Supplementary information

Design, synthesis, and biological evaluation of 1,2,4-oxadiazole based derivatives as multitarget Anti-Alzheimer agents

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1.Copy of NMR

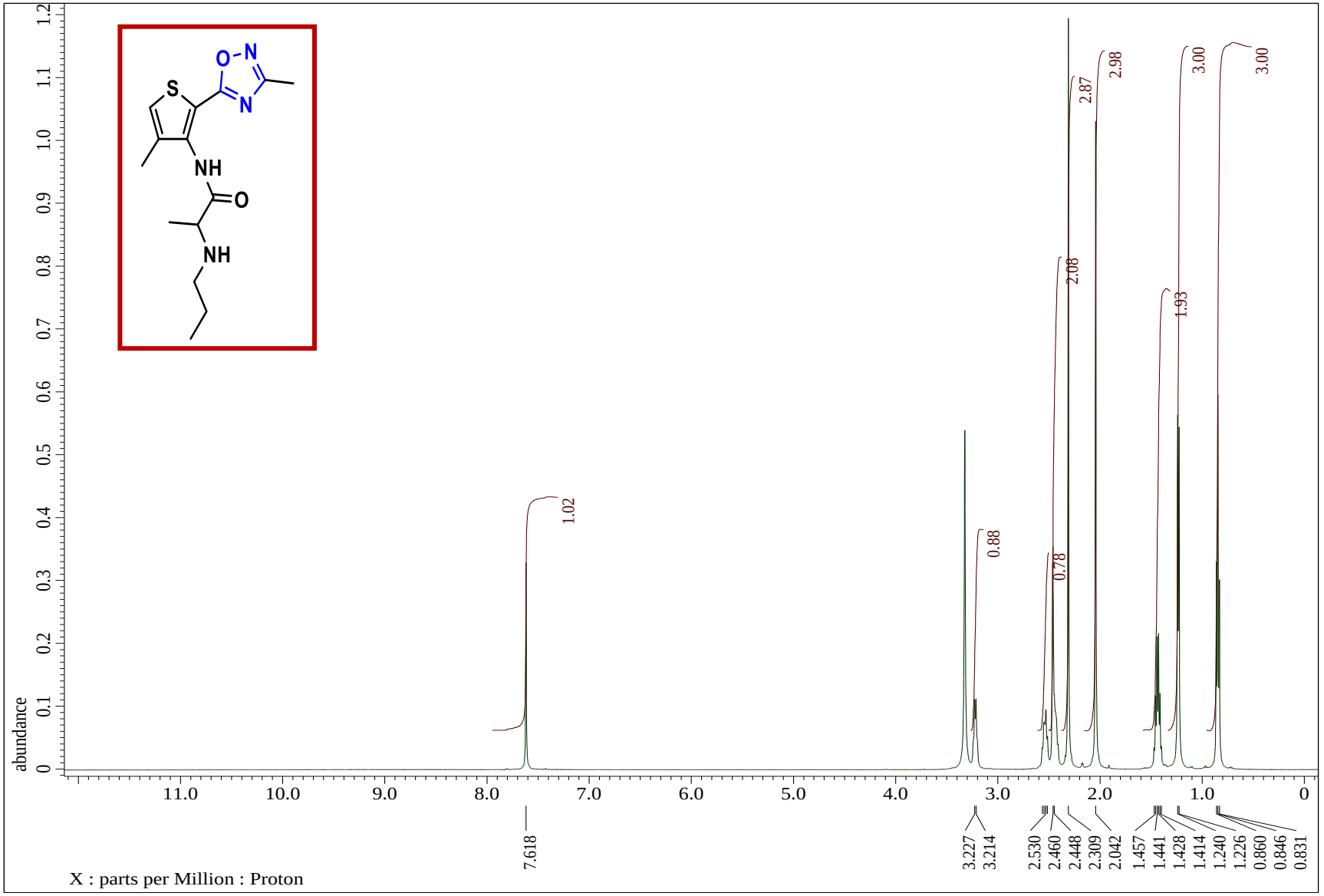

Figure 1. ^{1}H NMR of **2a** (DMSO-d6)

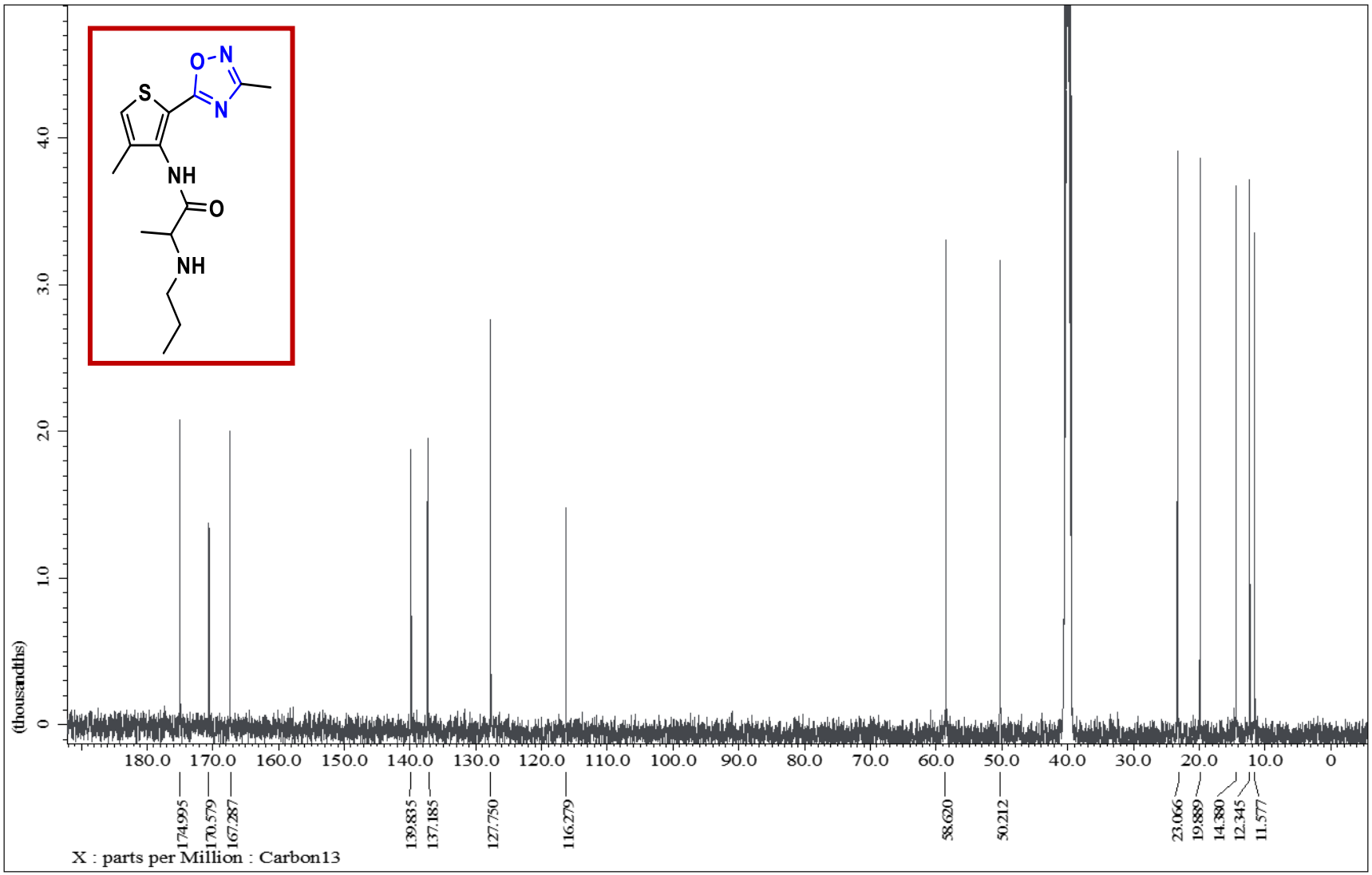

Figure 2. ^{13}C NMR of **2a** (DMSO-d6).

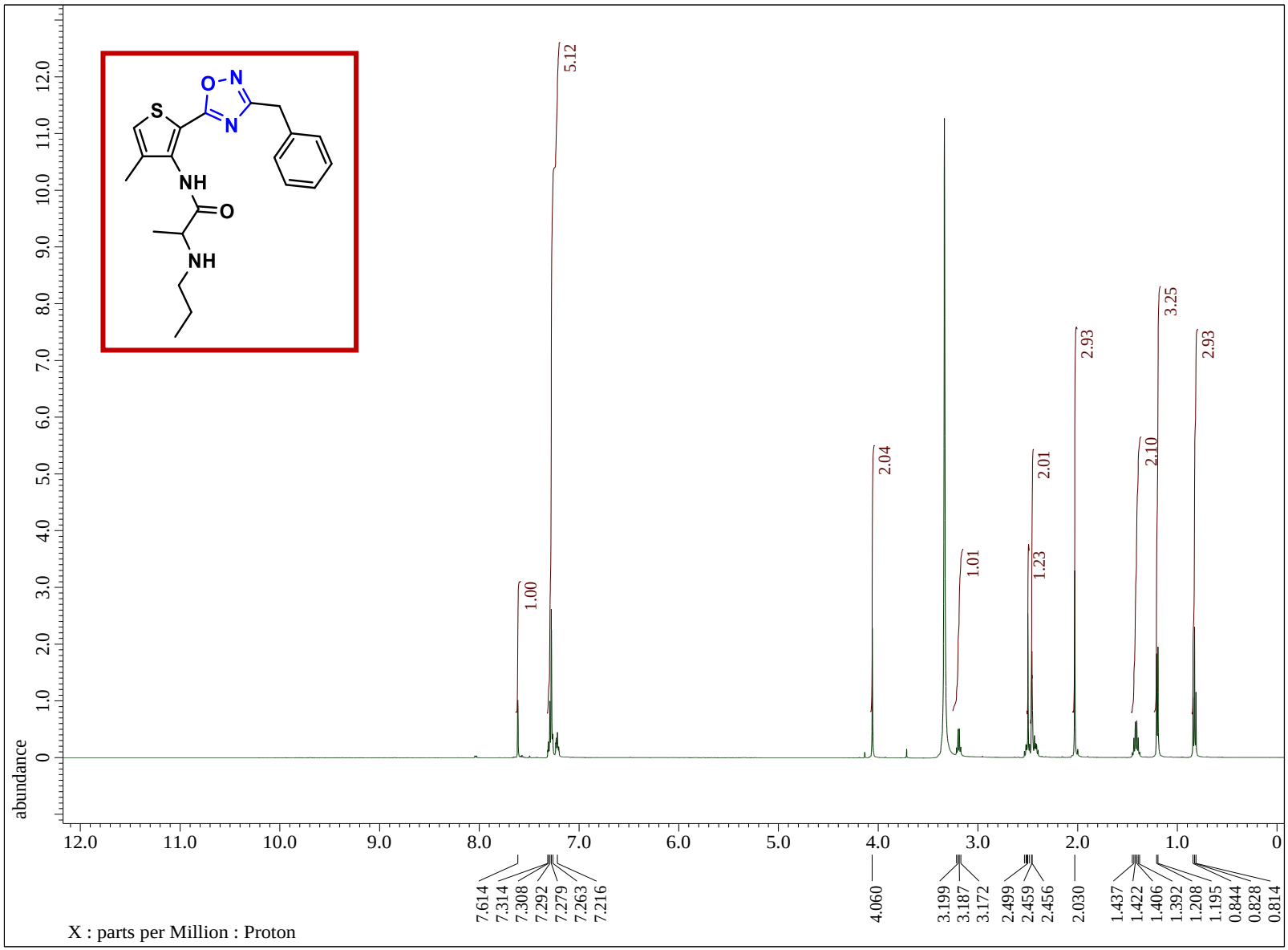

Figure 3. ^{1}H NMR of **2b** (DMSO-d6)

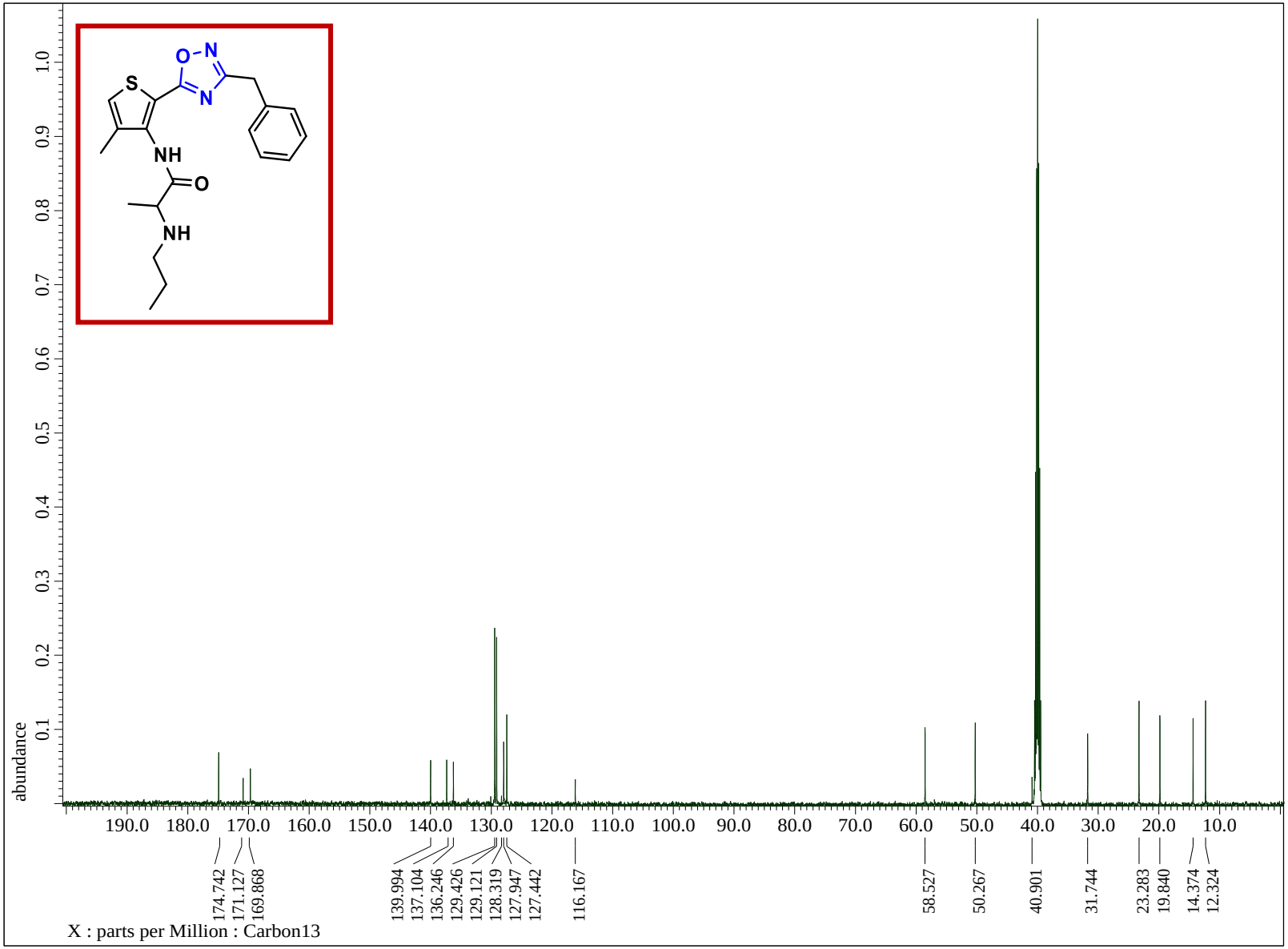

Figure 4. ^{13}C NMR of **2b** (DMSO-d6)

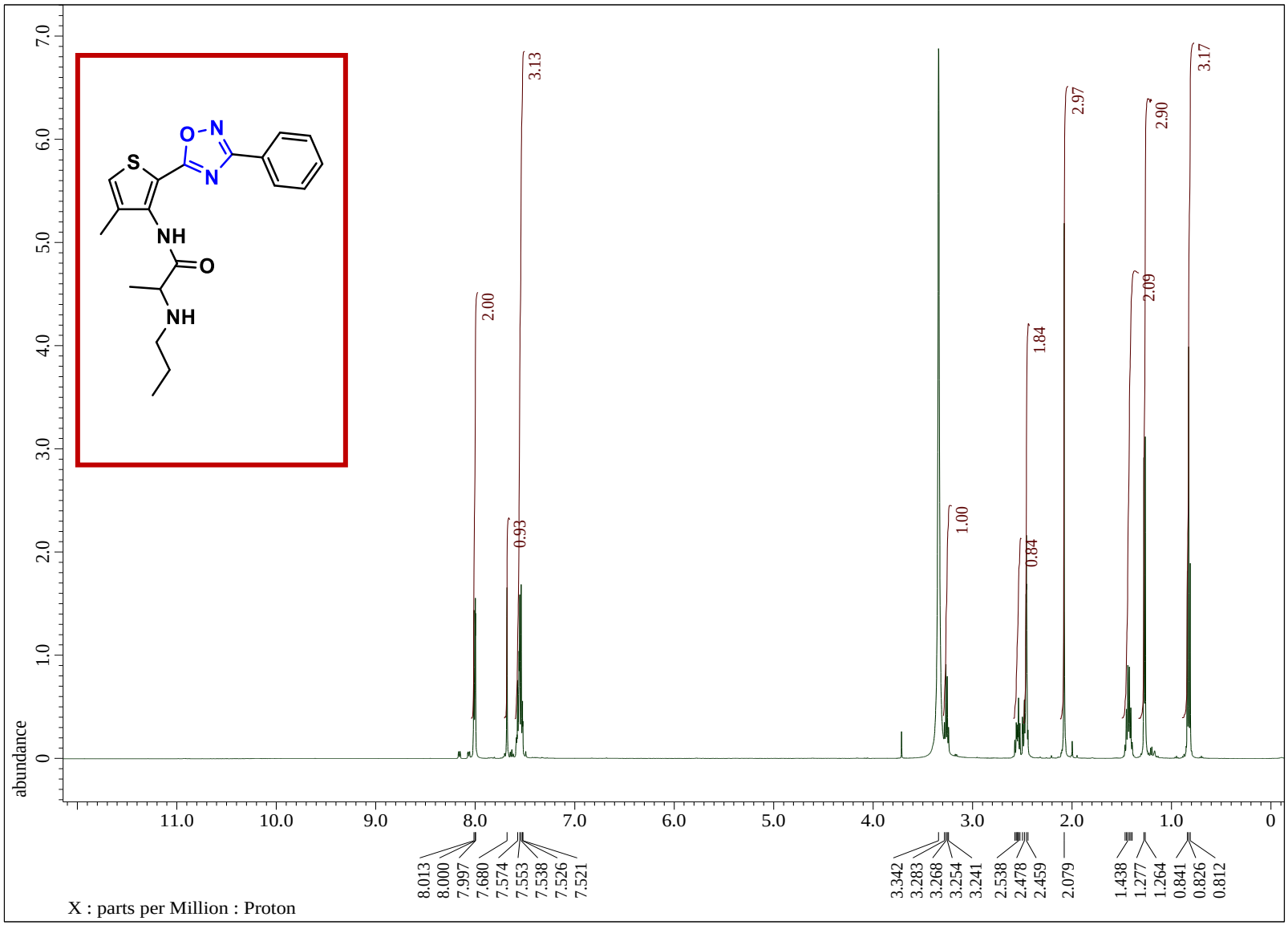

Figure 5. ^{1}H NMR of **2c** (DMSO-d6)

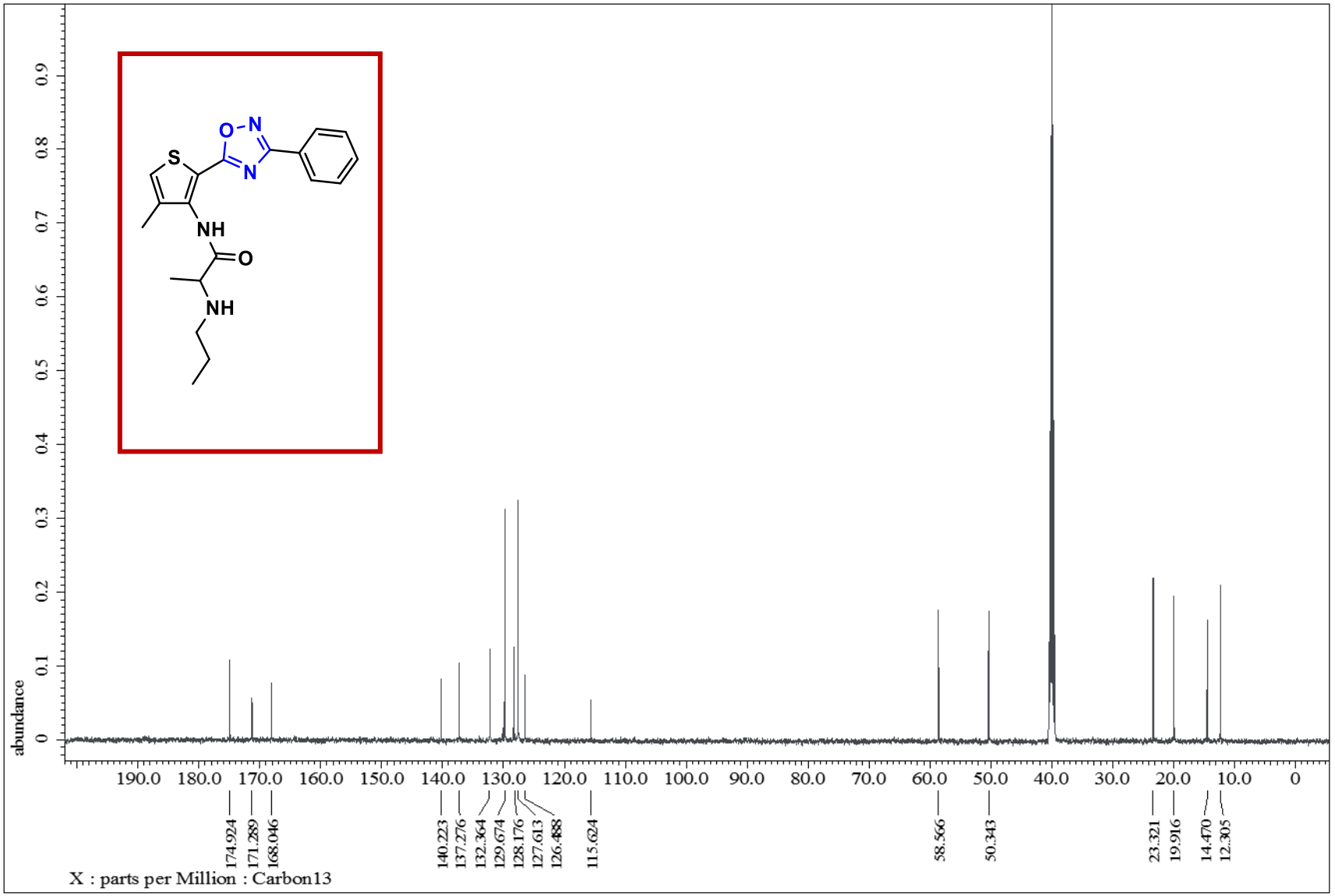

Figure 6. ^{13}C NMR of **2c** (DMSO-d6)

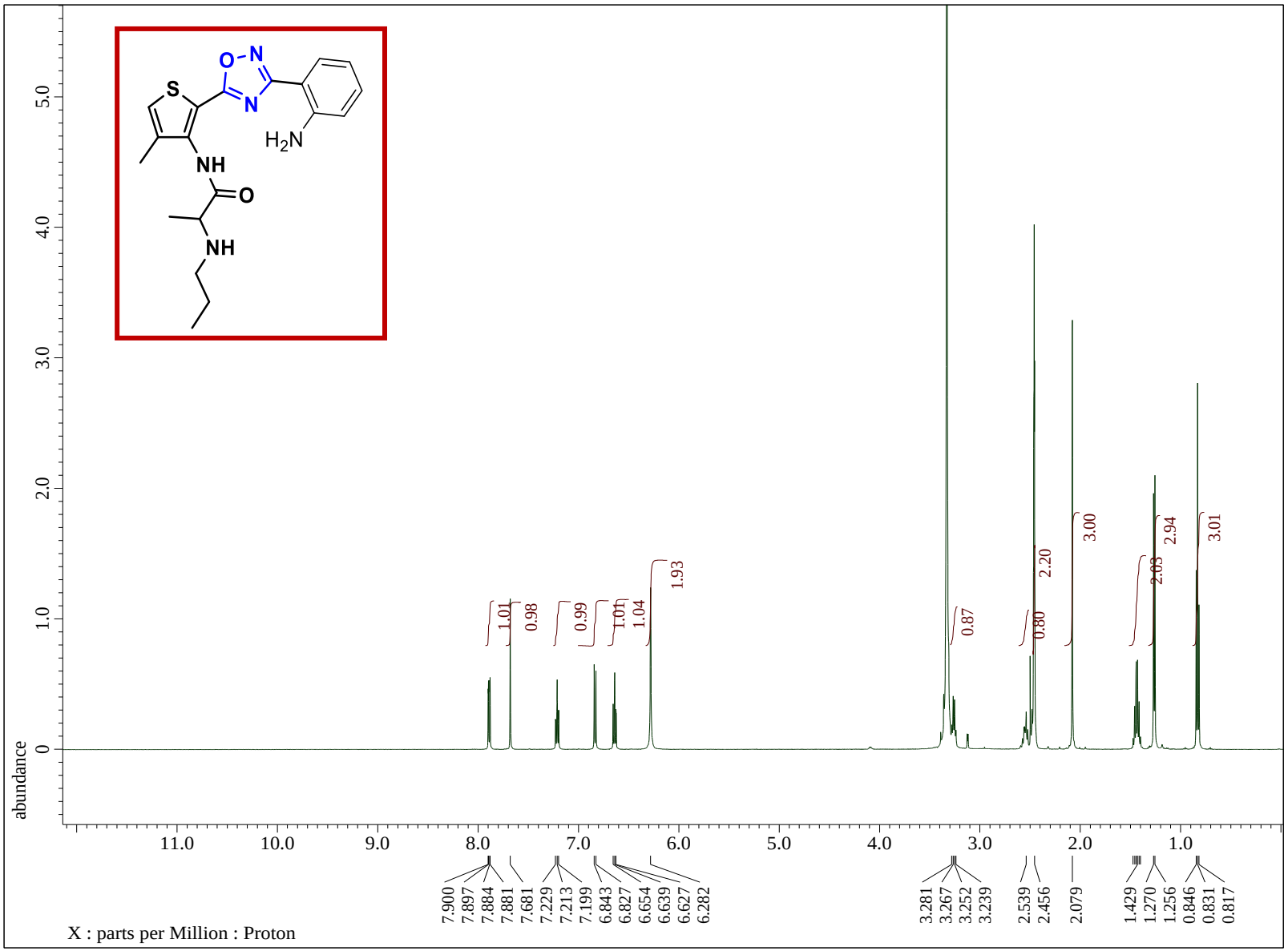

Figure 7. ^{1}H NMR of **2d** (DMSO-d6)

