

[Supplementary Materials]

3-Methoxy-5-methyl-12-phenylbenzacridinium Iodide

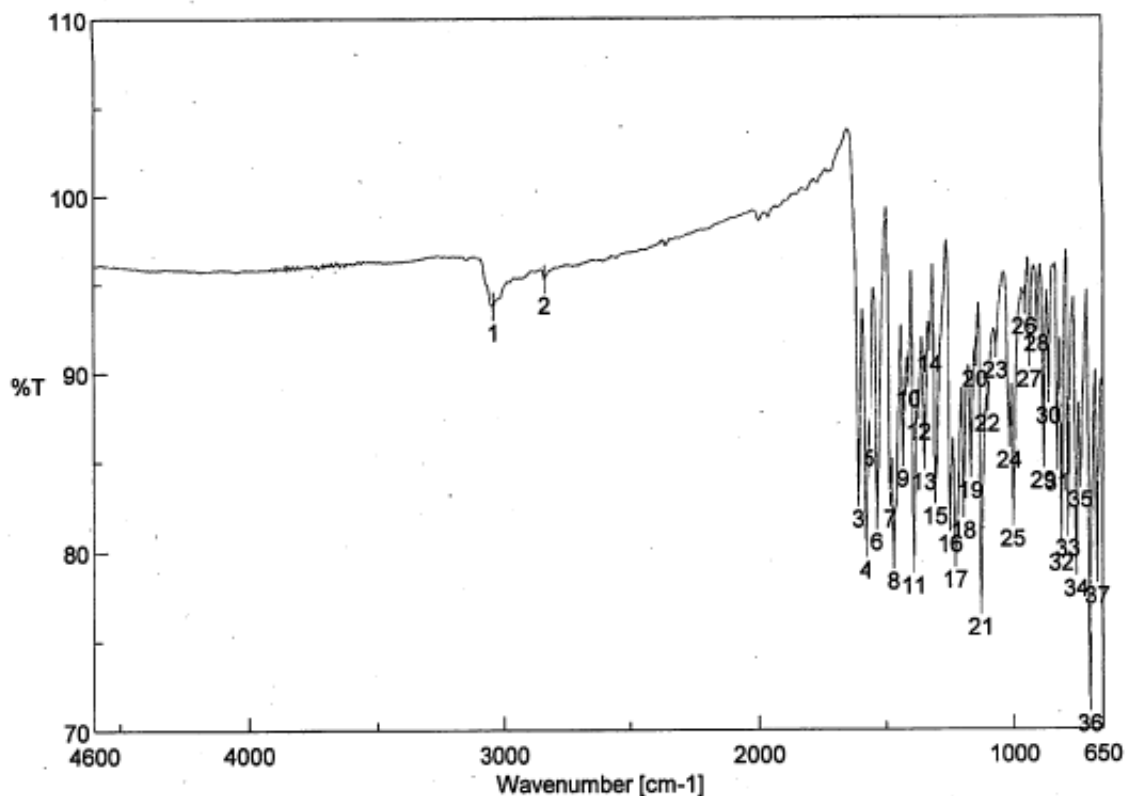
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[データ情報]		[測定情報]	
作成日時	2020/10/05 20:02	機種名	FT/IR-4100typeA
		シリアル番号	B184561016
データタイプ	等間隔データ	付属品名	ATR PRO450-S
横軸	Wavenumber [cm-1]	付属品シリアルNo.	A077261272
縦軸	%T	入射角	45度
スタート	649.893 cm-1	測定日時	2020/10/05 20:00
エンド	4600.36 cm-1	光源	標準光源
データ間隔	0.964233 cm-1	検出器	TGS
データ数	4098	積算回数	64
		分解	4 cm-1
		ゼロフィリング	On
		アポダイゼーション	Cosine
		ゲイン	Auto (4)
		アパーチャ	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]								
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3041.19	93.7341	2	2836.77	95.2589	3	1613.16	83.2256
4	1584.24	80.4185	5	1566.88	86.6183	6	1534.1	81.9617
7	1482.99	83.2361	8	1469.49	79.7921	9	1432.85	85.4784
10	1412.6	89.9256	11	1390.42	79.5507	12	1372.1	88.0893
13	1349.93	85.2899	14	1329.68	91.8979	15	1306.54	83.363
16	1248.68	81.838	17	1228.43	79.8688	18	1196.61	82.5911
19	1168.65	84.8036	20	1150.33	91.05	21	1128.15	77.2358
22	1102.12	88.5567	23	1071.26	91.5517	24	1017.27	86.4988
25	1001.84	82.1221	26	957.484	93.9824	27	938.199	91.0253
28	909.272	93.012	29	883.238	85.3619	30	862.989	88.9651
31	829.241	85.2215	32	812.849	80.7786	33	786.815	81.5641

Figure S1. IR spectrum (neat)

