

Supplementary Material

Synthesis, photophysical and redox properties of the 2,5,7-tri(het)aryl-[1,2,4]triazolo[1,5-*a*]pyrimidines

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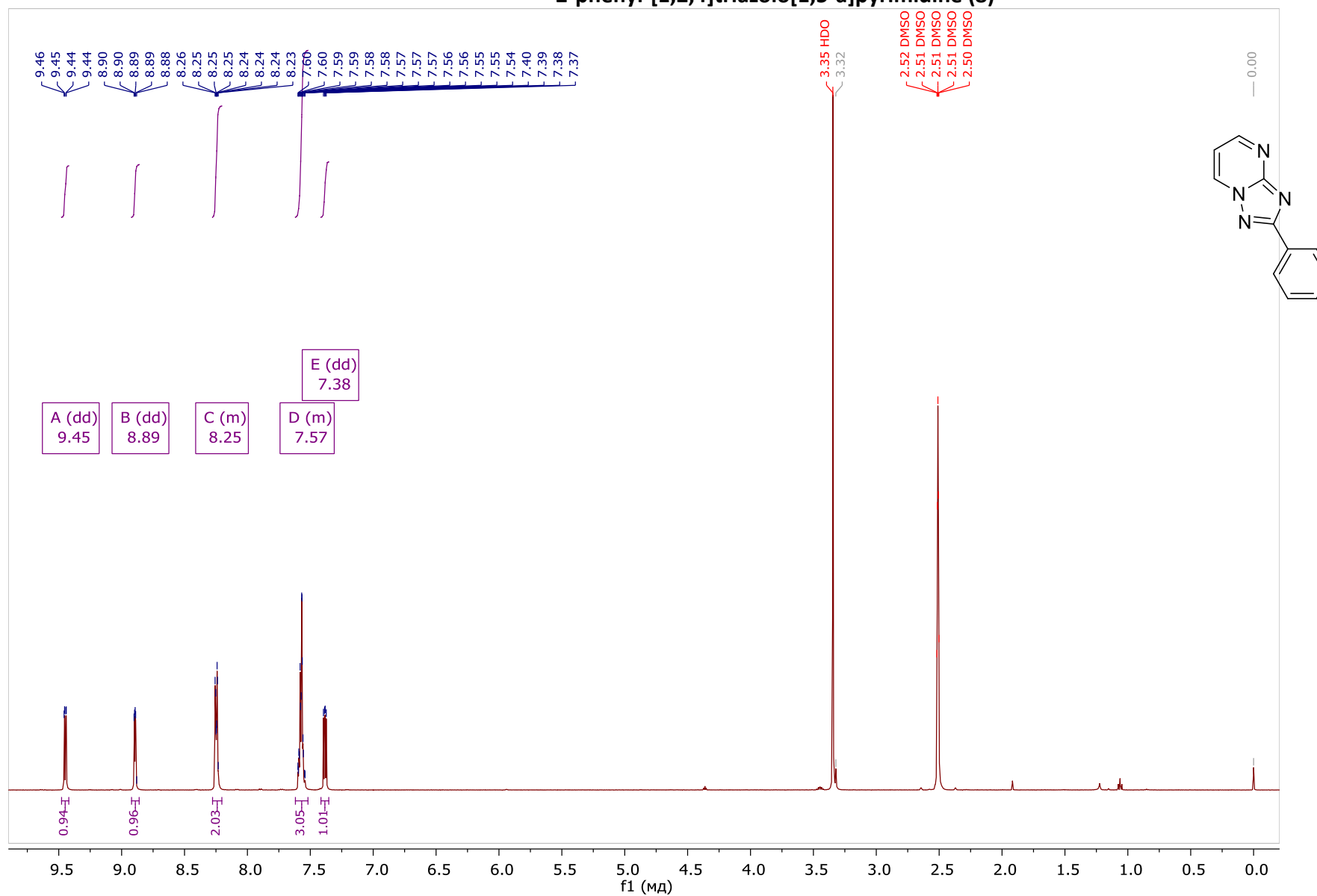
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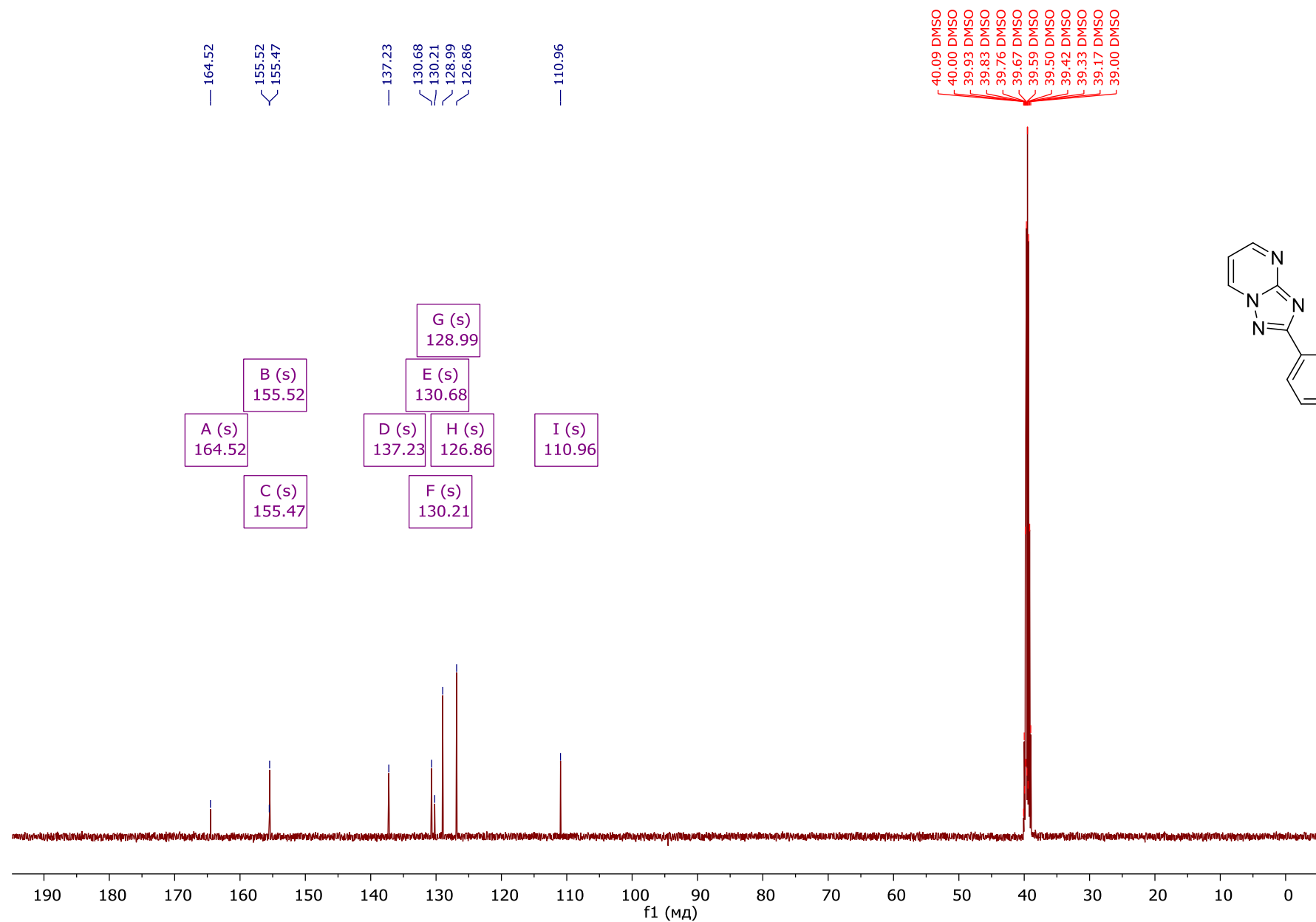
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I. Copies of ^{13}C and ^1H NMR spectra
2-phenyl-[1,2,4]triazolo[1,5-a]pyrimidine (8)

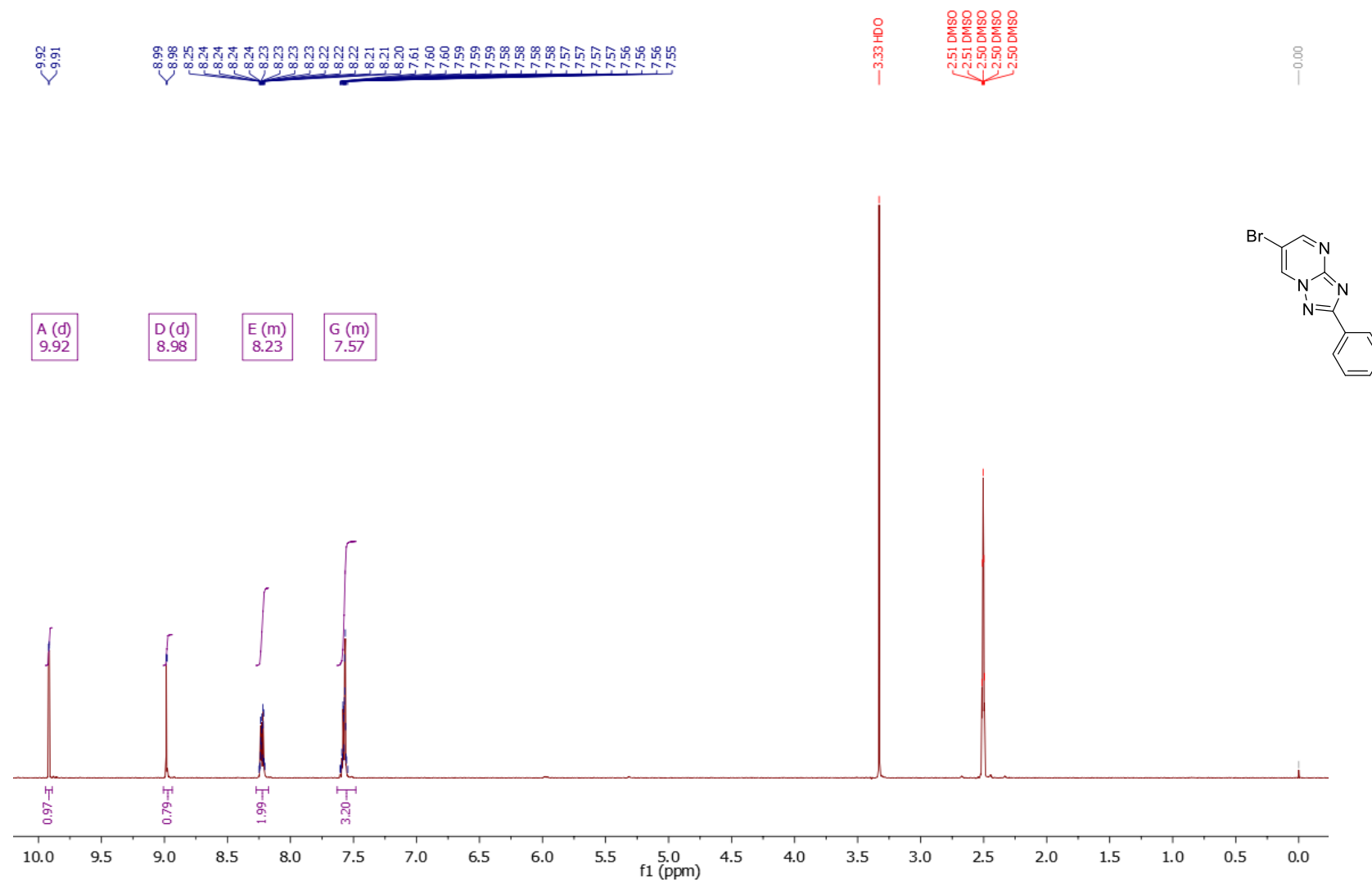


^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 9.45 (dd, $J = 6.8, 1.9$ Hz, 1H), 8.89 (dd, $J = 4.3, 1.9$ Hz, 1H), 8.28 – 8.20 (m, 2H), 7.62 – 7.52 (m, 3H), 7.38 (dd, $J = 6.8, 4.3$ Hz, 1H).

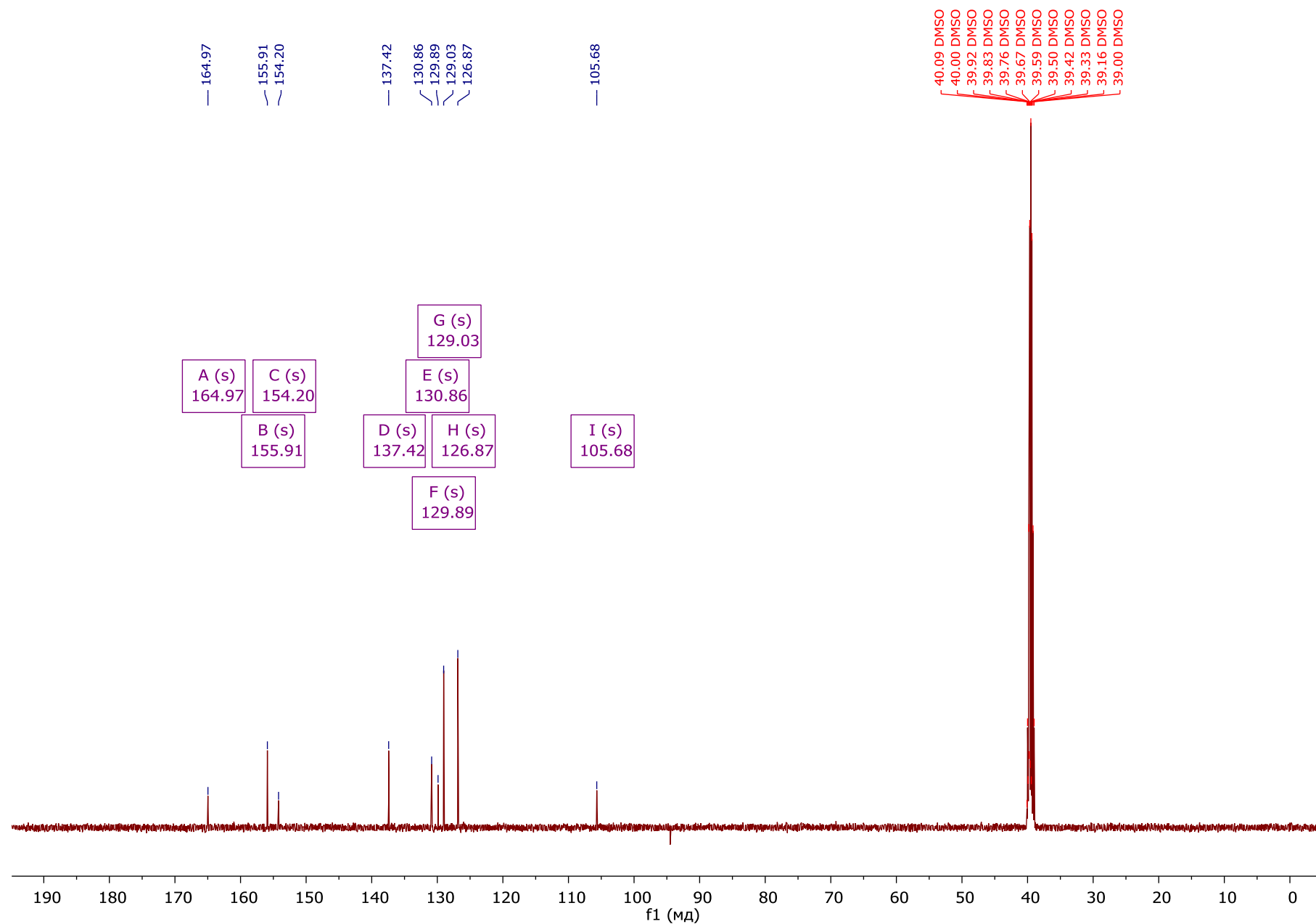


¹³C NMR (126 MHz, DMSO-*d*₆) δ 164.5 , 155.5 , 155.5 , 137.2 , 130.7 , 130.2 , 129.0 , 126.9 , 110.9 .

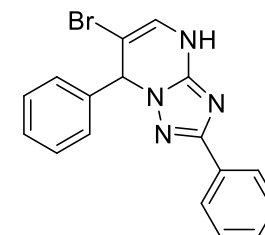
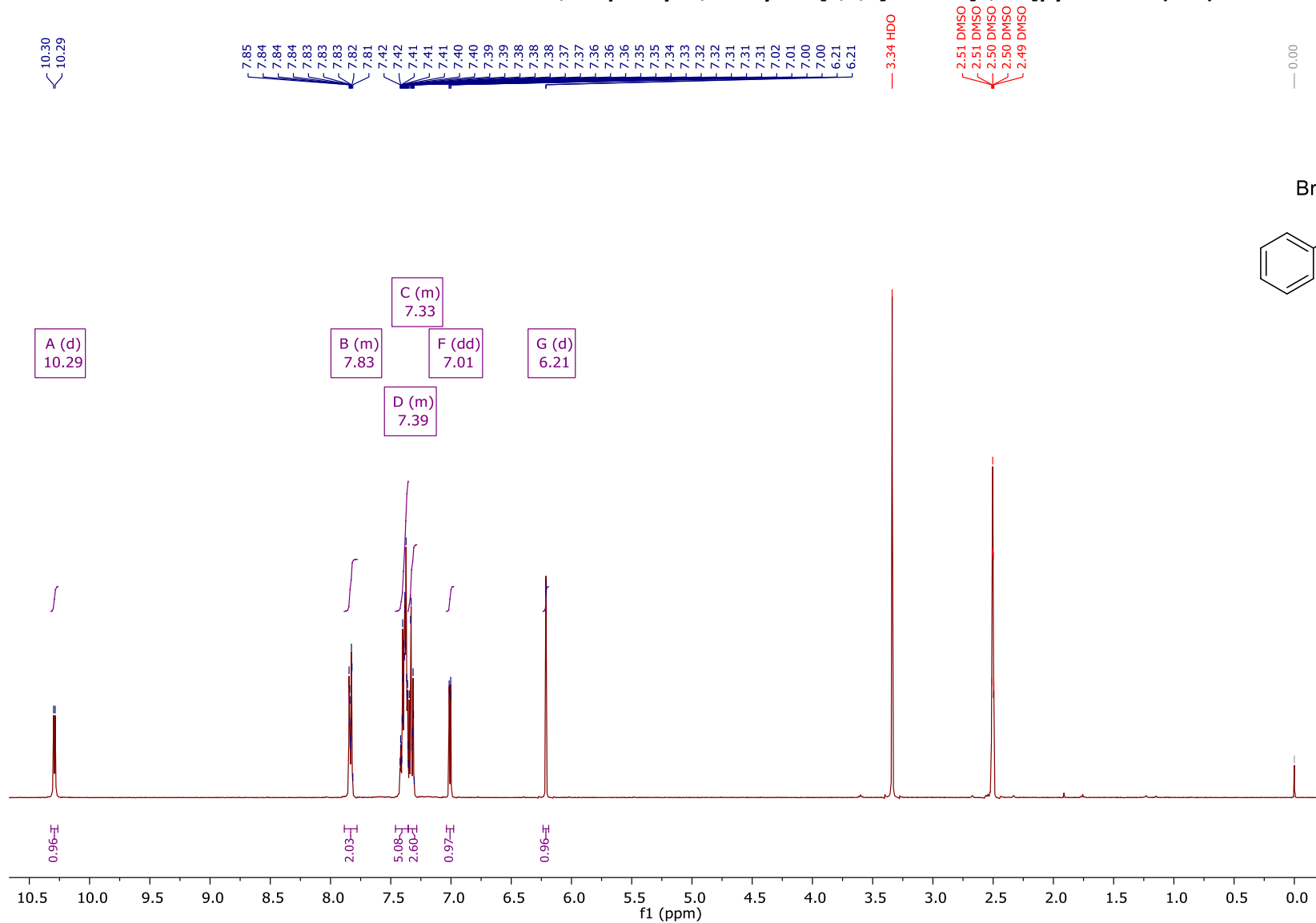
6-Bromo-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (9)

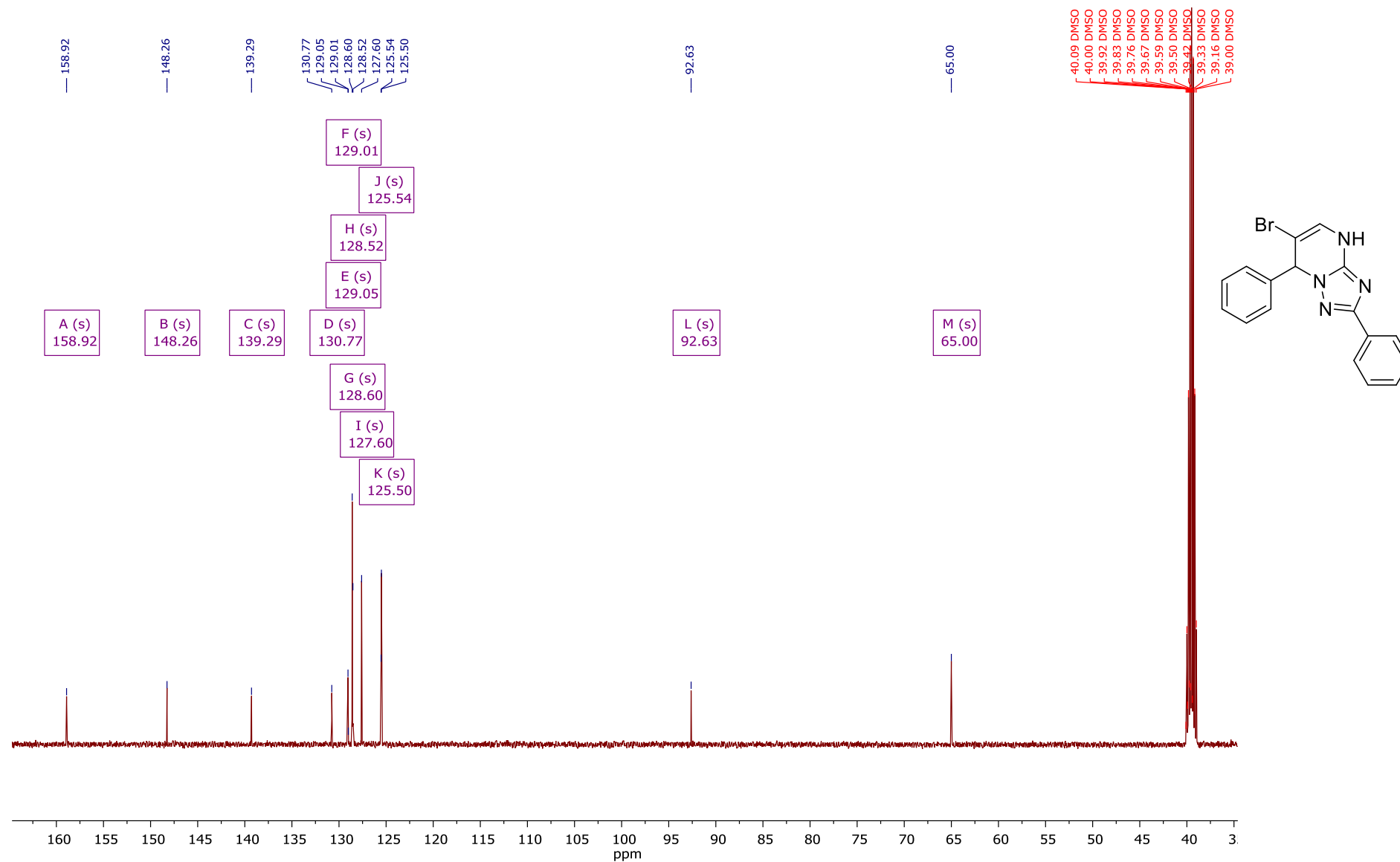


¹H NMR (400 MHz, DMSO-*d*₆) δ 9.92 (d, J = 2.4 Hz, 1H), 8.98 (d, J = 2.4 Hz, 1H), 8.27 – 8.17 (m, 2H), 7.63 – 7.48 (m, 3H).

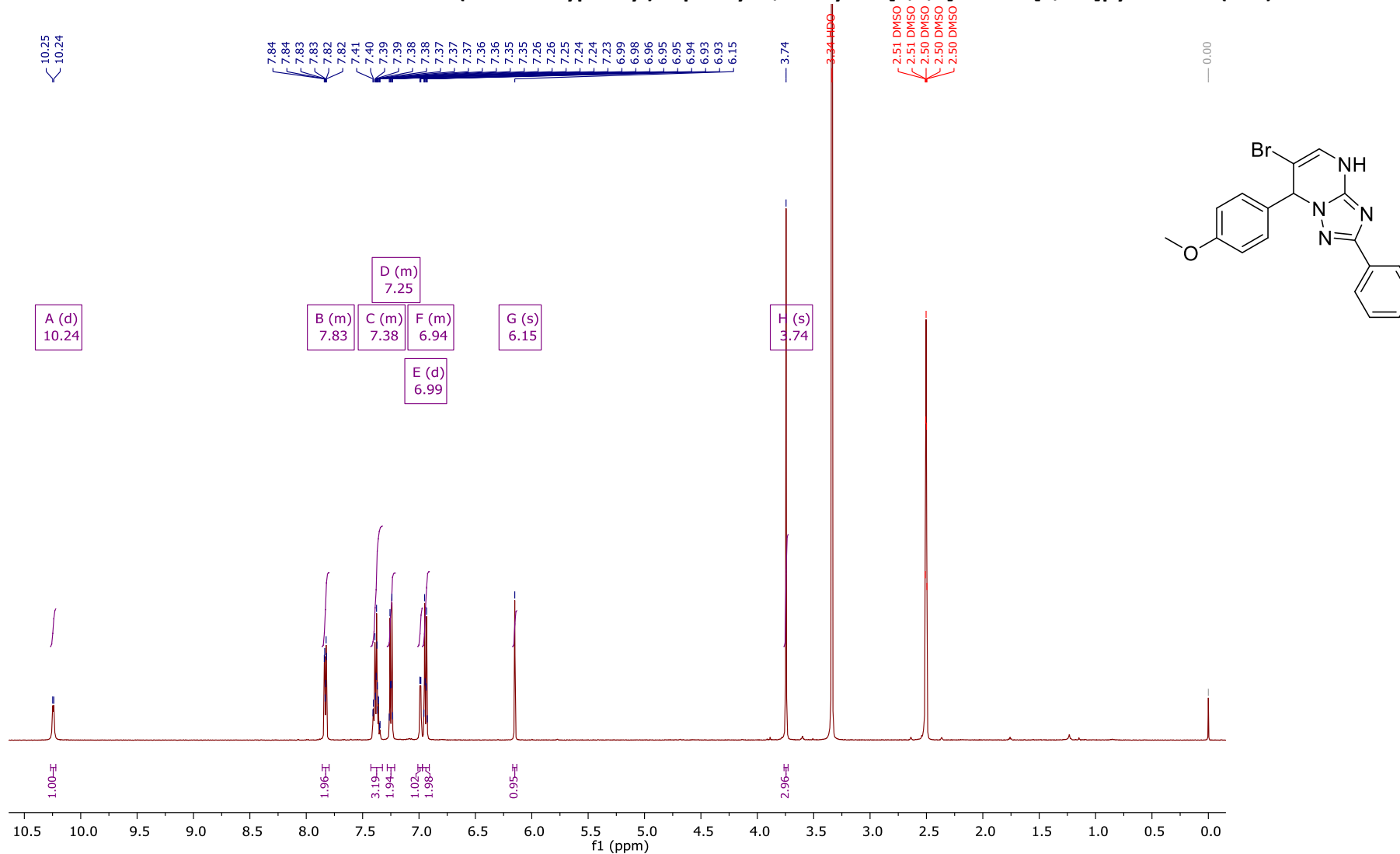


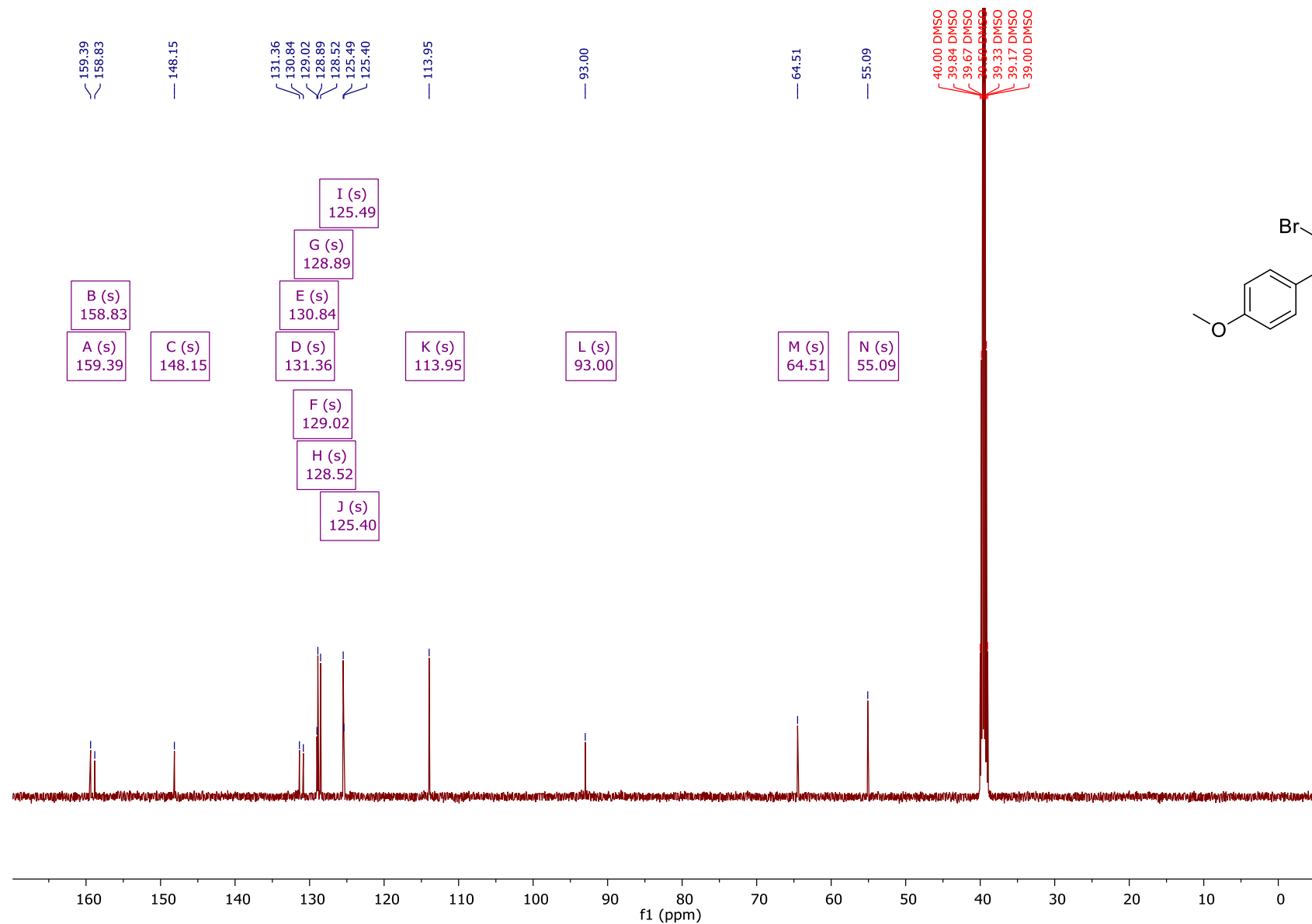
¹³C NMR (126 MHz, DMSO-*d*₆) δ 165.0 , 155.9 , 154.2 , 137.4 , 130.9 , 129.9 , 129.0 , 126.9 , 105.7 .

6-bromo-2,7-diphenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine (10a)



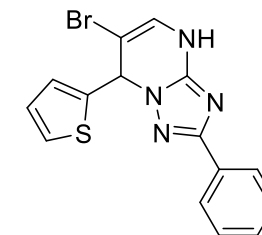
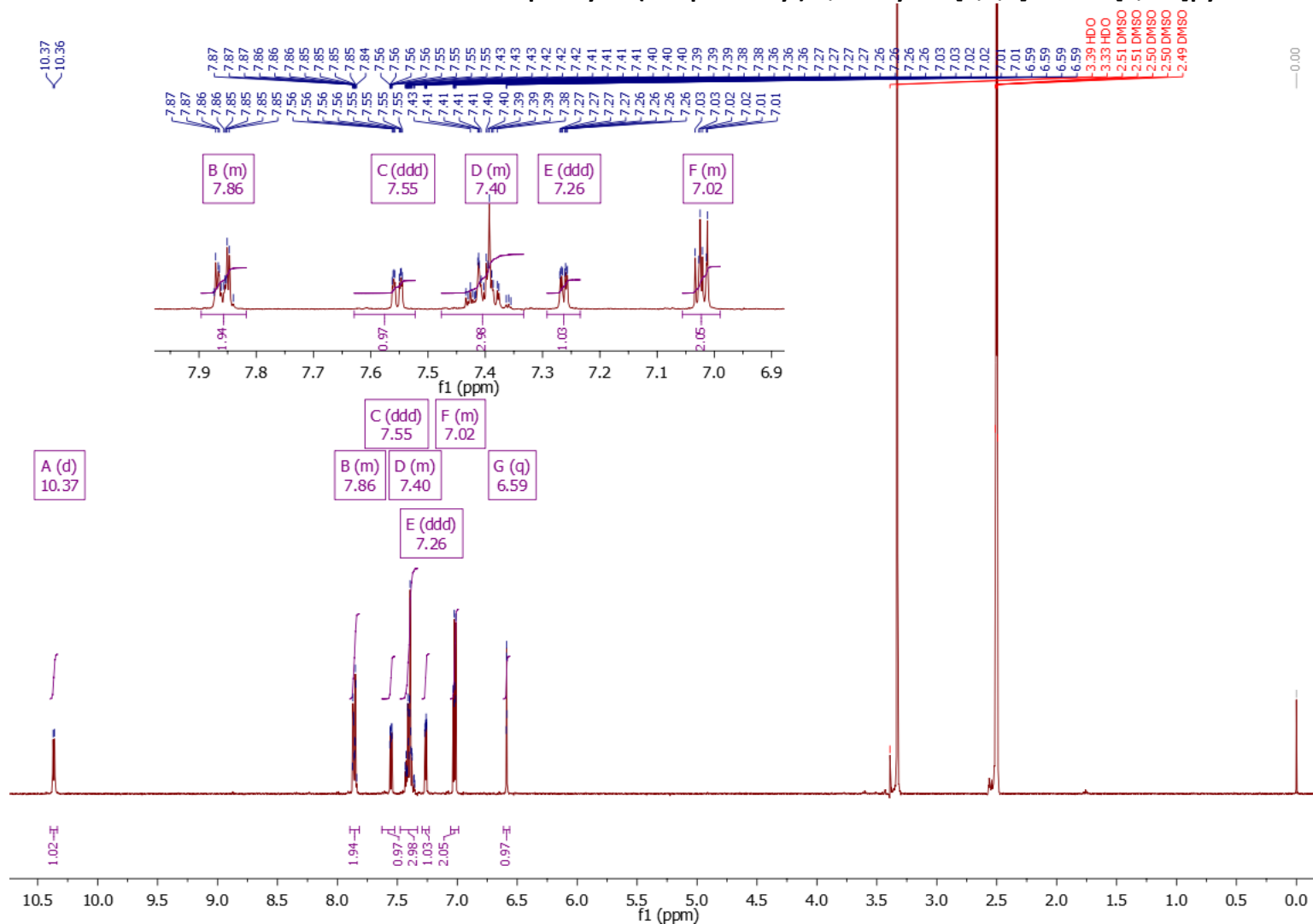
¹³C NMR (126 MHz, DMSO-*d*₆) δ 158.9, 148.3, 139.3, 130.8, 129.1, 129.0, 128.6, 128.5, 127.6, 125.5, 125.5, 92.6, 65.0.

