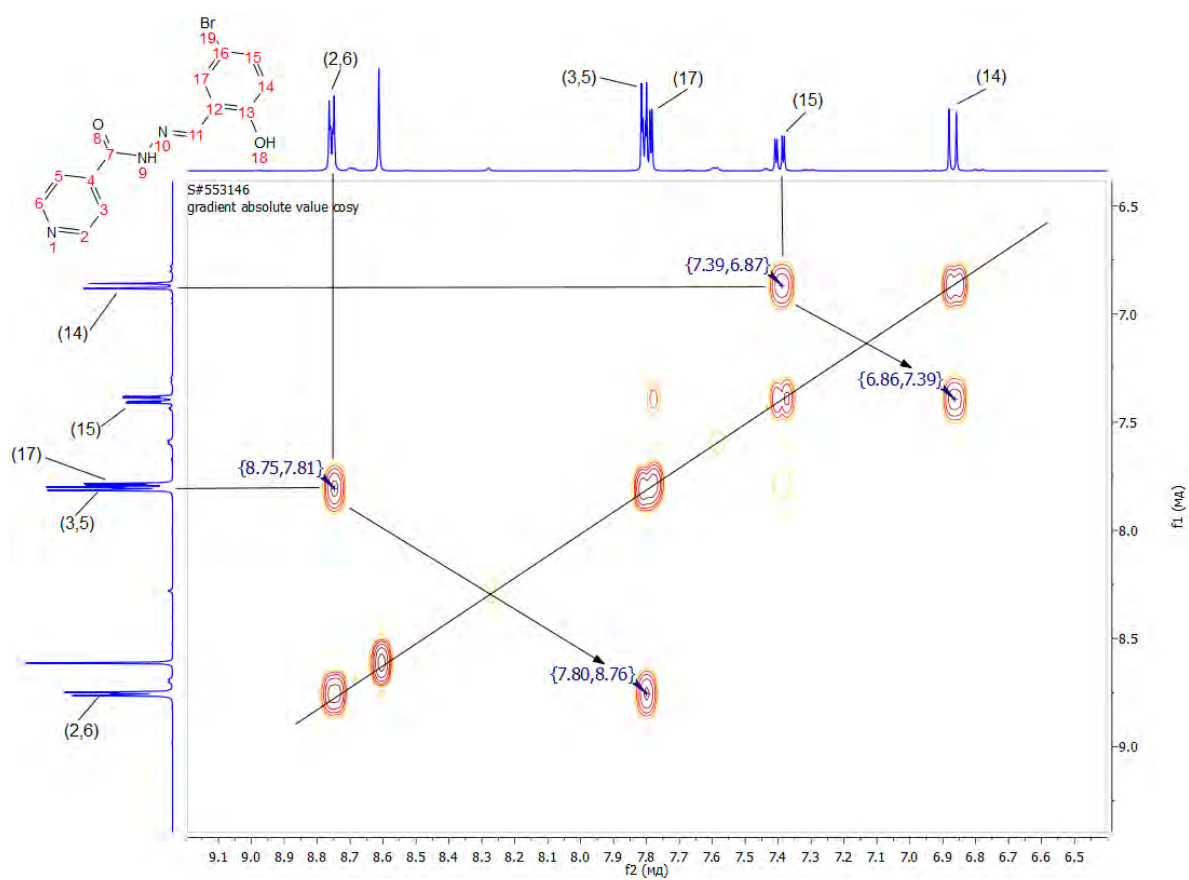


Fig. S-31. COSY ^1H - ^1H -NMR-spectrum of **8** (399.78 MHz, DMSO-d_6)

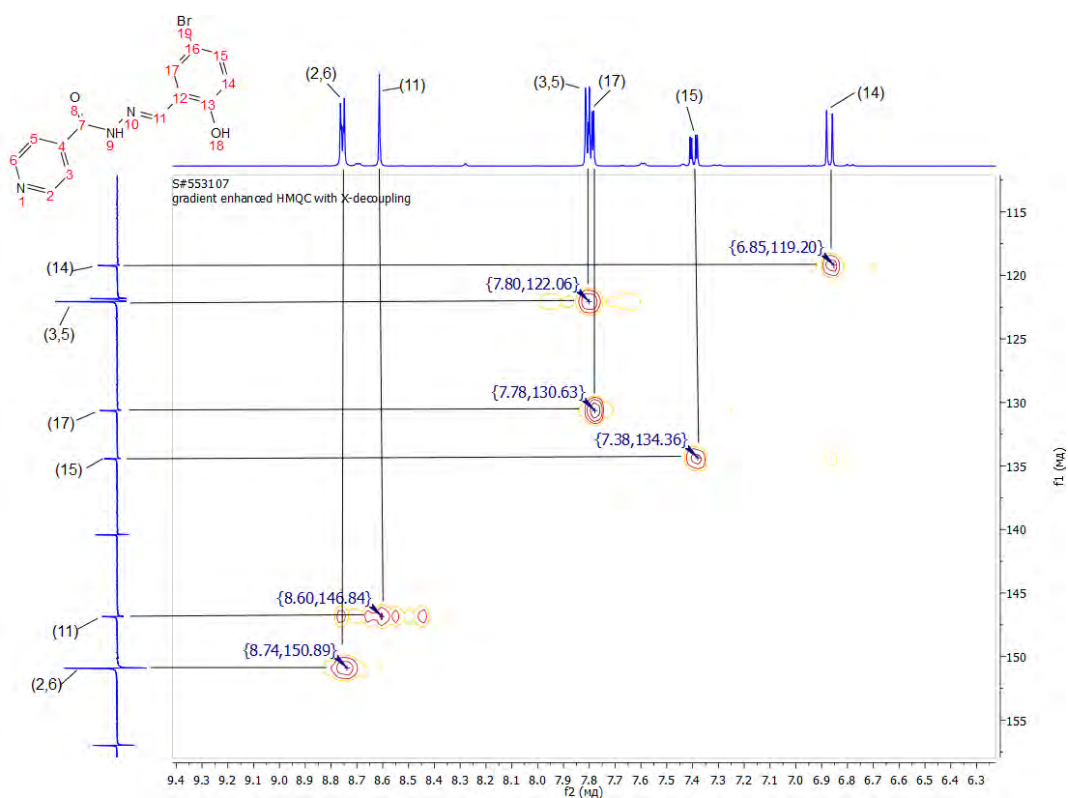


Fig. S-32. HMQC ^1H - ^{13}C -NMR-spectrum of **8** (399.78 MHz, 100.53 MHz, DMSO- d_6)

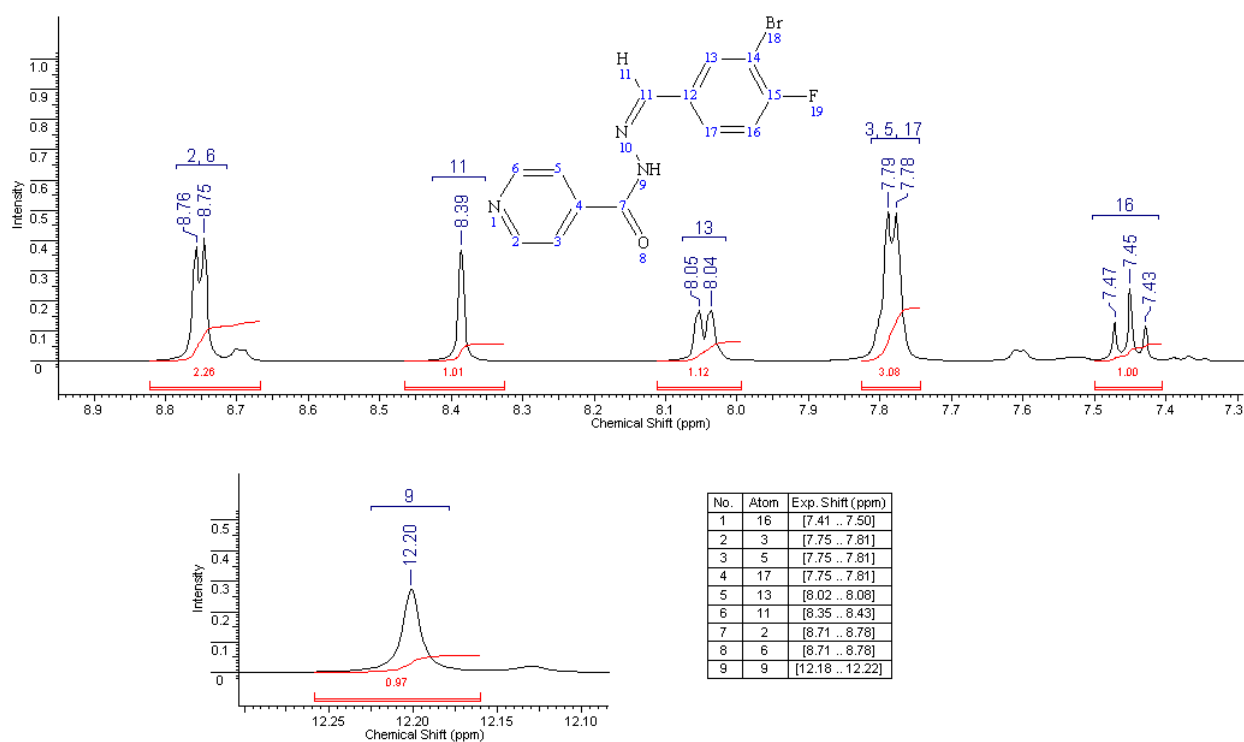


Fig. S-33. ^1H -NMR-spectrum of **9** (399.78 MHz, DMSO- d_6)

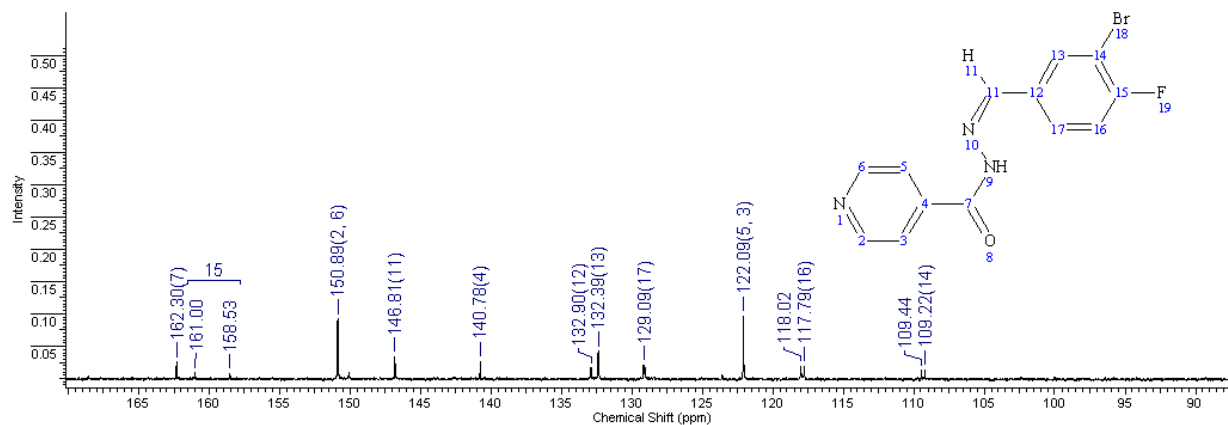


Fig. S-34. ^{13}C -NMR-spectrum of **9** (100.53 MHz, DMSO-d_6)

