Supplementary Information

Marine Natural Products-Inspired Phenylmethylene Hydantoins with Potent *in Vitro* and *in Vivo* Antitumor Activities via Suppression of Brk and FAK Signaling

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Table S1. ^{1}H NMR data of compounds **3**-**7**[a]

Position	δ_H				
	3	**4**	**5**	**6**	**7**
6	6.25, s	6.24, s	6.38, s	6.39, s	6.41, s
7	-------	-------	-------	-------	-------
8	6.87, brs	7.73, dd (9.2, 1.1)	7.44, d (8.2)	8.07, d (2.2)	7.65, d (8.7)
9	-------	6.73, d (9.2)	7.58, d (8.2)	-------	7.68, d (8.7)
10	-------	-------	-------	-------	-------
11	-------	-------	7.58, d (8.2)	7.42, d (8.8)	7.68, d (8.7)
12	7.05, dd (2.3, 11.9)	-------	7.44, d (8.2)	7.80, dd (2.2,8.8)	7.65, d (8.7)
1`	-------	-------	-------	5.30, 2H, s	-------
2`	-------	-------	-------	-------	7.27, t (8.7)
3`	-------	-------	-------	7.21, t (8.7)	7.73, dd (8.7, 6.0)
4`	-------	-------	-------	7.47, dd (8.7, 6.0)	-------
5`	-------	-------	-------	-------	7.73, dd (8.7, 6.0)
6`	-------	-------	-------	7.47, dd (8.7, 6.0)	7.27, t (8.7)
7`	-------	-------	-------	7.21, t (8.7)	-------
-OCH_3	3.78, 3H, s	-------	-------	-------	--------
-$N(CH_3)_2$	-------	3.10, 6H, s	-------	-------	-------
-$SC(\mathbf{CH_3})_3$	-------	-------	1.21, 9H, s	-------	-------

[a]In DMSO, 400 MHz. Coupling constants (*J*) are in Hertz.

Table S2. ^{1}H NMR data of compounds **8**-**11**[a]

Position	δ_H			
	8	**9**	**10**	**11**
6	6.39, s	6.41, s	6.40, s	6.10, s
7	-------	-------	-------	-------
8	7.57, d (8.7)	7.70, d (8.7)	7.71, d (8.2)	-------
9	7.04, d (8.7)	7.27, d (8.7)	7.67, d (8.2)	-------
10	-------	-------	-------	-------
11	7.04, d (8.7)	7.27, d (8.7)	7.67, d (8.2)	-------
12	7.57, d (8.7)	7.70, d (8.7)	7.71, d (8.2)	-------
1`	5.15, 2H, s	-------	-------	-------
2`	-------	6.81, m	-------	-------
3`	-------	-------	-------	-------
4`	7.48, m	-------	-------	-------
5`	7.29, dd (9.3, 8.7)	-------	-------	-------
6`	7.39, dd (8.7, 8.2)	-------	-------	6.10, s
7`	-------	-------	-------	-------
-OCH_3 (C-9)	-------	-------	-------	-------
-OCH_3 (C-10)	-------	-------	-------	-------
-$N(CH_3)_2$	-------	-------	-------	-------

[a]In DMSO, 400 MHz. Coupling constants (*J*) are in Hertz.

Table S3. ^{1}H NMR data of compounds **12**-**13**[a]

Position	δ_H	
	12	**13**
6	6.29, s	6.36, s
7	-------	-------
8	7.26, dd (6.8, 1.8)	6.98, d (12.4)
9	6.65, dd (6.8, 1.8)	-------
10	-------	-------
11	-------	7.05, d (7.3)
12	-------	-------
1`	-------	-------
2`	-------	-------
3`	-------	-------
4`	-------	-------
5`	-------	-------
6`	-------	-------
`	-------	-------
-OCH_3 (C-9)	--------	3.80, s
-OCH_3 (C-10)	-------	3.78, s
-$N(CH_3)_2$	-------	-------

[a]In DMSO, 400 MHz. Coupling constants (*J*) are in Hertz.