6-Bromo-7-(4-methoxyphenyl)-2-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine (10b)

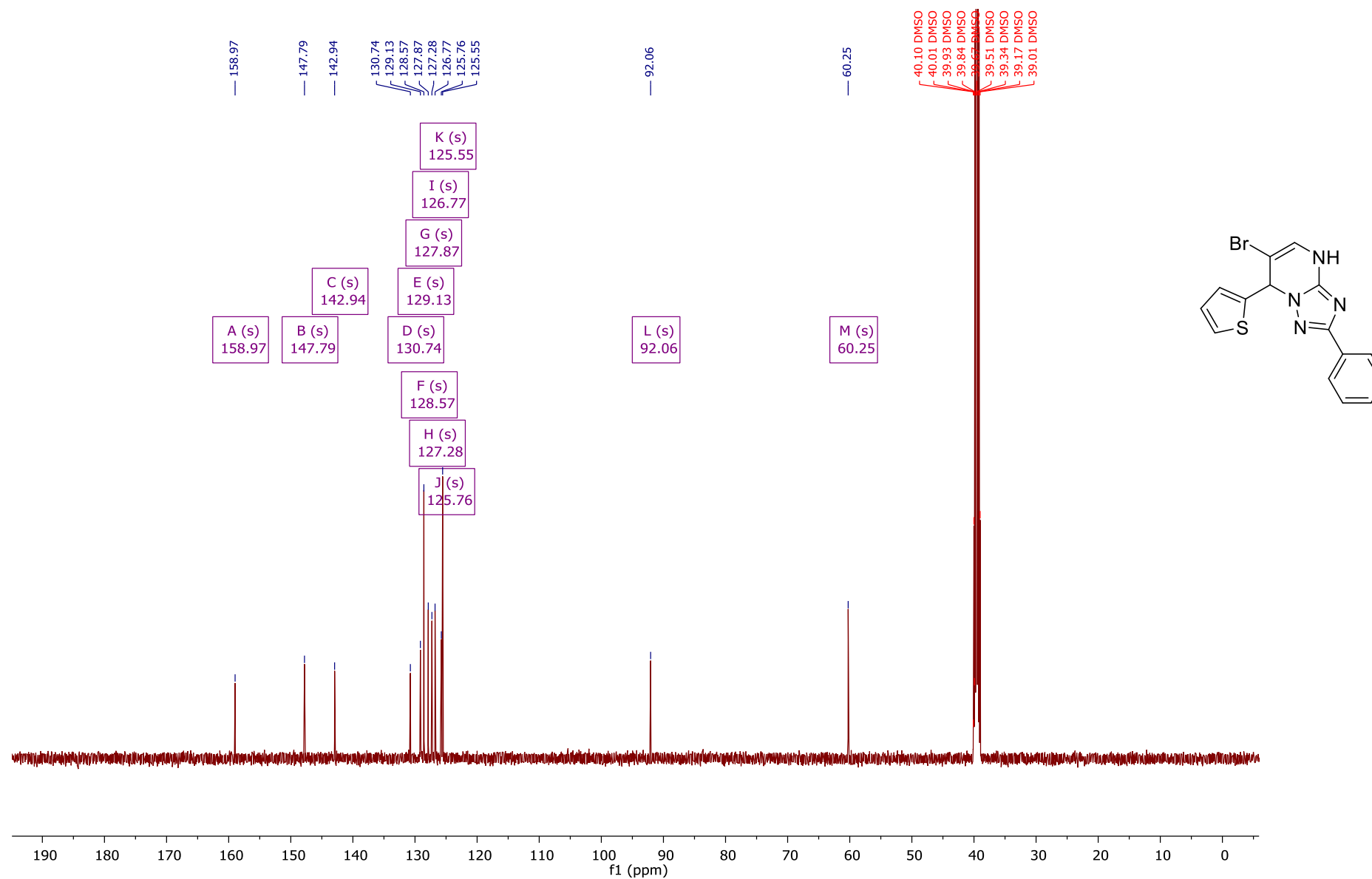


¹³C NMR (126 MHz, DMSO-*d*₆) δ 159.4, 158.8, 148.1, 131.4, 130.8, 129.0, 128.9, 128.5, 125.5, 125.4, 113.9, 93.0, 64.5, 55.1.

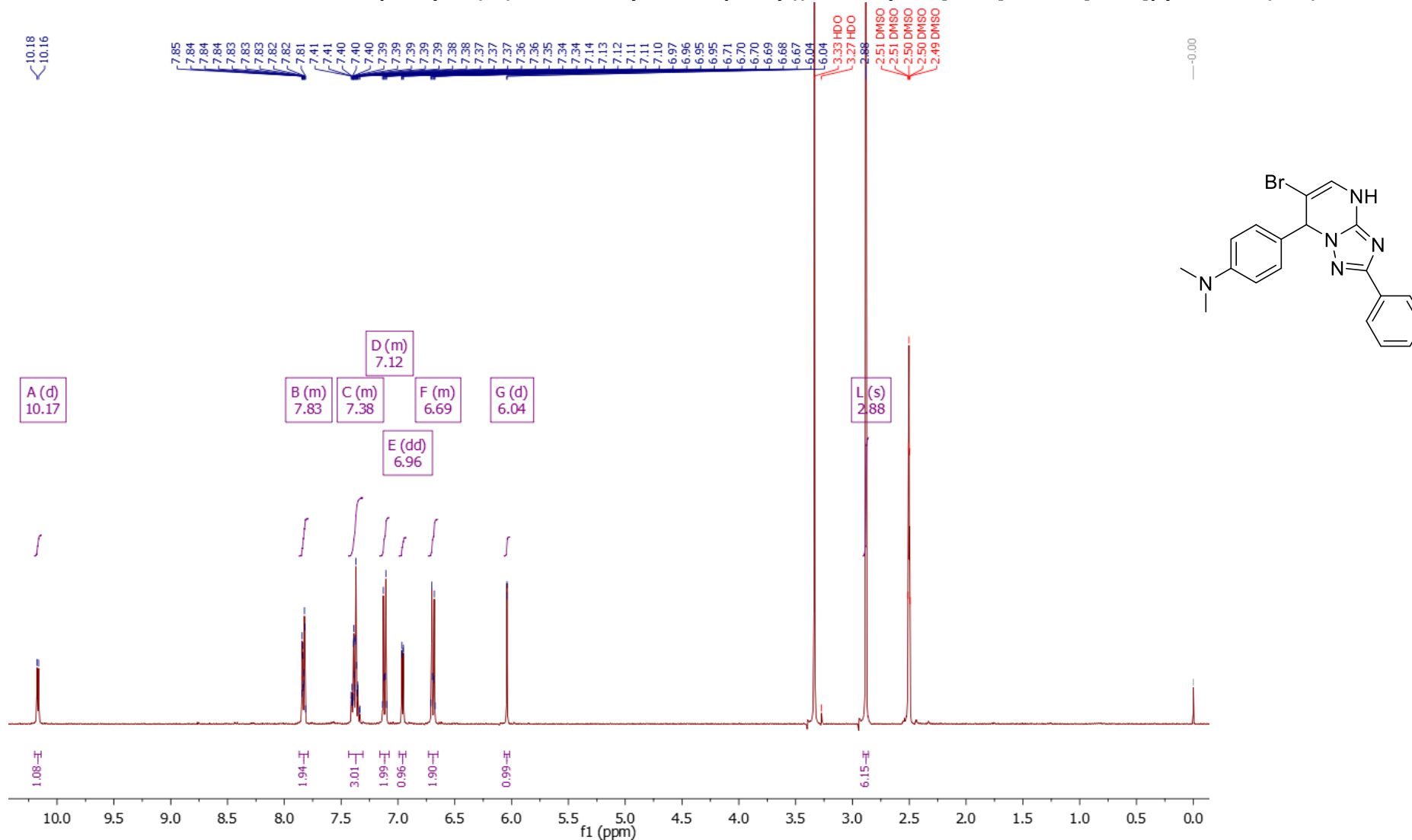
6-Bromo-2-phenyl-7-(thiophen-2-yl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine (10c)



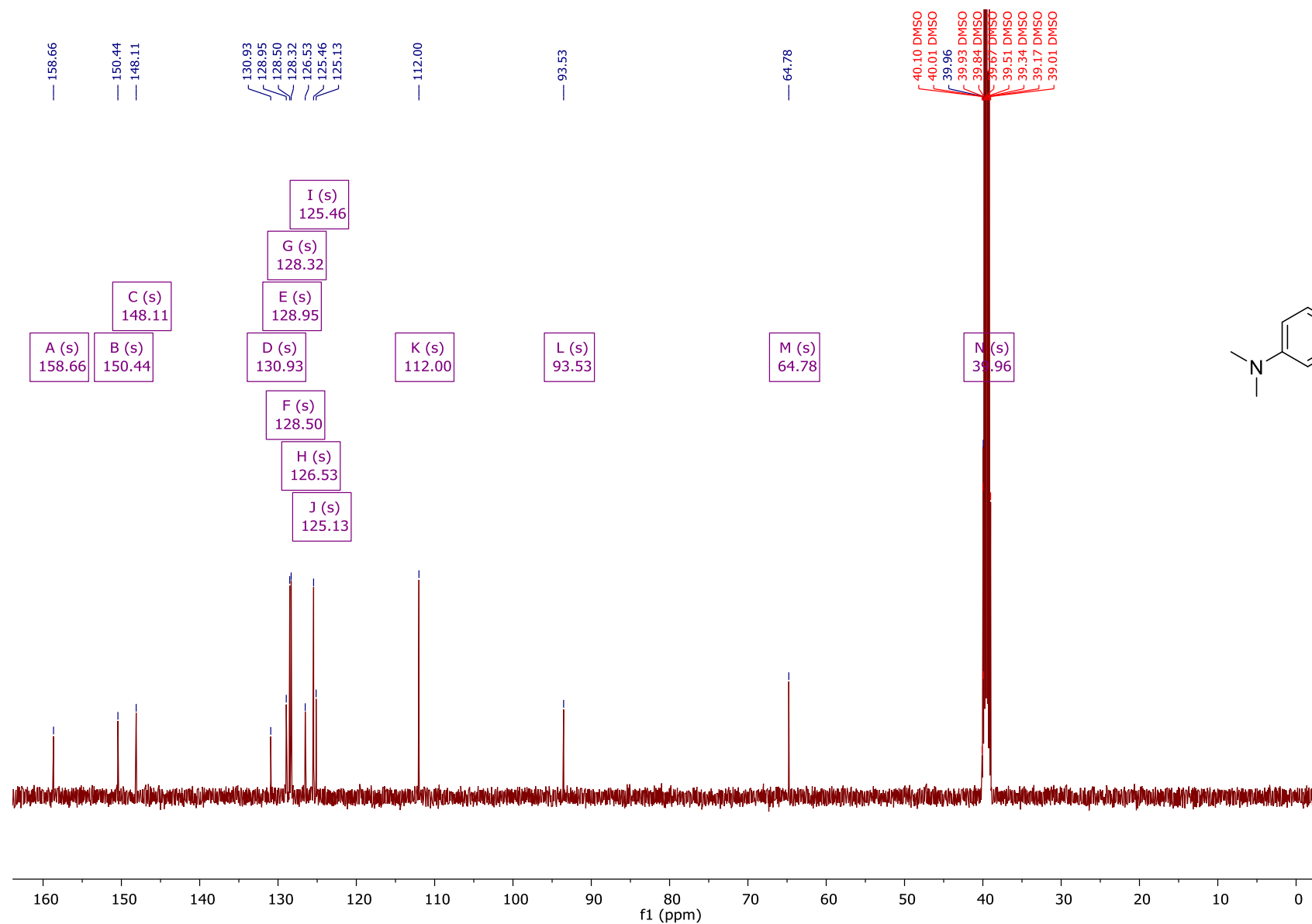
¹H NMR (400 MHz, DMSO-*d*₆) δ 10.37 (d, *J* = 5.1 Hz, 1H), 7.90 – 7.82 (m, 2H), 7.55 (ddd, *J* = 5.1, 1.3, 0.7 Hz, 1H), 7.48 – 7.33 (m, 3H), 7.26 (ddd, *J* = 3.5, 1.3, 0.5 Hz, 1H), 7.06 – 6.99 (m, 2H), 6.59 (q, *J* = 0.7 Hz, 1H).



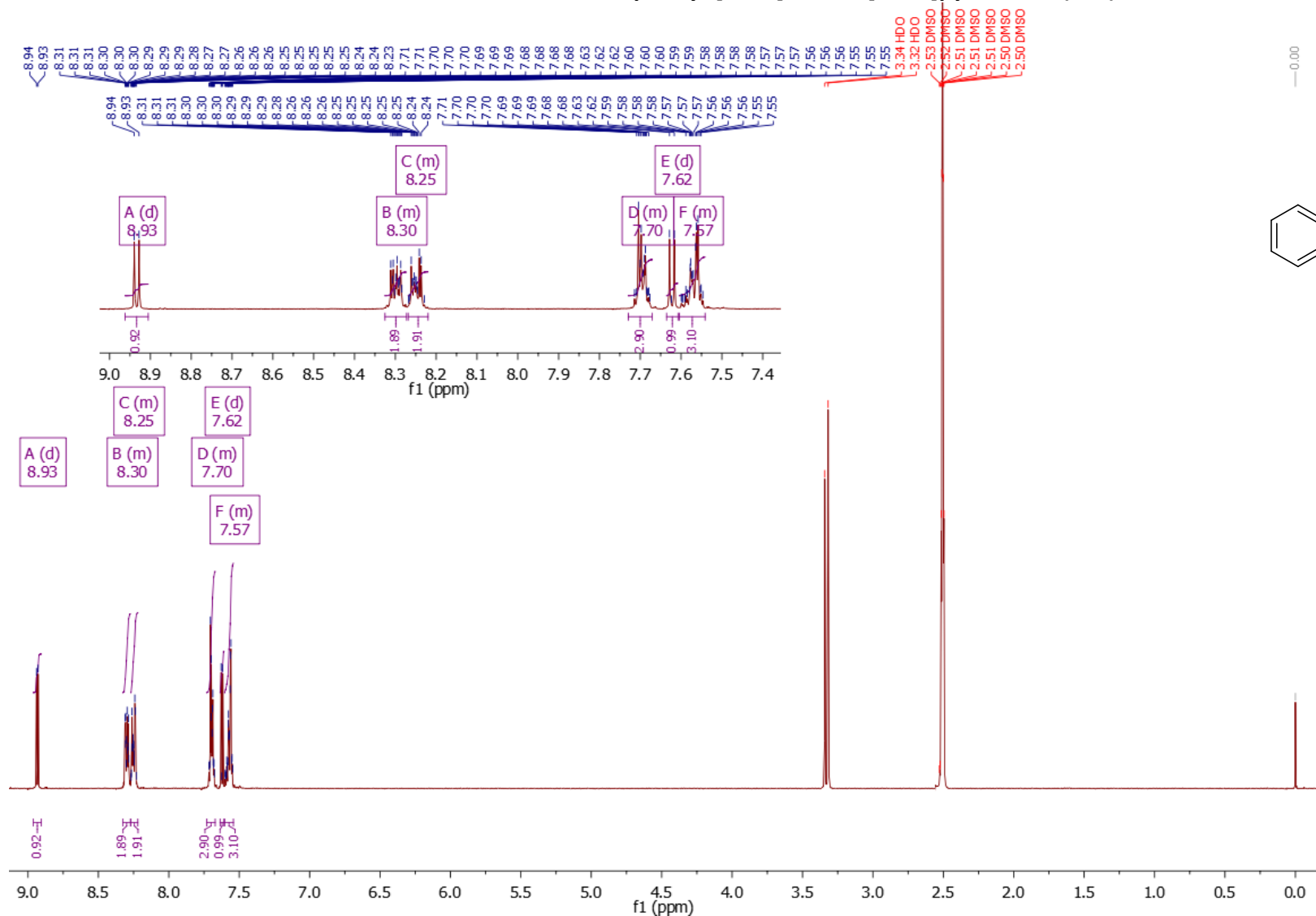
¹³C NMR (126 MHz, DMSO-*d*₆) δ 159.0, 147.8, 142.9, 130.7, 129.1, 128.6, 127.9, 127.3, 126.8, 125.8, 125.5, 92.1, 60.2.

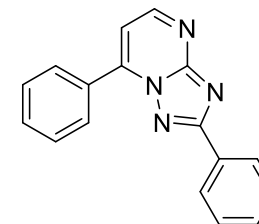
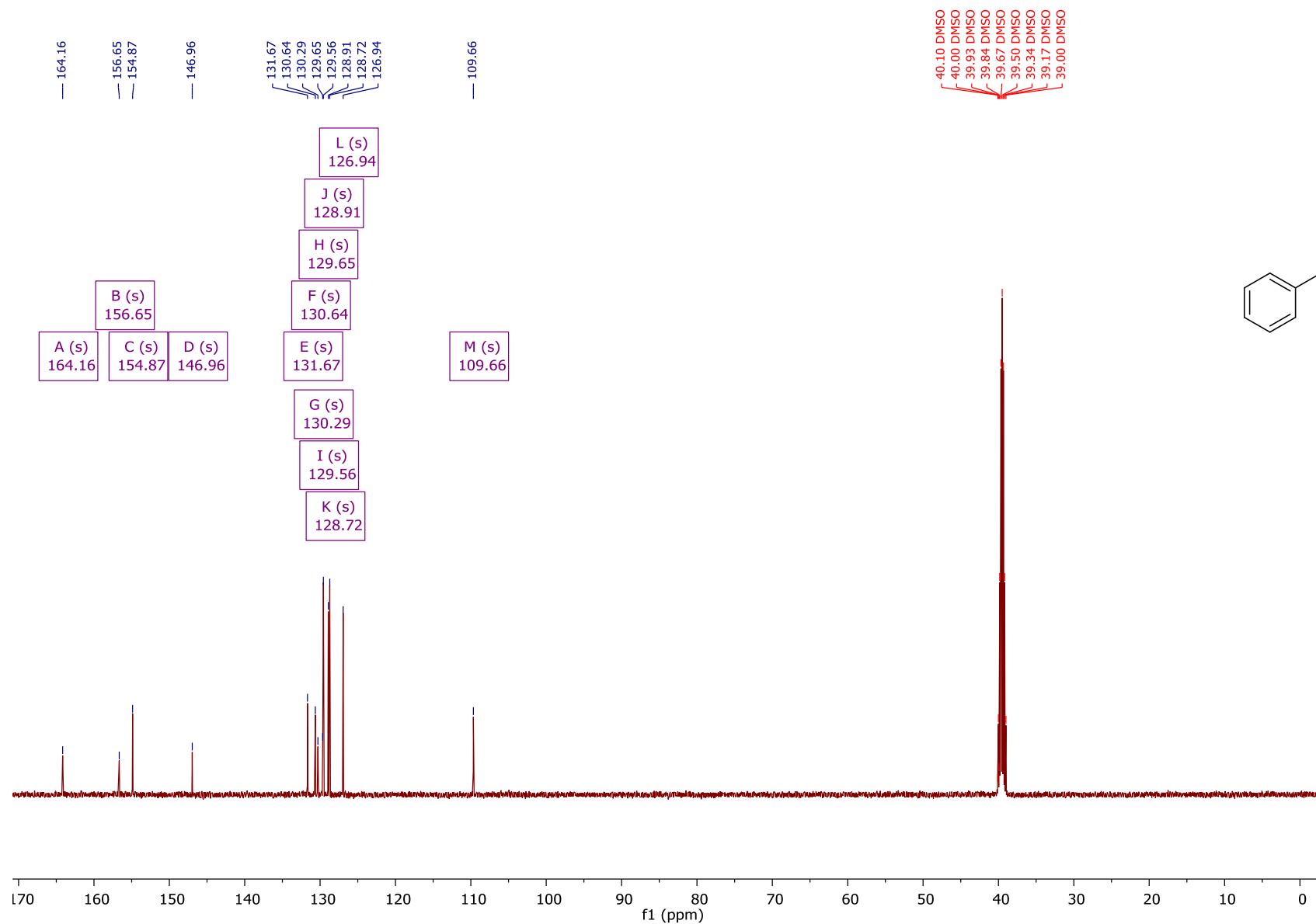
6-Bromo-2-phenyl-7-(4-(N,N-dimethylamionophenyl))-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine (10d)

¹H NMR (400 MHz, DMSO-*d*₆) δ 10.17 (d, *J* = 5.0 Hz, 1H), 7.87 – 7.79 (m, 2H), 7.43 – 7.31 (m, 3H), 7.16 – 7.08 (m, 2H), 6.96 (dd, *J* = 5.0, 0.8 Hz, 1H), 6.73 – 6.65 (m, 2H), 6.04 (d, *J* = 0.7 Hz, 1H), 2.88 (s, 6H).

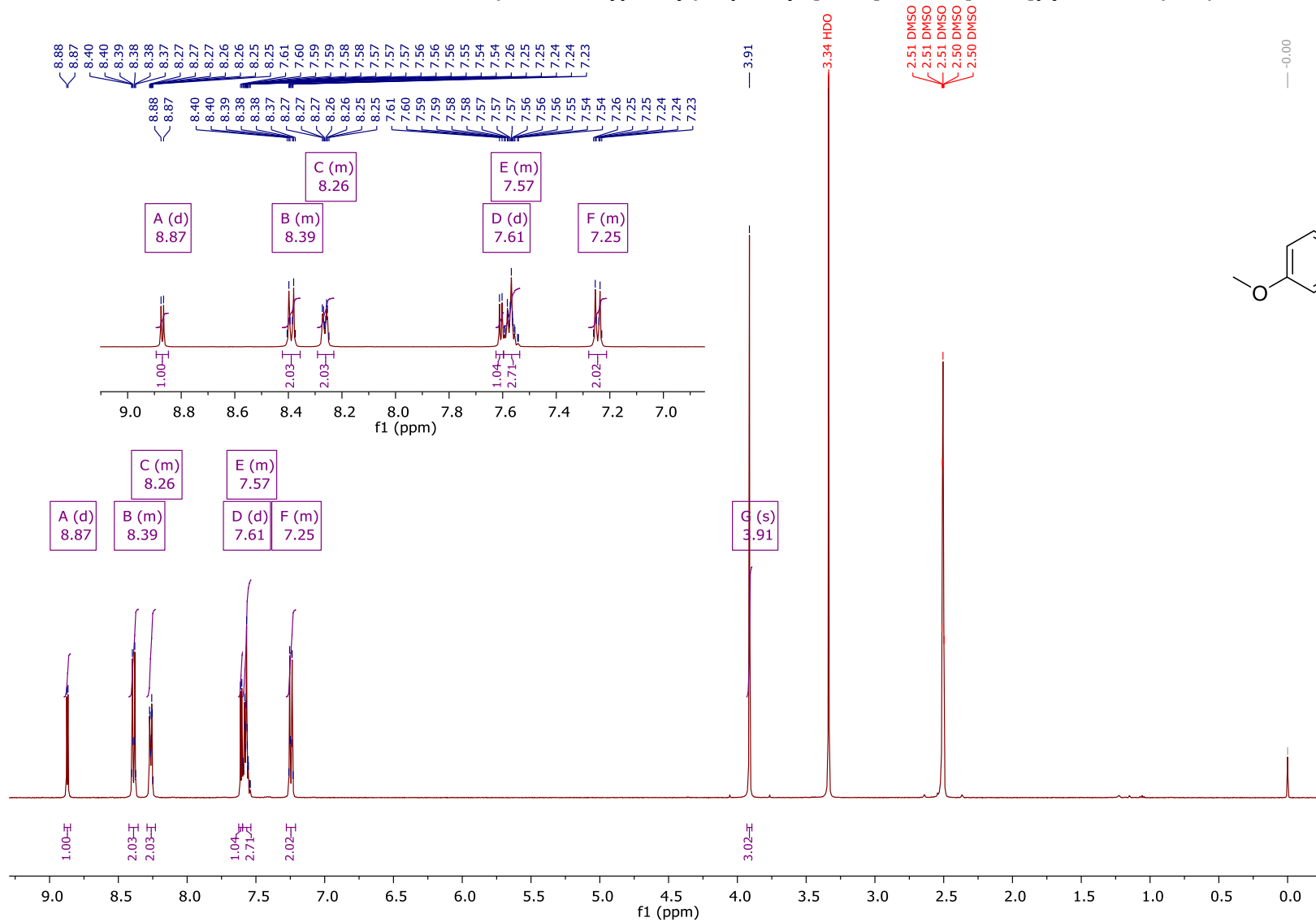


¹³C NMR (126 MHz, DMSO-*d*₆) δ 158.7, 150.4, 148.1, 130.9, 128.9, 128.5, 128.3, 126.5, 125.5, 125.1, 112.0, 93.5, 64.8, 40.0.

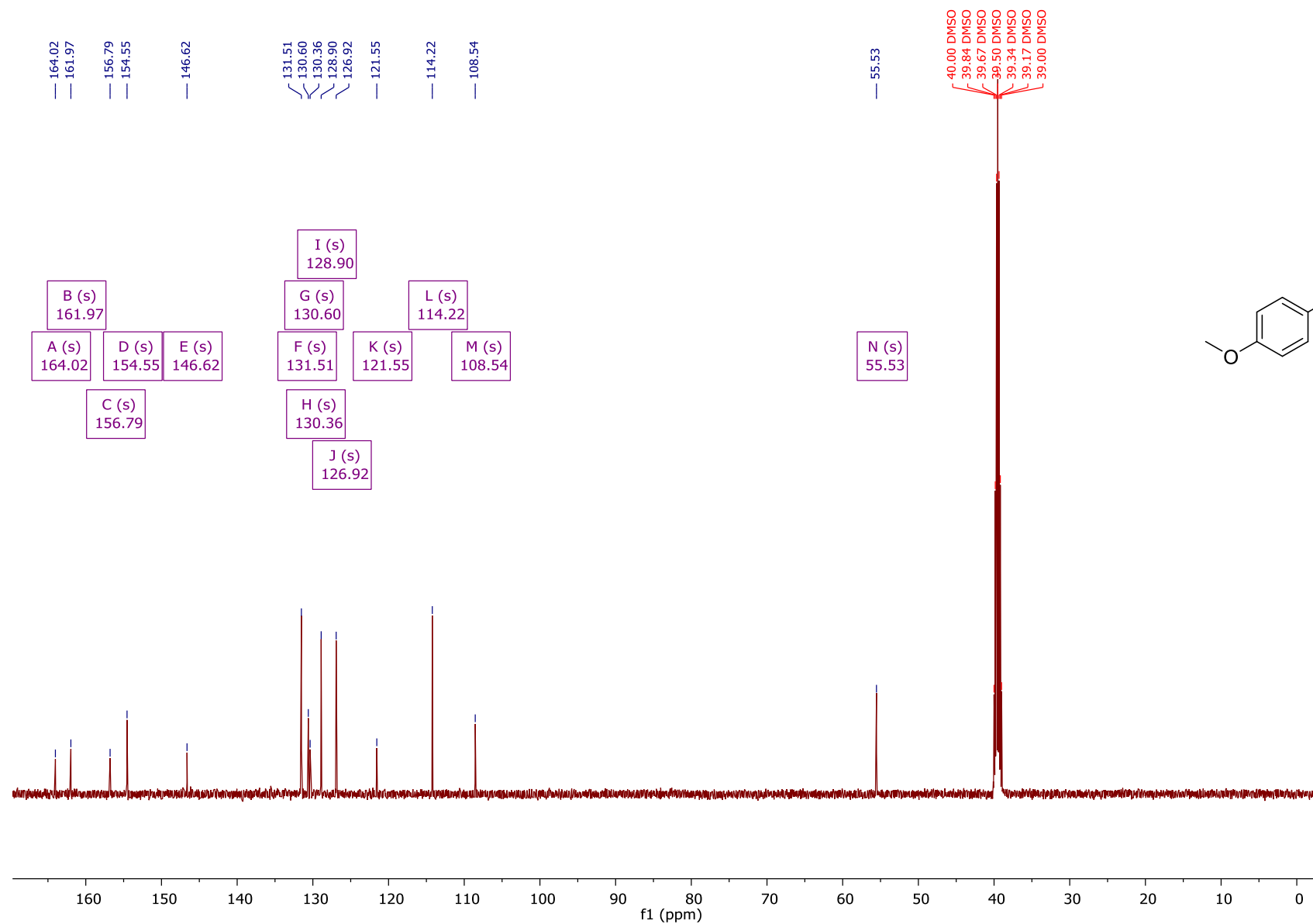
2,7-Diphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (11a)



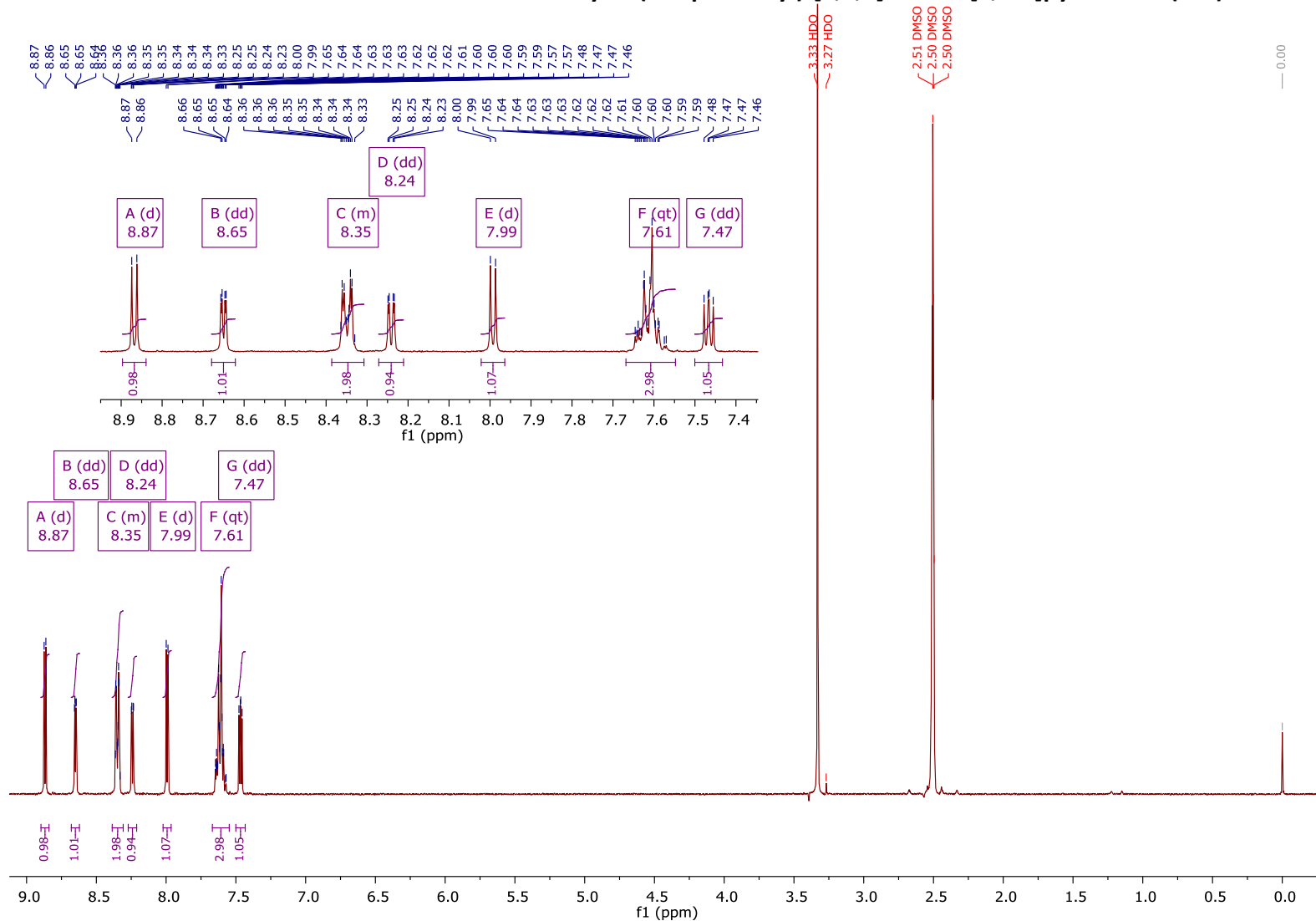
¹³C NMR (126 MHz, DMSO-*d*₆) δ 164.16, 156.65, 154.87, 146.96, 131.67, 130.64, 130.29, 129.65, 129.56, 128.91, 128.72, 126.94, 109.66.

7-(4-Methoxyphenyl)-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (11b)

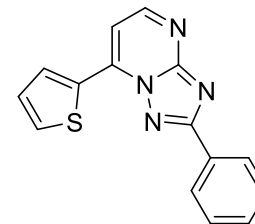
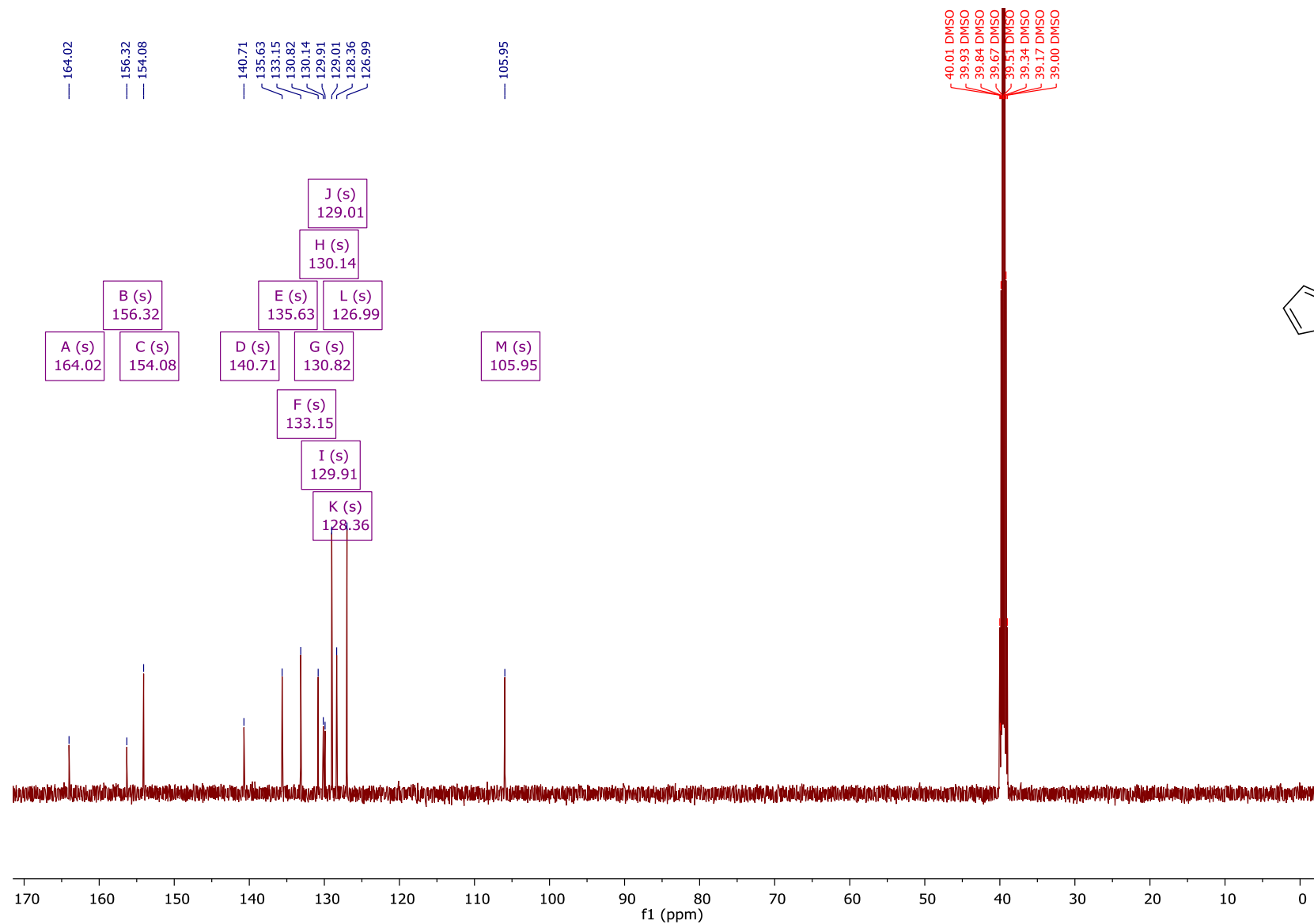
^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 8.87 (d, J = 4.8 Hz, 1H), 8.42 – 8.36 (m, 2H), 8.29 – 8.23 (m, 2H), 7.61 (d, J = 4.8 Hz, 1H), 7.60 – 7.54 (m, 3H), 7.28 – 7.21 (m, 2H), 3.91 (s, 3H).