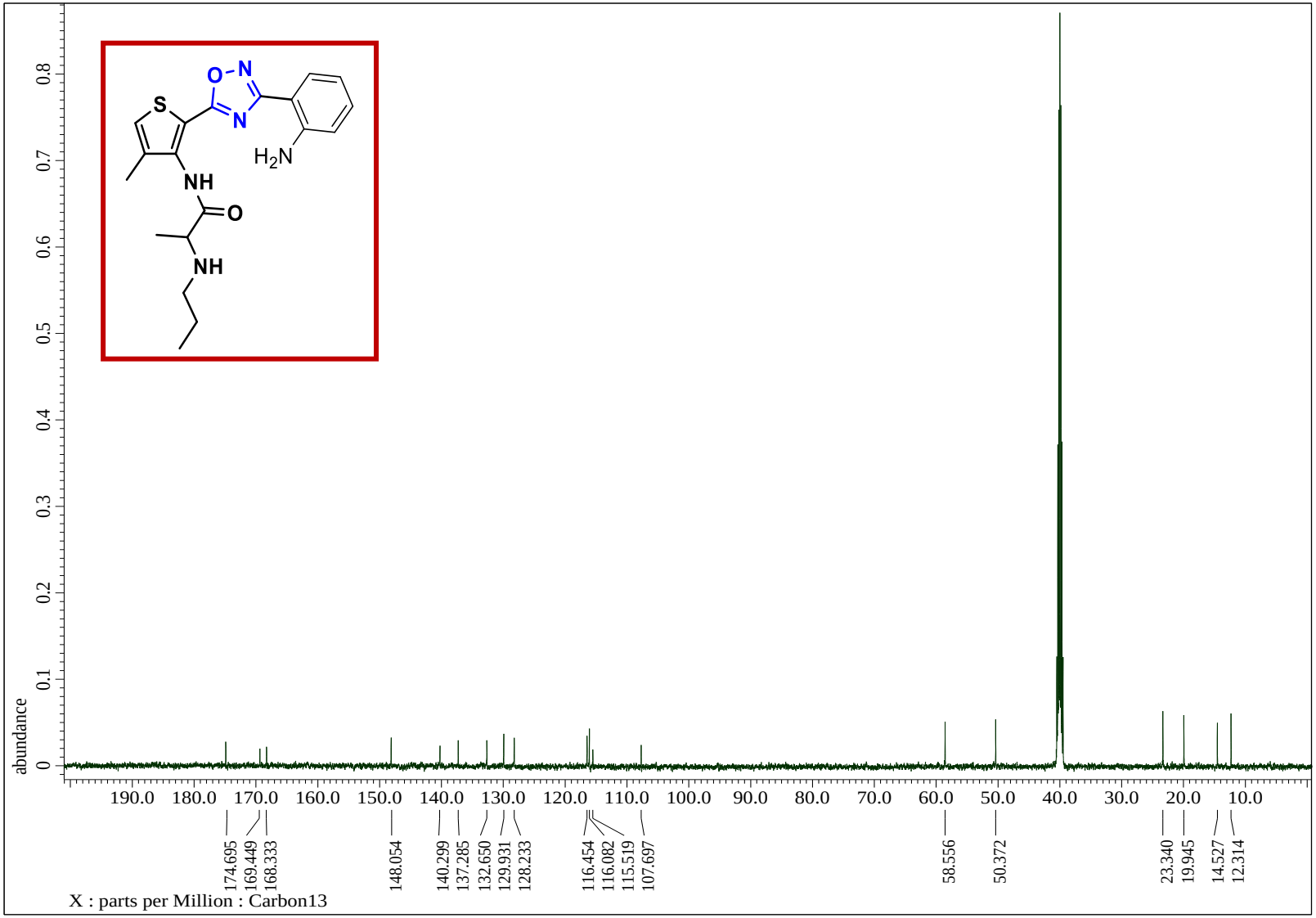

Figure 8. ^{13}C NMR of **2d** (DMSO-d6)

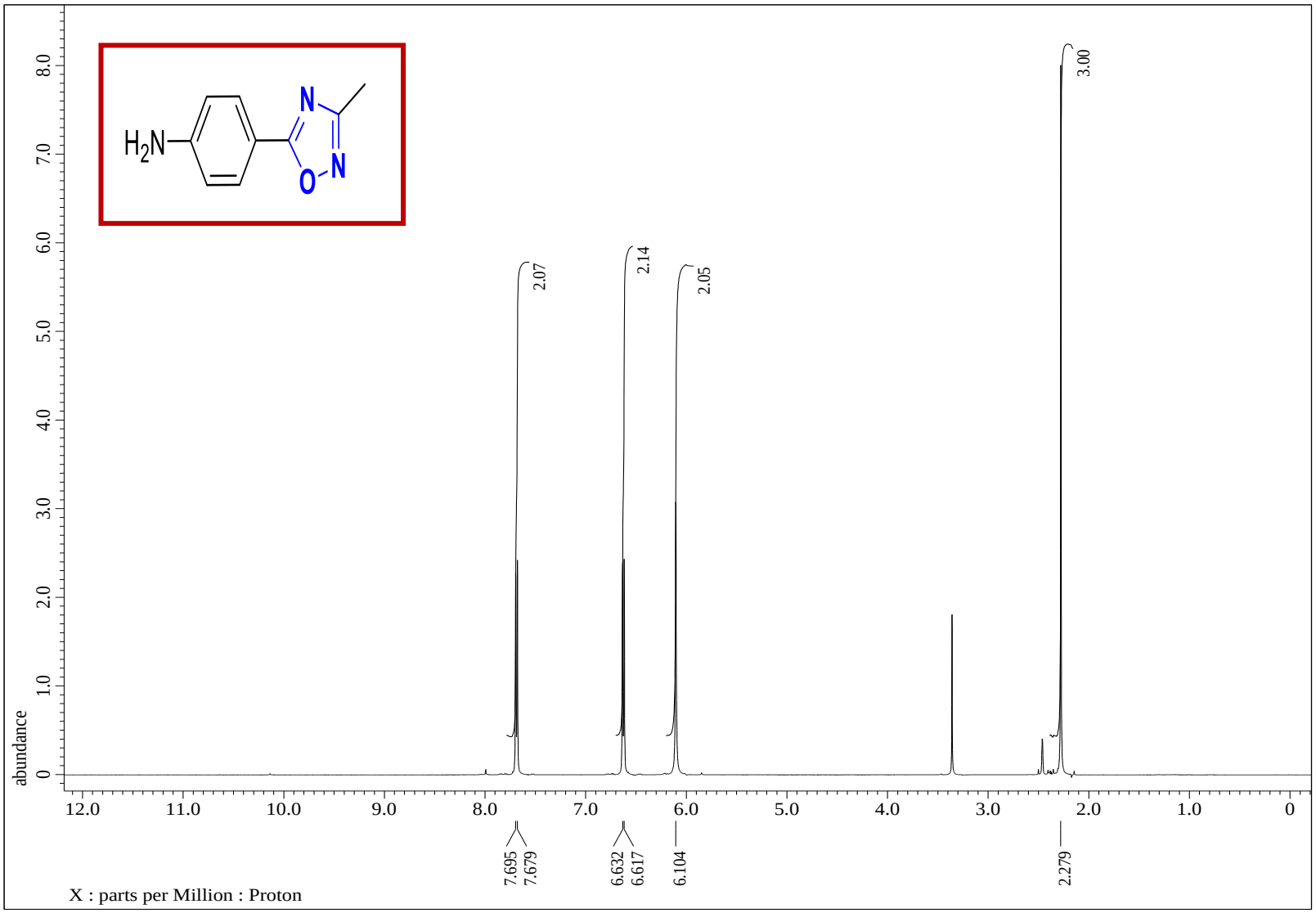

Figure 9. ^{1}H NMR of **3b** (DMSO-d6)

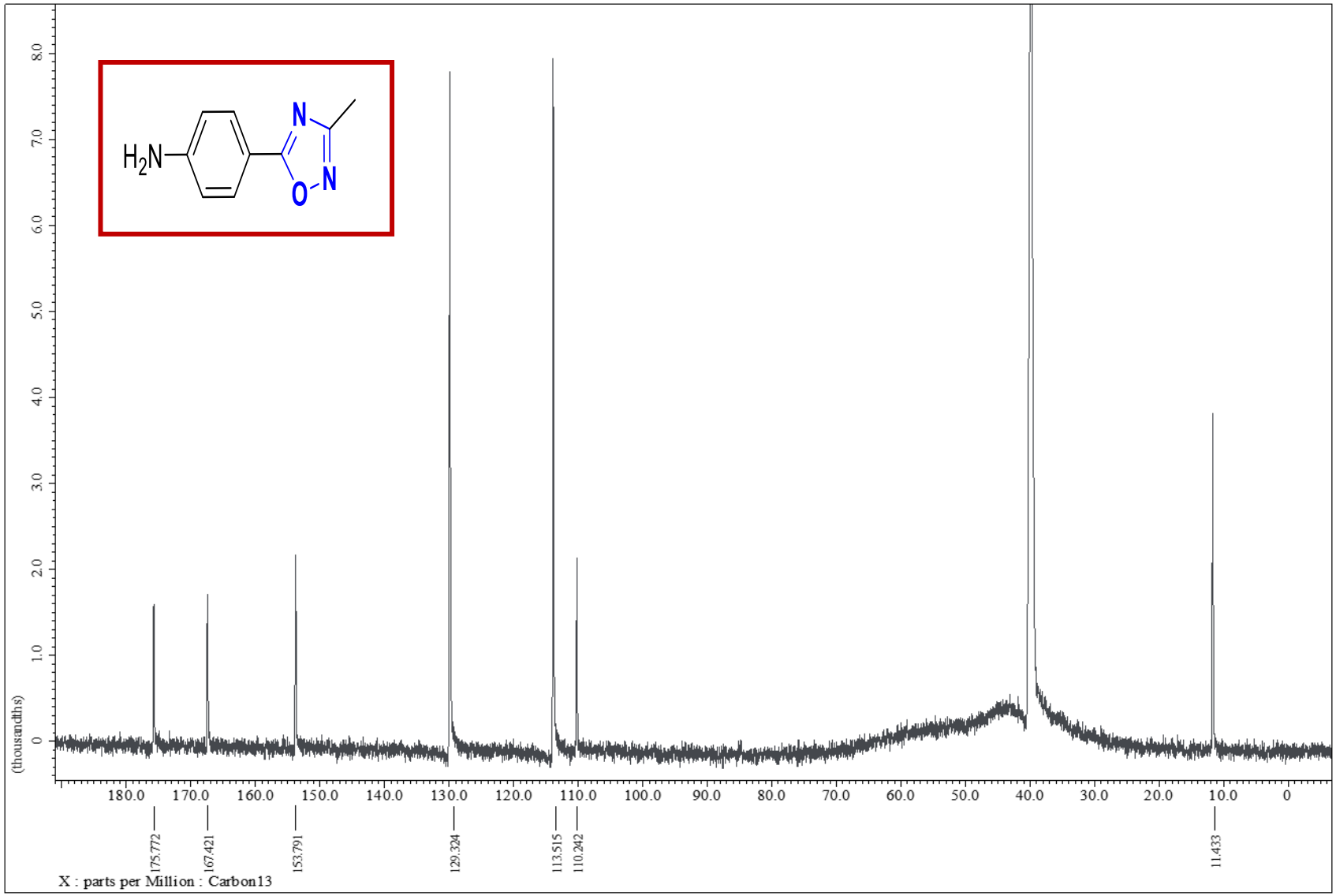

Figure 10. ^{13}C NMR of **3b** (DMSO-d6)

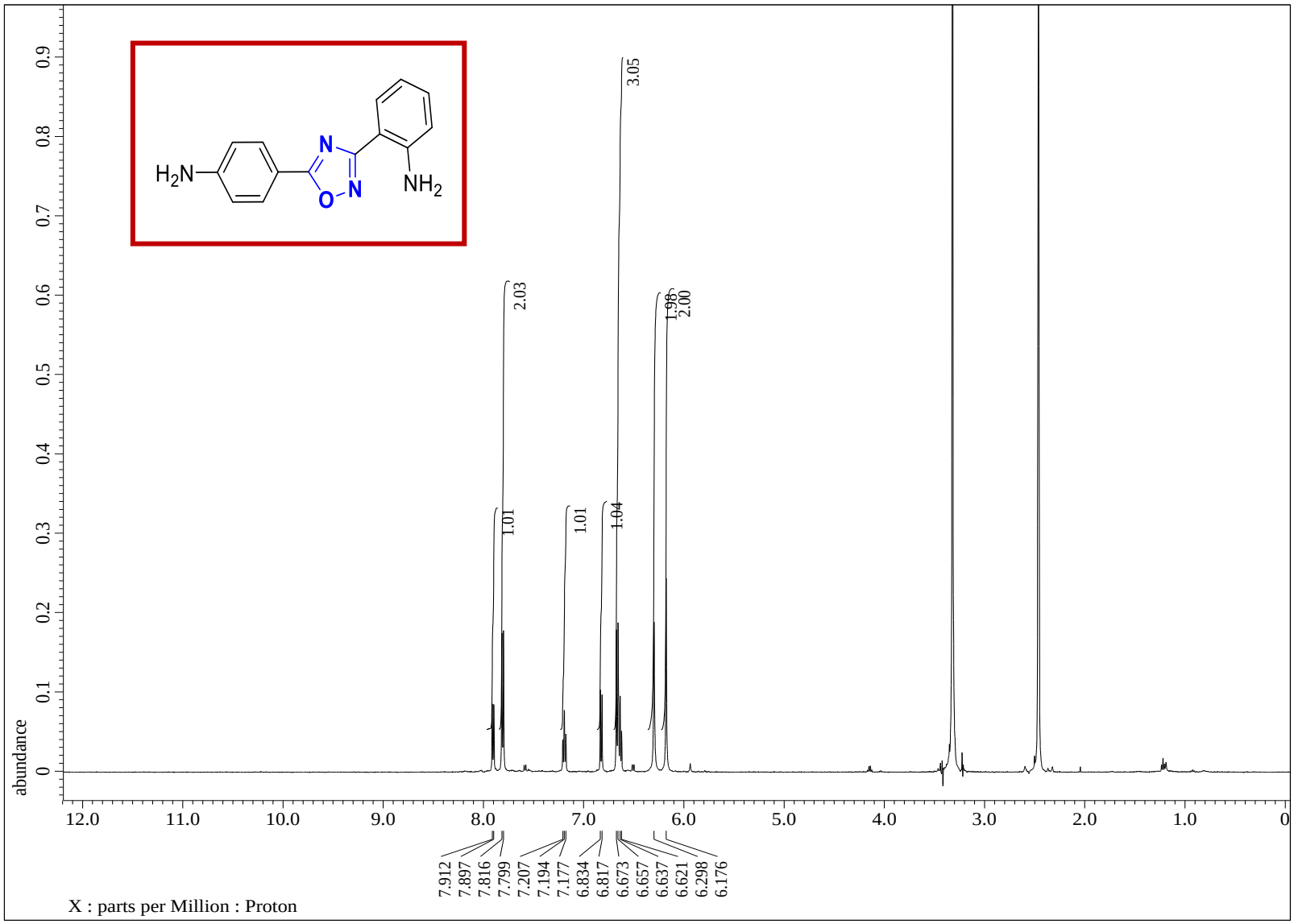

Figure 11. ^{1}H NMR of **3d** (DMSO-d6)

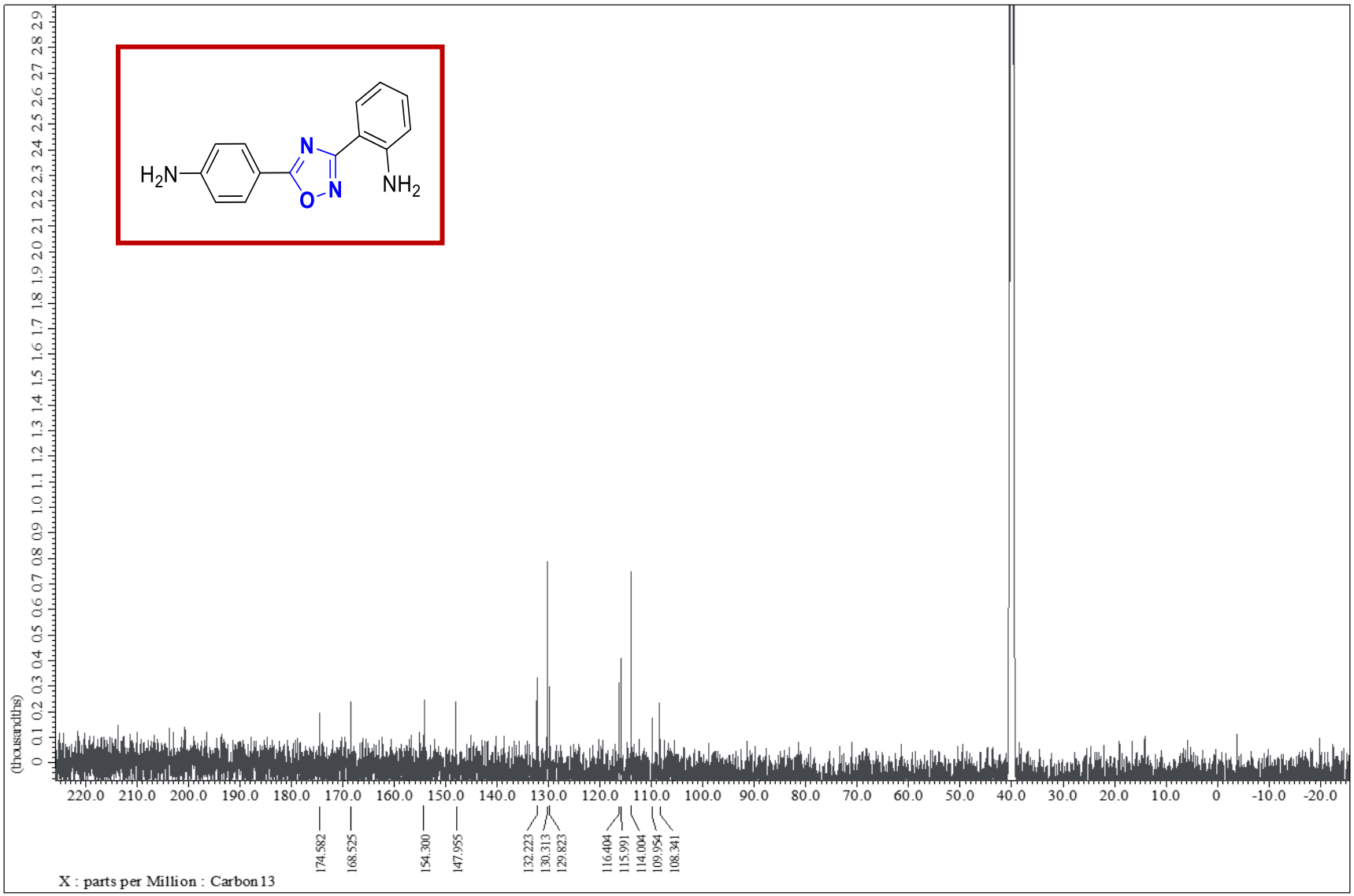

Figure 12. ^{13}C NMR of **3b** (DMSO-d6)

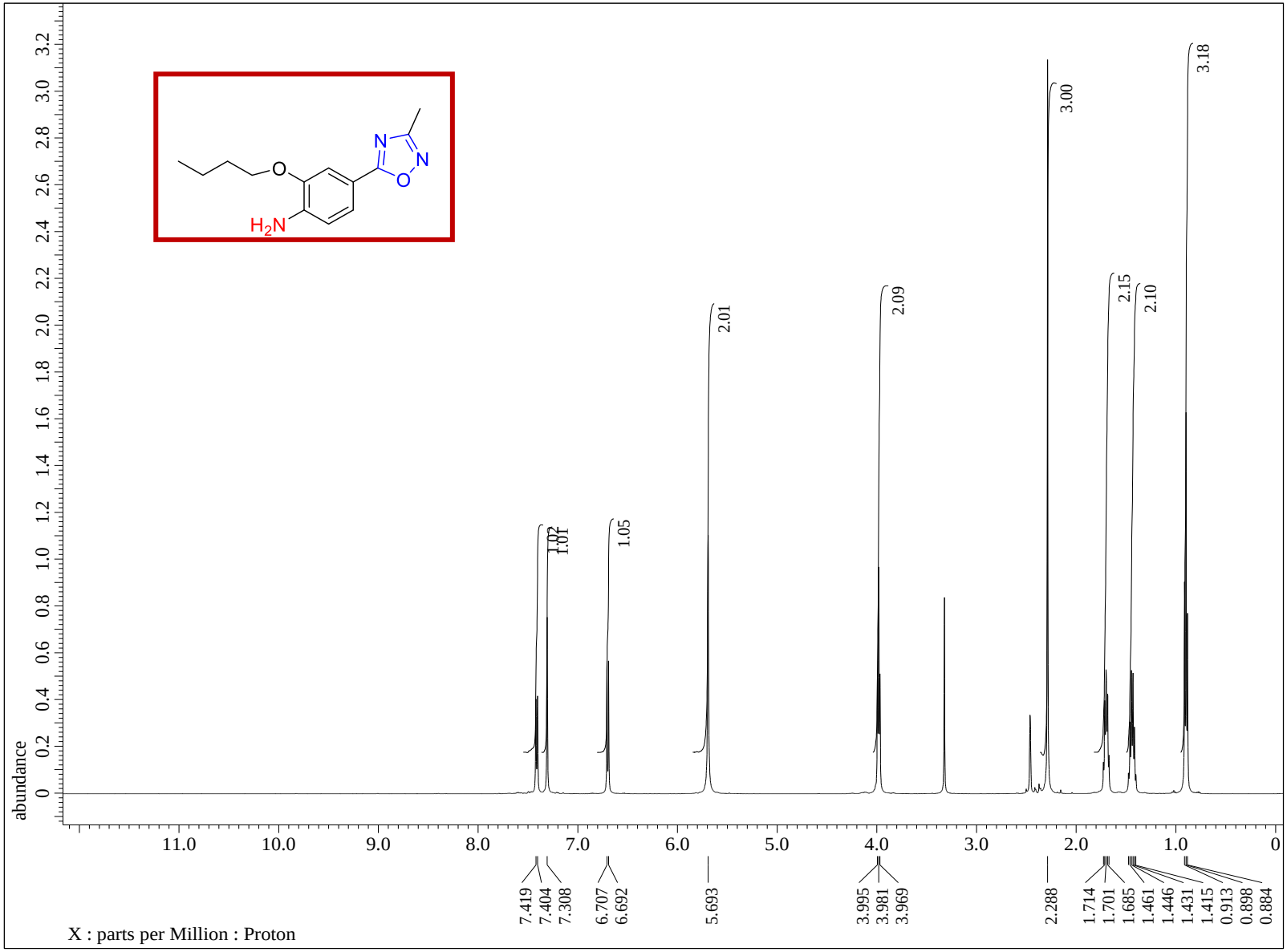

Figure 13. ^{1}H NMR of **4a** (DMSO-d6)

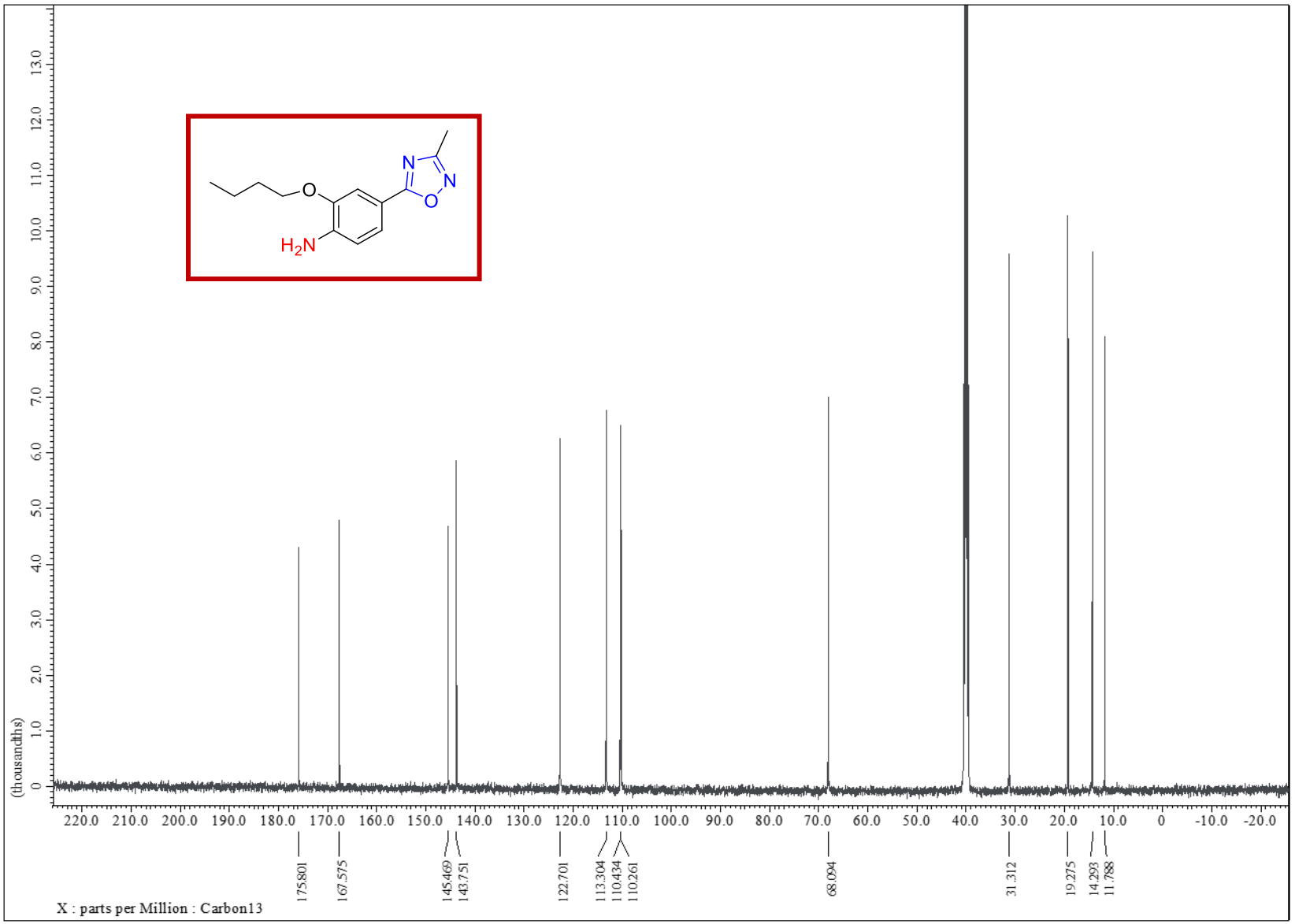

Figure 14 ^{13}C NMR of **4a** (DMSO-d6)