Table S4. ^{13}C NMR data of compounds **3**-**8**[a]

Position	δ_C					
	3	**4**	**5**	**6**	**7**	**8**
2	156.7, qC	156.0, qC	156.2, qC	156.3, qC	156.3, qC	156.2, qC
4	166.5, qC	165.7, qC	166.0, qC	165.9, qC	166.2, qC	166.2, qC
5	126.1, qC	128.5, qC	129.2, qC	126.5, qC	128.6, qC	126.6, qC
6	110.6, CH	98.8, CH	107.7, CH	106.3, CH	108.3, CH	109.0, CH
7	121.1, qC	109.8, qC	134.1, qC	128.8, qC	132.7, qC	126.9, qC
8	109.9, CH	134.4, CH	130.0, CH	125.4, CH	127.3, CH	131.7, CH
9	151.3, qC	112.5, CH	137.5, CH	140.6, qC	130.5, CH	115.4, CH
10	150.7, qC	161, qC	132.7, qC	150.5, qC	139.2, qC	160.7, qC
11	153.7, qC	154.7, qC	137.5, CH	115.9, CH	130.5, CH	115.4, CH
12	109.7, CH	163.2, qC	130.0, CH	135.4, CH	127.3, CH	131.7, CH
1`	-------	-------	-------	70.4, CH_2	136.3, qC	70.4, CH_2
2`	-------	-------	-------	132.6, qC	129.2, CH	136.0, qC
3`	-------	-------	-------	130.4, CH	116.4, CH	163.2, qC
4`	-------	-------	-------	116.1, CH	161.4, qC	126.6, CH
5`	-------	-------	-------	163.7, qC	116.4, CH	132.5, CH
6`	-------	-------	-------	116.1, CH	129.2, CH	132.4, CH
7`	-------	-------	-------	130.4, CH	-------	158.9, qC
-OCH_3	56.7, CH_3	-------	-------	-------	-------	-------
-$N(CH3)_2$	-------	42.8, CH_3	-------	-------	-------	-------
-CN	-------	115.1, qC	-------	-------	-------	-------
-S**C**$(CH_3)_3$	-------	-------	46.8, qC	-------	-------	-------
-SC(**CH_3**)$_3$	-------	-------	31.2, CH_3	-------	-------	-------

[a]In DMSO, 100 MHz. Carbon multiplicities were determined by pendant experiments. qC = quaternary. CH = methine, CH_2 = methylene, CH_3 =methyl carbons.

Table S5. ^{13}C NMR data of compounds **9**-**13**[a]

Position	δ_C				
	9	**10**	**11**	**12**	**13**
2	156.4, qC	156.3, qC	156.4, qC	156.0, qC	156.2, qC
4	166.1, qC	166.0, qC	165.6, qC	165.8, qC	166.2, qC
5	132.4, qC	122.7, qC	135.3, qC	127.8, qC	128.3, qC
6	107.9, CH	106.6, CH	91.2, CH	100.1, CH	111.5, CH
7	129.2, qC	128.5, qC	115.0, qC	111.1, qC	111.9, qC
8	131.8, CH	136.8, CH	142.7, qC	124.3, CH	100.4, CH
9	122.3, CH	131.0, CH	142.7, qC	114.3, CH	145.8, qC
10	148.1, qC	130.3, qC	115.0, qC	148.7, qC	154.3, qC
11	122.3, CH	131.0, CH	142.7, qC	142.1, qC	101.0, CH
12	131.8, CH	136.8, CH	142.7, qC	139.7, qC	150.8, qC
1`	117.0, qC	-------	-------	-------	-------
2`	108.7, CH	-------	156.4, qC	-------	-------
3`	-------	-------	-------	-------	-------
4`	-------	-------	165.6, qC	-------	-------
5`	-------	-------	135.3, qC	-------	-------
6`	-------	-------	91.2, CH	-------	-------
7`	-------	-------	-------	-------	-------
-OCH_3	-------	-------	-------	-------	56.6, CH_3
-$N(CH3)_2$	-------	-------	-------	-------	56.7, CH_3
-SCF_3	-------	136.7, qC	-------	-------	-------

[a]In DMSO, 100 MHz. Carbon multiplicities were determined by pendant experiments. qC = quaternary. CH = methine, CH_2 = methylene, CH_3 =methyl carbons.