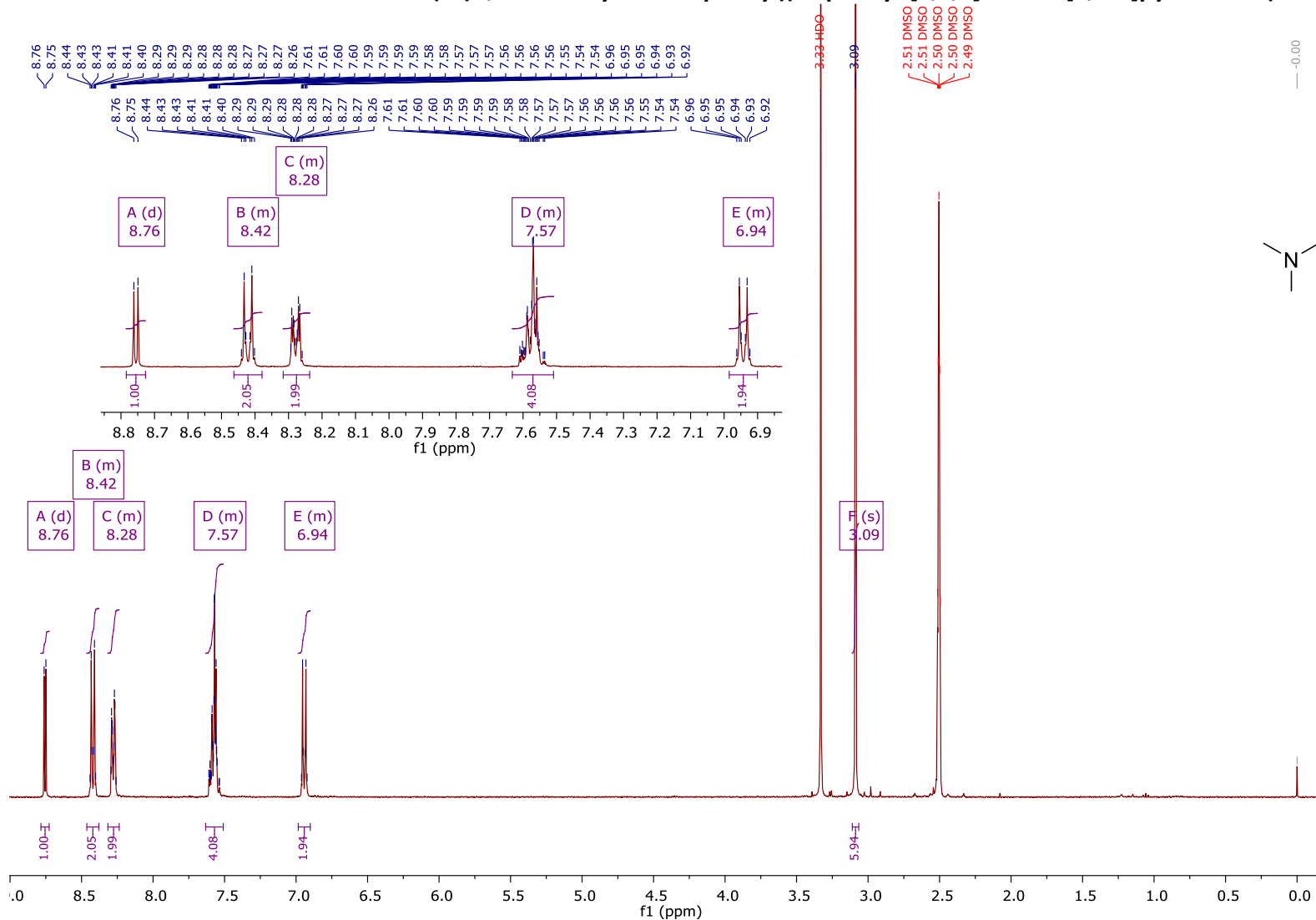
¹³C NMR (126 MHz, DMSO-*d*₆) δ 164.02, 161.97, 156.79, 154.55, 146.62, 131.51, 130.60, 130.36, 128.90, 126.92, 121.55, 114.22, 108.54, 55.53.

2-Phenyl-7-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (11c)

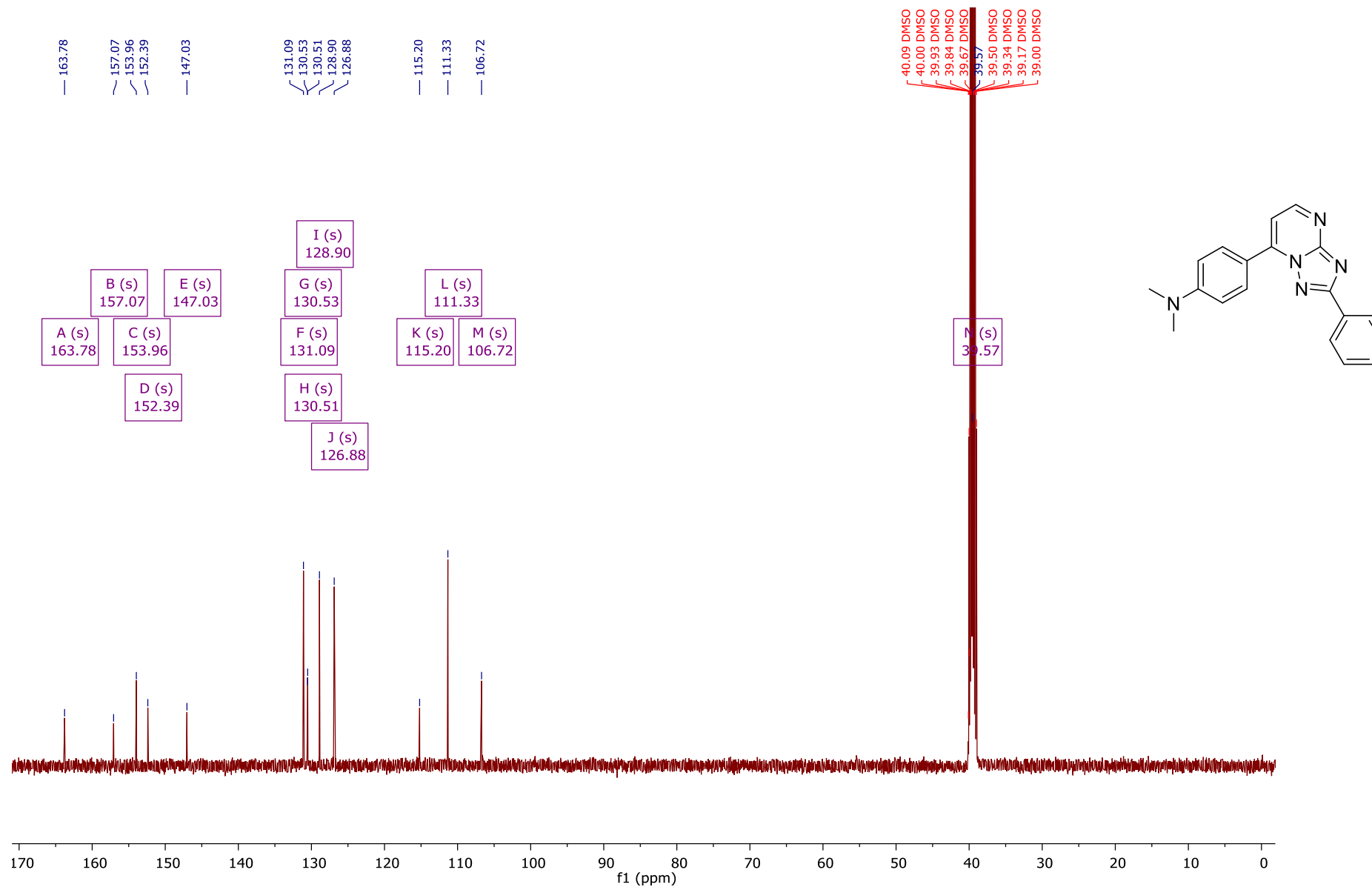
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.87 (d, J = 5.0 Hz, 1H), 8.65 (dd, J = 4.0, 1.2 Hz, 1H), 8.39 – 8.31 (m, 2H), 8.24 (dd, J = 5.0, 1.2 Hz, 1H), 7.99 (d, J = 5.0 Hz, 1H), 7.61 (qt, J = 5.0, 2.0 Hz, 3H), 7.47 (dd, J = 5.0, 3.9 Hz, 1H).



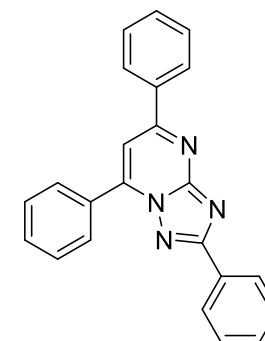
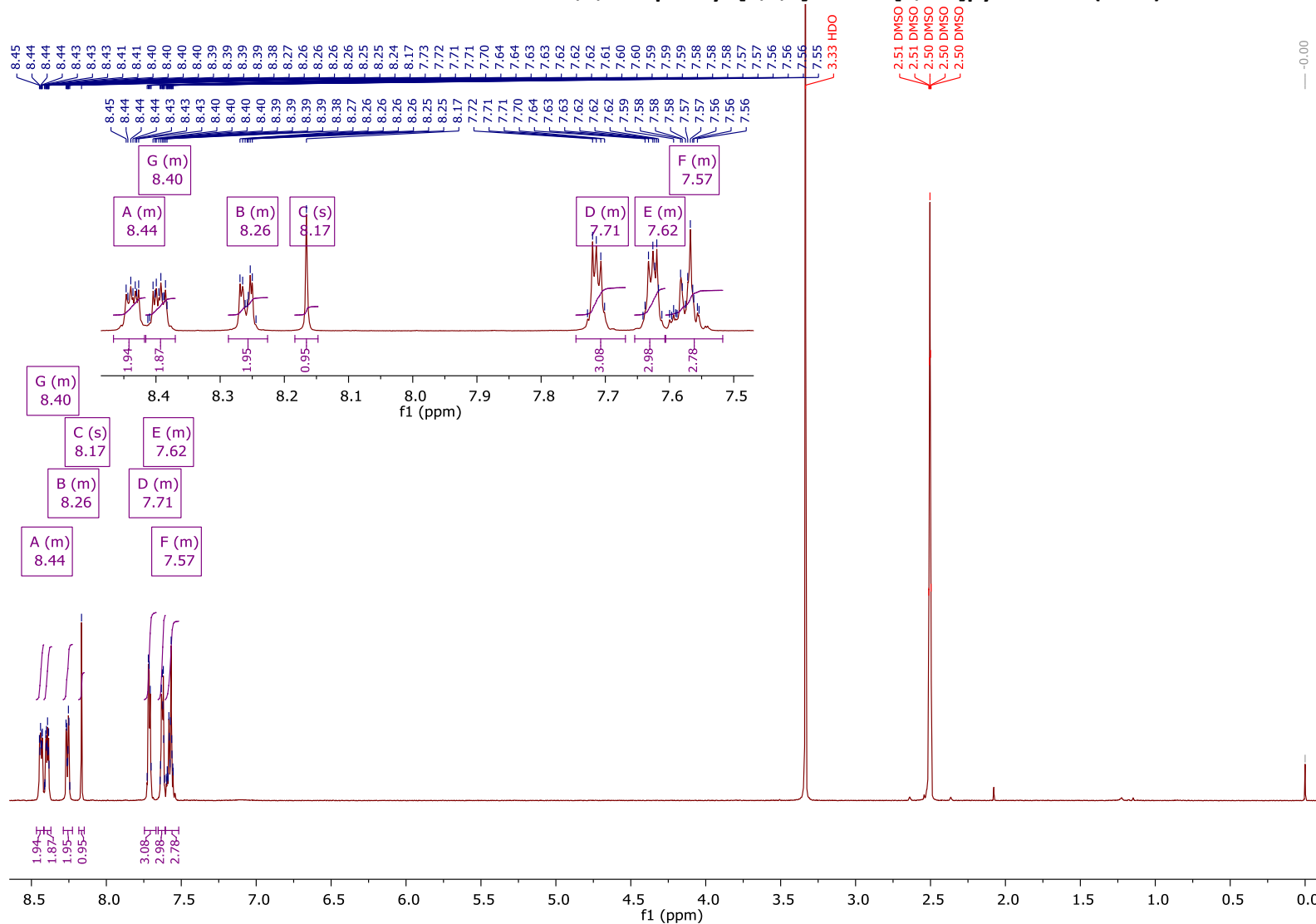
¹³C NMR (126 MHz, DMSO-*d*₆) δ 164.02, 156.32, 154.08, 140.71, 135.63, 133.15, 130.82, 130.14, 129.91, 129.01, 128.36, 126.99, 105.95.

7-(4-(N,N-dimethylamionophenyl))-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (11d)

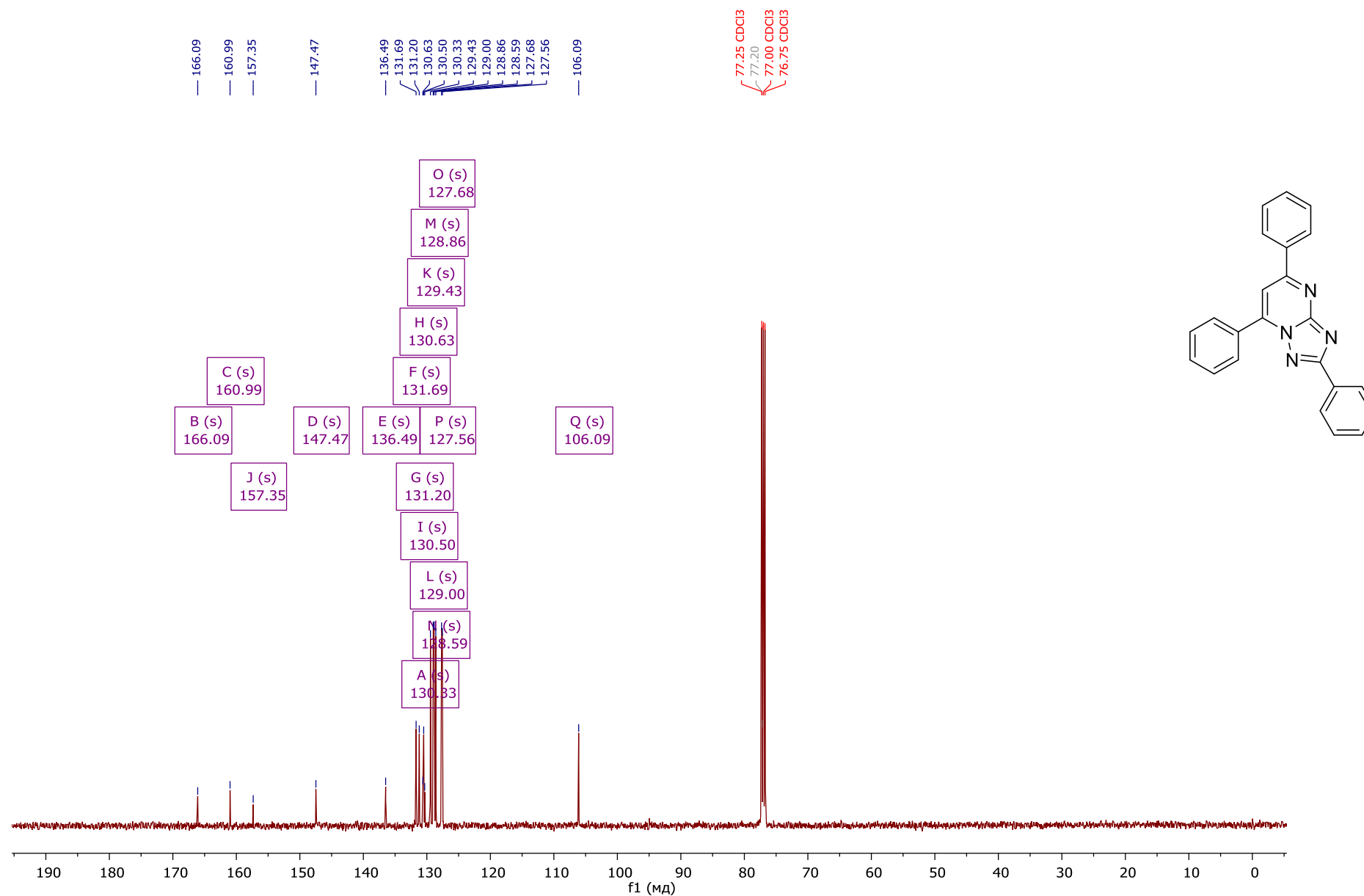
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.76 (d, *J* = 5.0 Hz, 1H), 8.46 – 8.38 (m, 2H), 8.32 – 8.24 (m, 2H), 7.63 – 7.51 (m, 4H), 6.98 – 6.90 (m, 2H), 3.09 (s, 6H).



¹³C NMR (126 MHz, DMSO-*d*₆) δ 163.78, 157.07, 153.96, 152.39, 147.03, 131.09, 130.53, 130.51, 128.90, 126.88, 115.20, 111.33, 106.72, 39.57.

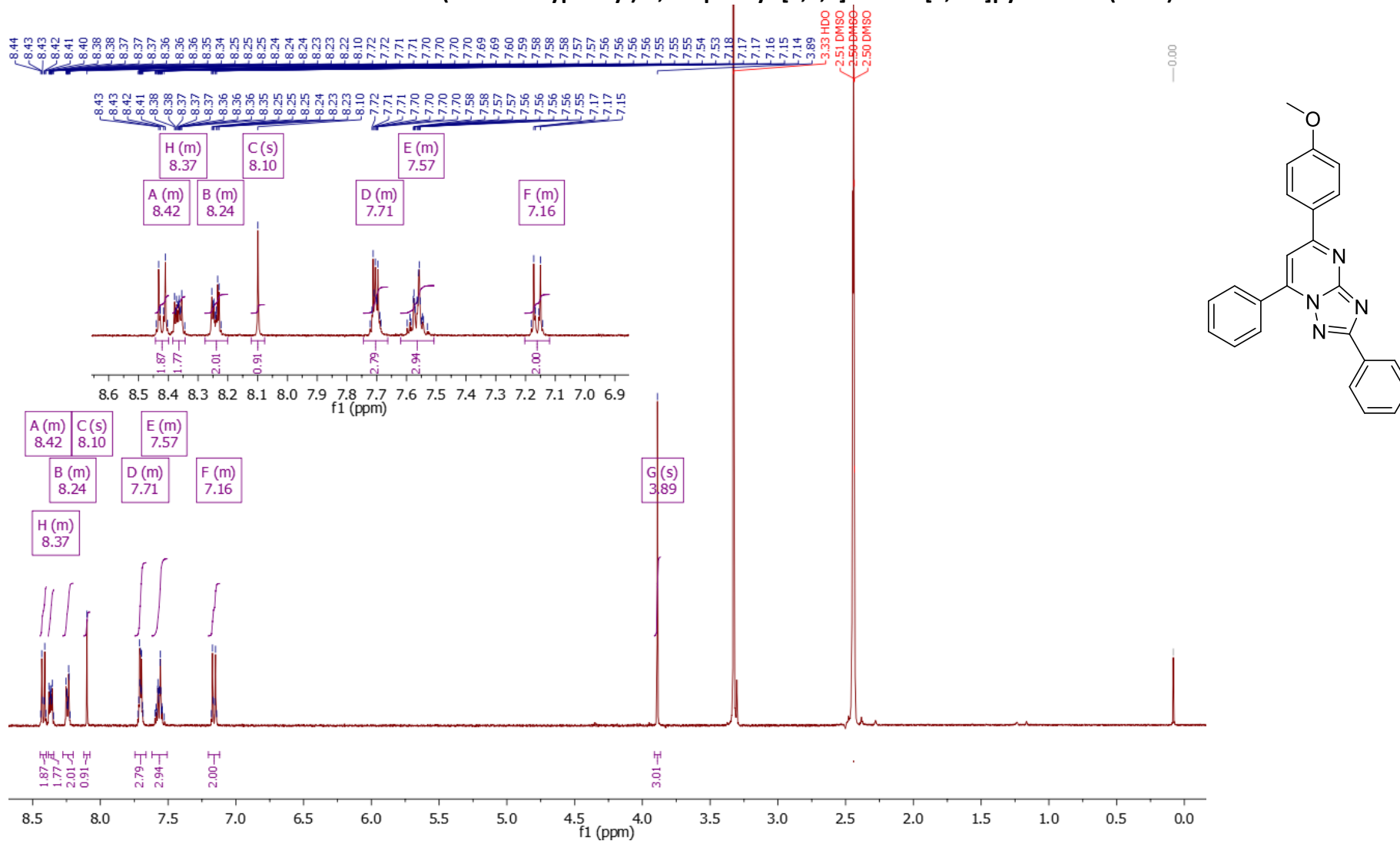
2,5,7-Triphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12aa)

¹H NMR (500 MHz, DMSO-*d*₆) δ 8.47 – 8.42 (m, 2H), 8.42 – 8.37 (m, 2H), 8.29 – 8.23 (m, 2H), 8.17 (s, 1H), 7.75 – 7.67 (m, 3H), 7.65 – 7.61 (m, 3H), 7.61 – 7.52 (m, 3H).

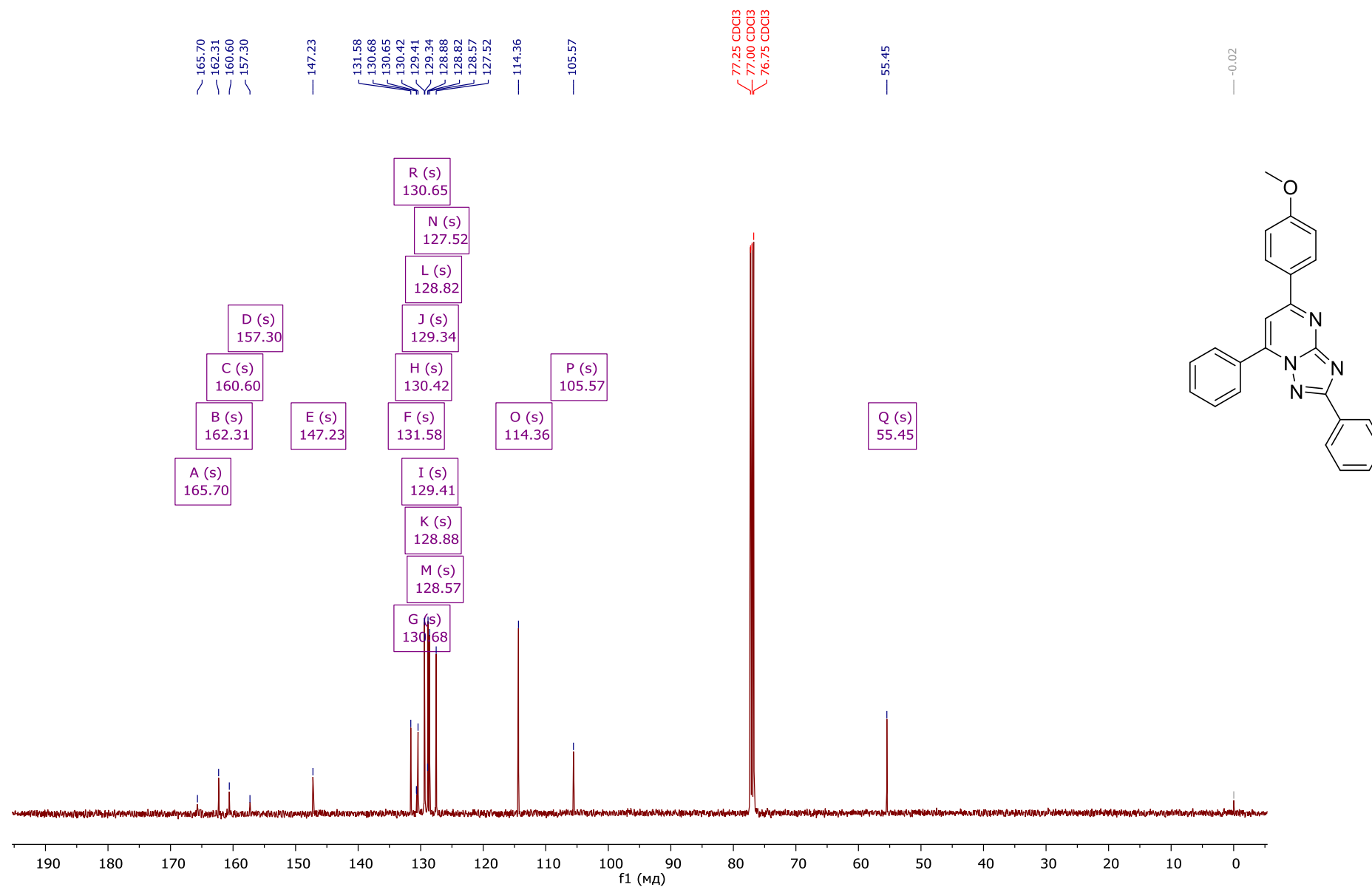


¹³C NMR (126 MHz, Chloroform-d) δ 166.09, 160.99, 157.35, 147.47, 136.49, 131.69, 131.20, 130.63, 130.50, 130.33, 129.43, 129.00, 128.86, 128.59, 127.68, 127.56, 106.09.

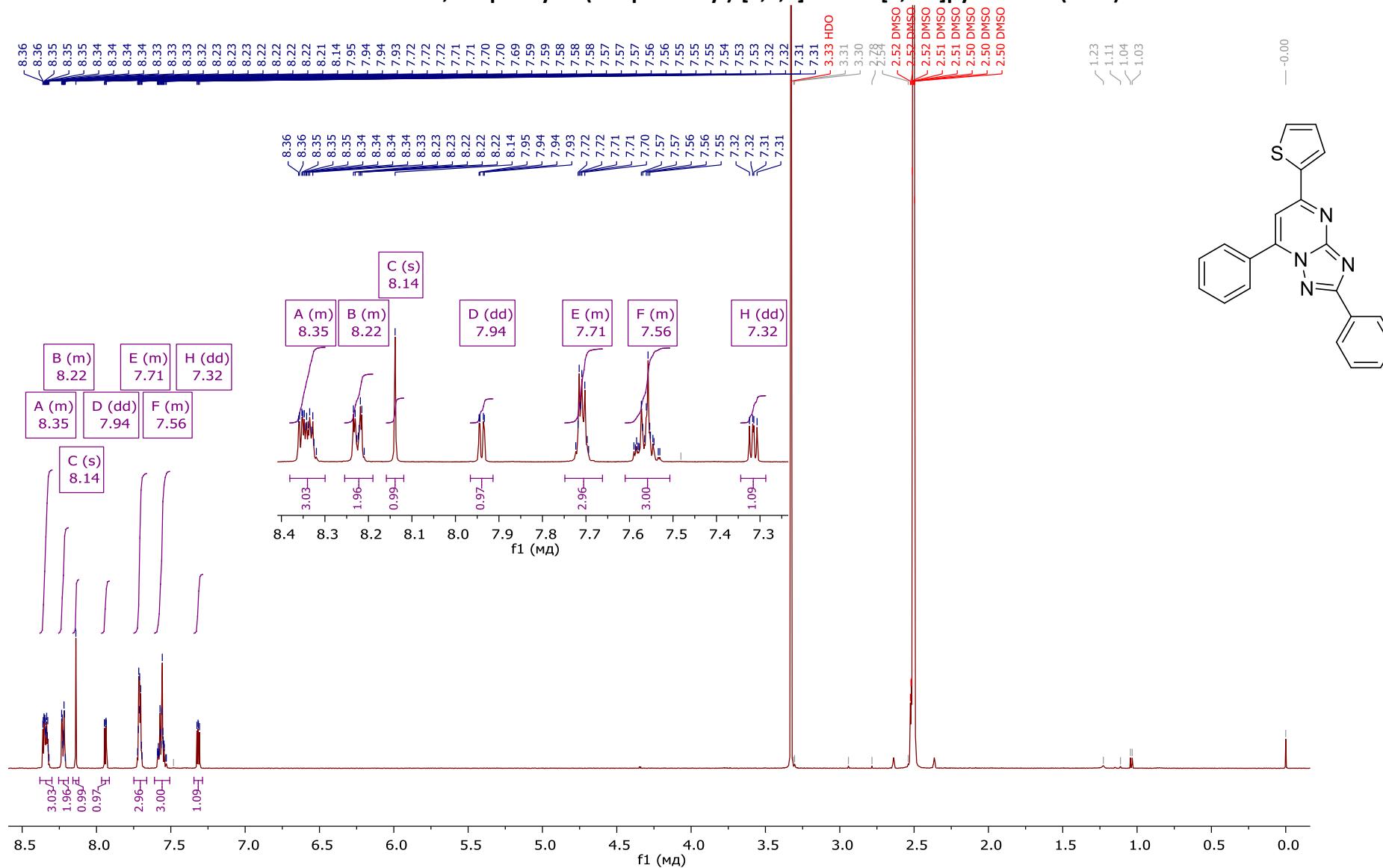
5-(4-Methoxyphenyl)-2,7-diphenyl-[1,2,4]triazolo[1,5-a]pyrimidine (12ab)



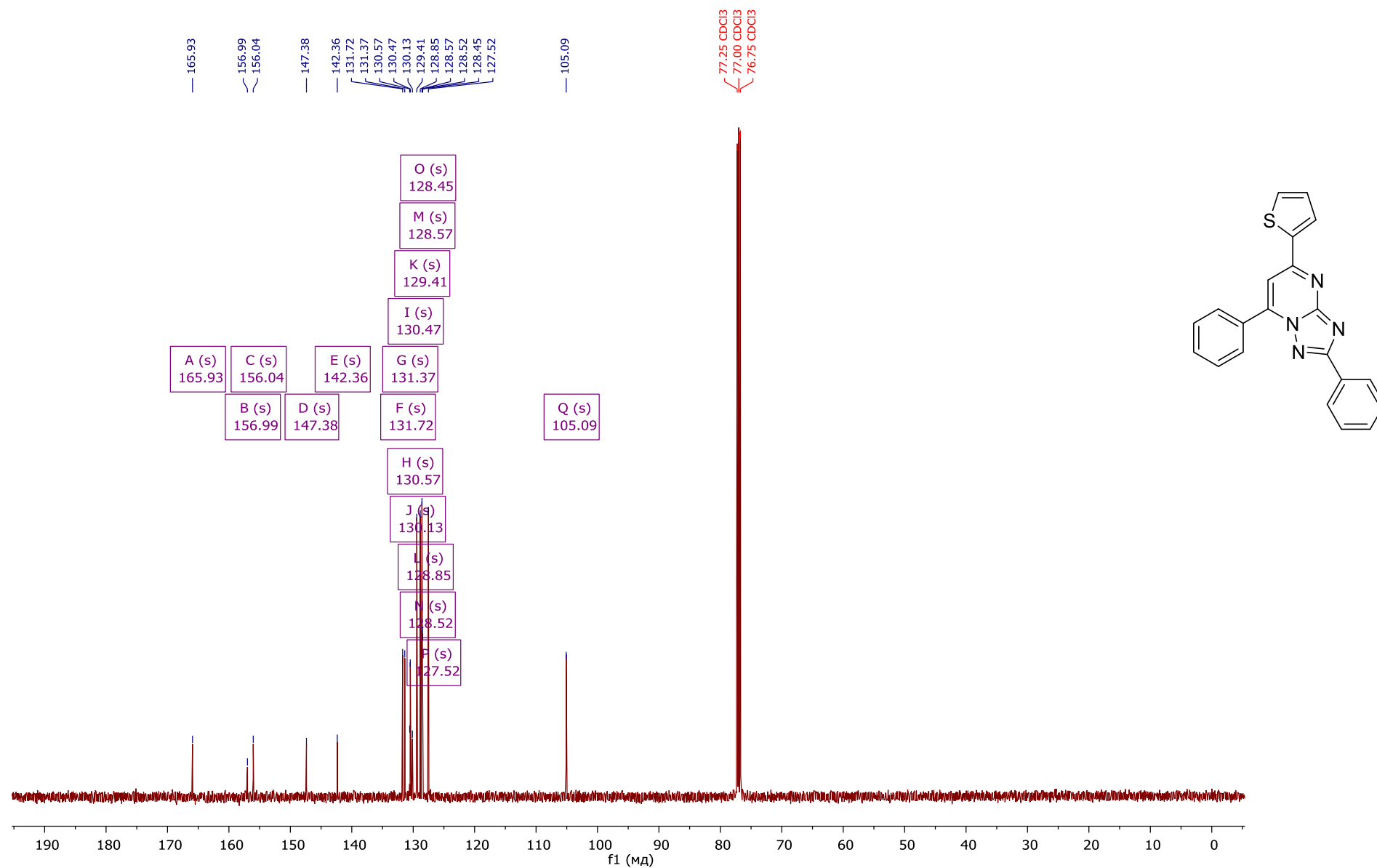
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.44 – 8.40 (m, 2H), 8.38 – 8.34 (m, 2H), 8.28 – 8.20 (m, 2H), 8.10 (s, 1H), 7.74 – 7.66 (m, 3H), 7.62 – 7.51 (m, 3H), 7.20 – 7.12 (m, 2H), 3.89 (s, 3H).



