Supplementary Material

Synthesis of some oxazolo[4,5-*d*]pyrimidine derivatives and evaluation of their antiviral activity and cytotoxicity

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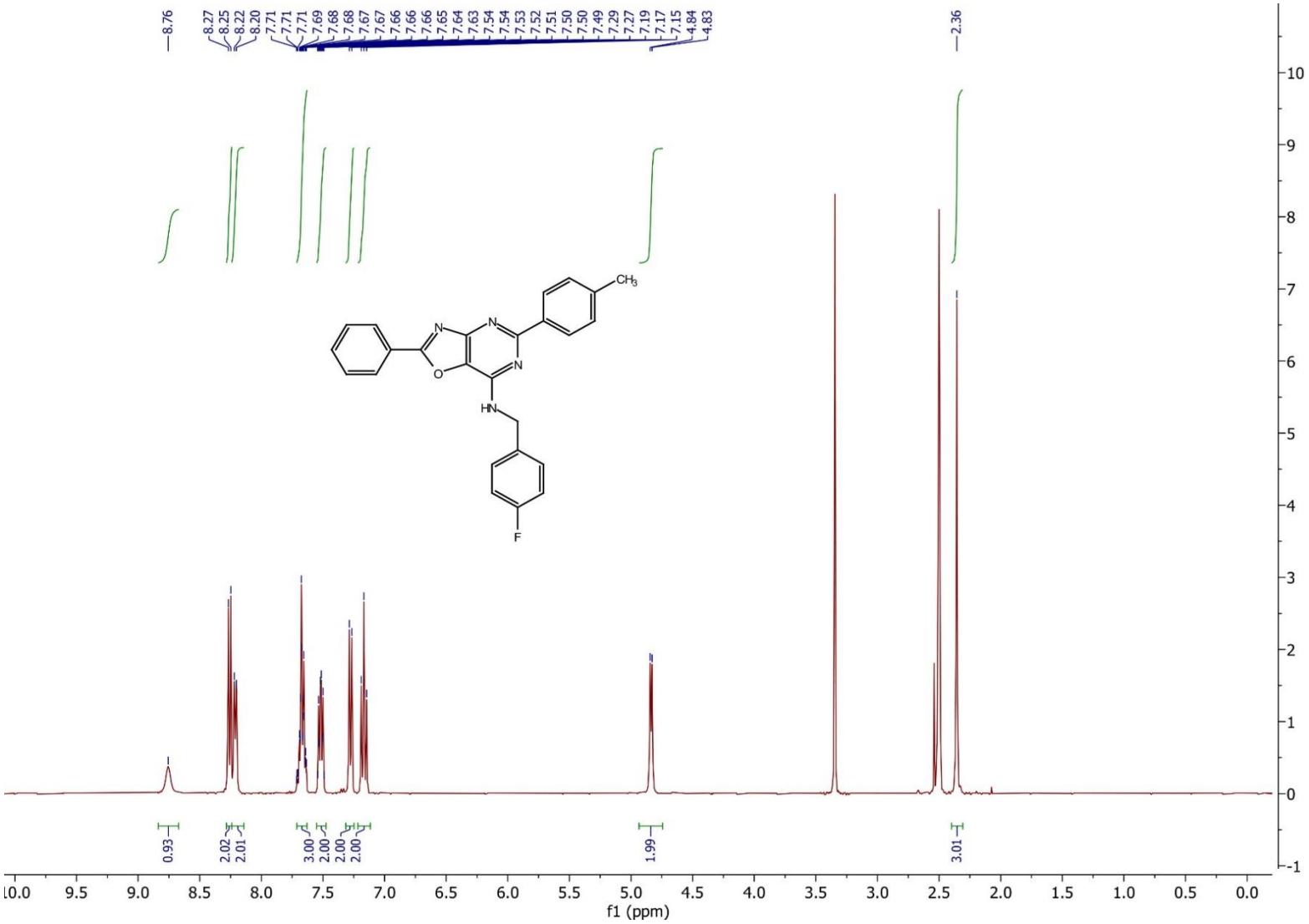

Figure S1. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**1**).

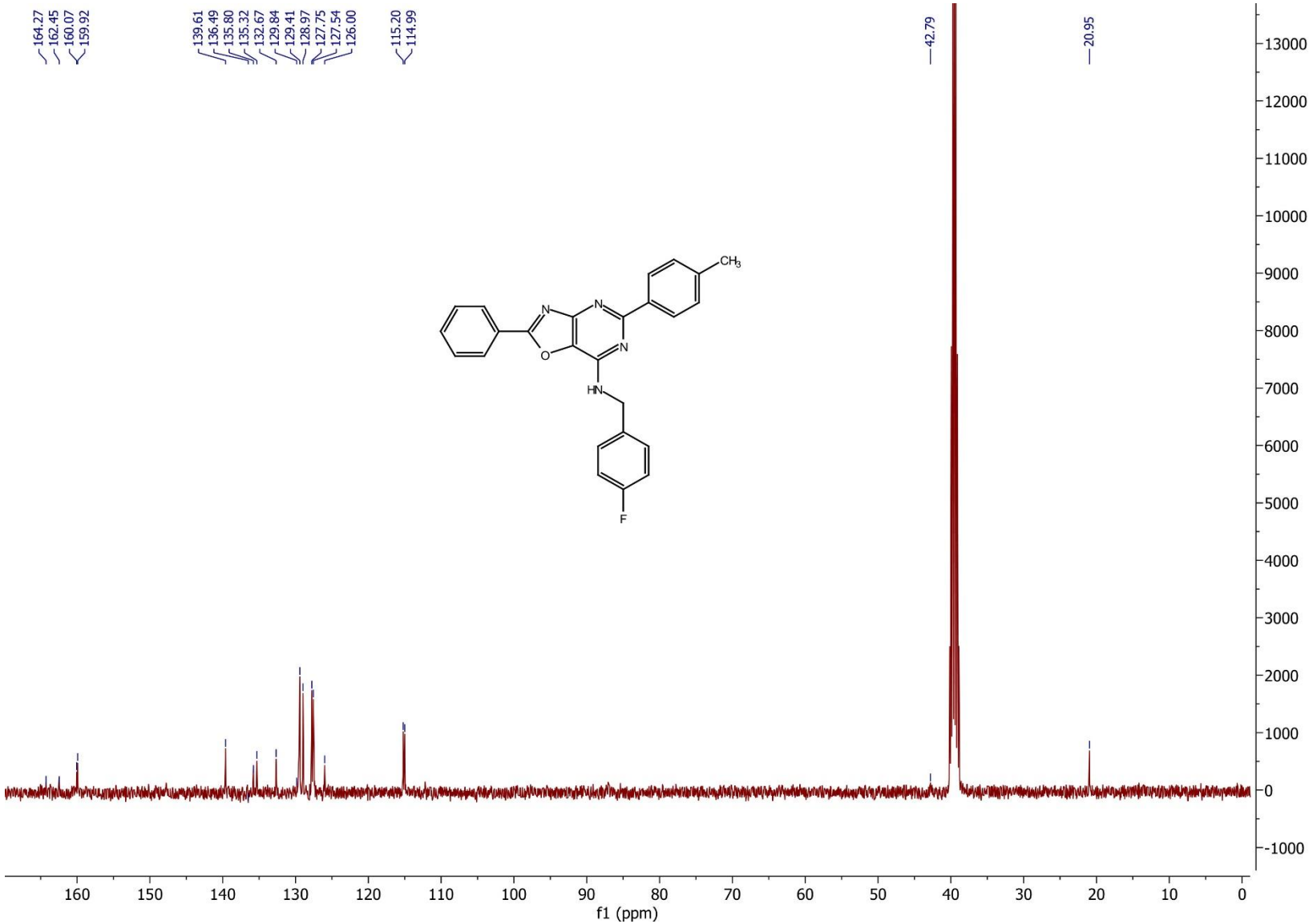

Figure S2. ^{13}C NMR (101 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**1**).

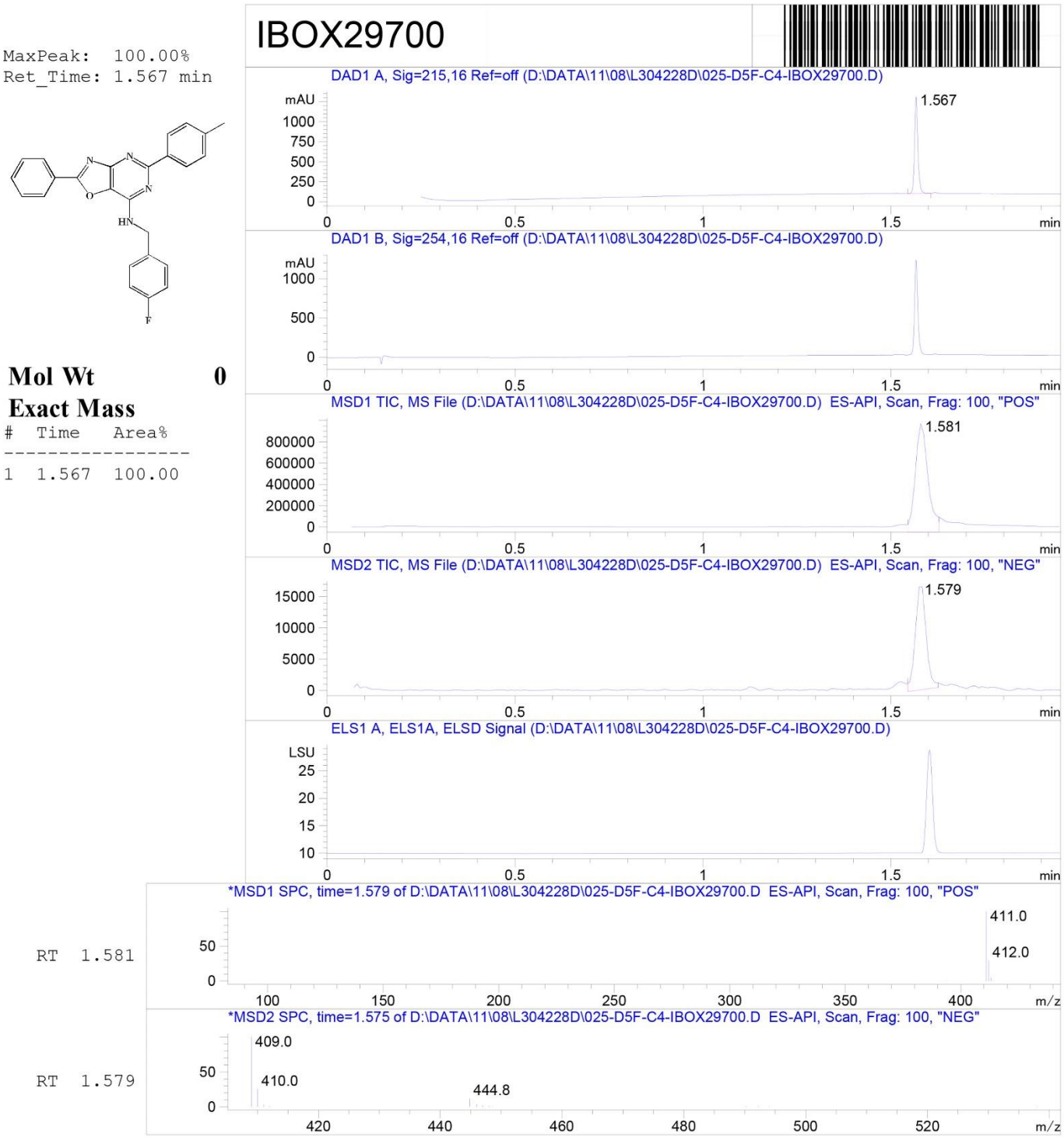

Figure S3. LCMS spectrum of compound (**1**).

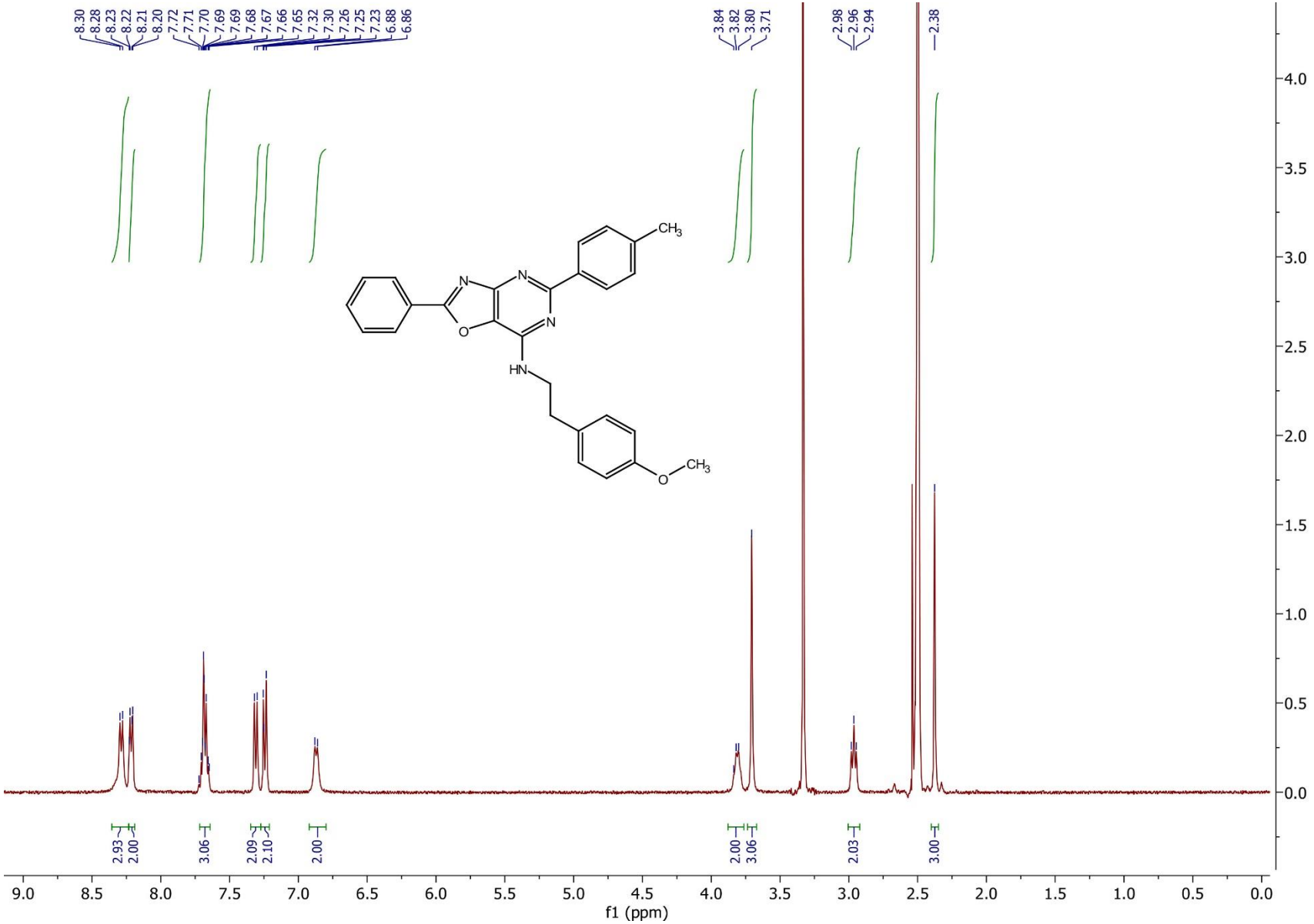

Figure S4. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**2**).

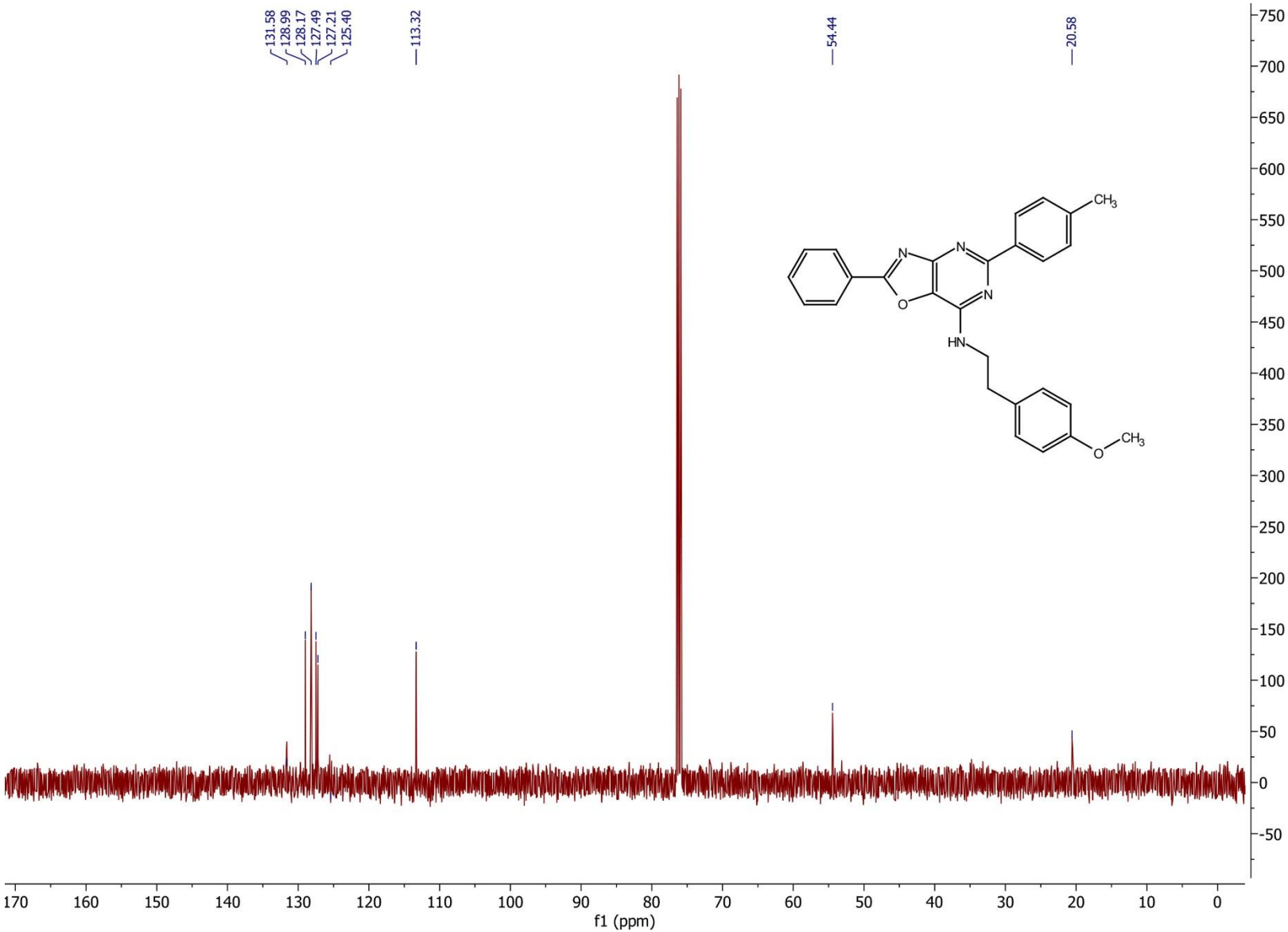

Figure S5. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**2**).

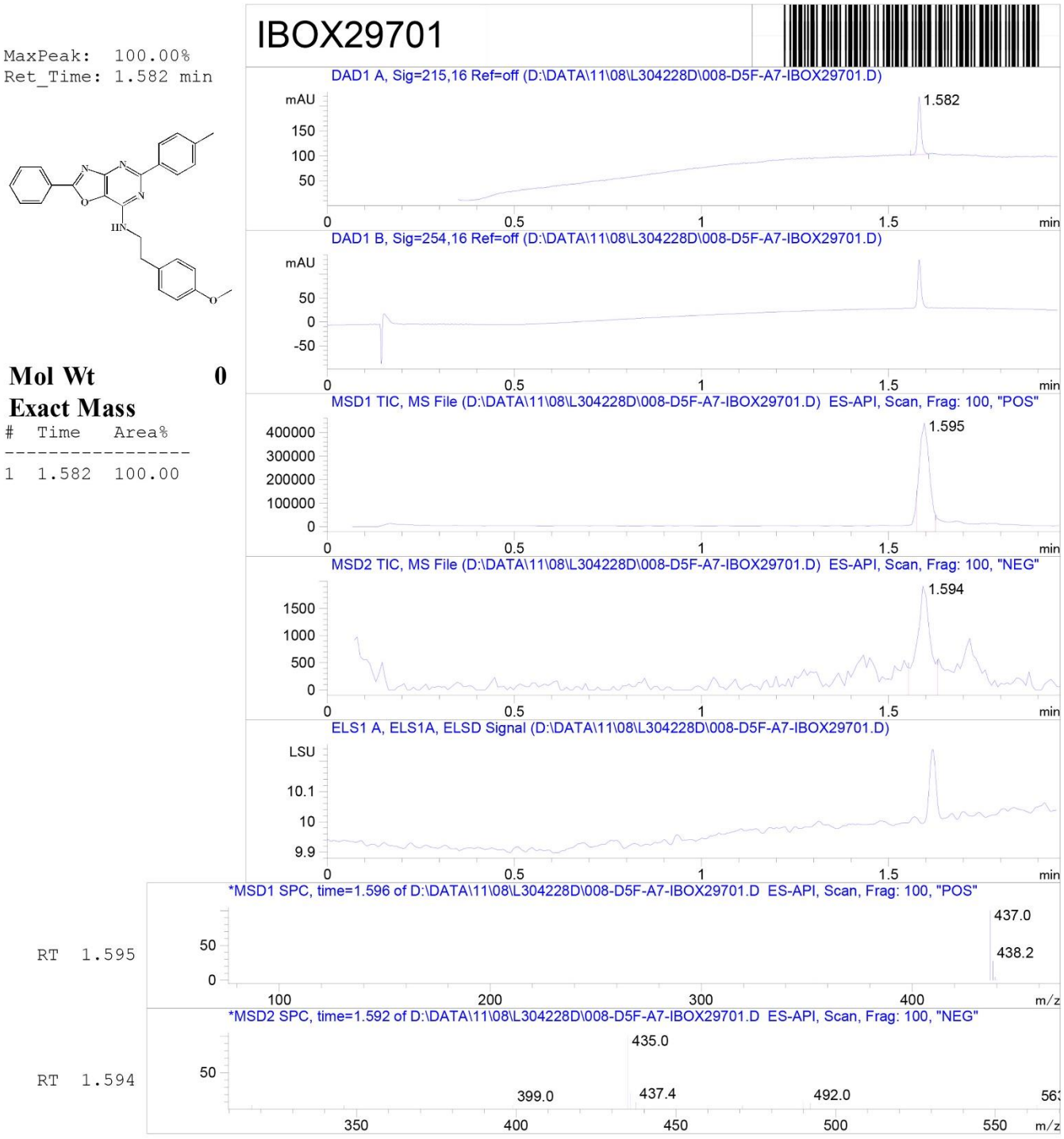

Figure S6. LCMS spectrum of compound (**2**).