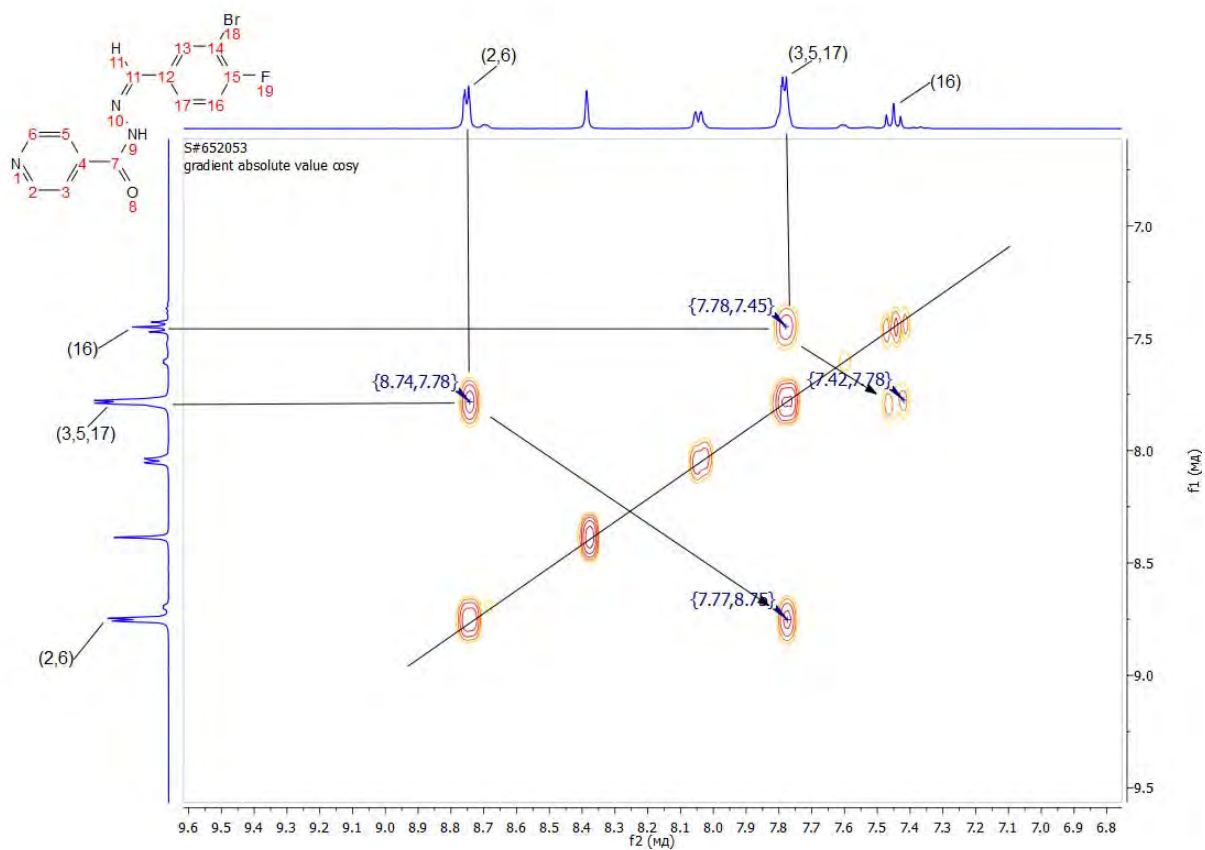


Fig. S-35. COSY ^1H - ^1H -NMR-spectrum of **9** (399.78 MHz, DMSO-d_6)

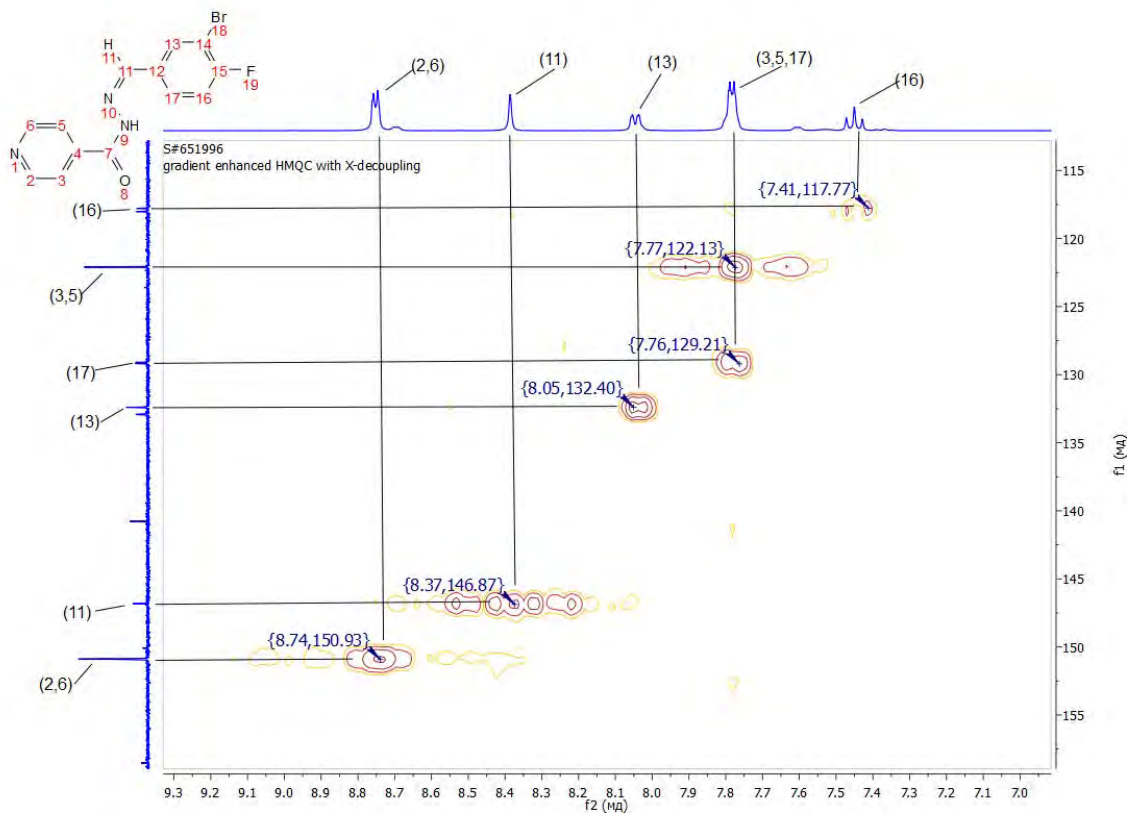


Fig. S-36. HMQC ^1H - ^{13}C -NMR-spectrum of **9** (399.78 MHz, 100.53 MHz, DMSO- d_6)

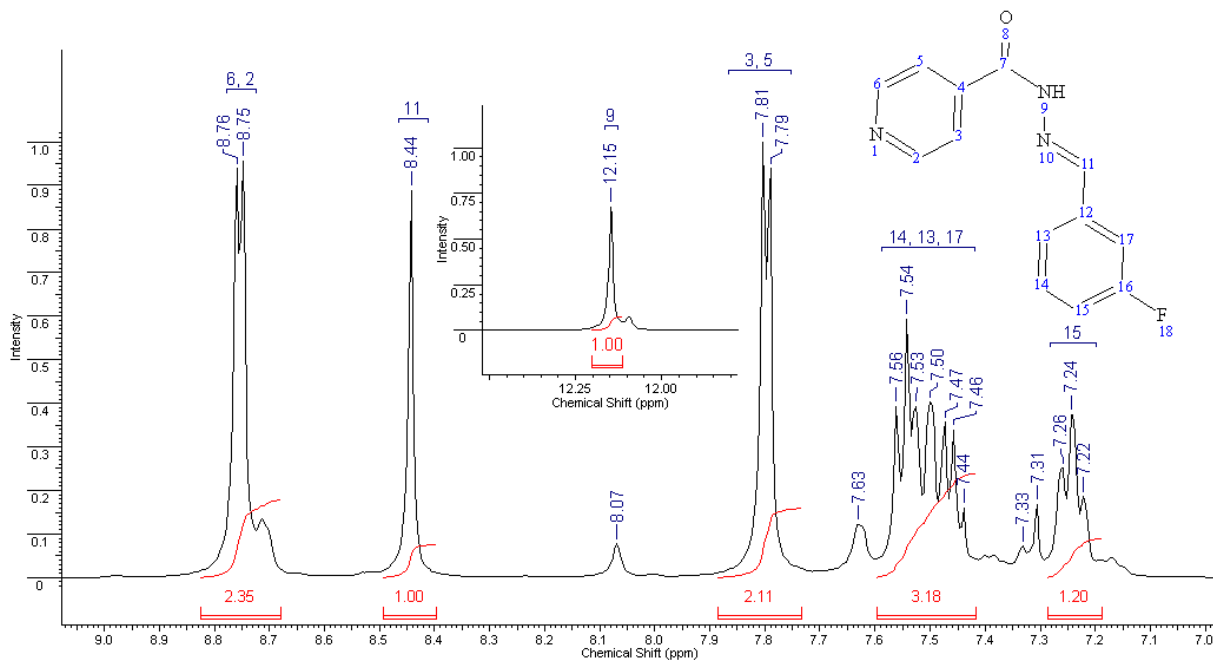


Fig. S-37. ^1H -NMR-spectrum of **10** (399.78 MHz, DMSO- d_6)