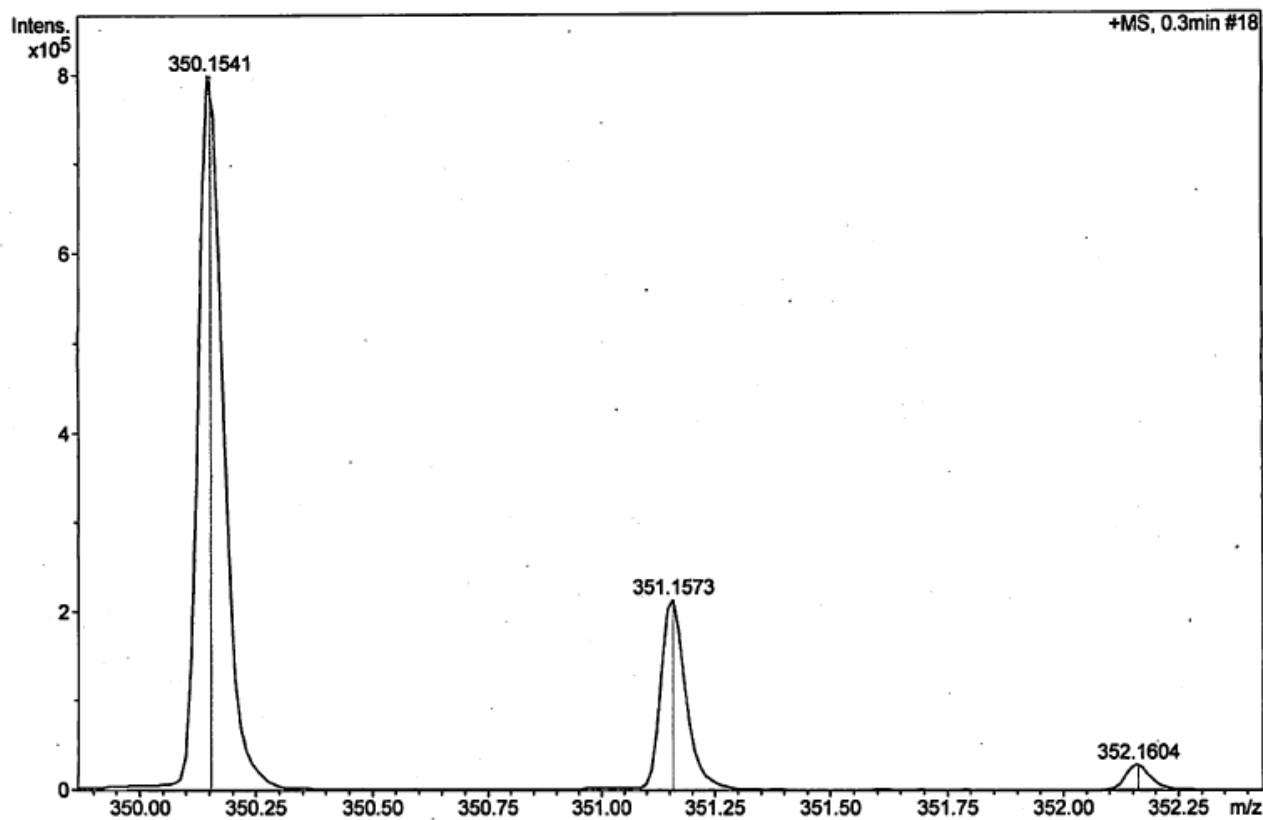
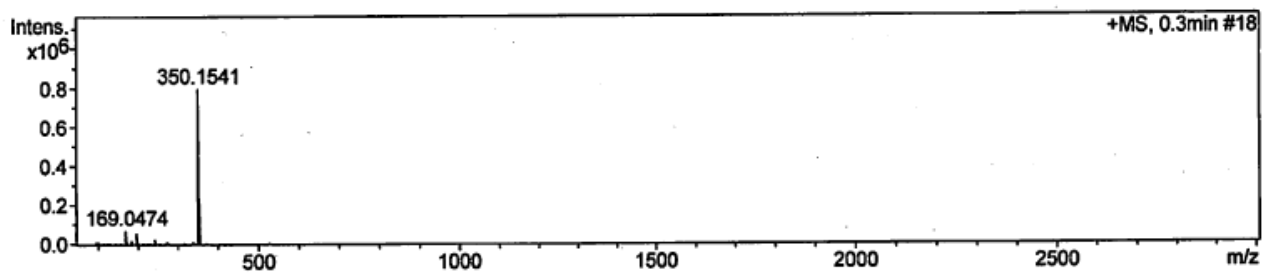


Figure S2. HRMS (ESI-TOF) spectrum

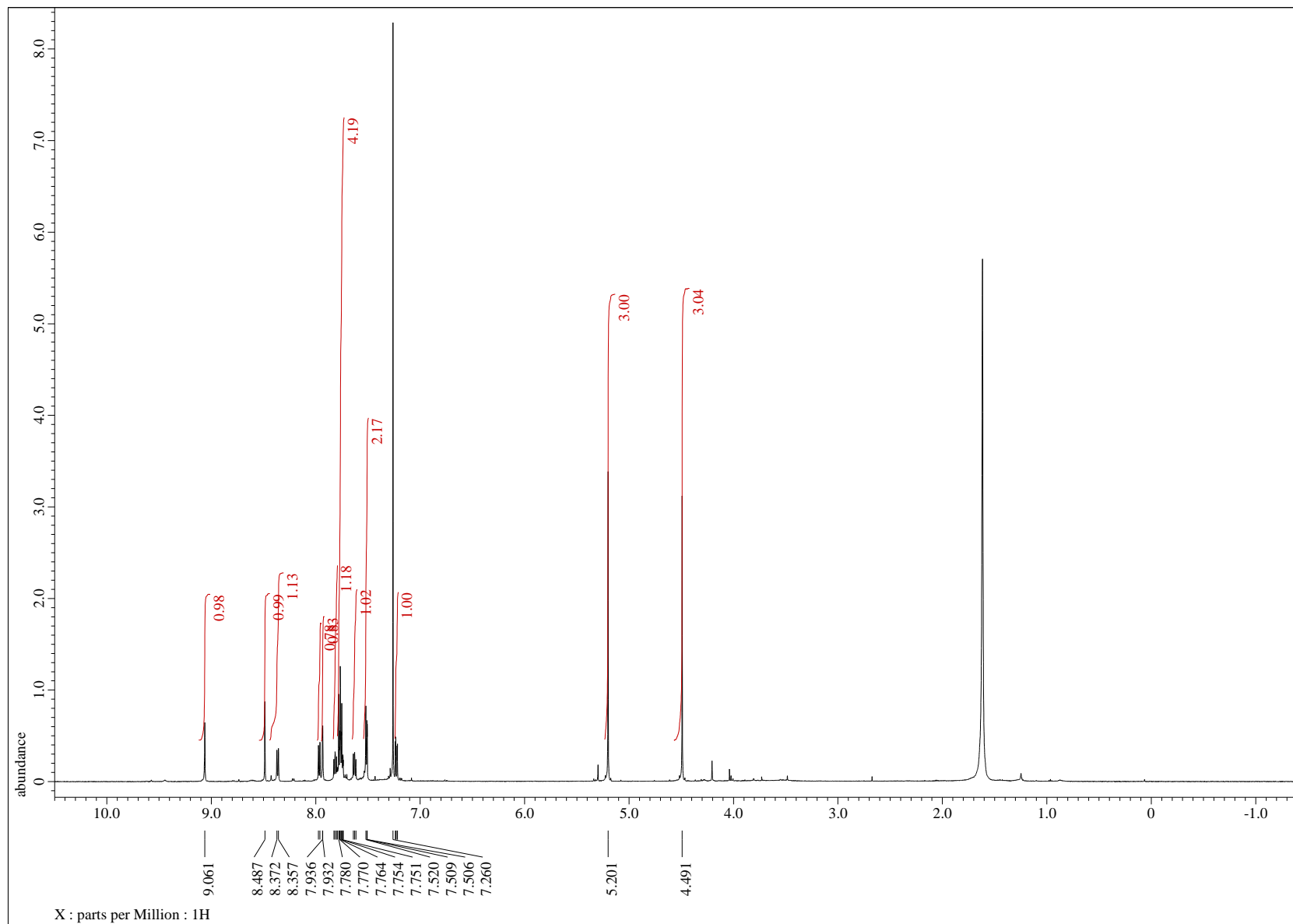


Figure S3. ^1H NMR spectrum (600 MHz, CDCl_3)