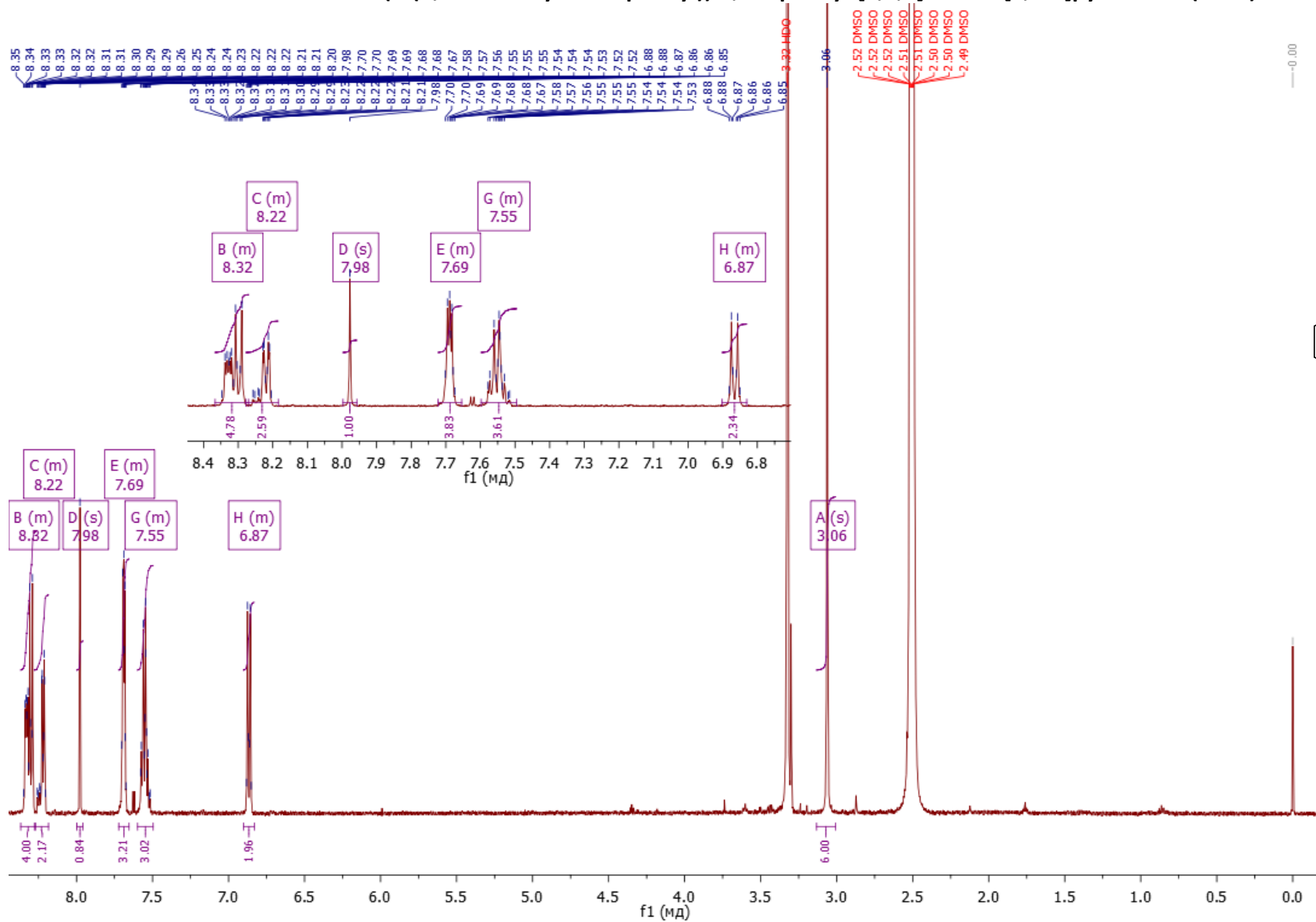
¹³C NMR (126 MHz, Chloroform-*d*) δ 165.70, 162.31, 160.60, 157.30, 147.23, 131.58, 130.68, 130.65, 130.42, 129.41, 129.34, 128.88, 128.82, 128.57, 127.52, 114.36, 105.57, 55.45.

2,7-Diphenyl-5-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (12ac)

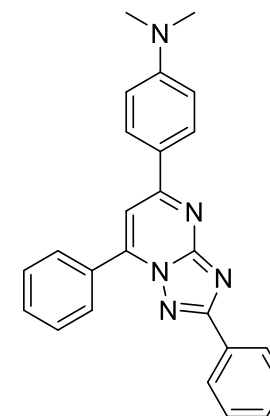
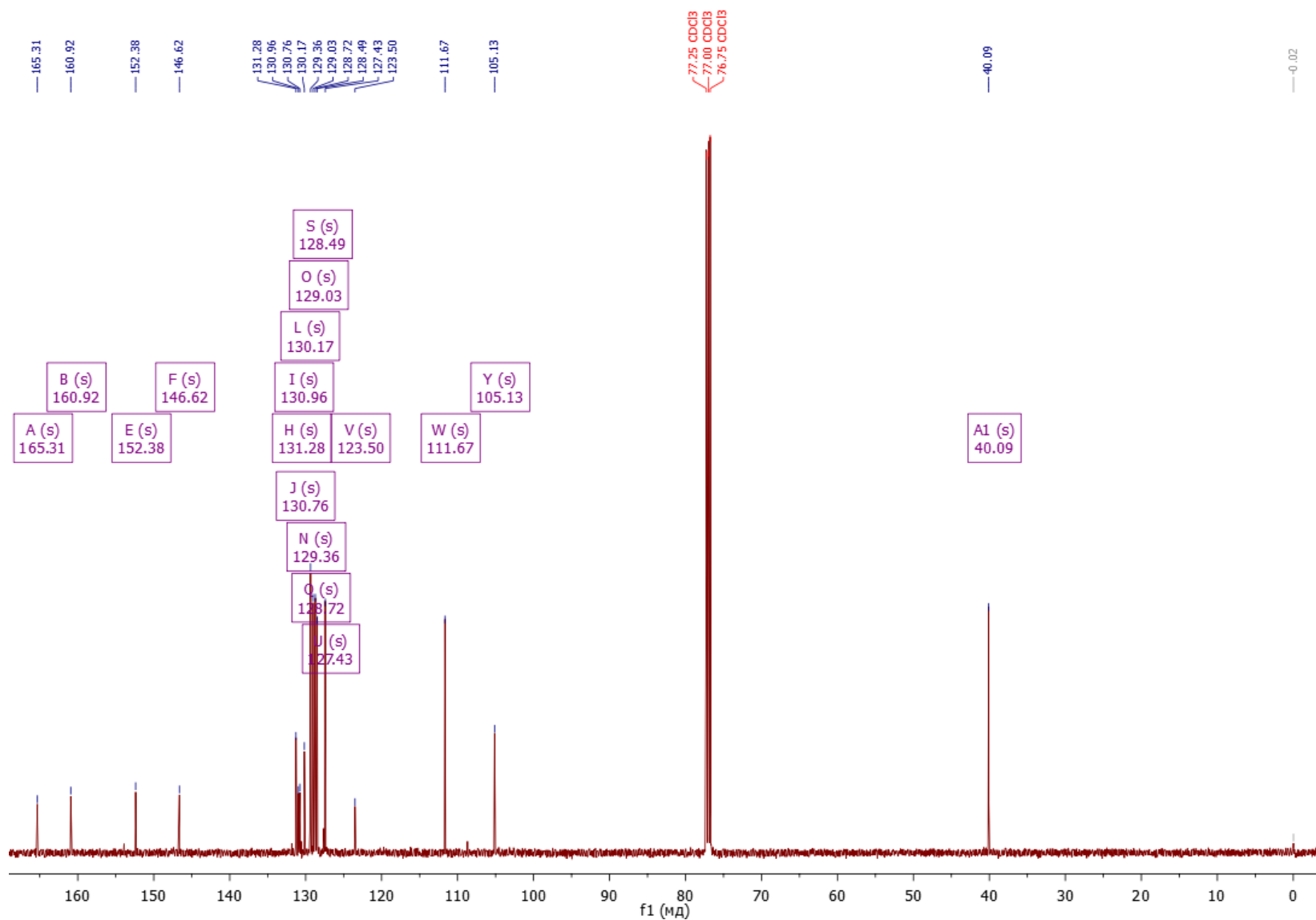
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.38 – 8.30 (m, 3H), 8.25 – 8.19 (m, 2H), 8.14 (s, 1H), 7.94 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.75 – 7.66 (m, 3H), 7.61 – 7.51 (m, 3H), 7.32 (dd, *J* = 5.0, 3.7 Hz, 1H).



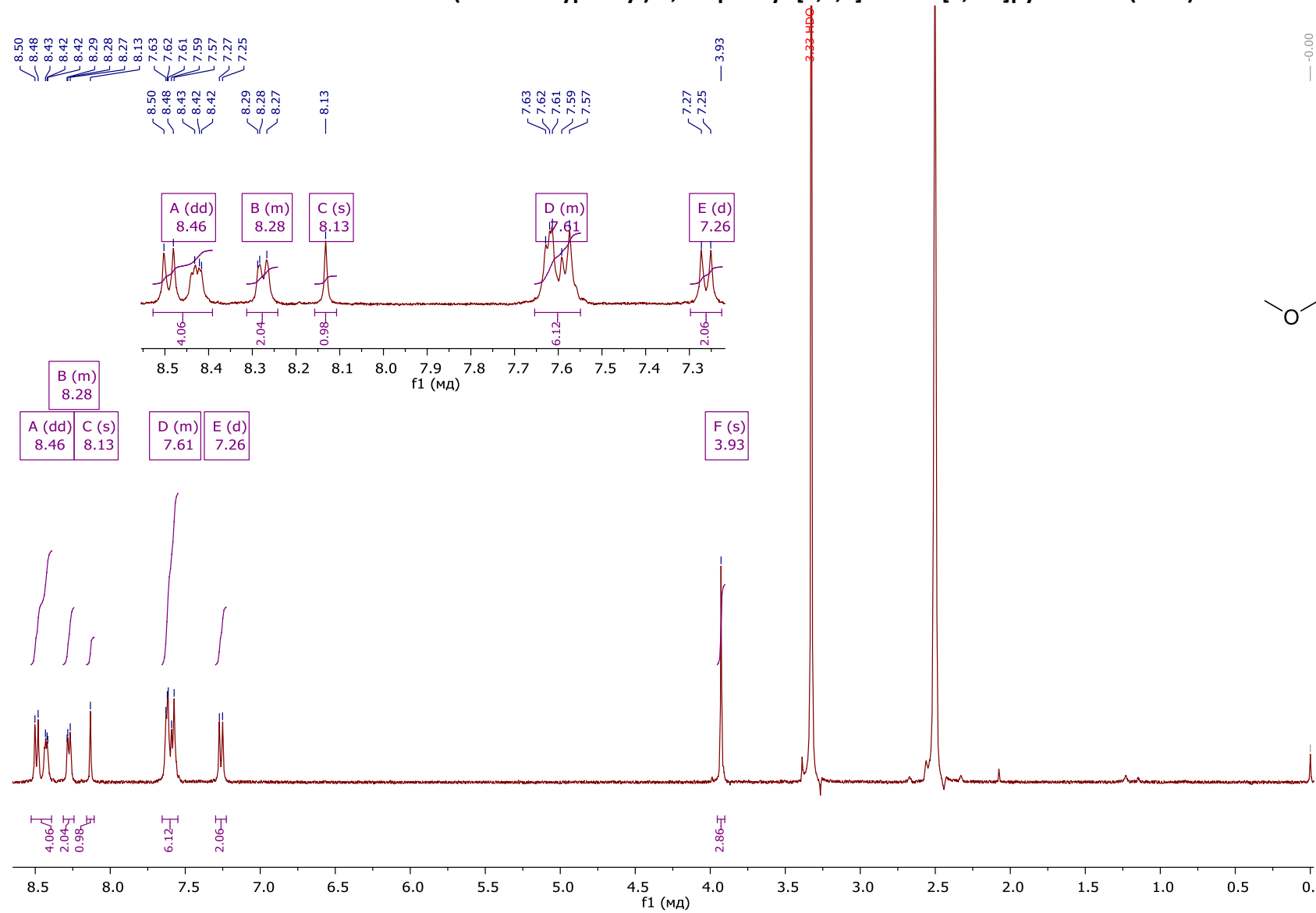
¹³C NMR (126 MHz, Chloroform-*d*) δ 165.93, 156.99, 156.04, 147.38, 142.36, 131.72, 131.37, 130.57, 130.47, 130.13, 129.41, 128.85, 128.57, 128.52, 128.45, 127.52, 105.09.

5-(4-(*N,N*-Dimethylaminophenyl))-2,7-diphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12ad)

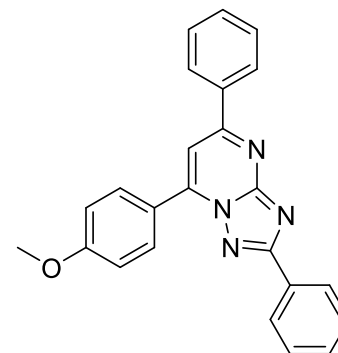
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.37 – 8.27 (m, 4H), 8.28 – 8.18 (m, 2H), 7.98 (s, 1H), 7.72 – 7.65 (m, 3H), 7.60 – 7.50 (m, 3H), 6.90 – 6.83 (m, 2H), 3.06 (s, 6H).

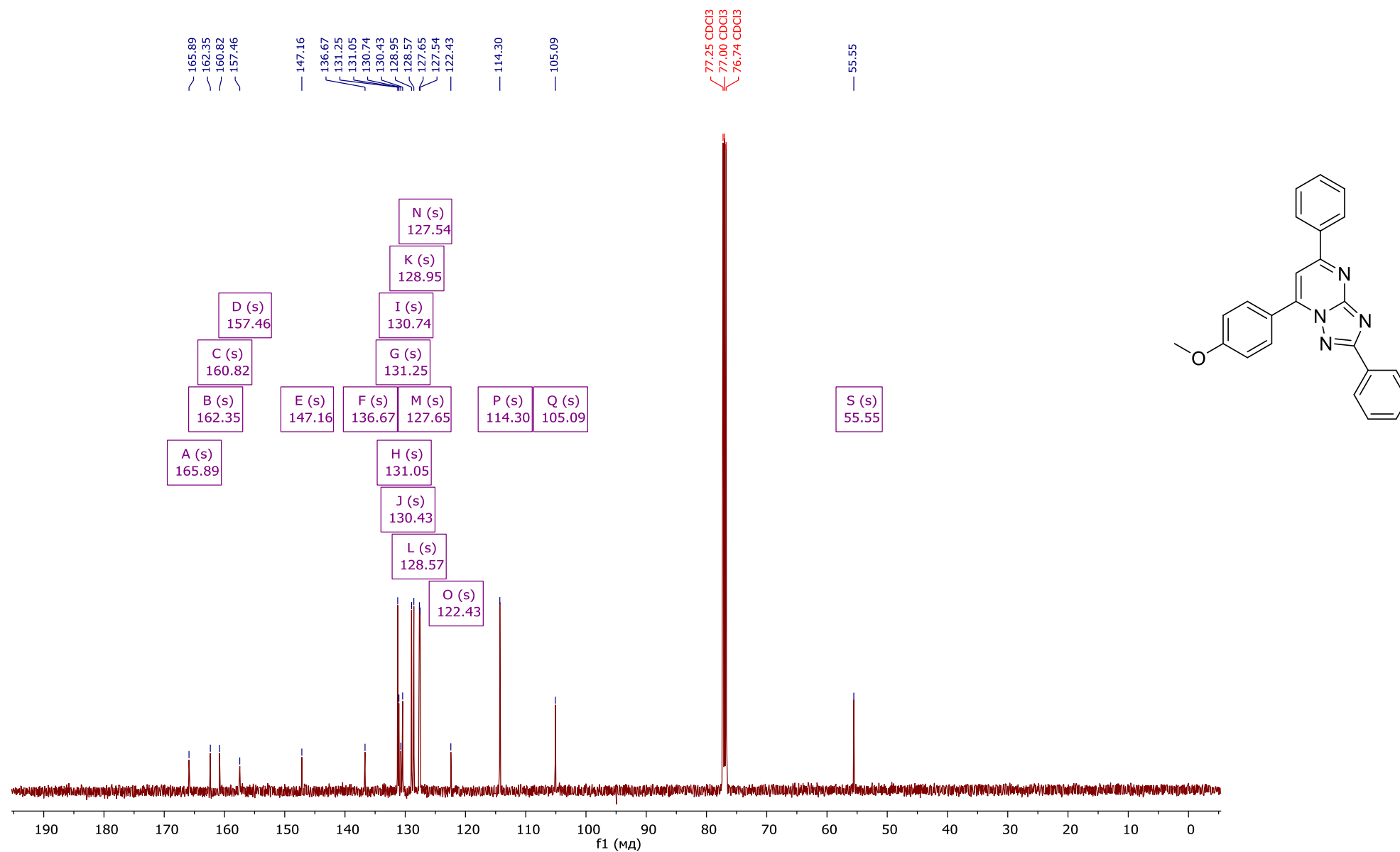


¹³C NMR (126 MHz, Chloroform-d) δ 165.31, 160.92, 152.38, 146.62, 131.28, 130.96, 130.76, 130.17, 129.36, 129.03, 128.85, 128.72, 128.49, 127.43, 123.50, 111.67, 105.13, 40.09.

7-(4-methoxyphenyl)-2,5-diphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12ba)

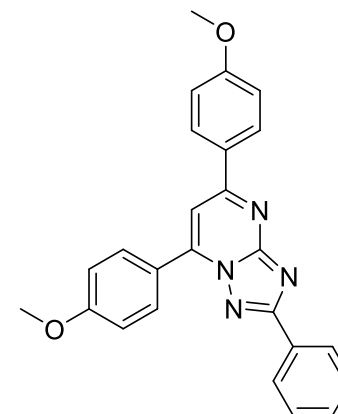
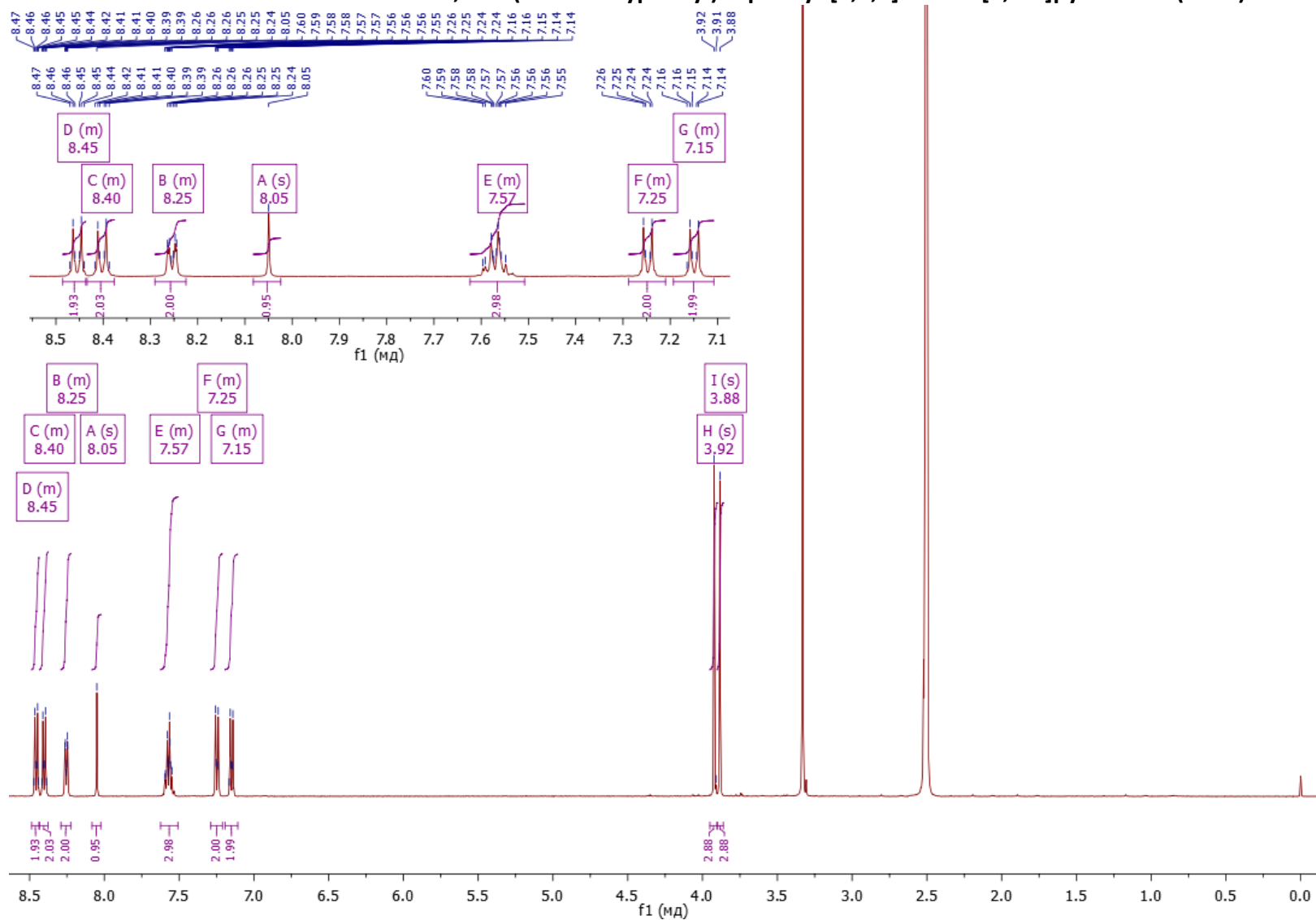
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.46 (dd, *J* = 26.0, 6.4 Hz, 4H), 8.31 – 8.24 (m, 2H), 8.13 (s, 1H), 7.65 – 7.55 (m, 6H), 7.26 (d, *J* = 8.5 Hz, 2H), 3.93 (s, 3H).



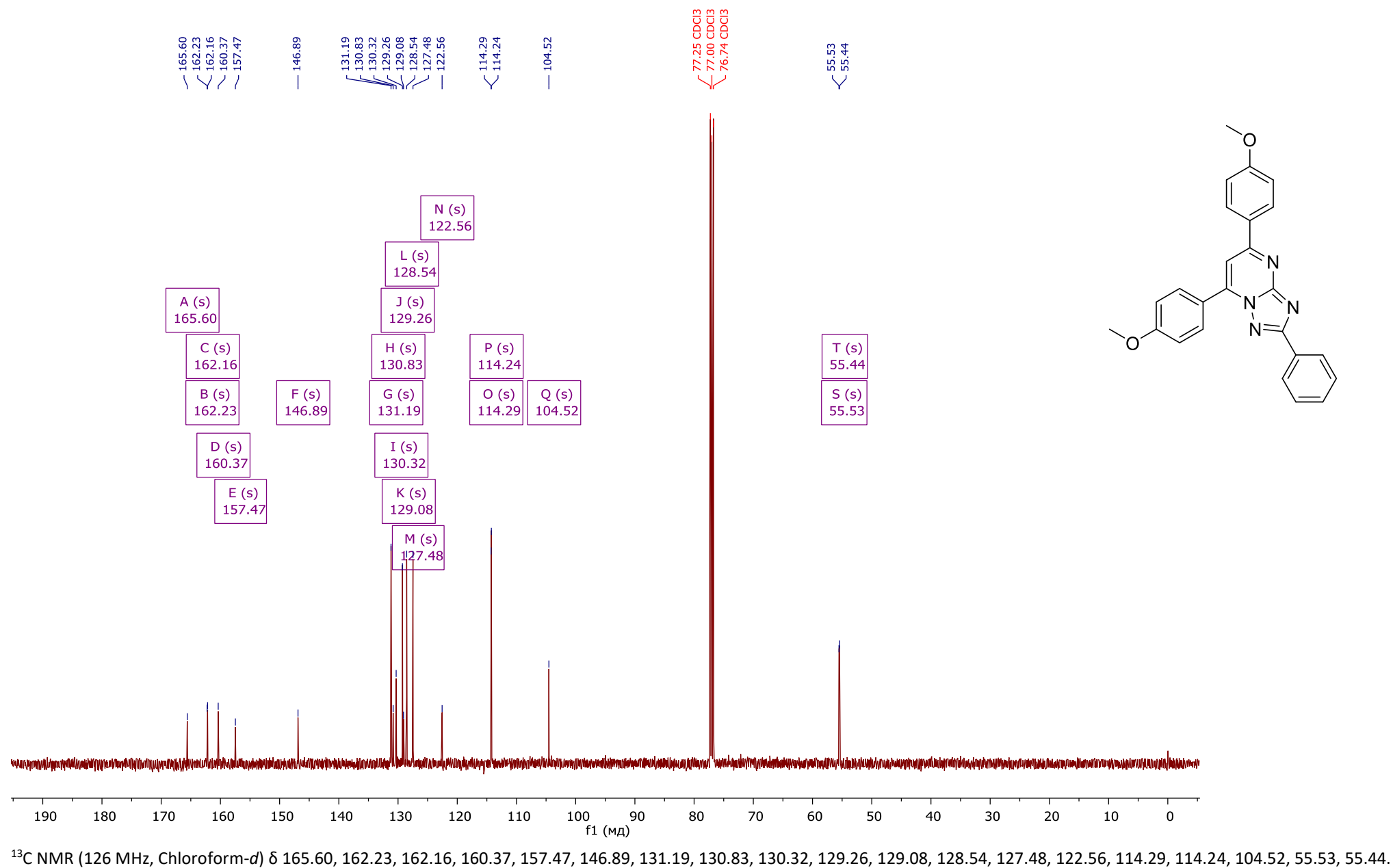


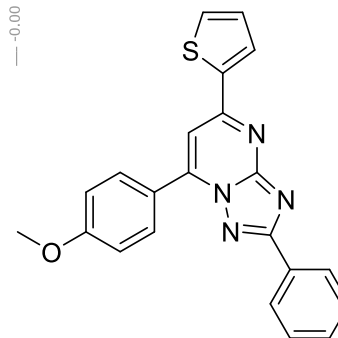
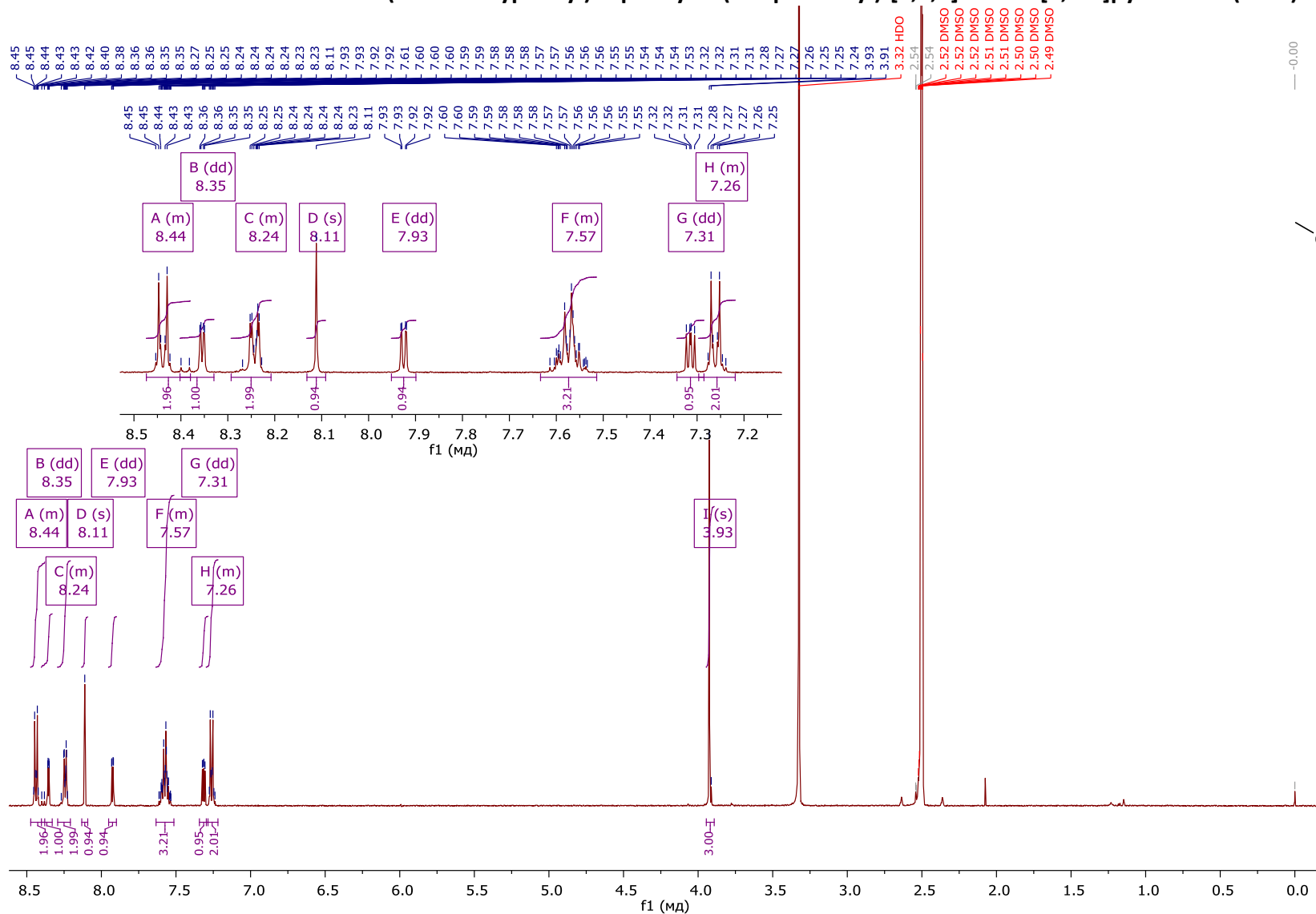
¹³C NMR (126 MHz, Chloroform-*d*) δ 165.89, 162.35, 160.82, 157.46, 147.16, 136.67, 131.25, 131.05, 130.74, 130.43, 128.95, 128.57, 127.65, 127.54, 122.43, 114.30, 105.09, 55.55.

5,7-bis(4-methoxyphenyl)-2-phenyl-[1,2,4]triazolo[1,5-a]pyrimidine (12bb)

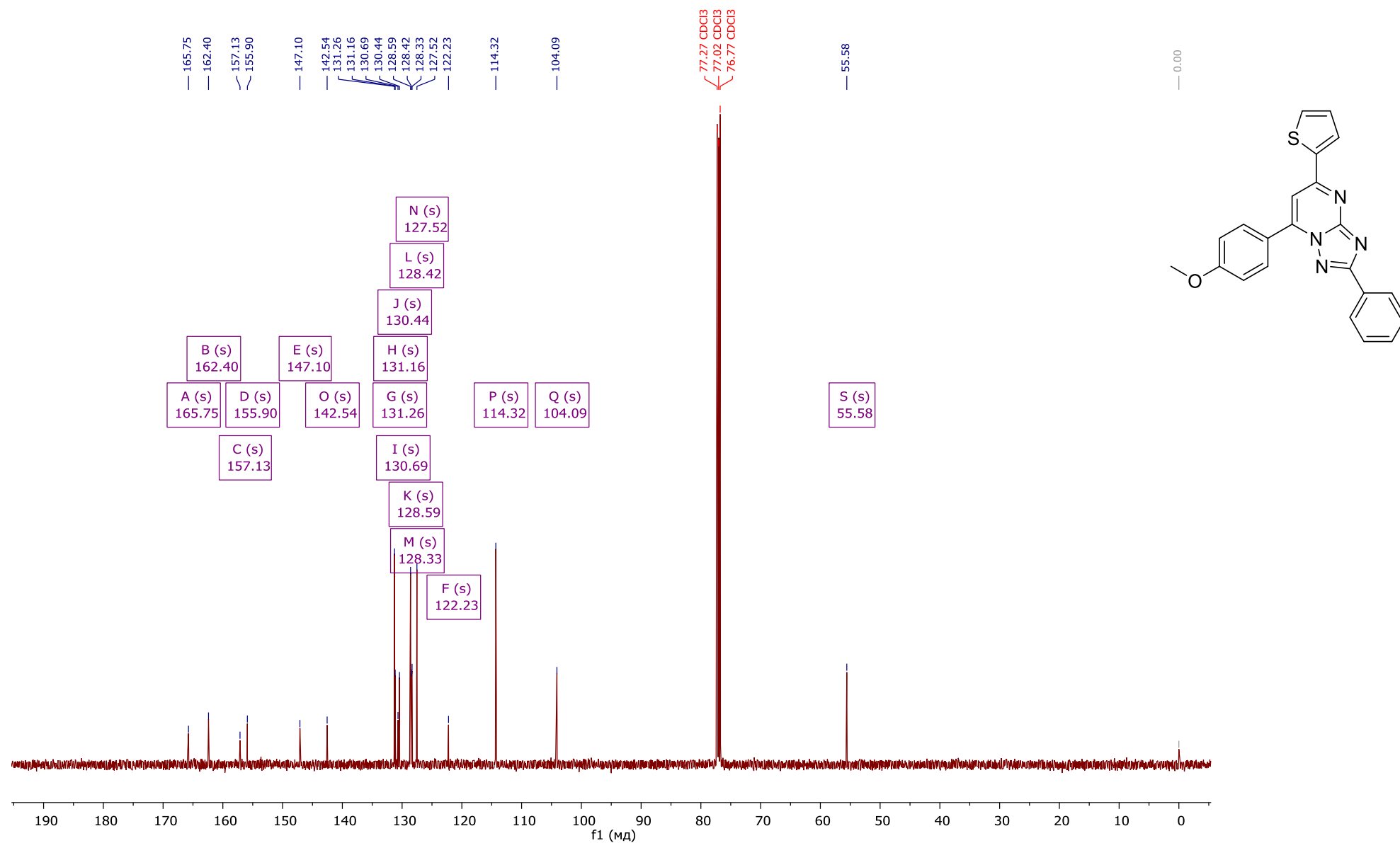


¹H NMR (500 MHz, DMSO-*d*₆) δ 8.49 – 8.44 (m, 2H), 8.43 – 8.38 (m, 2H), 8.29 – 8.22 (m, 2H), 8.05 (s, 1H), 7.62 – 7.51 (m, 3H), 7.29 – 7.21 (m, 2H), 7.19 – 7.11 (m, 2H), 3.92 (s, 3H), 3.88 (s, 3H).