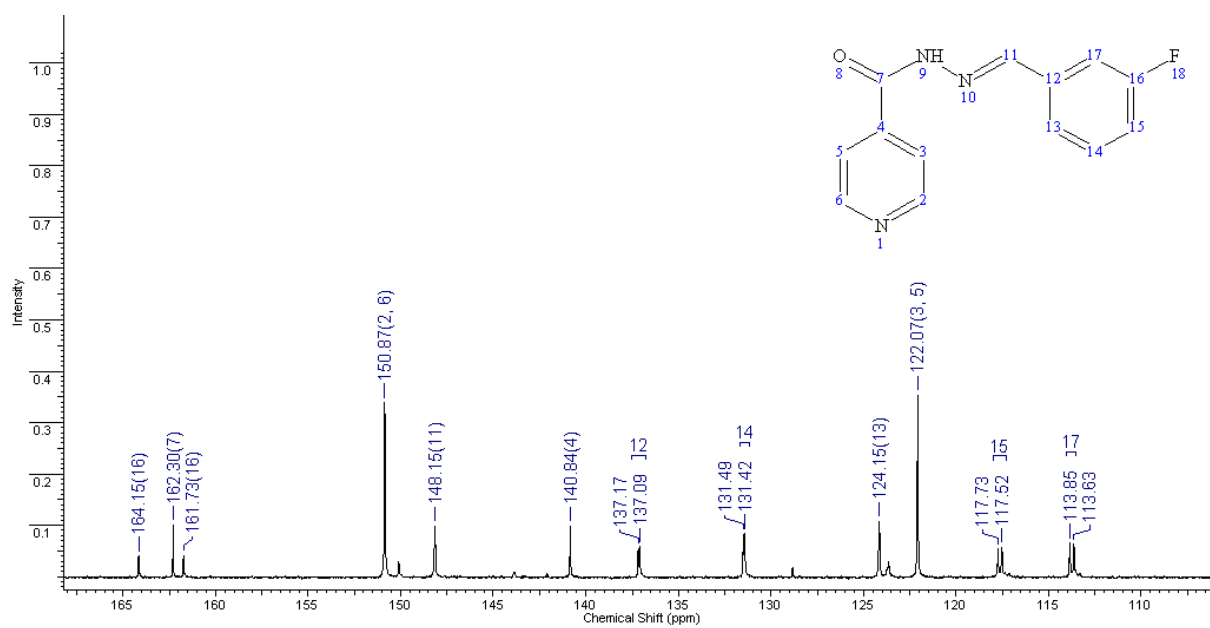


Fig. S-38. ¹³C-NMR-spectrum of **10** (100.53 MHz, DMSO-d₆)

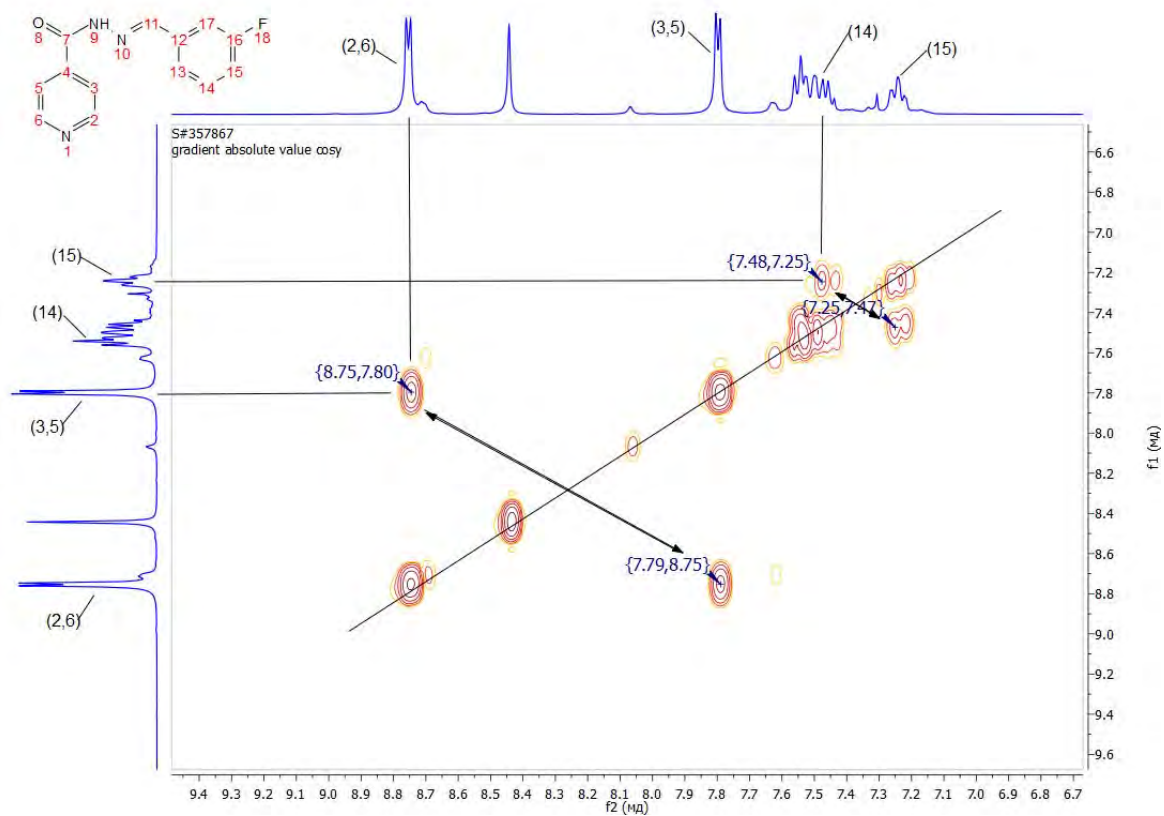


Fig. S-39. COSY ¹H-¹H-NMR-spectrum of **10** (399.78 MHz, DMSO-d₆)

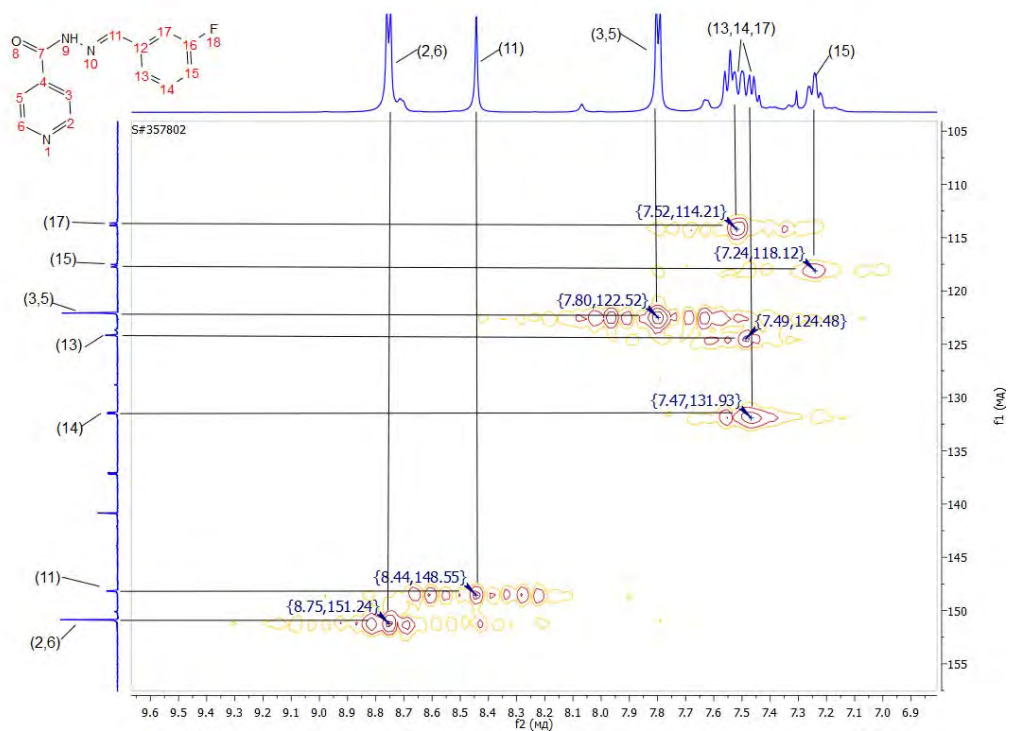


Fig. S-40. HMQC ^1H - ^{13}C -NMR-spectrum of **10** (399.78 MHz, 100.53 MHz, DMSO- d_6)

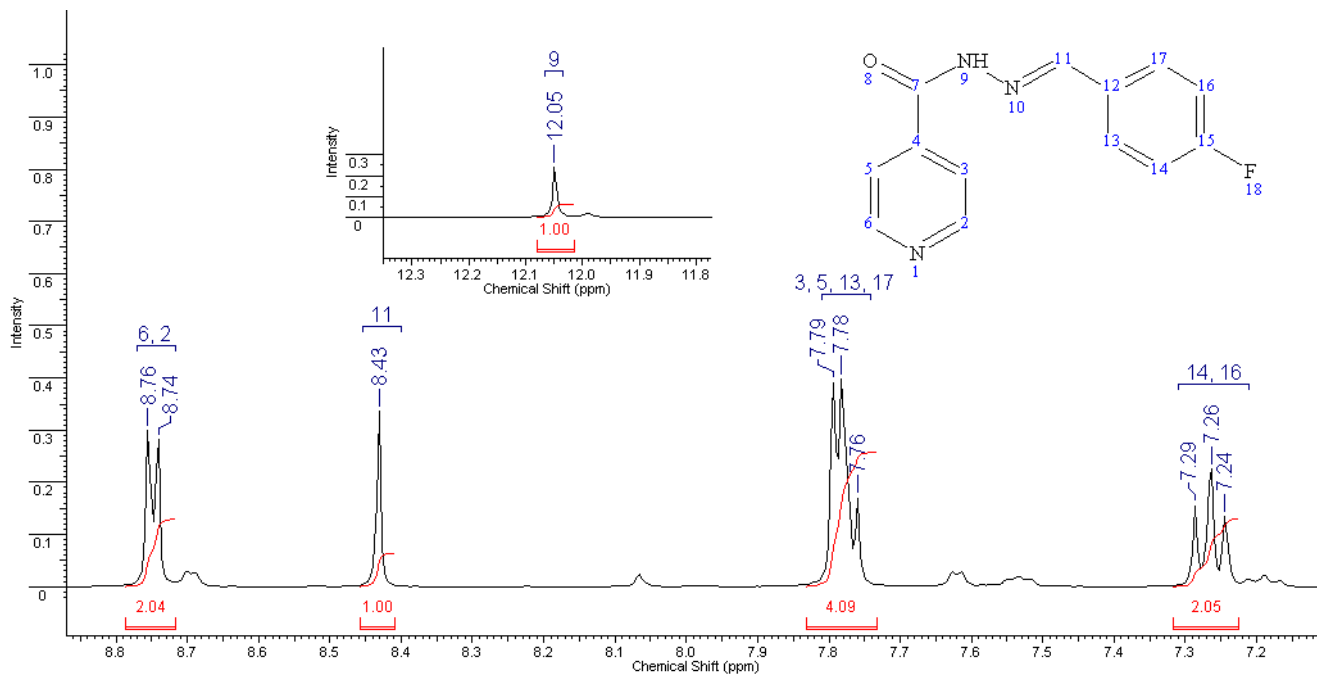


Fig. S-41. ^1H -NMR-spectrum of **11** (399.78 MHz, DMSO- d_6)