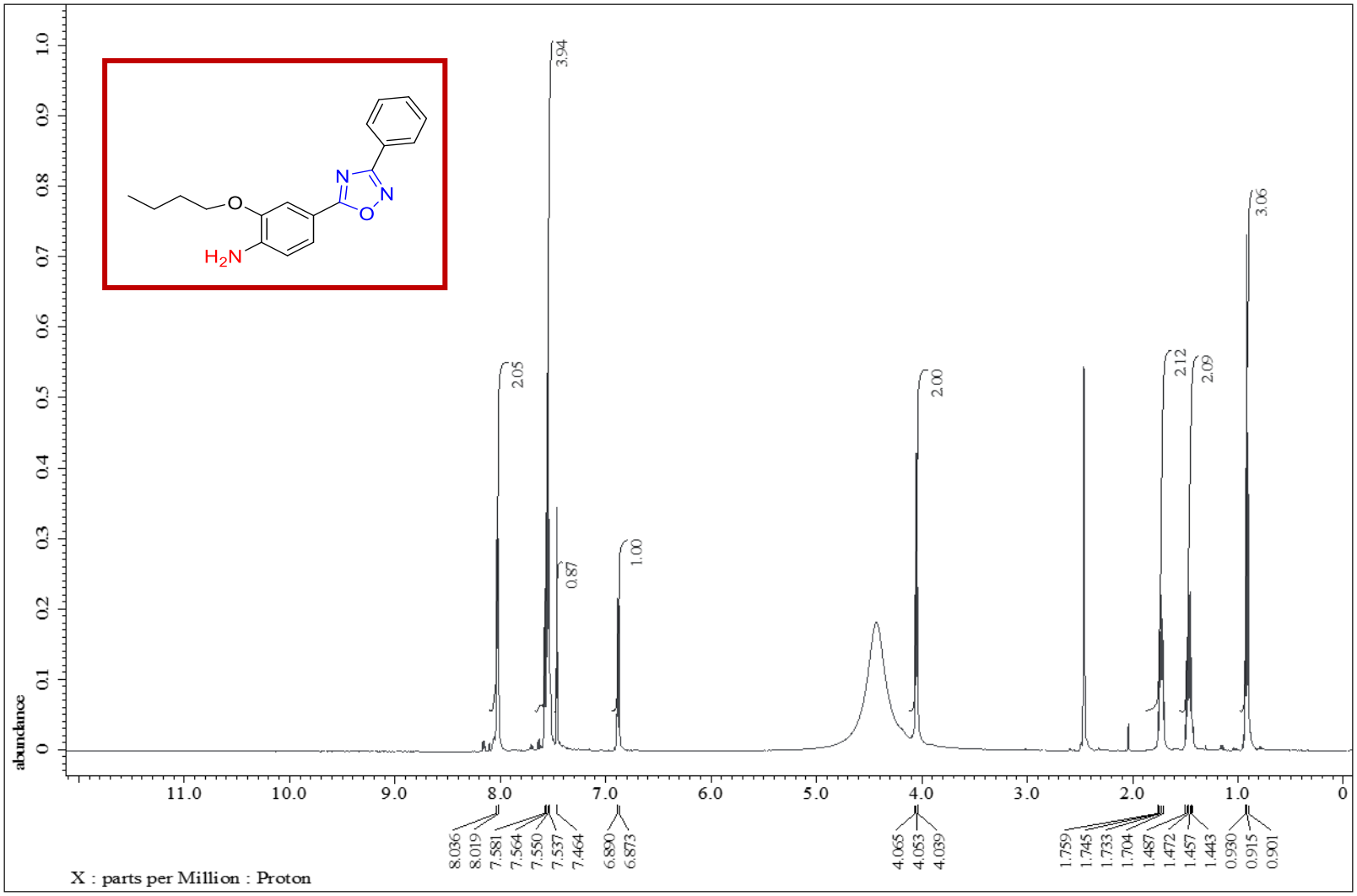

Figure 15. ^{1H} NMR of **4b** (DMSO-d6

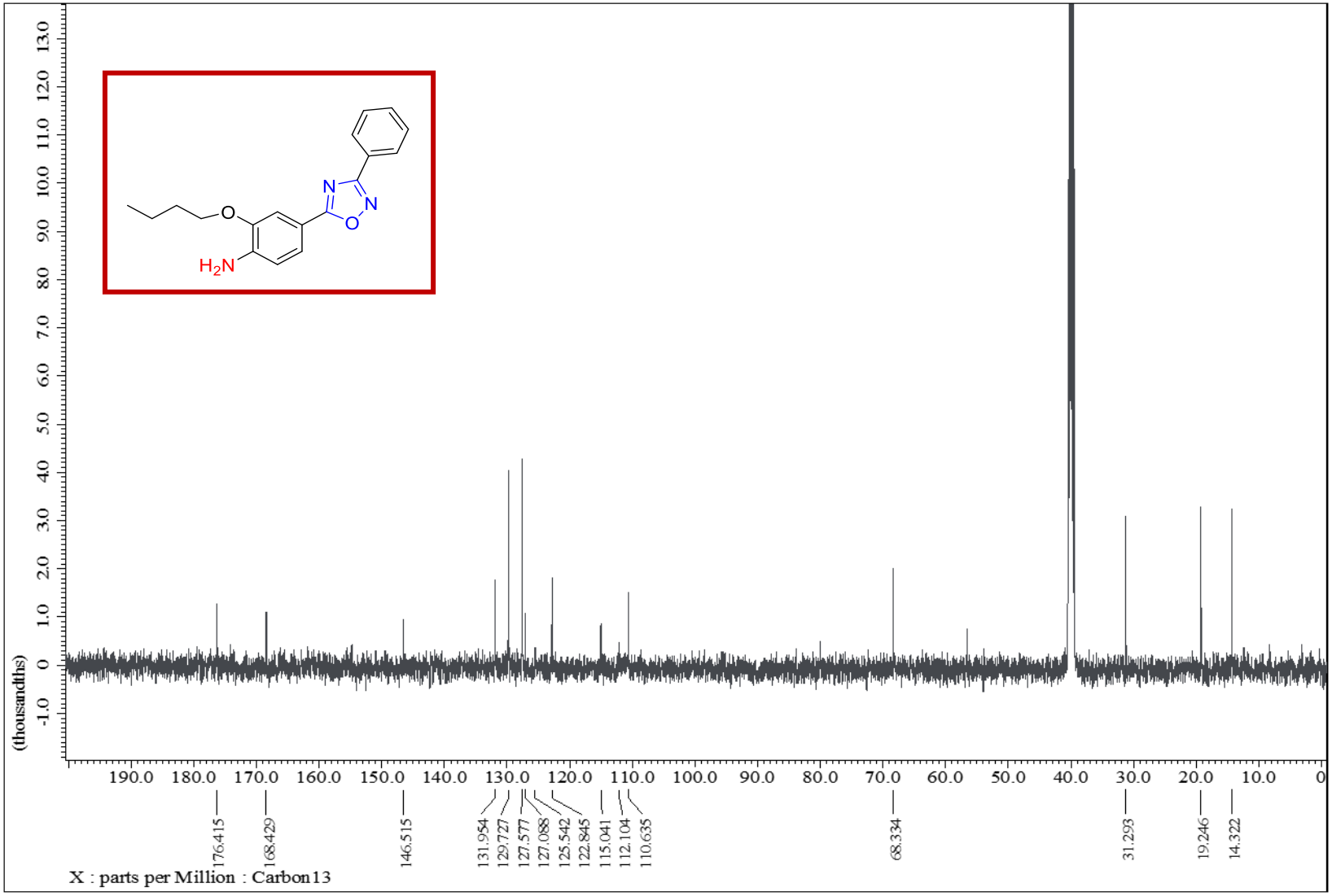

Figure 16. ^{13}C NMR of **4b** (DMSO-d6)

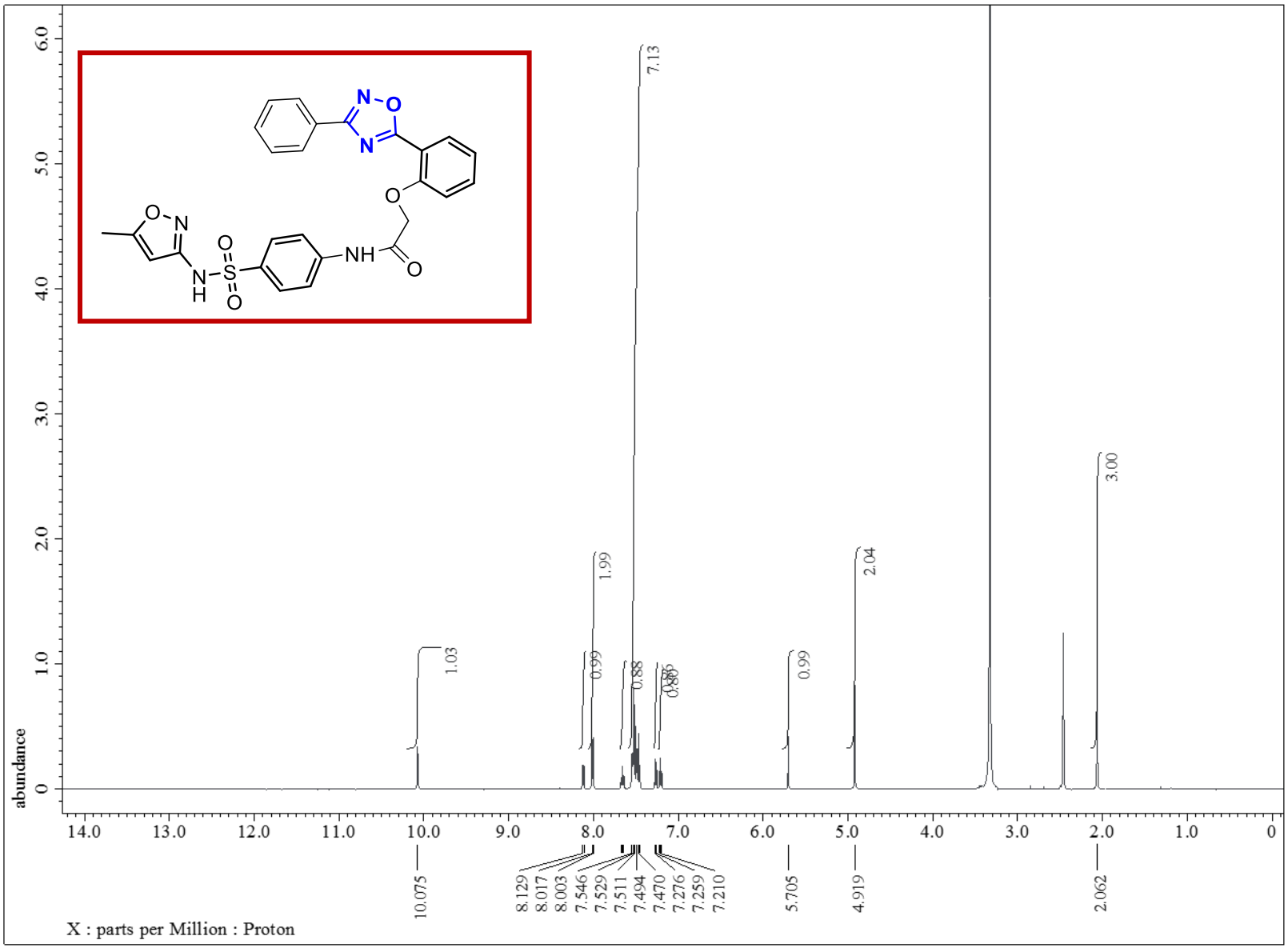

Figure 17. [1] H NMR of **6** (DMSO-d6)

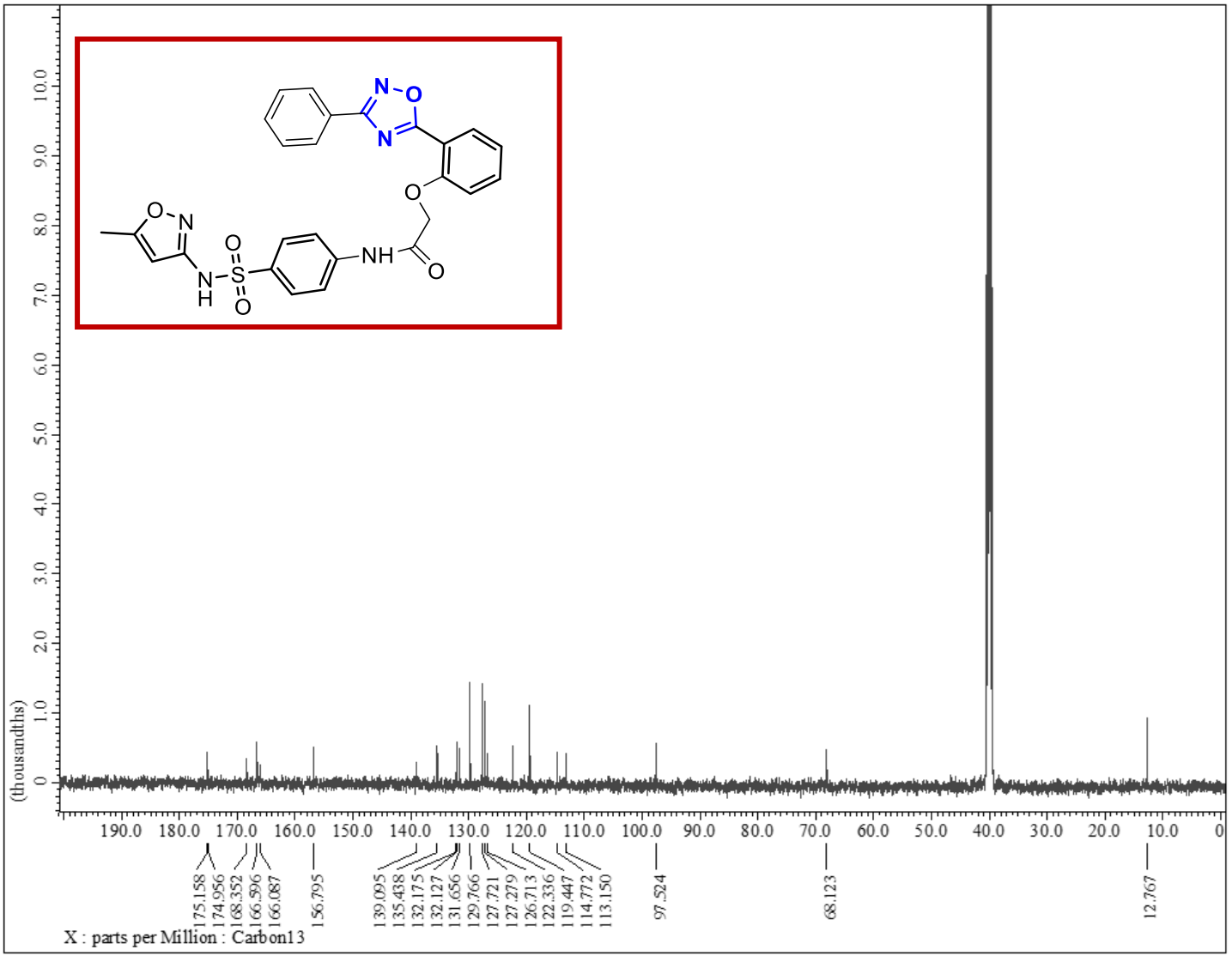

Figure 18. ^{13}C NMR of **6** (DMSO-d6)

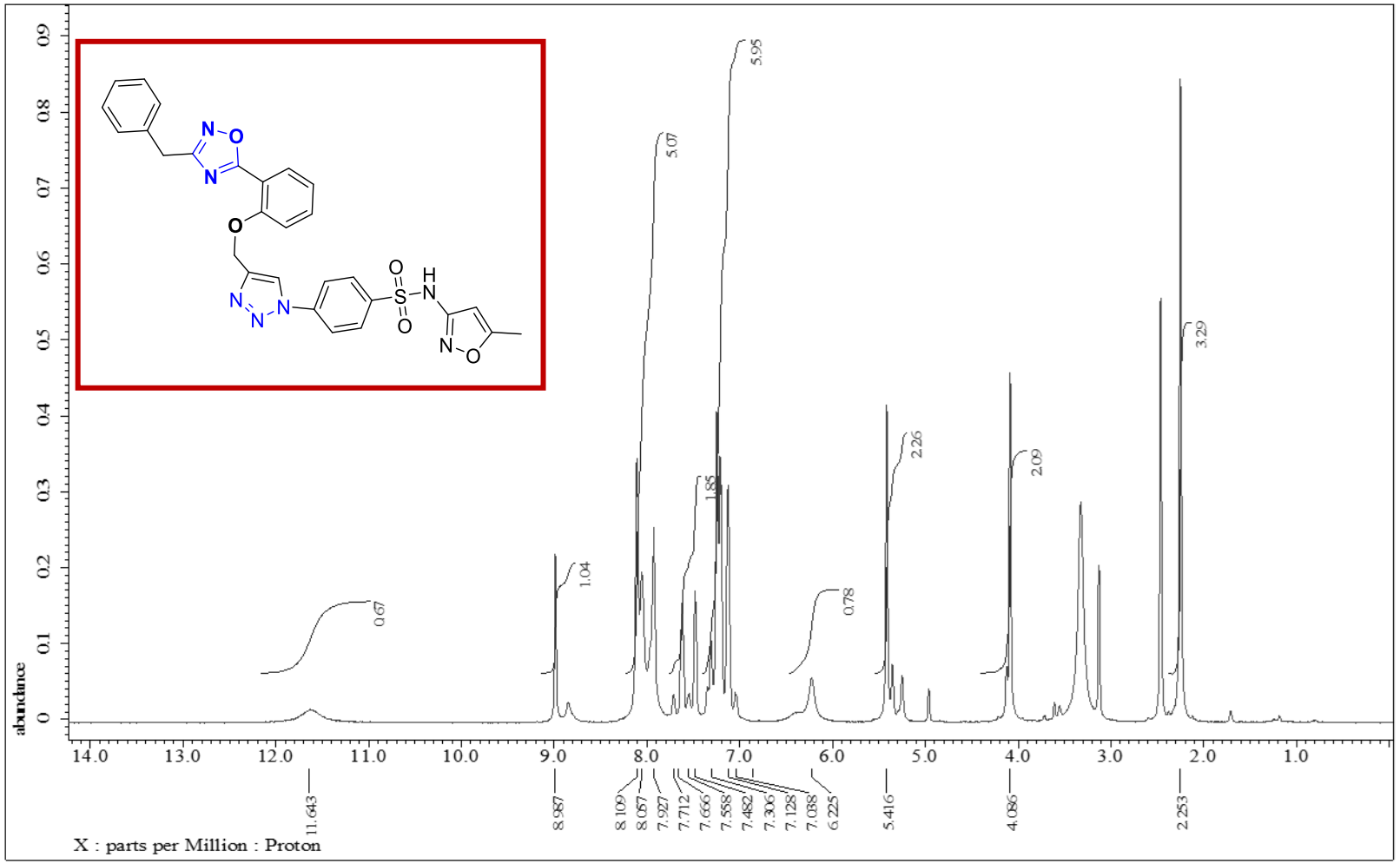

Figure 19. ^{1}H NMR of **9a** (DMSO-d6)

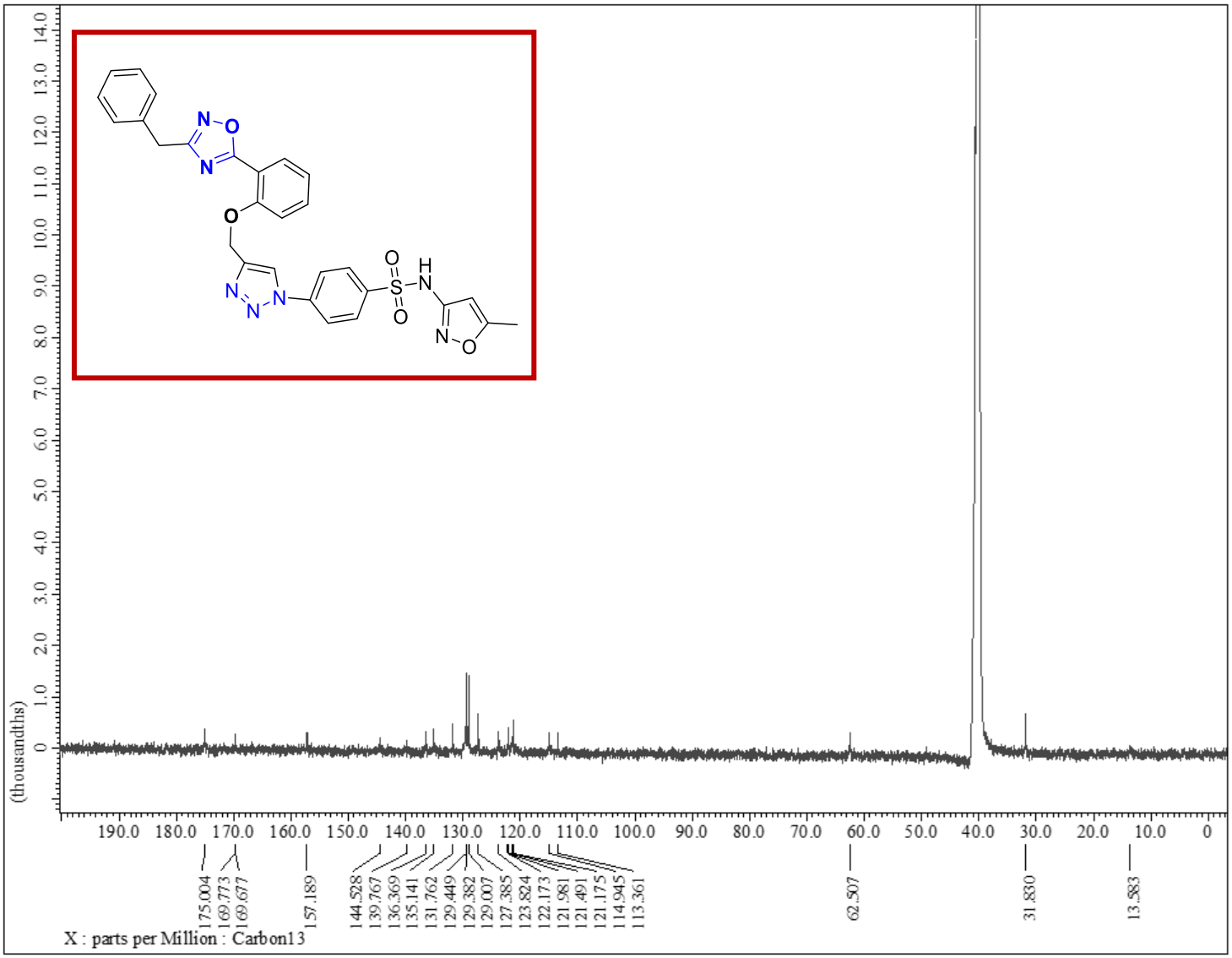

Figure 20. ^{13}C NMR of **9a** (DMSO-d6)

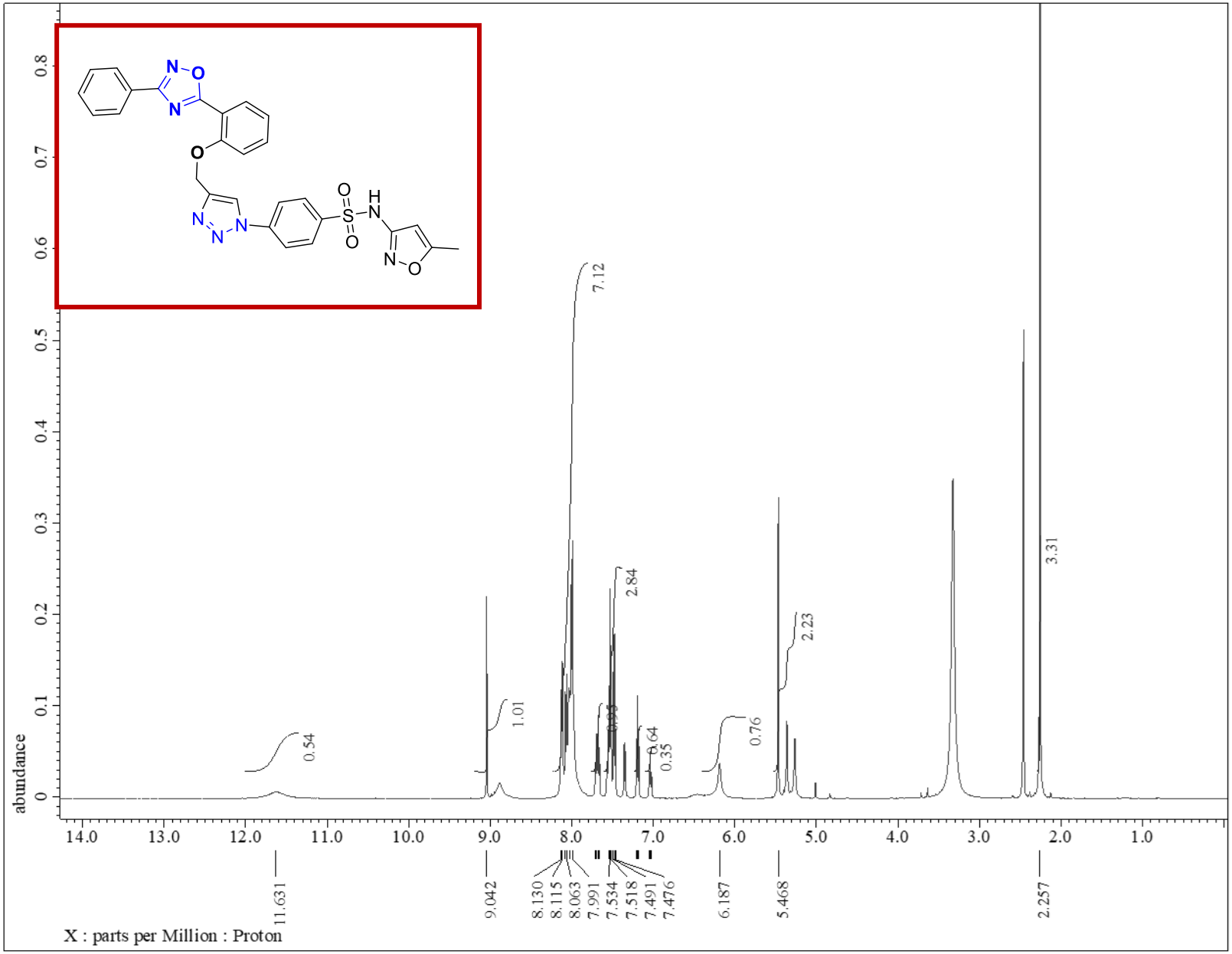

Figure 21. ^{1}H NMR of **9b** (DMSO-d6)

