

Reinvestigation of the Room Temperature Photochemical Reaction Between *N*-Methyl-1,2,4-triazoline-3,5-dione (MeTAD) and Benzene

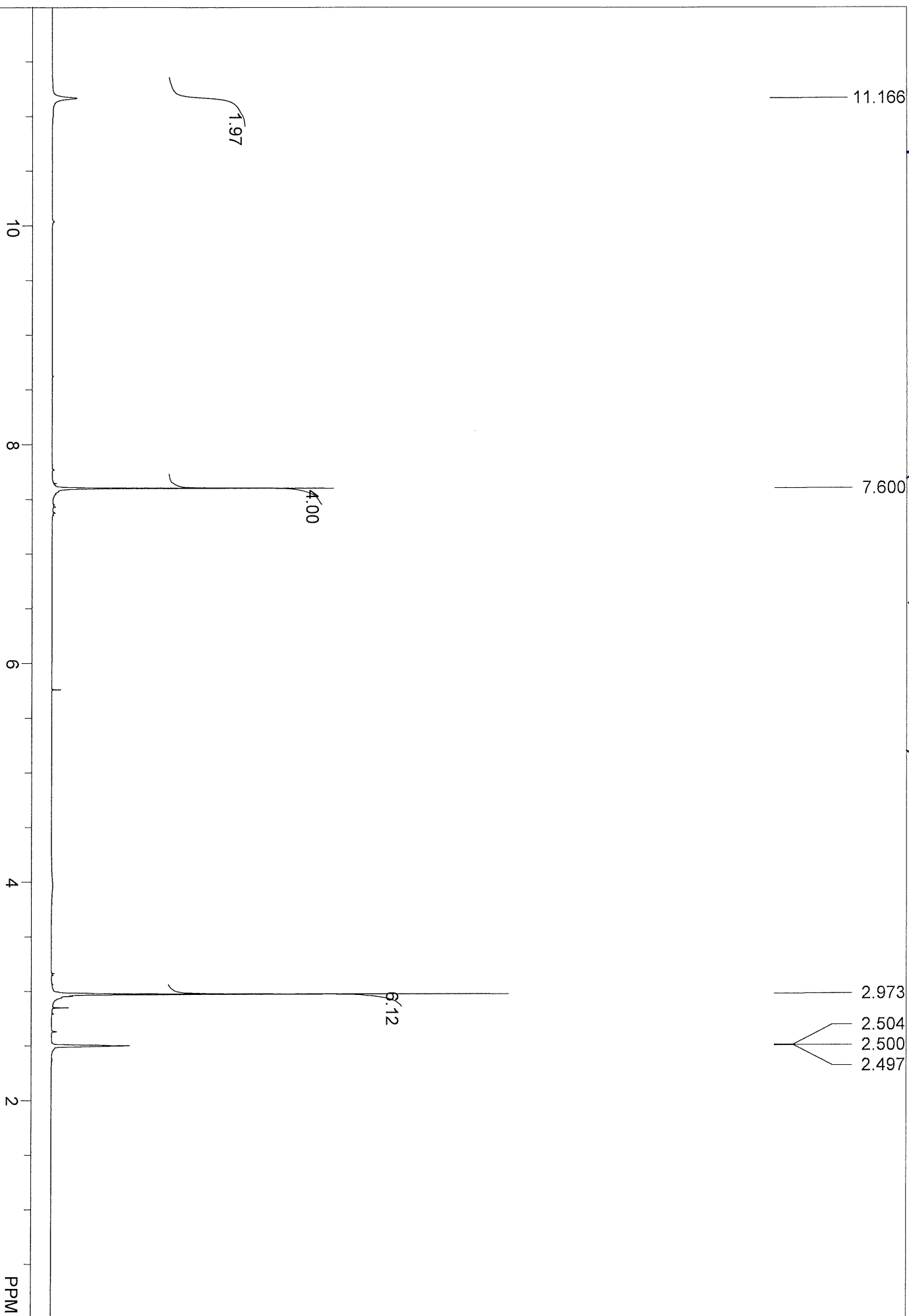
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Supplementary Materials