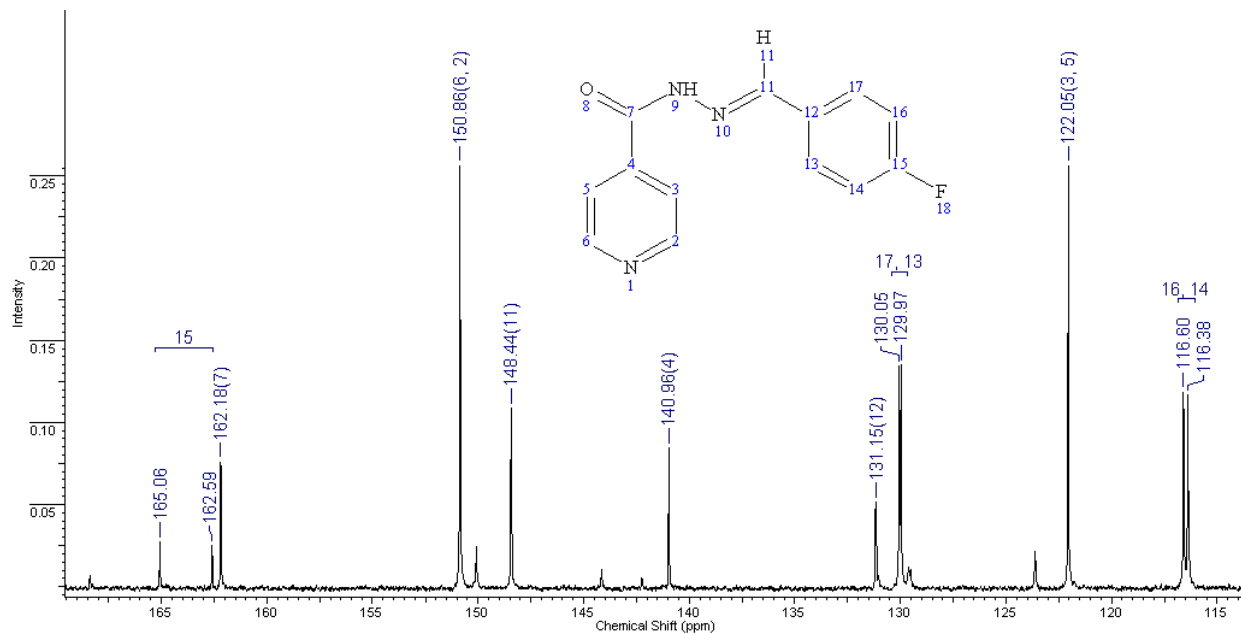


Fig. S-42. ^{13}C -NMR-spectrum of **11** (100.53 MHz, DMSO-d_6)

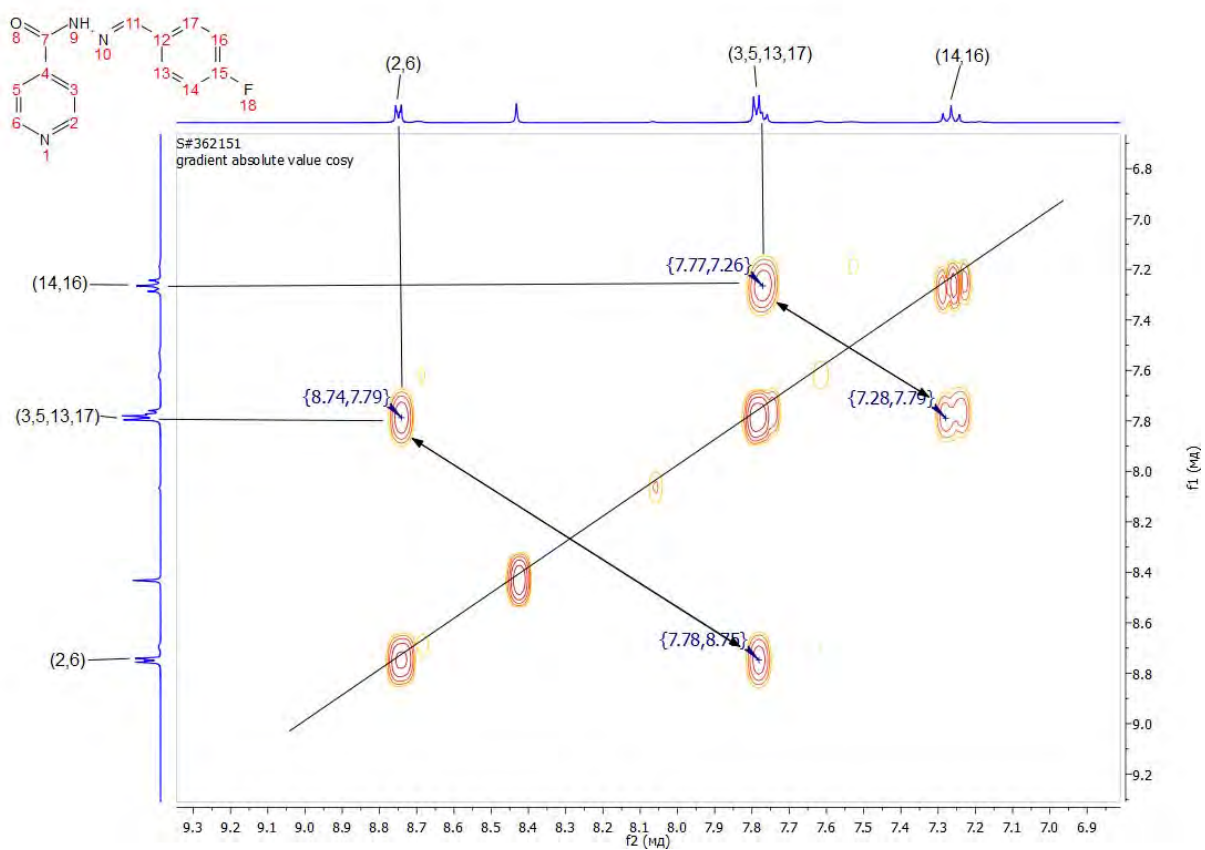


Fig. S-43. COSY ^1H - ^1H -NMR-spectrum of **11** (399.78 MHz, DMSO-d_6)

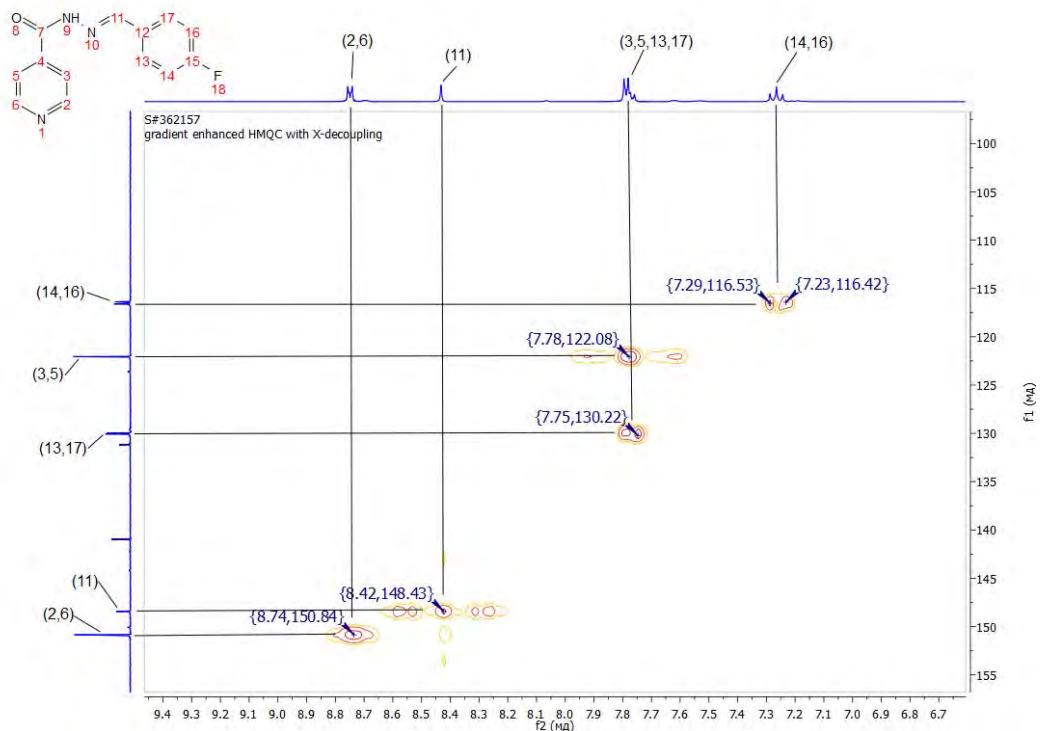


Fig. S-44. HMQC ^1H - ^{13}C -NMR-spectrum of **11** (399.78 MHz, 100.53 MHz, DMSO- d_6)

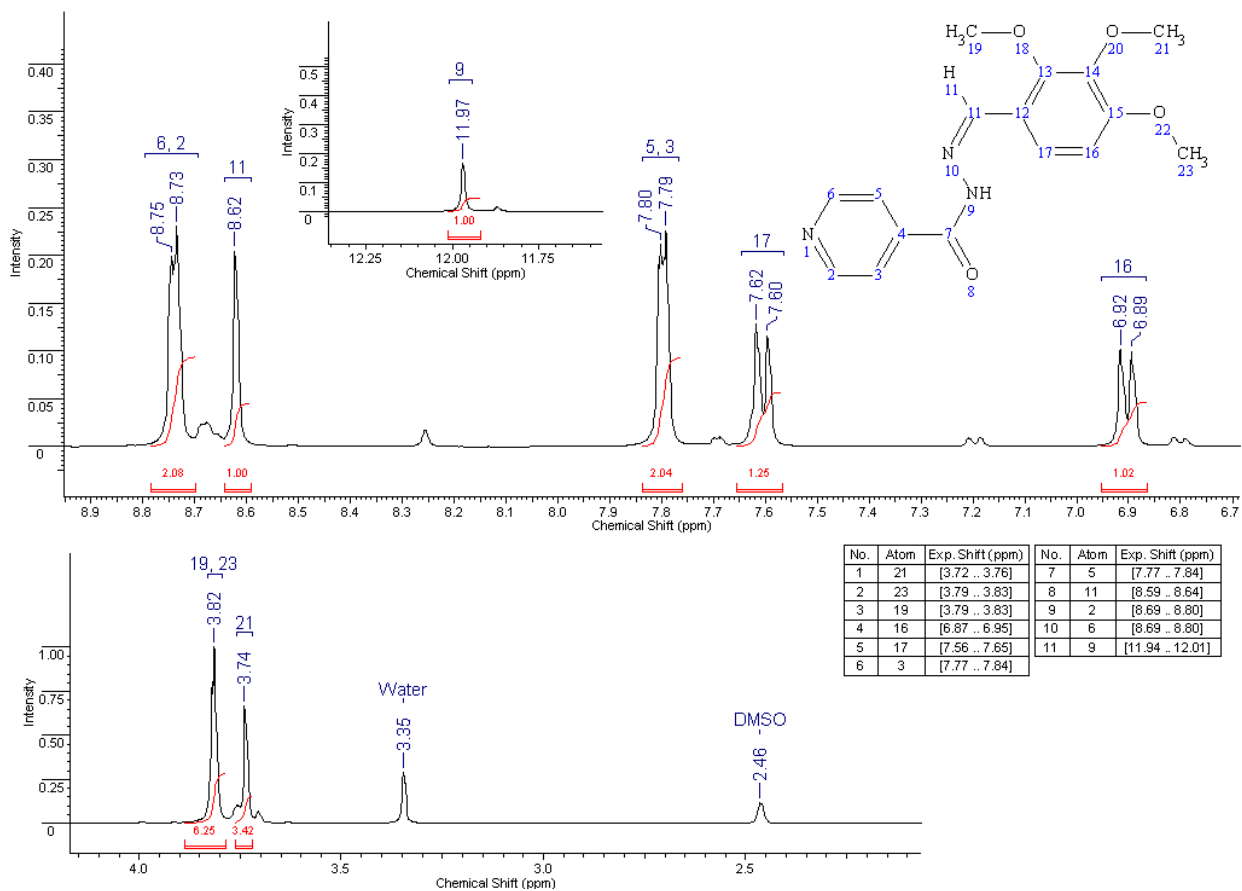


Fig. S-45. ^1H -NMR-spectrum of **12** (399.78 MHz, DMSO- d_6)