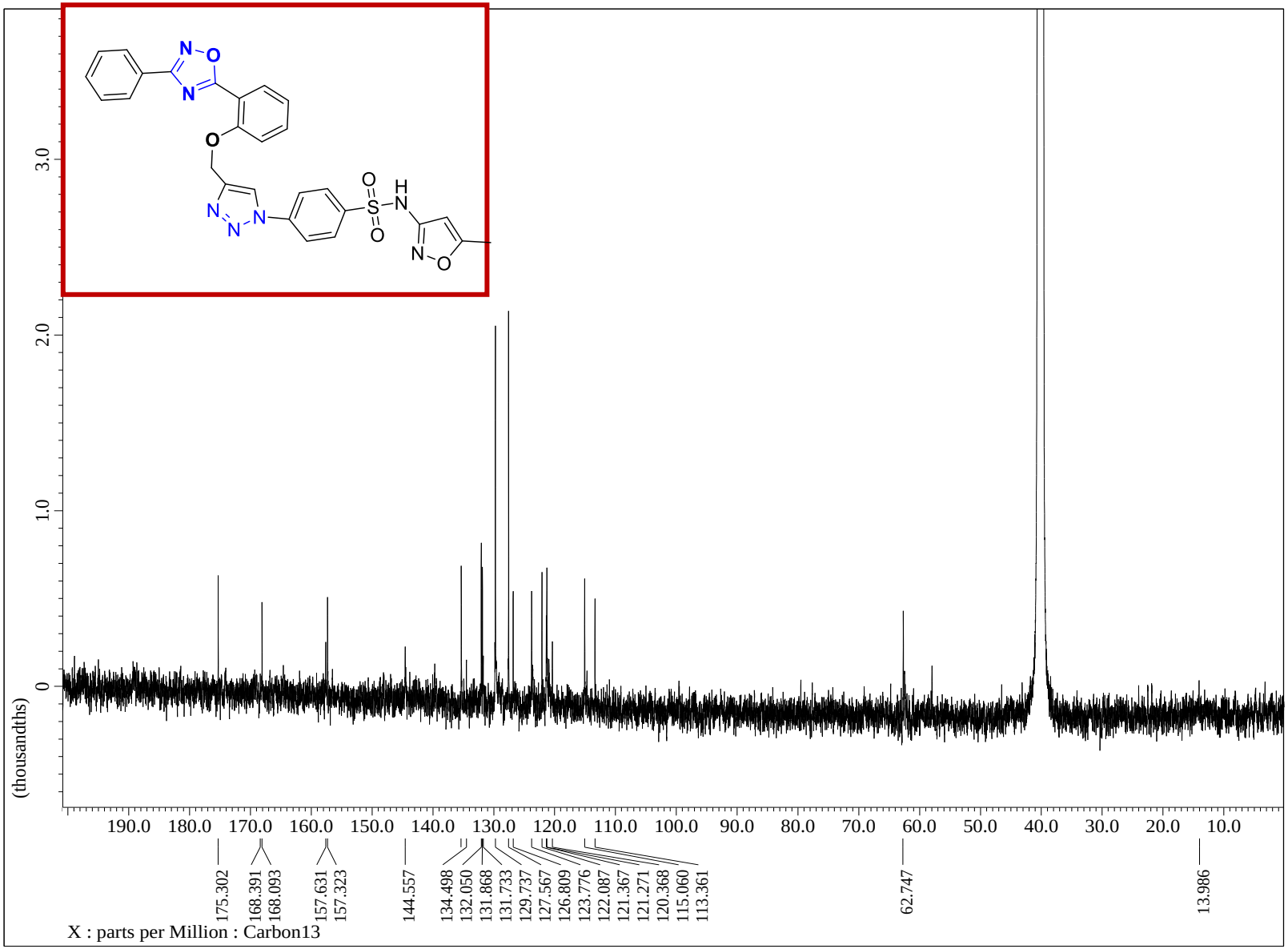

Figure 22. ^{13}C NMR of **9b** (DMSO-d6)

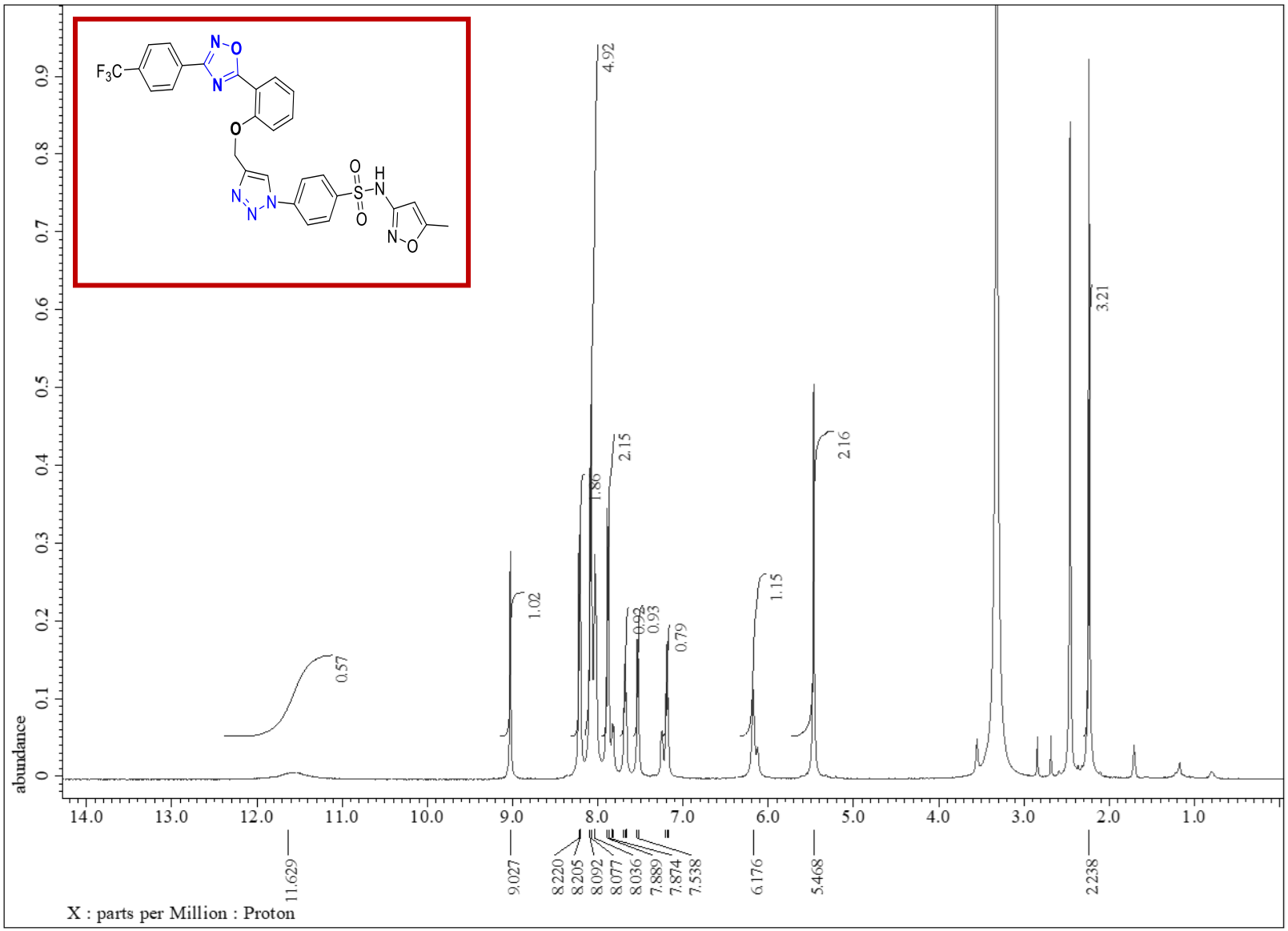

Figure 23. ^{1}H NMR of **9c** (DMSO-d6)

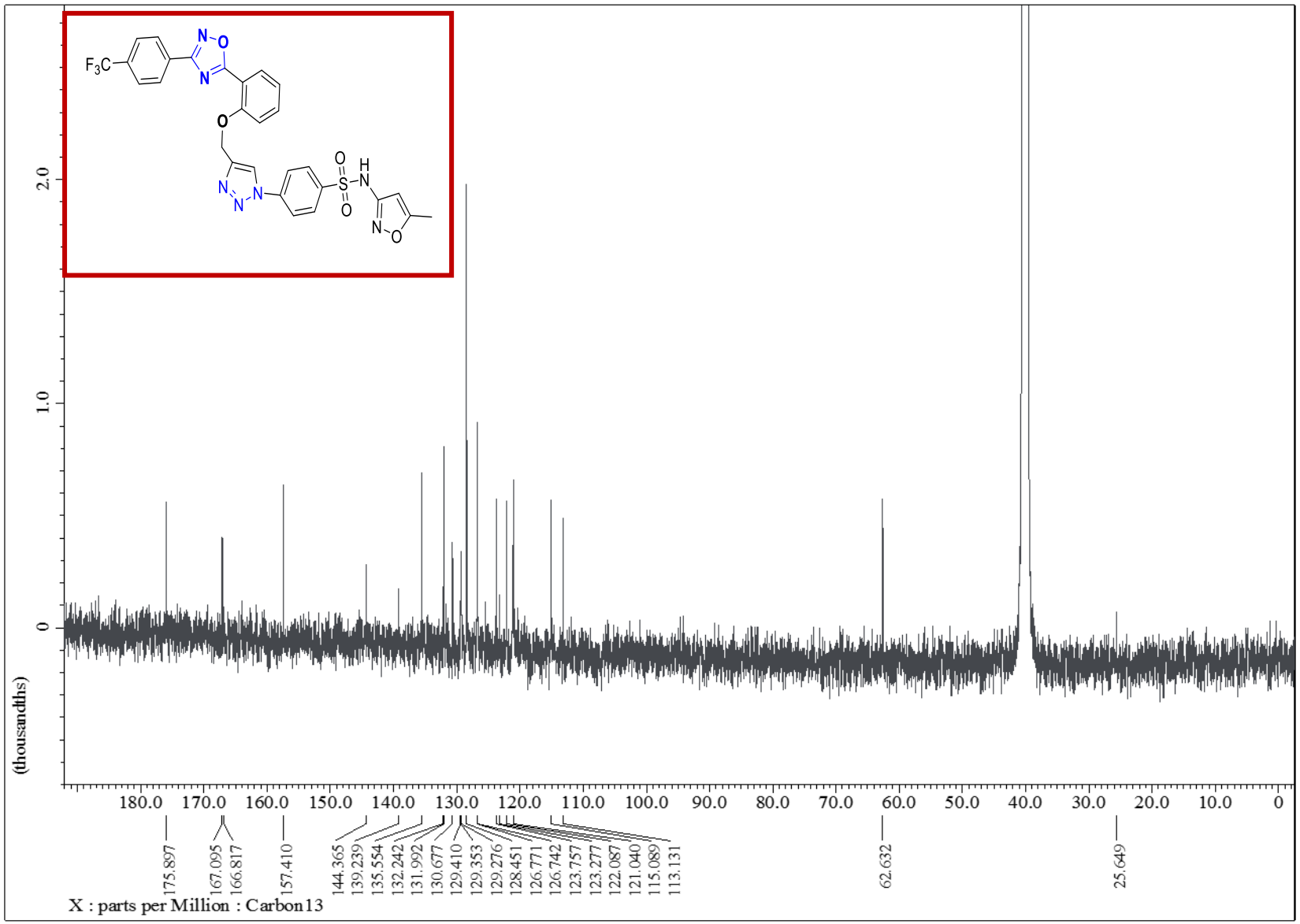

Figure 24. ^{13}C NMR of **9c** (DMSO-d6)

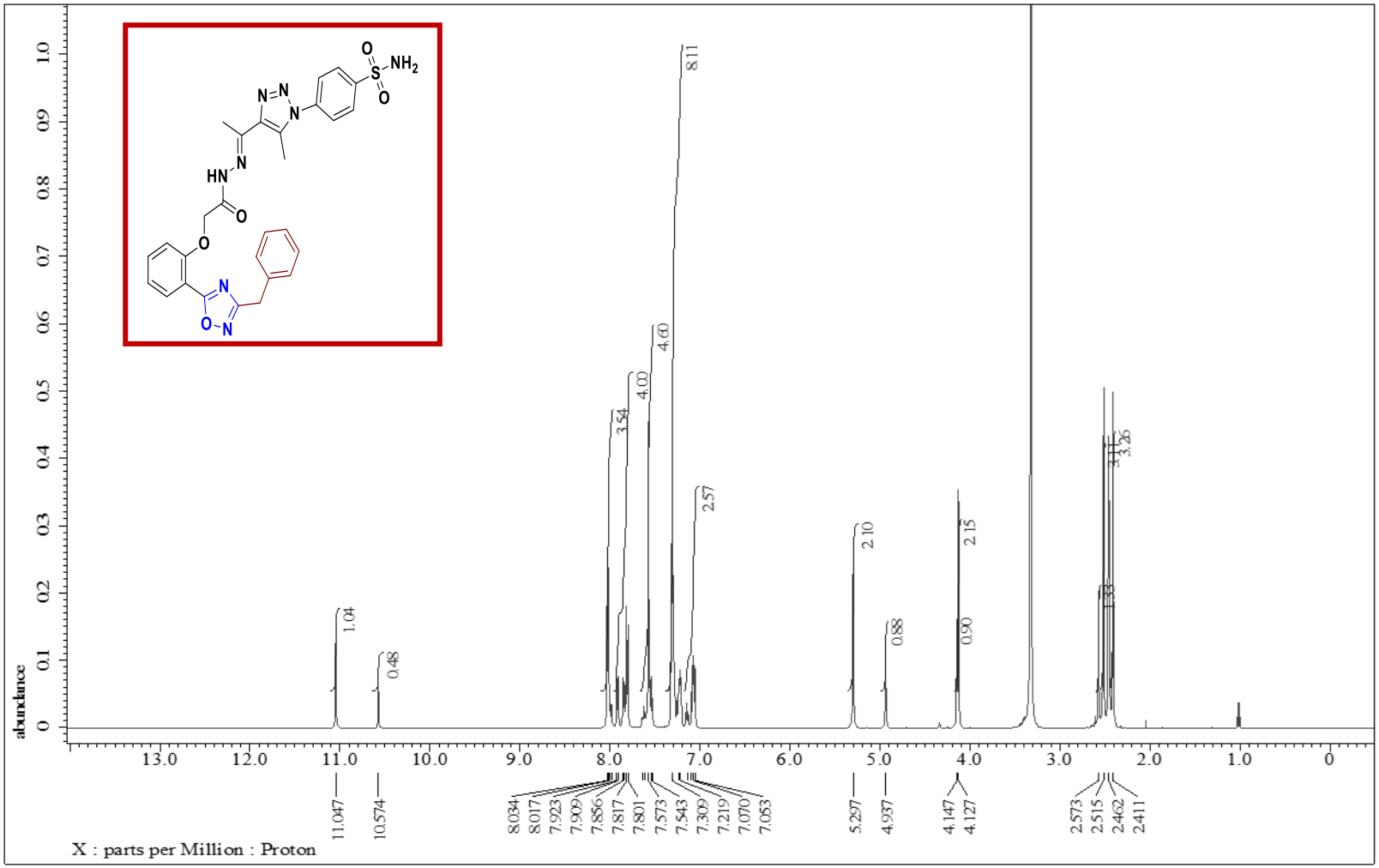

Figure 25. ^{1}H NMR of **12** (DMSO-d6)

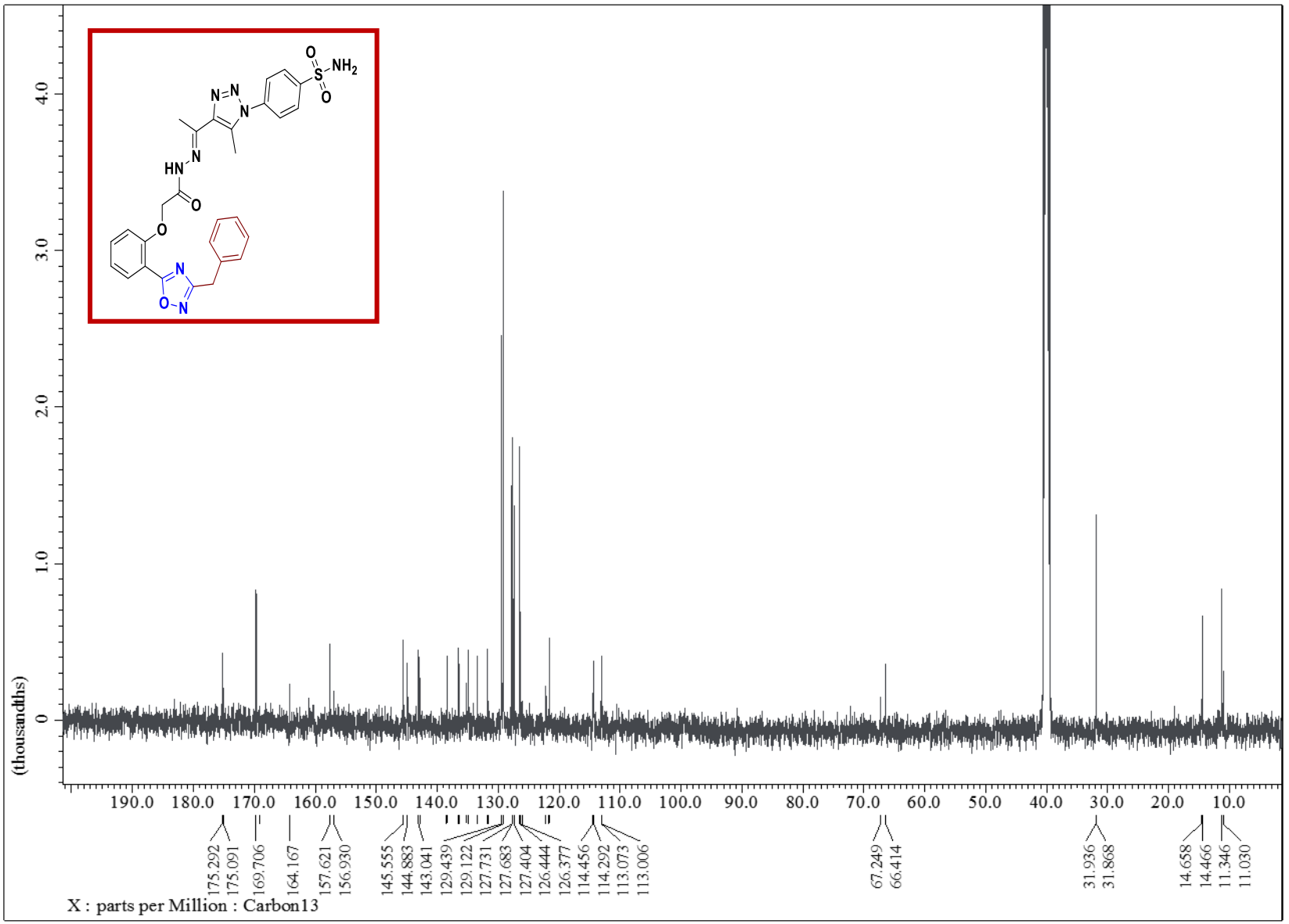

Figure 26. ^{13}C NMR of **12** (DMSO-d6)

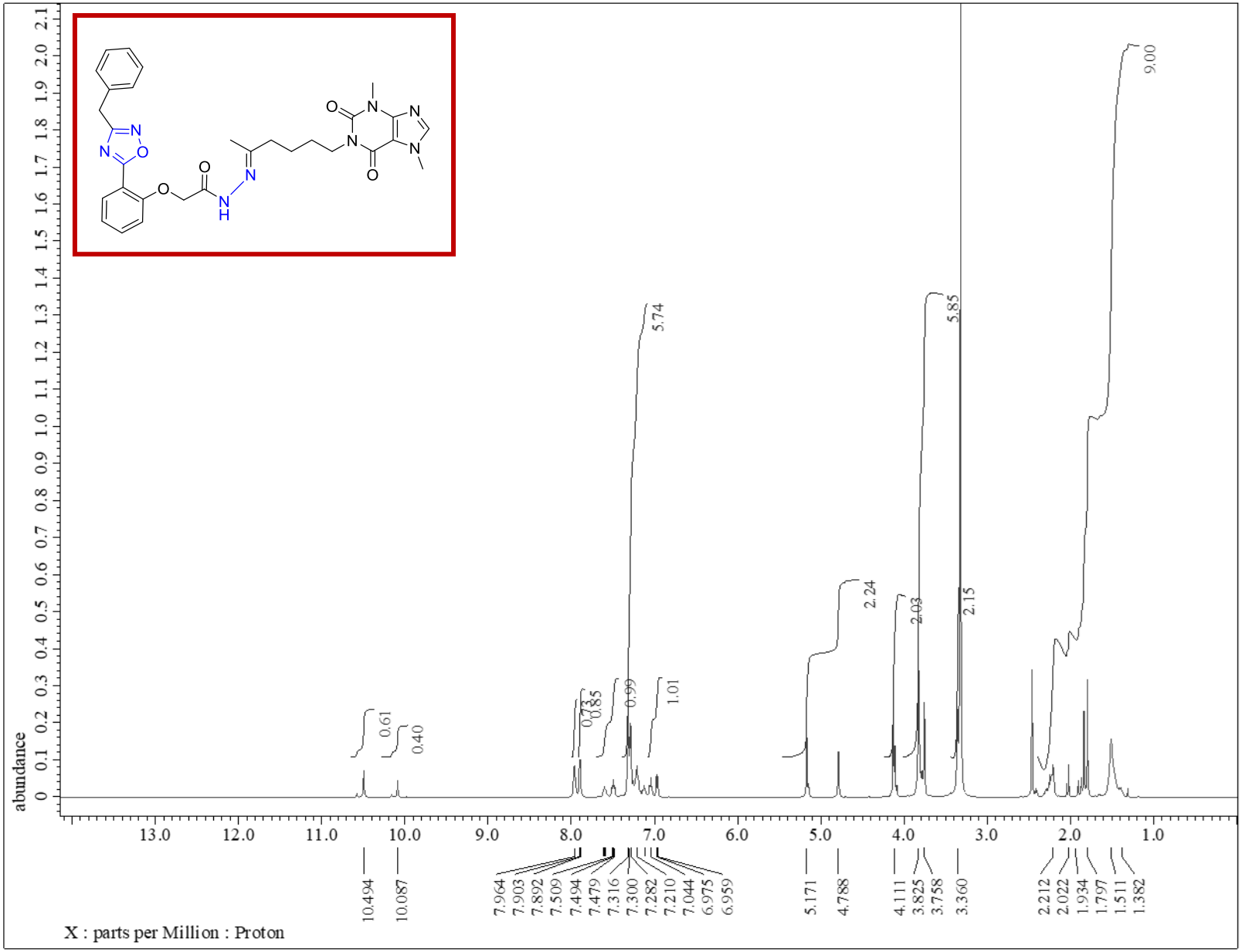

Figure 27[1]H NMR of **13a** (DMSO-d6)