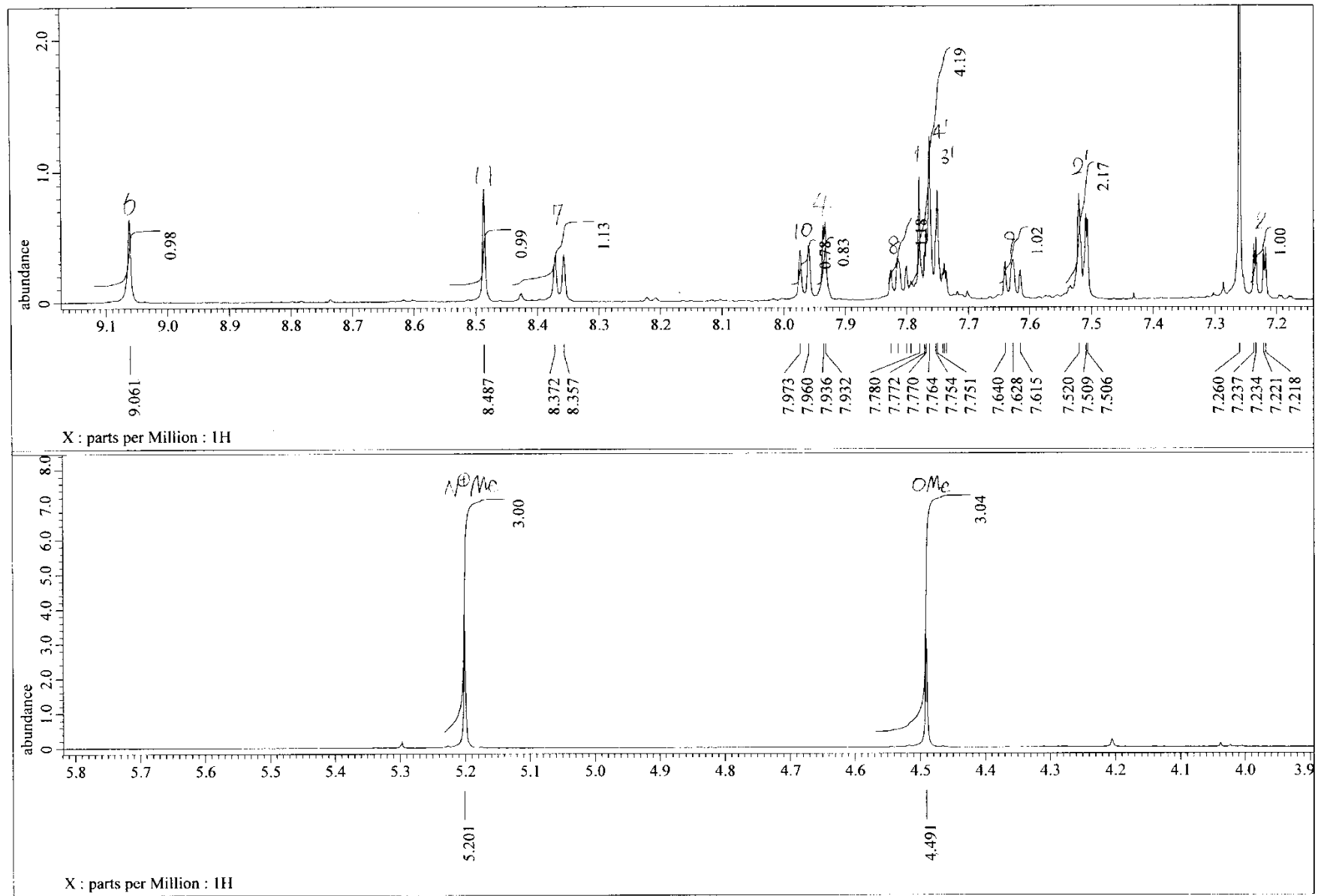


Figure S4. Assignment of ^1H NMR

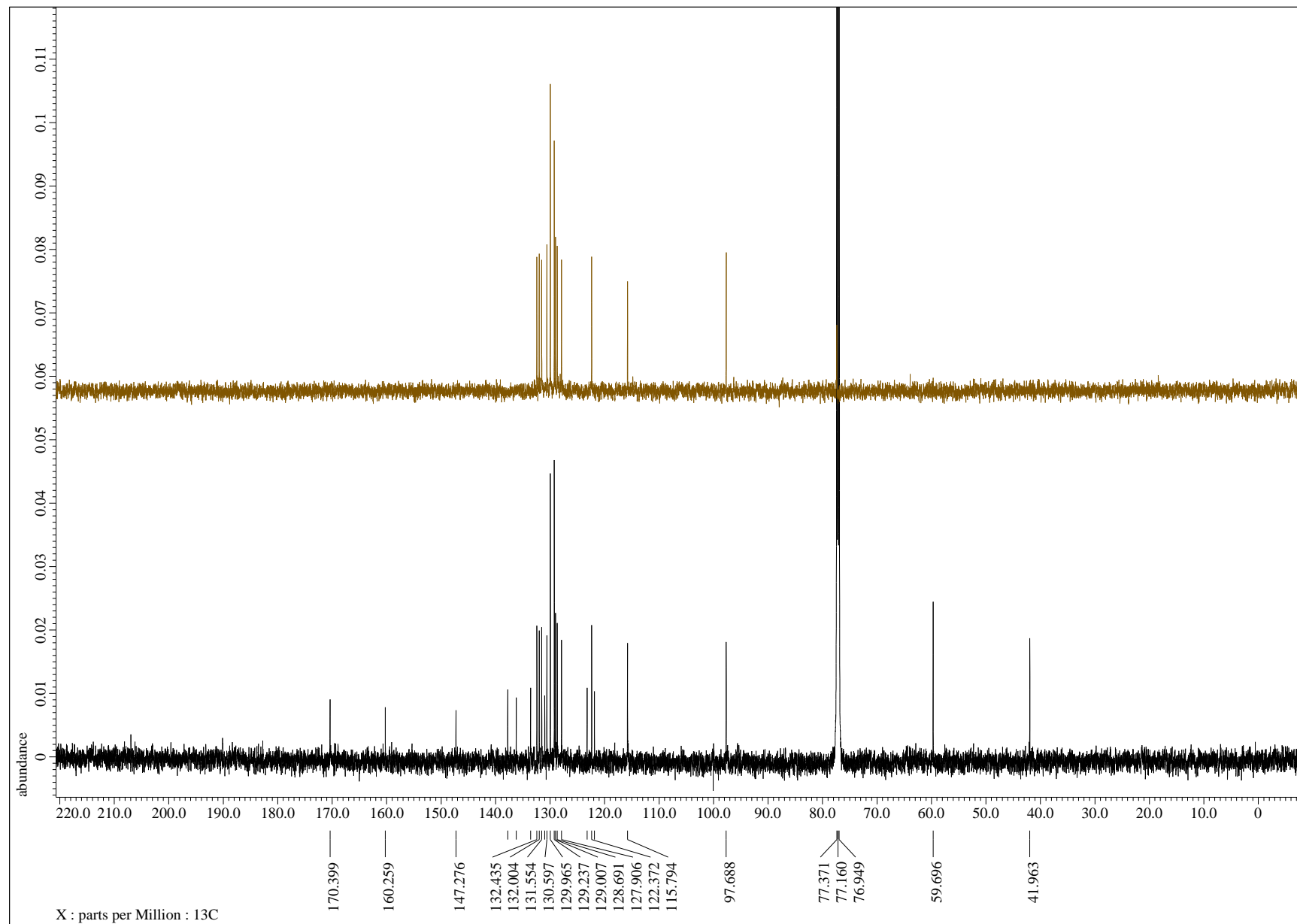


Figure S5. DEPT 90 (150 MHz, CDCl₃, top) and ¹³C NMR (150 MHz, CDCl₃, bottom)