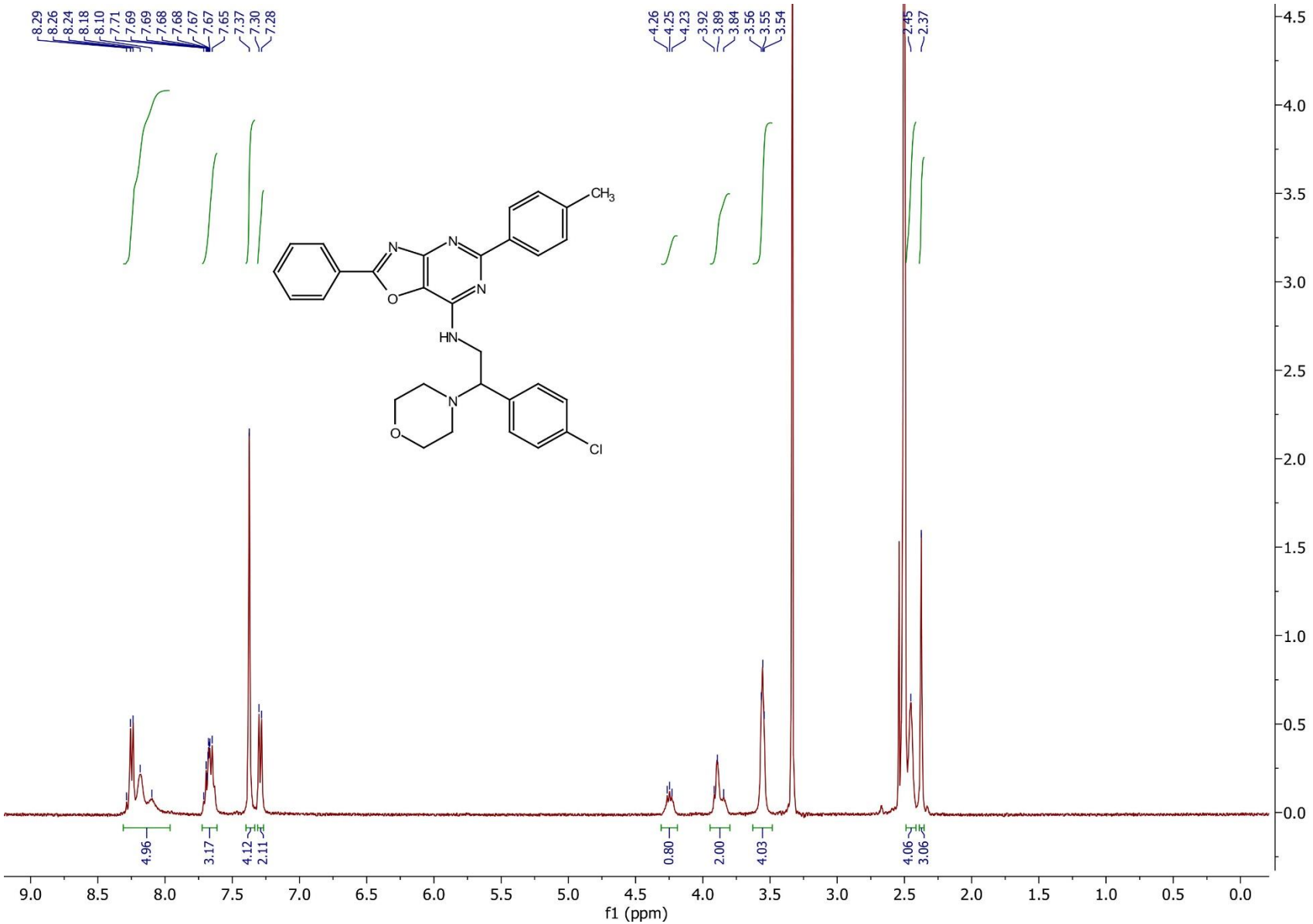

Figure S7. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**3**).

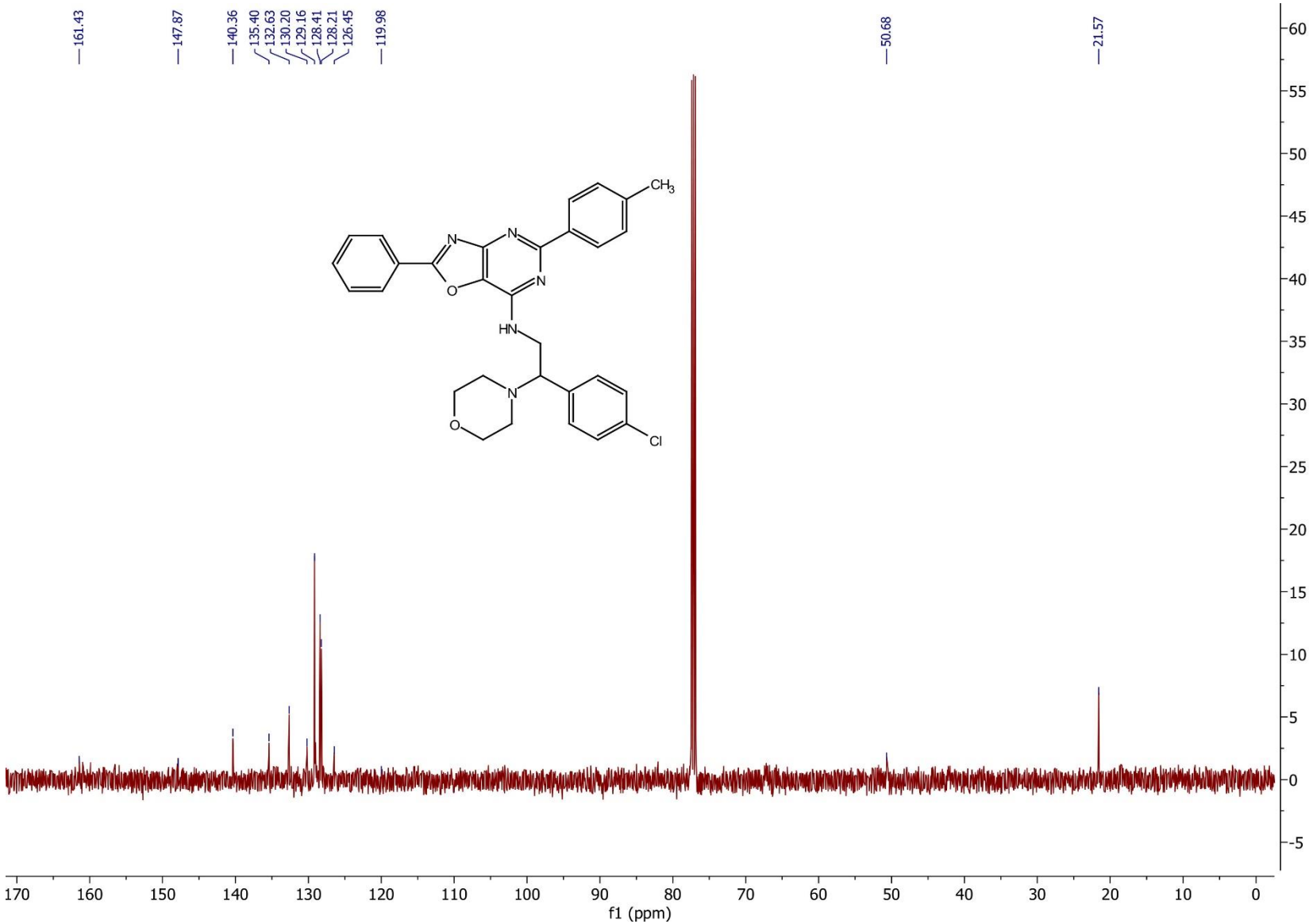

Figure S8. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**3**).

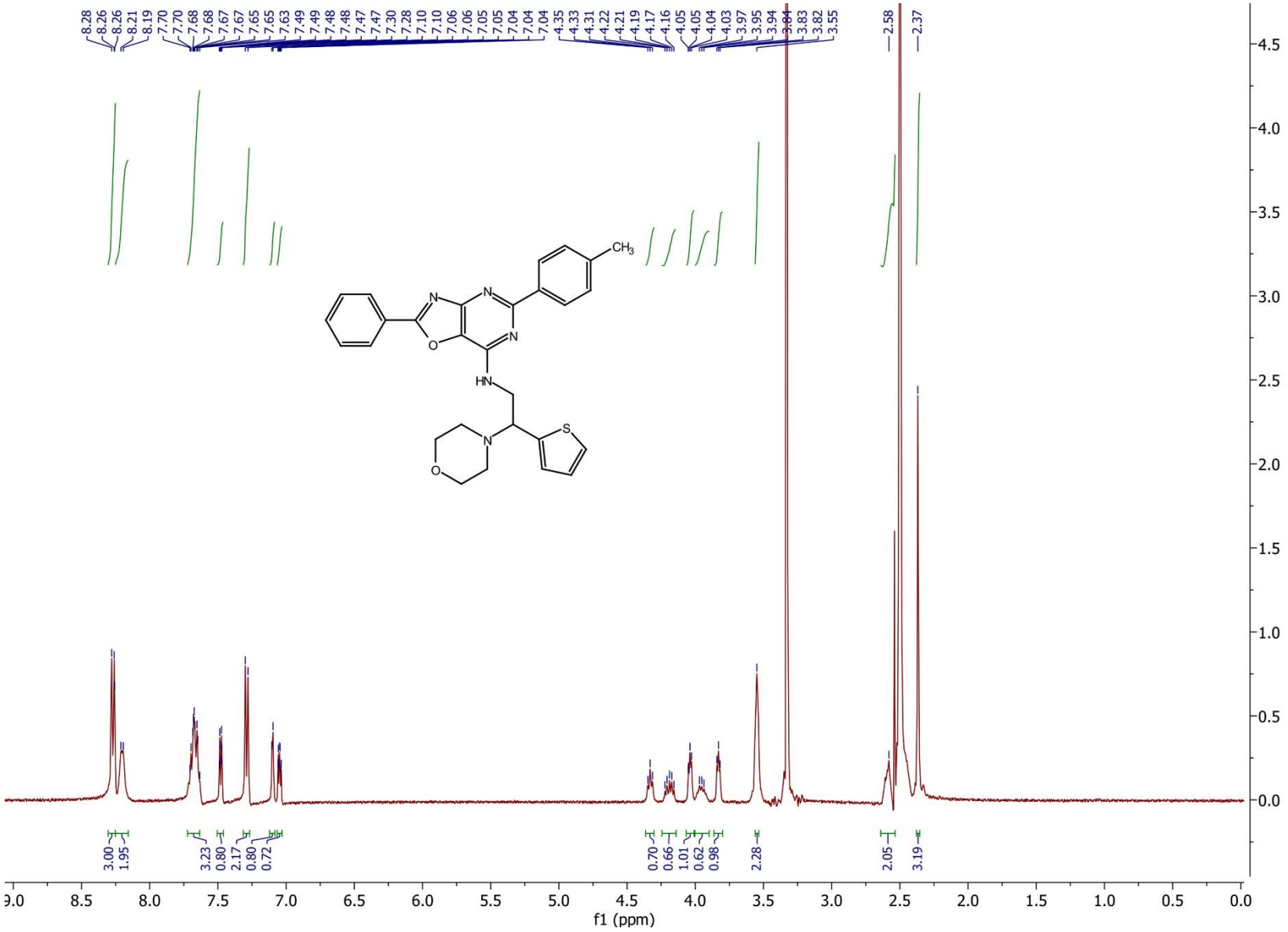

Figure S9. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**4**).

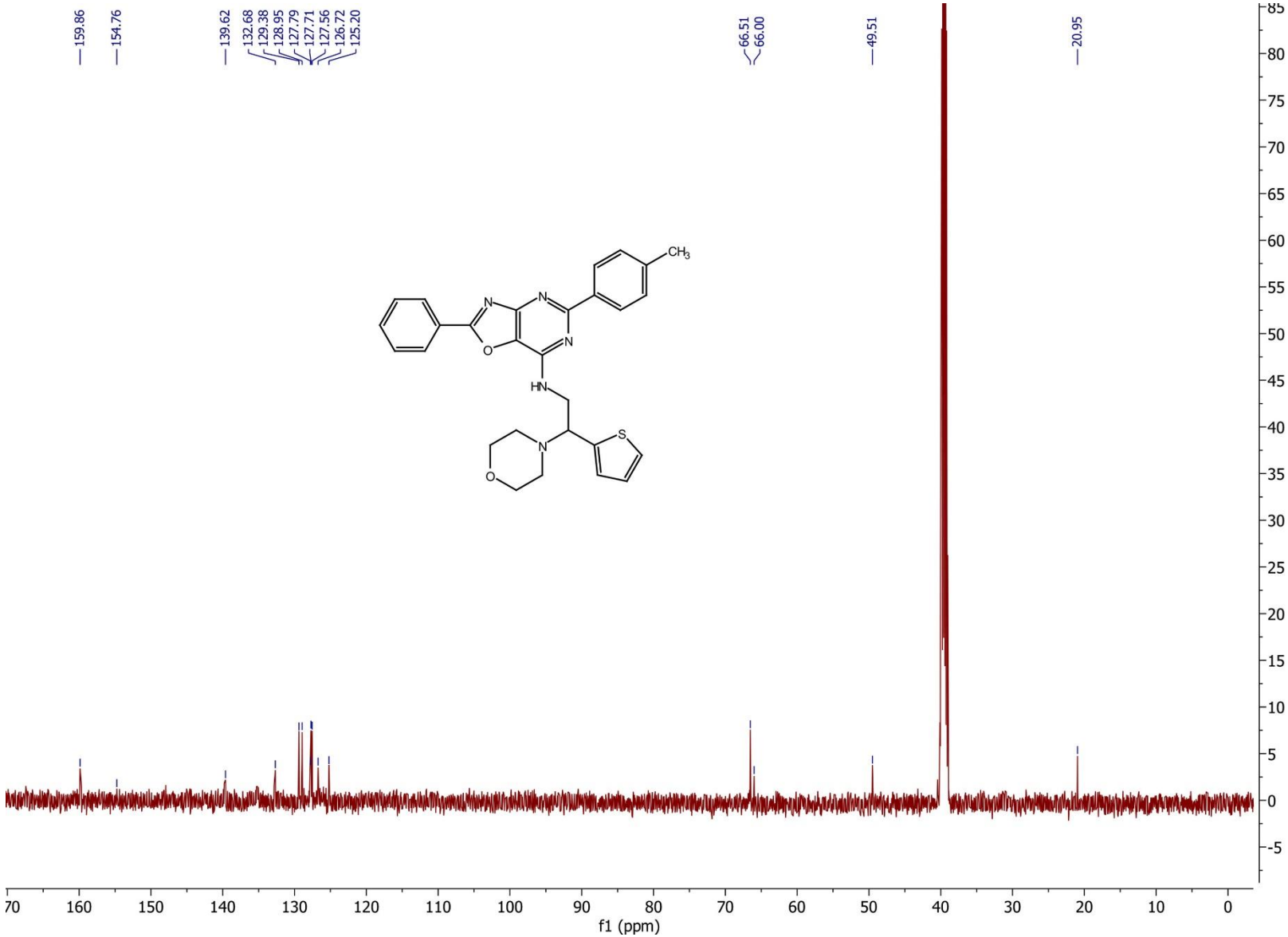

Figure S10. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**4**).

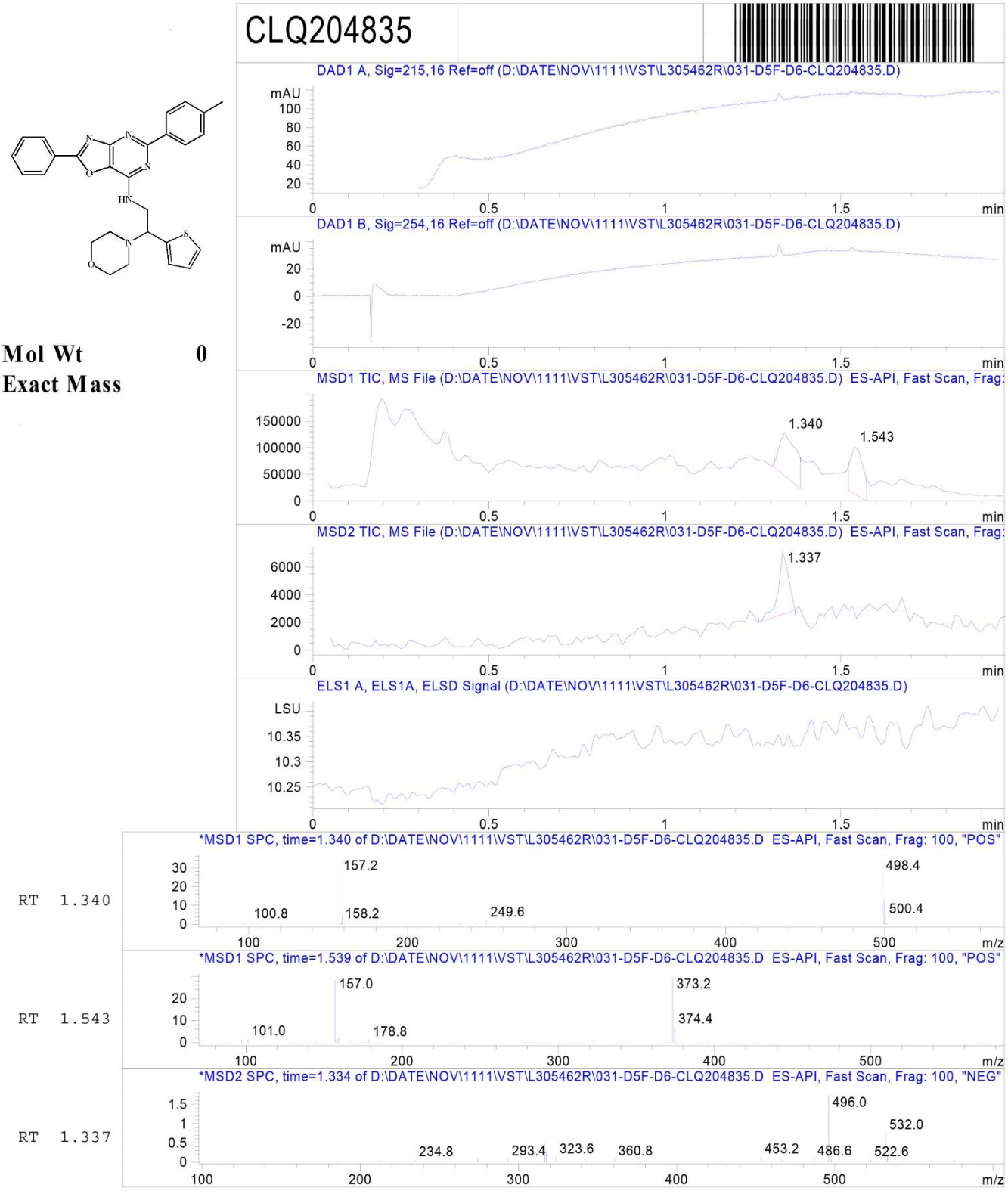

Figure S11. LCMS spectrum of compound (**4**).