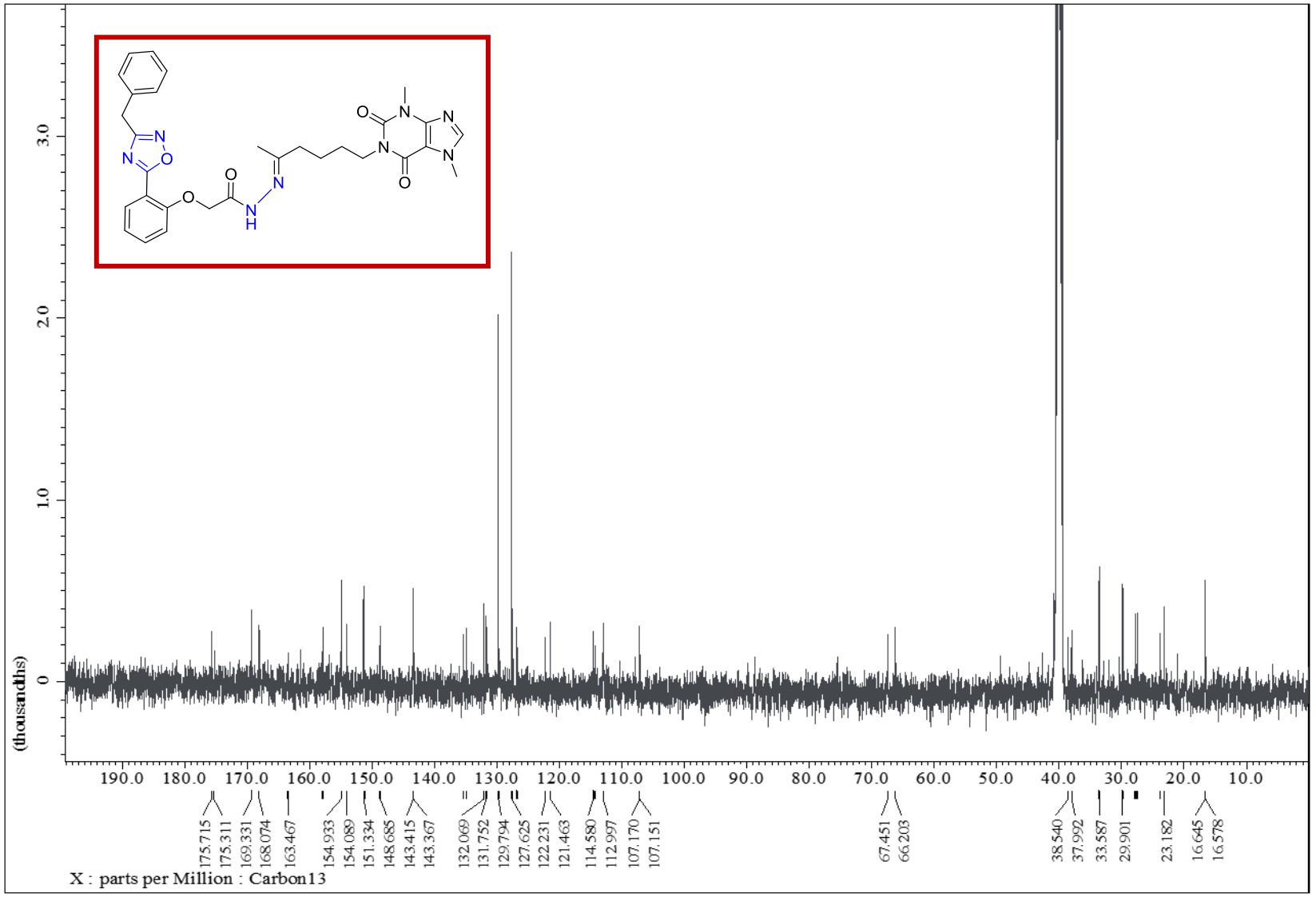

Figure 28. ^{13}C NMR of **13a** (DMSO-d6)

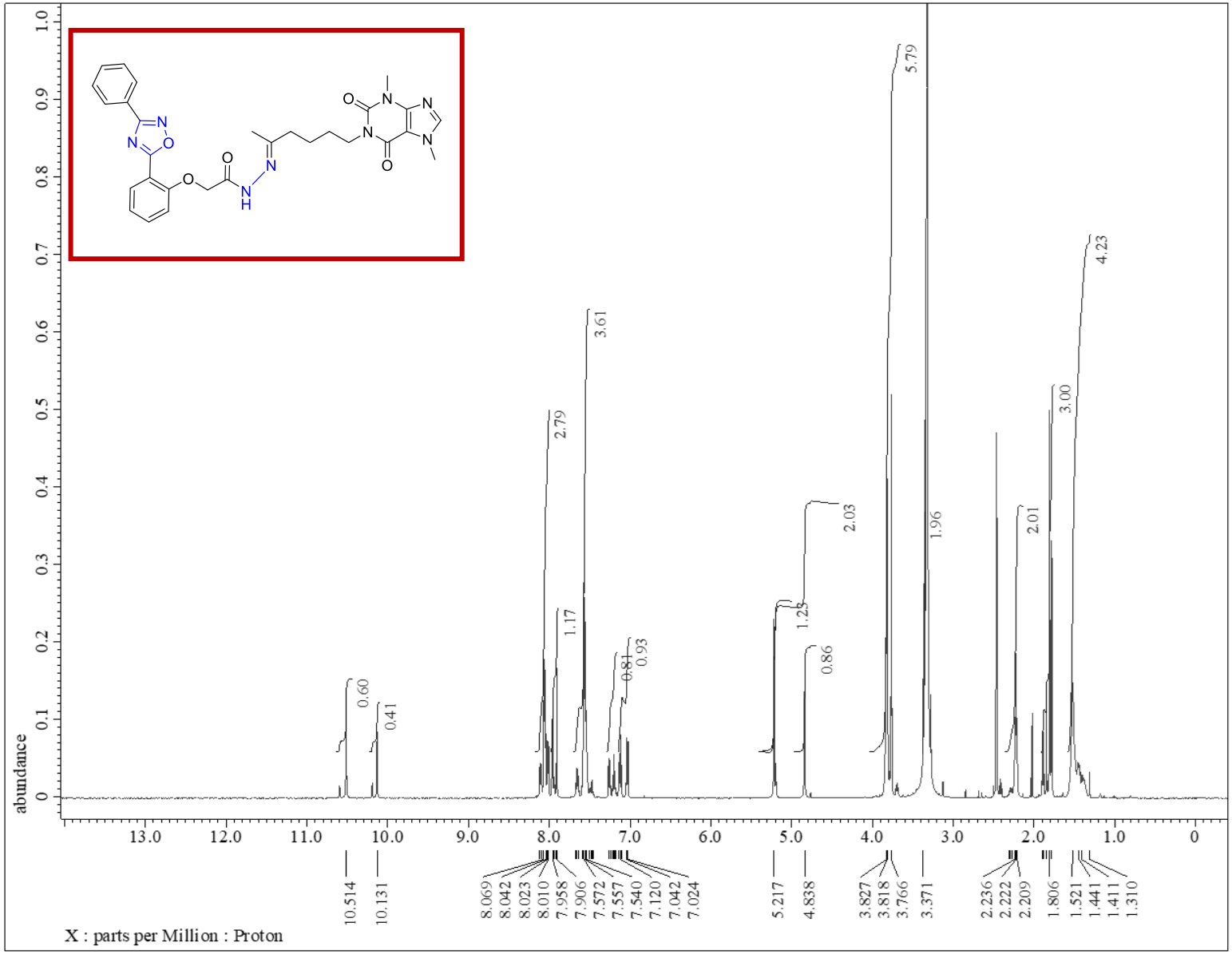

Figure 29. ^{1}H NMR of **13b** (DMSO-d6)

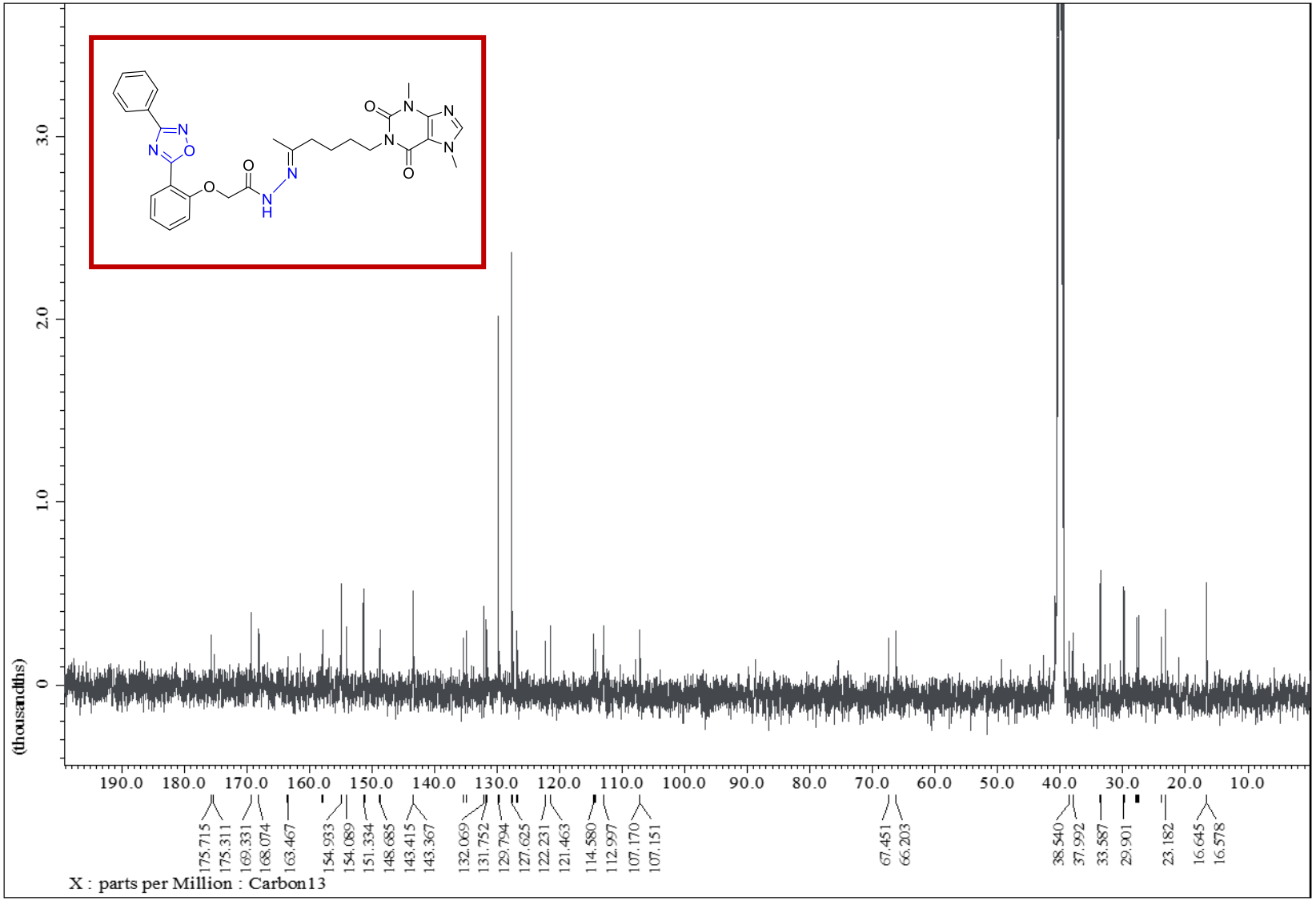

Figure 30. ^{13}C NMR of **13b** (DMSO-d6)