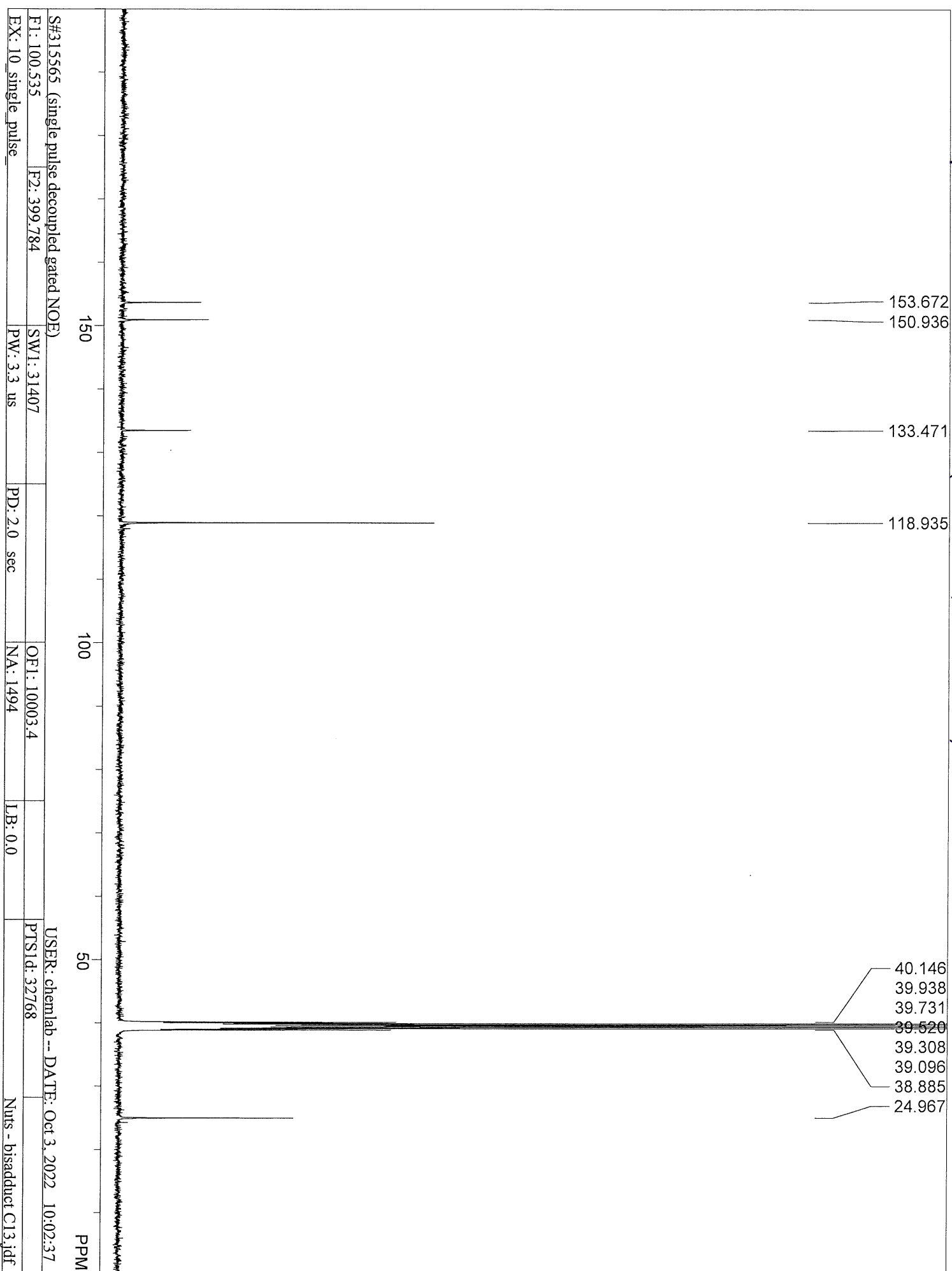
- ¹H NMR spectrum for **6** (page S2)
- ¹³C NMR spectrum for **6** (page S3)
- IR spectrum for **6** (page S4)
- HRMS spectra for **6** (page S5-S6)
- ¹H NMR spectrum for **5** (page S7)
- ¹³C NMR spectrum for **5** (page S8)
- ¹H NMR spectrum for **7** (page S9)
- ¹³C NMR spectrum for **7** (page S10)