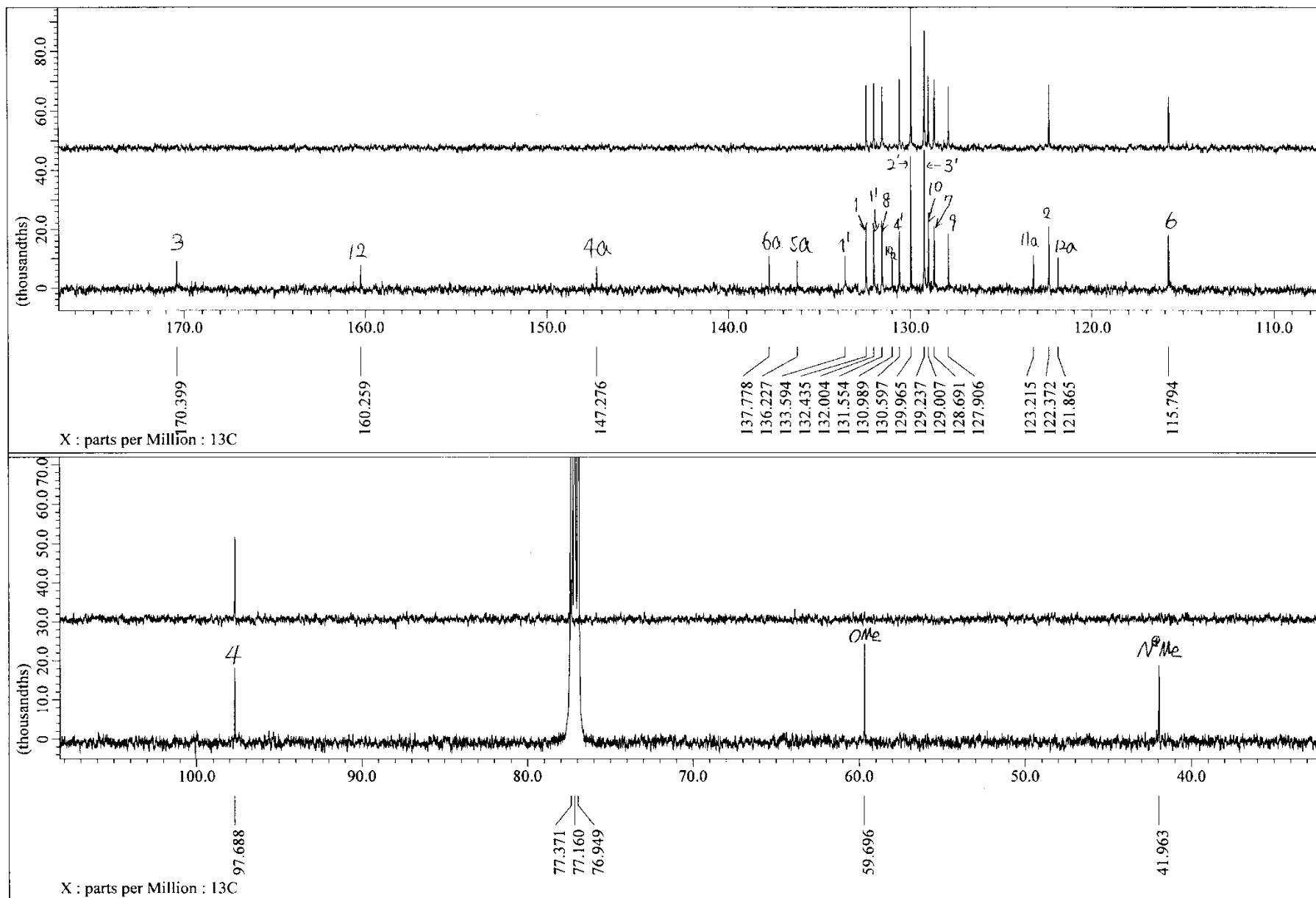


Figure S6. Assignment of ^{13}C NMR

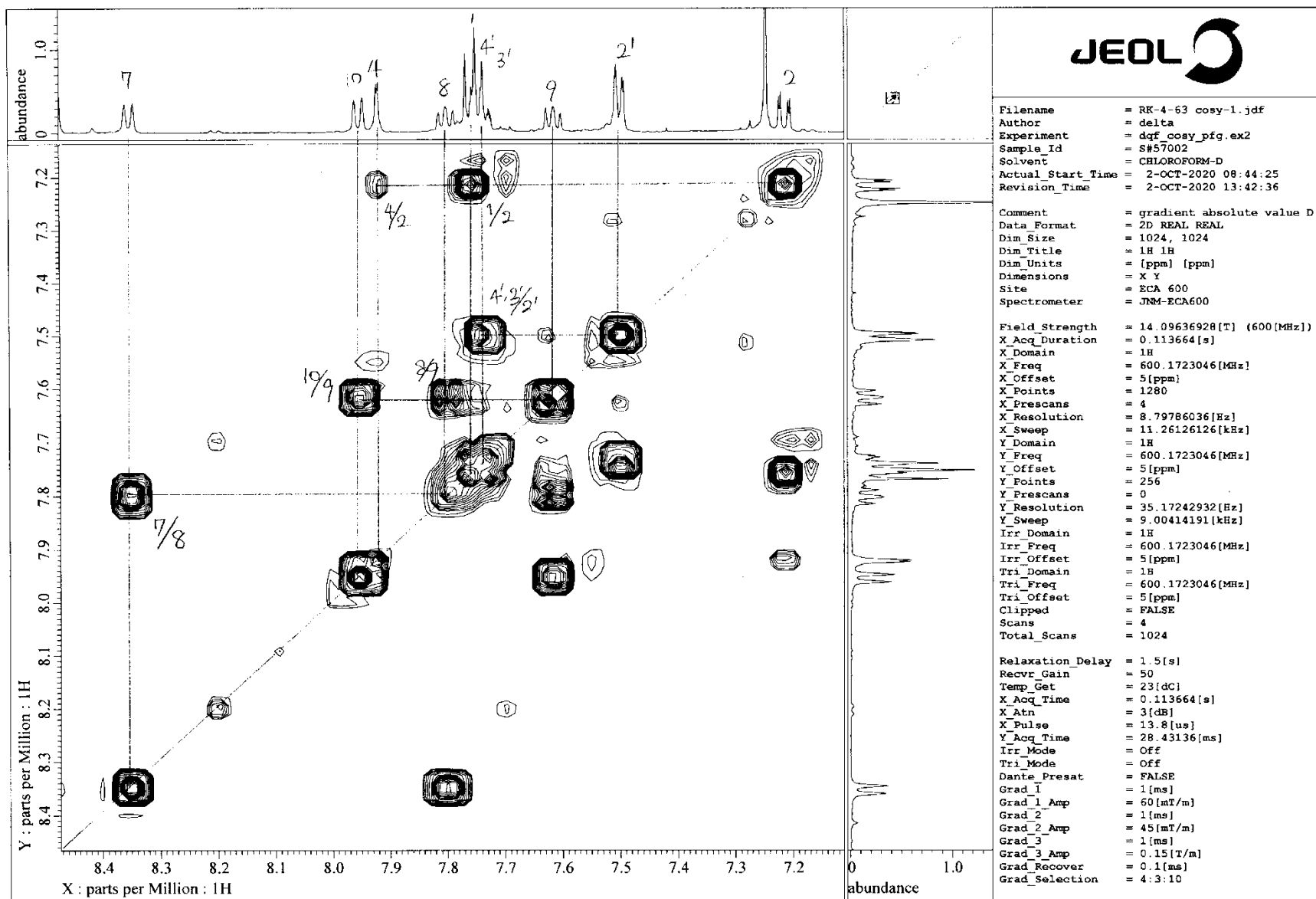


Figure S7. Assignment