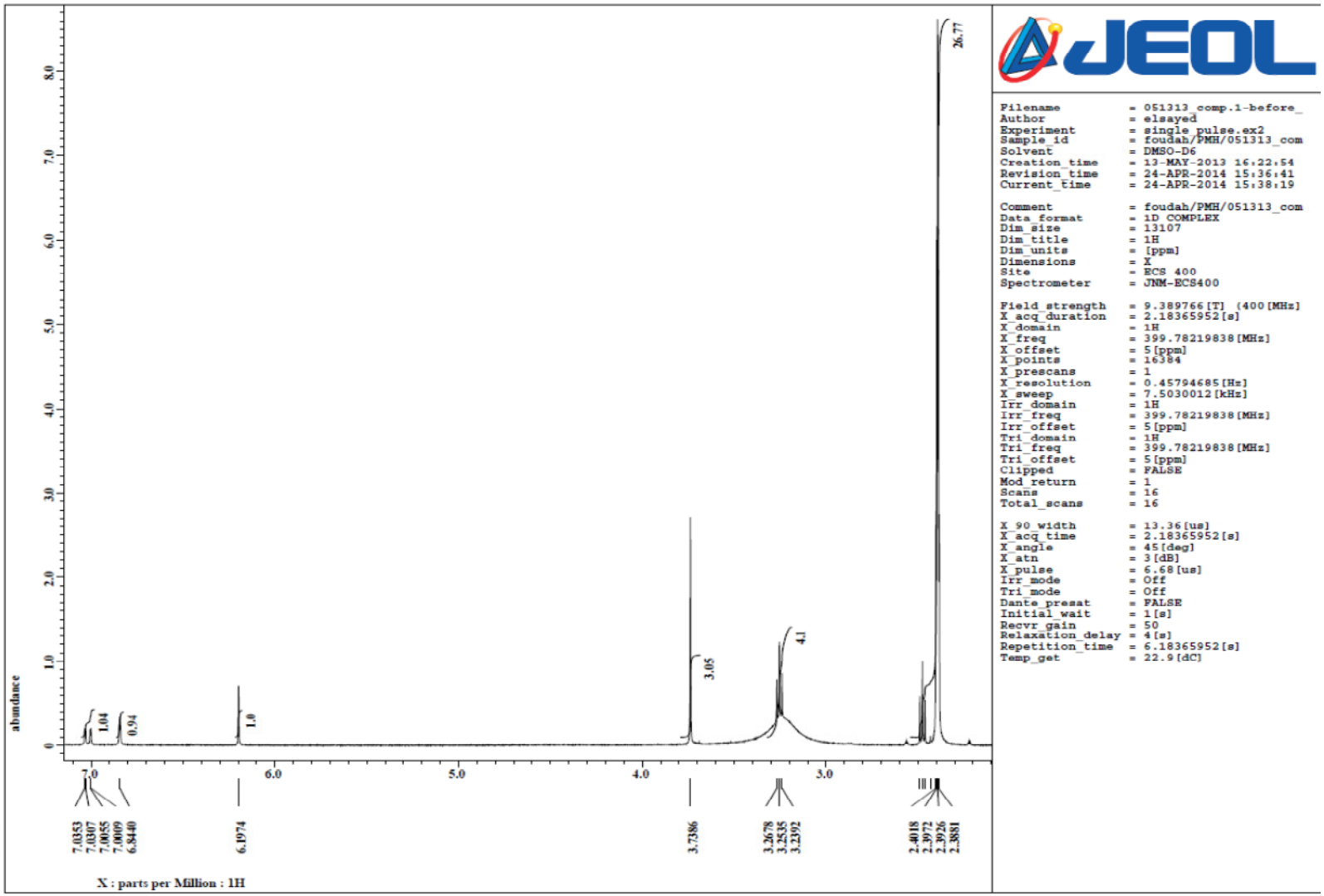

Figure SI1. ^{1}H NMR Spectrum of **3**.