IR spectra of the synthesized compounds

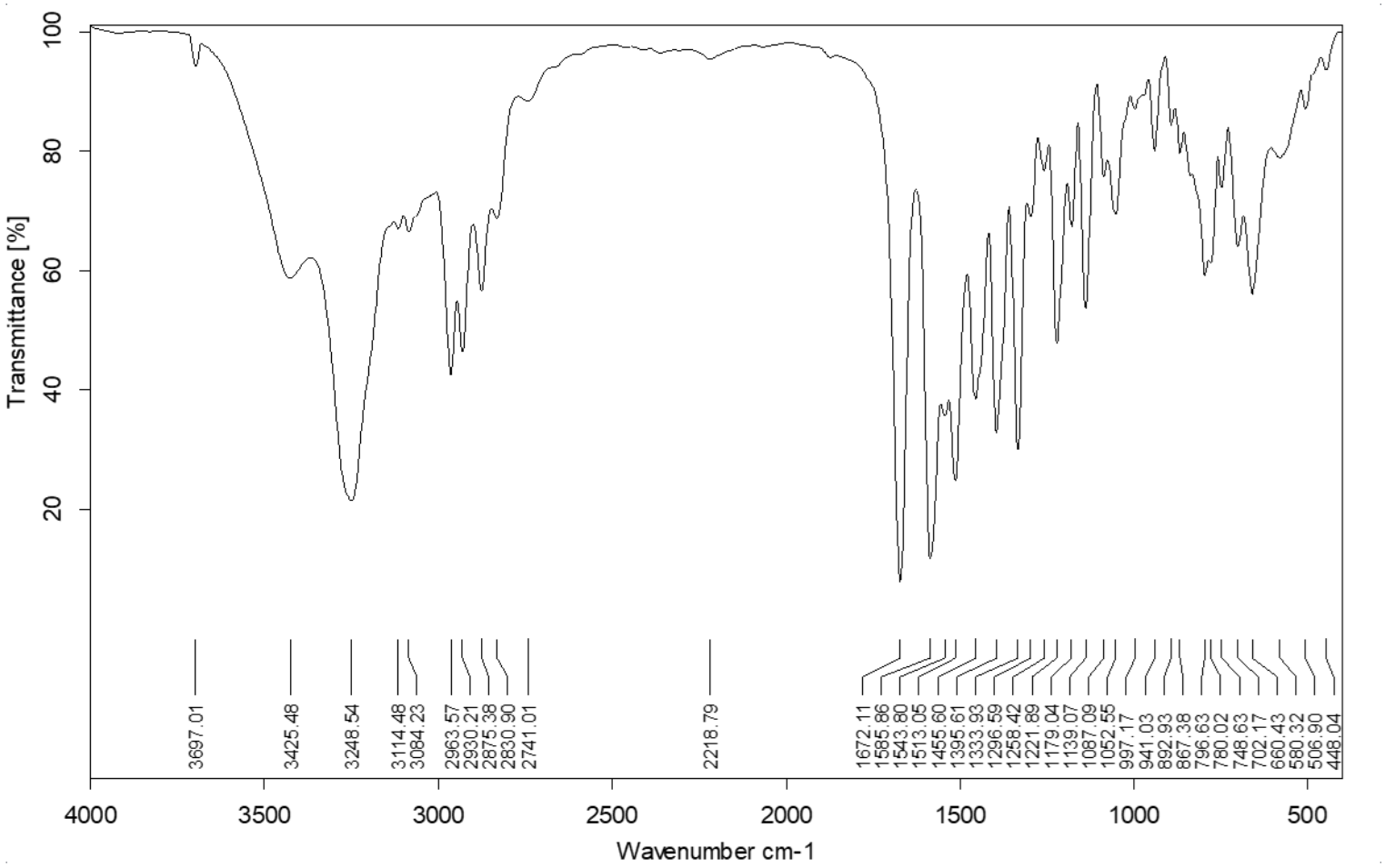

Figure 31. IR of **2a**

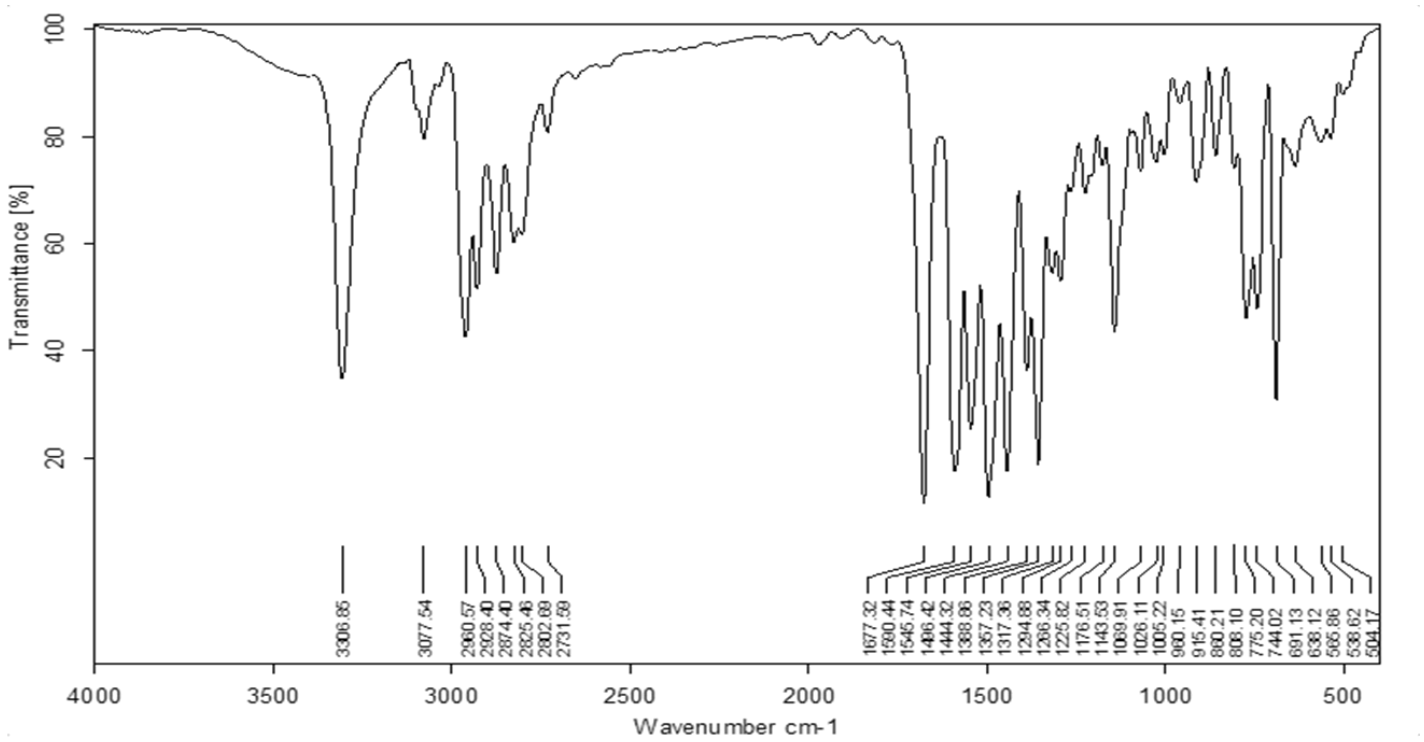

Figure 32. IR of **2b**

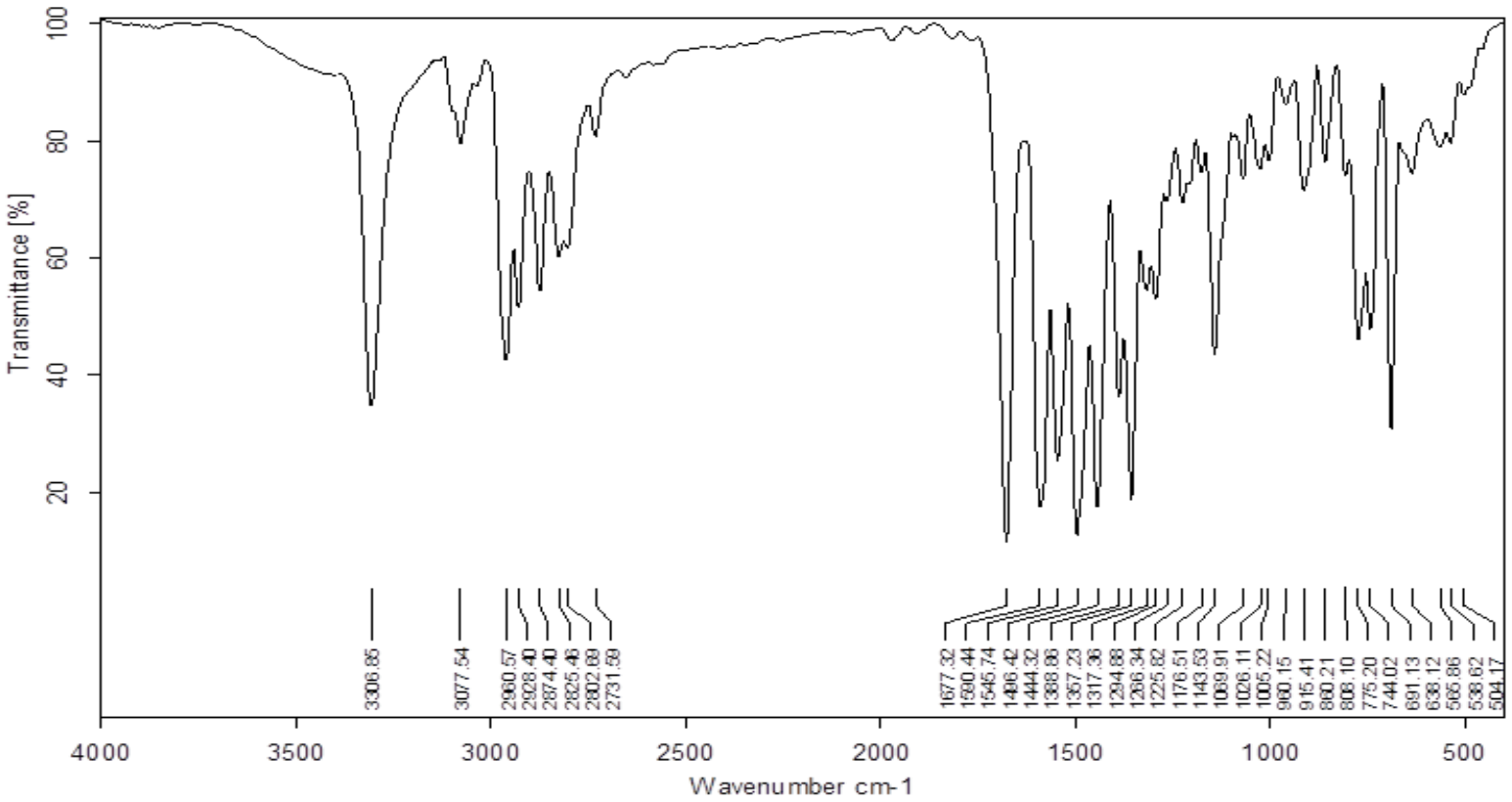

Figure 33. IR of **2c**

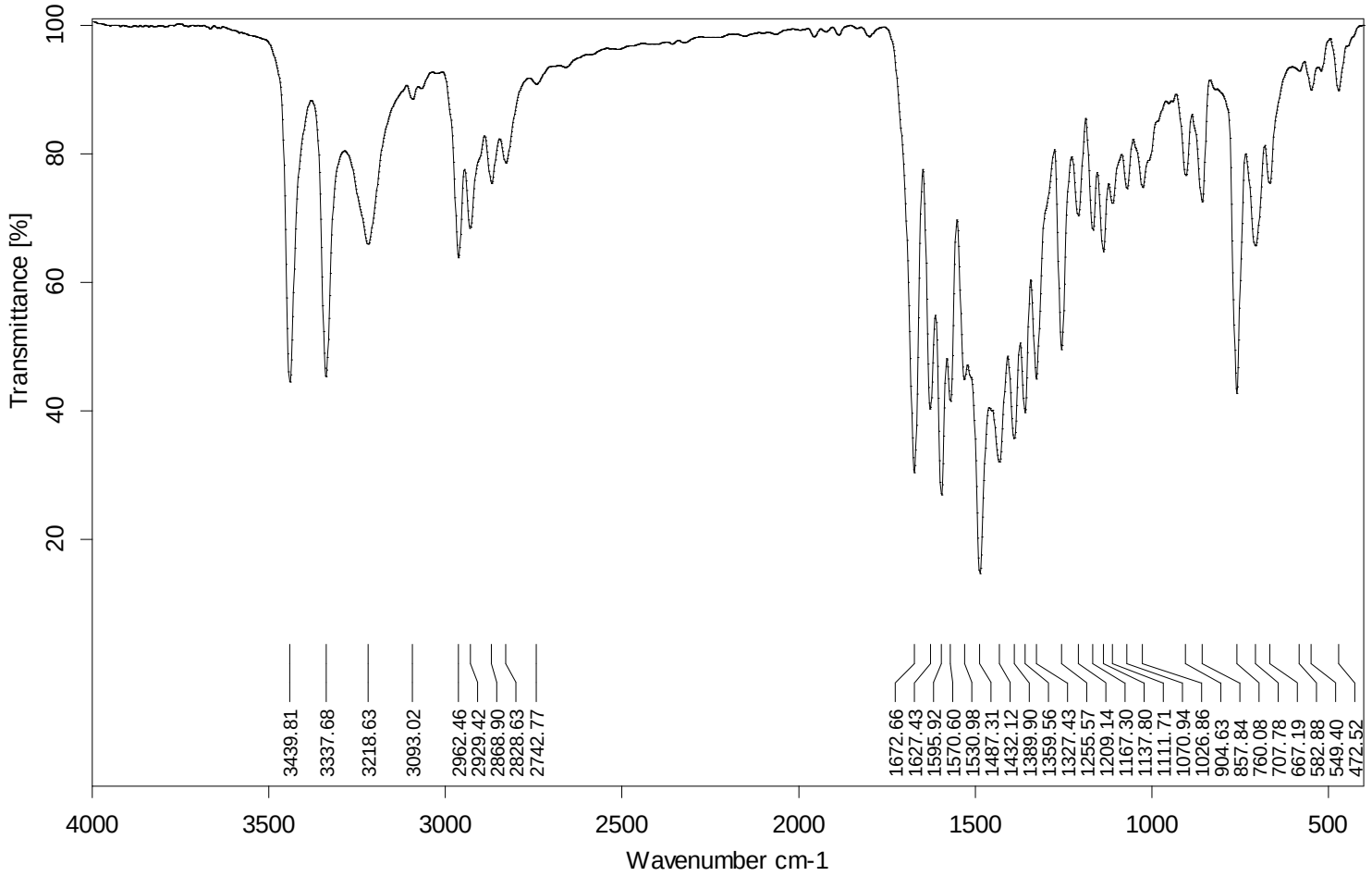

Figure 34. IR of **2d**

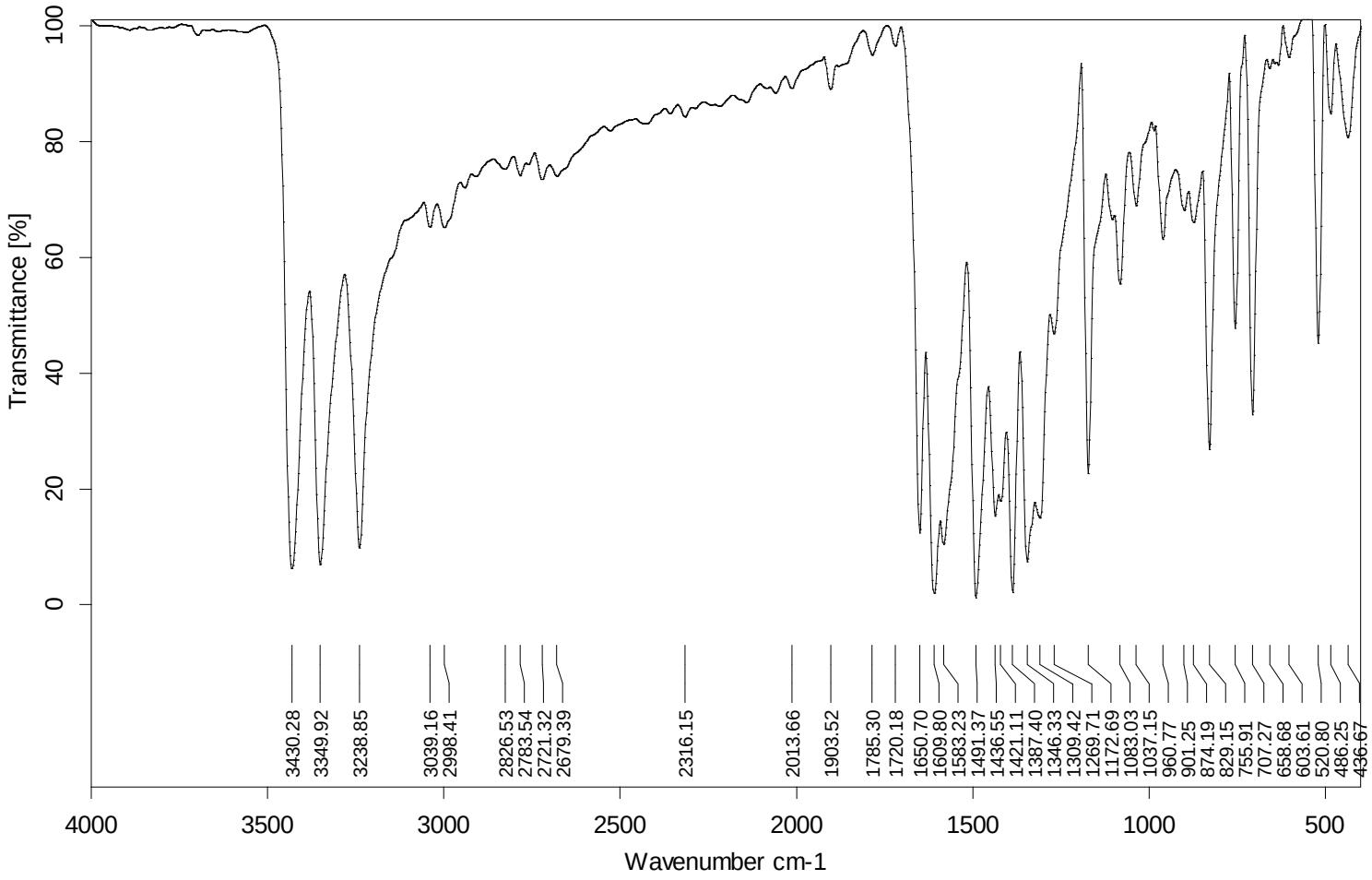

Figure 35. IR of **3a**

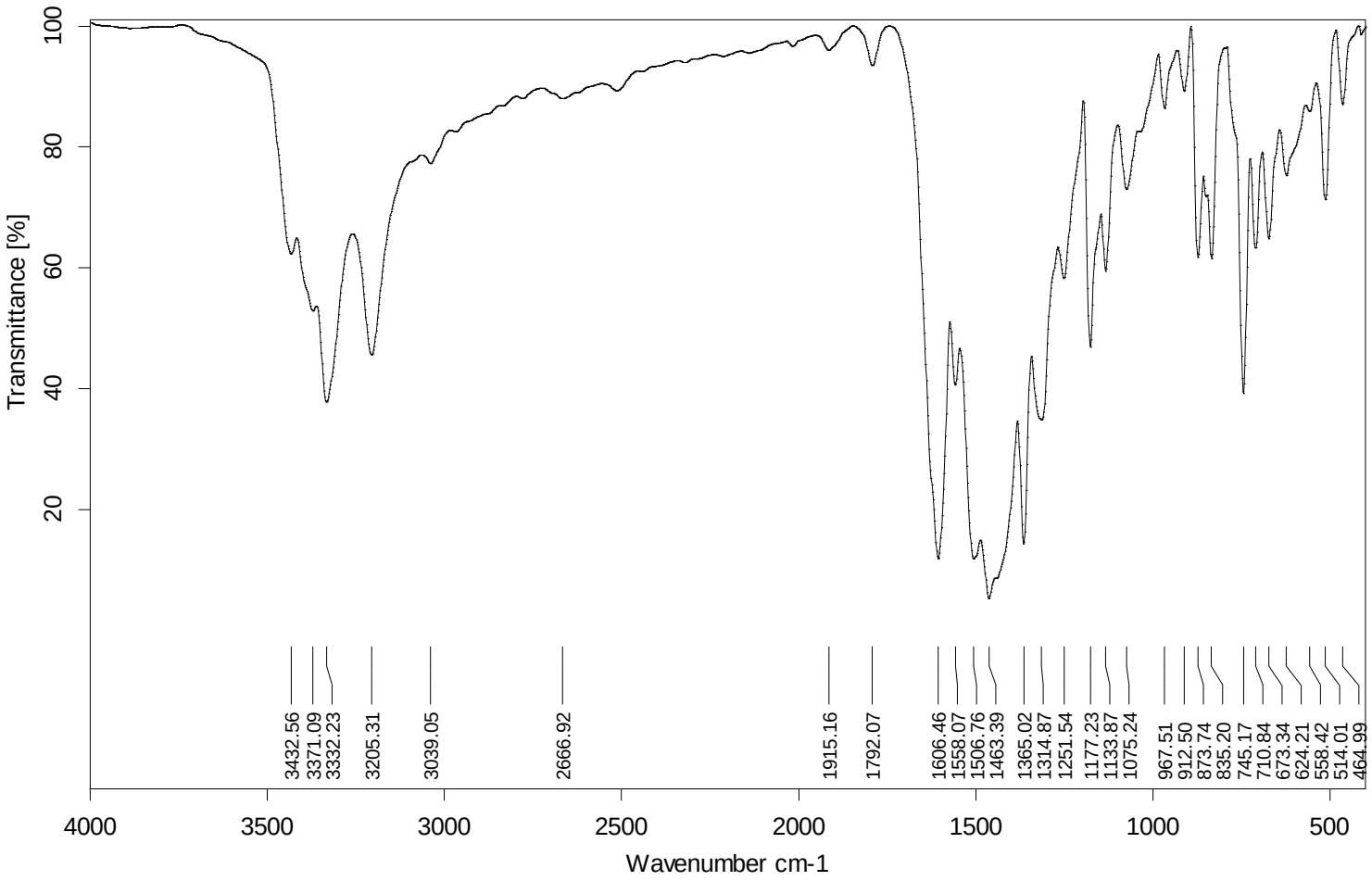

Figure 36. IR of **3b**

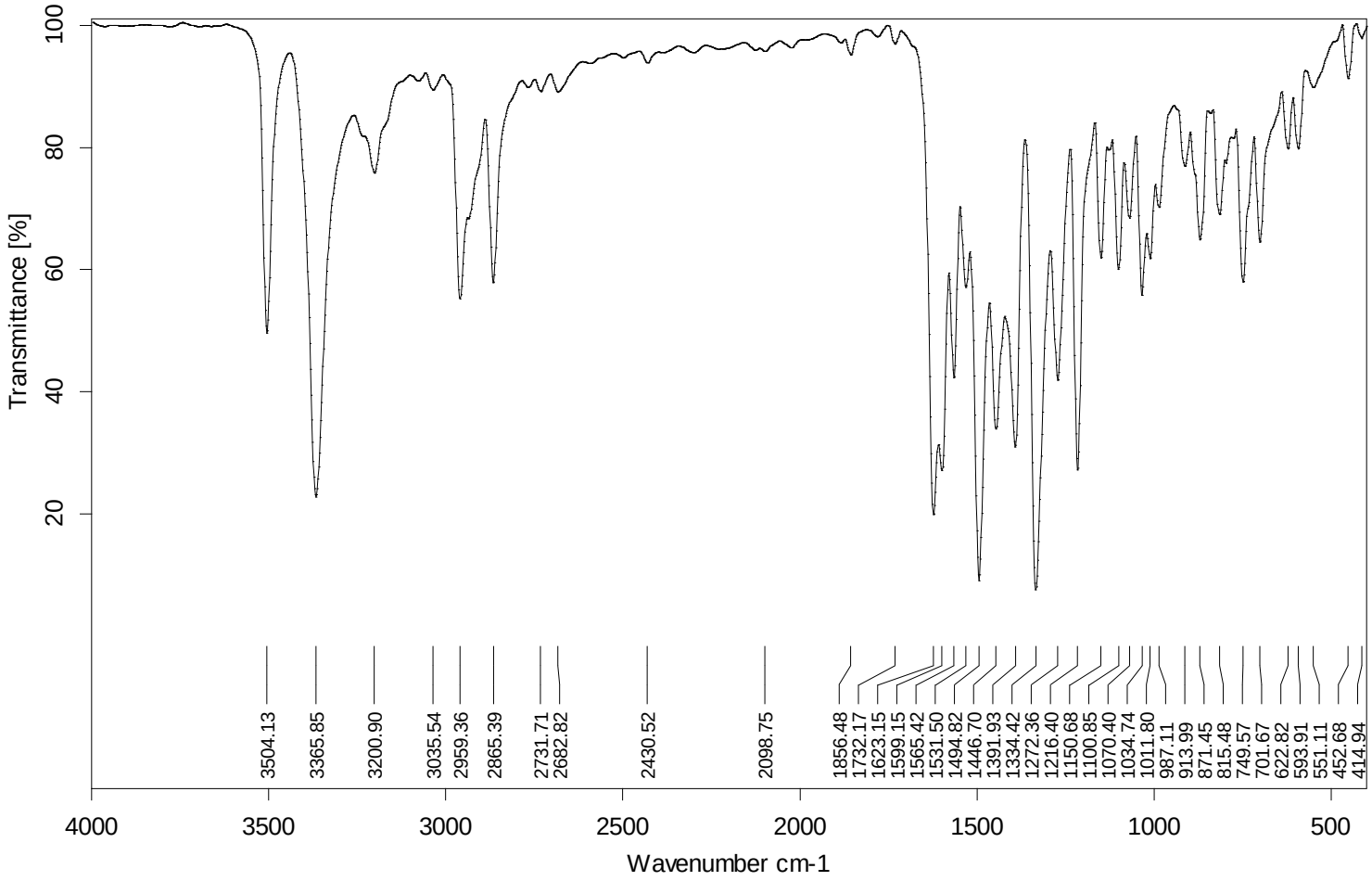

Figure 37. IR of **4a**

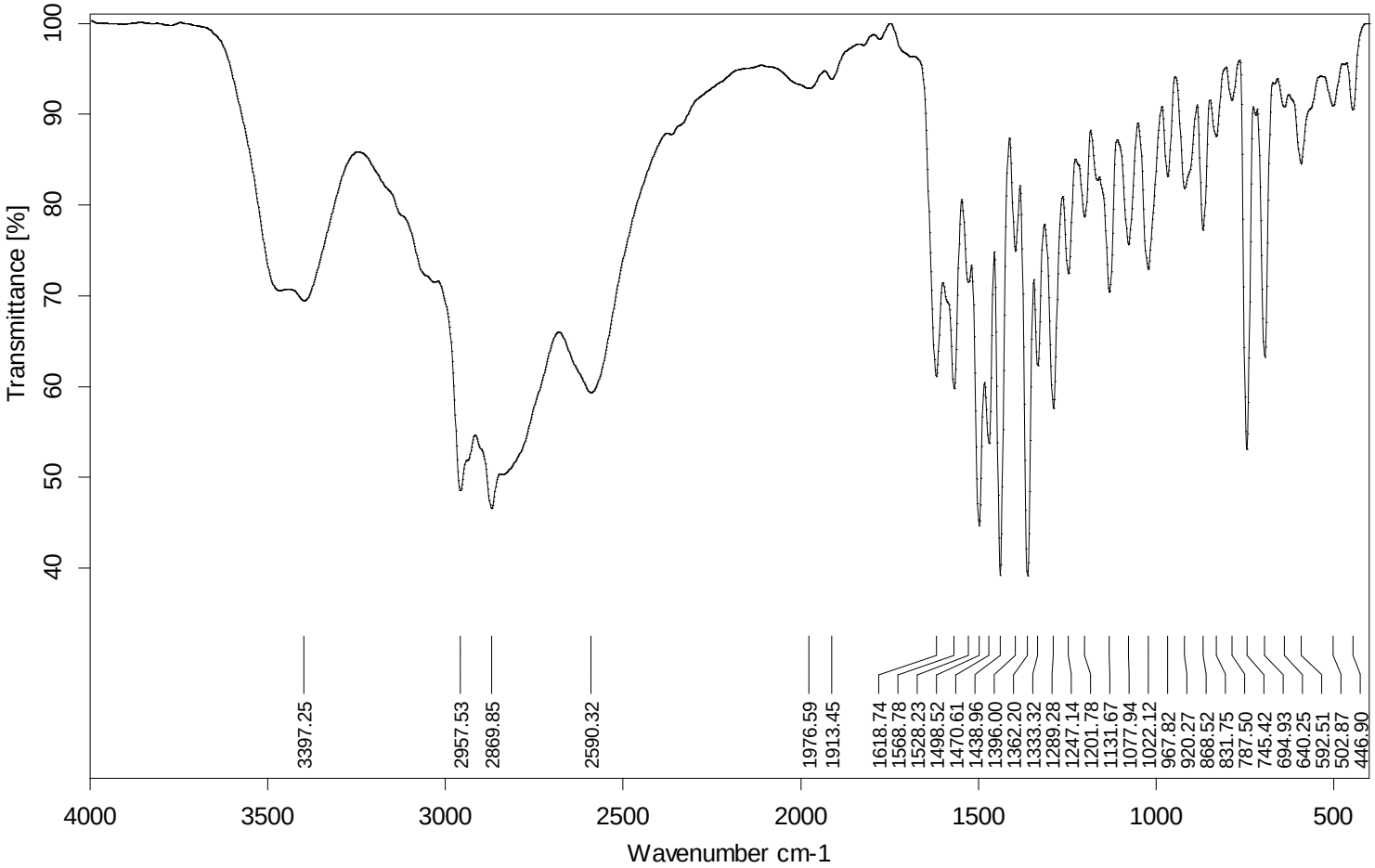

Figure 38. IR of **4b**

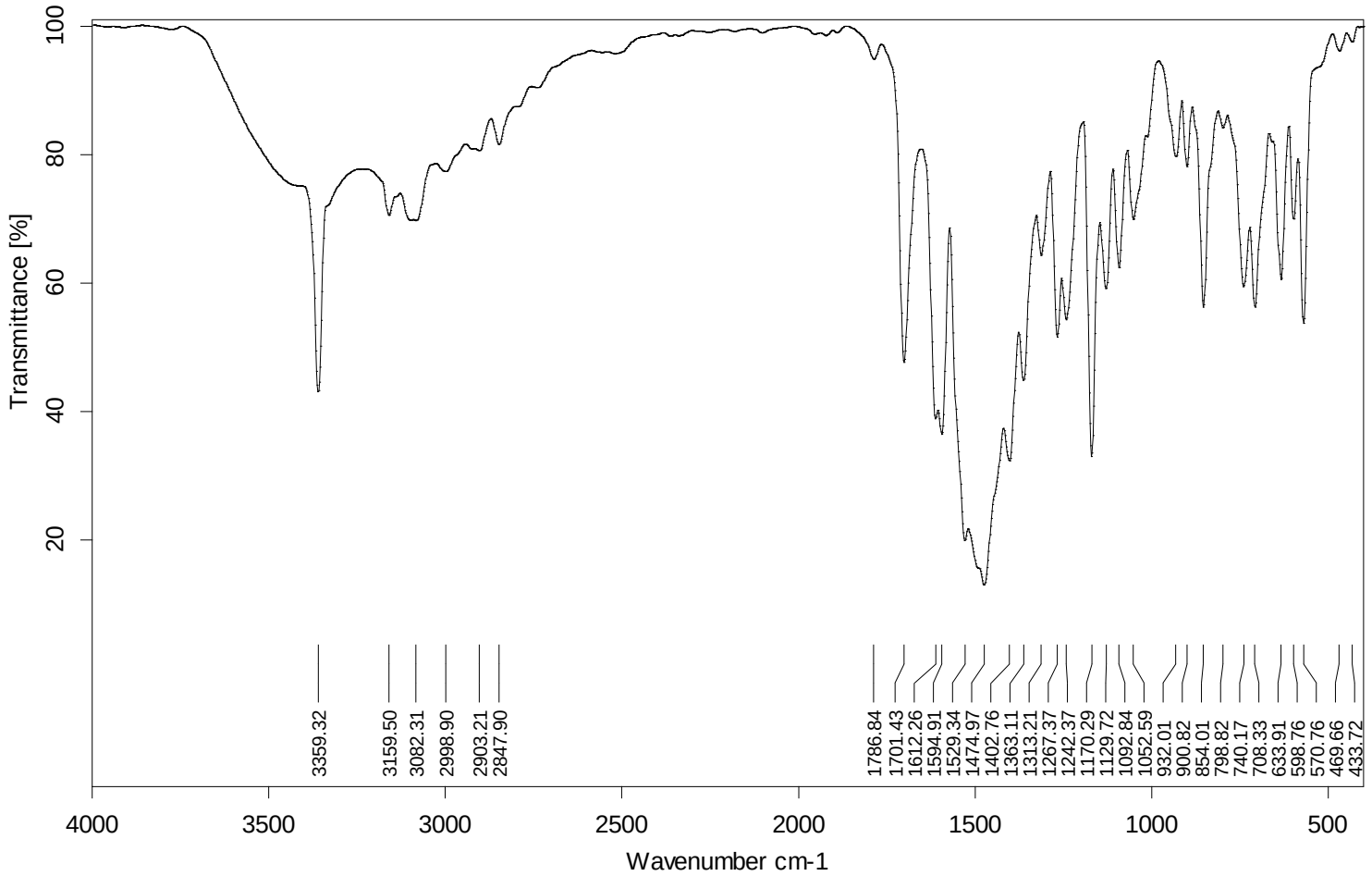

Figure 39. IR of **6**

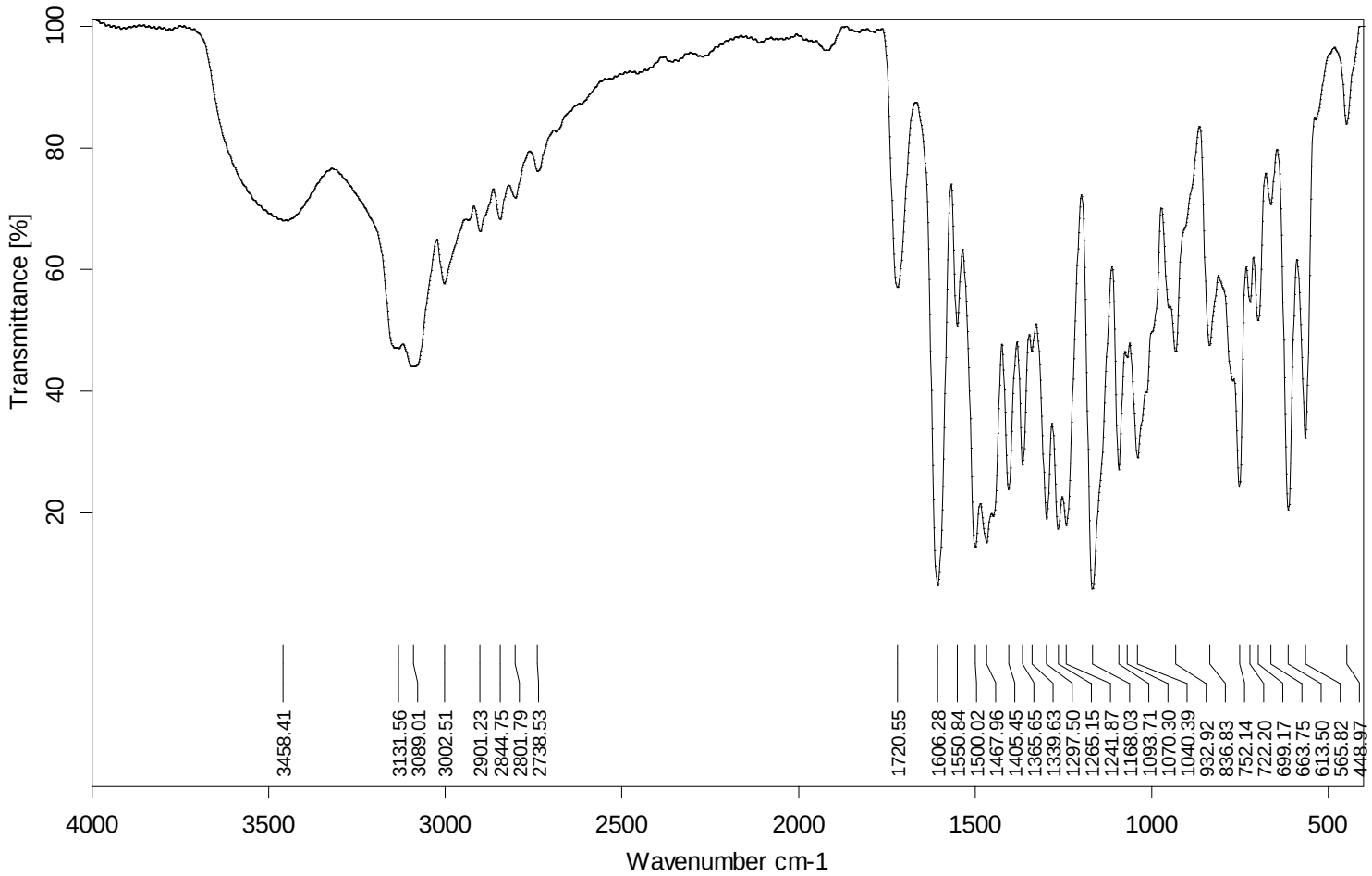

Figure 40. IR of **9a**

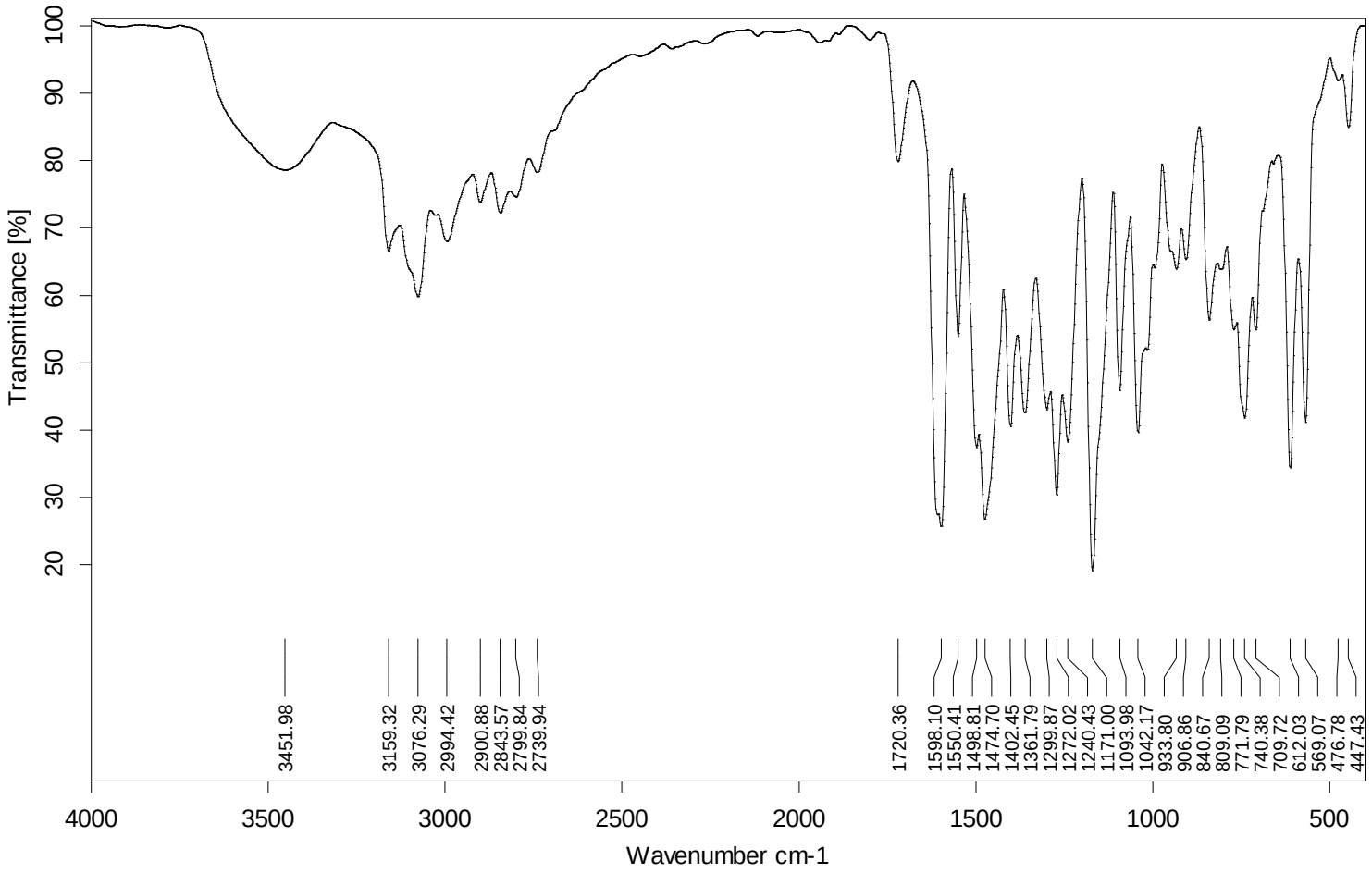

Figure 41. IR of **9b**

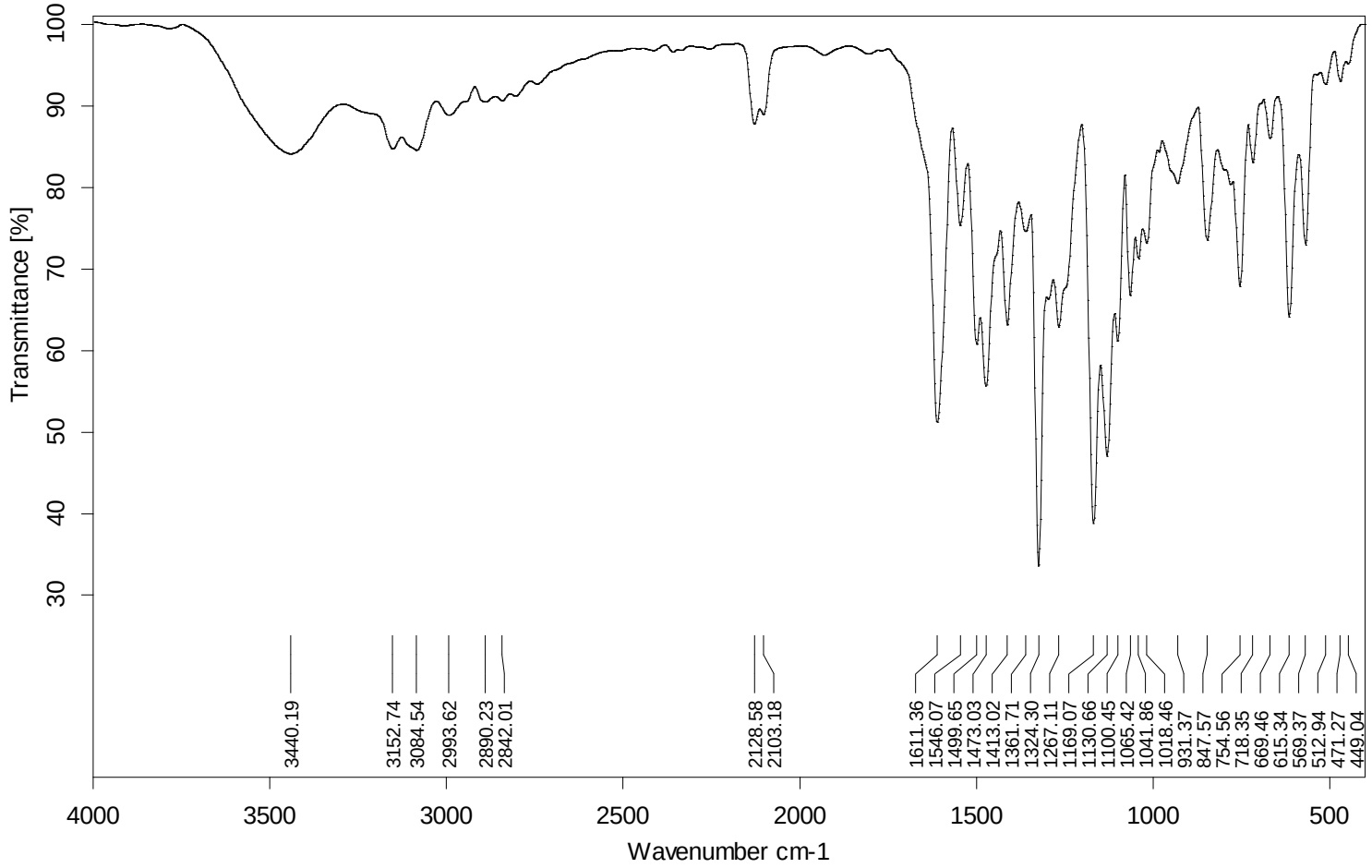

Figure 42. IR of **3b**

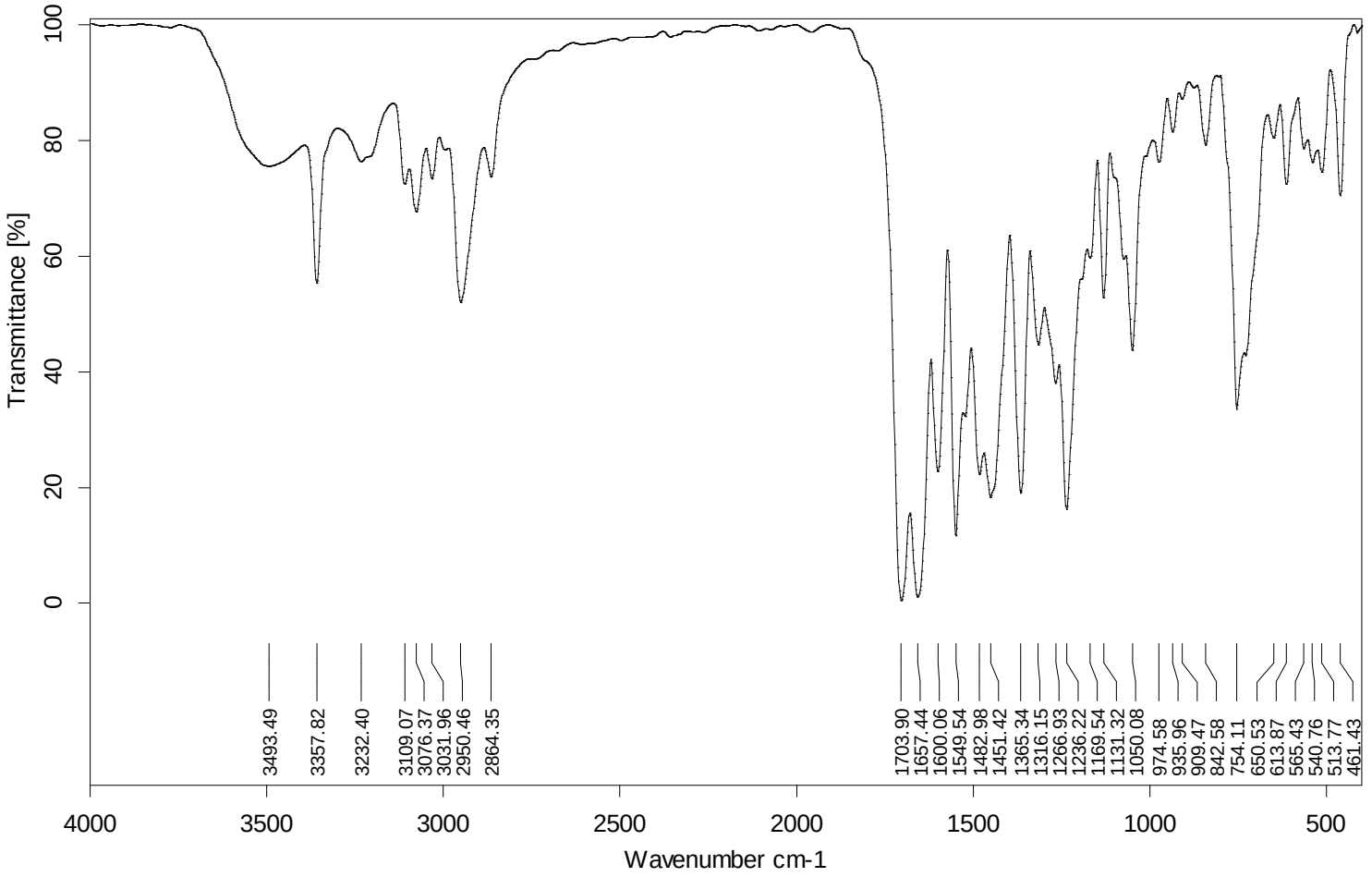

Figure 43. IR of **12**

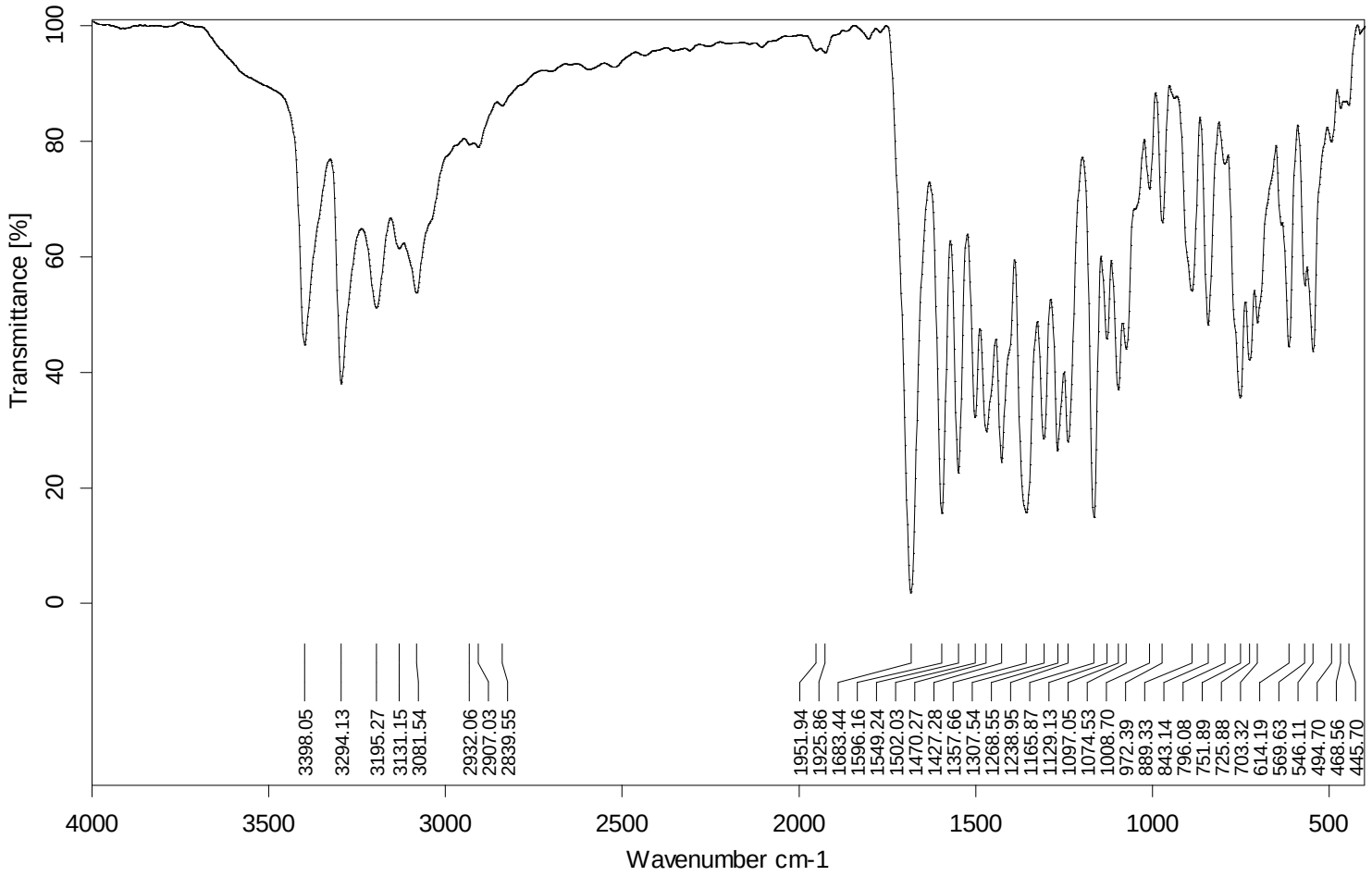

Figure 44. IR of **13a**

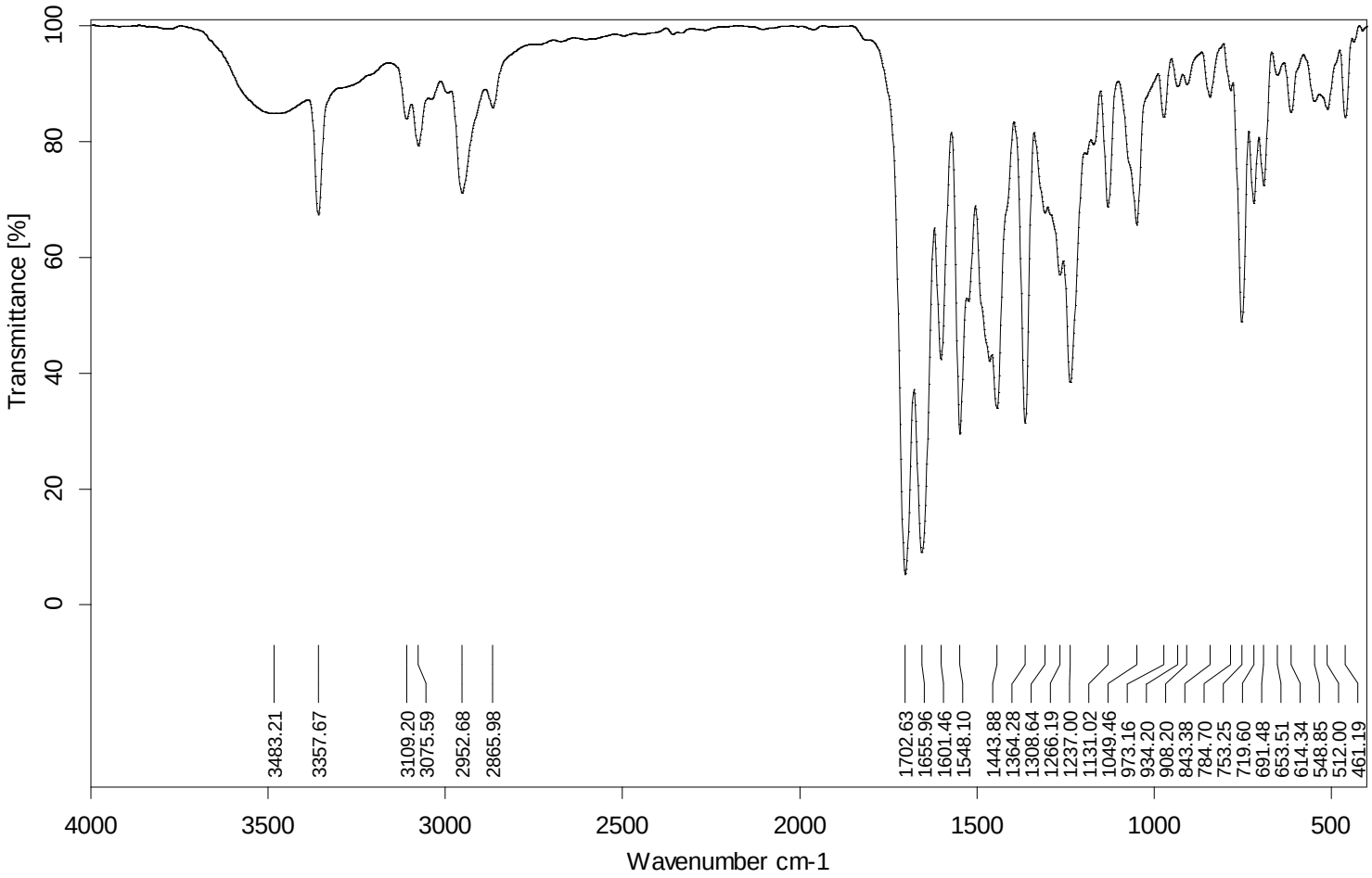

Figure 45. IR of **13b**

3. Molecular modelling

Table 1: 2D diagram and 3D representation of molecular docking of all compounds in the binding pocket (PDB: 7E3H).

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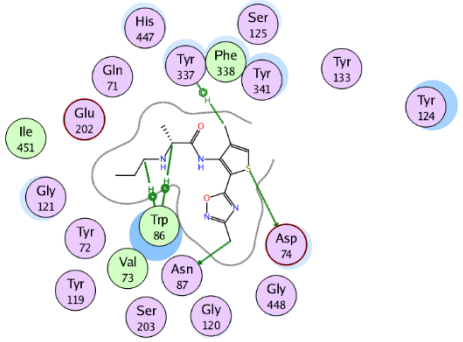