of COSY spectrum (600 MHz, CDCl₃)

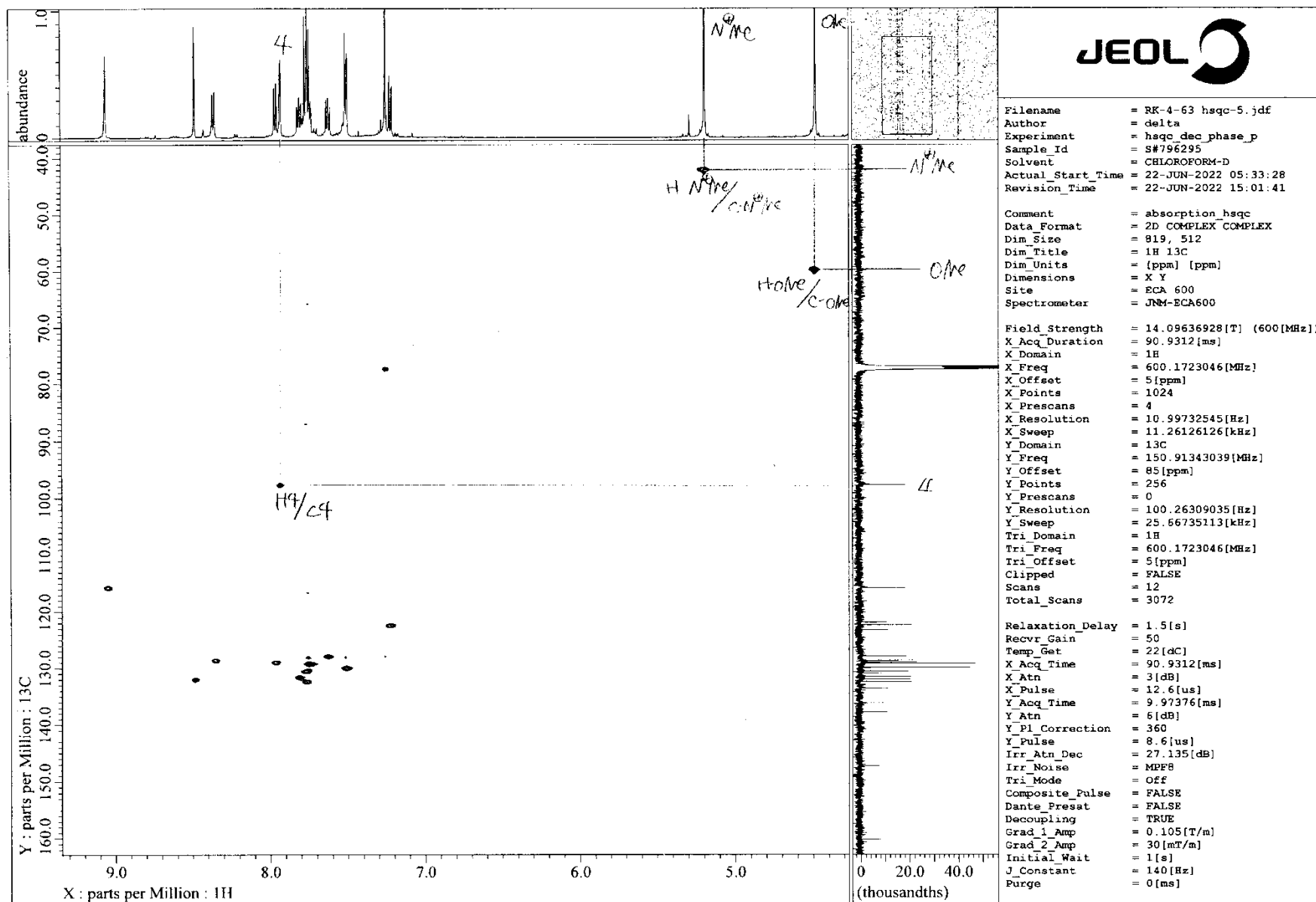


Figure S8. Assignment of HSQC spectrum (part 1, 600/150 MHz, CDCl_3)