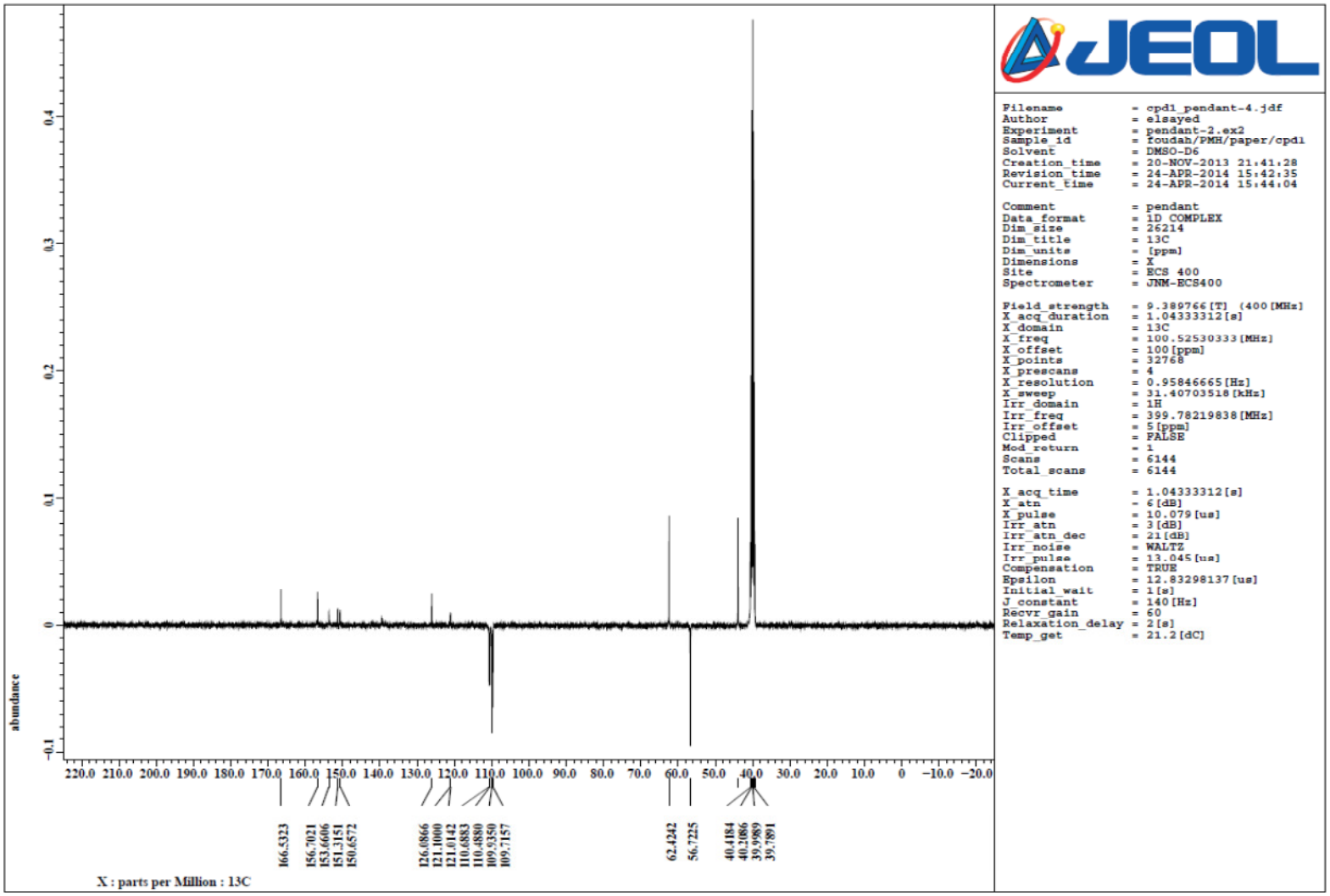

Figure SI2. ^{13}C NMR (PENDANT) Spectrum of **3**.