¹H NMR Spectrum of Bisurazole 6 (400 MHz, DMSO-d₆)

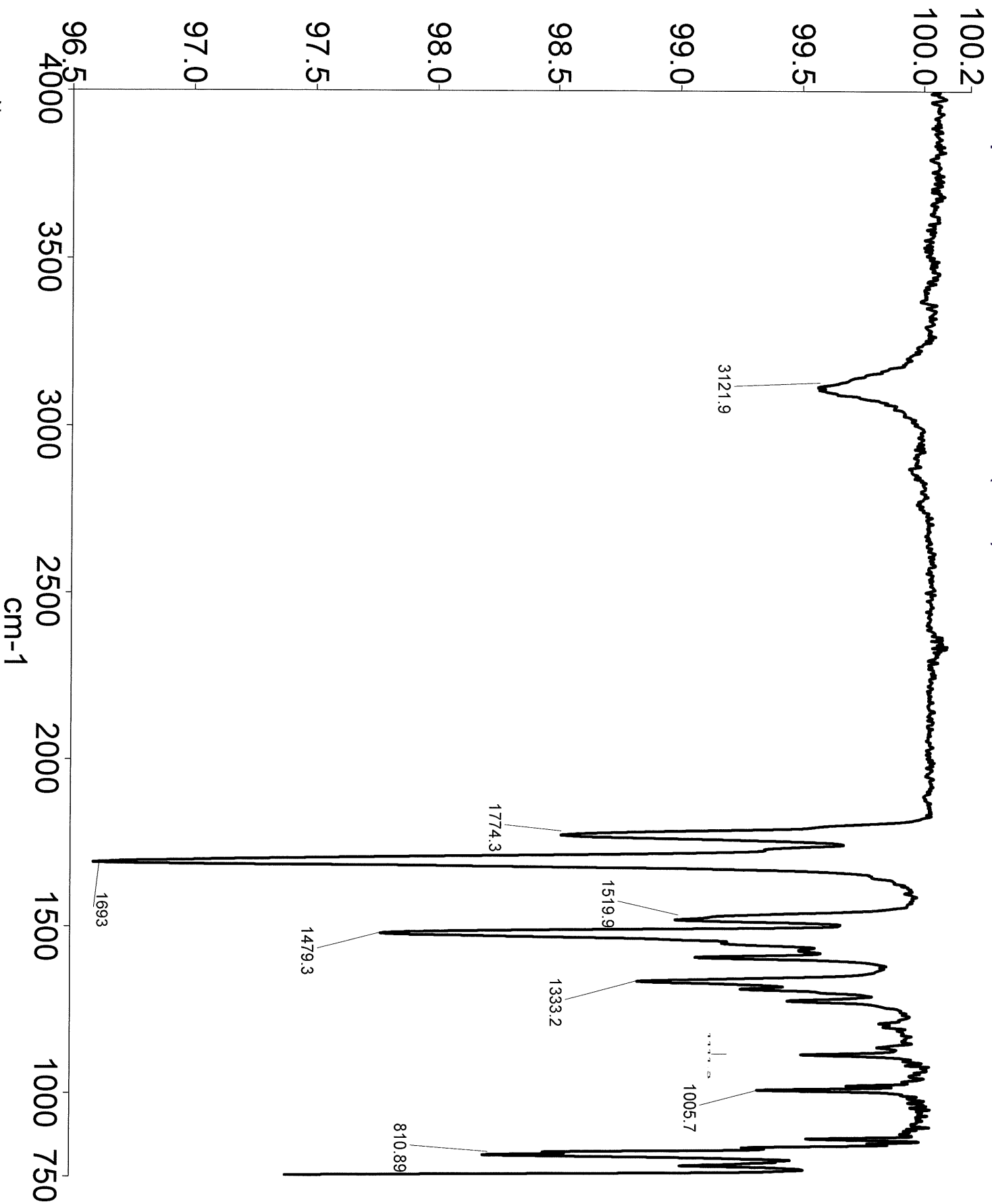


S#314441 (single_pulse)					USER: chemlab -- DATE: Oct 3, 2022 08:46:19				
F1: 399.784	F2: 399.784	SW1: 7503			PTSD: 16384				