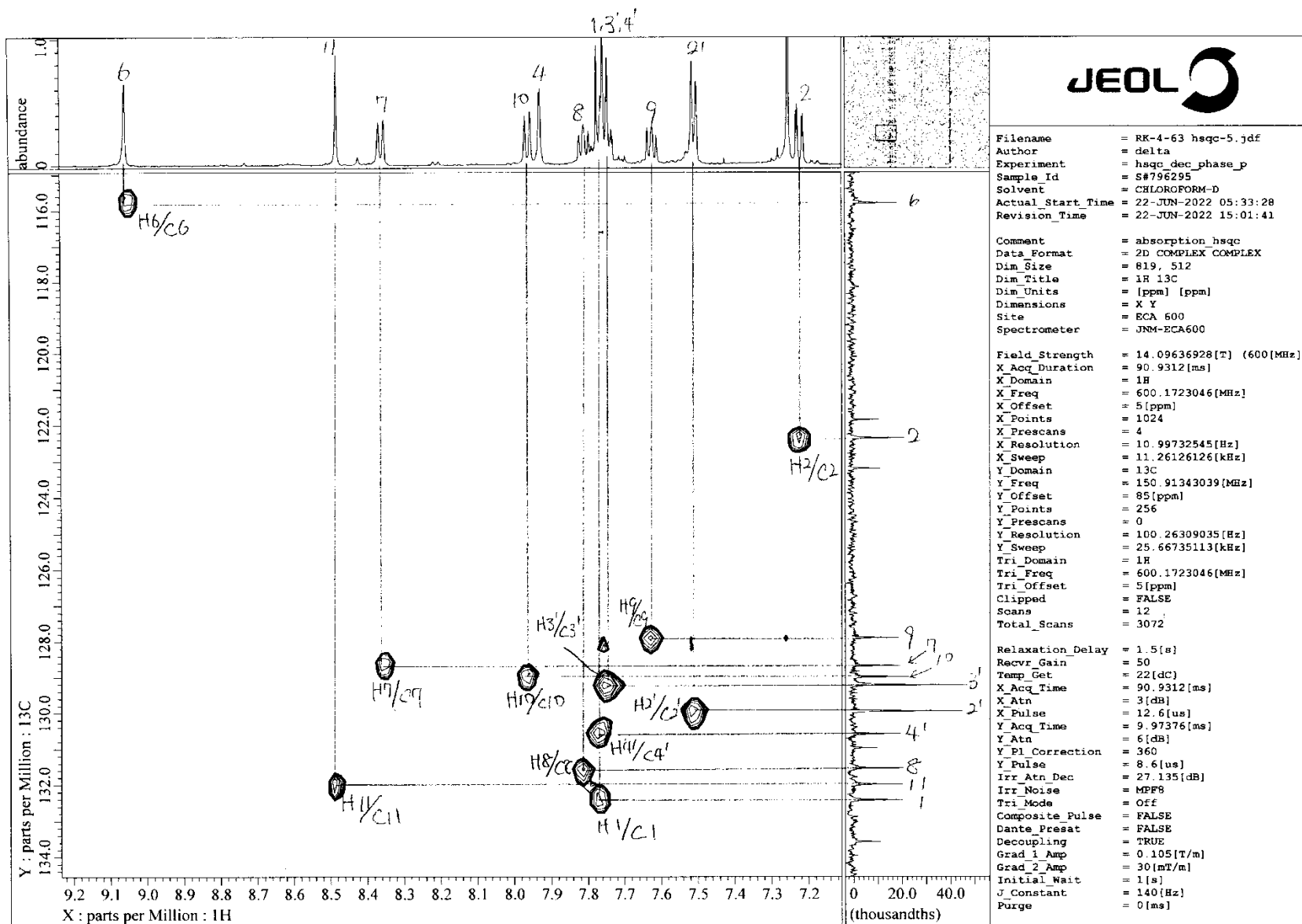


Figure S9. Assignment of HSQC spectrum (part 2, 600/150 MHz, CDCl₃)

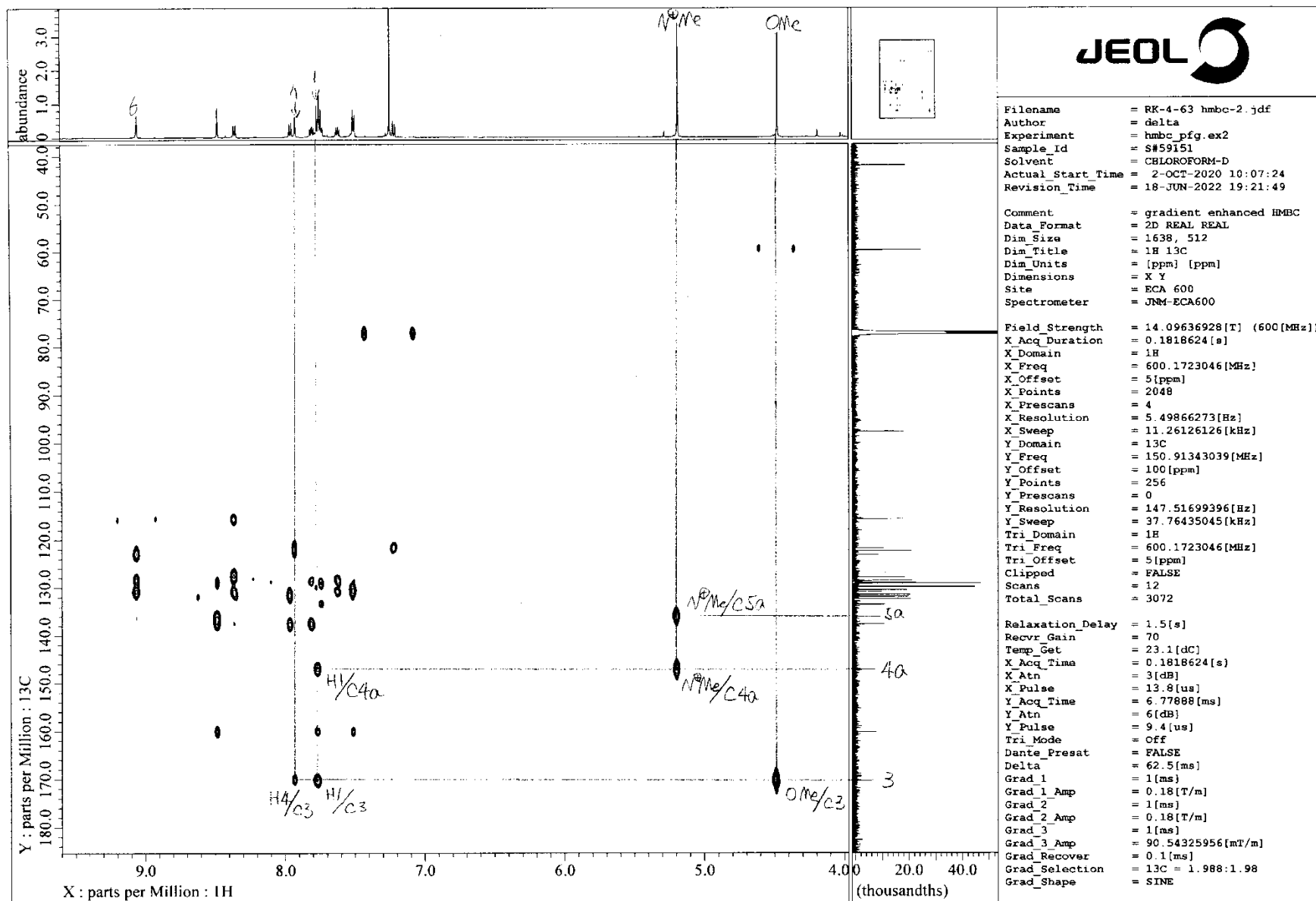


Figure S10. Assignment of HMBC spectrum (part 1, 600/150 MHz, CDCl₃)