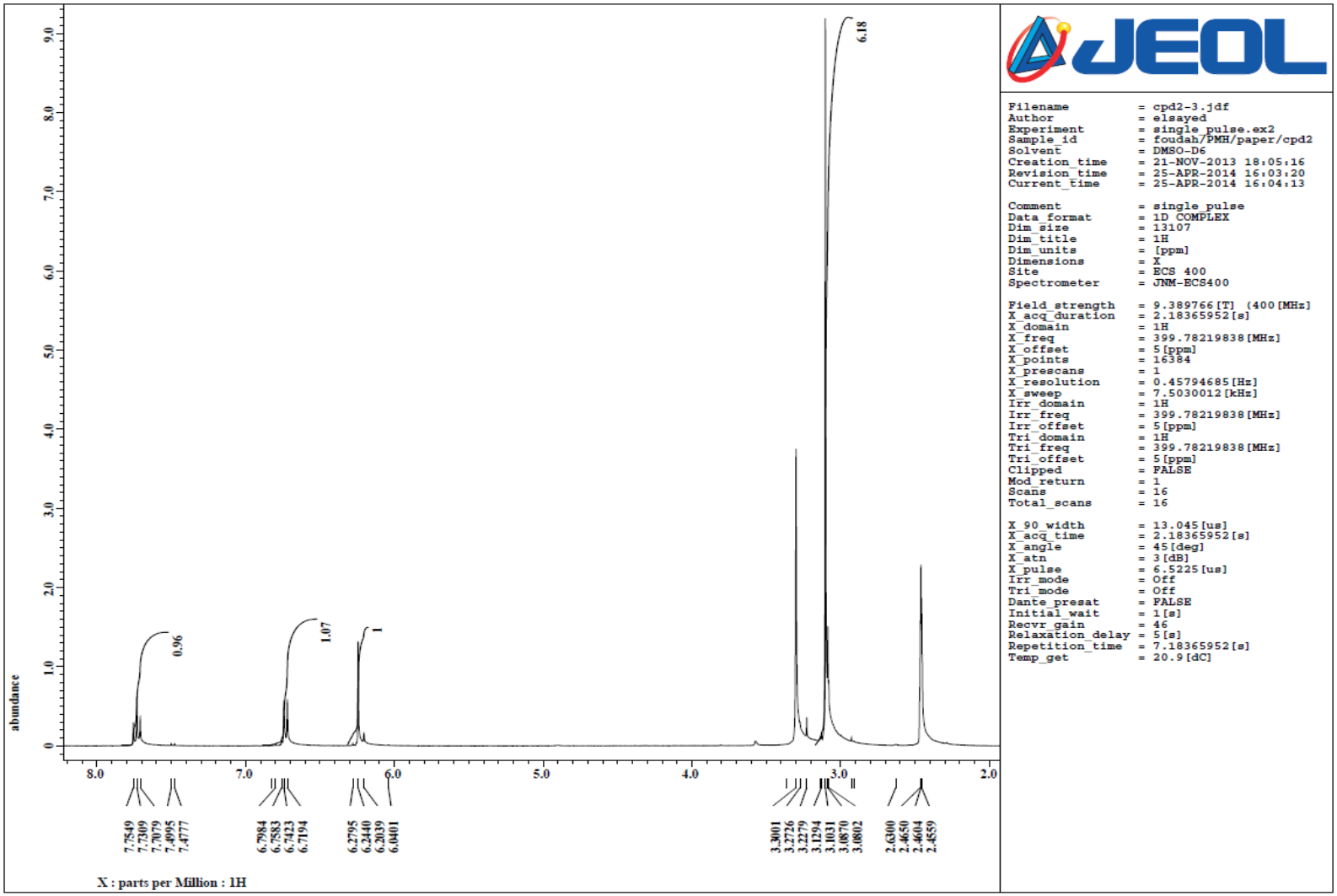

Figure SI3. ^{1}H NMR Spectrum of **4**.