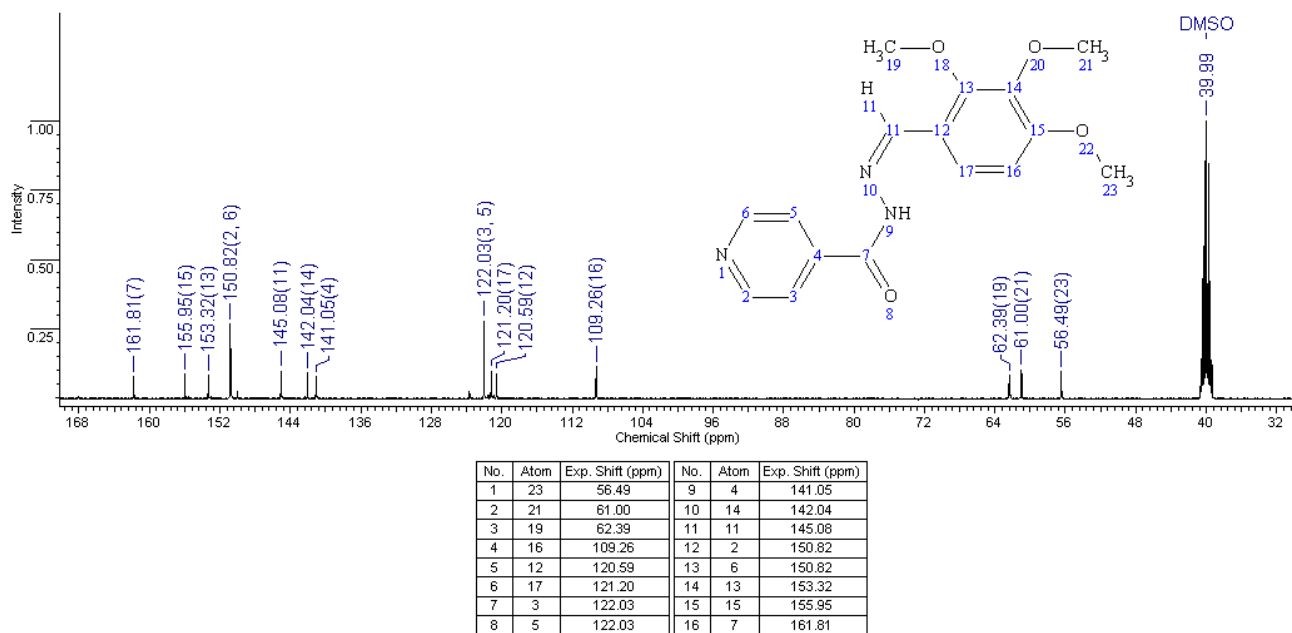


Fig. S-46. ^{13}C -NMR-spectrum of **12** (100.53 MHz, DMSO-d_6)

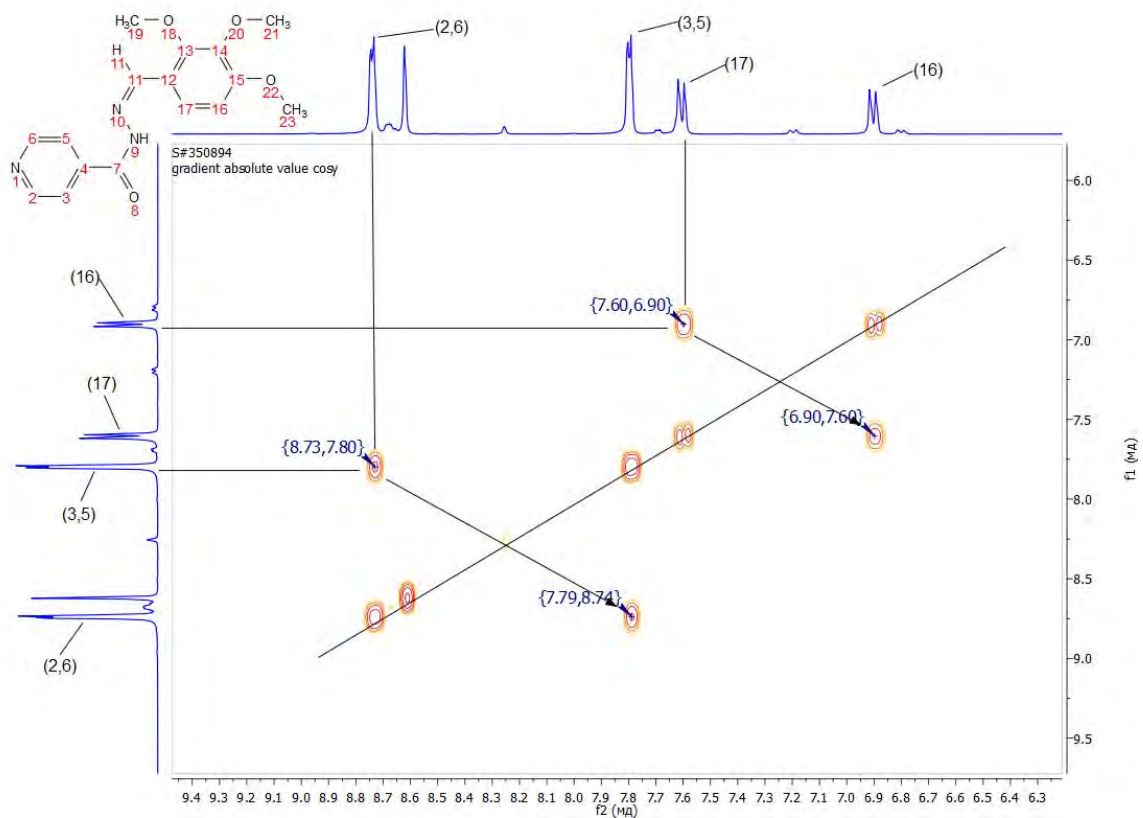


Fig. S-47. COSY ^1H - ^1H -NMR-spectrum of **12** (399.78 MHz, DMSO-d_6)

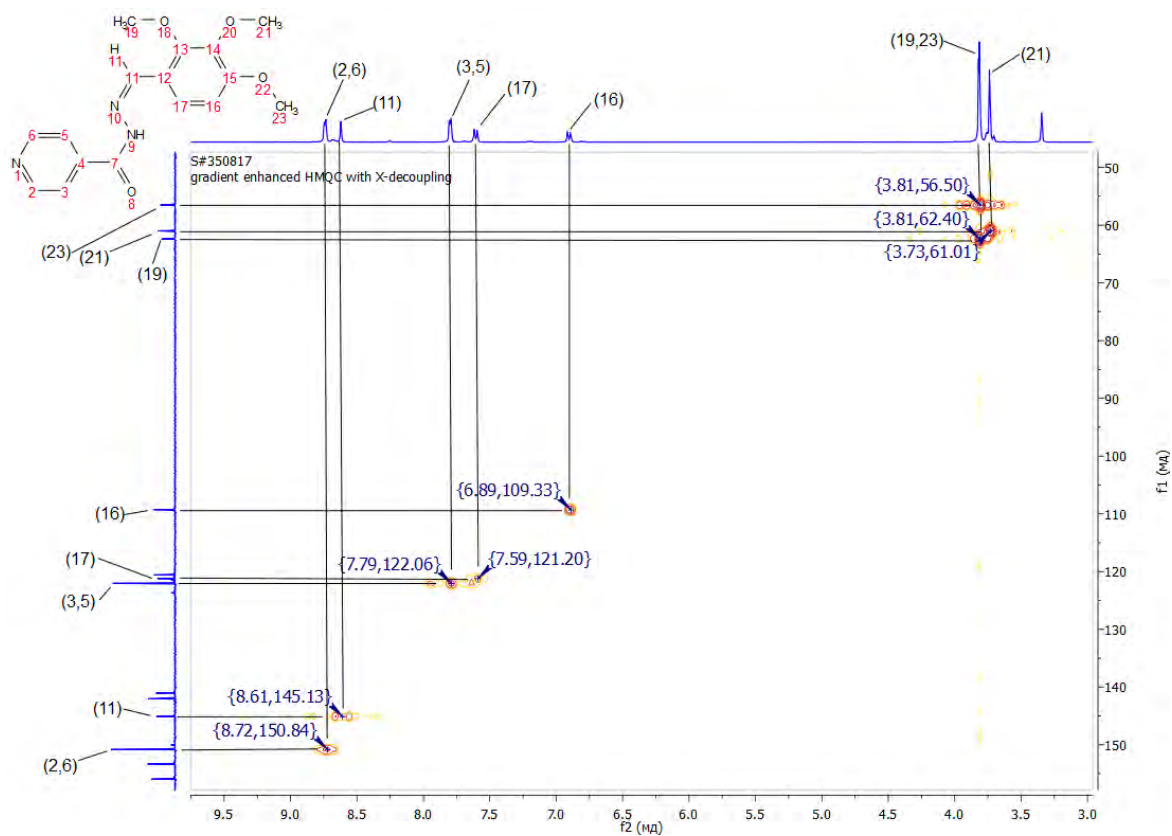


Fig. S-48. HMOC ^1H - ^{13}C -NMR-spectrum of **12** (399.78 MHz, 100.53 MHz, DMSO- d_6)