EX: 10_single_pulse.		PW: 6.8 us	PD: 5.0 sec	NA: 8	LB: 0.0				Nuts - bisaduct.jif

¹³C NMR Spectrum of Bisurazole 6 (100 MHz, DMSO-d6)



IR Spectrum of Bisurazole 6 (ATR)



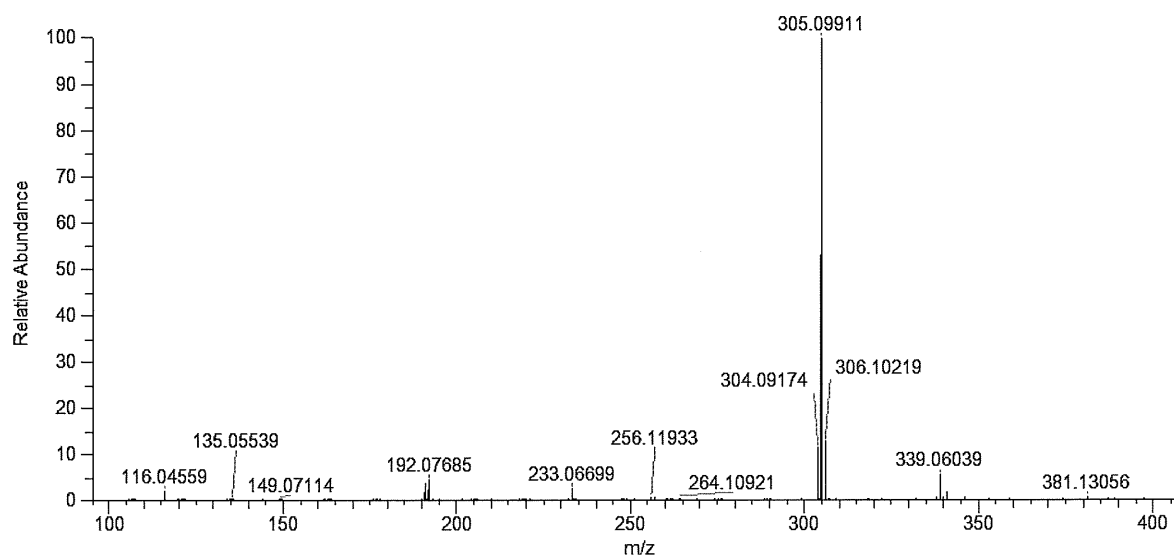
High Resolution Mass Spectrometry Data for Bisurazole 6