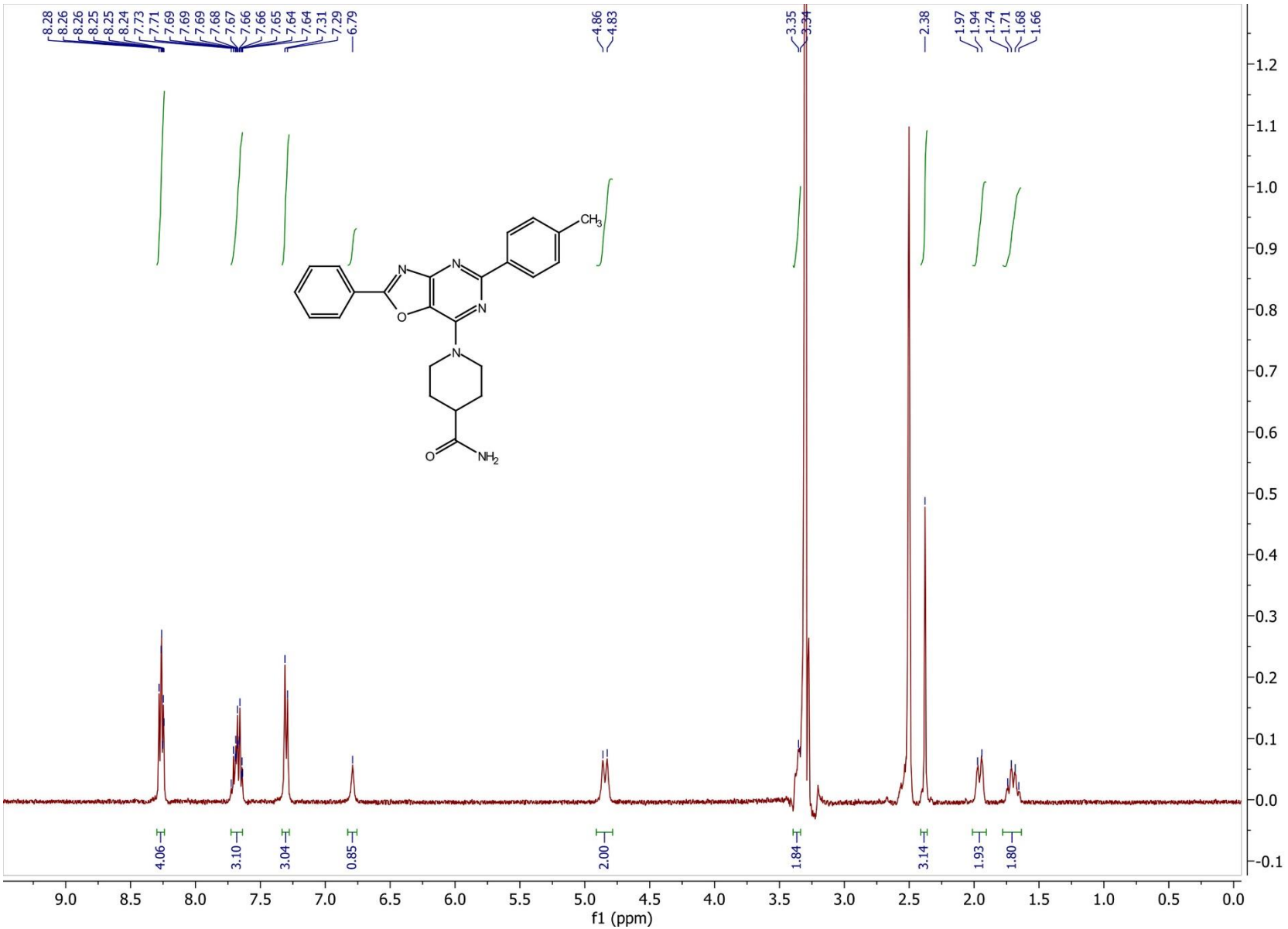

Figure S12. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound **(5).**

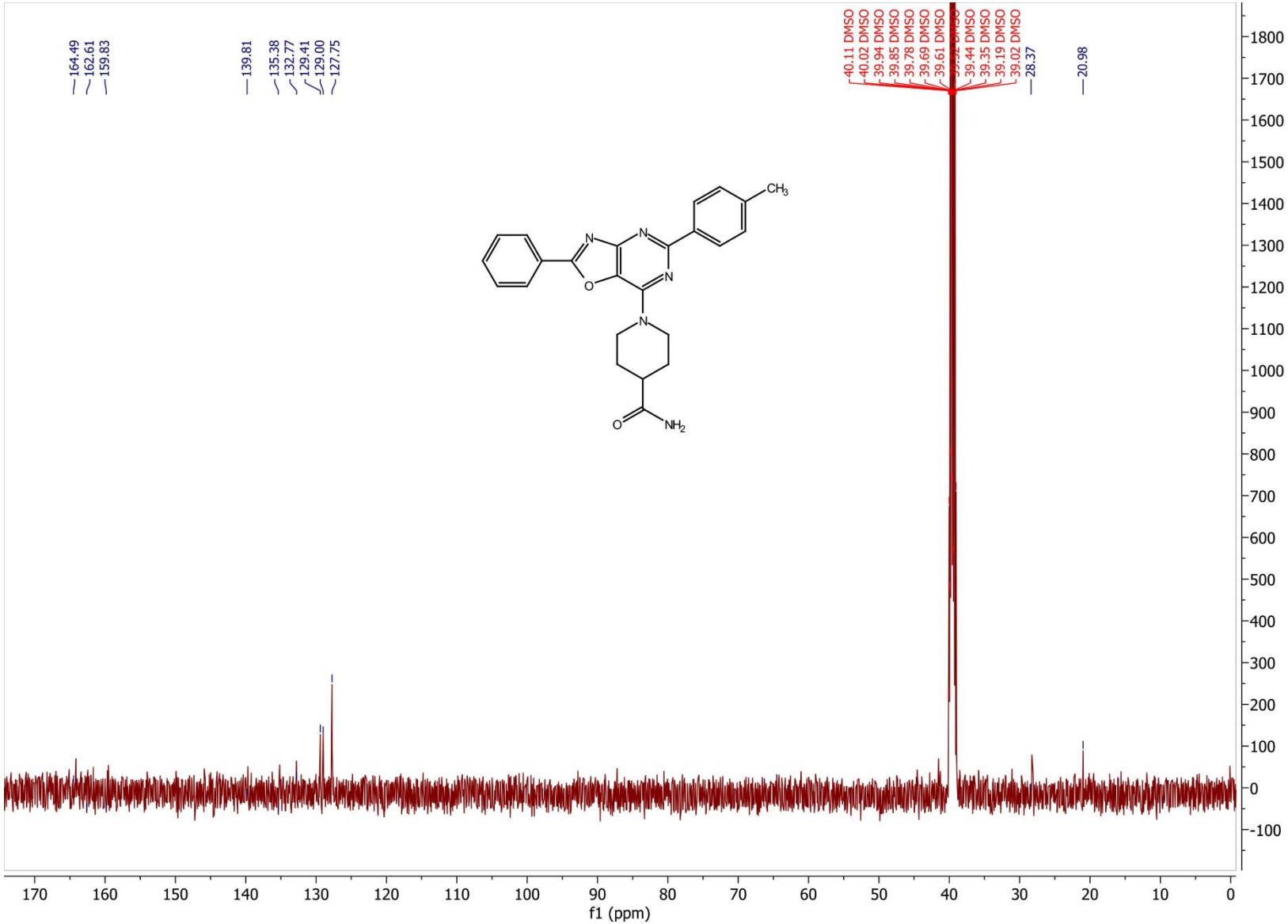

Figure S13. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound **(5).**

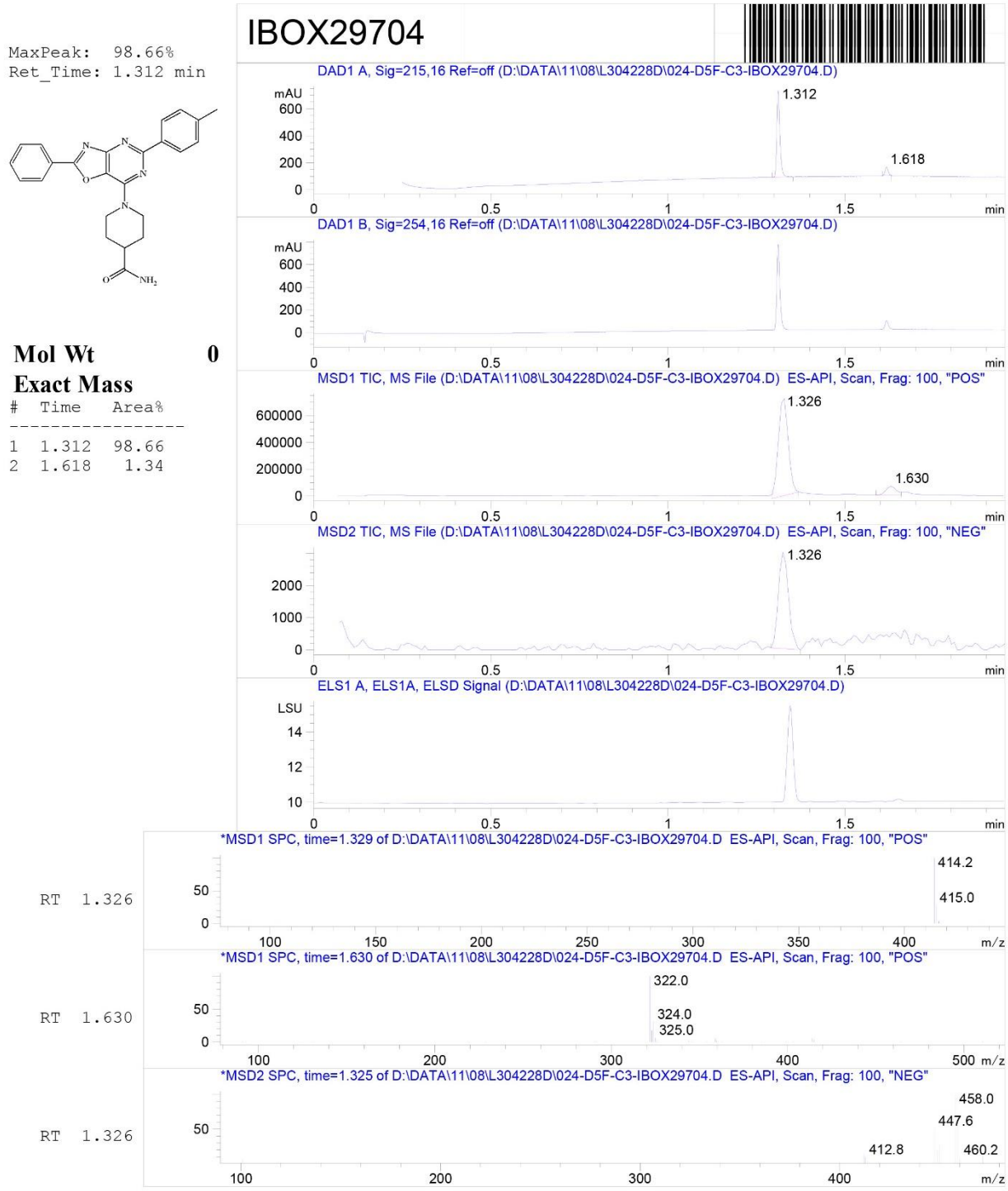

Figure S14. LCMS spectrum of compound **(5).**

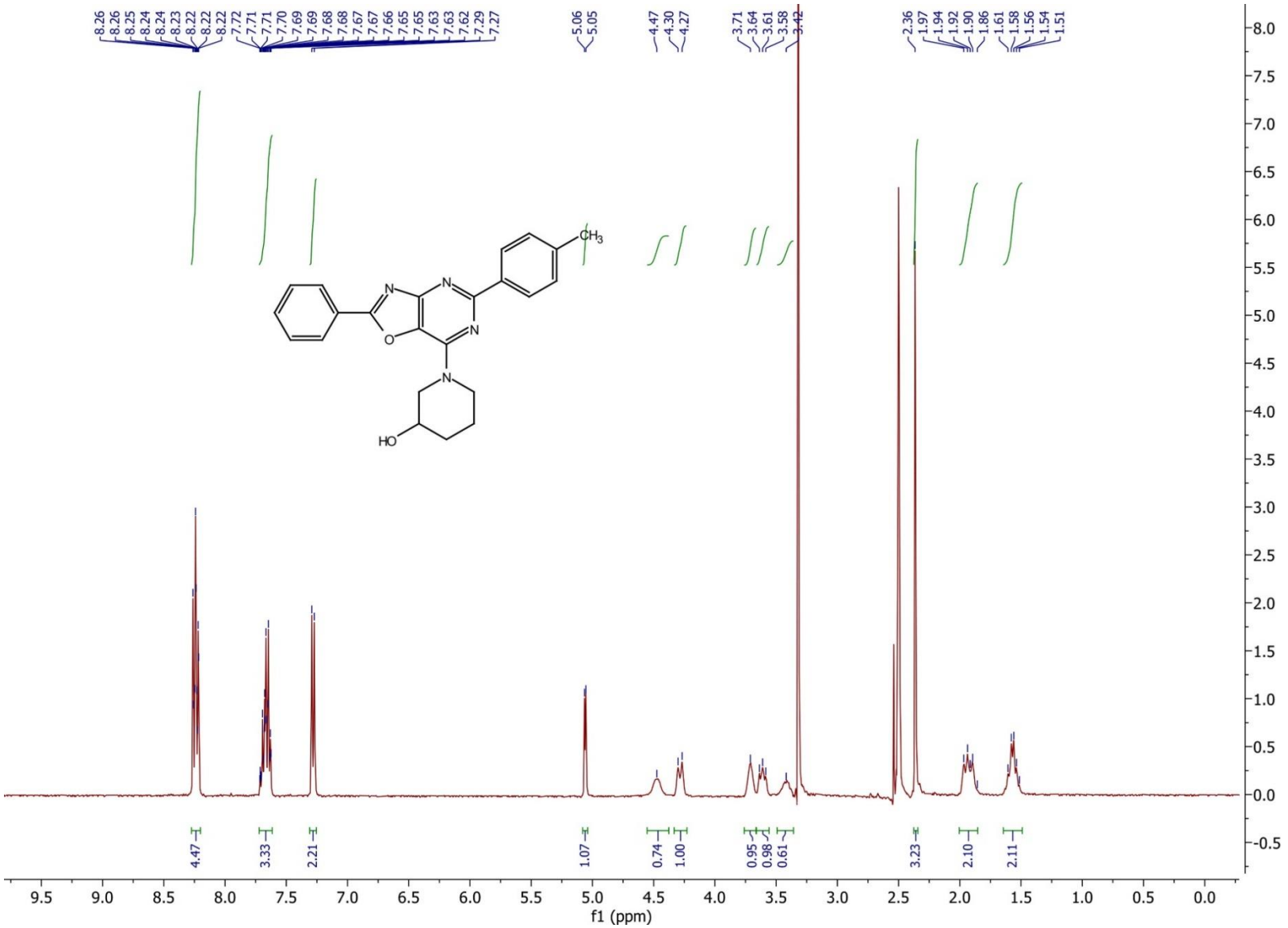

Figure S15. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**6).**

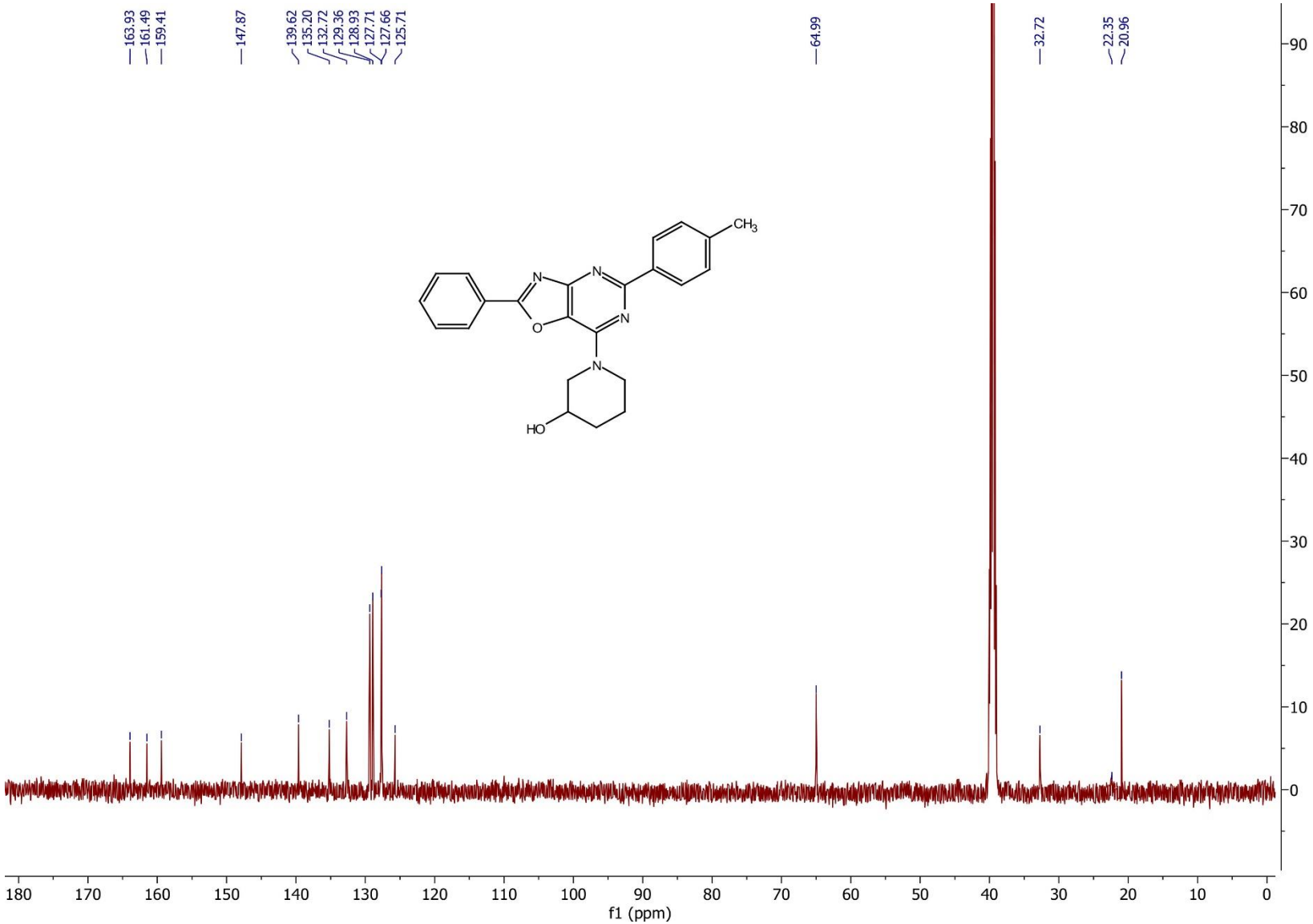

Figure S16. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**6**).

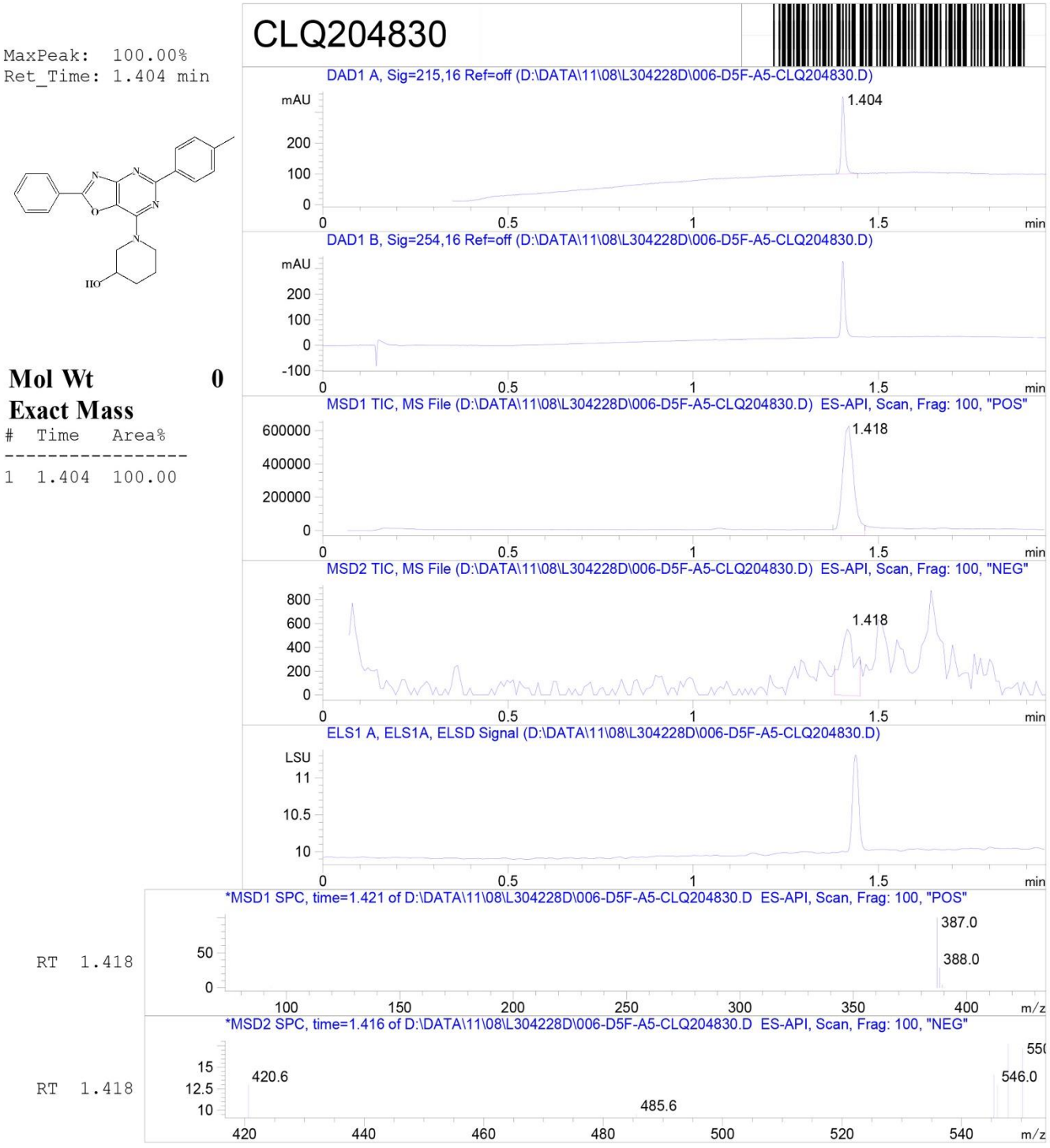

Figure S17. LCMS spectrum of compound (**6**).