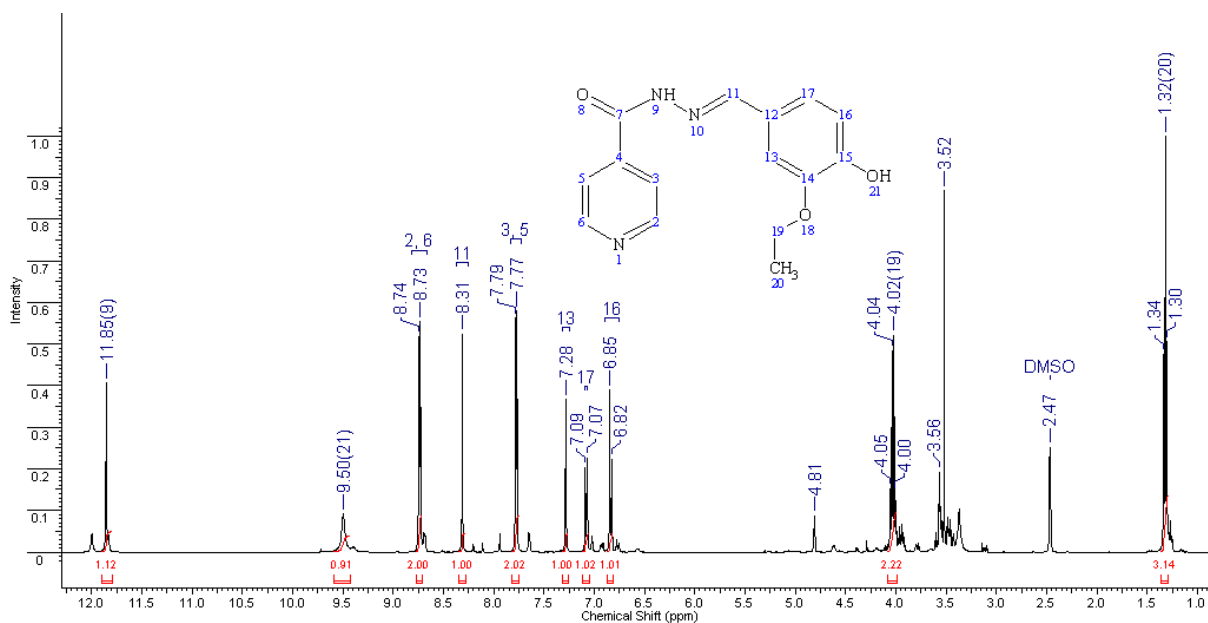


Fig. S-49. ^1H -NMR-spectrum of **13** (399.78 MHz, DMSO- d_6)

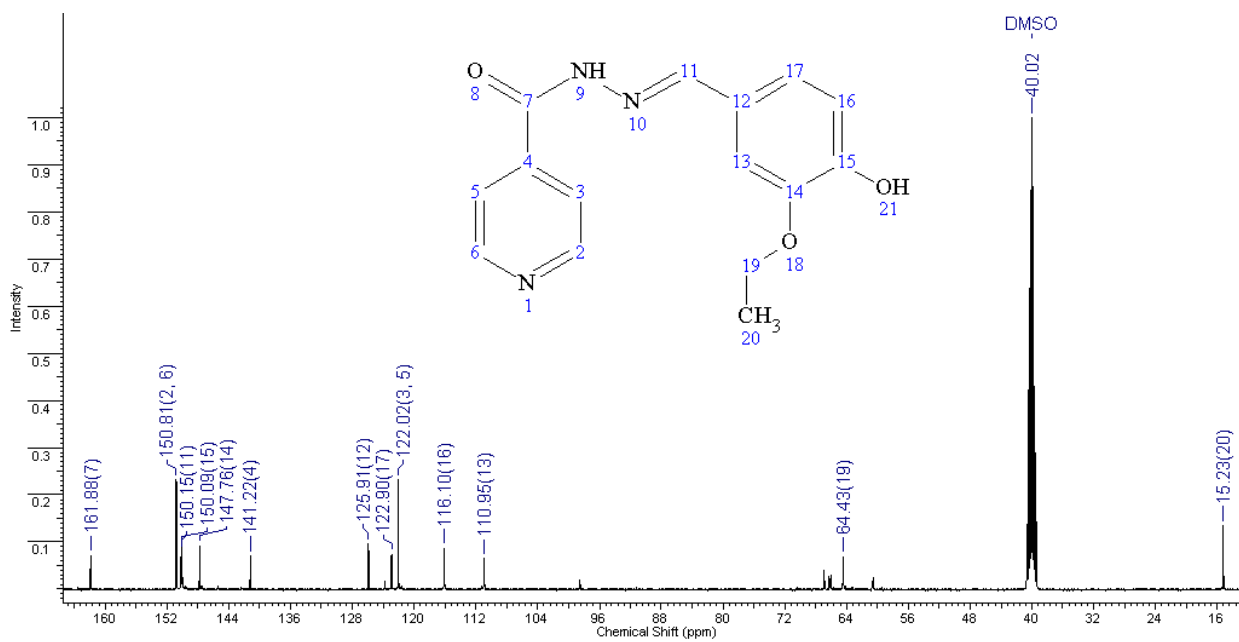


Fig. S-50. ¹³C-NMR-spectrum of **13** (100.53 MHz, DMSO-d₆)

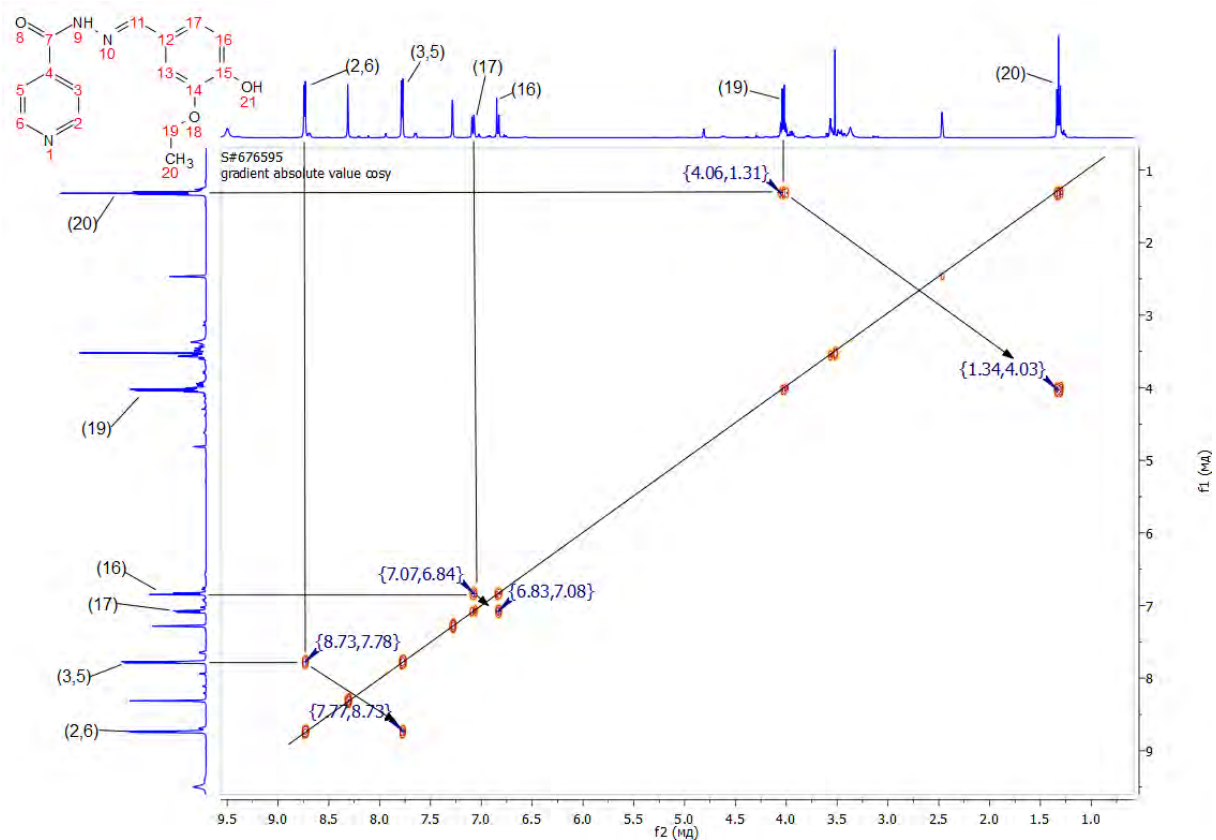


Fig. S-51. COSY ¹H-¹H-NMR-spectrum of **13** (399.78 MHz, DMSO-d₆)

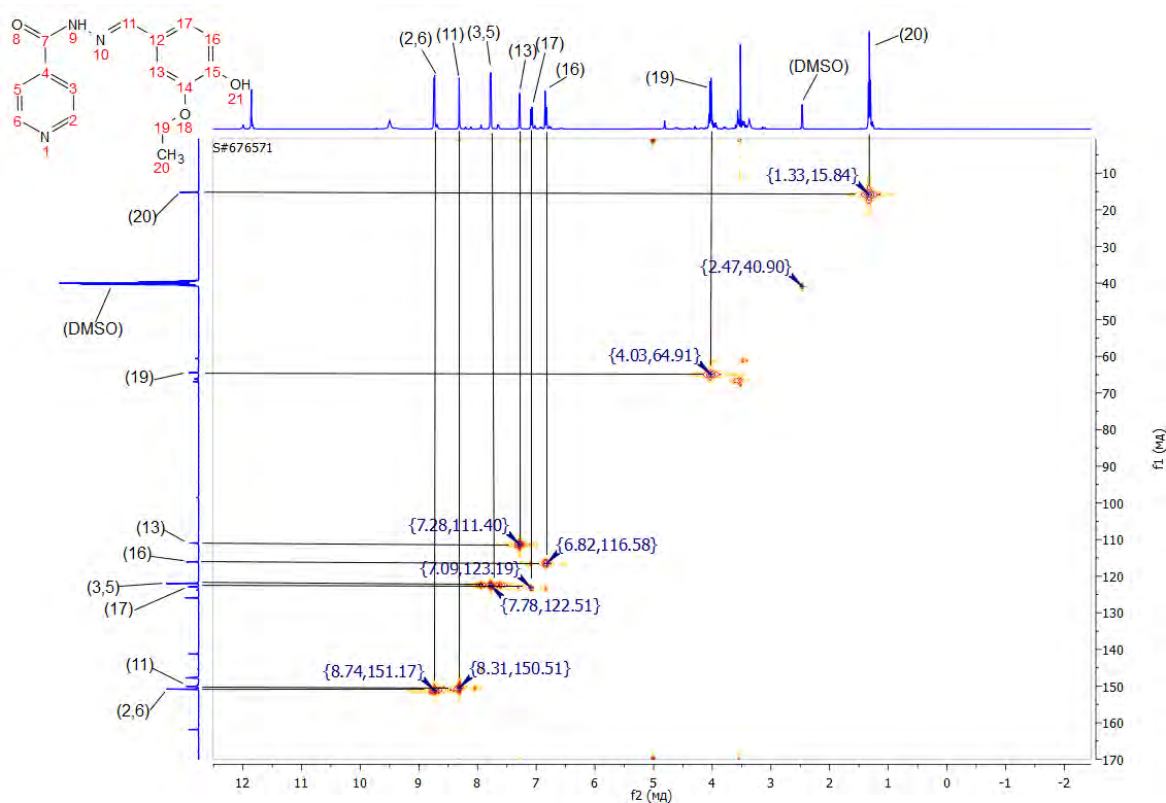


Fig. S-52. HMQC ^1H - ^{13}C -NMR-spectrum of **13** (399.78 MHz, 100.53 MHz, DMSO- d_6)