Brenton100522

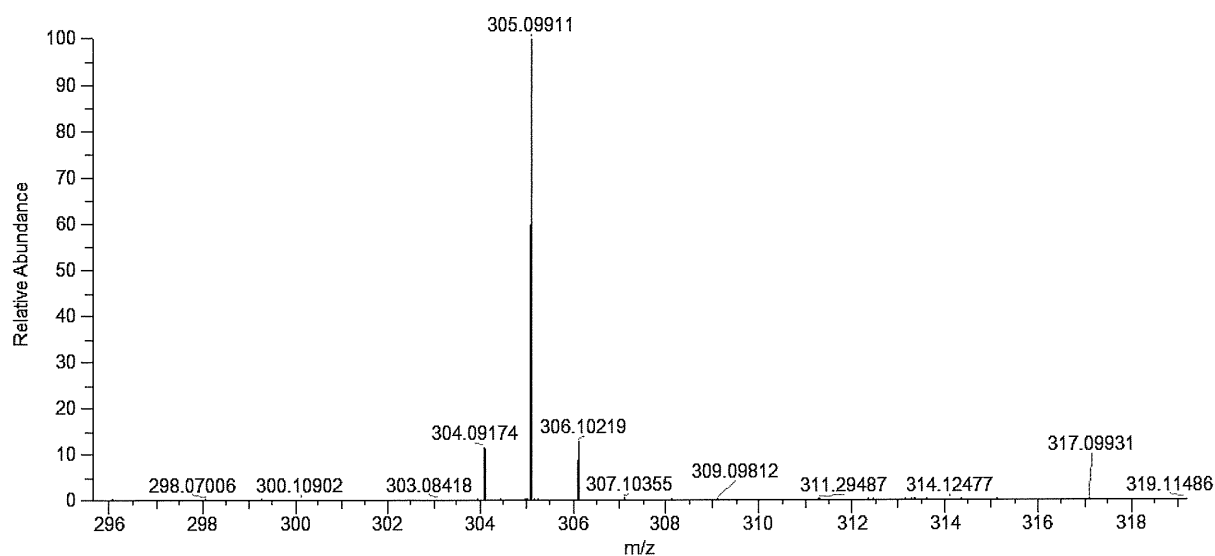
GB-2022-9

Peak Mass	Display Formula	RDB	Delta [ppm]	Delta [mmu]	Theo. mass	Combined Score	MS Cov. [%]
305.09911	C ₁₂ H ₁₃ O ₄ N ₆	9.5	-0.56	-0.17	305.09928	95.02	99.1
305.09911	C ₁₁ H ₁₇ O ₈ N ₂	4.5	3.82	1.17	305.09794	93.19	97.44
305.09911	C ₁₃ H ₉ N ₁₀	14.5	-4.95	-1.51	305.10062	82.42	86.71

EX4804 #113-146 RT: 0.98-1.28 AV: 34 SB: 4 0.02-0.04 NL: 1.92E8
T: FTMS + p APCI corona Full ms [100.0000-400.0000]