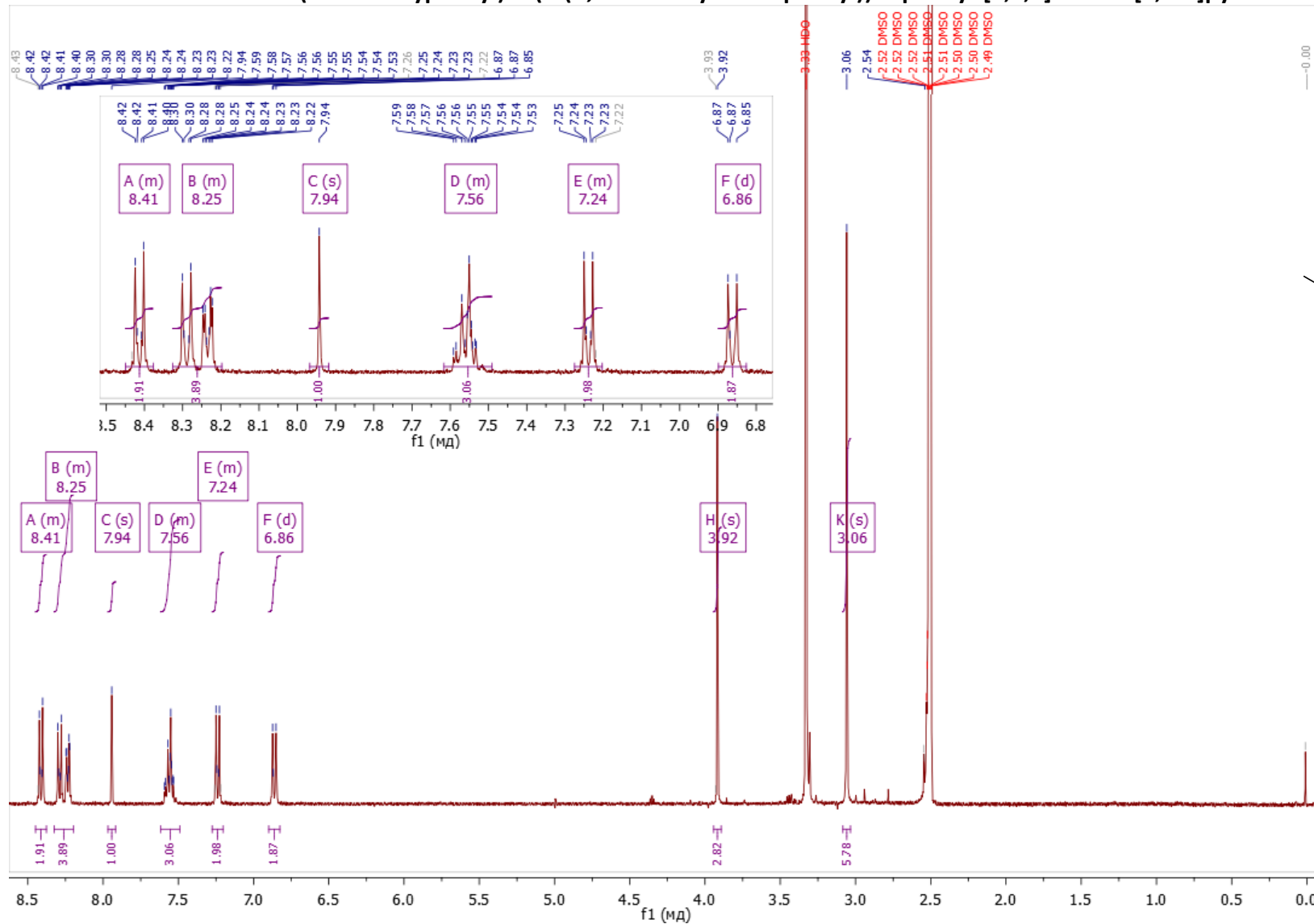


7-(4-Methoxyphenyl)-2-phenyl-5-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (12bc)

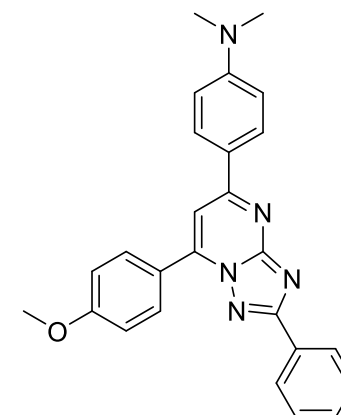
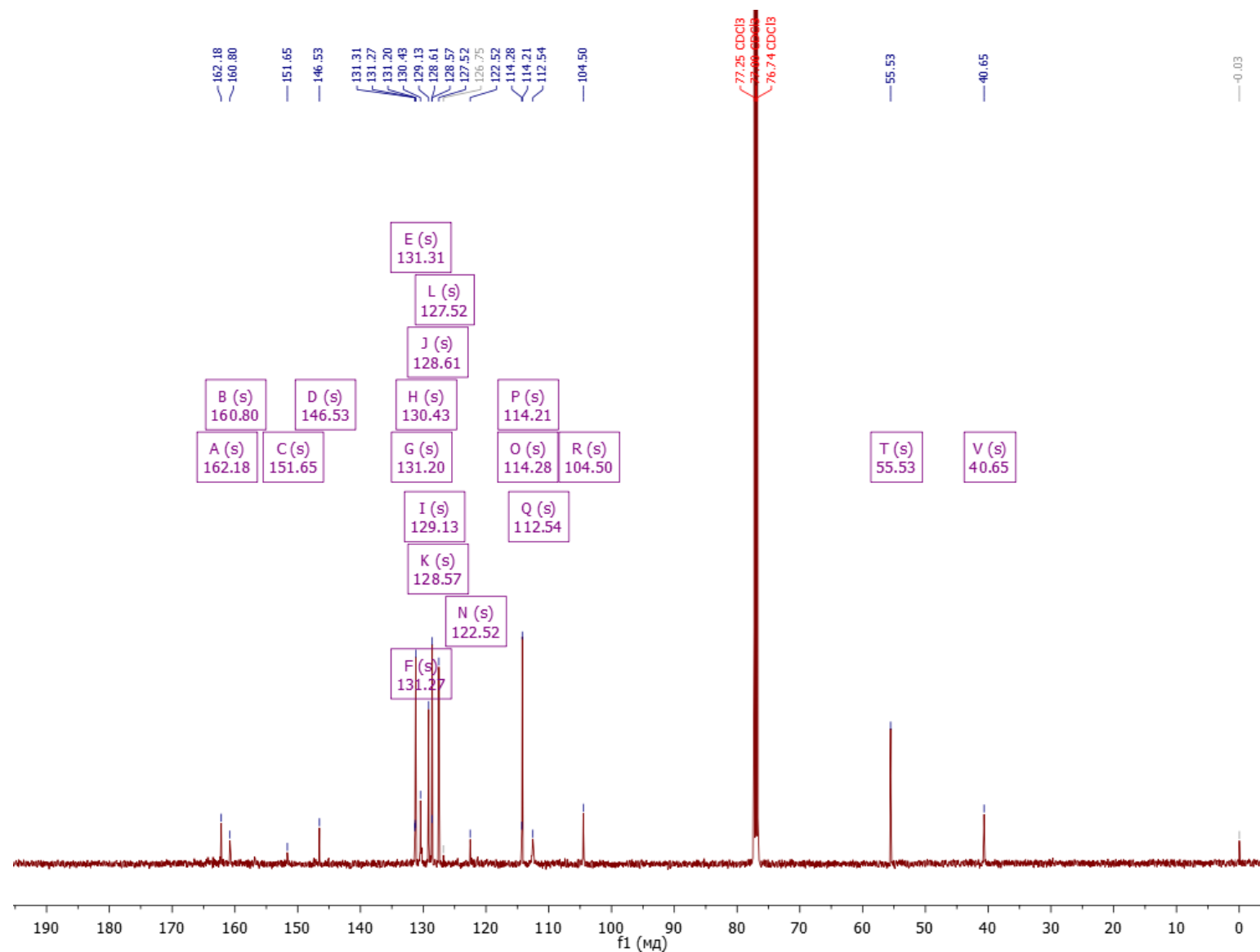
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.47 – 8.38 (m, 2H), 8.35 (dd, *J* = 3.8, 1.2 Hz, 1H), 8.29 – 8.21 (m, 2H), 8.11 (s, 1H), 7.93 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.63 – 7.51 (m, 3H), 7.31 (dd, *J* = 5.0, 3.7 Hz, 1H), 7.30 – 7.22 (m, 2H), 3.93 (s, 3H).



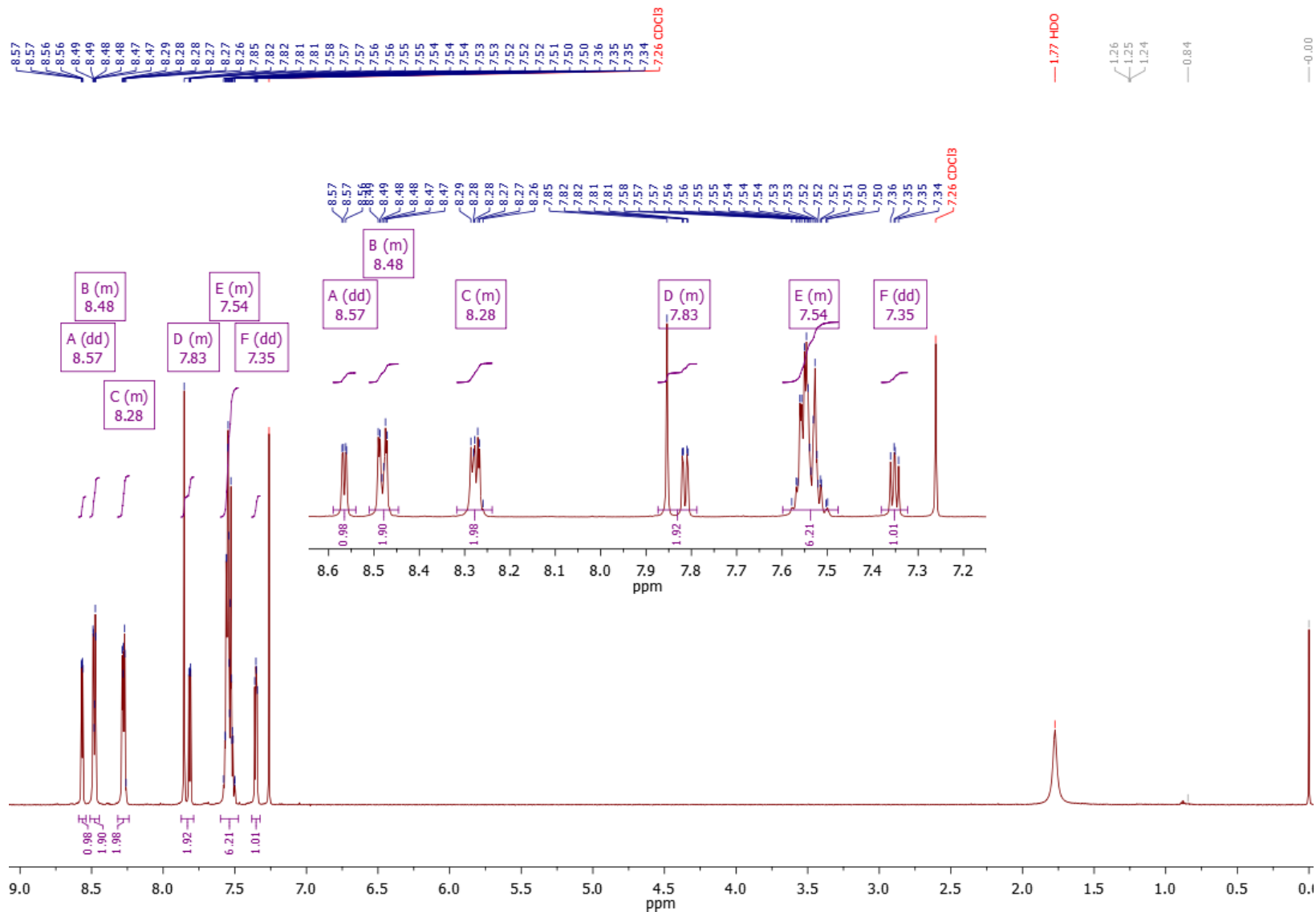
¹³C NMR (126 MHz, Chloroform-*d*) δ 165.75, 162.40, 157.13, 155.90, 147.10, 142.54, 131.26, 131.16, 130.69, 130.44, 128.59, 128.42, 128.33, 127.52, 122.23, 114.32, 104.09, 55.58.

7-(4-Methoxyphenyl)-5-(4-(*N,N*-dimethylaminophenyl))-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12bd)

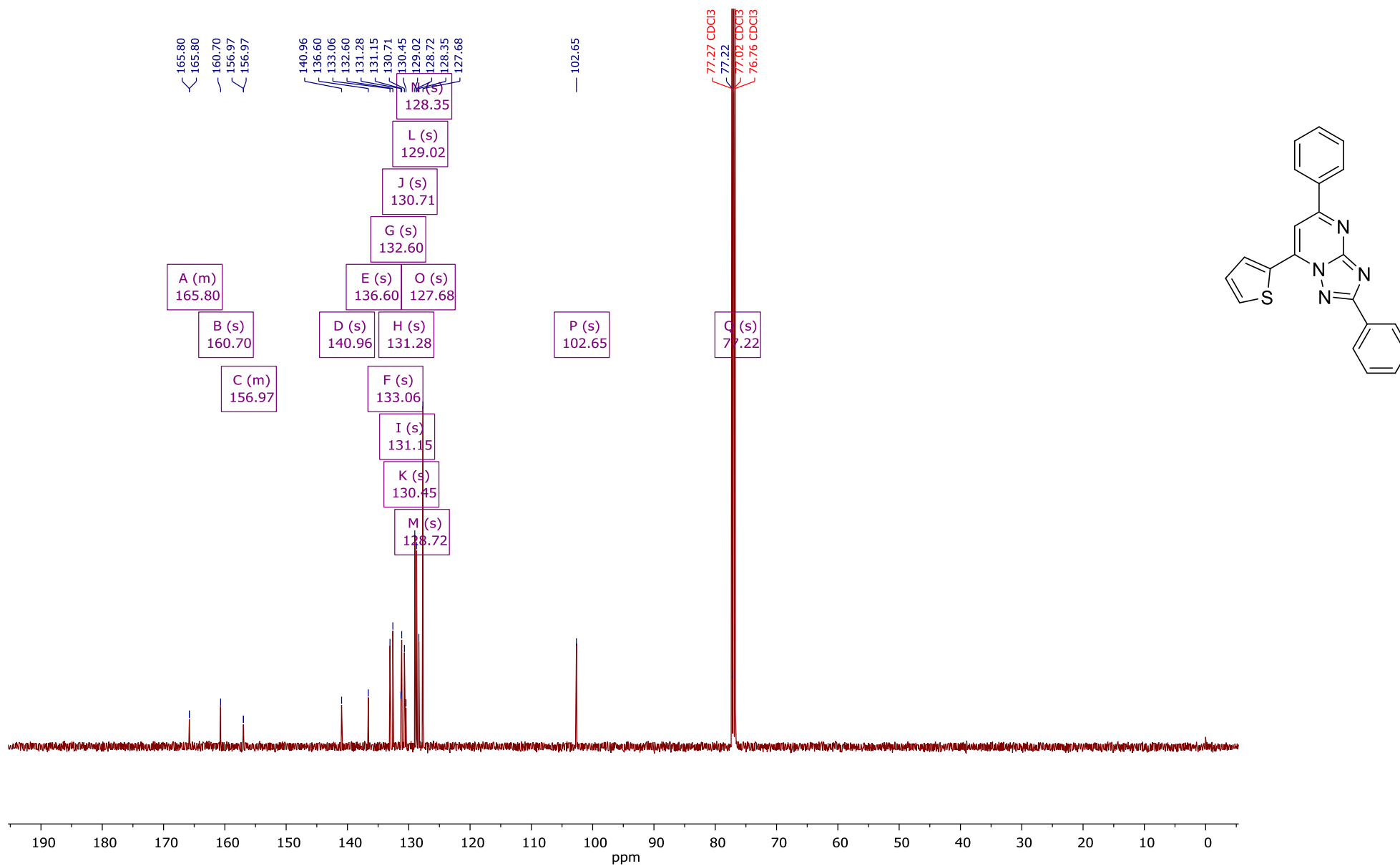
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.45 – 8.38 (m, 2H), 8.33 – 8.20 (m, 4H), 7.94 (s, 1H), 7.62 – 7.49 (m, 3H), 7.27 – 7.20 (m, 2H), 6.86 (d, *J* = 9.1 Hz, 2H), 3.92 (s, 3H), 3.06 (s, 6H).

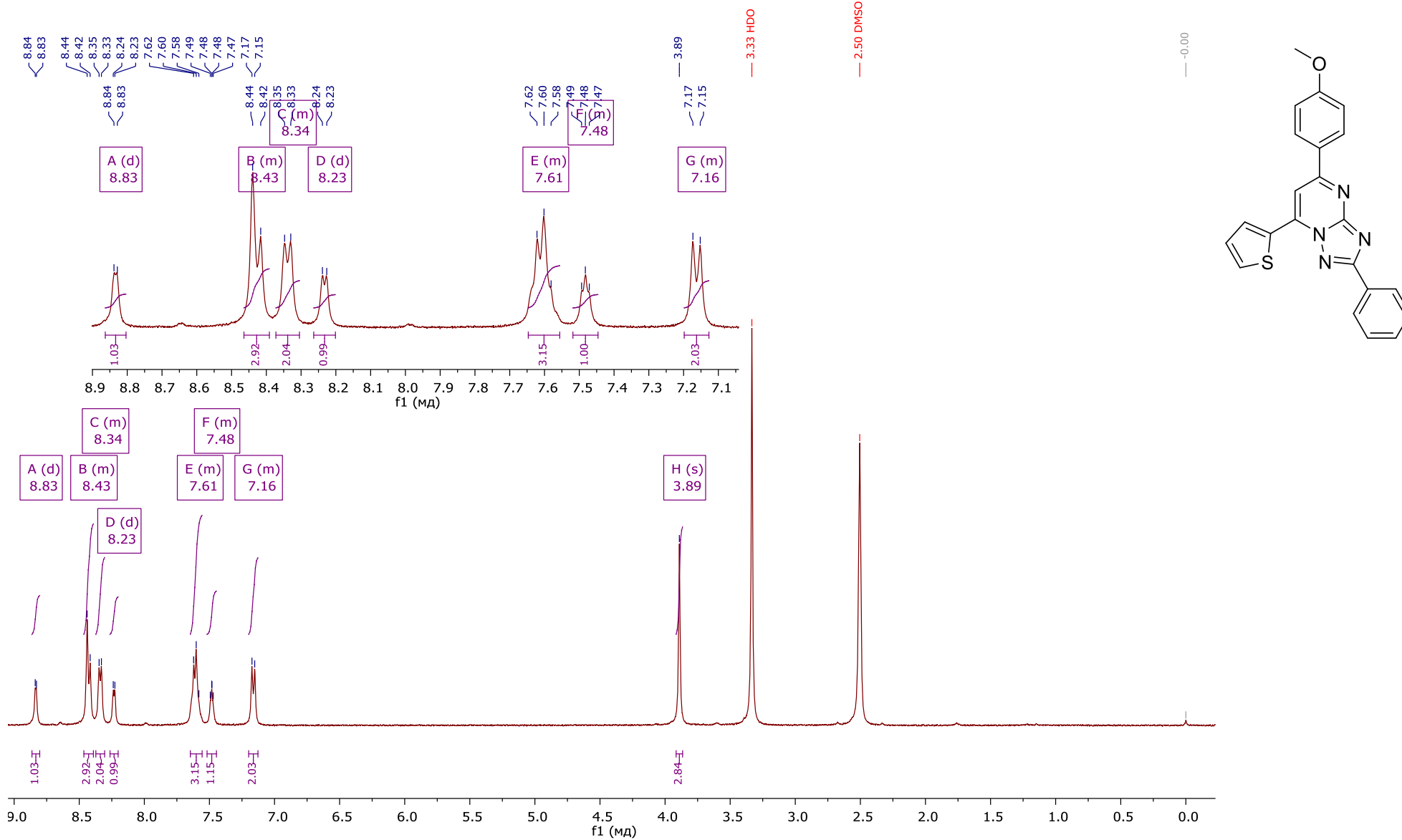


¹³C NMR (126 MHz, Chloroform-*d*) δ 162.18, 160.80, 151.65, 146.53, 131.31, 131.27, 131.20, 130.43, 129.13, 128.61, 128.57, 127.52, 122.52, 114.28, 114.21, 112.54, 104.50, 55.53, 40.65.

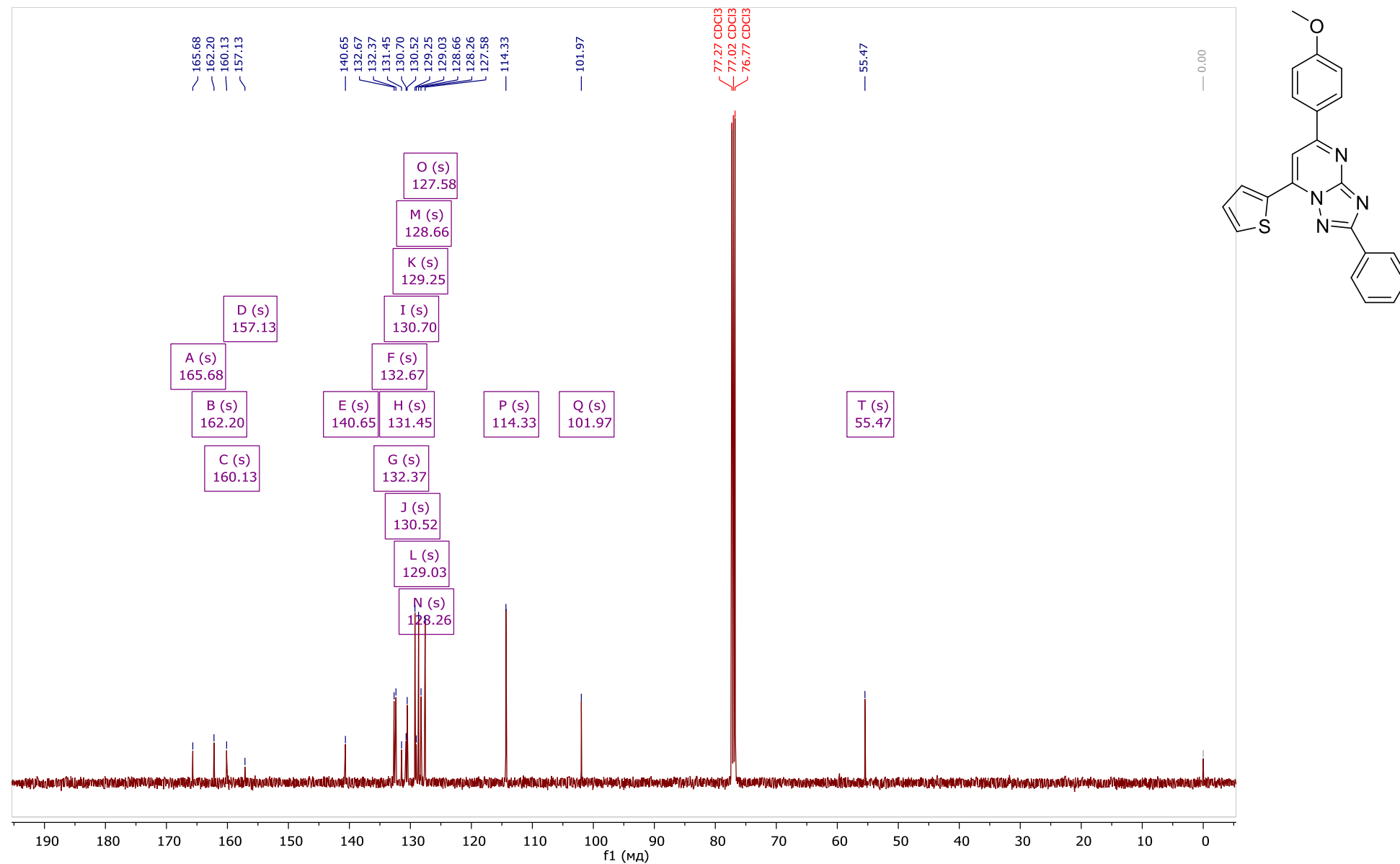
2,5-Diphenyl-7-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (12ca)

¹H NMR (500 MHz, Chloroform-*d*) δ 8.57 (dd, *J* = 3.9, 1.2 Hz, 1H), 8.51 – 8.45 (m, 2H), 8.32 – 8.24 (m, 2H), 7.87 – 7.79 (m, 2H), 7.60 – 7.48 (m, 6H), 7.35 (dd, *J* = 5.0, 3.9 Hz, 1H).

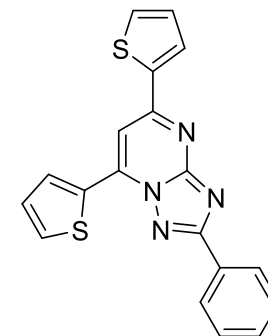
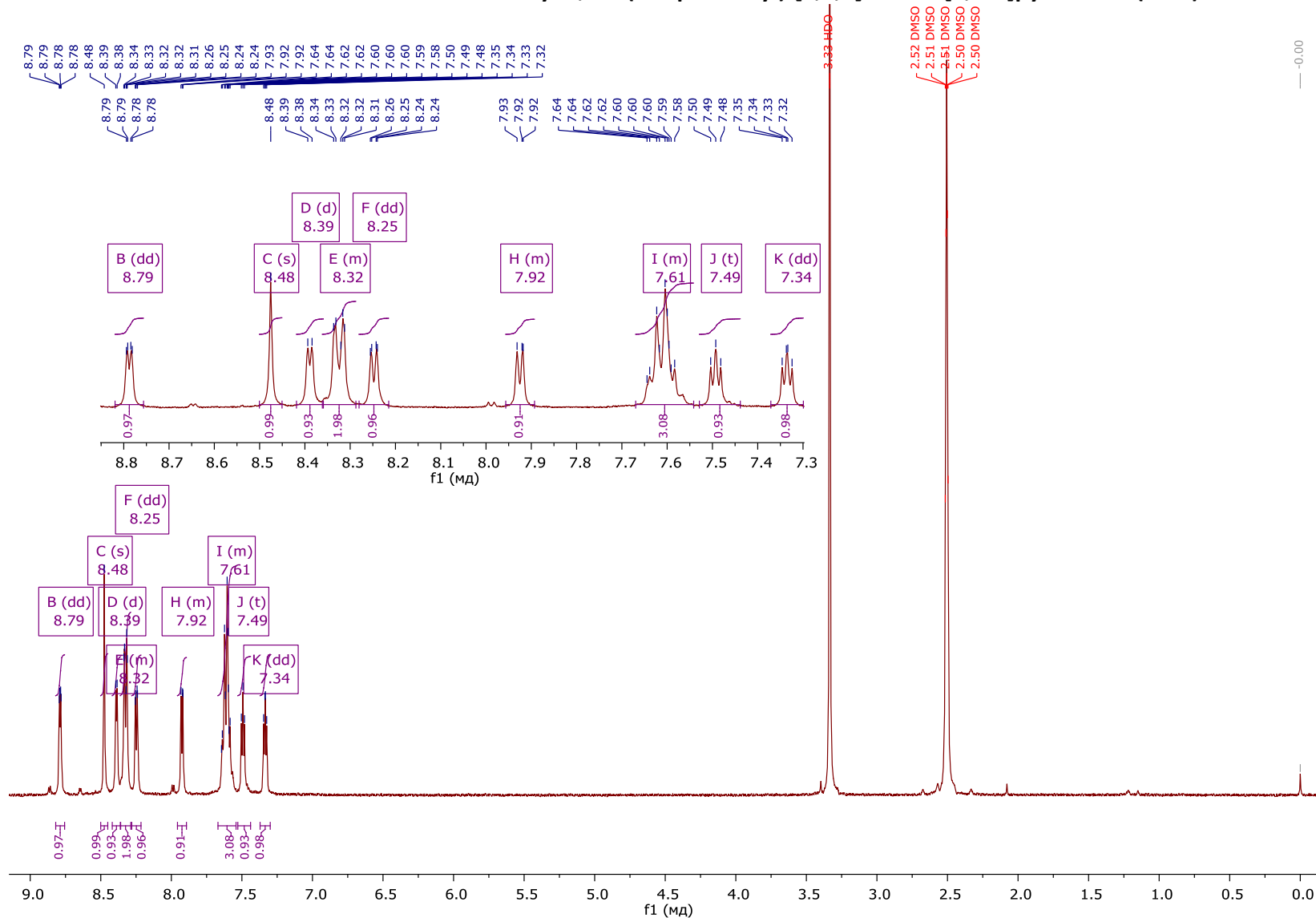


5-(4-Methoxyphenyl)-2-phenyl-7-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (12cb)

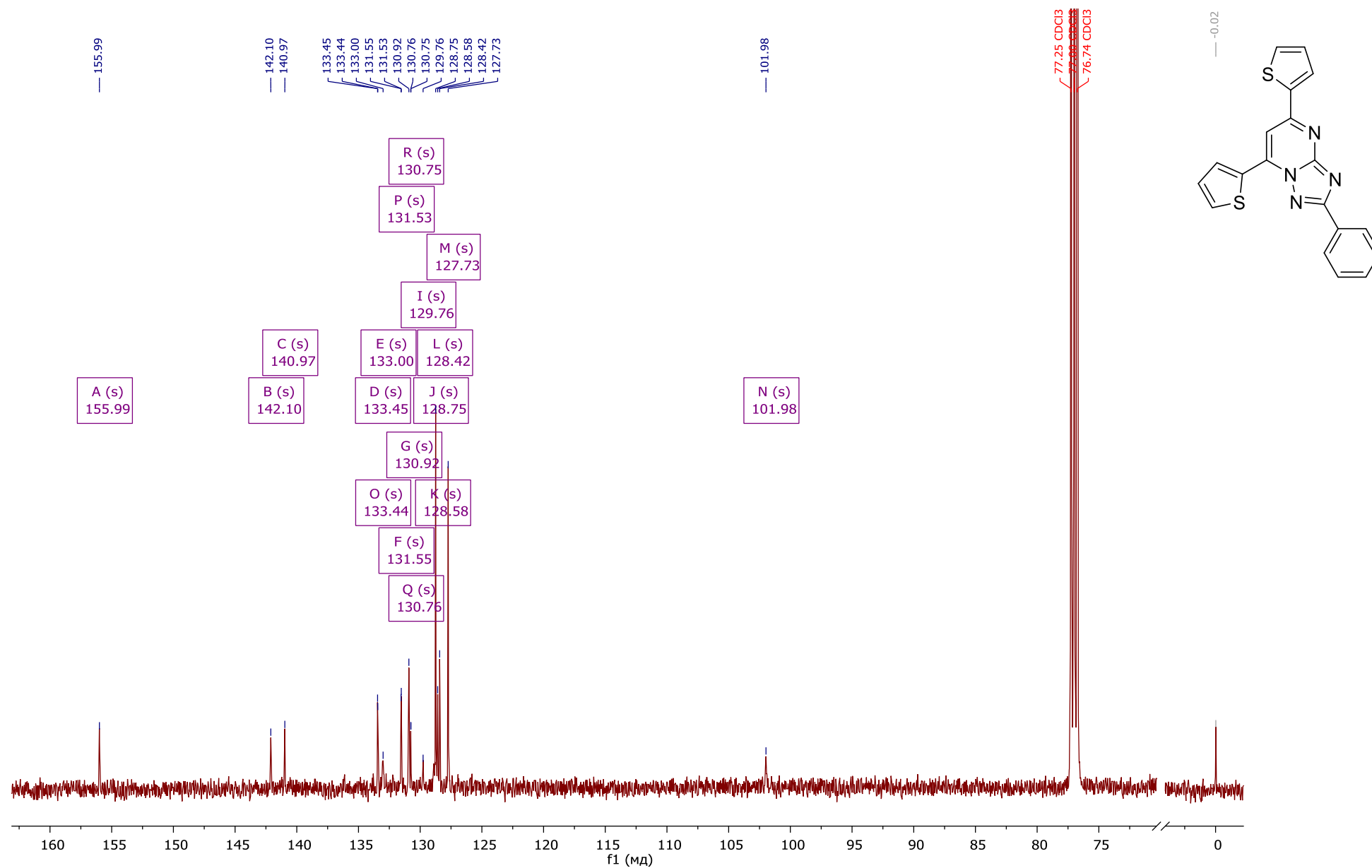
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.83 (d, *J* = 3.9 Hz, 1H), 8.46 – 8.39 (m, 3H), 8.37 – 8.30 (m, 2H), 8.23 (d, *J* = 5.0 Hz, 1H), 7.65 – 7.56 (m, 3H), 7.52 – 7.45 (m, 1H), 7.20 – 7.13 (m, 2H), 3.89 (s, 3H).



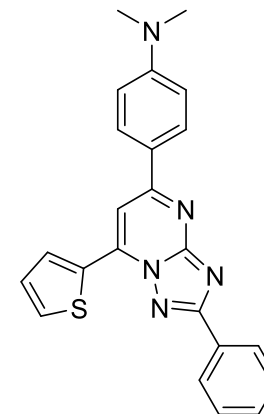
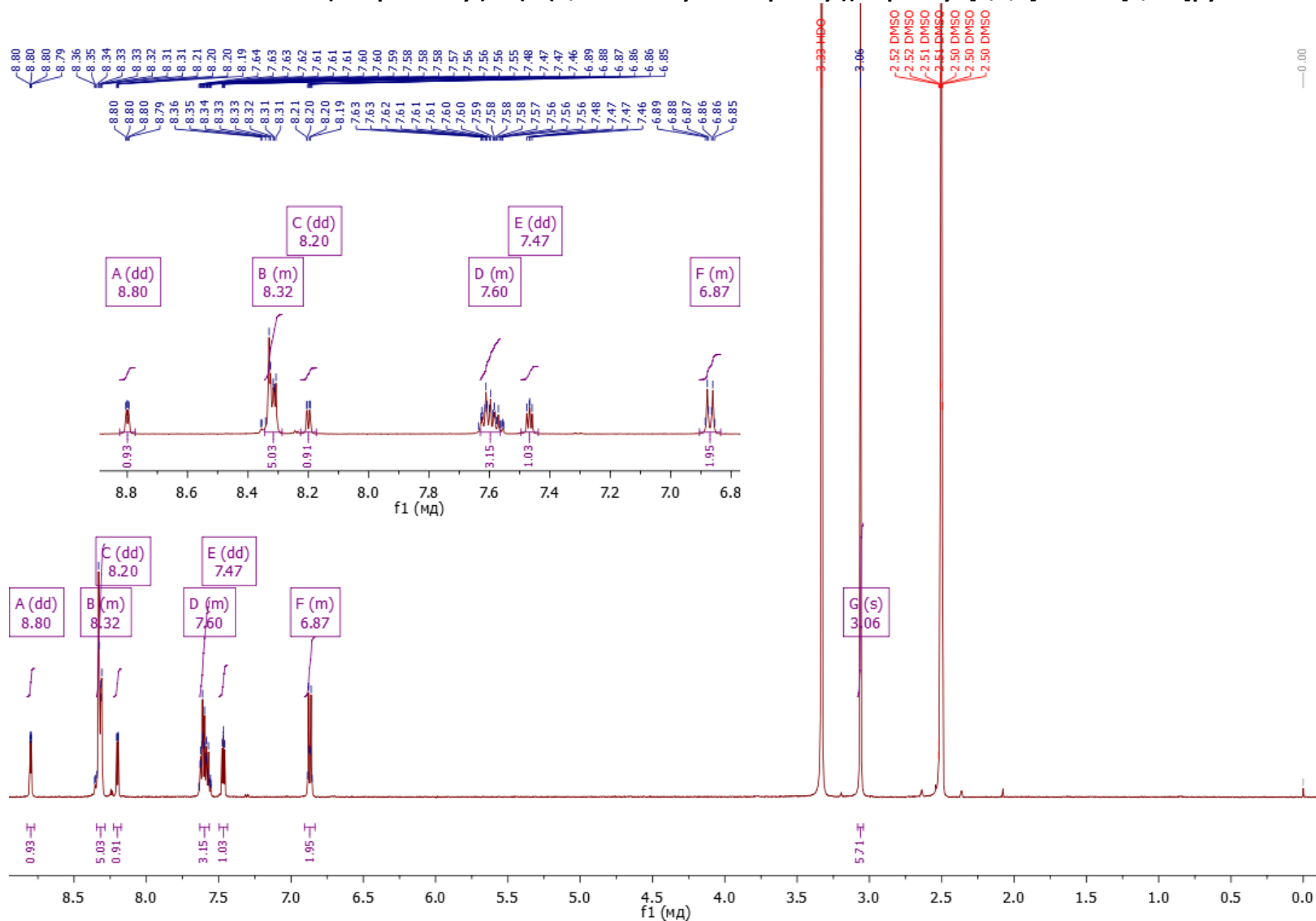
^{13}C NMR (126 MHz, Chloroform-d) δ 165.68, 162.20, 160.13, 157.13, 140.65, 132.67, 132.37, 131.45, 130.70, 130.52, 129.25, 129.03, 128.66, 128.26, 127.58, 114.33, 101.97, 55.47.