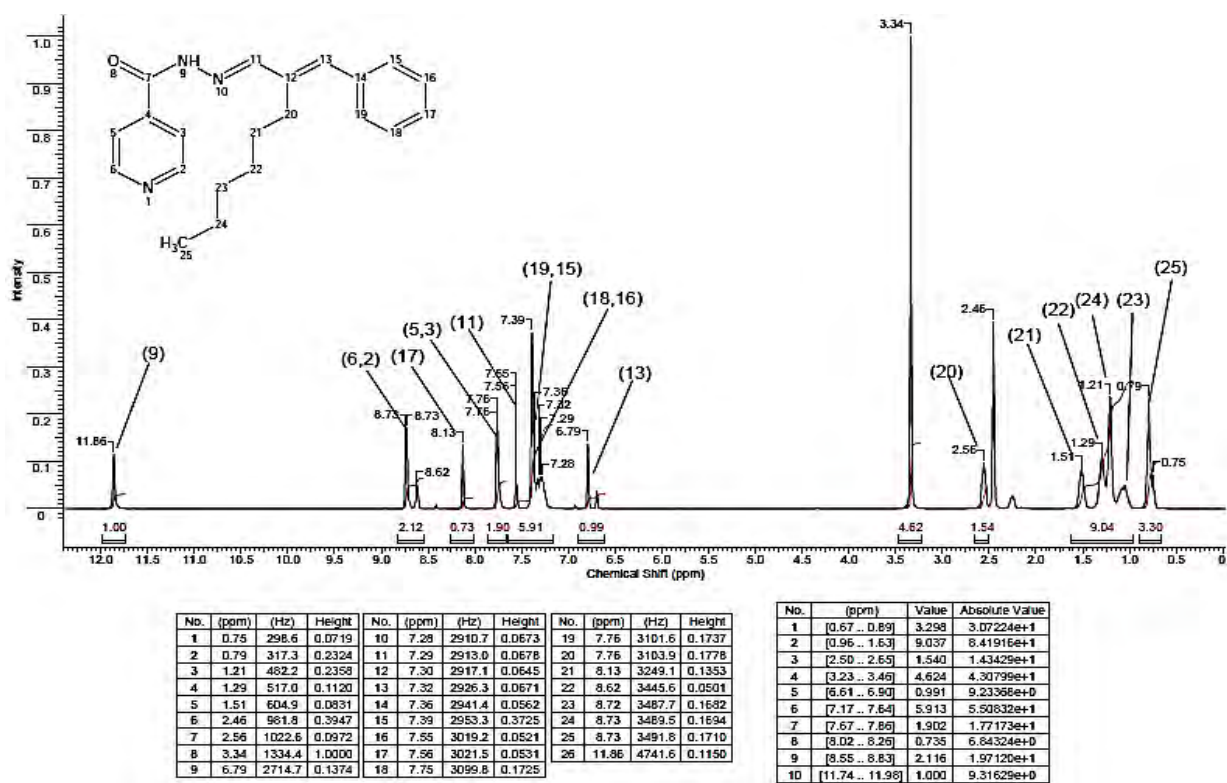
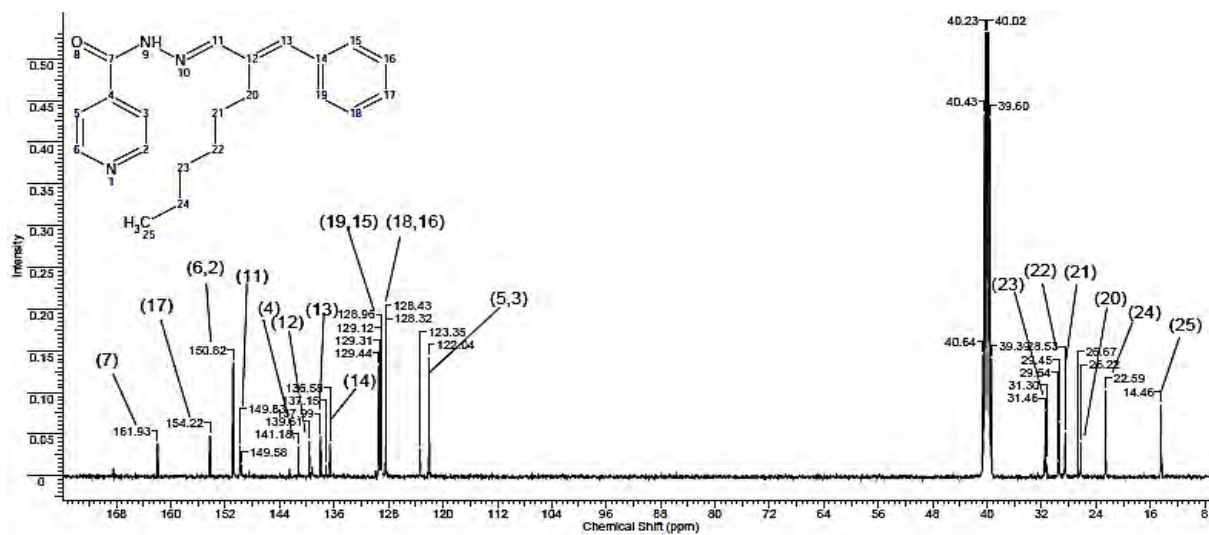


Fig. S-53. ^1H -NMR-spectrum of **14** (399.78 MHz, DMSO- d_6)



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.46	1453.2	0.0653	13	39.81	4001.7	0.8547	25	129.44	13012.3	0.1314
2	22.59	2270.7	0.1022	14	40.02	4022.8	1.0000	26	136.58	13730.2	0.0390
3	26.22	2635.9	0.0404	15	40.23	4043.9	0.8494	27	137.15	13766.7	0.0127
4	26.67	2681.0	0.0122	16	40.43	4064.0	0.4336	28	137.99	13871.1	0.0473
5	28.53	2867.9	0.0520	17	40.64	4085.1	0.1455	29	139.61	14034.0	0.0418
6	28.62	2877.4	0.0158	18	122.04	12268.5	0.1419	30	141.18	14182.1	0.0344
7	29.45	2960.8	0.0641	19	123.35	12399.8	0.0323	31	149.58	15036.6	0.0128
8	29.64	2980.0	0.0160	20	128.32	12899.2	0.0133	32	149.83	15061.5	0.0357
9	31.30	3146.8	0.0199	21	128.43	12910.7	0.0408	33	150.82	15161.2	0.1358
10	31.46	3162.1	0.0776	22	128.96	12963.4	0.0135	34	154.22	15503.3	0.0477
11	39.39	3959.6	0.1409	23	129.12	12979.7	0.1447	35	161.93	16277.8	0.0384
12	39.60	3980.6	0.4287	24	129.31	12998.9	0.0392				

Fig. S-54. ¹³C-NMR-spectrum of **14** (100.53 MHz, DMSO-d₆)

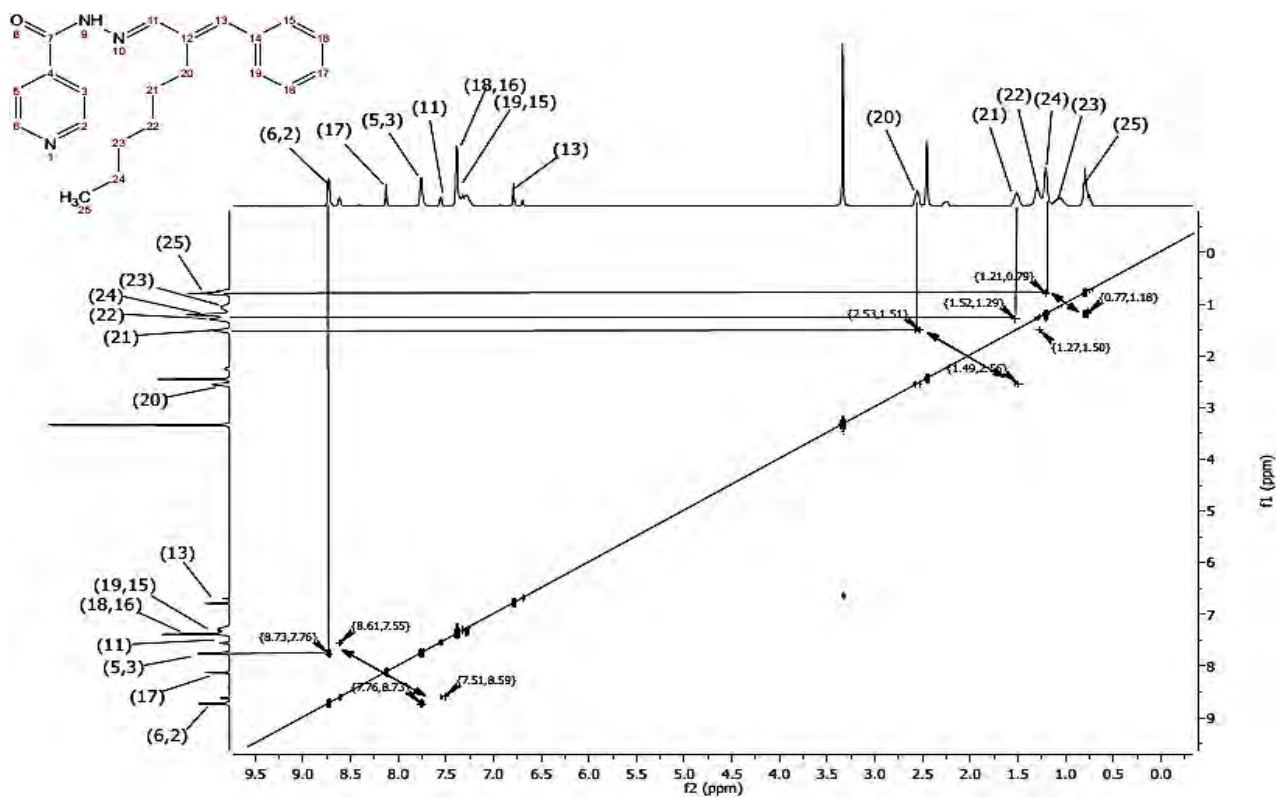


Fig. S-55. COSY ¹H-¹H-NMR-spectrum of **14** (399.78 MHz, DMSO-d₆)