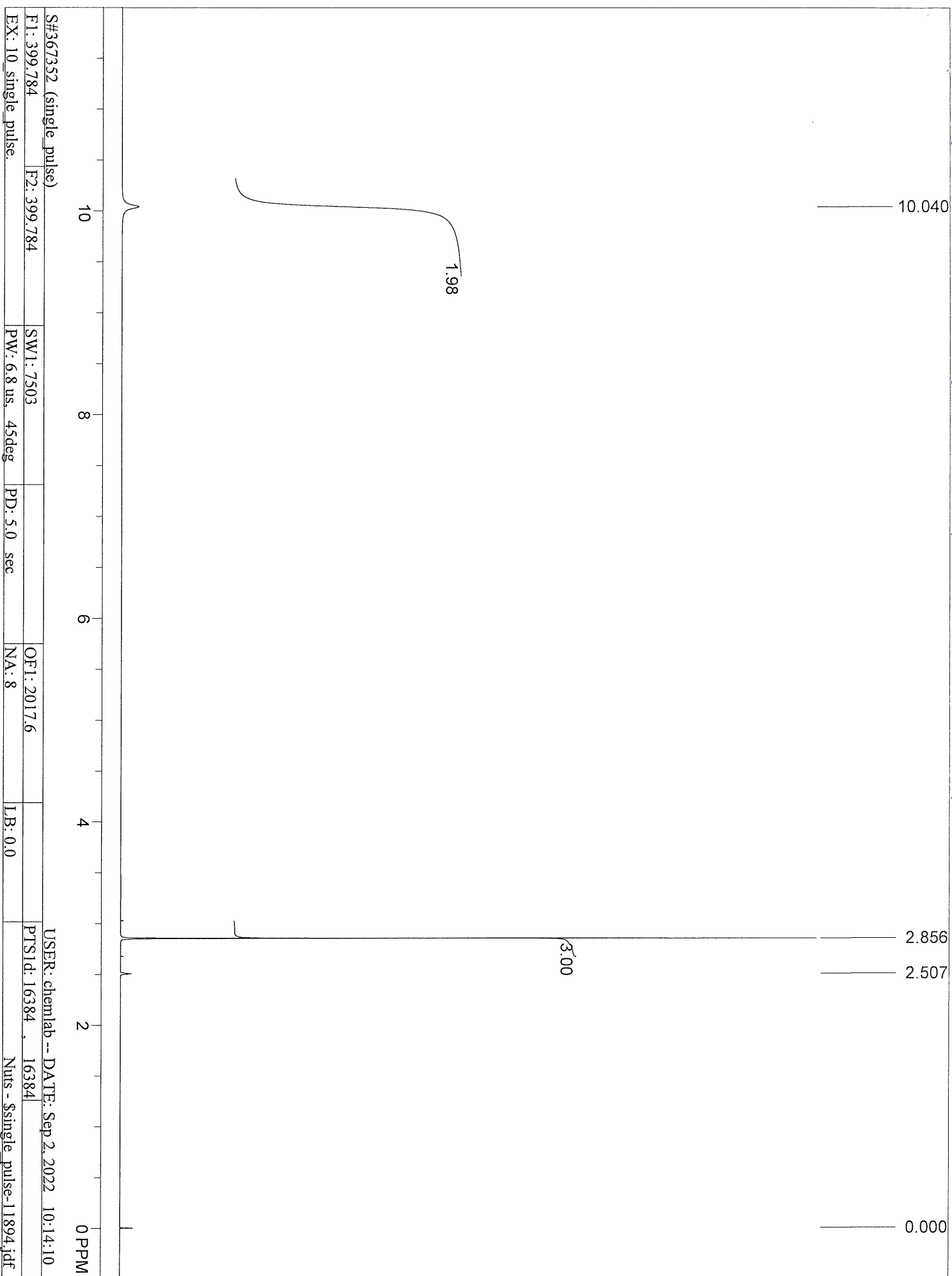
EX4804 #113-146 RT: 0.98-1.28 AV: 34 SB: 4 0.02-0.04 NL: 1.92E+008
T: FTMS + p APCI corona Full ms [100.0000-400.0000]