2-Phenyl-5,7-di(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidine (12cc)

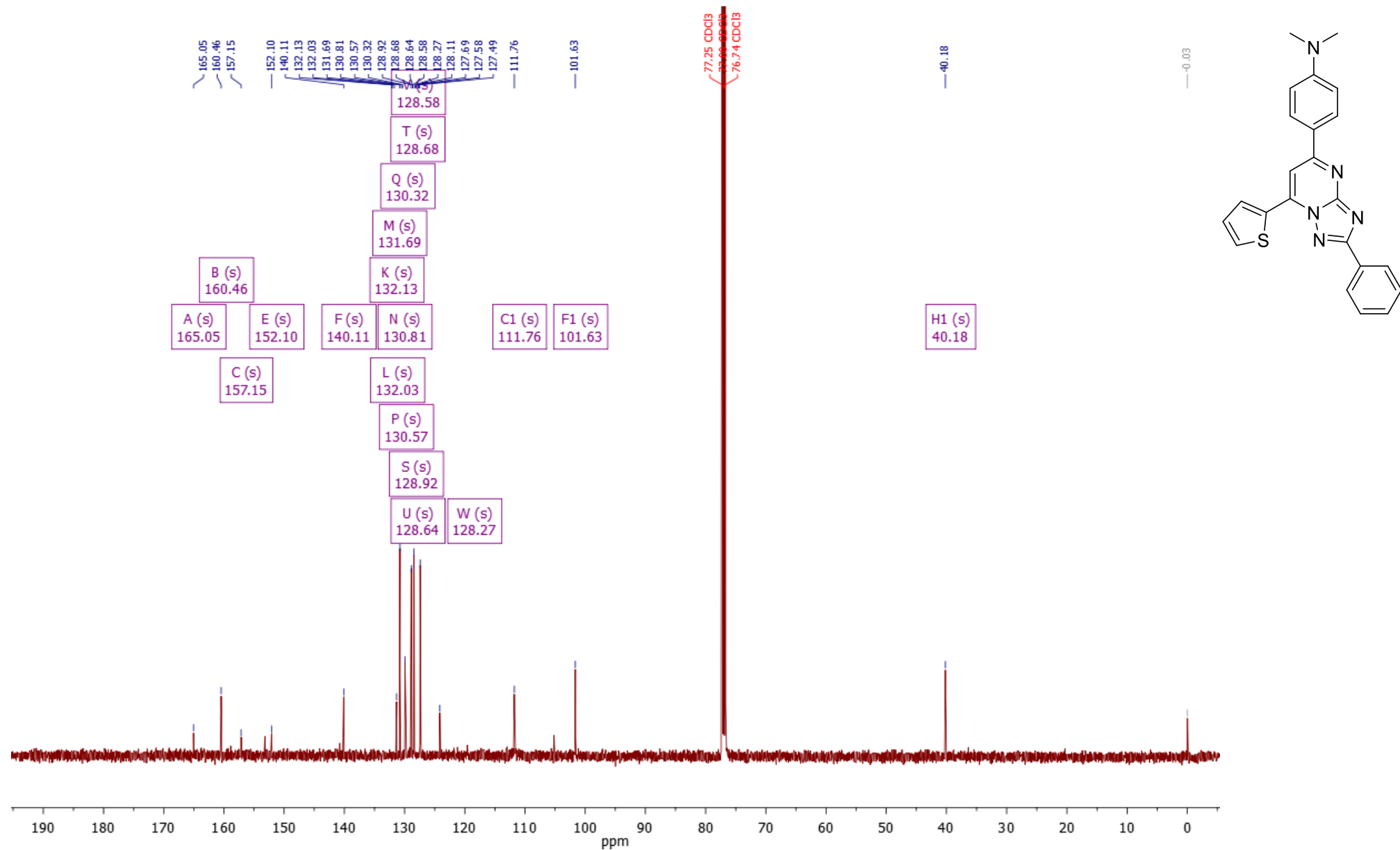
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.79 (dd, J = 4.0, 1.2 Hz, 1H), 8.48 (s, 1H), 8.39 (d, J = 3.8 Hz, 1H), 8.36 – 8.29 (m, 2H), 8.25 (dd, J = 5.1, 1.1 Hz, 1H), 7.96 – 7.89 (m, 1H), 7.67 – 7.54 (m, 3H), 7.49 (t, J = 4.5 Hz, 1H), 7.34 (dd, J = 5.0, 3.7 Hz, 1H).



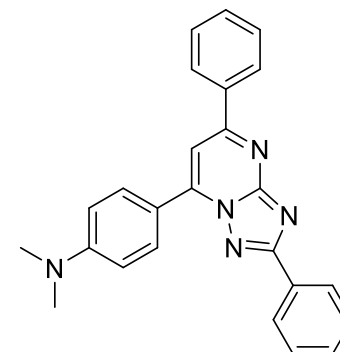
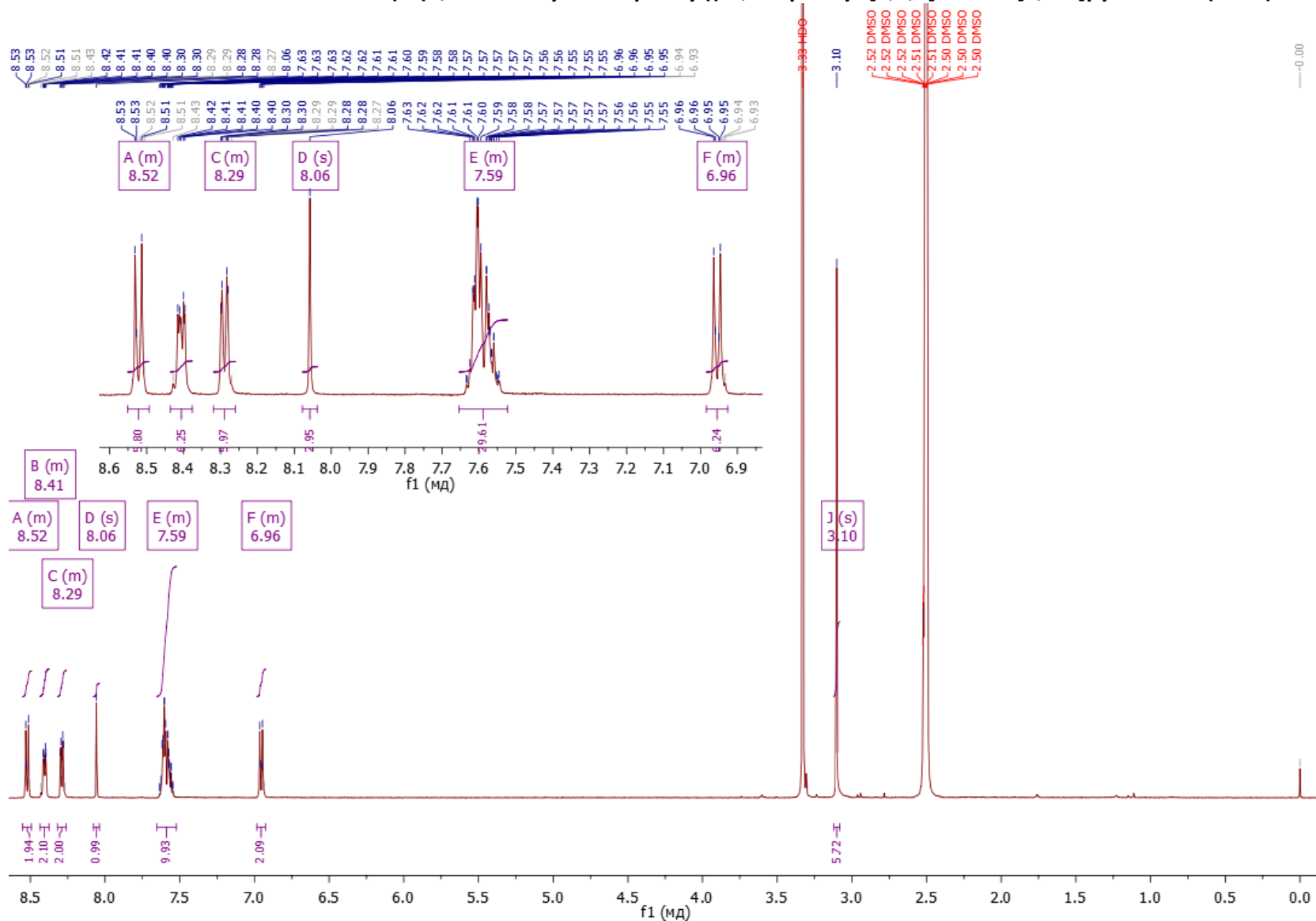
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.99, 142.10, 140.97, 133.45, 133.44, 133.00, 131.55, 131.53, 130.92, 130.76, 130.75, 129.76, 128.75, 128.58, 128.42, 127.73, 101.98.

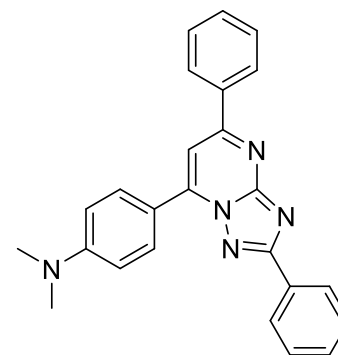
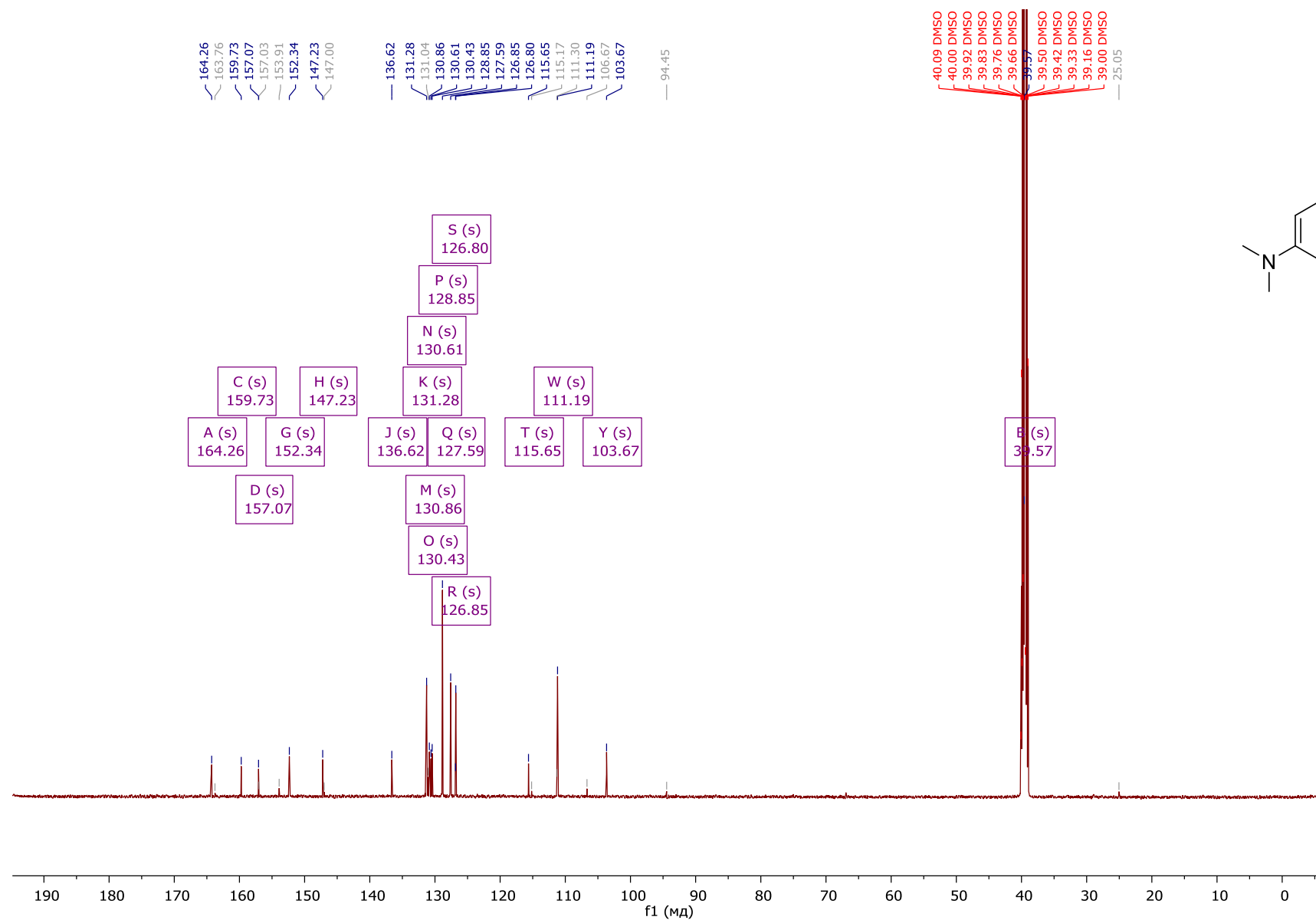
7-(thiophen-2-yl)-5-(4-(*N,N*-dimethylaminophenyl))-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12cd)

¹H NMR (500 MHz, DMSO-*d*₆) δ 8.80 (dd, J = 4.0, 1.2 Hz, 1H), 8.34 – 8.29 (m, 5H), 8.20 (dd, J = 5.0, 1.1 Hz, 1H), 7.63 – 7.56 (m, 3H), 7.47 (dd, J = 5.1, 3.9 Hz, 1H), 6.91 – 6.83 (m, 2H), 3.06 (s, 6H).

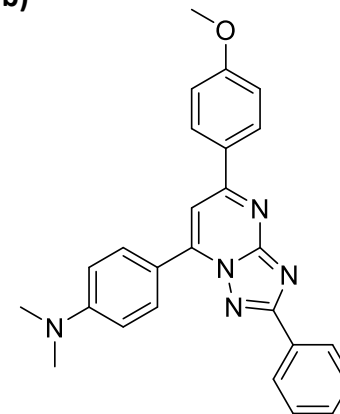
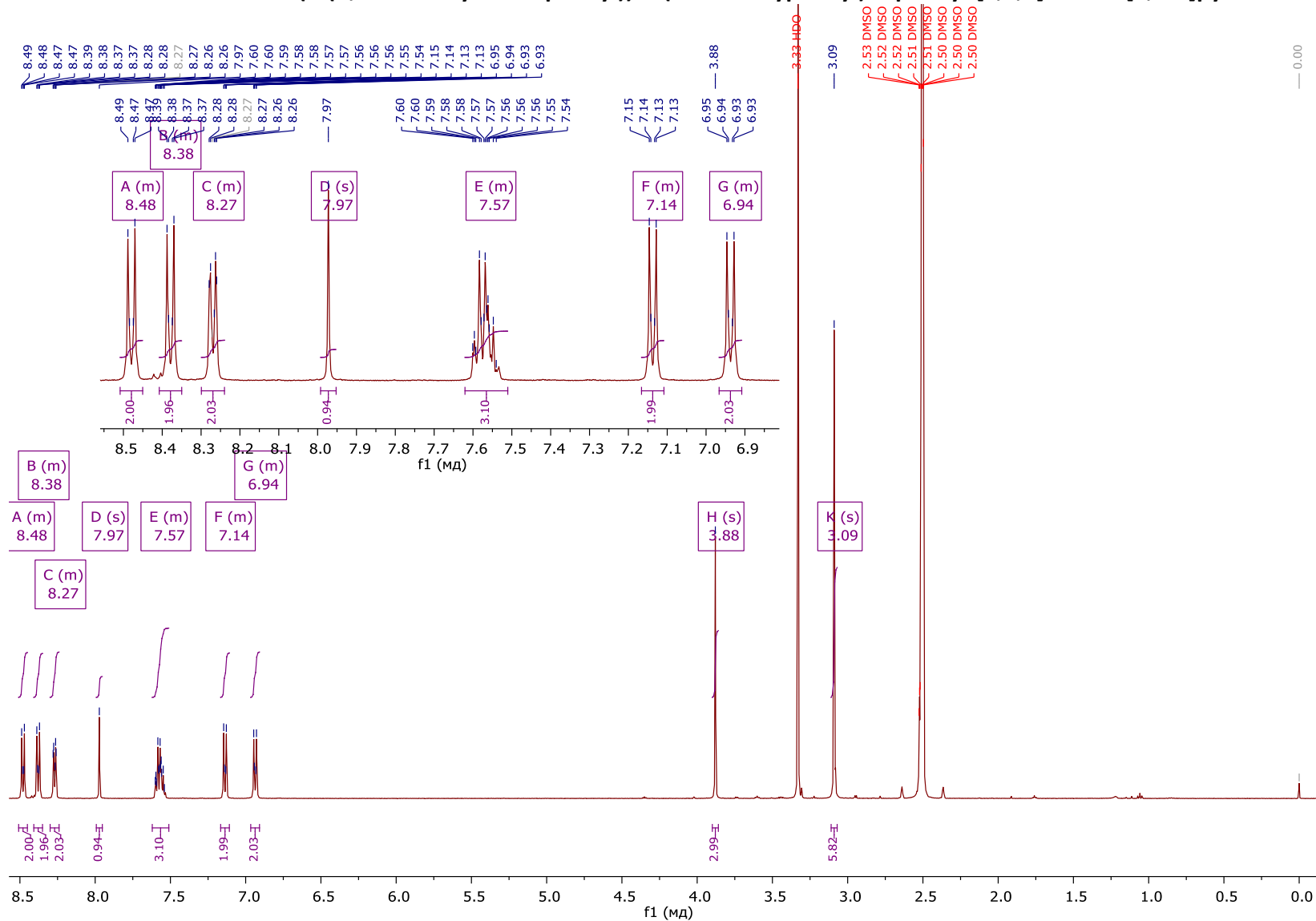


¹³C NMR (126 MHz, Chloroform-*d*) δ 165.05, 160.46, 157.15, 152.10, 140.11, 132.13, 132.03, 131.69, 130.81, 130.57, 130.32, 128.92, 128.68, 128.64, 128.58, 128.27, 128.11, 127.69, 127.58, 127.49, 111.76, 101.63, 40.18.

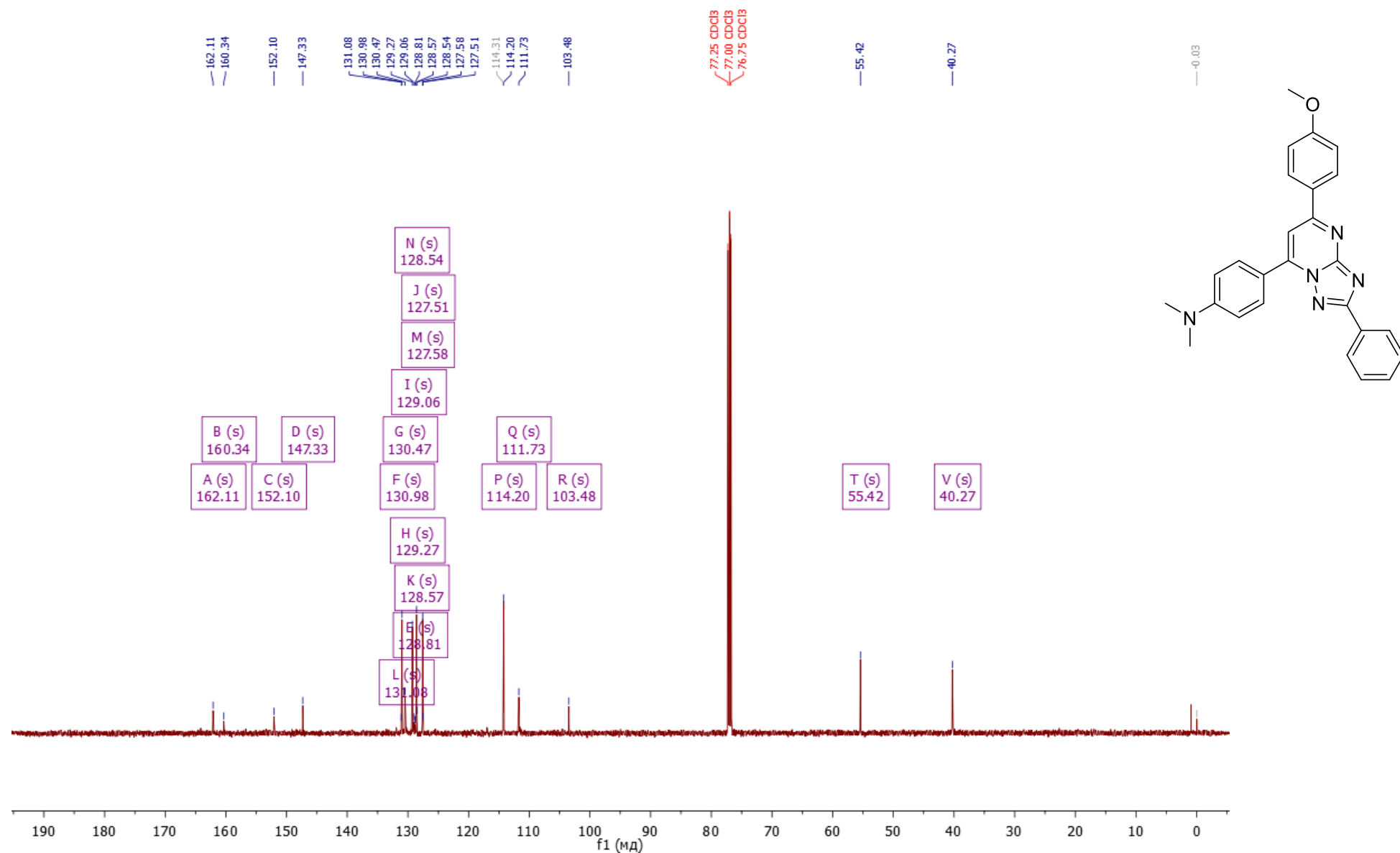
7-(4-(*N,N*-dimethylaminophenyl))-2,5-diphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12da)



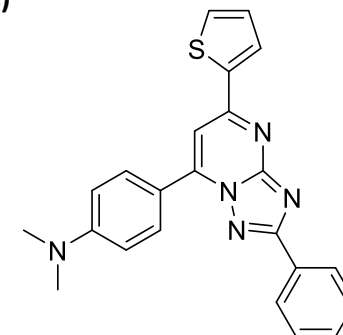
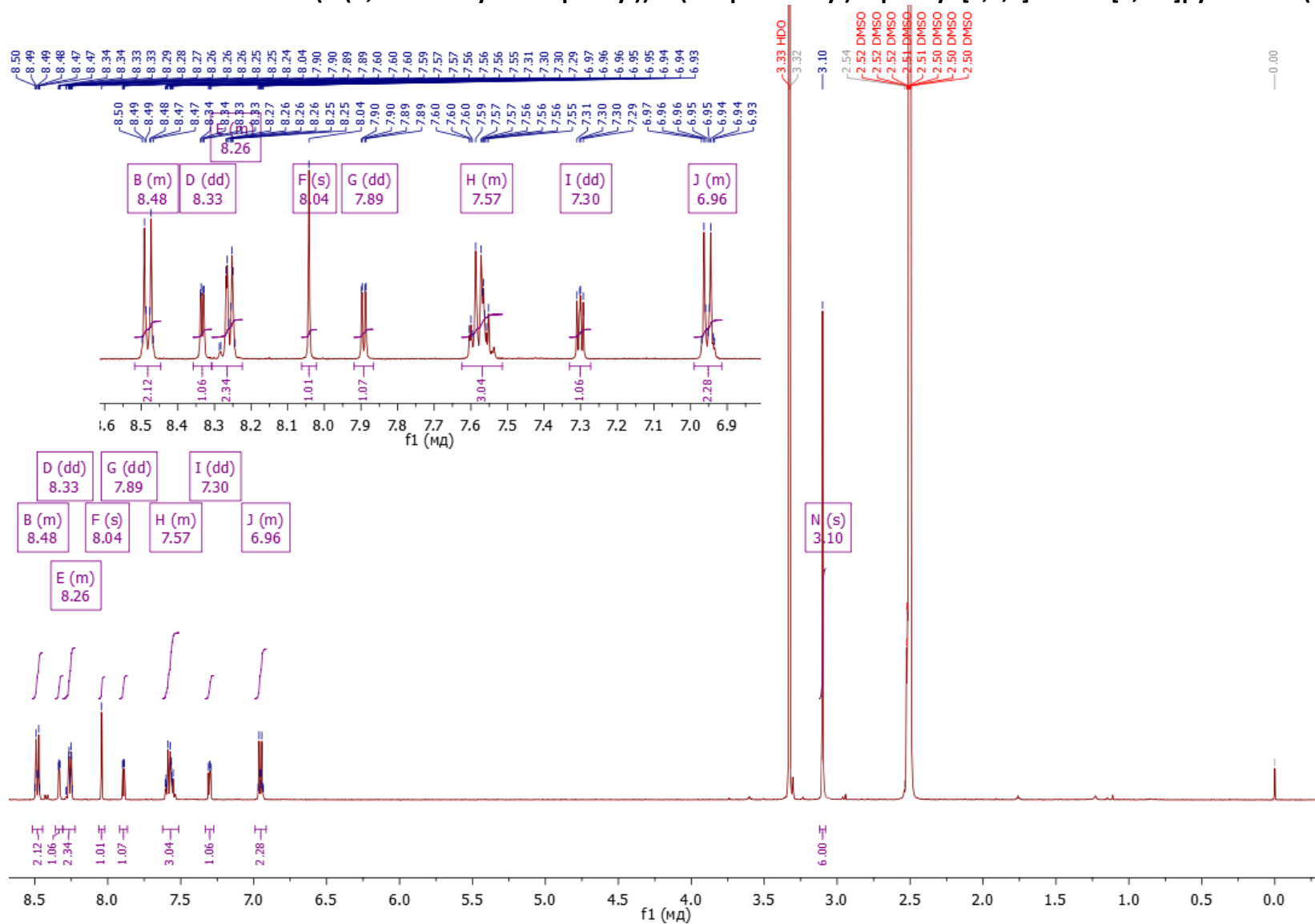
^{13}C NMR (126 MHz, $\text{DMSO}-d_6$) δ 164.26, 159.73, 157.07, 152.34, 147.23, 136.62, 131.28, 130.86, 130.61, 130.43, 128.85, 127.59, 126.85, 126.80, 115.65, 111.19, 103.67, 39.57.

7-(4-(*N,N*-dimethylaminophenyl))-5-(4-methoxyphenyl)-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12db)

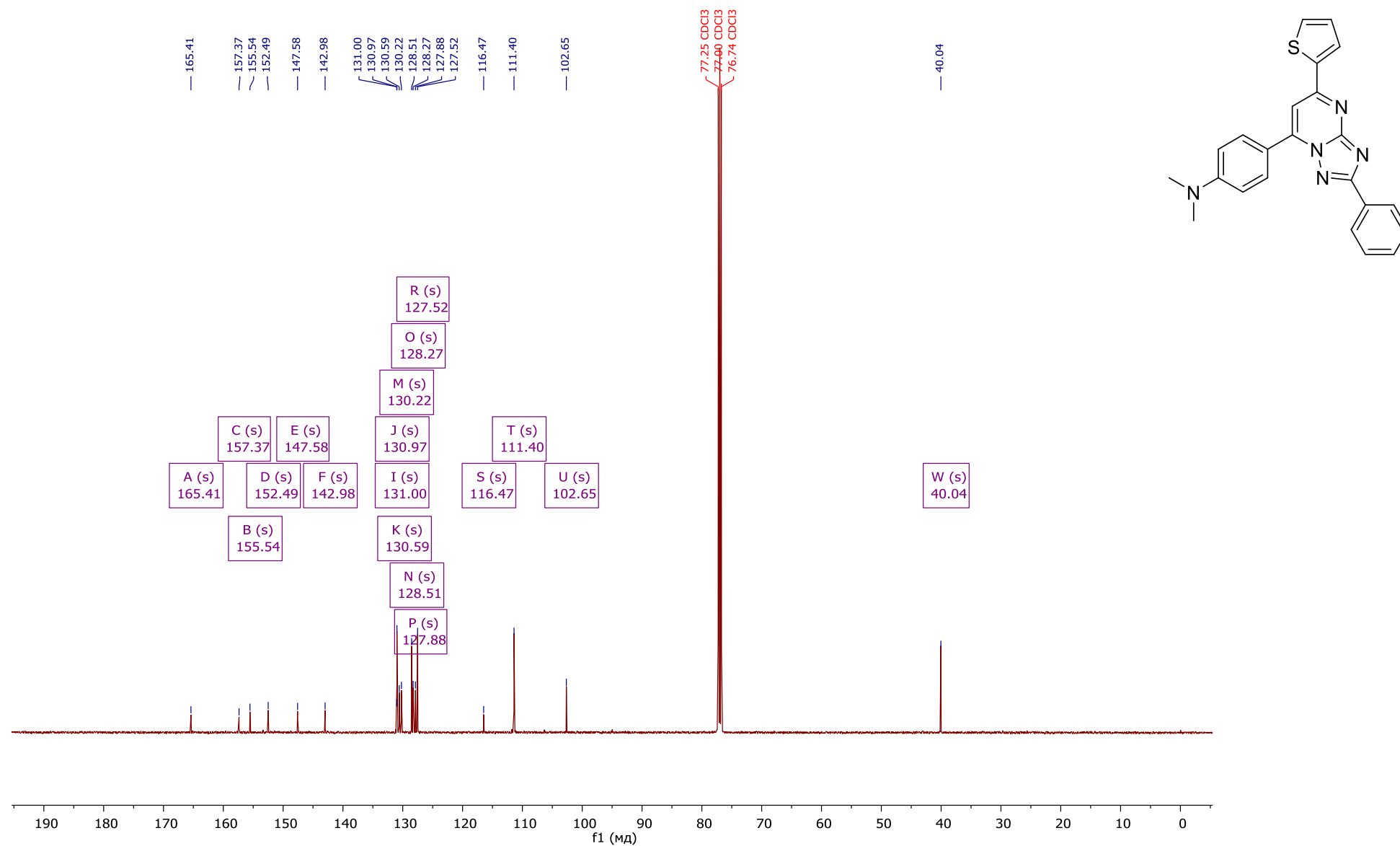
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.51 – 8.45 (m, 2H), 8.41 – 8.35 (m, 2H), 8.30 – 8.24 (m, 2H), 7.97 (s, 1H), 7.62 – 7.51 (m, 3H), 7.17 – 7.11 (m, 2H), 6.97 – 6.91 (m, 2H), 3.88 (s, 3H), 3.09 (s, 6H).



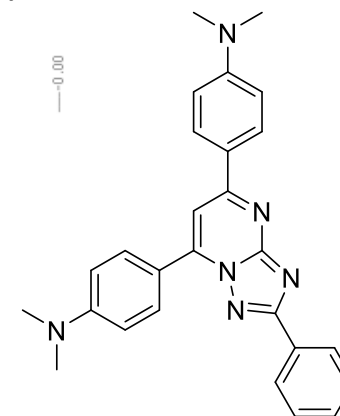
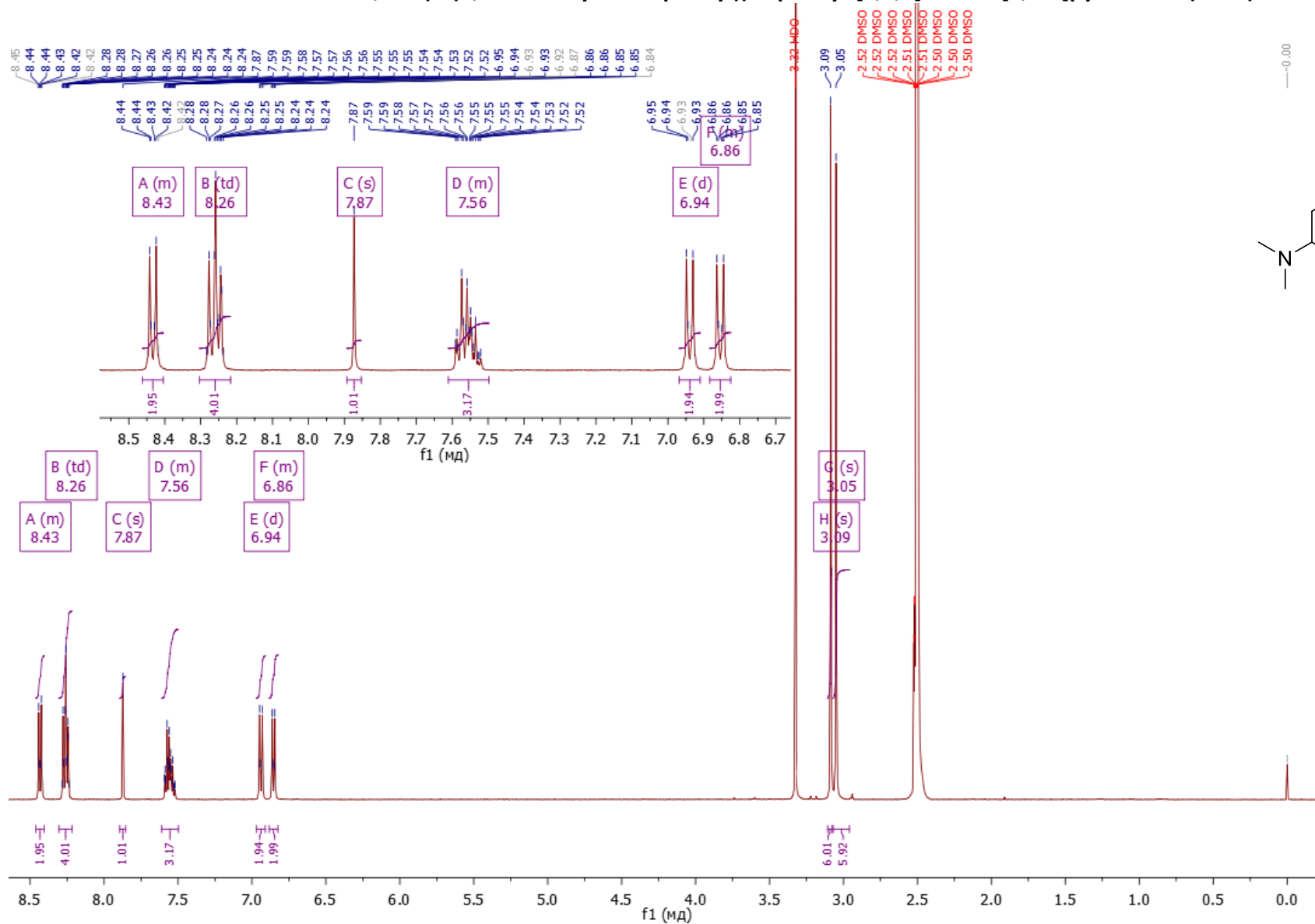
¹³C NMR (126 MHz, Chloroform-*d*) δ 162.11, 160.34, 152.10, 147.33, 131.08, 130.98, 130.47, 129.27, 129.06, 128.81, 128.57, 128.54, 127.58, 127.51, 114.20, 111.73, 103.48, 55.42, 40.27.

7-(4-(*N,N*-dimethylaminophenyl))-5-(thiophene-2-yl)-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12dc)

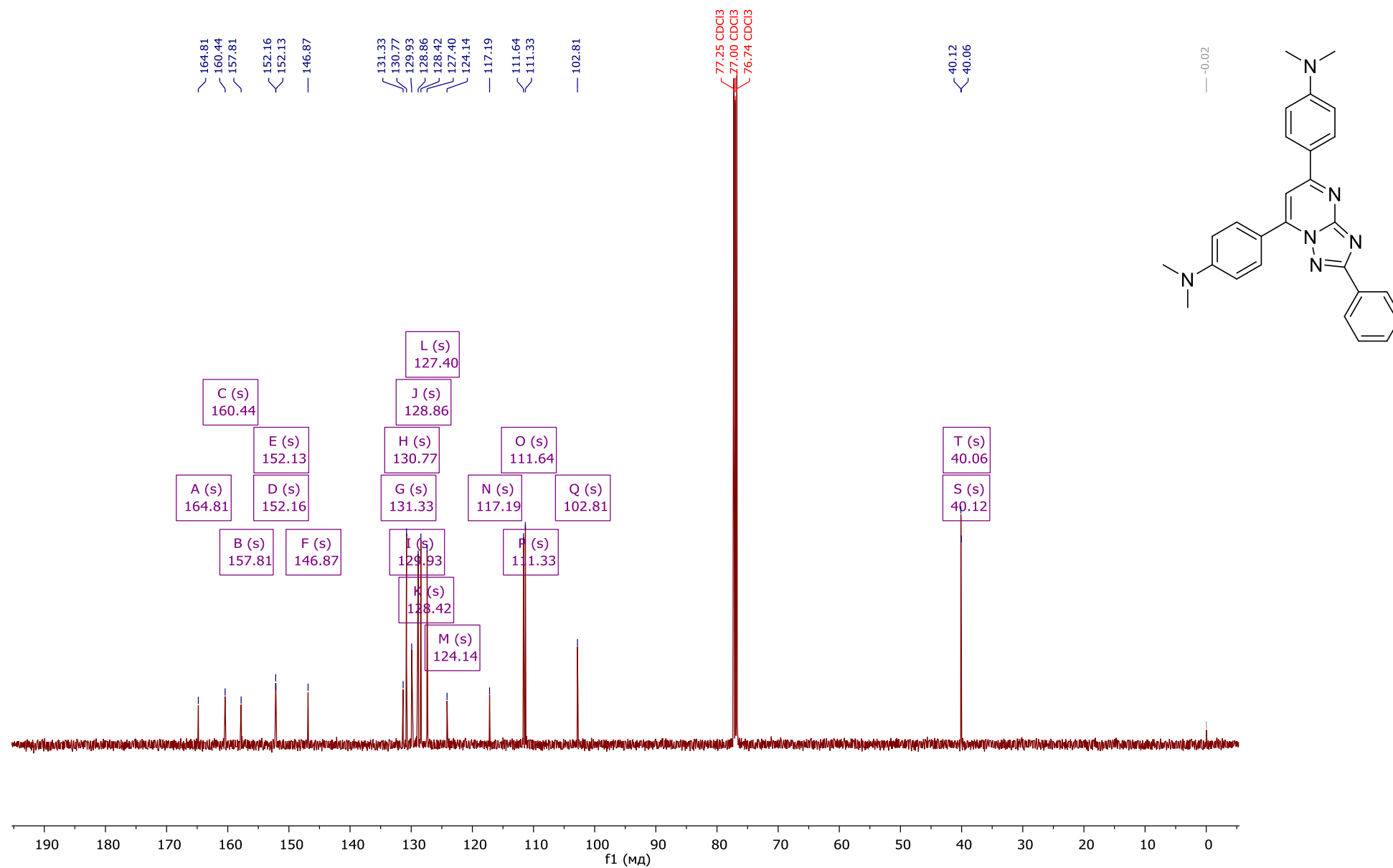
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.52 – 8.45 (m, 2H), 8.33 (dd, *J* = 3.8, 1.1 Hz, 1H), 8.31 – 8.22 (m, 2H), 8.04 (s, 1H), 7.89 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.62 – 7.51 (m, 7H), 7.30 (dd, *J* = 5.0, 3.7 Hz, 1H), 6.99 – 6.91 (m, 2H), 3.10 (s, 6H).