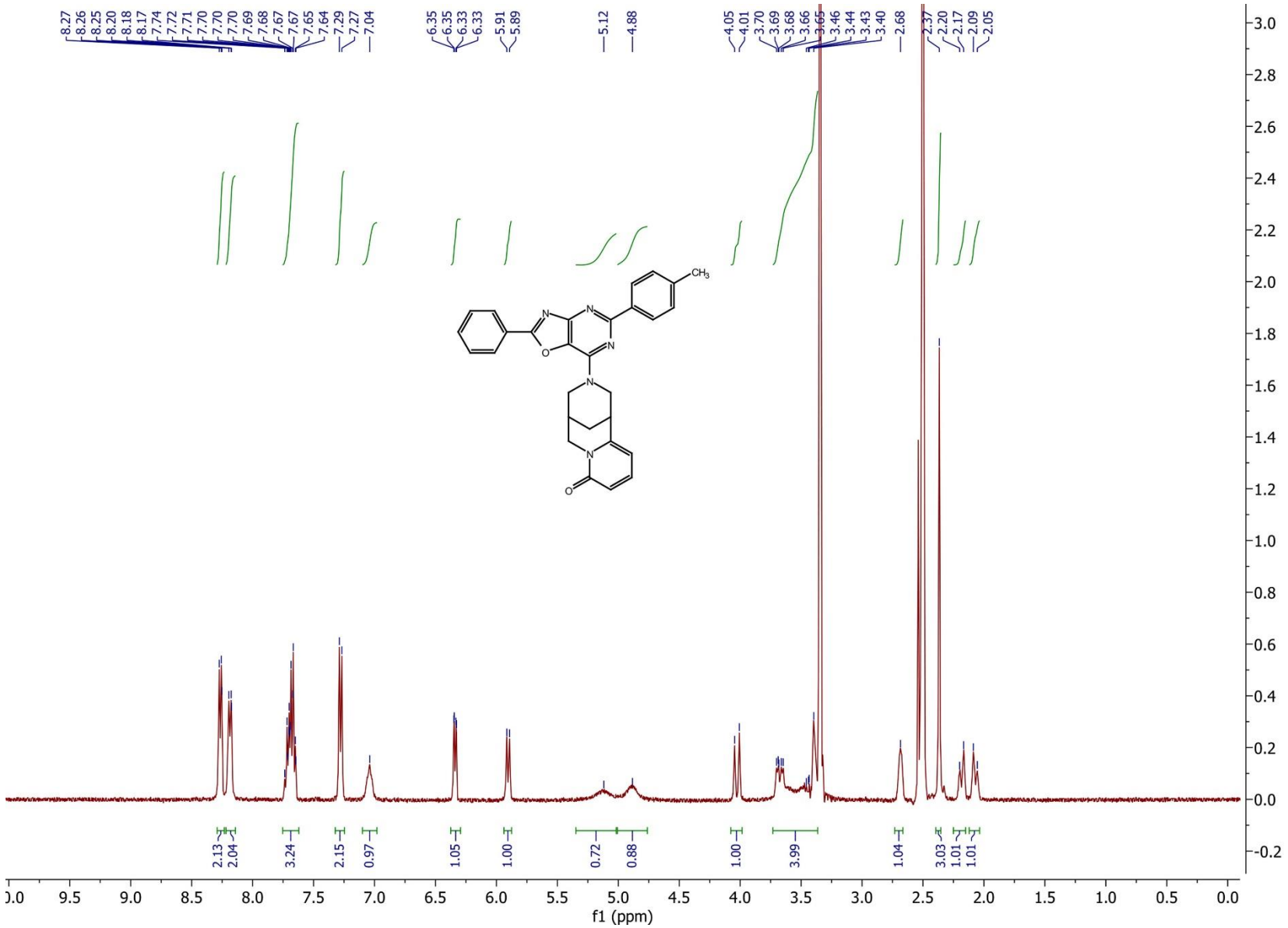

Figure S18. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**7**).

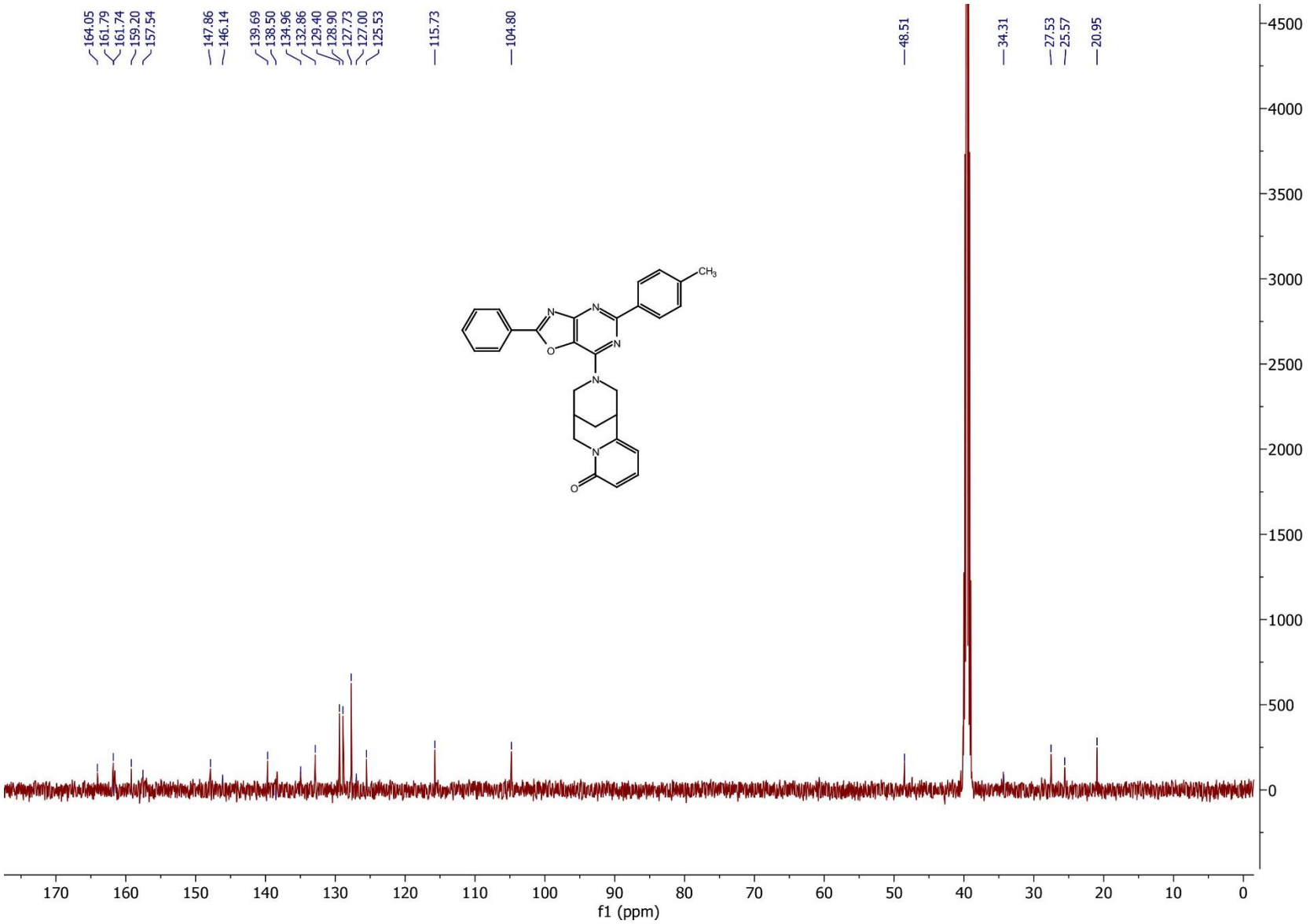

Figure S19. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**7**).

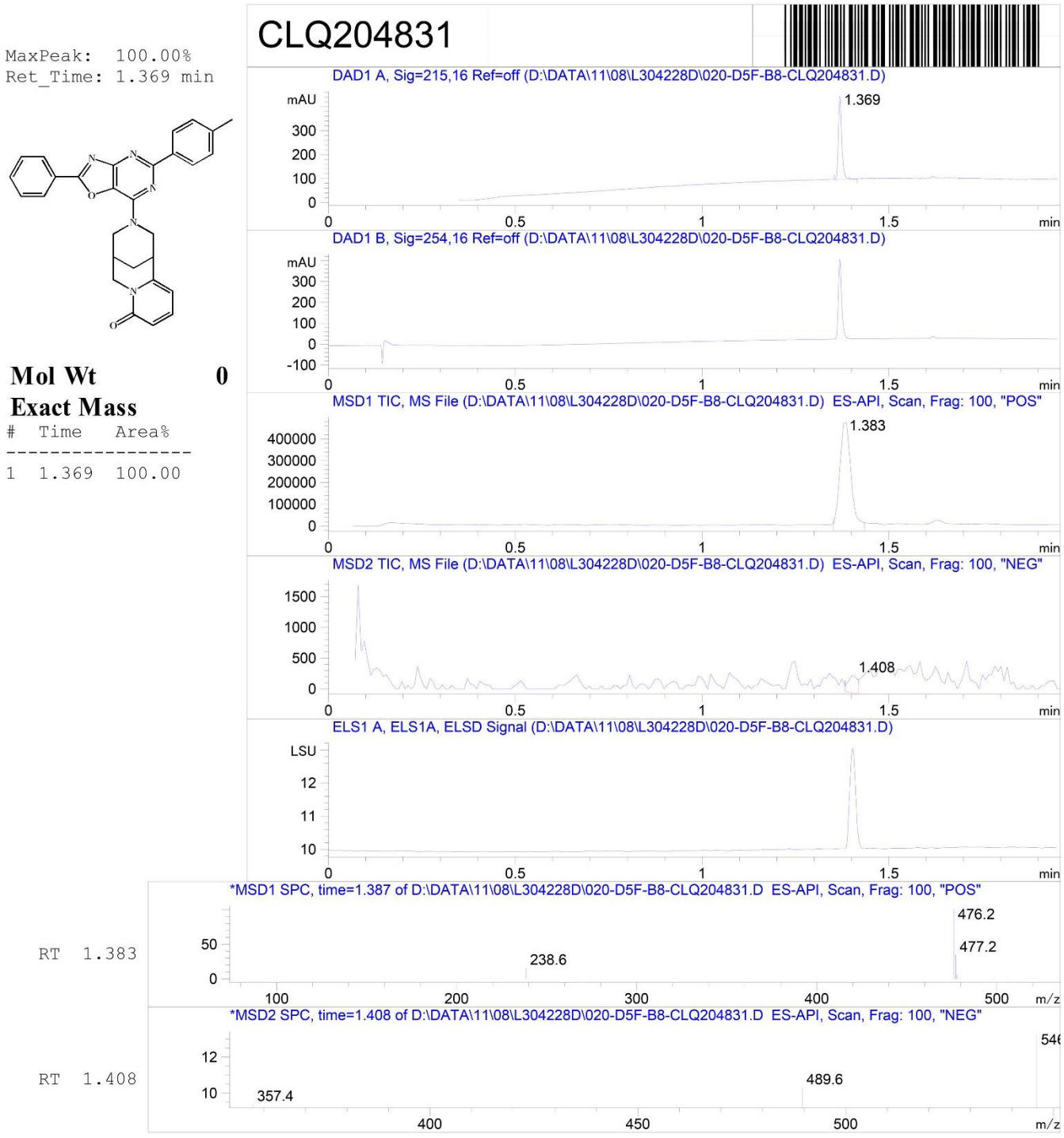

Figure S20. LCMS spectrum of compound (**7**).

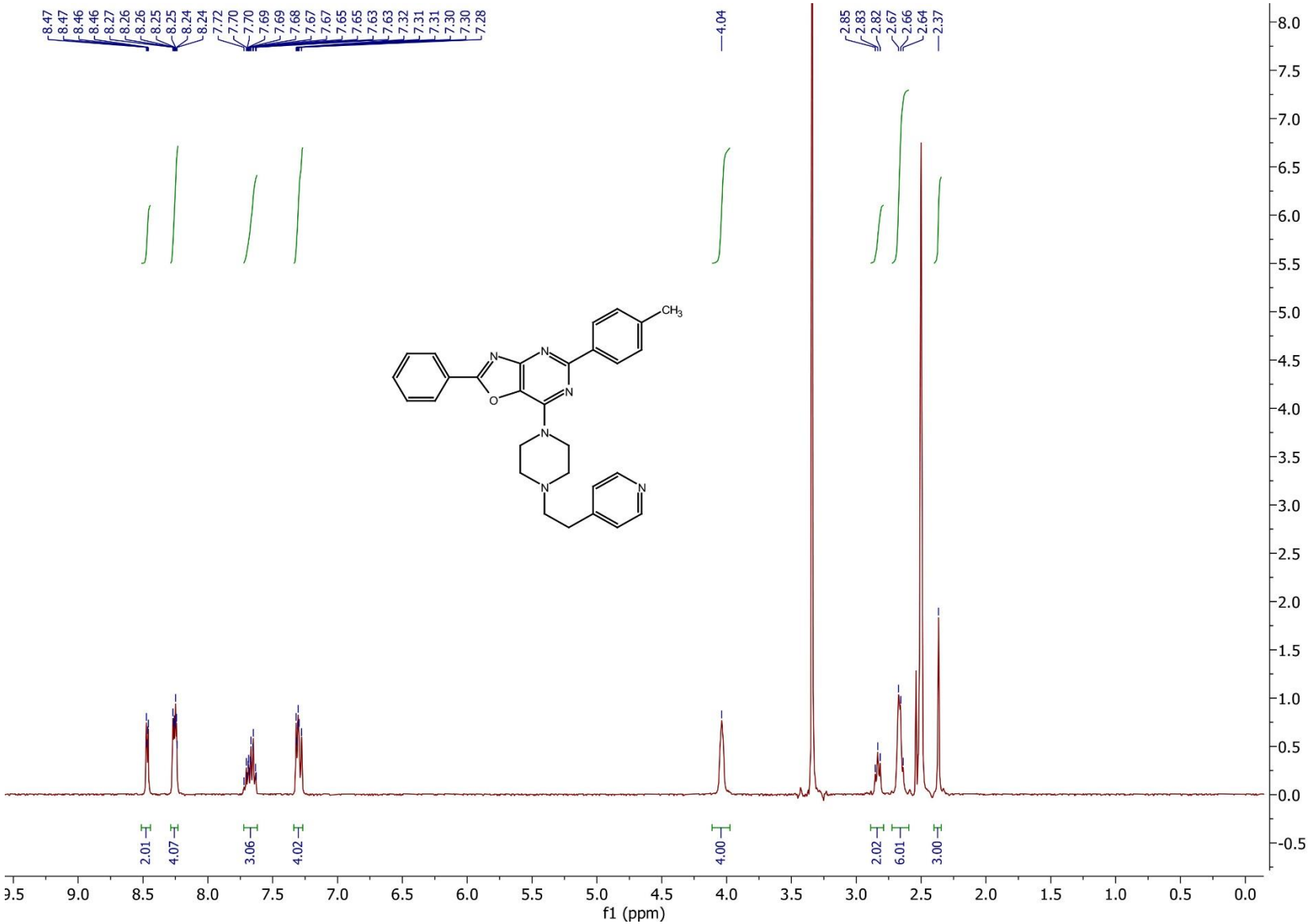

Figure S21. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**8**).

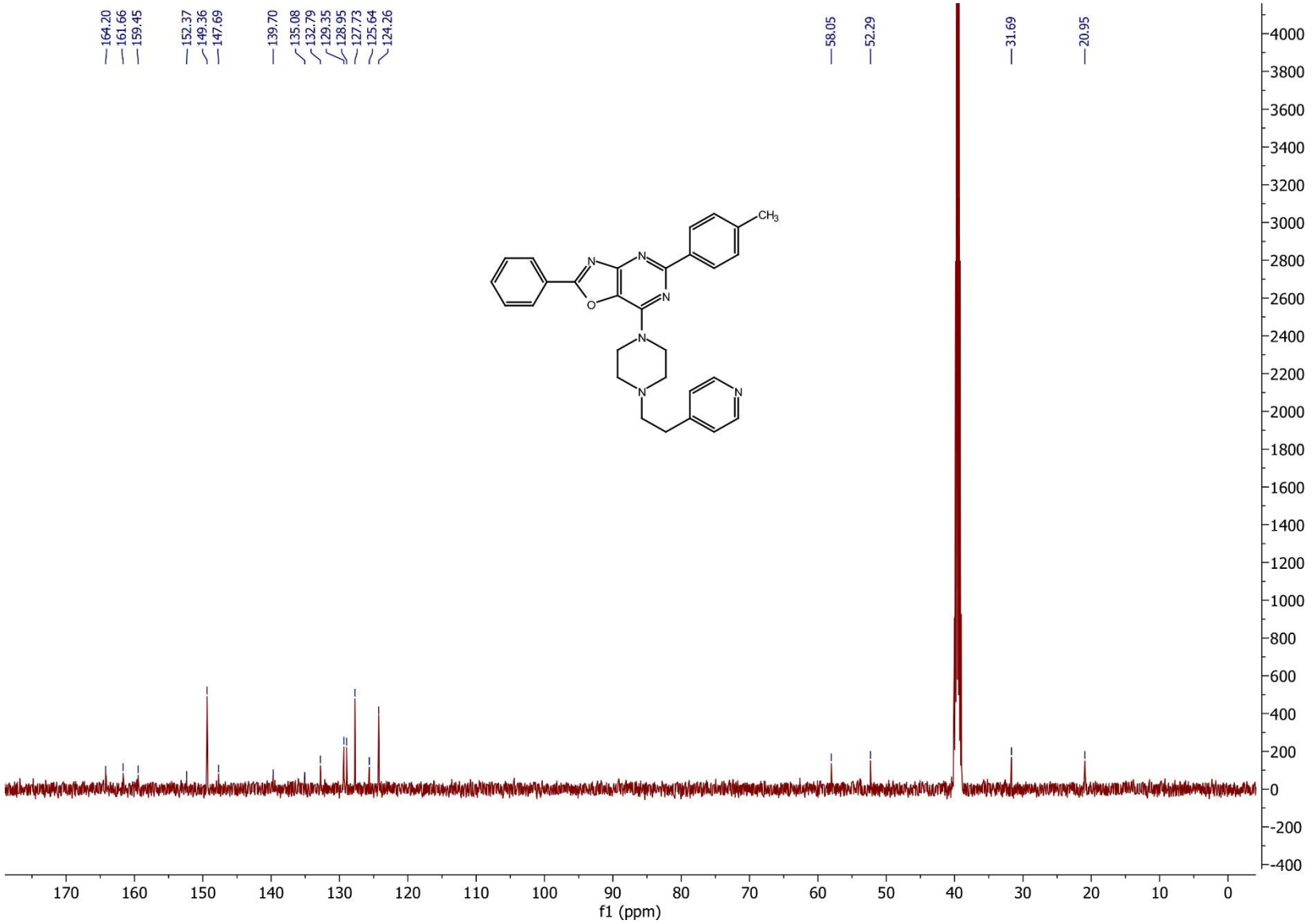

Figure S22. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**8**).