m/z Intensity Relative

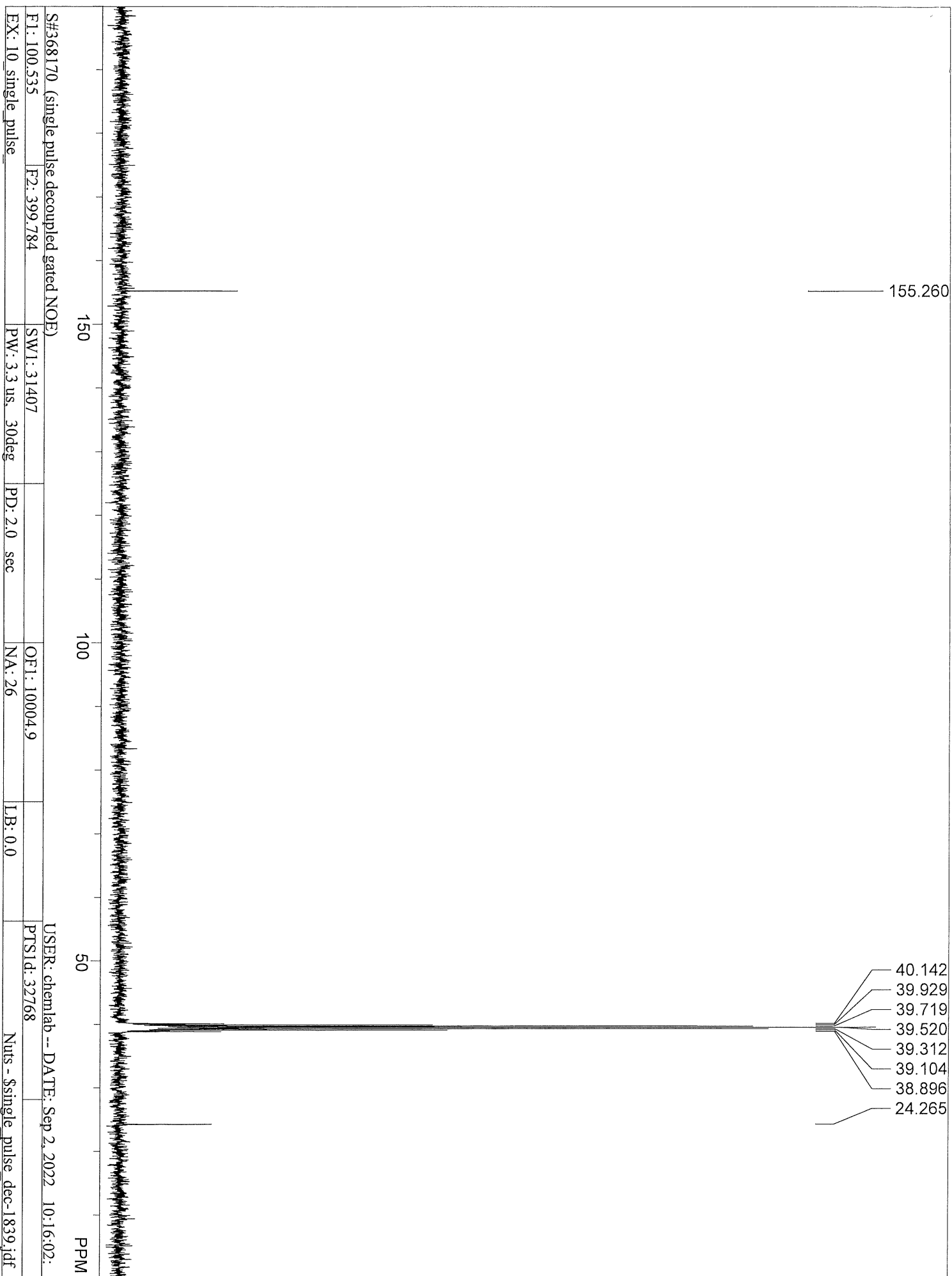
116.0456	3977103	2.009315
191.069	6950804	3.51169
192.0769	8553698	4.321506
193.0803	756091.1	0.381993
233.067	4784681	2.41732
256.1193	1487949	0.751743
257.2476	1270101	0.641681
264.1092	939770.7	0.474792
304.0917	22659621	11.44811
305.0991	1.98E+08	100
306.0971	3788609	1.914084
306.1022	24478848	12.36722
307.1035	824091.2	0.416348
307.1052	713252.3	0.36035
338.0524	1067582	0.539364
339.0604	10898045	5.505918
340.0636	1235395	0.624147
341.0574	3352012	1.693506
346.0895	844044.4	0.426429
381.1306	1255856	0.634484

¹H NMR spectrum of N-Methylurazole 5 (400 MHz, DMSO-d6)