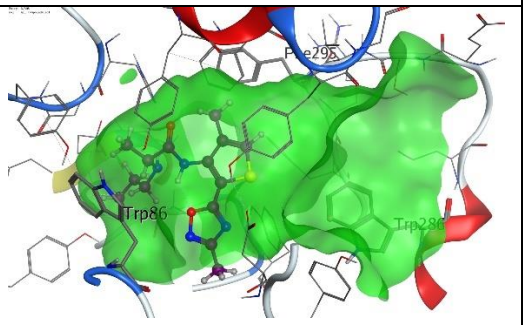
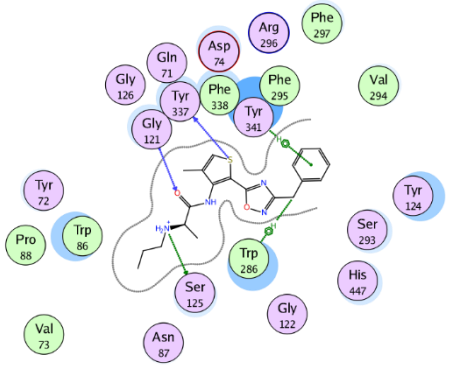
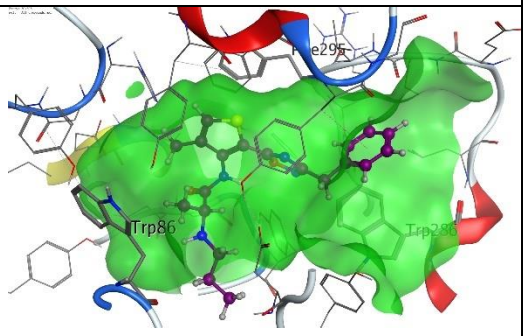
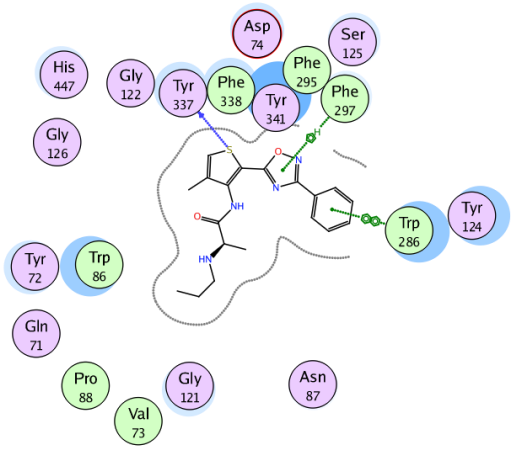
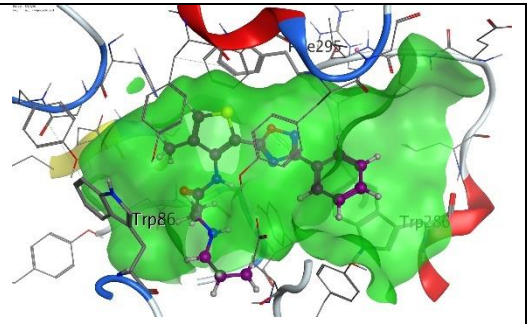
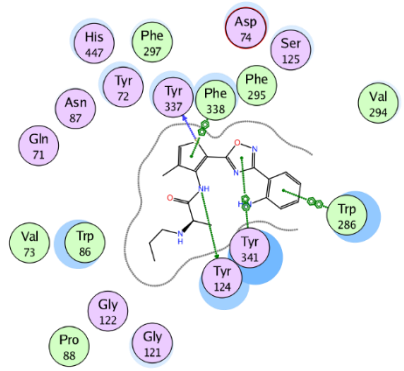
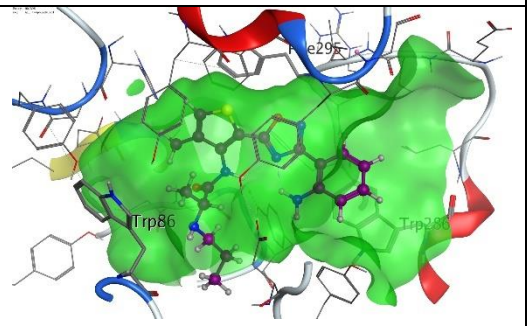
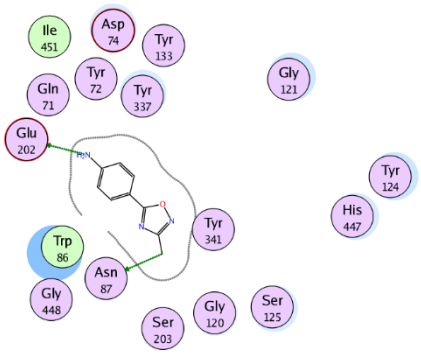
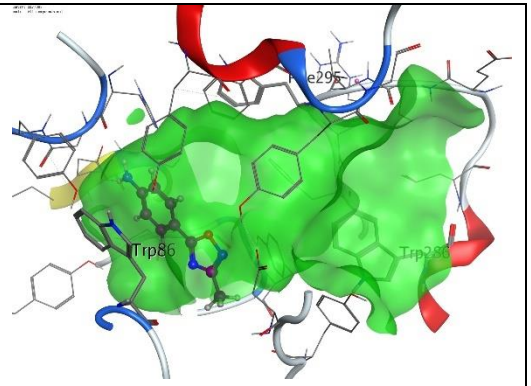
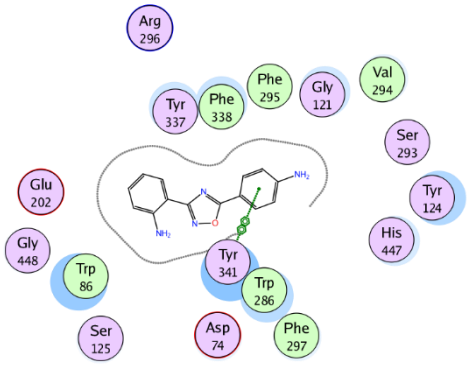
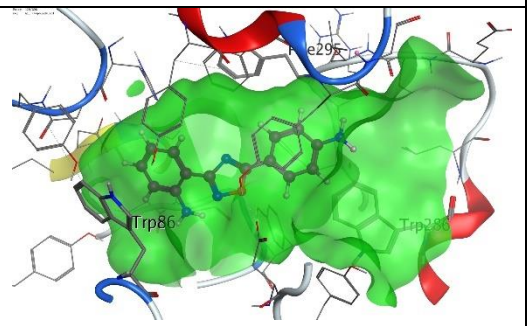
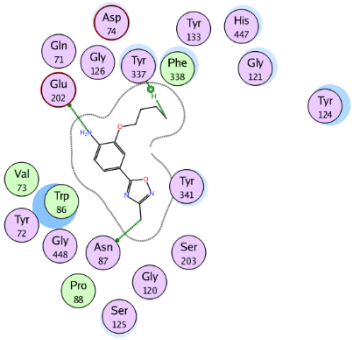
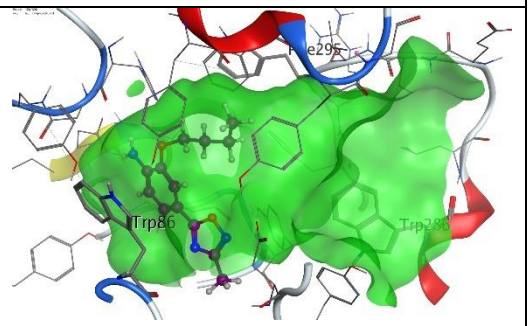
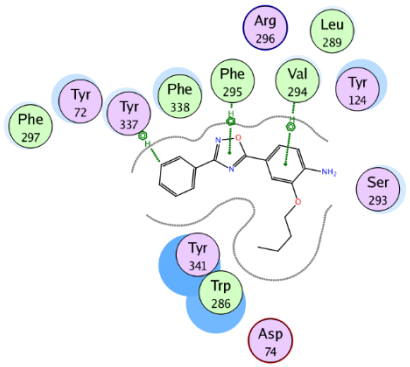
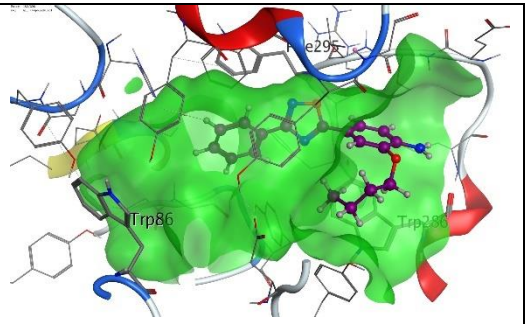
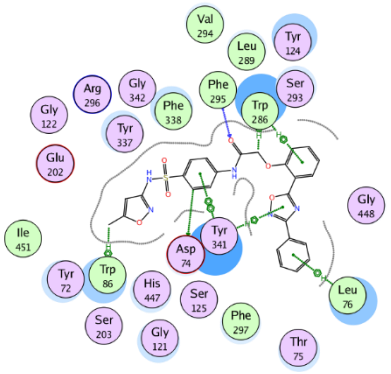
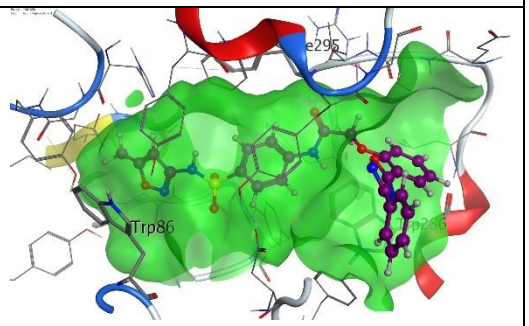
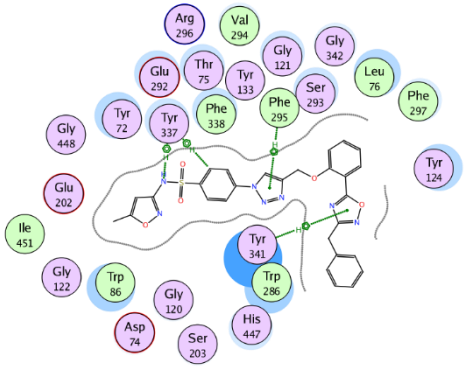
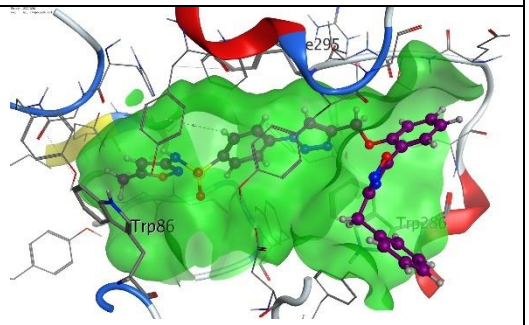
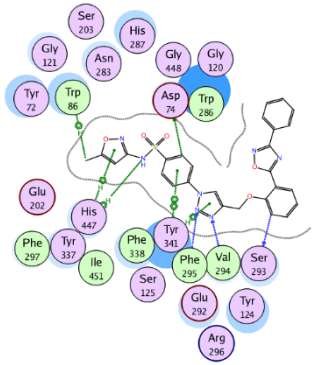
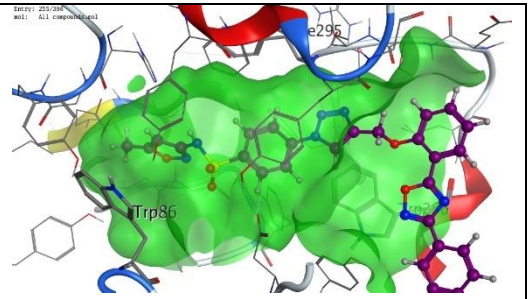
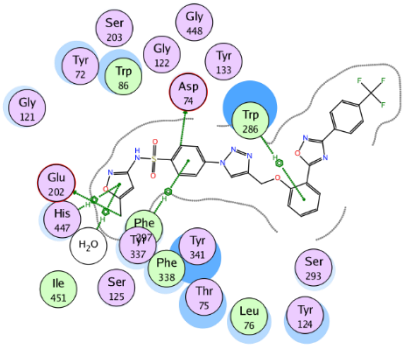
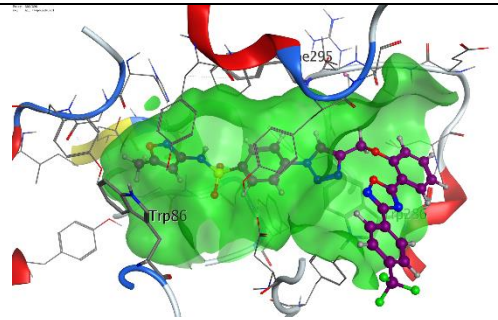
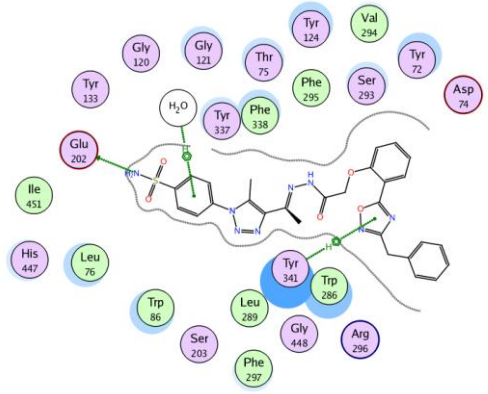
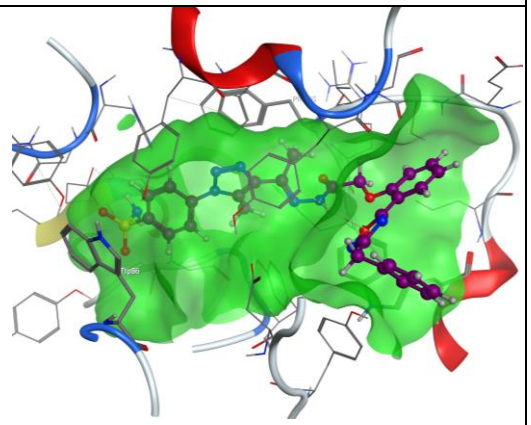
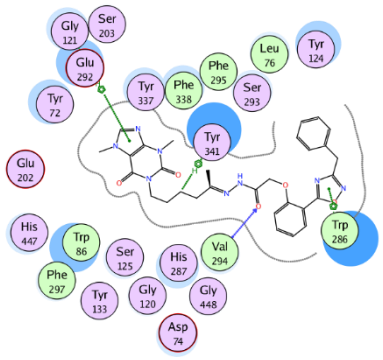
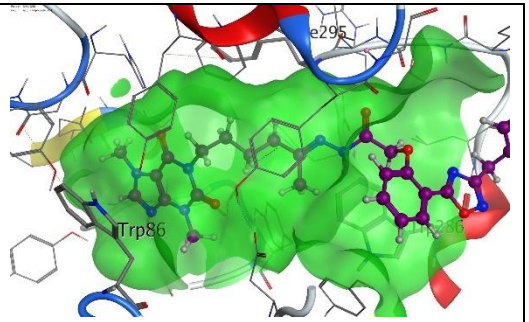
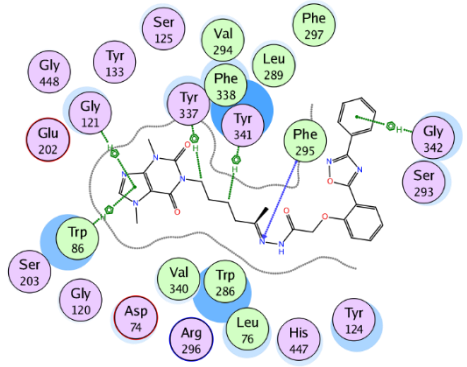
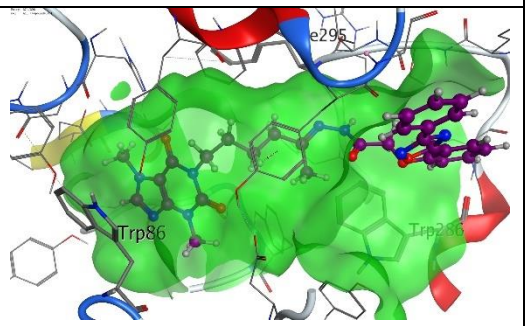
2a		
2b		