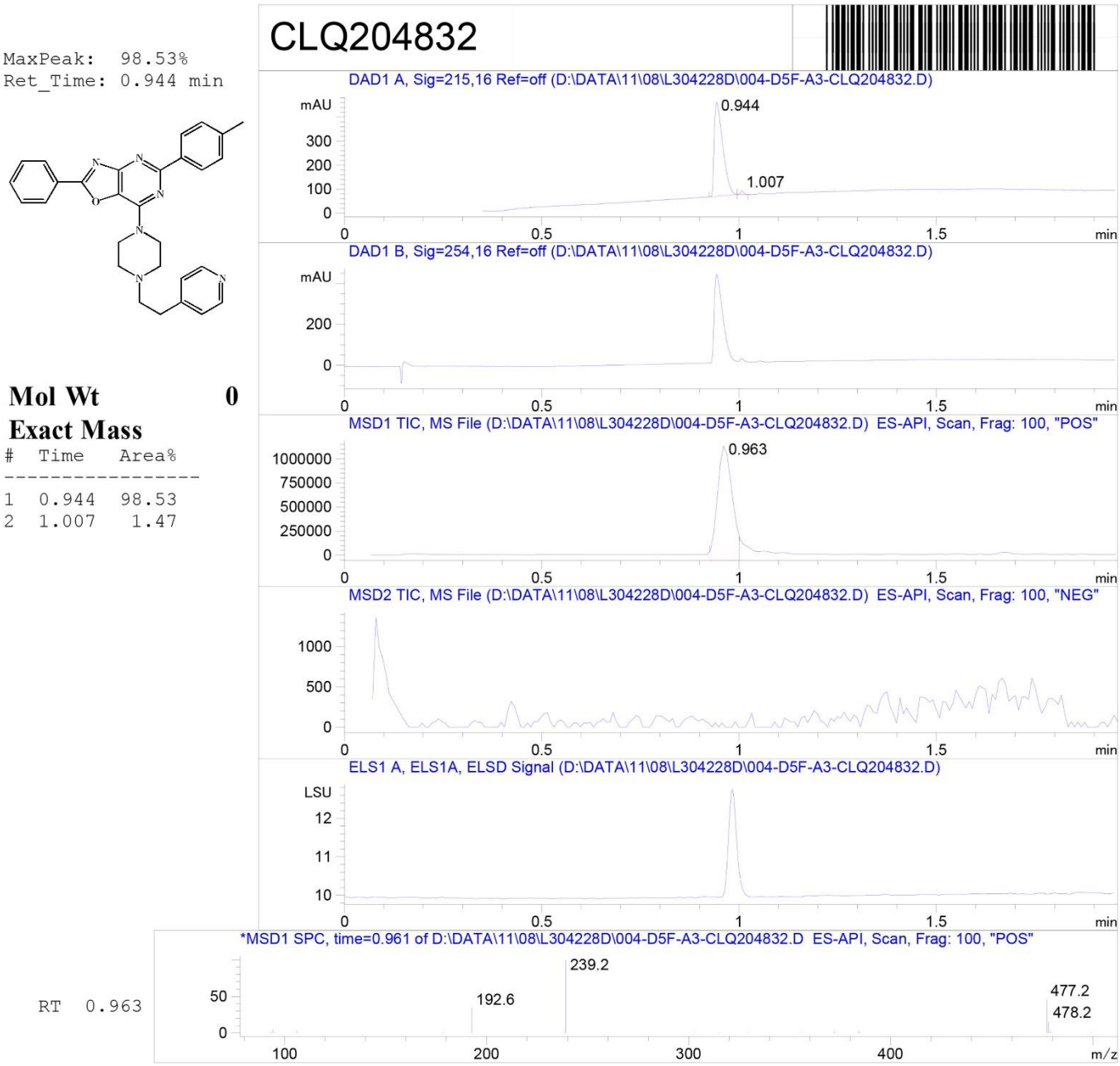

Figure S23. LCMS spectrum of compound (**8**).

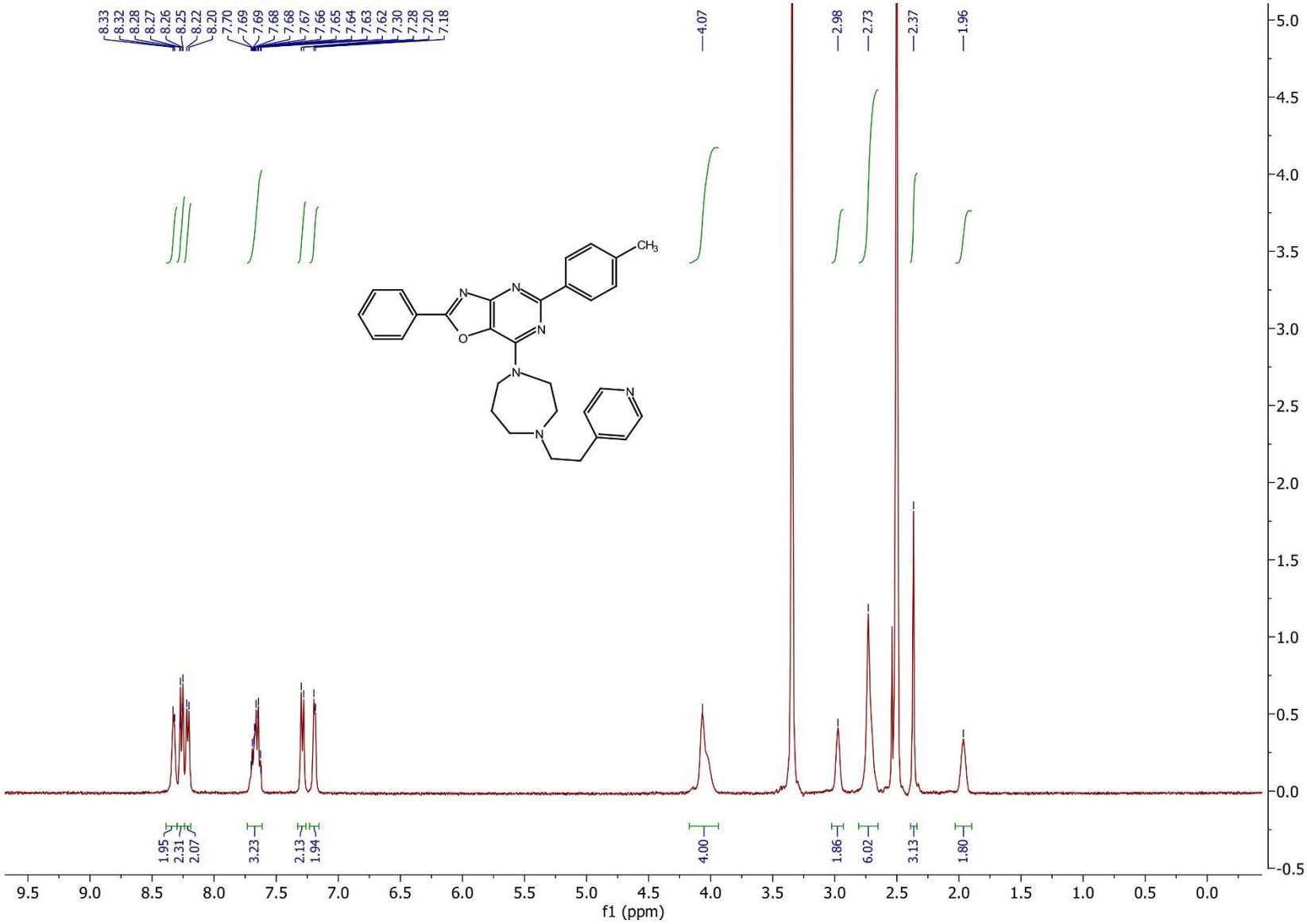

Figure S24. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**9**).

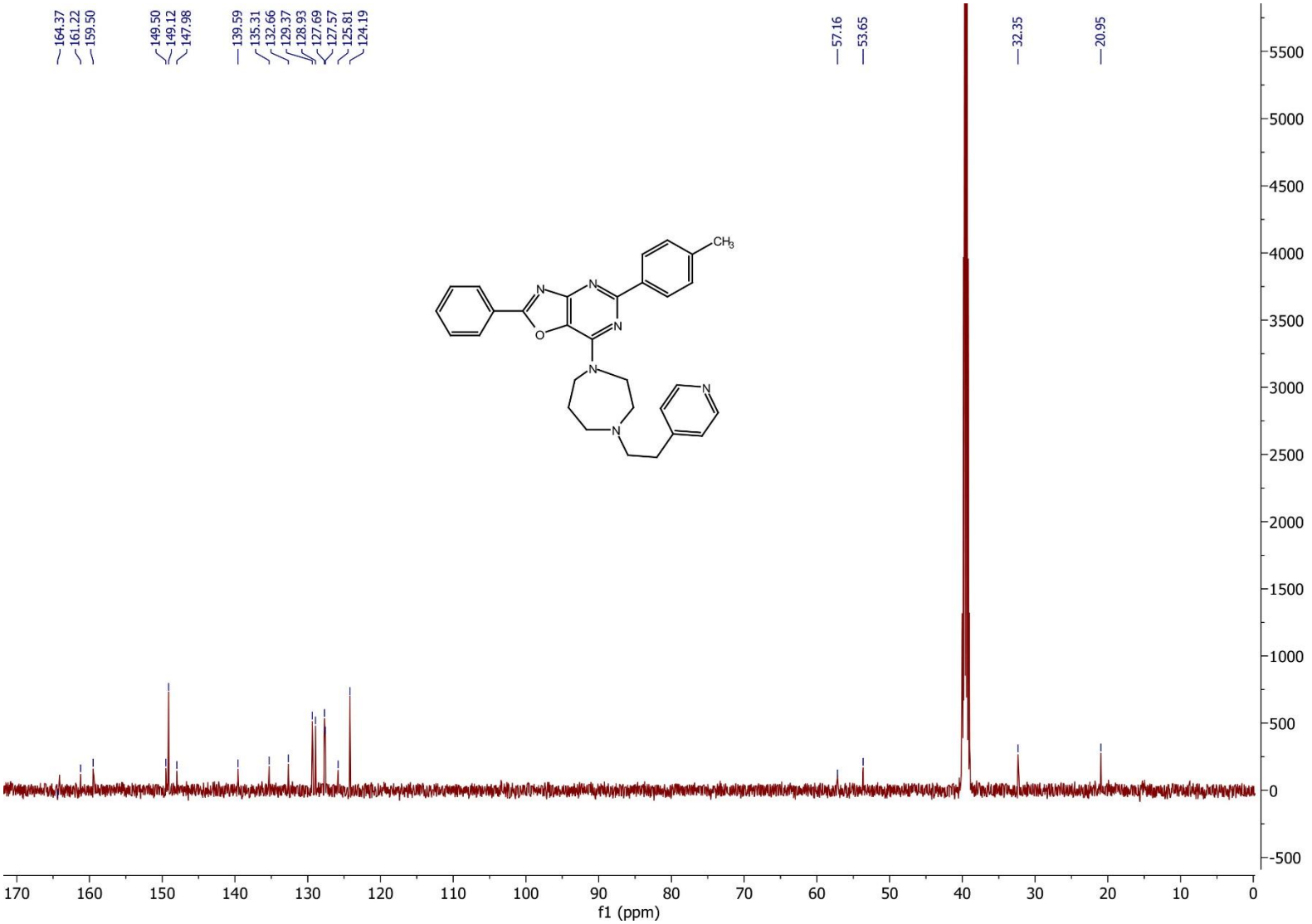

Figure S25. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**9**).

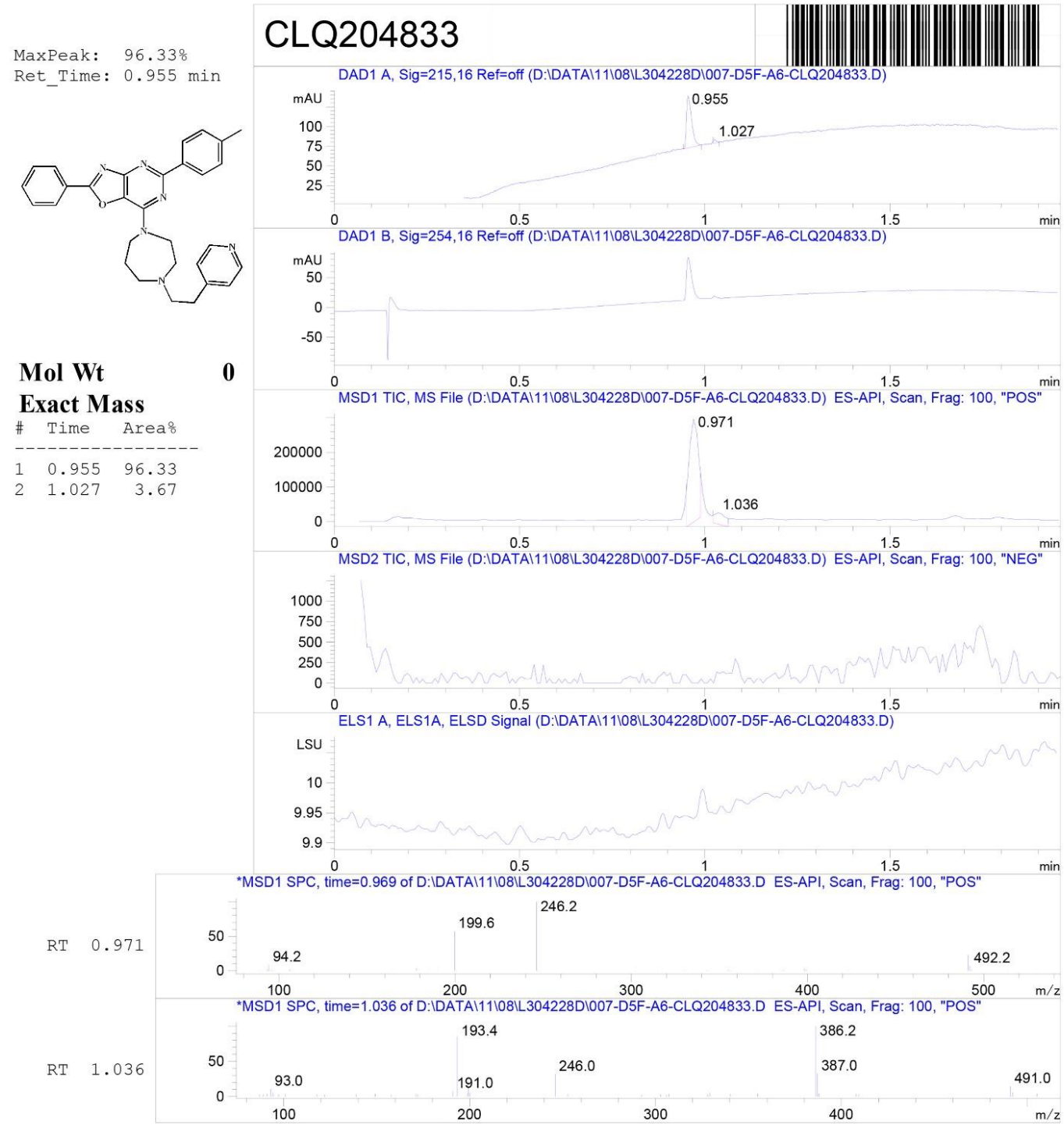

Figure S26. LCMS spectrum of compound (**9**).

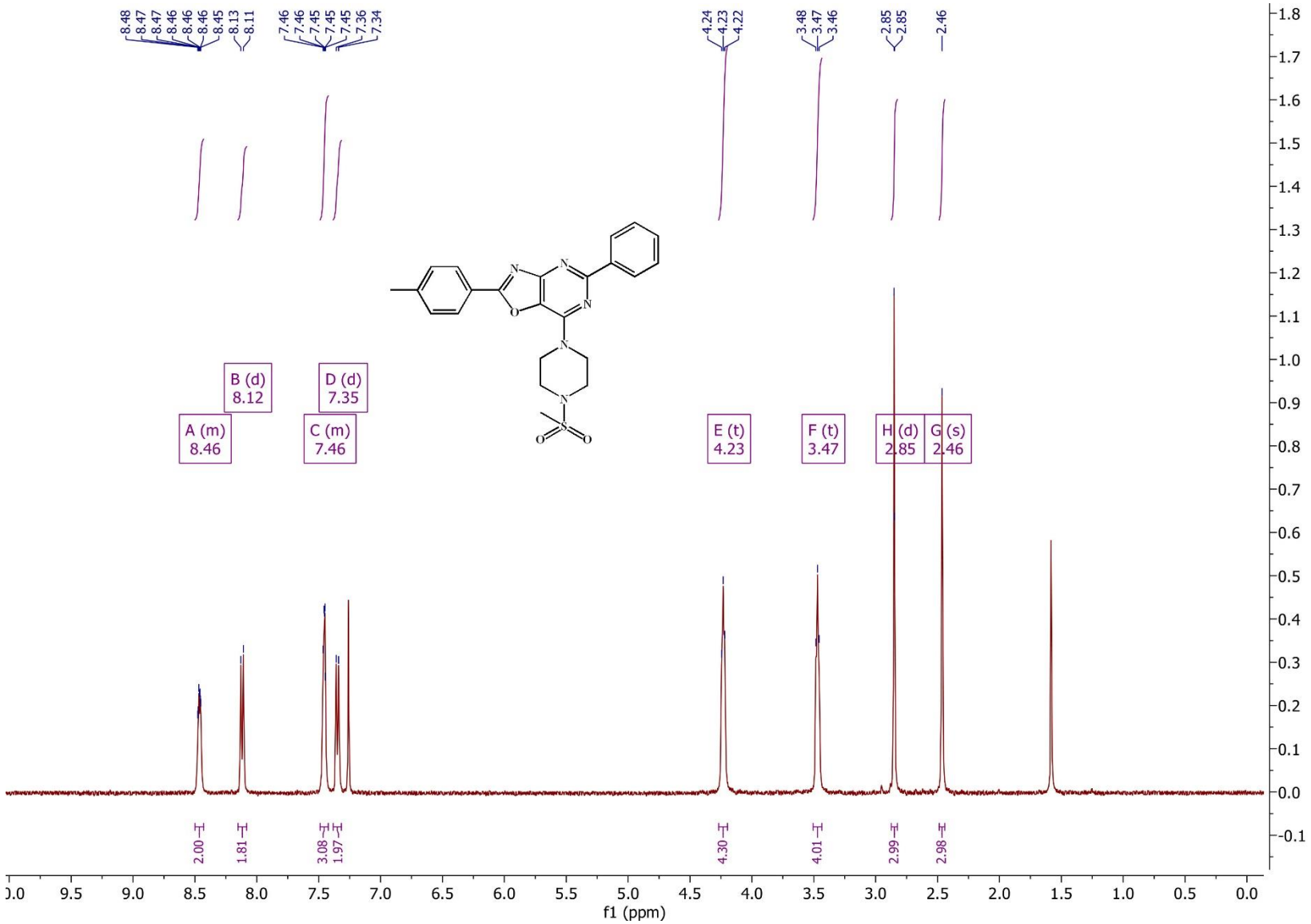

Figure S27. ^{1}H NMR (400 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**10**).

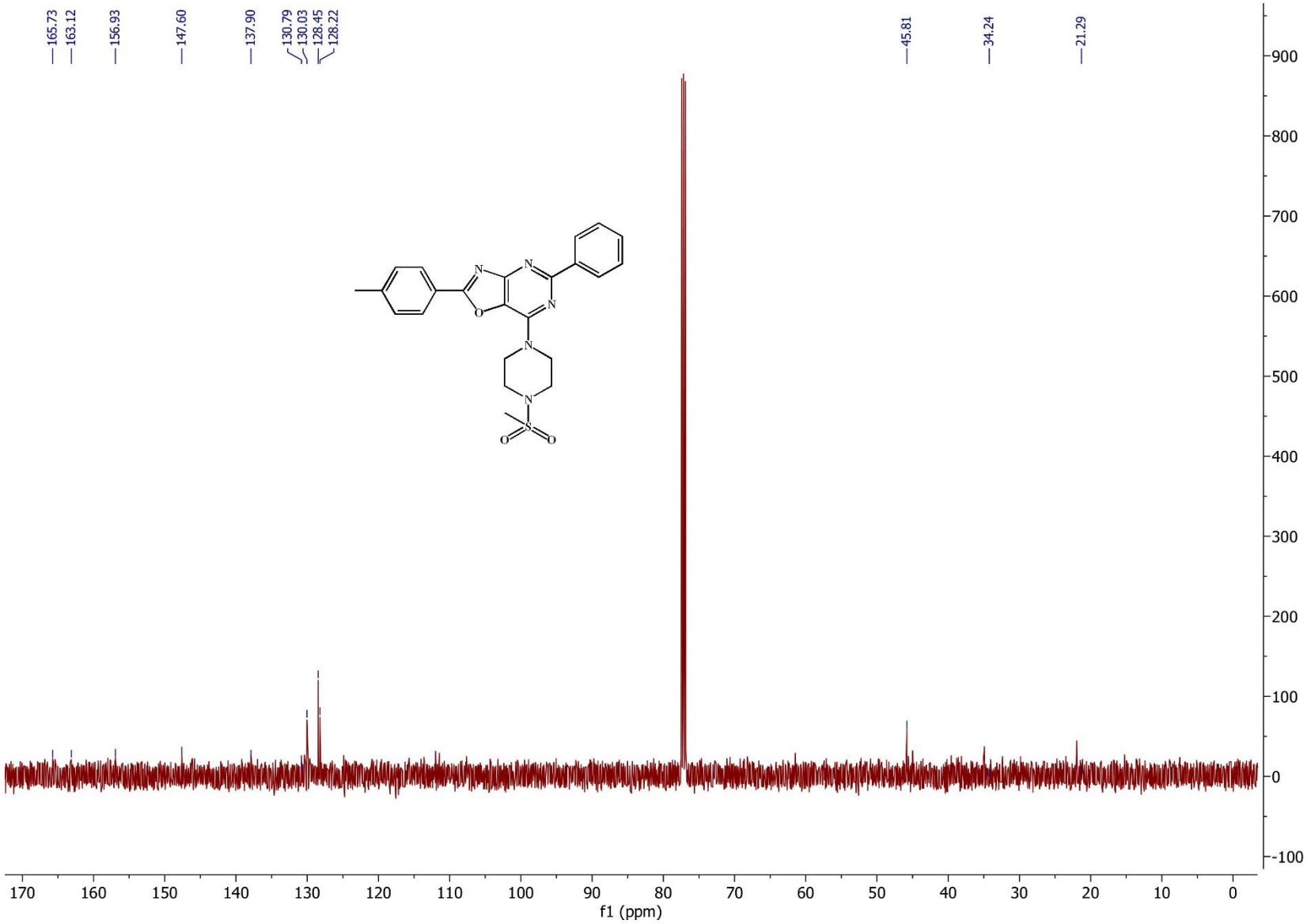

Figure S28. ^{13}C NMR (126 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**10**).