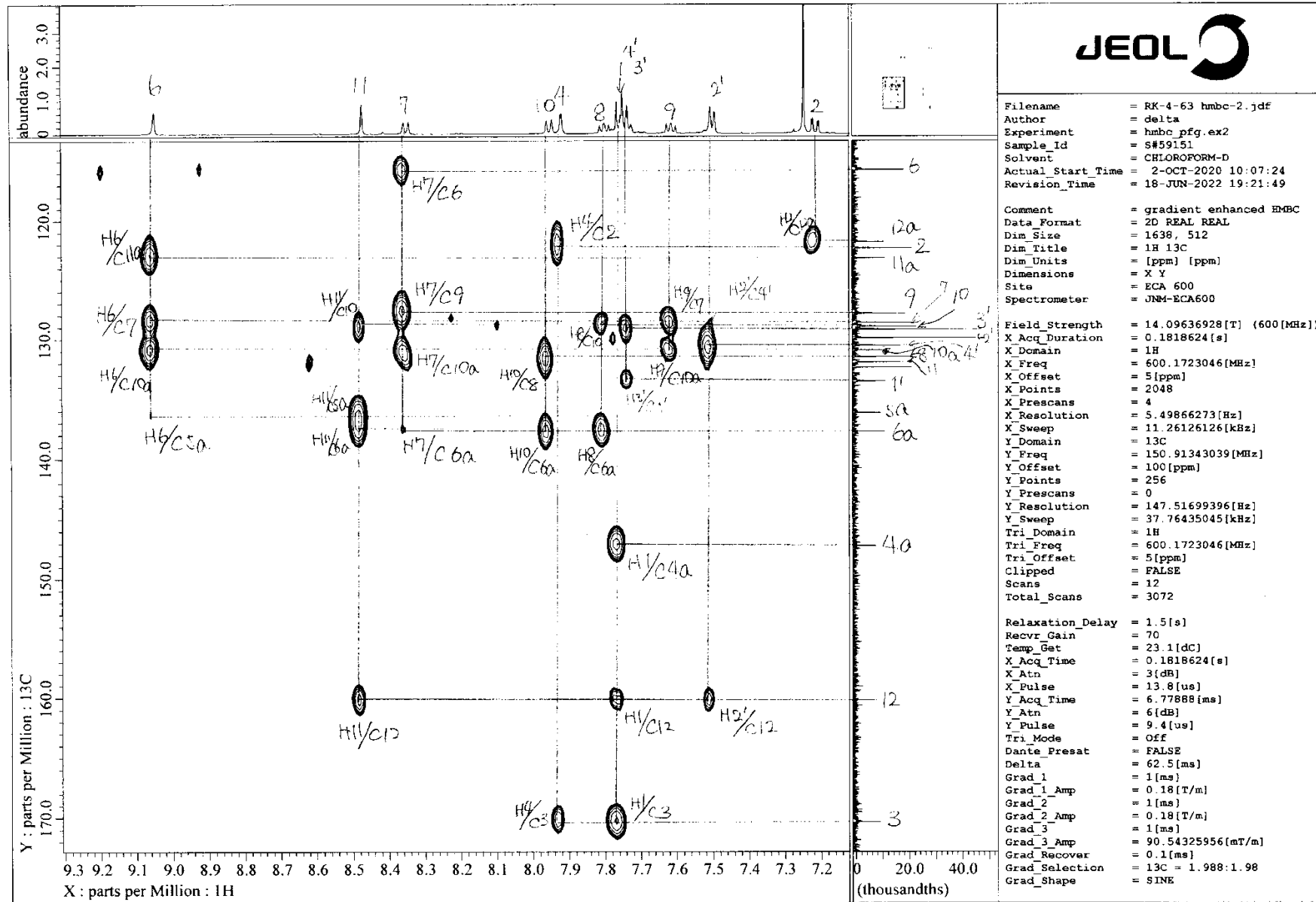


Figure S11. Assignment of HMBC spectrum (part 2, 600/150 MHz, CDCl₃)

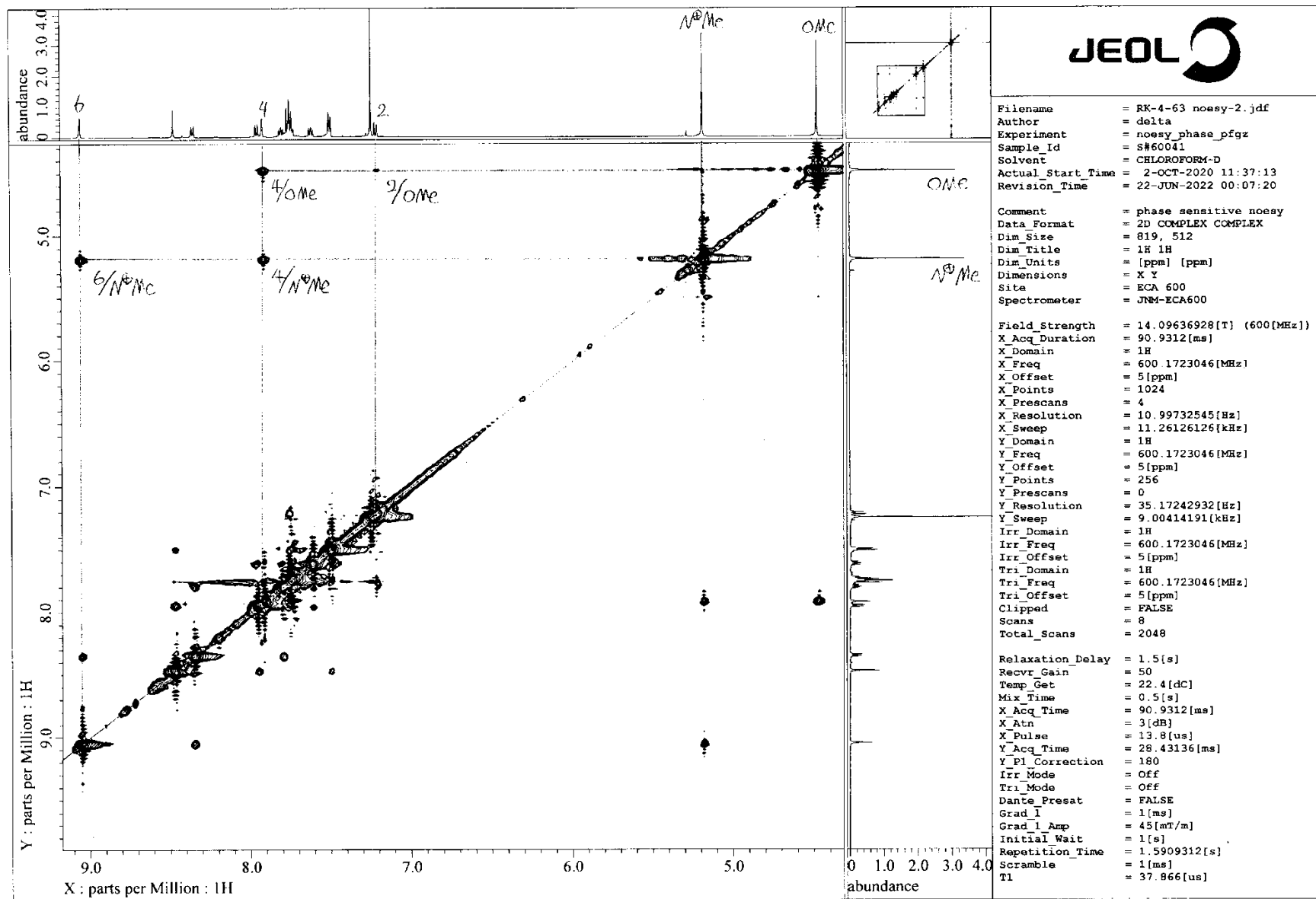


Figure S12. Assignment of NOESY spectrum (part 1, 600 MHz, CDCl₃)