¹³C NMR (126 MHz, Chloroform-d) δ 165.41, 157.37, 155.54, 152.49, 147.58, 142.98, 131.00, 130.97, 130.59, 130.22, 128.51, 128.27, 127.88, 127.52, 116.47, 111.40, 102.65, 40.04.

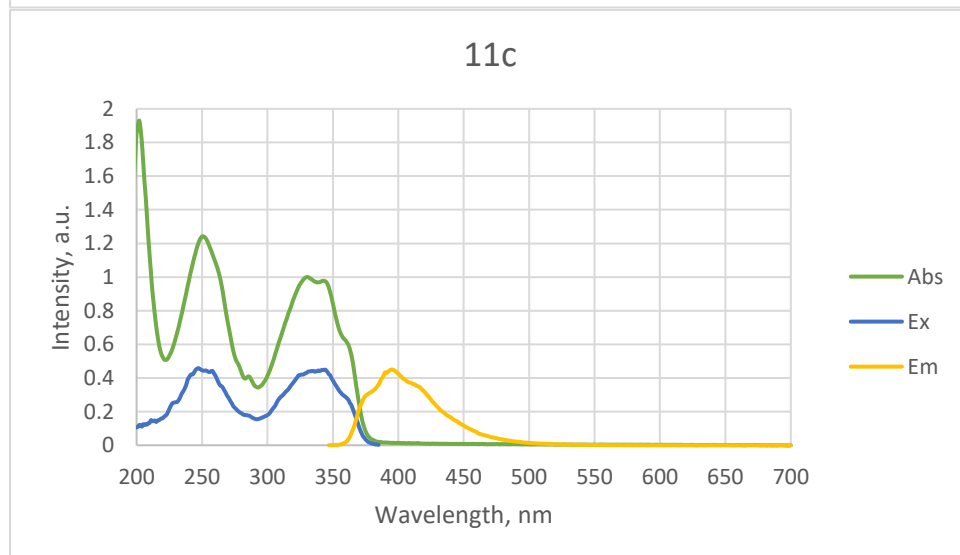
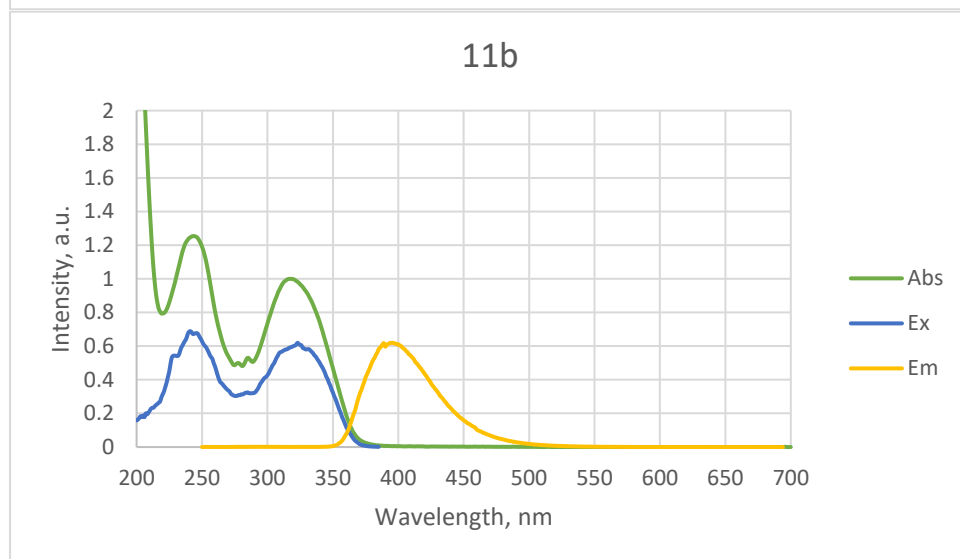
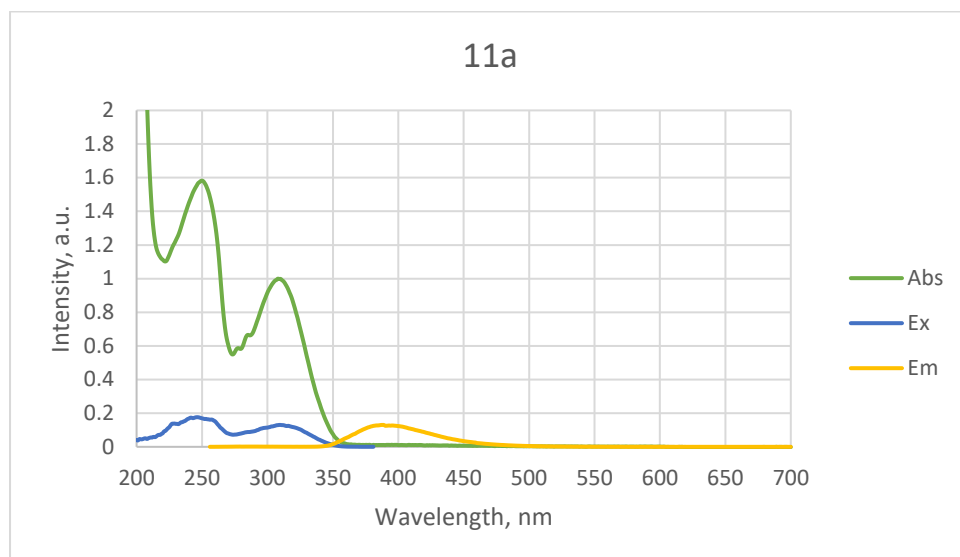
5,7-Di(4-(*N,N*-dimethylaminophenyl))-2-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (12dd)

¹H NMR (500 MHz, DMSO-*d*₆) δ 8.46 – 8.40 (m, 2H), 8.30 – 8.22 (m, 4H), 7.87 (s, 1H), 7.61 – 7.50 (m, 3H), 6.97 – 6.91 (m, 2H), 6.88 – 6.83 (m, 2H), 3.09 (s, 12H), 3.05 (s, 6H).

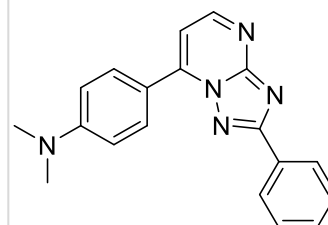
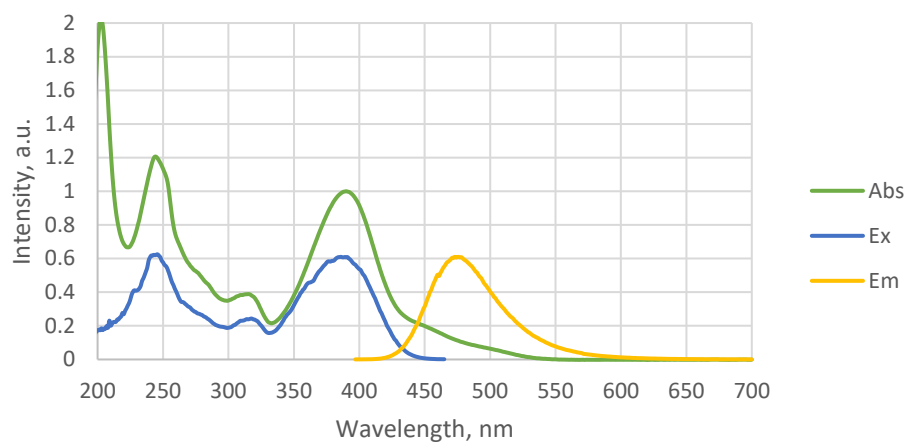


¹³C NMR (126 MHz, Chloroform-*d*) δ 164.81, 160.44, 157.81, 152.16, 152.13, 146.87, 131.33, 130.77, 129.93, 128.86, 128.42, 127.40, 124.14, 117.19, 111.64, 111.33, 102.81, 40.12, 40.06.

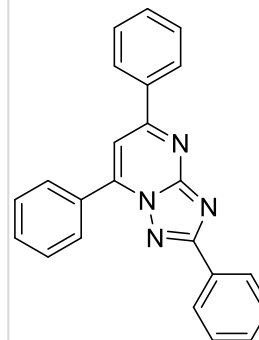
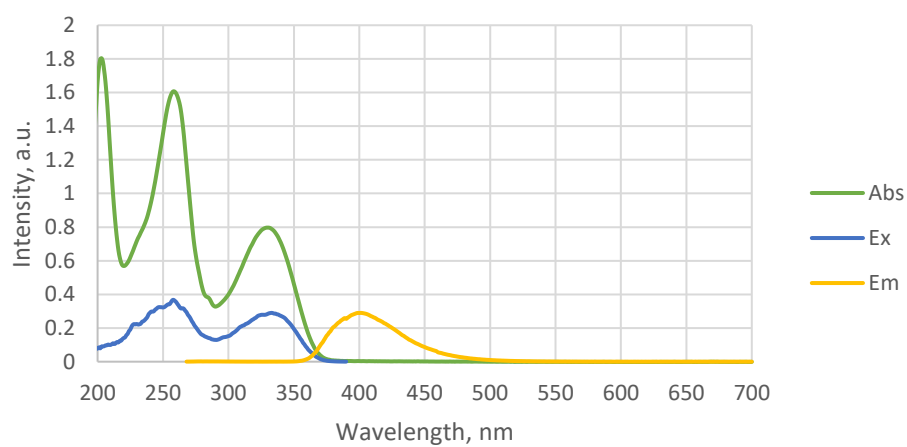
II. Absorption, excitation and emission spectra of 11 and 12 compounds



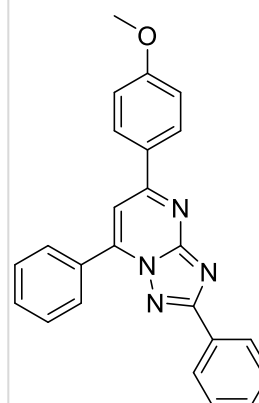
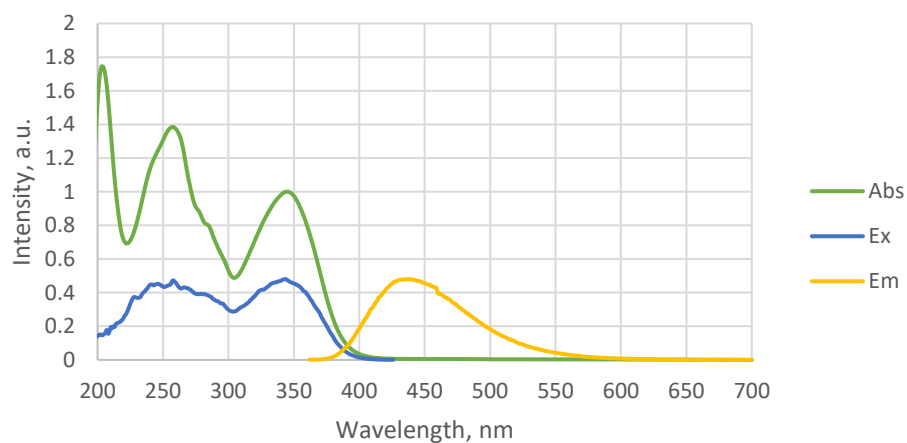
11d



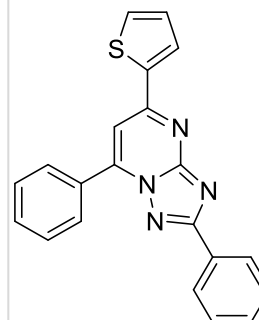
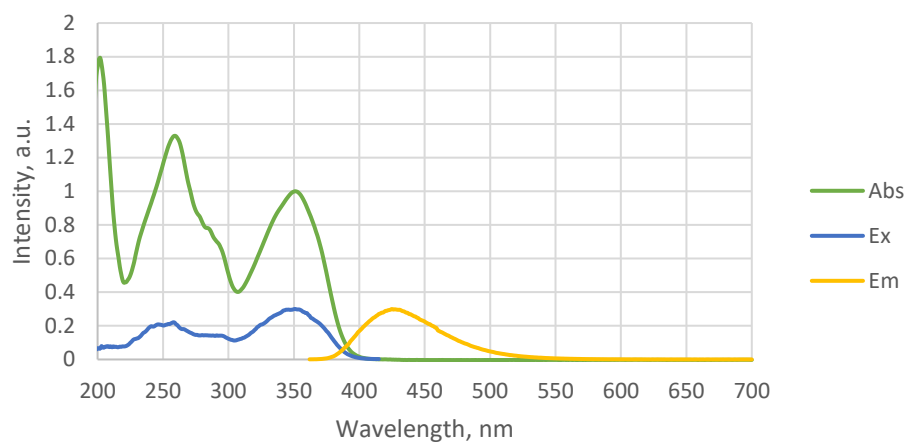
12aa



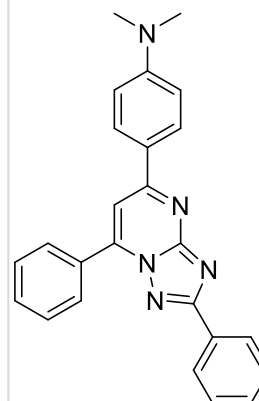
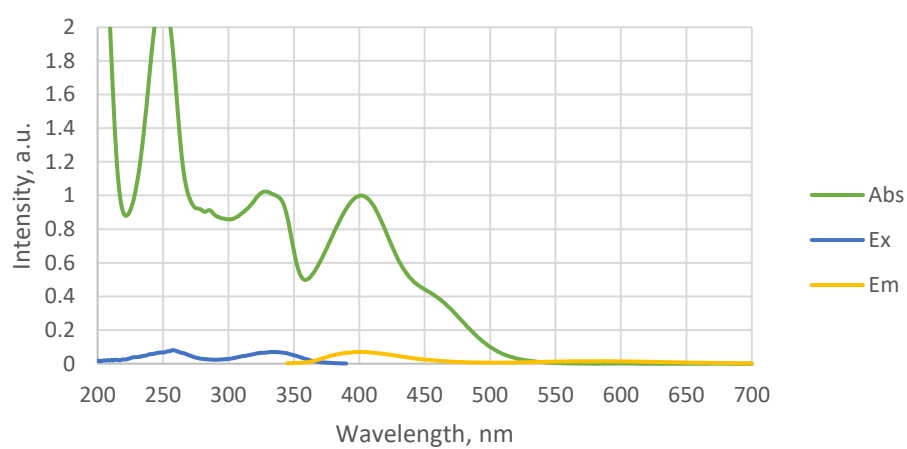
12ab



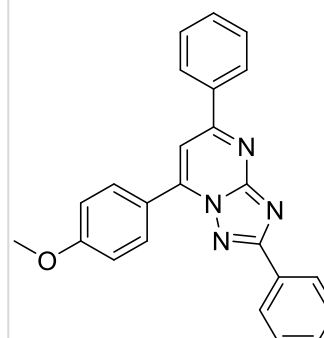
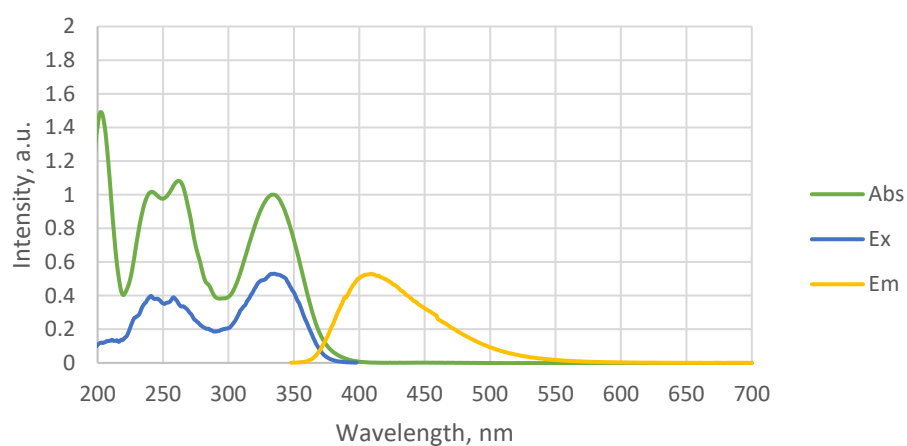
12ac



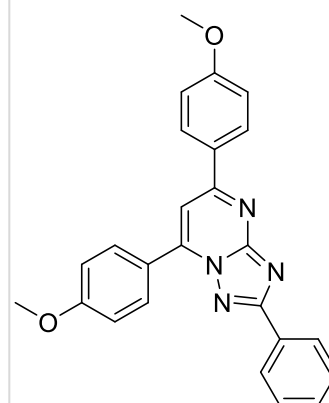
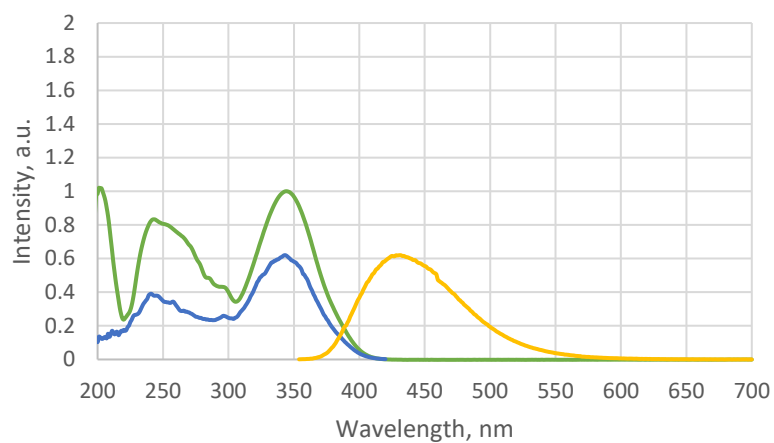
12ad



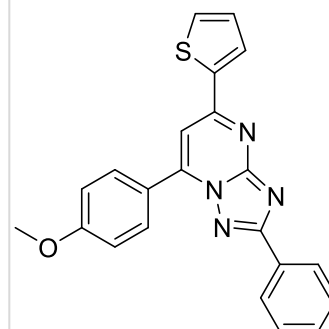
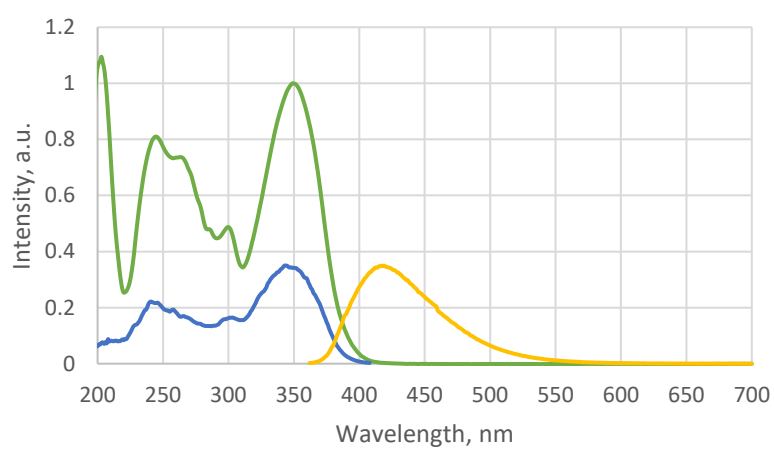
12ba



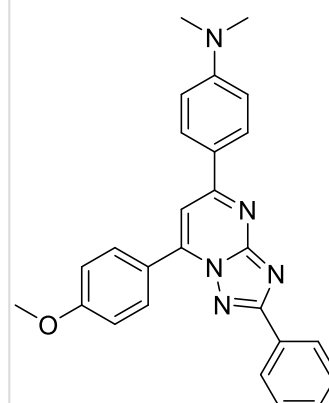
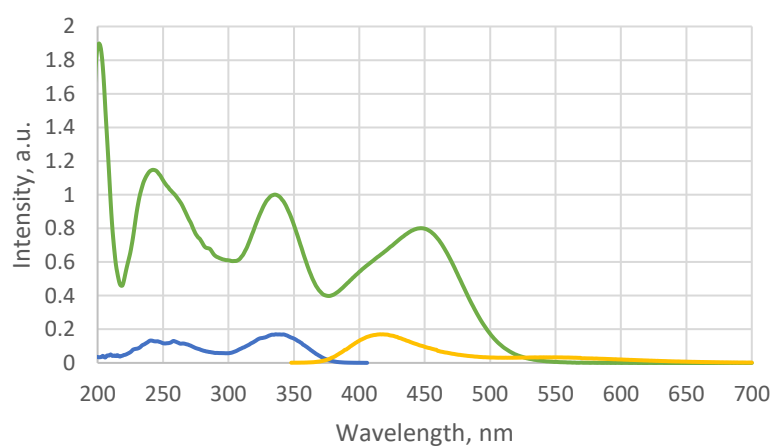
12bb



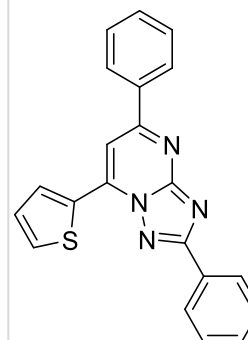
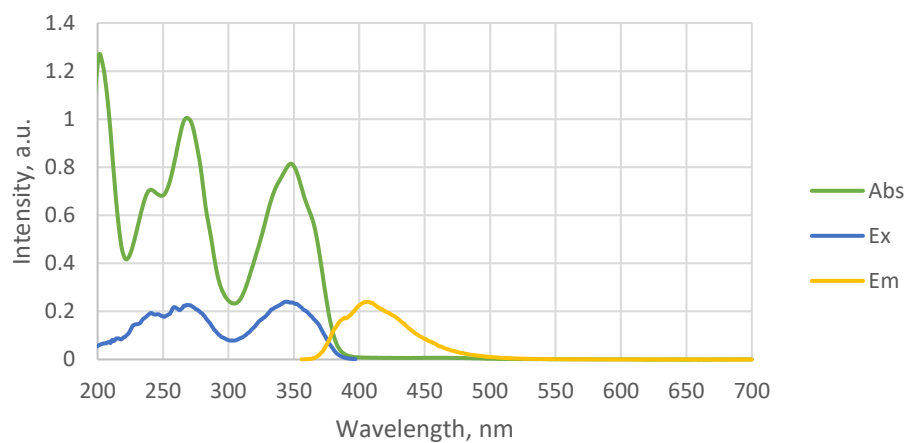
12bc



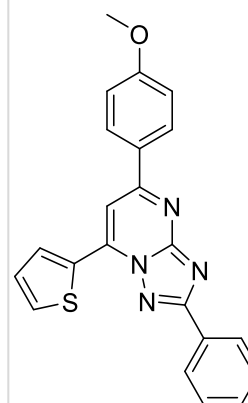
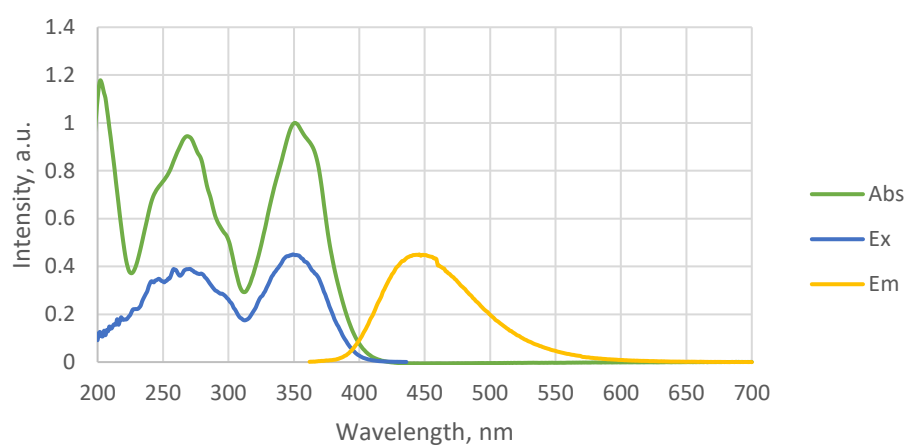
12bd



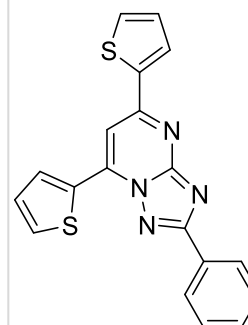
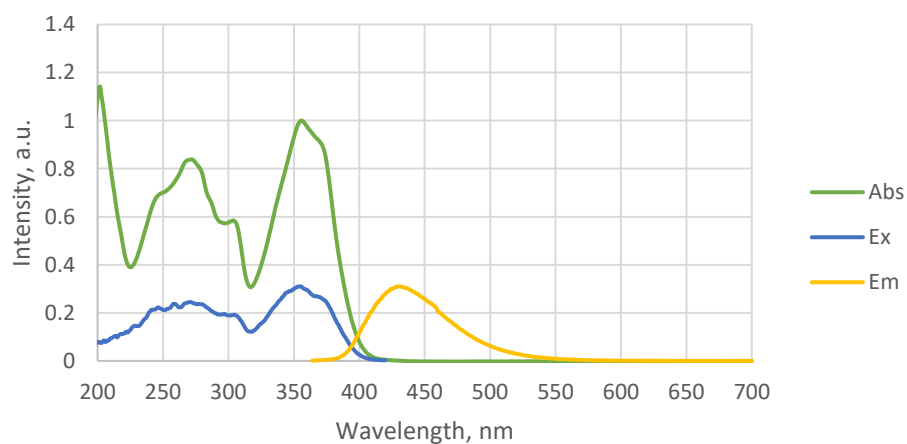
12ca



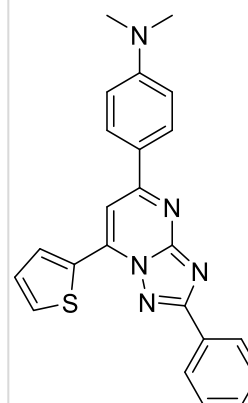
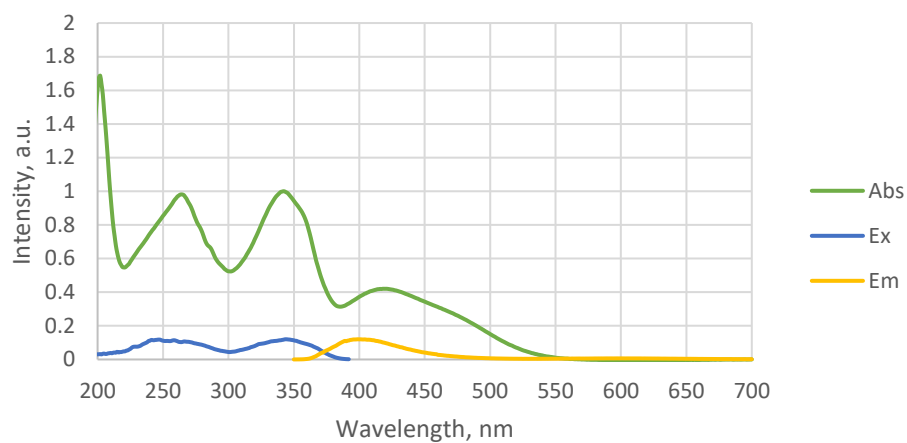
12cb



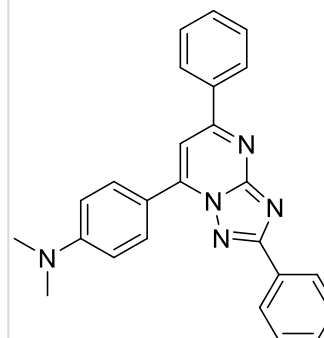
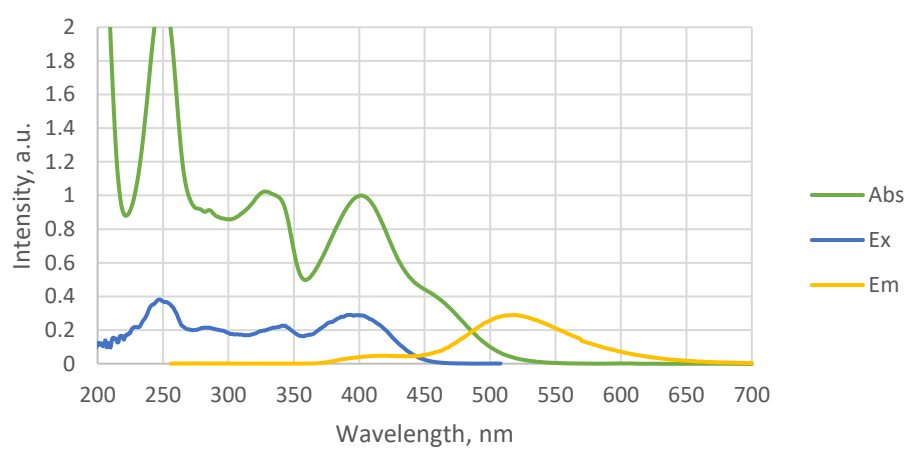
12cc



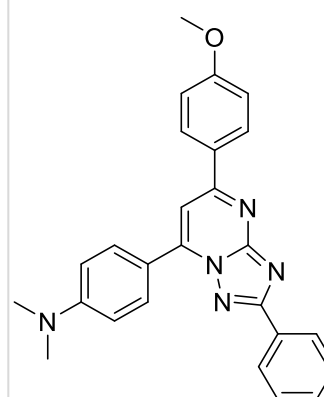
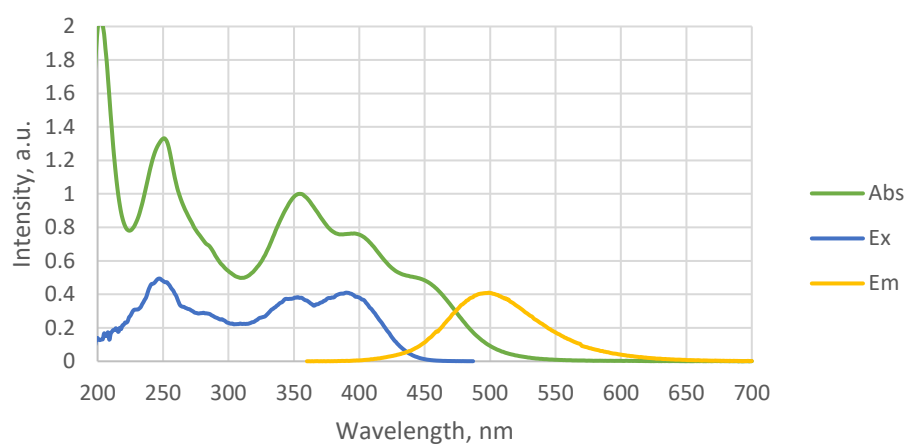
12cd



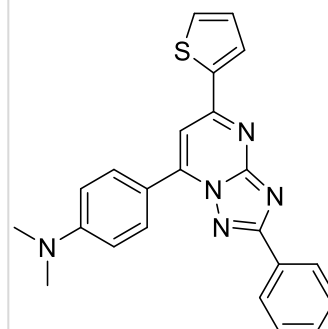
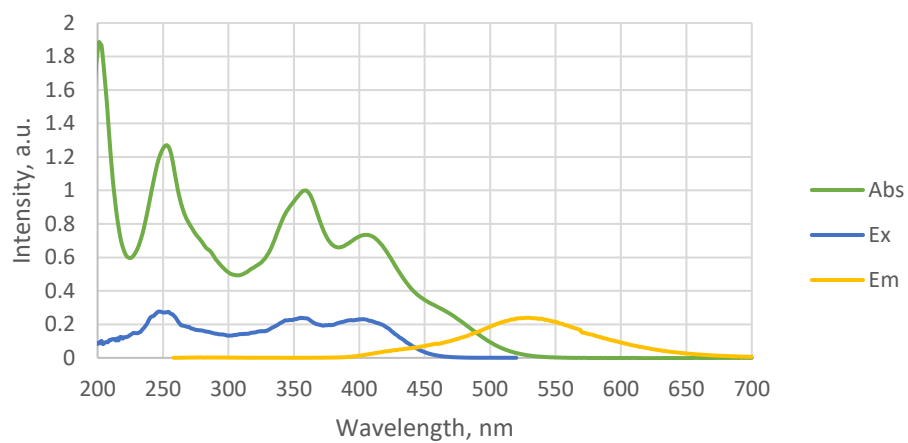
12da



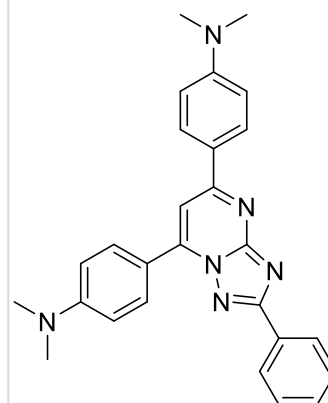
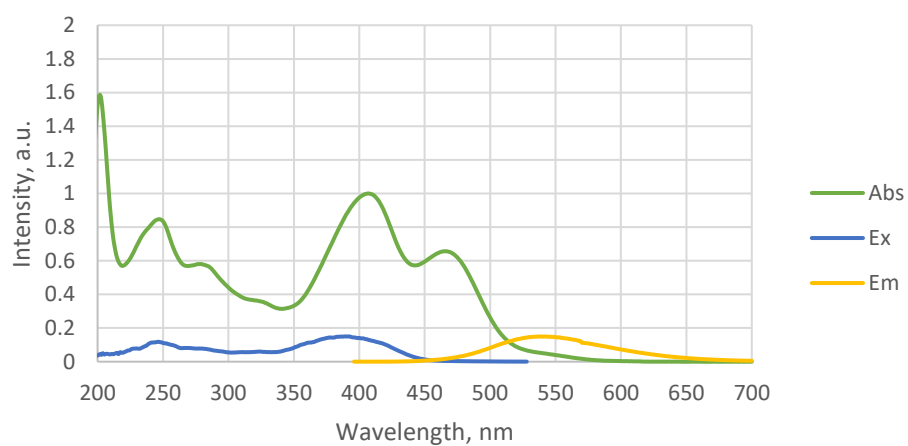
12db



12dc



12dd



III. The data of UV-visible spectroscopy of 11 and 12 compounds

The maxima of absorption, excitation and emission spectra, Stokes shifts, quantum yields and values of calculated energy gaps of compounds **6** and **7**.