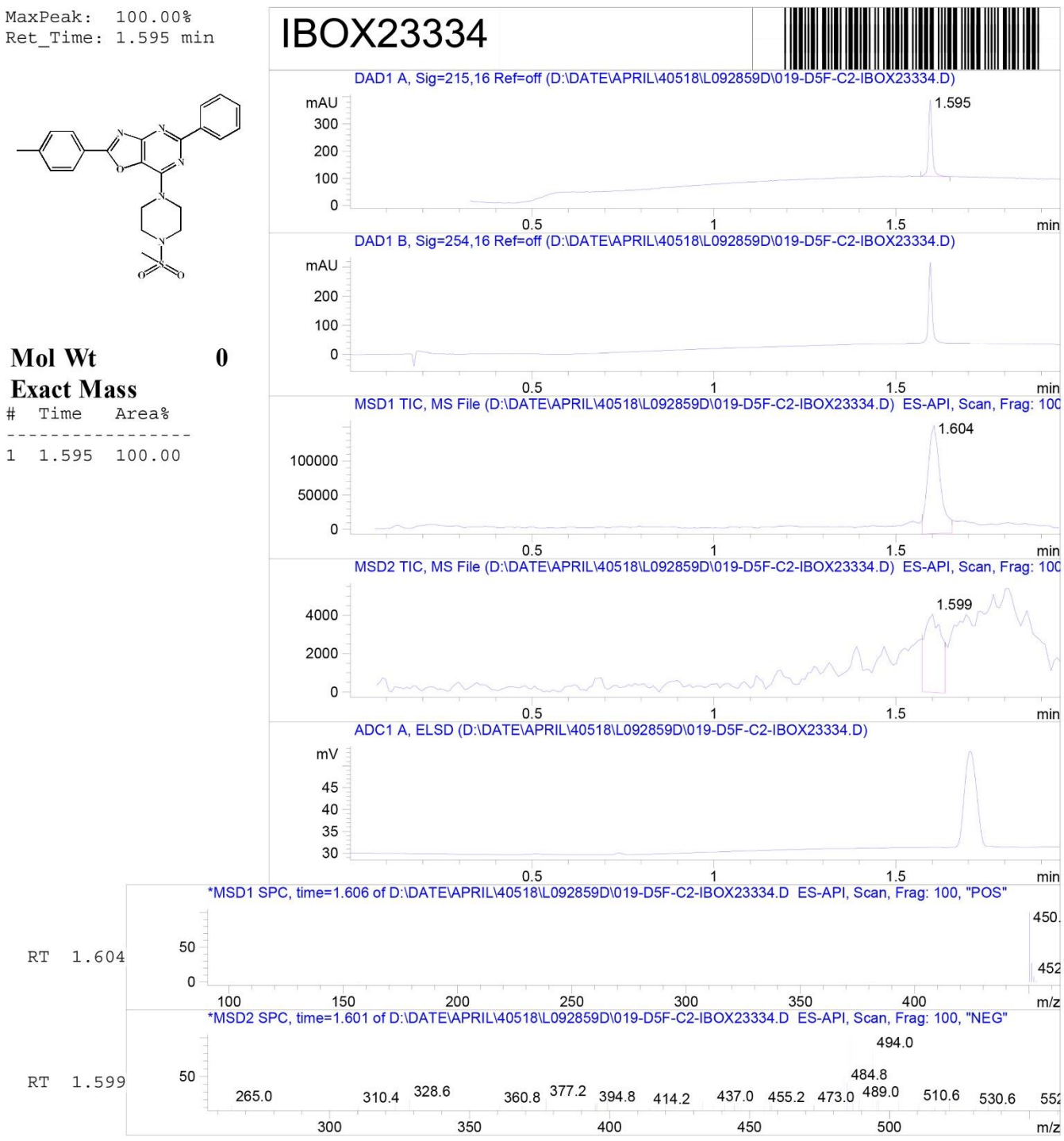

Figure S29. LCMS spectrum of compound (**10**).

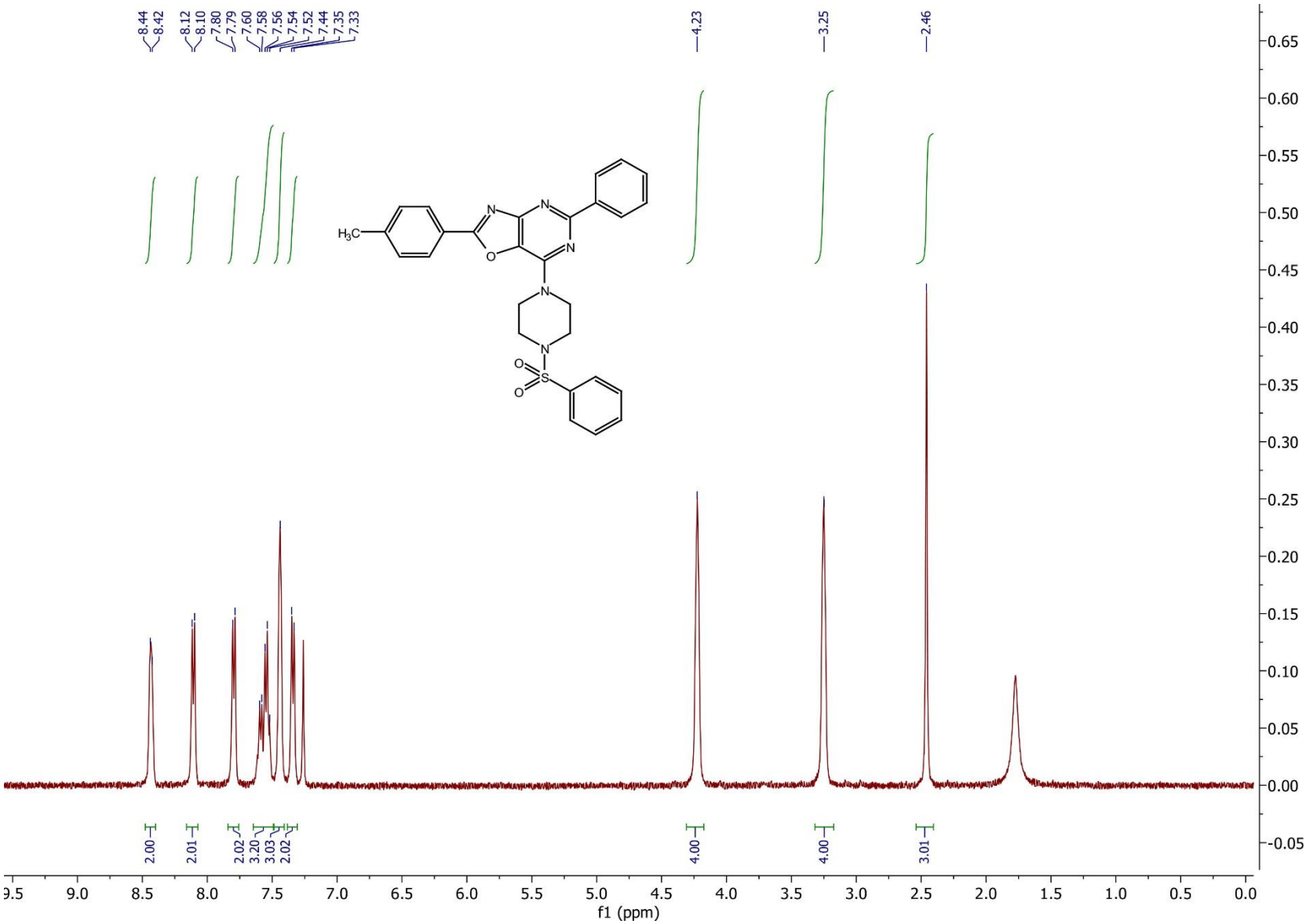

Figure S30. ^{1}H NMR (400 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**11**).

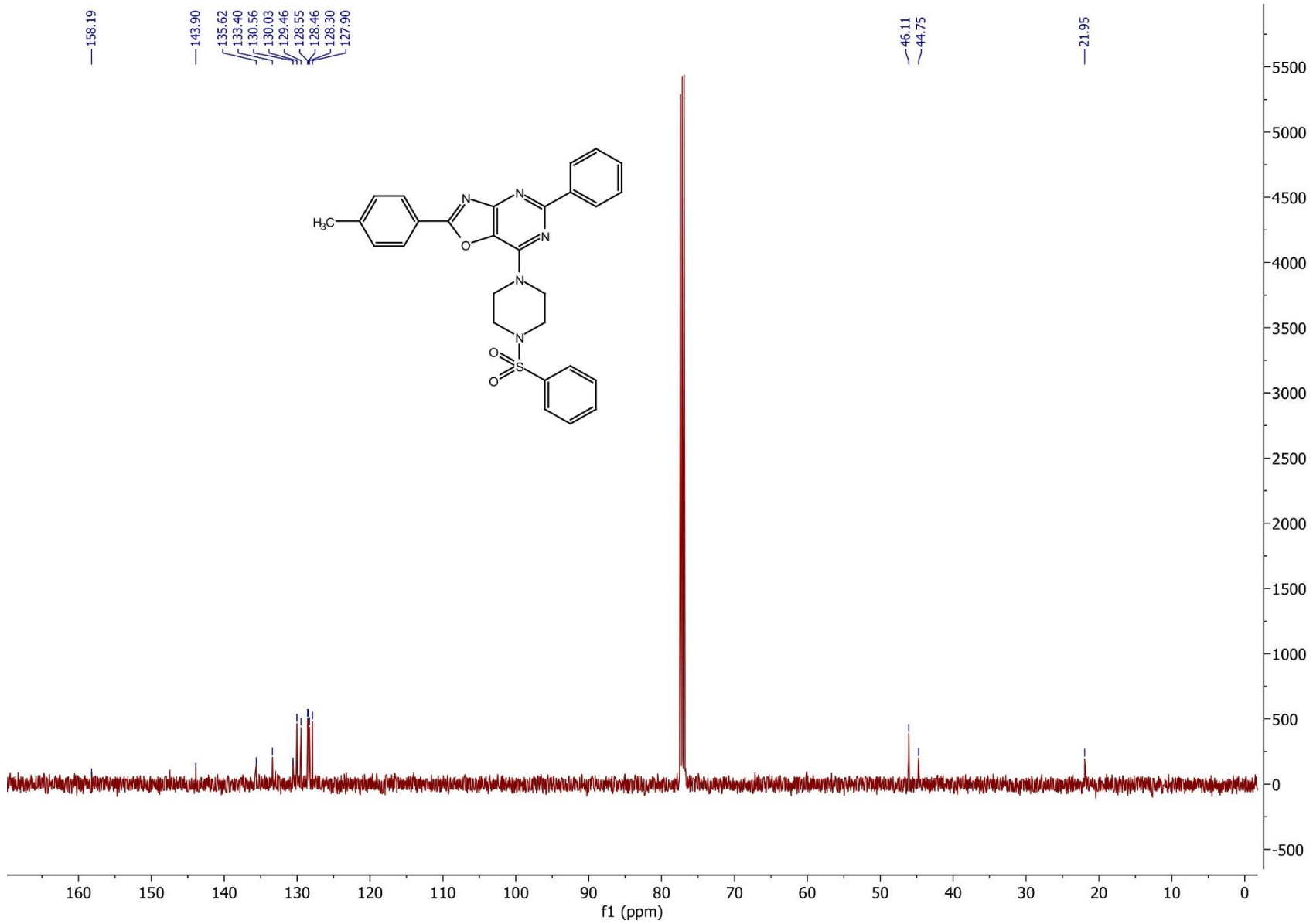

Figure S31. ^{13}C NMR (126 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**11**).

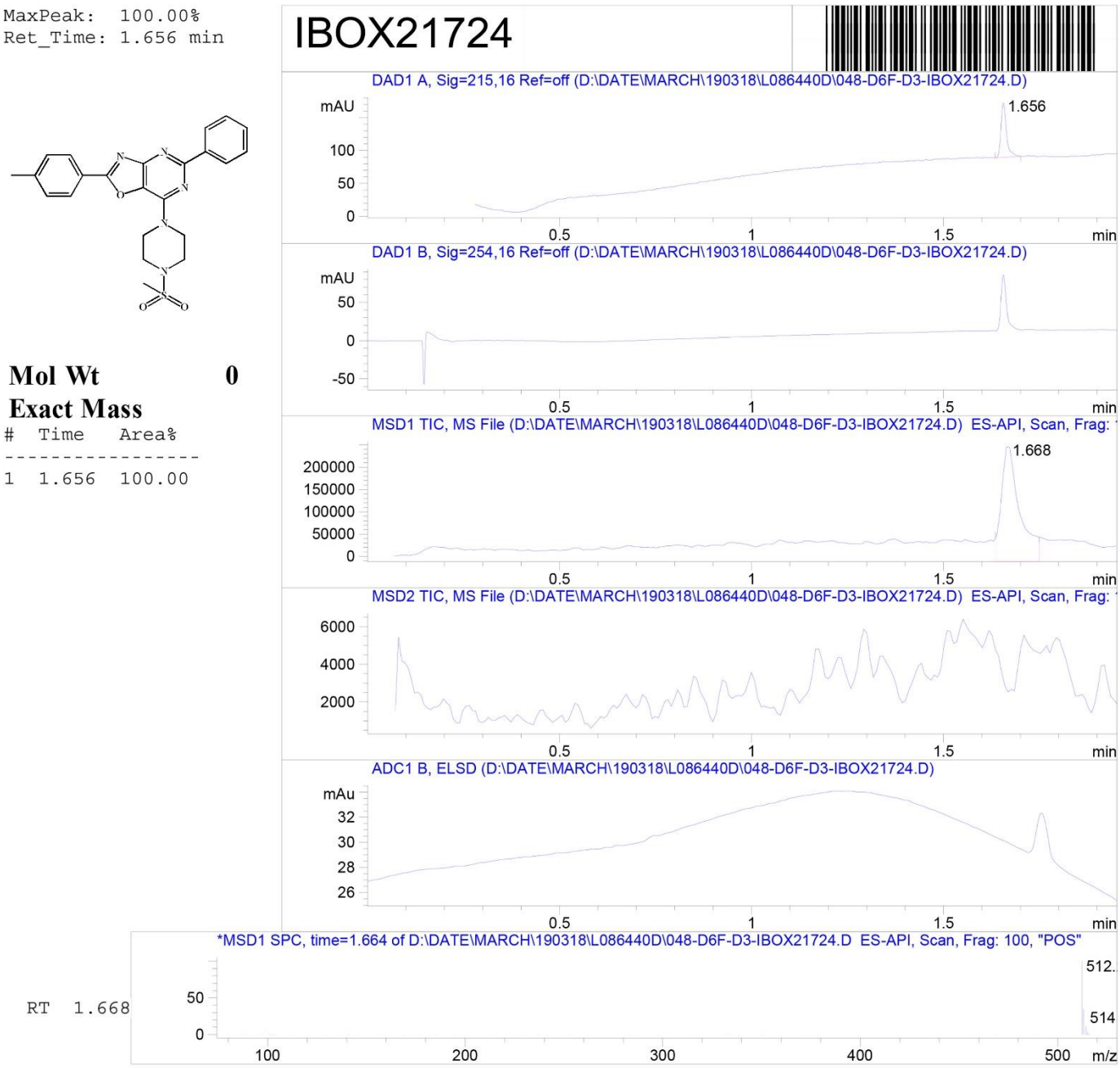

Figure S32. LCMS spectrum of compound (**11**).

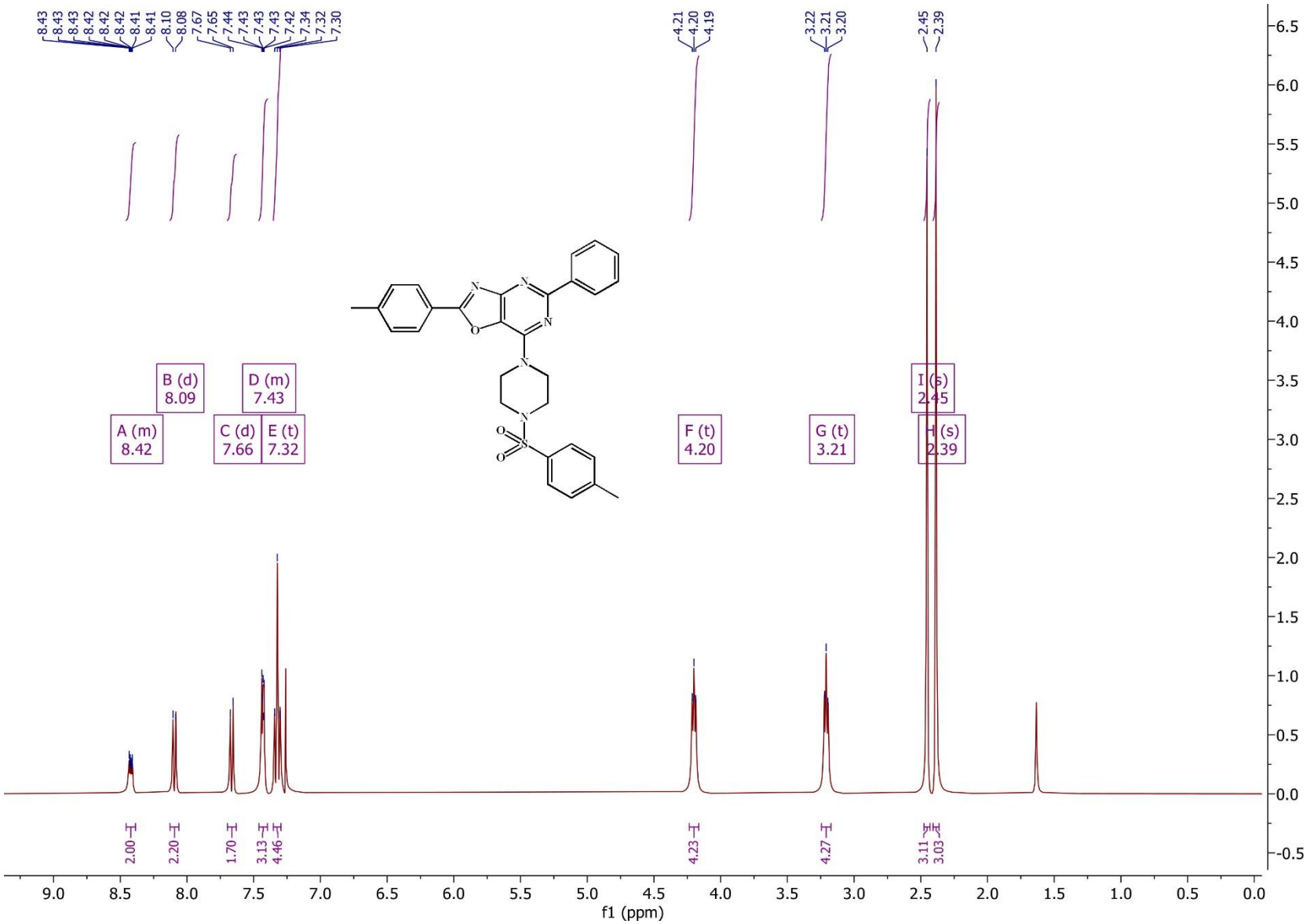

Figure S33. ^{1}H NMR (400 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**12**).