2c	 Asp 74 Ser 125 His 447 Gly 122 Tyr 337 Phe 338 Phe 295 Tyr 341 Phe 297 Gly 126 Tyr 124 Trp 286 Tyr 72 Trp 86 Gln 71 Pro 88 Gly 121 Asn 87 Val 73	 Phe295 Trp86 Trp286
2d	 Asp 74 His 447 Phe 297 Ser 125 Tyr 72 Tyr 337 Phe 338 Phe 295 Asn 87 Val 294 Gln 71 Trp 286 Val 73 Trp 86 Tyr 341 Tyr 124 Gly 122 Pro 88 Gly 121	 Phe295 Trp86 Trp286

3a	 Ile 451 Asp 74 Tyr 133 Tyr 72 Tyr 337 Gly 121 Gln 71 Glu 202 Tyr 124 His 447 Tyr 341 Trp 86 Asn 87 Gly 448 Gly 120 Ser 125 Ser 203	 Phe295 Trp86 Trp286
3b	 Arg 296 Phe 295 Gly 121 Val 294 Tyr 337 Phe 338 Ser 293 Glu 202 Tyr 124 His 447 Gly 448 Tyr 341 Trp 86 Trp 286 Ser 125 Asp 74 Phe 297	 Phe295 Trp86 Trp286
4a	 Asp 74 Tyr 133 His 447 Gln 71 Gly 126 Tyr 337 Phe 338 Gly 121 Glu 202 Tyr 124 Val 73 Trp 86 Tyr 341 Tyr 72 Gly 448 Asn 87 Ser 203 Gly 120 Pro 88 Ser 125	 Phe295 Trp86 Trp286

4b	 Arg 296 Leu 289 Phe 295 Val 294 Tyr 72 Tyr 337 Phe 338 Tyr 124 Phe 297 Ser 293 Tyr 341 Trp 286 Asp 74	 Phe295 Trp86 Trp286
6	 Val 294 Leu 289 Tyr 124 Arg 296 Gly 342 Phe 295 Ser 293 Gly 122 Phe 338 Trp 286 Tyr 337 Glu 202 Gly 448 Ile 451 Tyr 341 Asp 74 Tyr 72 Trp 86 His 447 Ser 125 Leu 76 Ser 203 Phe 297 Gly 121 Thr 75	 e295 Trp86
9a	 Arg 296 Val 294 Gly 342 Gly 121 Glu 292 Thr 75 Tyr 133 Leu 76 Ser 293 Phe 297 Tyr 72 Tyr 337 Phe 295 Phe 338 Gly 448 Tyr 124 Glu 202 Ile 451 Tyr 341 Gly 122 Trp 86 Trp 286 Gly 120 His 447 Asp 74 Ser 203	 e295 Trp86

9b	 Ser 203 His 287 Gly 121 Asn 283 Gly 448 Gly 120 Tyr 72 Trp 86 Asp 74 Trp 286 Glu 202 His 447 Phe 297 Tyr 337 Ile 451 Phe 338 Tyr 341 Phe 295 Val 294 Ser 293 Ser 125 Glu 292 Tyr 124 Arg 296	 e295 Trp86
9c	 Ser 203 Gly 448 Tyr 72 Gly 122 Tyr 133 Trp 86 Gly 121 Asp 74 Trp 286 Glu 202 His 447 Phe 297 Tyr 337 Tyr 341 Phe 338 Ser 293 Ile 451 Ser 125 Thr 75 Leu 76 Tyr 124	 e295 Trp86
12	 Tyr 124 Val 294 Gly 120 Gly 121 Thr 75 Tyr 72 Tyr 133 Phe 295 Ser 293 Asp 74 Tyr 337 Phe 338 Glu 202 Ile 451 His 447 Leu 76 Tyr 341 Trp 286 Trp 86 Leu 289 Gly 448 Arg 296 Ser 203 Phe 297	

13a	 Gly 121 Ser 203 Glu 292 Tyr 72 Tyr 337 Phe 338 Phe 295 Ser 293 Leu 76 Tyr 124 Tyr 341 Glu 202 His 447 Trp 86 Ser 125 His 287 Val 294 Trp 286 Phe 297 Tyr 133 Gly 120 Gly 448 Asp 74	 e295 Trp86
13b	 Ser 125 Val 294 Phe 297 Gly 448 Tyr 133 Leu 289 Phe 338 Tyr 337 Gly 121 Tyr 341 Phe 295 Gly 342 Glu 202 Ser 293 Trp 86 Ser 203 Val 340 Trp 286 Gly 120 Asp 74 Leu 76 Tyr 124 Arg 296 His 447	 e295 Trp86

4. ADME study

Table 2. Physicochemical properties and ADME properties of the target compounds.

Compd.	MW (g/mol) <500	#H-bond acceptors <10	#H-bond donors <5	TPSA (Å^2) <140	Log P o/w <5	GI absorption	BBB permeant	Lipinski #violations	Bioavailability Score	PAINS #alerts
2a	308.4	5	2	108.29	1.21	High	No	0	0.55	0
2b	385.5	4	2	112.87	-1.26	High	No	0	0.55	0
2c	370.47	5	2	108.29	2.47	High	No	0	0.55	0
2d	385.48	5	3	134.31	1.94	Low	No	0	0.55	0
3a	175.19	3	1	64.94	1.08	High	Yes	0	0.55	0
3b	252.27	3	2	90.96	1.96	High	No	0	0.55	0
4a	247.29	4	1	74.17	1.67	High	Yes	0	0.55	0
4b	309.36	4	1	74.17	2.95	High	Yes	0	0.55	0
6	531.54	9	2	157.83	1.82	Low	No	2	0.17	0
9a	569.59	10	1	159.44	2.58	Low	No	2	0.17	0
9b	555.56	10	1	159.44	2.38	Low	No	2	0.17	0
9c	623.56	13	1	159.44	2.87	Low	No	2	0.17	0
12	586.62	11	2	188.86	1.87	Low	No	2	0.17	0
13a	584.63	9	1	151.43	2.29	Low	No	2	0.17	0
13b	570.6	9	1	151.43	2.09	Low	No	2	0.17	0
Donepezil HCl	379.49	4	0	38.77	3.06	High	Yes	0	0.55	0

5. Biological activities detailed results.

a) AChE inhibitory assay results

SAMPLE	%AChE INHIBITION	SD	ng/ml	nmole	nM
2c_1	0	0	2.083333	0.005623	5.623487
2c_2	0.436681223	0.202	4.166667	0.011247	11.24697
2c_3	5.676855895	0.274	8.333333	0.022494	22.49395
2c_4	24.45414847	0.214	16.66667	0.044988	44.9879
2c_5	41.92139738	0.237	33.33333	0.089976	89.9758
2b_1	0	0	2.083333	0.005418	5.418292
2b_2	6.986899563	0.21	4.166667	0.010837	10.83658
2b_3	24.45414847	0.242	8.333333	0.021673	21.67317
2b_4	70.74235808	0.28	16.66667	0.043346	43.34634
2b_5	75.98253275	0.302	33.33333	0.086693	86.69267
2d_1	18.77729258	0.234	2.083333	0.005404	5.404377
2d_2	23.58078603	0.217	4.166667	0.010809	10.80875
2d_3	31.44104803	0.283	8.333333	0.021618	21.61751
2d_4	36.24454148	0.261	16.66667	0.043235	43.23502
2d_5	39.30131004	0.237	33.33333	0.08647	86.47003
2a_1	2.183406114	0.216	2.083333	0.006755	6.755296
2a_2	3.056768559	0.225	4.166667	0.013511	13.51059
2a_3	8.296943231	0.234	8.333333	0.027021	27.02118
2a_4	16.59388646	0.234	16.66667	0.054042	54.04237
2a_5	26.20087336	0.237	33.33333	0.108085	108.0847
3a_1	2.620087336	0.236	2.083333	0.008258	8.25802
3a_2	10.48034934	0.221	4.166667	0.016516	16.51604
3a_3	24.45414847	0.259	8.333333	0.033032	33.03208
3a_4	51.09170306	0.294	16.66667	0.066064	66.06416
3a_5	53.27510917	0.276	33.33333	0.132128	132.1283
3b_1	0	0.23	2.083333	0.011892	11.89185

3b_2	0	0.22	4.166667	0.023784	23.7837
3b_3	0	0.201	8.333333	0.047567	47.5674
3b_4	33.18777293	0.238	16.66667	0.095135	95.13481
3b_5	43.23144105	0.239	33.33333	0.19027	190.2696
4a_1	18.34061135	0.279	2.083333	0.008424	8.424316
4a_2	25.76419214	0.236	4.166667	0.016849	16.84863
4a_3	47.59825328	0.272	8.333333	0.033697	33.69726
4a_4	54.14847162	0.255	16.66667	0.067395	67.39453
4a_5	86.02620087	0.428	33.33333	0.134789	134.7891
4b_1	24.01746725	0.502	2.083333	0.006742	6.742179
4b_2	47.16157205	0.256	4.166667	0.013484	13.48436
4b_3	79.91266376	0.499	8.333333	0.026969	26.96872
4b_4	84.71615721	0.388	16.66667	0.053937	53.93743
4b_5	85.15283843	0.317	33.33333	0.107875	107.8749
9a_1	0	0	2.083333	0.00375	3.749903
9a_2	0	0	4.166667	0.0075	7.499805
9a_3	3.930131004	0.241	8.333333	0.015	14.99961
9a_4	13.5371179	0.265	16.66667	0.029999	29.99922
9a_5	26.63755459	0.394	33.33333	0.059998	59.99844
9c_1	42.79475983	0.264	2.083333	0.003658	3.657537
9c_2	13.5371179	0.279	4.166667	0.007315	7.315075
9c_3	-1.746724891	0.25	8.333333	0.01463	14.63015
9c_4	-37.99126638	0.312	16.66667	0.02926	29.2603
9c_5	-82.96943231	0.433	33.33333	0.058521	58.5206
6_1	4.366812227	0.244	2.083333	0.003341	3.340977
6_2	4.366812227	0.203	4.166667	0.006682	6.681955
6_3	6.550218341	0.228	8.333333	0.013364	13.36391
6_4	21.83406114	0.217	16.66667	0.026728	26.72782
6_5	32.31441048	0.222	33.33333	0.053456	53.45564
12_1	0	0	2.083333	0.003919	3.919429

12_2	-2.183406114	0.265	4.166667	0.007839	7.838858
12_3	-12.66375546	0.321	8.333333	0.015678	15.67772
12_4	-17.03056769	0.39	16.66667	0.031355	31.35543
12_5	-32.7510917	0.537	33.33333	0.062711	62.71087
3b_1	33.18777293	0.228	2.083333	0.003551	3.551358
3b_2	21.39737991	0.23	4.166667	0.007103	7.102717
3b_3	11.79039301	0.252	8.333333	0.014205	14.20543
3b_4	9.170305677	0.23	16.66667	0.028411	28.41087
3b_5	3.493449782	0.42	33.33333	0.056822	56.82173
3a_1	0	0	2.083333	0.003563	3.563446
3a_2	0	0	4.166667	0.007127	7.126893
3a_3	-34.06113537	0.195	8.333333	0.014254	14.25379
3a_4	-55.45851528	0.212	16.66667	0.028508	28.50757
3a_5	-81.65938865	0.502	33.33333	0.057015	57.01514
9b_1	-13.5371179	0.268	2.083333	0.003651	3.651063
9b_2	-9.6069869	0.288	4.166667	0.007302	7.302127
9b_3	2.620087336	0.217	8.333333	0.014604	14.60425
9b_4	9.6069869	0.416	16.66667	0.029209	29.20851
9b_5	10.04	0.306	33.33333	0.058417	58.41702
donepezil HCl_1	3.930131004	0.241	2.083333	0.005008	5.008013
donepezil HCl_2	7.860262009	0.252	4.166667	0.010016	10.01603
donepezil HCl_3	45.85152838	0.472	8.333333	0.020032	20.03205
donepezil HCl_4	50.65502183	0.339	16.66667	0.040064	40.0641
donepezil HCl_5	51.52838428	1.327	33.33333	0.080128	80.12821

b) 1,1-Diphenyl-2-picrylhydrazyl (DPPH) radical scavenging activity results

SAMPLE	DPPH SCAVENGING%	SD	ug/ml	umole	uM
2c_1	2.88	0.1	6.25	0.005501	5.501422
2c_2	7.00	0.3	12.5	0.011003	11.00284
2c_3	11.11	0.4	25	0.022006	22.00569
2c_4	13.99	0.3	50	0.044011	44.01137
2c_5	14.20	0.5	100	0.088023	88.02275
2b_1	4.94	0.1	6.25	0.011219	11.21942
2b_2	6.38	0.05	12.5	0.022439	22.43883
2b_3	8.44	0.03	25	0.044878	44.87766
2b_4	10.91	0.8	50	0.089755	89.75533
2b_5	13.37	0.4	100	0.179511	179.5107
2d_1	4.32	0.01	6.25	0.004448	4.44824
2d_2	4.94	0.03	12.5	0.008896	8.896481
2d_3	9.67	0.08	25	0.017793	17.79296
2d_4	13.58	1.1	50	0.035586	35.58592
2d_5	15.64	1.2	100	0.071172	71.17184
2a_1	7.82	0.07	6.25	0.003361	3.360757
2a_2	8.02	0.08	12.5	0.006722	6.721514
2a_3	8.64	0.1	25	0.013443	13.44303
2a_4	10.08	1.1	50	0.026886	26.88606
2a_5	15.64	0.9	100	0.053772	53.77211
3a_1	2.47	0.02	6.25	0.00793	7.930063
3a_2	11.11	1.1	12.5	0.01586	15.86013
3a_3	12.55	0.9	25	0.03172	31.72025
3a_4	16.46	0.8	50	0.063441	63.44051
3a_5	21.40	1.8	100	0.126881	126.881

3b_1	0.00	0	6.25	0.005925	5.925294
3b_2	1.65	0.003	12.5	0.011851	11.85059
3b_3	7.61	0.1	25	0.023701	23.70118
3b_4	9.47	0.2	50	0.047402	47.40235
3b_5	11.52	0.4	100	0.094805	94.8047
4a_1	0.00	0	6.25	0.053355	53.35496
4a_2	6.17	0.03	12.5	0.10671	106.7099
4a_3	6.58	0.5	25	0.21342	213.4198
4a_4	13.17	0.3	50	0.42684	426.8397
4a_5	17.49	0.4	100	0.853679	853.6794
4b_1	31.69	0.1	6.25	0.003534	3.534168
4b_2	49.79	0.3	12.5	0.007068	7.068337
4b_3	60.29	0.6	25	0.014137	14.13667
4b_4	72.63	1.5	50	0.028273	28.27335
4b_5	78.81	1.9	100	0.056547	56.54669
9a_1	5.14	0.05	6.25	0.003534	3.534168
9a_2	8.02	0.03	12.5	0.007068	7.068337
9a_3	11.11	1.1	25	0.014137	14.13667
9a_4	11.93	0.03	50	0.028273	28.27335
9a_5	17.08	1.1	100	0.056547	56.54669
9c_1	0.00	0	6.25	0.010973	10.97261
9c_2	0.00	0	12.5	0.021945	21.94522
9c_3	4.12	0.01	25	0.04389	43.89045
9c_4	6.79	0.2	50	0.087781	87.7809
9c_5	9.47	0.3	100	0.175562	175.5618
6_1	0.00		6.25	0.00415	4.150397
6_2	0.00		12.5	0.008301	8.300794
6_3	0.00		25	0.016602	16.60159
6_4	2.06	0.03	50	0.033203	33.20318
6_5	5.76	0.05	100	0.066406	66.40635

12_1	10.49	0.06	6.25	0.011758	11.75829
12_2	13.58	0.4	12.5	0.023517	23.51657
12_3	17.08	0.9	25	0.047033	47.03315
12_4	17.28	0.8	50	0.094066	94.0663
12_5	18.72	1.1	100	0.188133	188.1326
3b_1	8.64	0.05	6.25	0.003782	3.781851
3b_2	10.91	0.03	12.5	0.007564	7.563701
3b_3	14.20	1.4	25	0.015127	15.1274
3b_4	15.43	1.2	50	0.030255	30.25481
3b_5	18.52	1.8	100	0.06051	60.50961
3a_1	10.70	0.8	6.25	0.01069	10.69034
3a_2	12.14	0.6	12.5	0.021381	21.38068
3a_3	14.40	0.9	25	0.042761	42.76136
3a_4	15.84	0.8	50	0.085523	85.52271
3a_5	21.60	2.1	100	0.171045	171.0454
9b_1	1.97	0.003	6.25	0.003594	3.59375
9b_2	4.18	0.1	12.5	0.007188	7.1875
9b_3	9.21	0.8	25	0.014375	14.375
9b_4	10.93	0.8	50	0.02875	28.75
9b_5	17.44	1.2	100	0.0575	57.5

c) MAO-B inhibitory assay results

SAMPLE	% INHIBITION	SD	**ug/ml**	**umole**	**uM**
2c_1	-8.67362E-14	3.00E-17	8.928571	0.024101	24.10066
2c_2	-8.67362E-14	7.00E-17	17.85714	0.048201	48.20132
2c_3	20	1.1	35.71429	0.096403	96.40264
2c_4	60	3.2	71.42857	0.192805	192.8053
2c_5	80	4.1	142.8571	0.385611	385.6106

2b_1	20	0.9	8.928571	0.023221	23.22125
2b_2	40	1.4	17.85714	0.046443	46.4425
2b_3	40	1.6	35.71429	0.092885	92.88501
2b_4	40	2.3	71.42857	0.18577	185.77
2b_5	40	3.7	142.8571	0.37154	371.54
2d_1	-8.67362E-14	4.00E-19	8.928571	0.023162	23.16162
2d_2	-8.67362E-14	3.00E-17	17.85714	0.046323	46.32323
2d_3	20	0.8	35.71429	0.092646	92.64646
2d_4	40	1.7	71.42857	0.185293	185.2929
2d_5	60	3.5	142.8571	0.370586	370.5859
2a_1	2.13371E-12	1.00E-17	8.928571	0.028951	28.95127
2a_2	-8.67362E-14	4.00E-16	17.85714	0.057903	57.90254
2a_3	-40	2.1	35.71429	0.115805	115.8051
2a_4	-60	3.1	71.42857	0.23161	231.6102
2a_5	-60	2.7	142.8571	0.46322	463.2203
3a_1	-8.67362E-14	3.00E-17	8.928571	0.035392	35.39152
3a_2	-8.67362E-14	4.00E-17	17.85714	0.070783	70.78303
3a_3	-20	1.7	35.71429	0.141566	141.5661
3a_4	-40	1.2	71.42857	0.283132	283.1321
3a_5	-80	2.4	142.8571	0.566264	566.2642
3b_1	-8.67362E-14	3.00E-17	8.928571	0.050965	50.96507
3b_2	-40	3.1	17.85714	0.10193	101.9301
3b_3	-100	3.5	35.71429	0.20386	203.8603
3b_4	-120	8.4	71.42857	0.407721	407.7206
3b_5	-140	6.3	142.8571	0.815441	815.4412

4a_1	-80	4.5	8.928571	0.036104	36.10421
4a_2	-80	4.7	17.85714	0.072208	72.20842
4a_3	-140	6.7	35.71429	0.144417	144.4168
4a_4	-140	6.7	71.42857	0.288834	288.8337
4a_5	-200	9.4	142.8571	0.577667	577.6674
4b_1	-8.67362E-14	3.00E-17	8.928571	0.028895	28.89505
4b_2	-40	3.4	17.85714	0.05779	57.79011
4b_3	-60	5.1	35.71429	0.11558	115.5802
4b_4	-140	11.3	71.42857	0.23116	231.1604
4b_5	-160	12.1	142.8571	0.462321	462.3209
9a_1	-40	0.8	8.928571	0.016071	16.07101
9a_2	-60	3.4	17.85714	0.032142	32.14202
9a_3	-140	9.7	35.71429	0.064284	64.28404
9a_4	-180	8.6	71.42857	0.128568	128.5681
9a_5	-180	10.6	142.8571	0.257136	257.1362
9c_1	-80	7.5	8.928571	0.015675	15.67516
9c_2	-80	6.8	17.85714	0.03135	31.35032
9c_3	-100	9.4	35.71429	0.062701	62.70064
9c_4	-160	8.7	71.42857	0.125401	125.4013
9c_5	-180	11.2	142.8571	0.250803	250.8026
6_1	-8.67362E-14	3.00E-17	8.928571	0.014318	14.31847
6_2	-20	1.1	17.85714	0.028637	28.63695
6_3	-80	2.5	35.71429	0.057274	57.2739
6_4	-120	6.4	71.42857	0.114548	114.5478
6_5	-200	11.7	142.8571	0.229096	229.0956
12_1	-80	4.5	8.928571	0.016798	16.79755
12_2	-100	6.3	17.85714	0.033595	33.59511
12_3	-120	12.3	35.71429	0.06719	67.19021
12_4	-120	10.4	71.42857	0.13438	134.3804

12_5	-140	10.6	142.8571	0.268761	268.7609
3b_1	-8.67362E-14	7.00E-17	8.928571	0.01522	15.22011
3b_2	-40	1.6	17.85714	0.03044	30.44021
3b_3	-100	7.8	35.71429	0.06088	60.88043
3b_4	-160	6.7	71.42857	0.121761	121.7609
3b_5	-180	11.3	142.8571	0.243522	243.5217
3a_1	-40	4.3	8.928571	0.015272	15.27191
3a_2	-60	6.4	17.85714	0.030544	30.54383
3a_3	-80	4.8	35.71429	0.061088	61.08765
3a_4	-80	6.8	71.42857	0.122175	122.1753
3a_5	-100	9.6	142.8571	0.244351	244.3506
9b_1	-20	1.2	8.928571	0.015647	15.64741
9b_2	-80	6.5	17.85714	0.031295	31.29483
9b_3	-100	8.7	35.71429	0.06259	62.58966
9b_4	-100	9.6	71.42857	0.125179	125.1793
9b_5	-120	8.7	142.8571	0.250359	250.3586