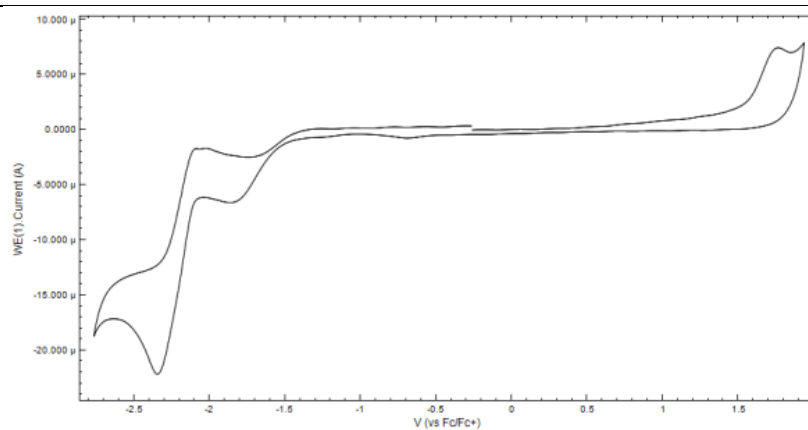
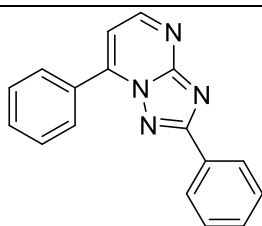
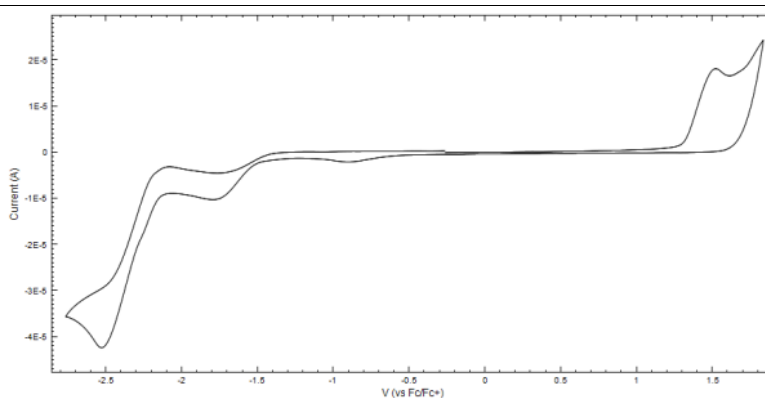
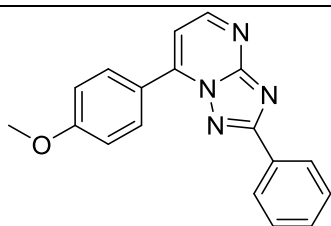
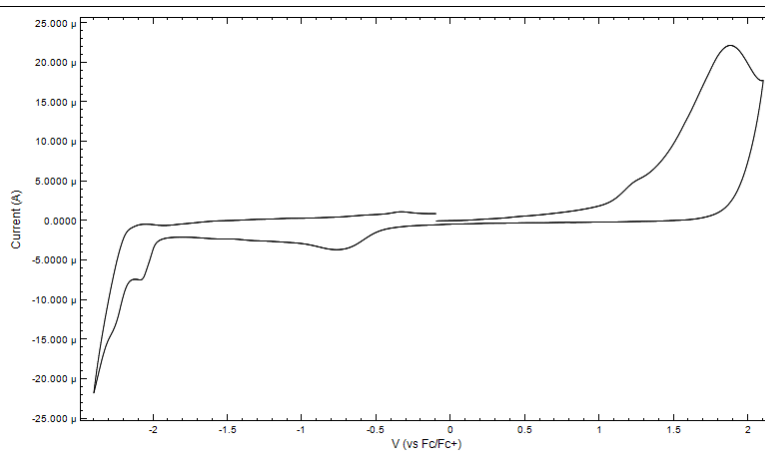
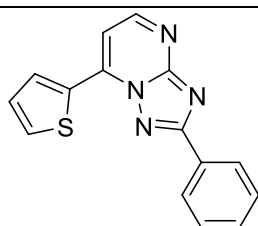
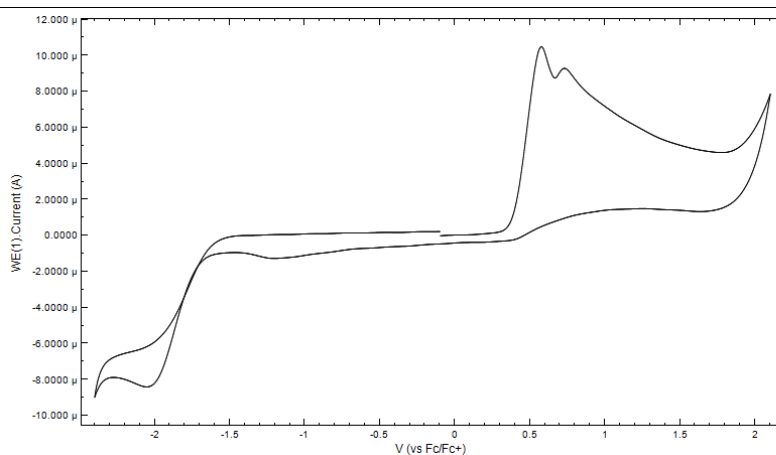
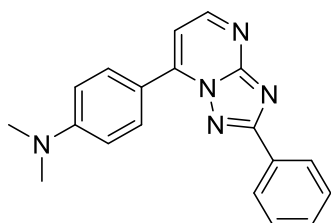
Entry	$^{abs}\lambda_{max}$ (nm)	$^{em}\lambda_{max}$ (nm)	Stokes shift (sm^{-1})	Φ (%)	E_g^{opt} (eV)
11a	250	391	14425	12.9%	3.36
	309	391	6787		
11b	243	395	15836	61.9%	3.19
	317	395	6229		
11c	251	395	14524	44.9%	3.06
	330	395	4987		
	343	395	3838		
	360	395	2461		
11d	244	475	19931	60.5%	2.69
	315	475	10693		
	390	475	4588		
	451	475	1120		
	500	—	—	—	
12aa	258	400	13760	28.8%	3.22
	330	400	5303		
12ab	257	436	14872	47.8%	3.01
	344	436	5031		
	391	436	7125		
12ac	259	425	15081	30.0%	3.01
	284	425	11682		
	351	425	4961		
12ad	251	400	14841	7.4%	2.53
	310	400	7258		
	409	580	7208	—	
	442	580	5383		
12ba	241	408	16984	53.2%	3.17
	261	408	13804		
	334	408	5430		
12bb	249	430	16905	61.5%	3.06
	344	430	5814		
12bc	245	418	16893	34.6%	2.97
	262	418	14244		
	300	418	9410		
	350	418	4648		
12bd	242	416	17284	16.5%	2.57
	336	416	5723		
	447	542	3921	—	
12ca	240	407	17097	23.5%	3.01
	268	407	12743		

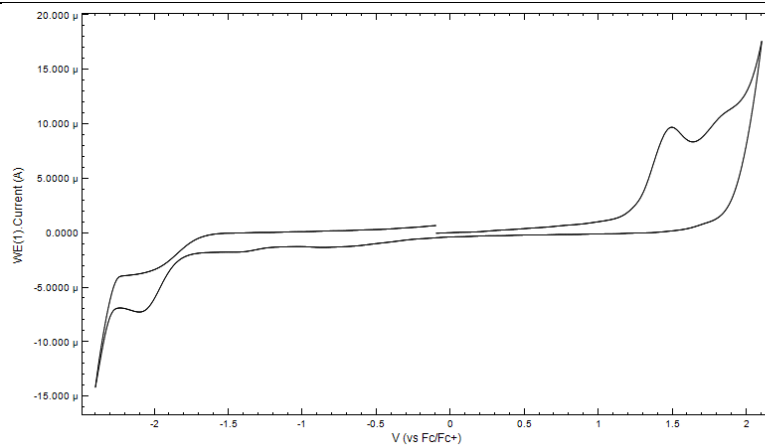
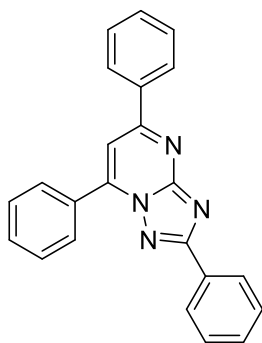
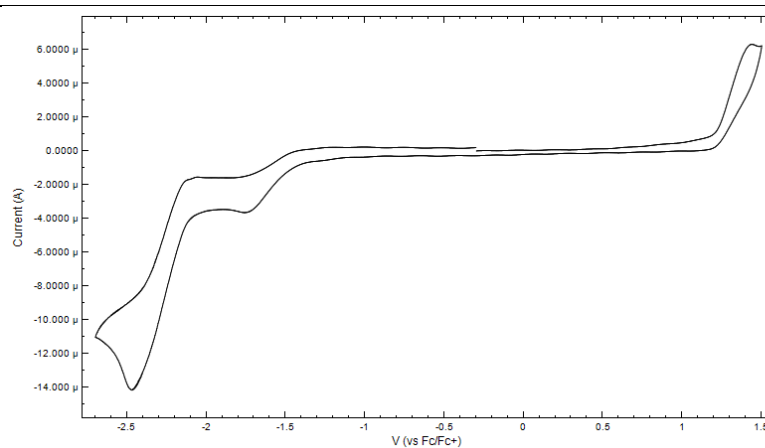
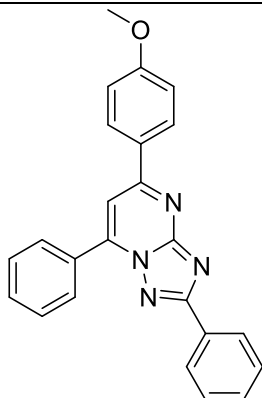
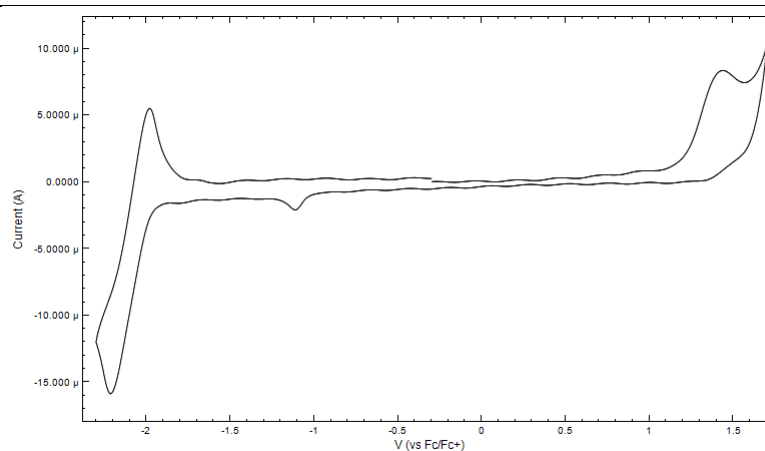
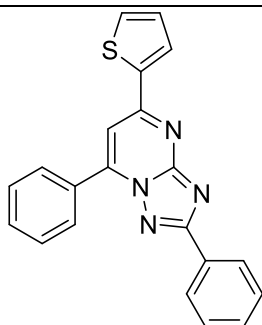
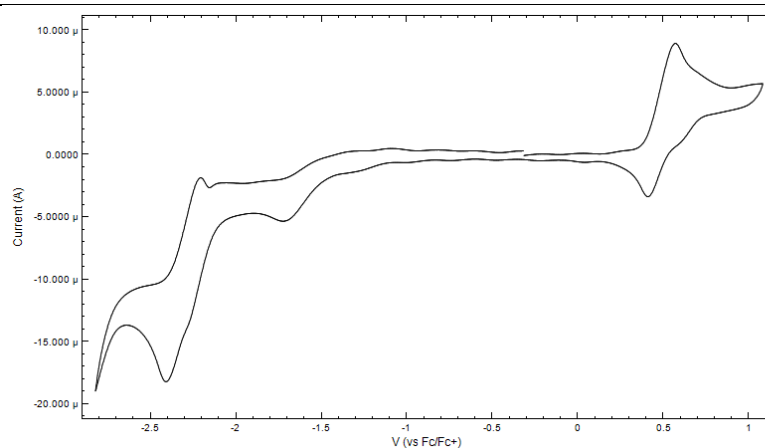
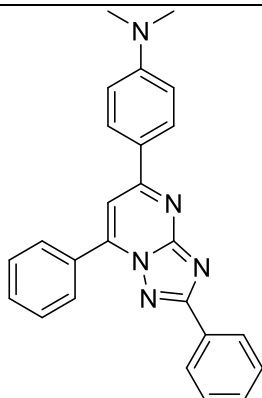
	348	407	4166		
12cb	<i>244</i>	<i>446</i>	<i>18562</i>	44.6%	2.89
	269	446	14753		
	<i>296</i>	<i>446</i>	<i>11362</i>		
	351	446	6069		
	363	446	5127		
12cc	246	430	17395	30.8%	2.85
	271	430	13645		
	302	430	9857		
	355	430	4913		
	370	430	3771		
12cd	264	402	13003	12.2%	2.38
	342	402	4364		
	420	600	7143	—	
	<i>480</i>	<i>600</i>	<i>4167</i>		
12da	349	518	9348	28.8%	2.53
	330	518	10998		
	402	518	5571		
	<i>460</i>	<i>518</i>	<i>2434</i>		
12db	250	497	19879	40.9%	2.33
	354	497	8128		
	400	497	4879		
	451	497	2052		
12dc	252	530	20815	24.2%	2.52
	359	530	8987		
	405	530	5823		
	<i>467</i>	<i>530</i>	<i>2545</i>		
12dd	246	538	22063	14.7%	2.53
	280	538	17127		
	<i>323</i>	<i>538</i>	<i>12372</i>		
	406	538	6043		
	464	538	2964		

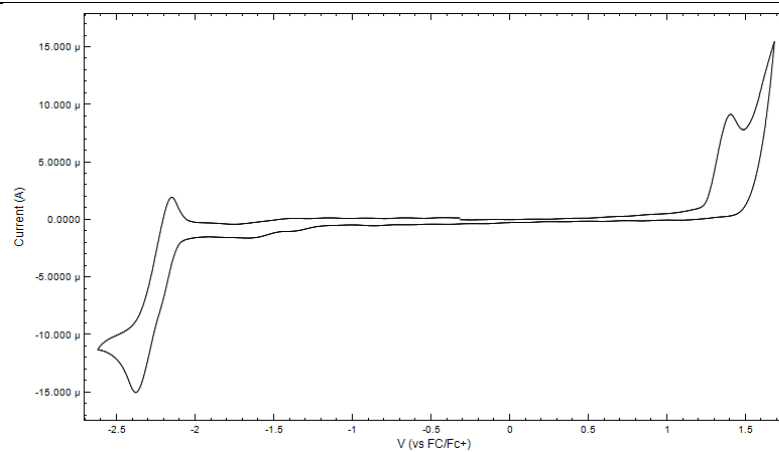
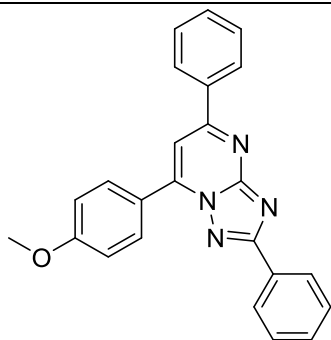
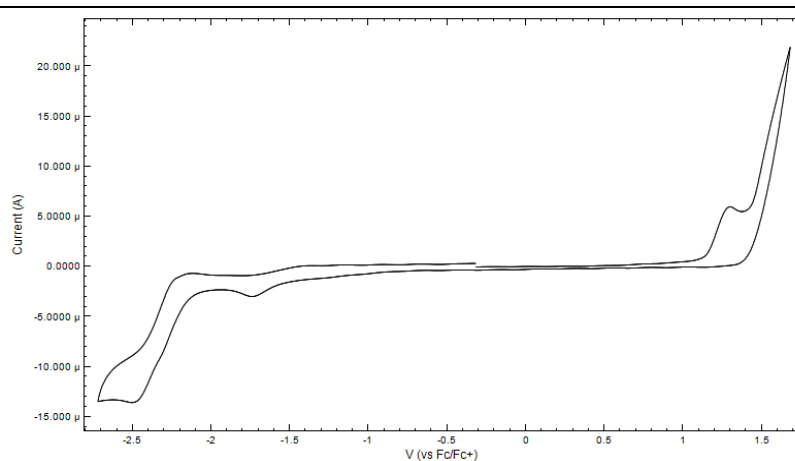
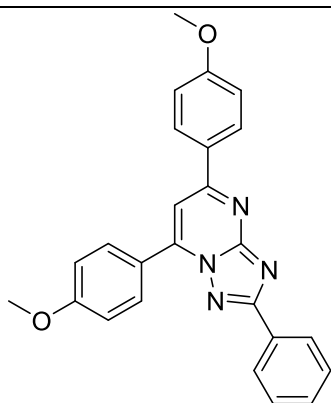
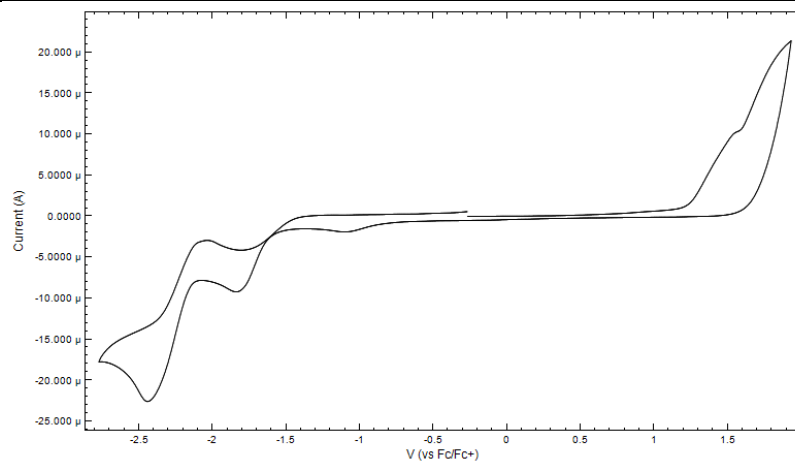
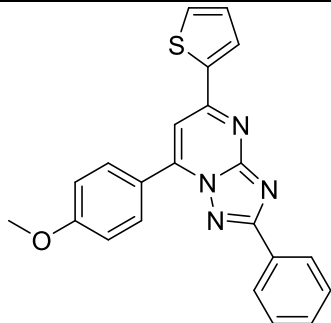
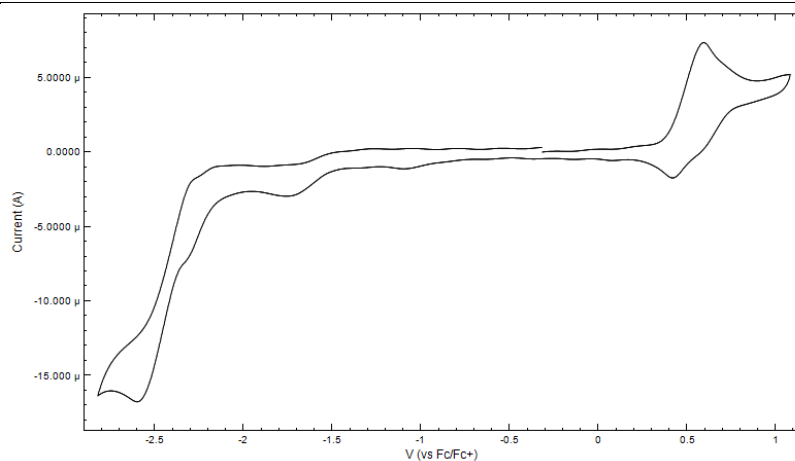
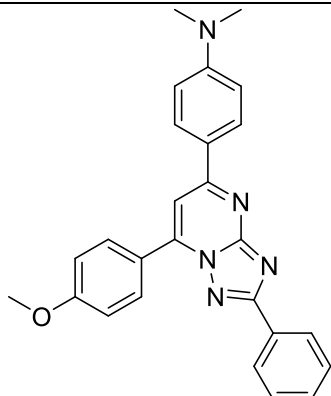
IV. Electrochemical studies of 11 and 12 compounds

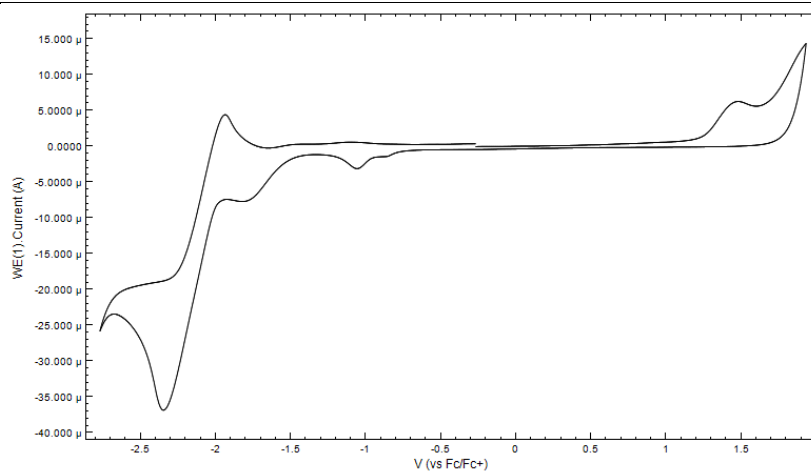
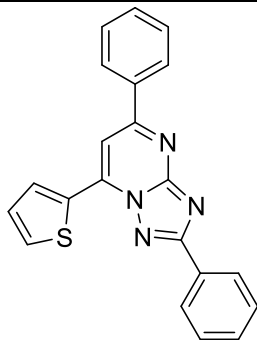
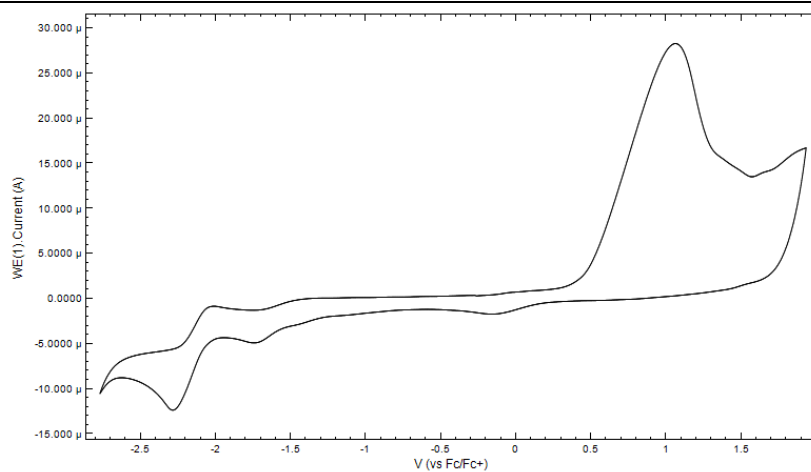
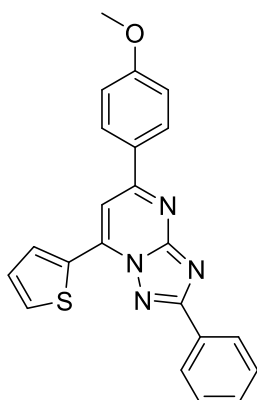
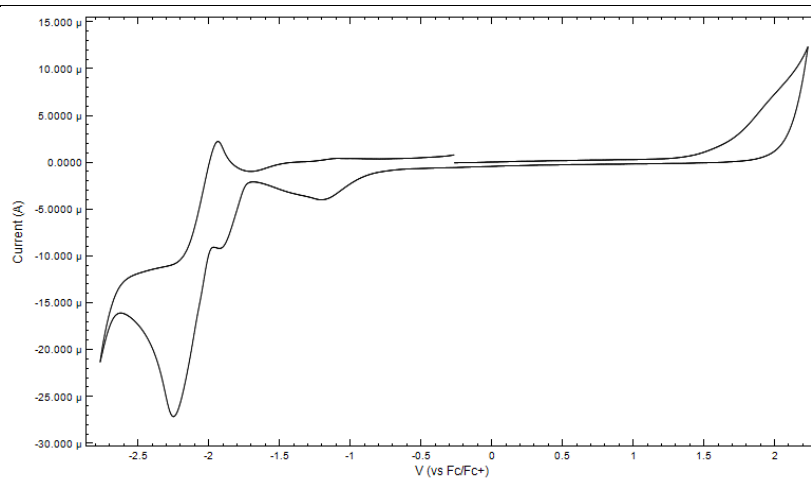
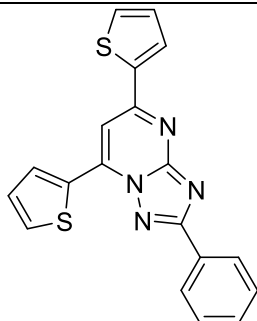
The HOMO energy levels (E_{HOMO}) were estimated from $E_{\text{ox}}^{\text{onset}}$ of the first oxidation peaks by the empirical equation: $E_{\text{HOMO}} = -[E_{[\text{onset,ox vs. Fc/Fc}^+]} + 5.10]$. The LUMO energy levels (E_{LUMO}) were estimated from $E_{\text{red}}^{\text{onset}}$ of the first reduction peaks by the empirical equation: $E_{\text{LUMO}} = -[E_{[\text{onset,red vs. Fc/Fc}^+]} + 5.10]$. We have used +5.10 eV value in the Fermi scale for the formal potential of the Fc/Fc^+ redox couple instead of +4.80 eV in accordance with a recent discussion of Bazan et al.¹ Energy gaps (E_{gap}) were calculated by the following equation: $E_{\text{gap}} = E_{\text{LUMO}} - E_{\text{HOMO}}$.

Compound	$E_{[\text{onset, red vs. Fc/Fc}^+]}$, V	E_{LUMO} , eV	$E_{[\text{onset, ox vs. Fc/Fc}^+]}$, V	E_{HOMO} , eV	E_{gap} , eV
11a	-2.09	-3.01	1.56	-6.66	3.65
11b	-2.15	-2.95	1.31	-6.41	3.46
11c	-1.82	-3.28	1.18	-6.28	3.00
11d	-1.81	-3.29	0.39	-5.49	2.20
12aa	-1.84	-3.26	1.28	-6.38	3.12
12ab	-2.09	-3.01	1.22	-6.32	3.31
12ac	-1.98	-3.12	1.20	-6.30	3.18
12ad	-2.09	-3.01	0.35	-5.45	2.44
12ba	-2.11	-2.99	1.24	-6.34	3.35
12bb	-2.16	-2.94	1.15	-6.25	3.31
12bc	-2.13	-2.97	1.21	-6.31	3.34
12bd	-2.20	-2.90	0.34	-5.44	2.54
12ca	-1.98	-3.12	1.24	-6.34	3.22
12cb	-2.00	-3.10	0.39	-5.49	2.39
12cc	-1.75	-3.35	-	-	-
12cd	-2.01	-3.09	0.36	-5.46	2.37
12da	-2.17	-2.93	0.52	-5.62	2.69
12db	-2.34	-2.76	0.51	-5.61	2.85
12dc	-2.10	-3.00	0.46	-5.56	2.56
12dd	-2.34	-2.76	0.30	-5.40	2.64

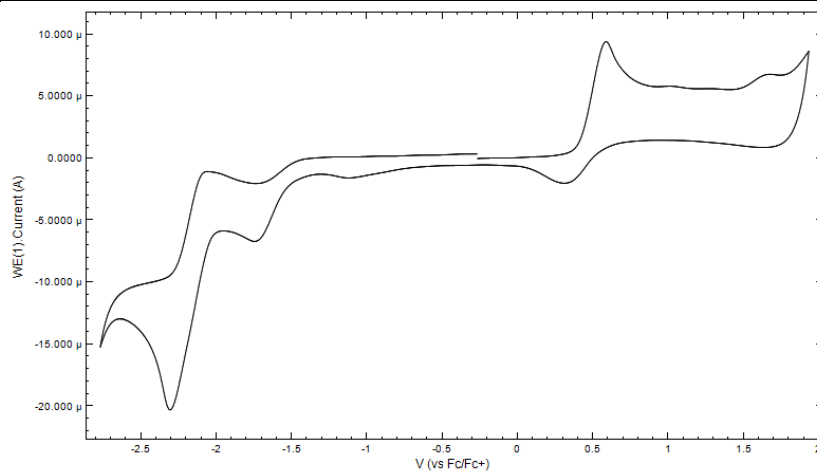
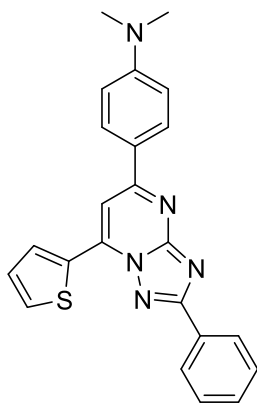
11a**11b****11c****11d**

12aa**12ab****12ac****12ad**

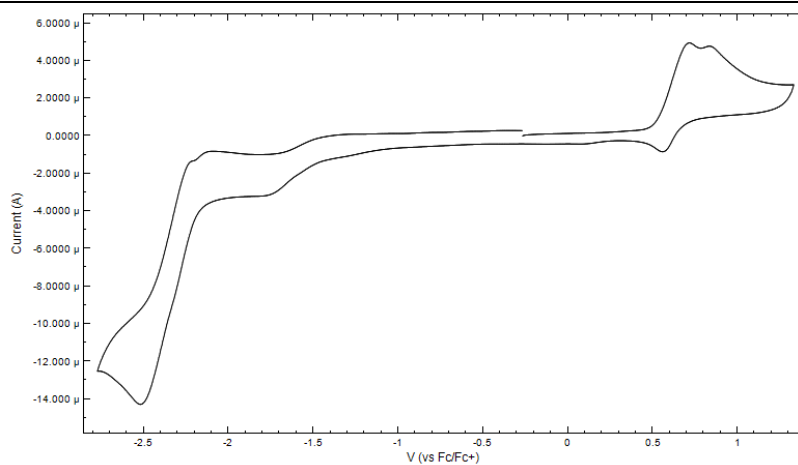
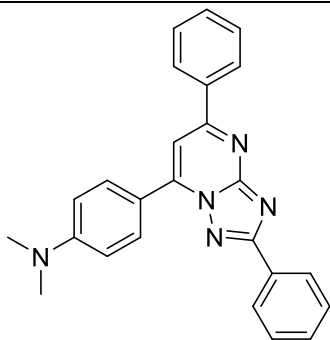
12ba**12bb****12bc****12bd**

12ca**12cb****12cc**

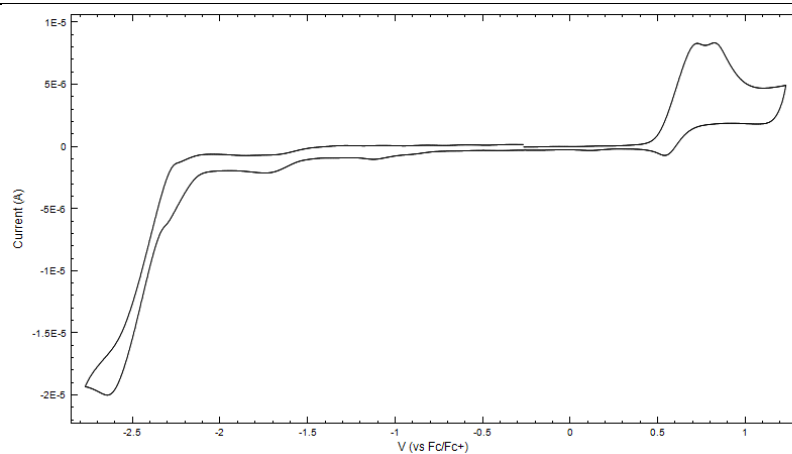
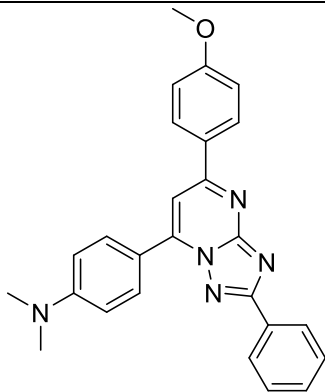
12cd

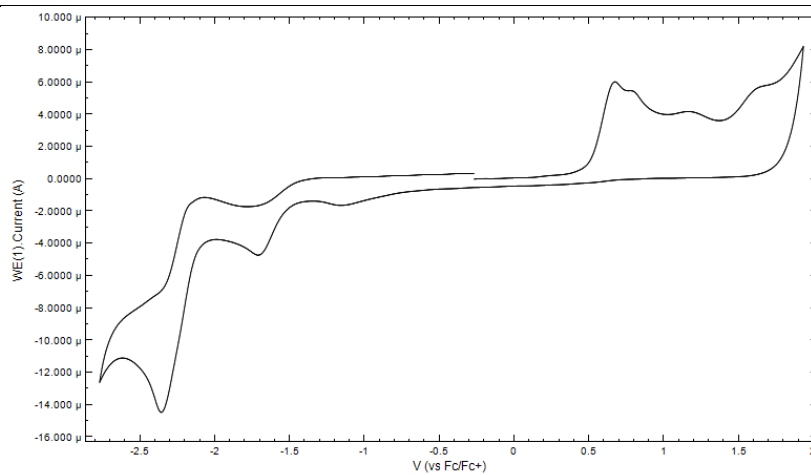
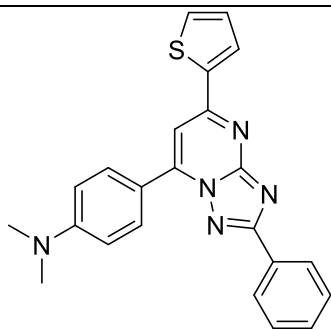
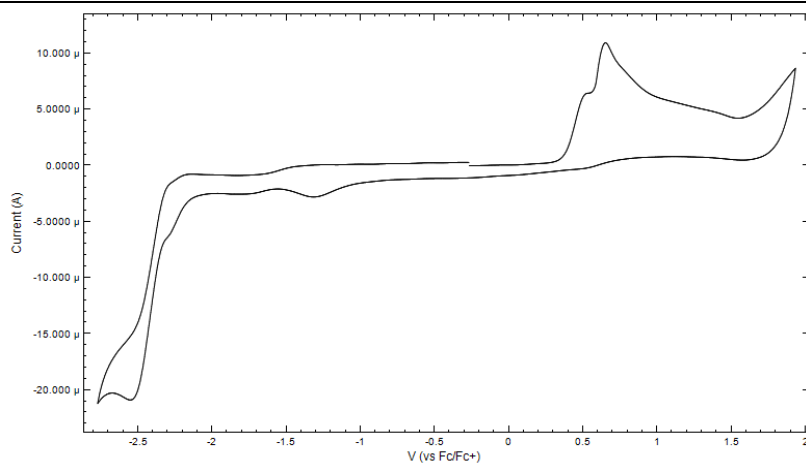
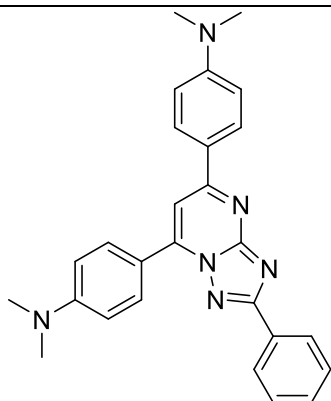


12da



12db



2dc**12dd**

References

1. Cardona CM, Li W, Kaifer AE, Stockdale D, Bazan GC. Electrochemical Considerations for Determining Absolute Frontier Orbital Energy Levels of Conjugated Polymers for Solar Cell Applications. *Adv Mater.* 2011;23(20):2367-2371. doi:10.1002/adma.201004554