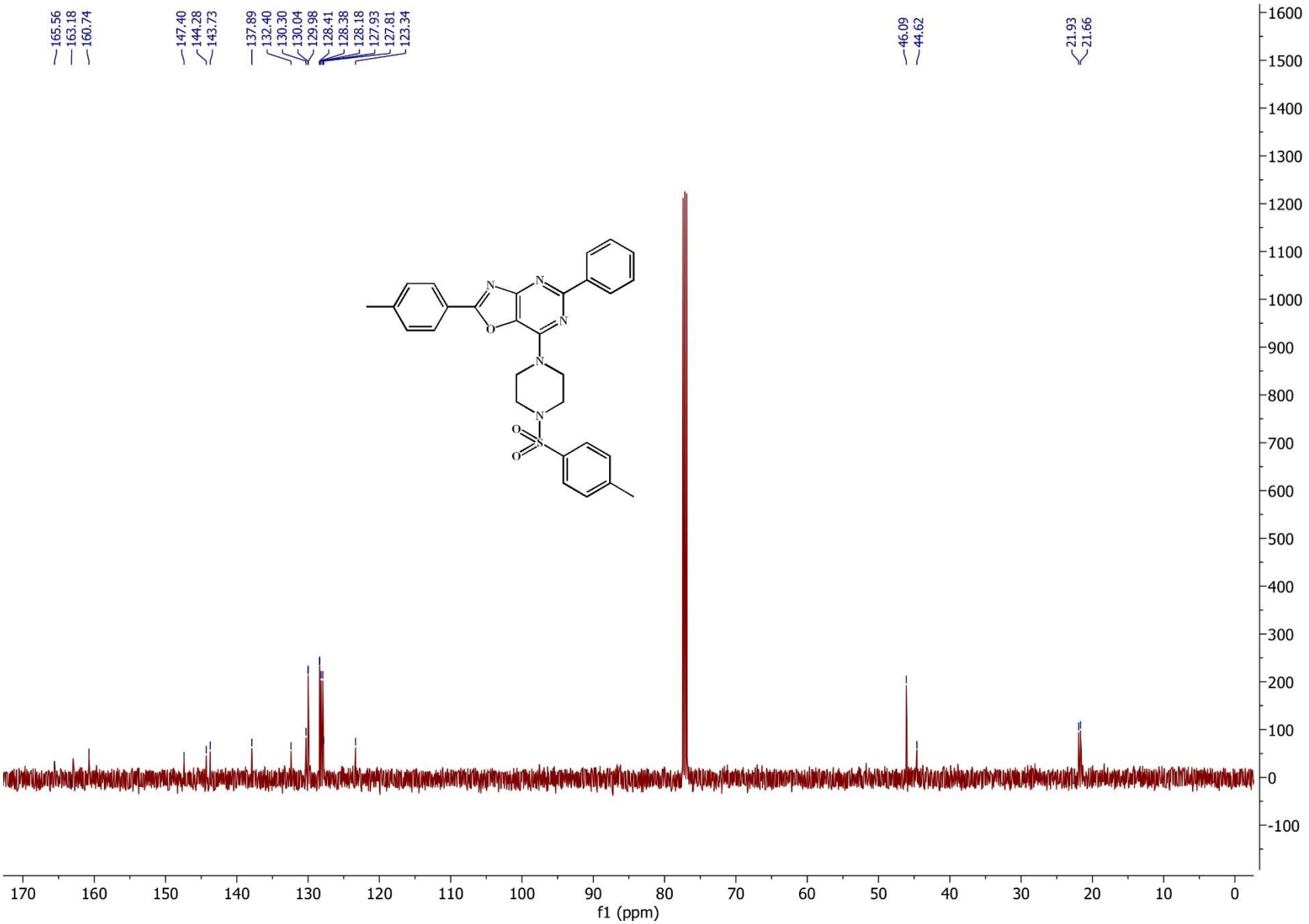

Figure S34. ^{13}C NMR (126 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**12**).

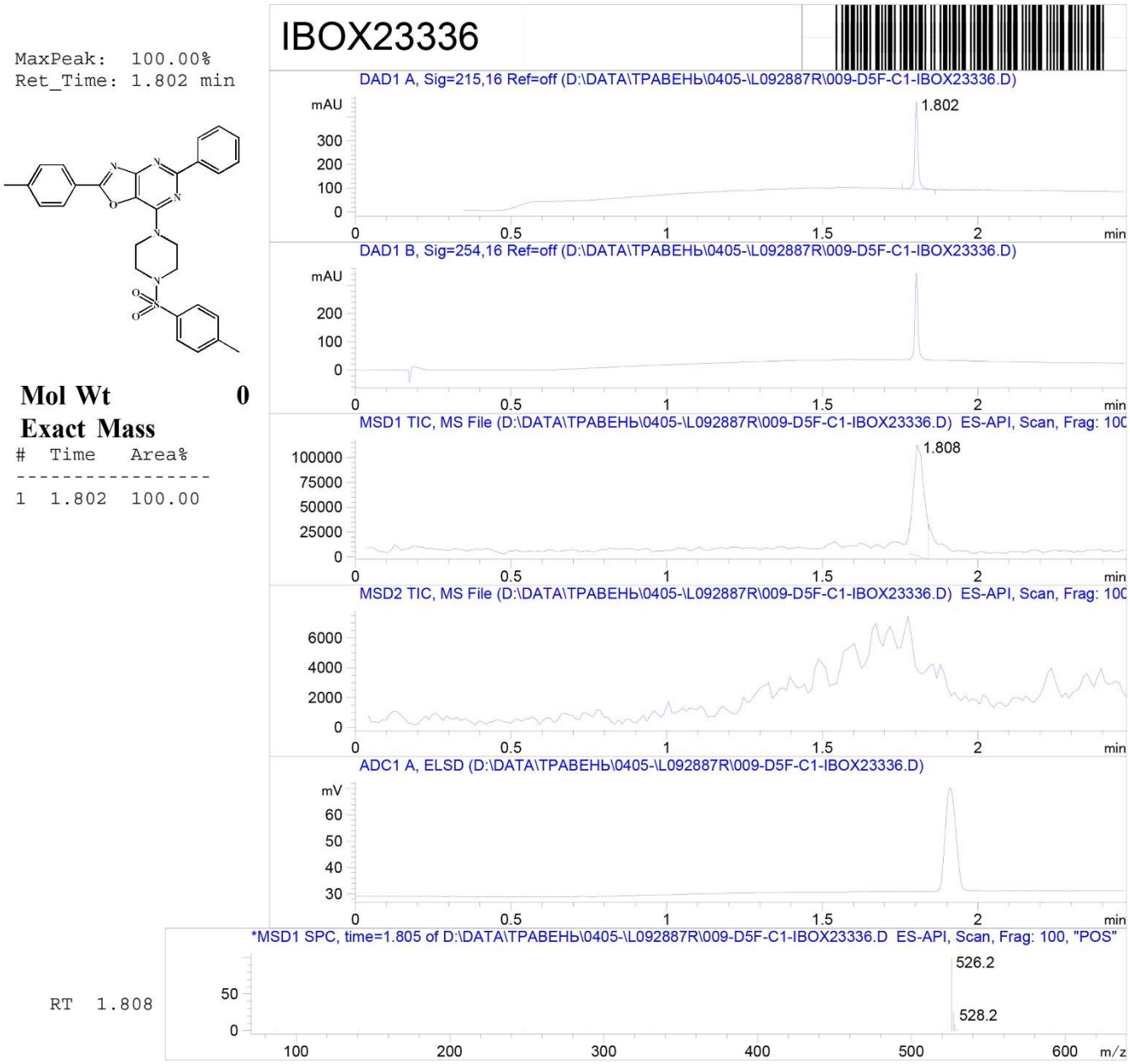

Figure S35. LCMS spectrum of compound (**12**).

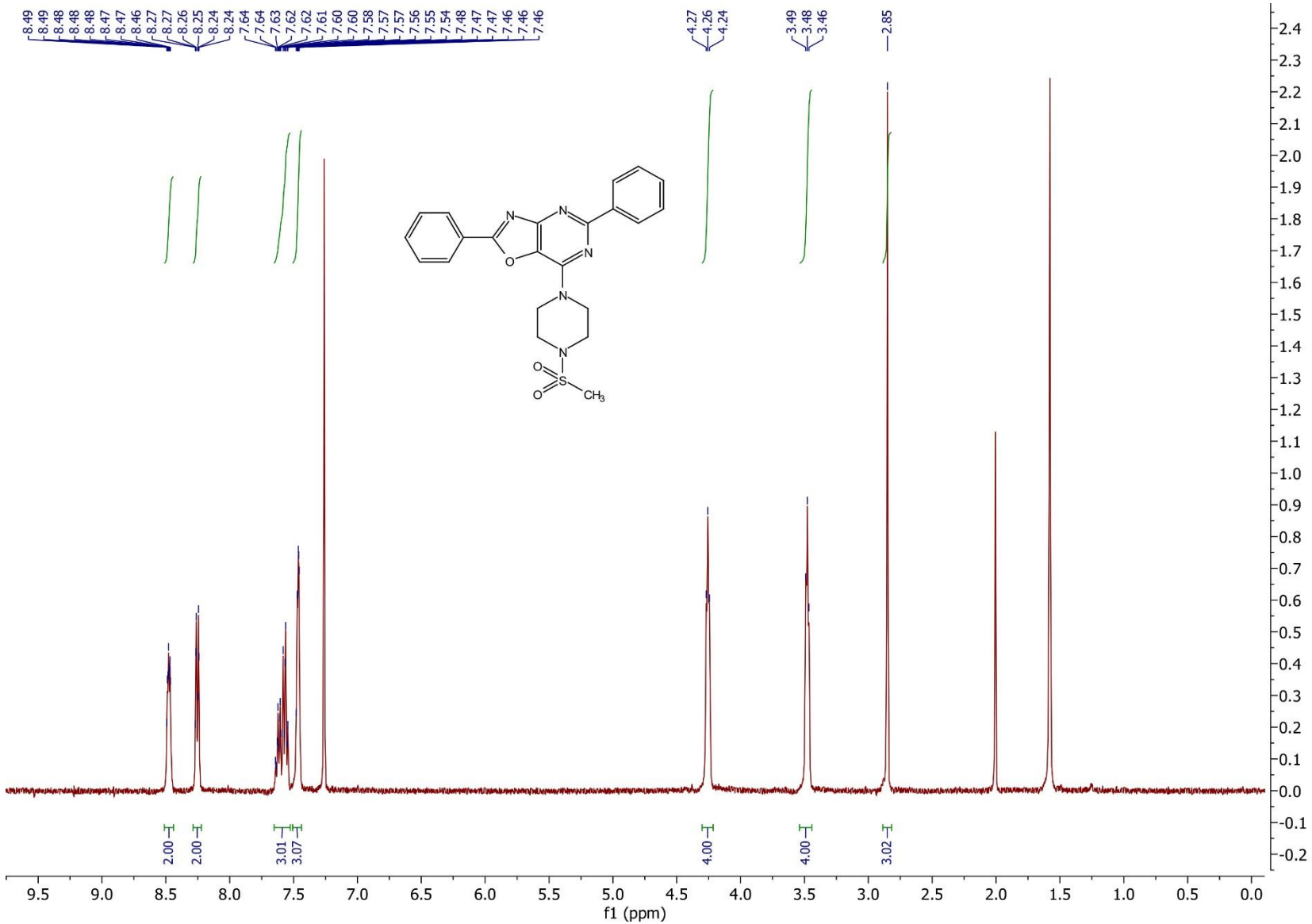

Figure S36. ^{1}H NMR (400 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**13**).

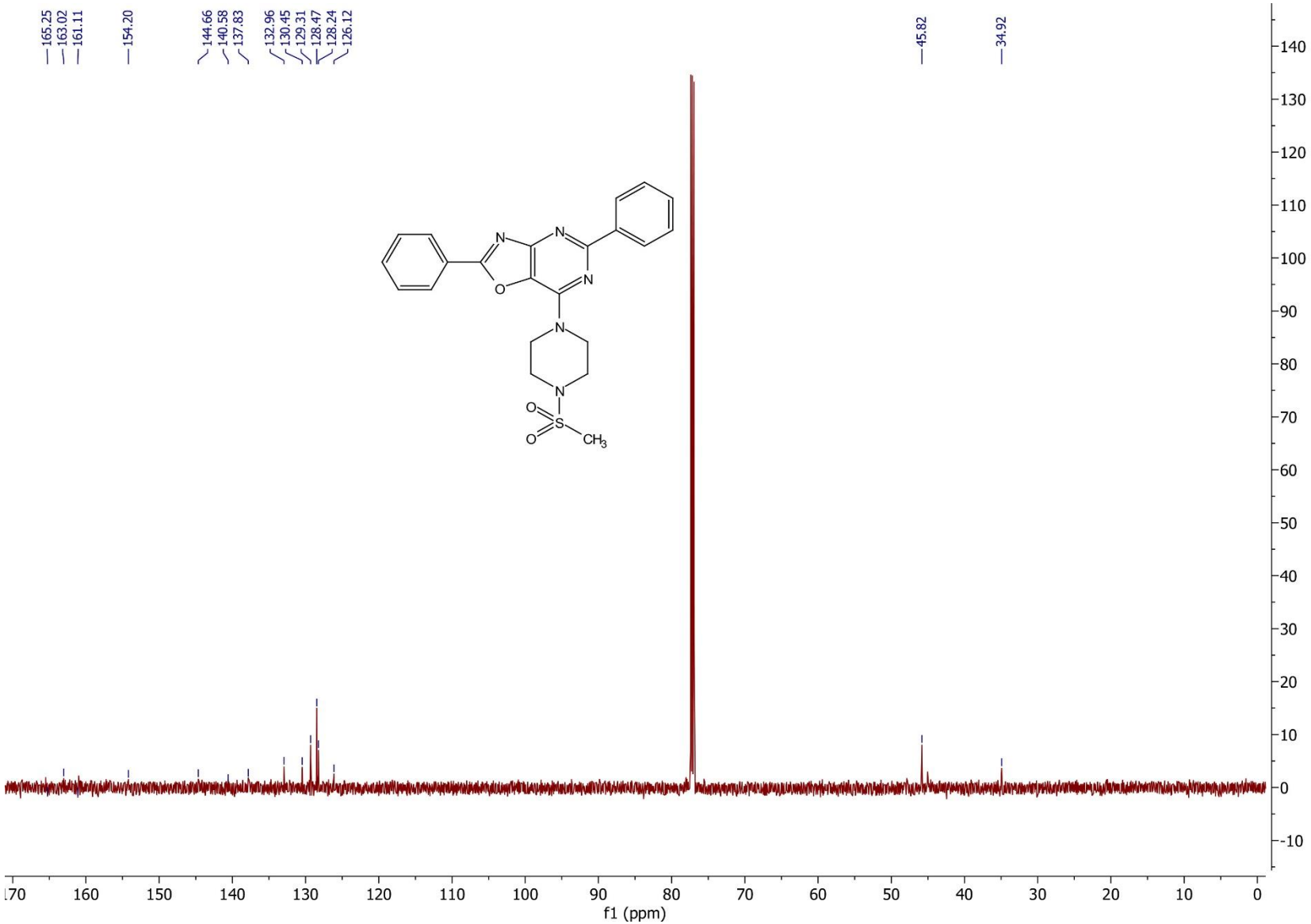

Figure S37. ^{13}C NMR (151 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**13**).

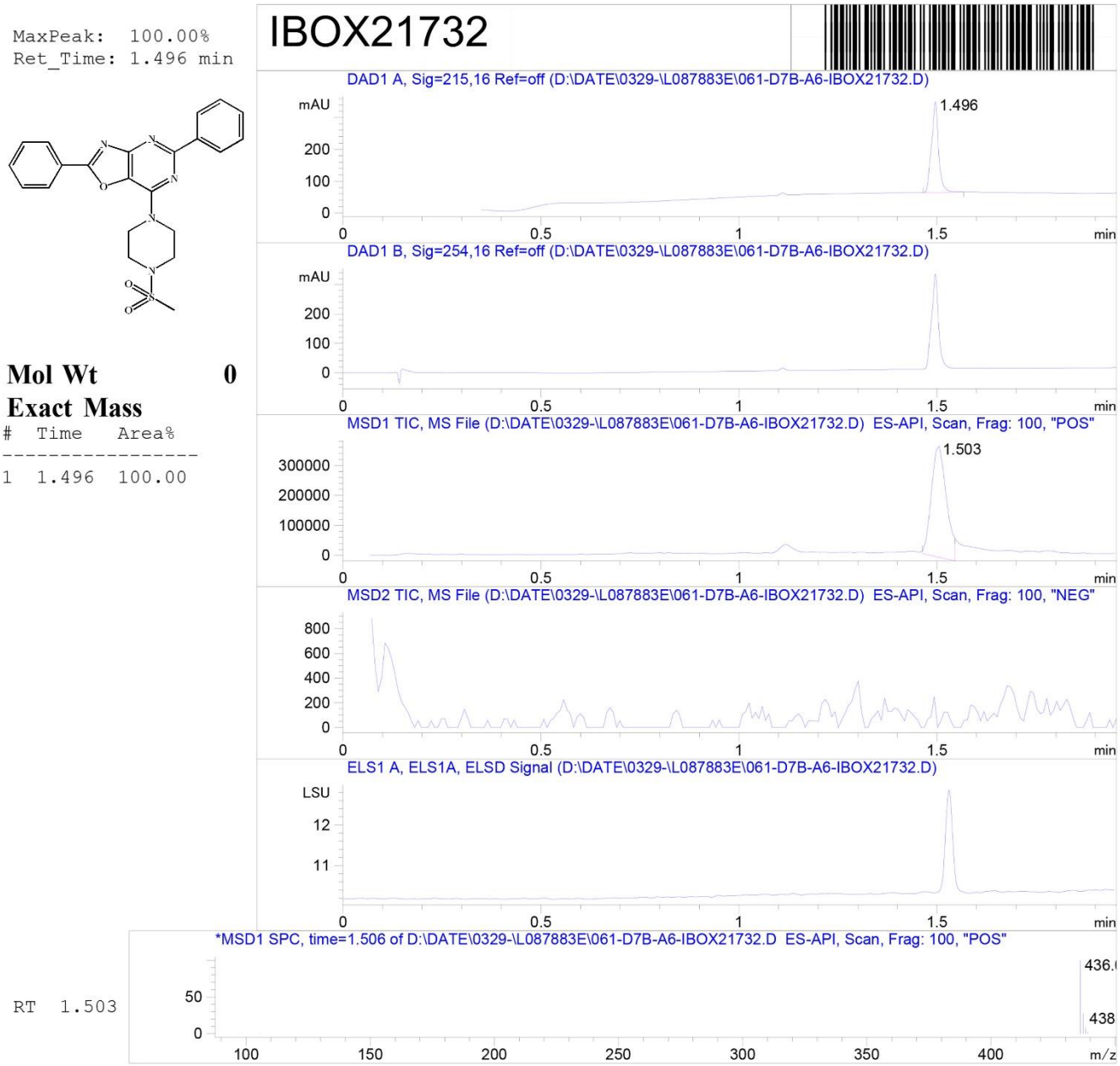

Figure S38. LCMS spectrum of compound (**13**).

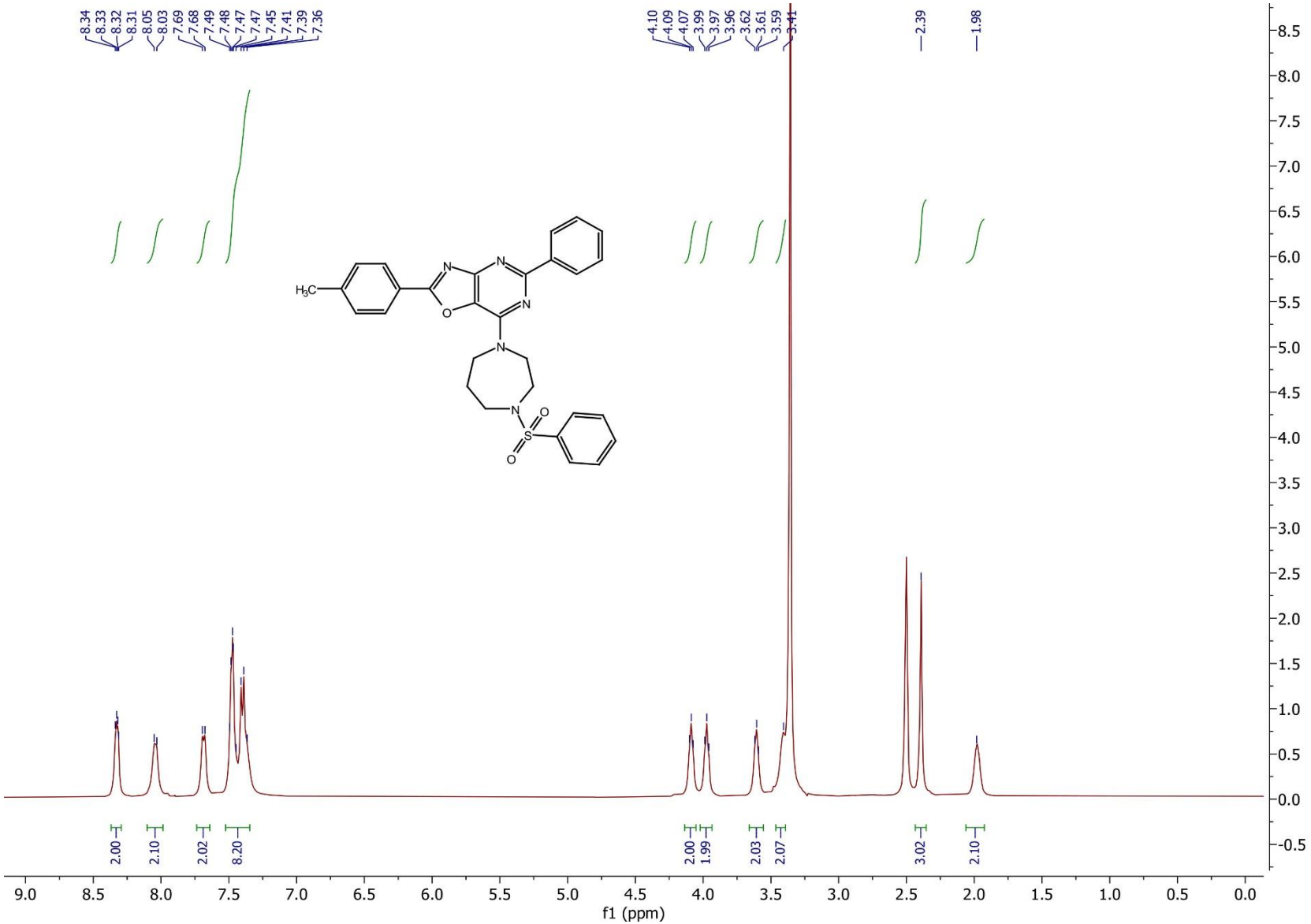

Figure S39. ^{1}H NMR (400 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**14**).