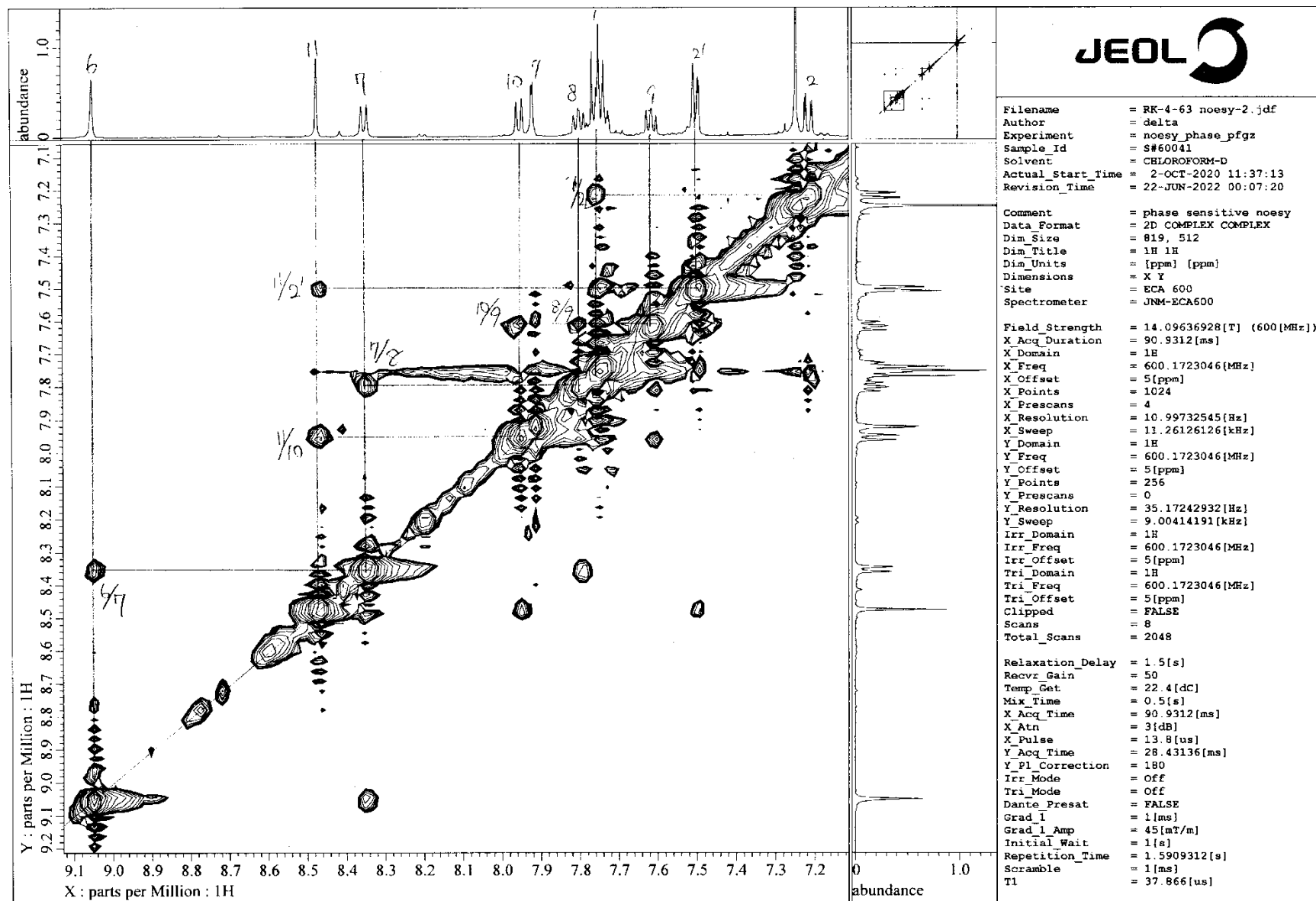


Figure S13. Assignment of NOESY spectrum (part 2, 600 MHz, CDCl₃)

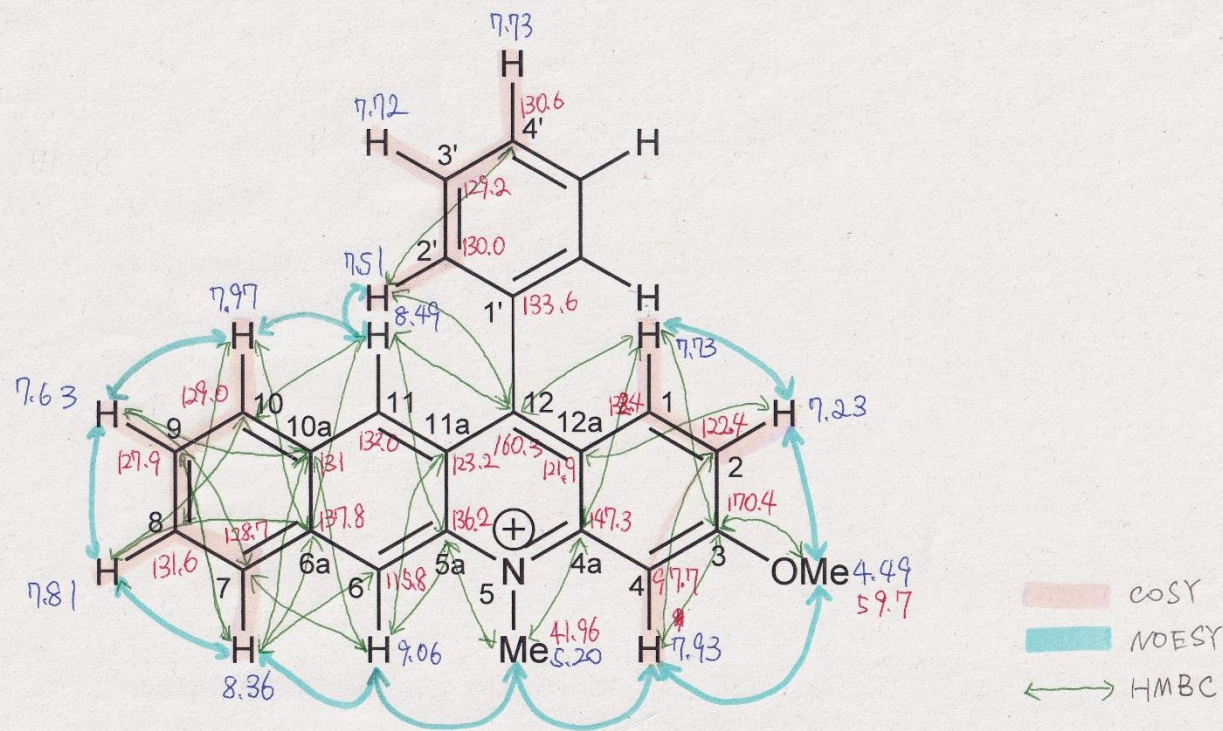


Figure S14. Summary of the assignments of ^1H NMR, ^{13}C NMR, COSY, HMBC and NOESY spectra