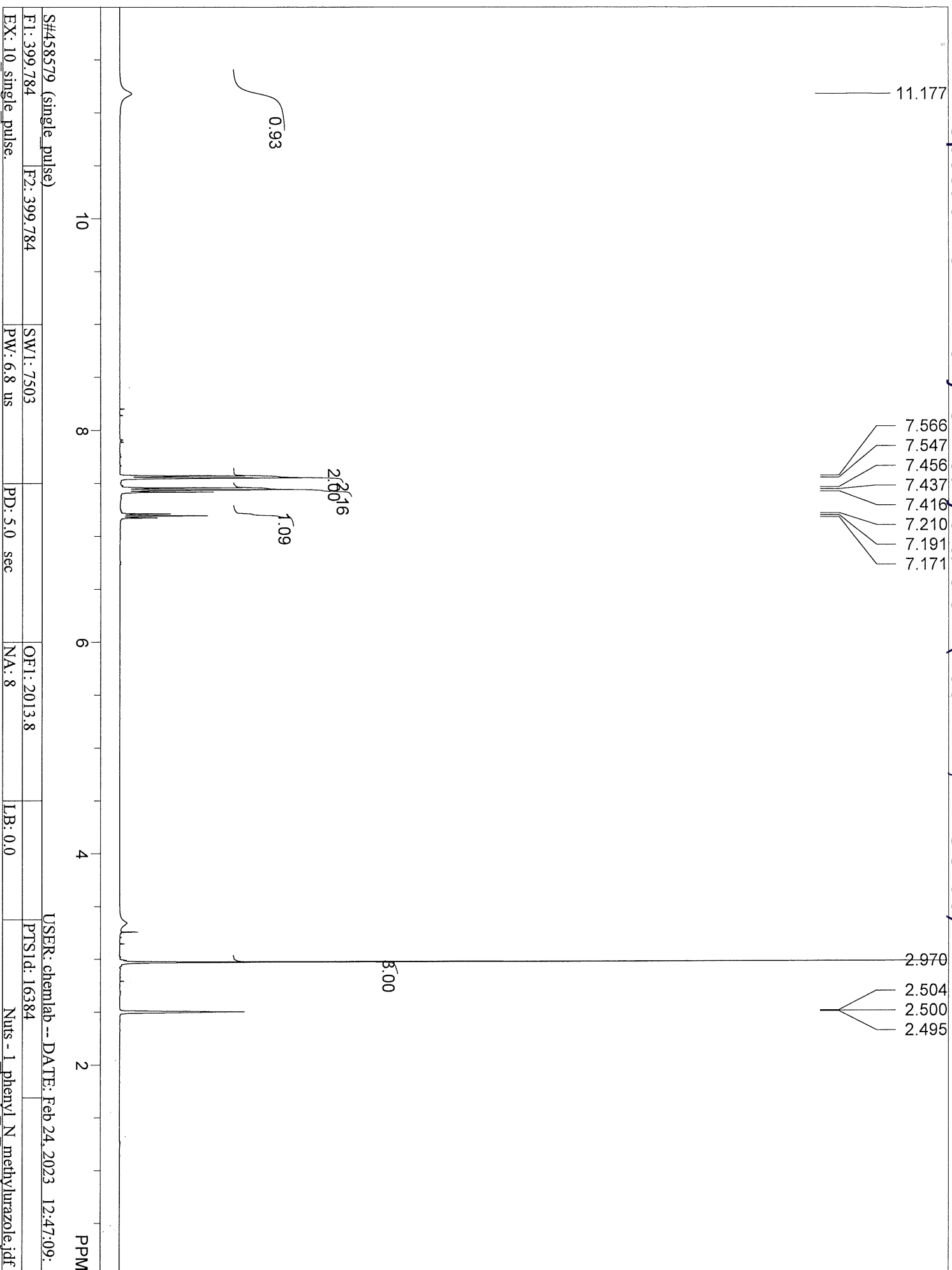


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¹³C NMR Spectrum of N-Methylurazole 5 (100 MHz, DMSO-d₆)



¹H NMR Spectrum of 1-Phenyl-3-Methylurazole 7 (400 MHz, DMSO-d6)



¹³C NMR Spectrum of 1-Phenyl-3-Methylurazole 7 (100 MHz, DMSO-d6)