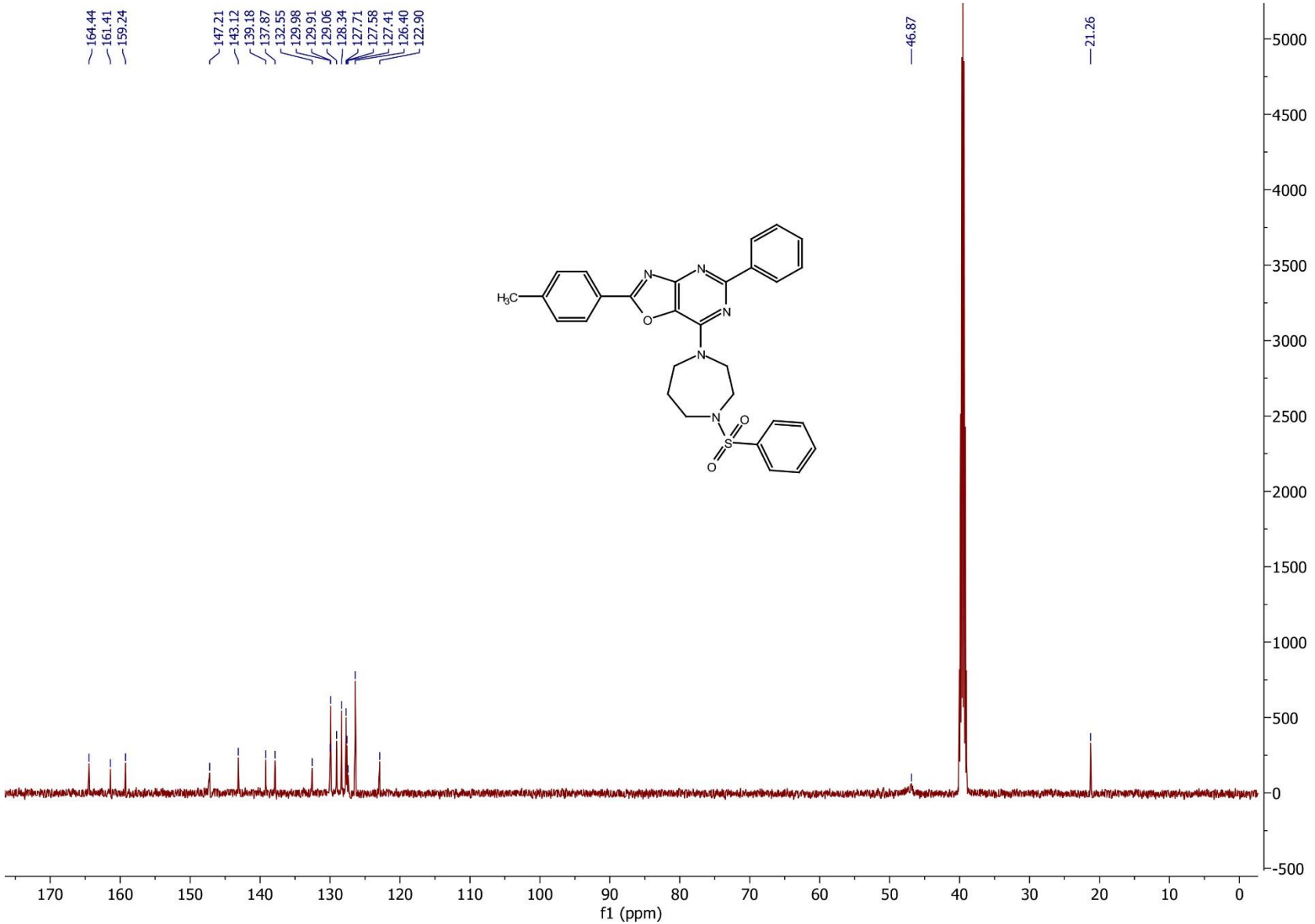

Figure S40. ^{13}C NMR (126 MHz, 296.2 K, DMSO-d_6) spectrum of compound (**14**).

Figure S41. LCMS spectrum of compound (**14**).

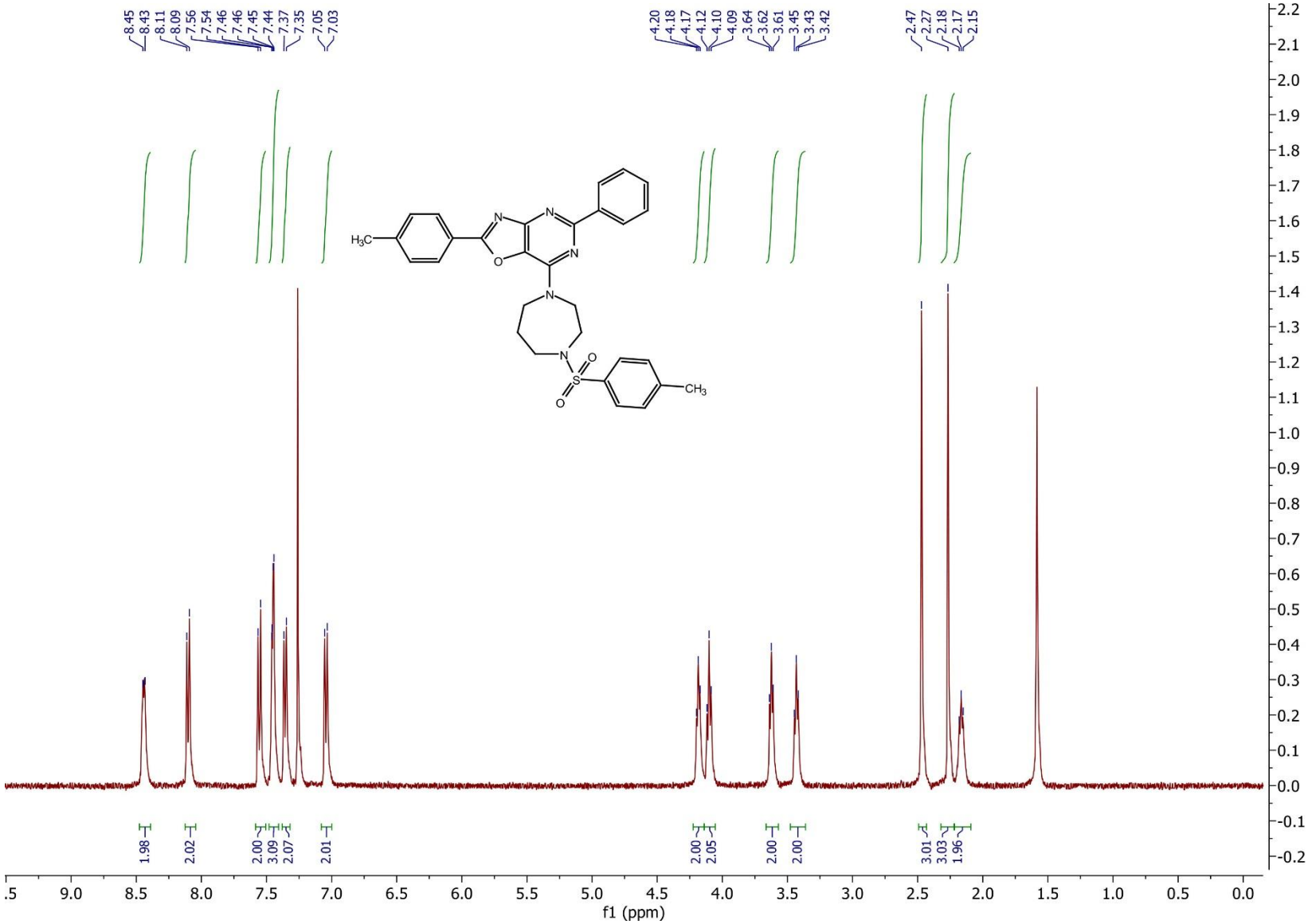

Figure S42. ^{1}H NMR (400 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**15**).

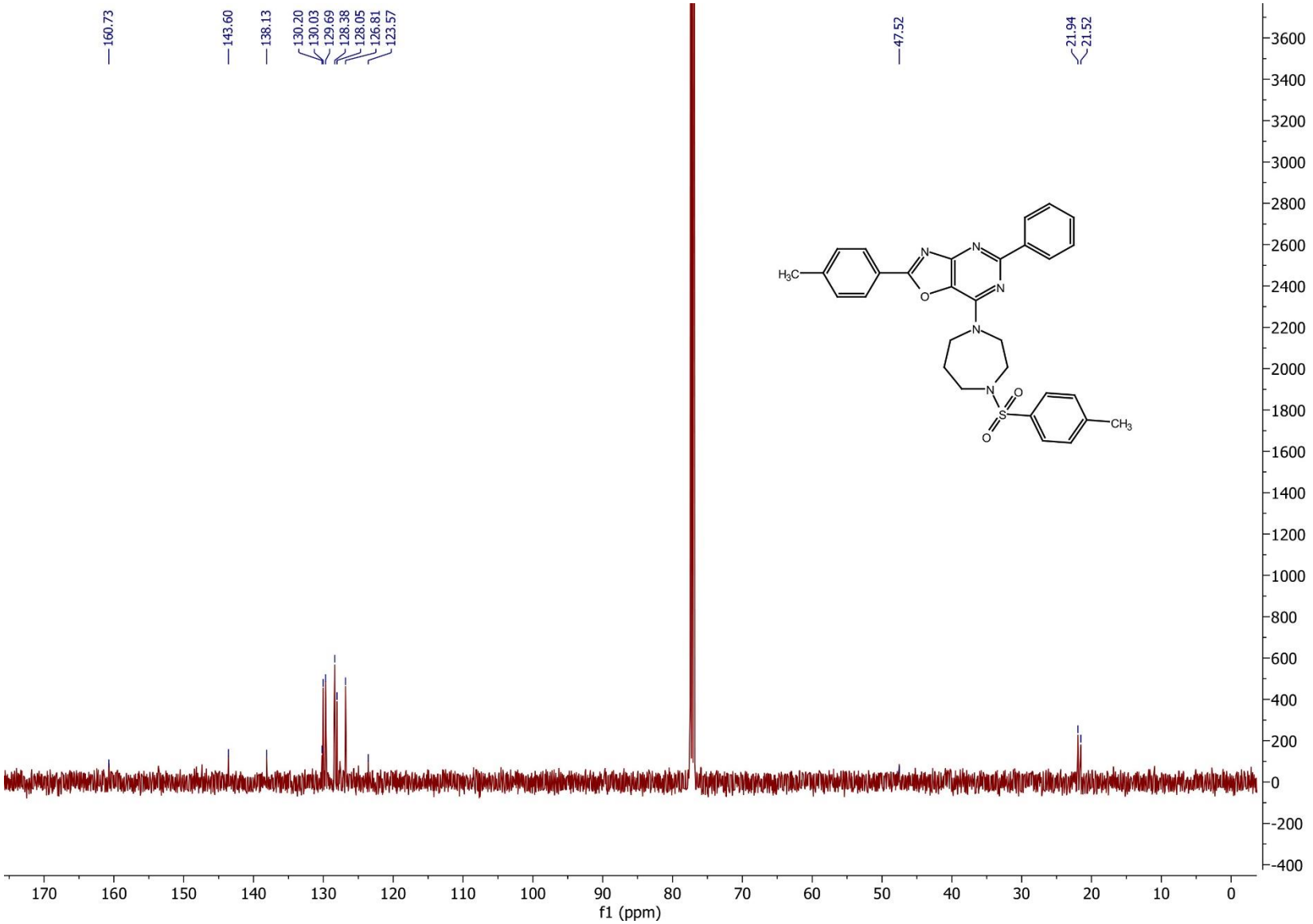

Figure S43. ^{13}C NMR (126 MHz, 296.2 K, $CDCl_3$) spectrum of compound (**15**).

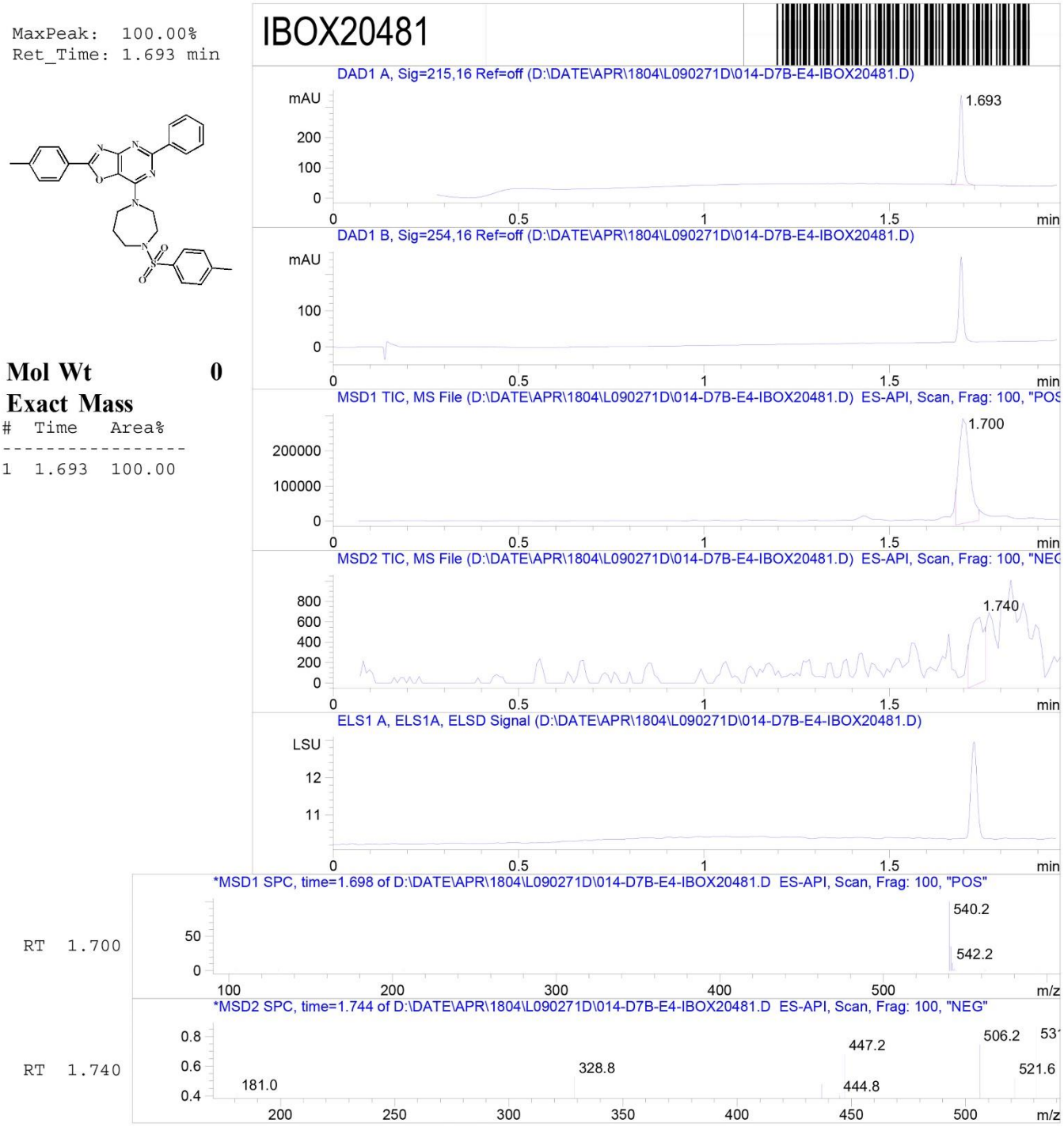

Figure S44. LCMS spectrum of compound (**15**).

Table S1. ADMET properties of oxazolo[4,5-*d*]pyrimidine derivatives predicted by pkCSM online server

Compd	Absorption						Distribution			Metabolism							Excretion		Toxicity									
	Water solubility	Caco2 permeability	Skin Permeability	P-glycoprotein substrate	P-glycoprotein I inhibitor	P-glycoprotein II inhibitor	VDss (human)	Fraction unbound (human)	CNS permeability	CYP2D6 substrate	CYP3A4 substrate	CYP1A2 inhibitior	CYP2C19 inhibitior	CYP2C9 inhibitior	CYP2D6 inhibitior	CYP3A4 inhibitior	Total Clearance	Renal OCT2 substrate	AMES toxicity	Max. tolerated dose (human)	hERG I inhibitor	hERG II inhibitor	Oral Rat Acute Toxicity (LD50)	Oral Rat Chronic Toxicity (LOAEL)	Hepatotoxicity	Skin Sensitisation	*T.Pyriformis* toxicity	Minnow toxicity
1	-3.793	0.991	-2.735	Yes	Yes	Yes	0.135	0.245	-1.586	No	Yes	Yes	No	Yes	No	No	0.404	No	No	0.693	No	Yes	3.098	0.793	Yes	No	0.285	-1.45
2	-3.382	1.299	-2.735	Yes	Yes	Yes	-0.237	0.329	-1.819	No	Yes	Yes	Yes	Yes	No	Yes	0.759	No	No	0.675	No	Yes	2.739	0.068	Yes	No	0.285	-1.626
3	-4.085	1	-2.735	Yes	Yes	Yes	0.642	0.154	-1.762	No	Yes	No	Yes	No	No	Yes	0.718	No	No	0.711	No	Yes	3.401	0.034	Yes	No	0.285	-2.273
4	-4.08	0.976	-2.735	Yes	Yes	Yes	0.666	0.13	-1.928	No	Yes	No	Yes	No	No	Yes	0.88	No	No	0.715	No	Yes	3.371	0.191	Yes	No	0.285	-1.61
5	-3.814	0.807	-2.727	No	Yes	Yes	0.432	0.205	-2.131	No	Yes	Yes	Yes	Yes	No	Yes	0.611	No	No	0.468	No	Yes	2.59	1.125	Yes	No	0.289	0.22
6	-3.629	1.121	-2.731	No	Yes	Yes	0.447	0.232	-1.99	No	Yes	Yes	Yes	Yes	No	Yes	0.668	No	No	0.484	No	Yes	2.683	1.179	Yes	No	0.288	0.711
7	-3.939	1.295	-2.734	No	Yes	Yes	0.733	0.229	-1.783	No	Yes	Yes	Yes	Yes	No	Yes	0.699	No	No	0.445	No	Yes	2.765	1.153	Yes	No	0.286	-0.501
8	-3.777	1.135	-2.735	Yes	Yes	Yes	1.097	0.248	-1.932	No	Yes	No	No	Yes	No	Yes	0.594	No	No	0.66	No	Yes	2.914	1.048	Yes	No	0.285	-0.436
9	-3.846	1.202	-2.735	No	Yes	Yes	1.182	0.25	-1.845	No	Yes	No	No	Yes	No	Yes	0.518	No	No	0.662	No	Yes	2.868	1.084	Yes	No	0.285	-0.298
10	-3.293	0.995	-2.734	No	Yes	Yes	0.415	0.169	-2.389	No	Yes	Yes	Yes	Yes	No	Yes	1.02	No	No	0.458	No	Yes	2.54	0.825	Yes	No	0.286	-2.013
11	-3.23	1.192	-2.735	No	Yes	Yes	0.167	0.261	-2.083	No	Yes	No	Yes	Yes	No	Yes	1.096	No	No	0.785	No	Yes	2.855	0.886	Yes	No	0.285	-6.516
12	-3.252	1.111	-2.735	No	Yes	Yes	0.209	0.267	-2.01	No	Yes	No	Yes	Yes	No	No	1.101	No	No	0.786	No	Yes	2.897	0.942	Yes	No	0.285	-6.497
13	-3.632	1.095	-2.735	No	Yes	Yes	-0.042	0.258	-2.584	No	Yes	Yes	No	No	No	No	1.016	No	No	0.778	No	Yes	2.999	0.508	Yes	No	0.285	-3.759
14	-3.239	1.191	-2.735	No	Yes	Yes	0.193	0.262	-1.991	No	Yes	No	Yes	Yes	No	Yes	1.104	No	No	0.787	No	Yes	2.86	0.907	Yes	No	0.285	-6.633
15	-3.261	1.11	-2.735	No	Yes	Yes	0.236	0.268	-1.919	No	Yes	No	Yes	Yes	No	No	1.108	No	No	0.789	No	Yes	2.903	0.963	Yes	No	0.285	-6.615