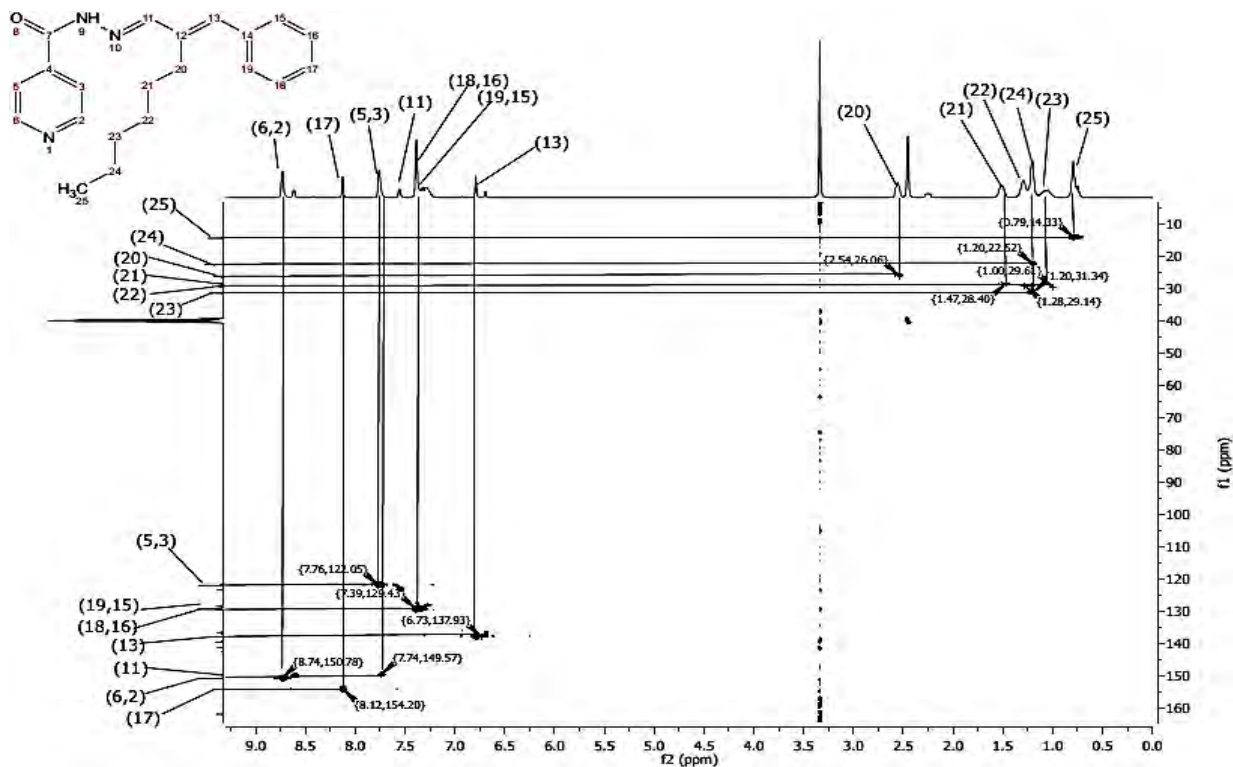


Fig. S-56. HMOC ^1H - ^{13}C -NMR-spectrum of **14** (399.78 MHz, 100.53 MHz, DMSO- d_6)

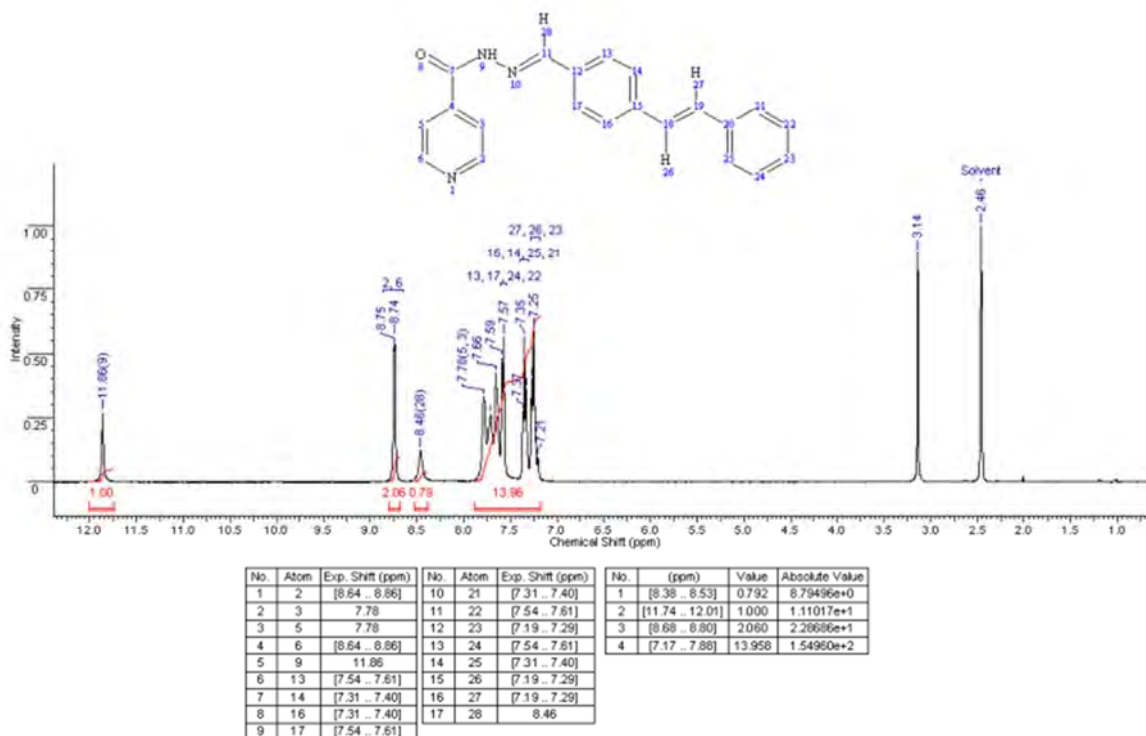
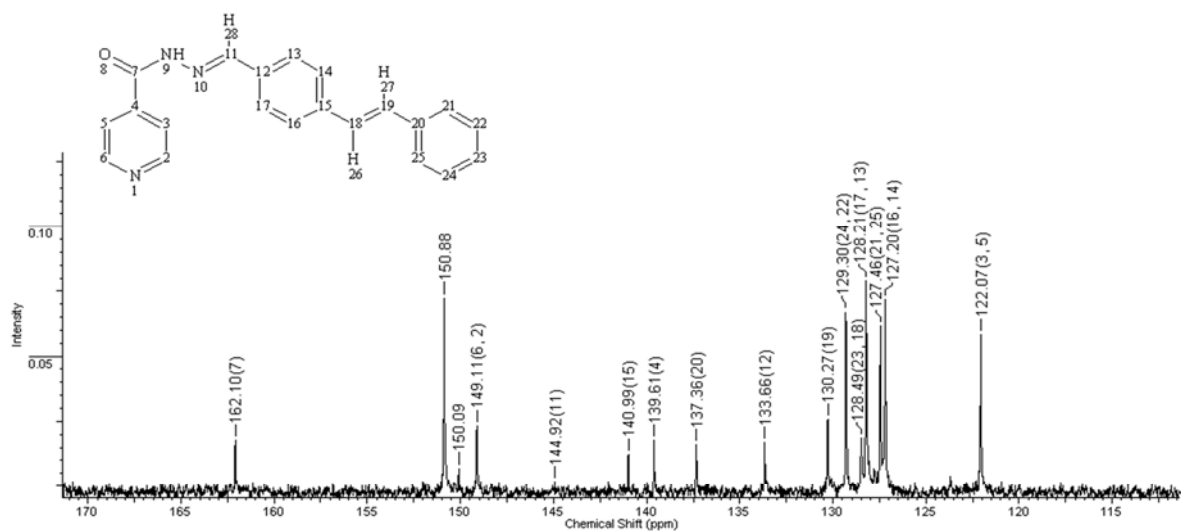


Fig. S-57. ^1H -NMR-spectrum of **15** (399.78 MHz, DMSO- d_6)



No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)	No.	Atom	Exp. Shift (ppm)	Calc. Shift (ppm)	Difference (ppm)
1	2	149.11	148.690	0.423	8	12	133.66	133.080	0.577	15	19	130.27	130.780	-0.508
2	3	122.07	126.050	-3.977	9	13	128.21	128.930	-0.717	16	20	137.36	137.960	-0.604
3	4	139.61	138.210	1.397	10	14	127.20	126.500	0.702	17	21	127.46	128.340	-0.880
4	5	122.07	126.050	-3.977	11	15	140.99	140.800	0.189	18	22	129.30	129.850	-0.550
5	6	149.11	148.690	0.423	12	16	127.20	126.500	0.702	19	23	128.49	128.460	0.029
6	7	162.10	162.470	-0.371	13	17	128.21	128.930	-0.717	20	24	129.30	129.850	-0.550
7	11	144.92	144.550	0.367	14	18	128.49	128.480	0.009	21	25	127.46	128.340	-0.880

Fig. S-58. ^{13}C -NMR-spectrum of **15** (100.53 MHz, DMSO-d_6)

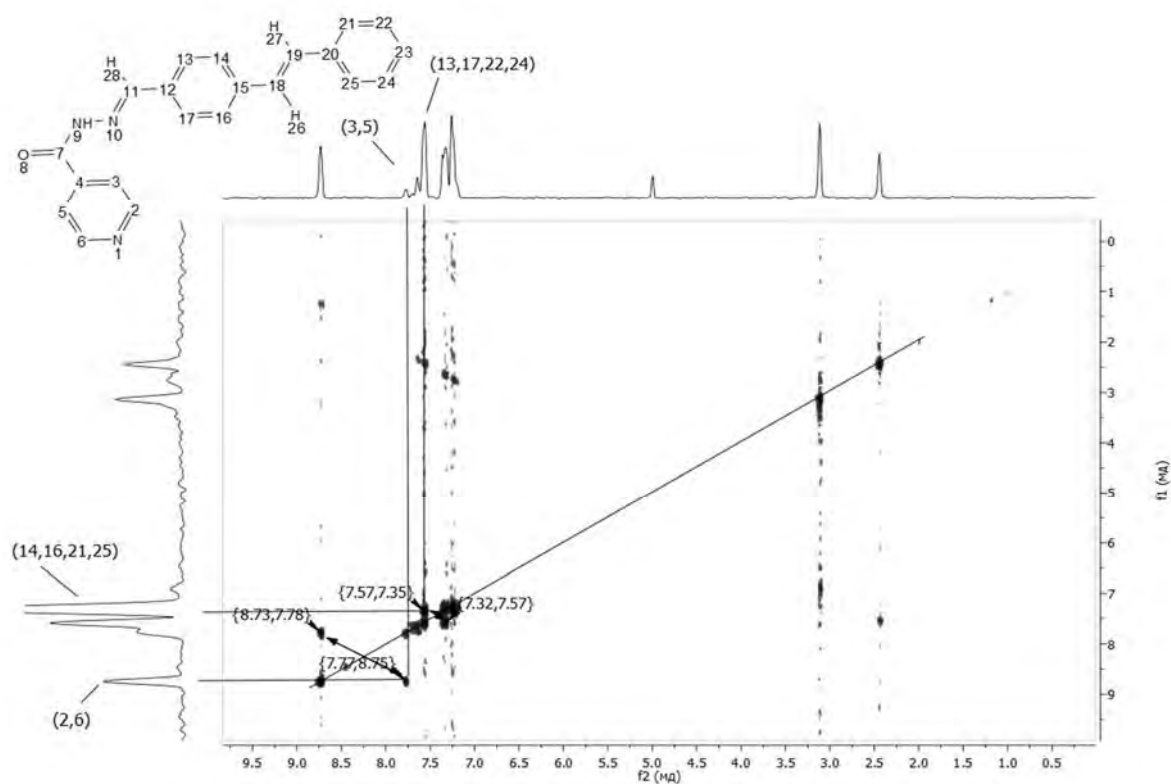


Fig. S-59. COSY ^1H - ^1H -NMR-spectrum of **15** (399.78 MHz, DMSO-d_6)