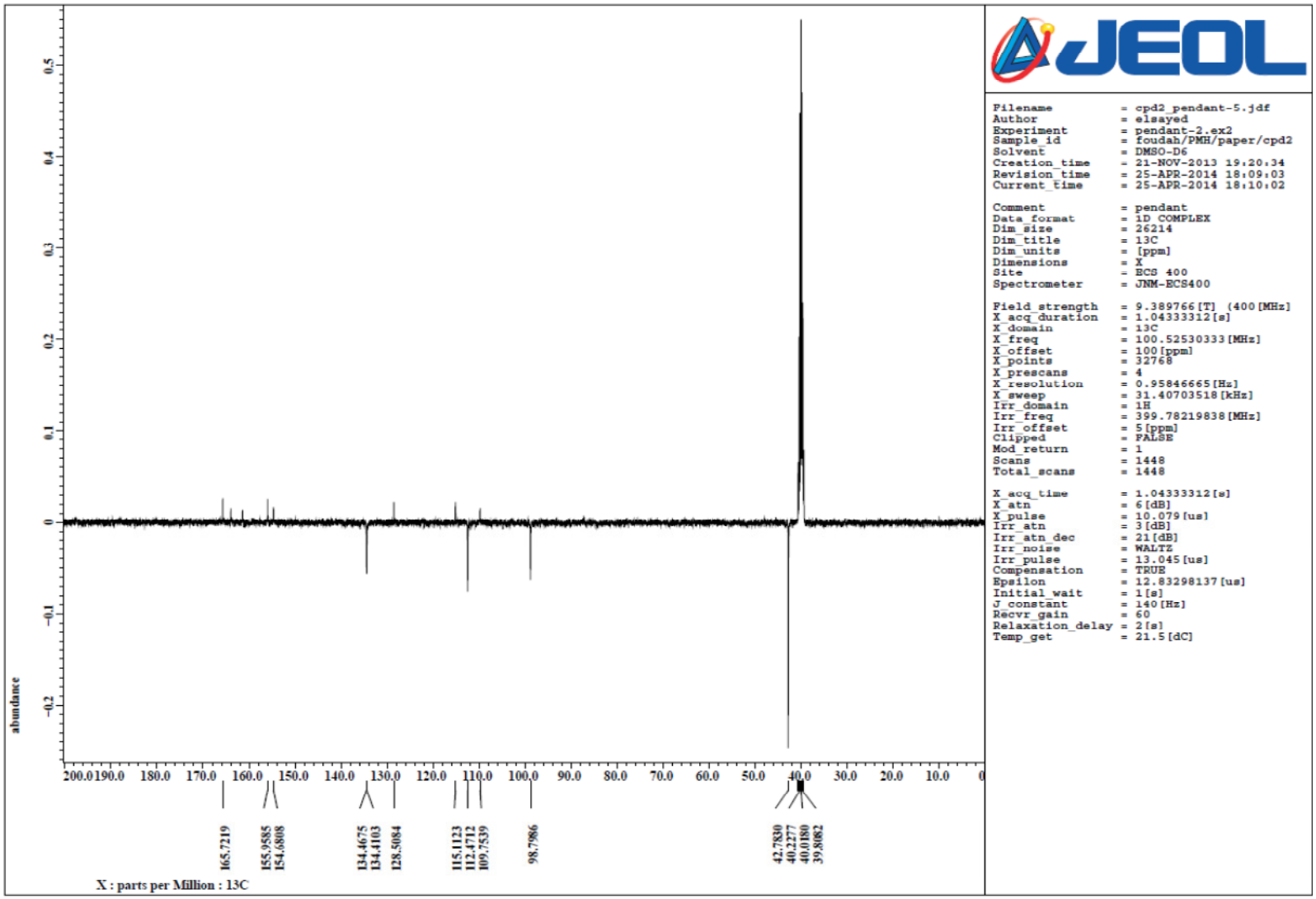

Figure SI4. ^{13}C NMR (PENDANT) Spectrum of **4**.

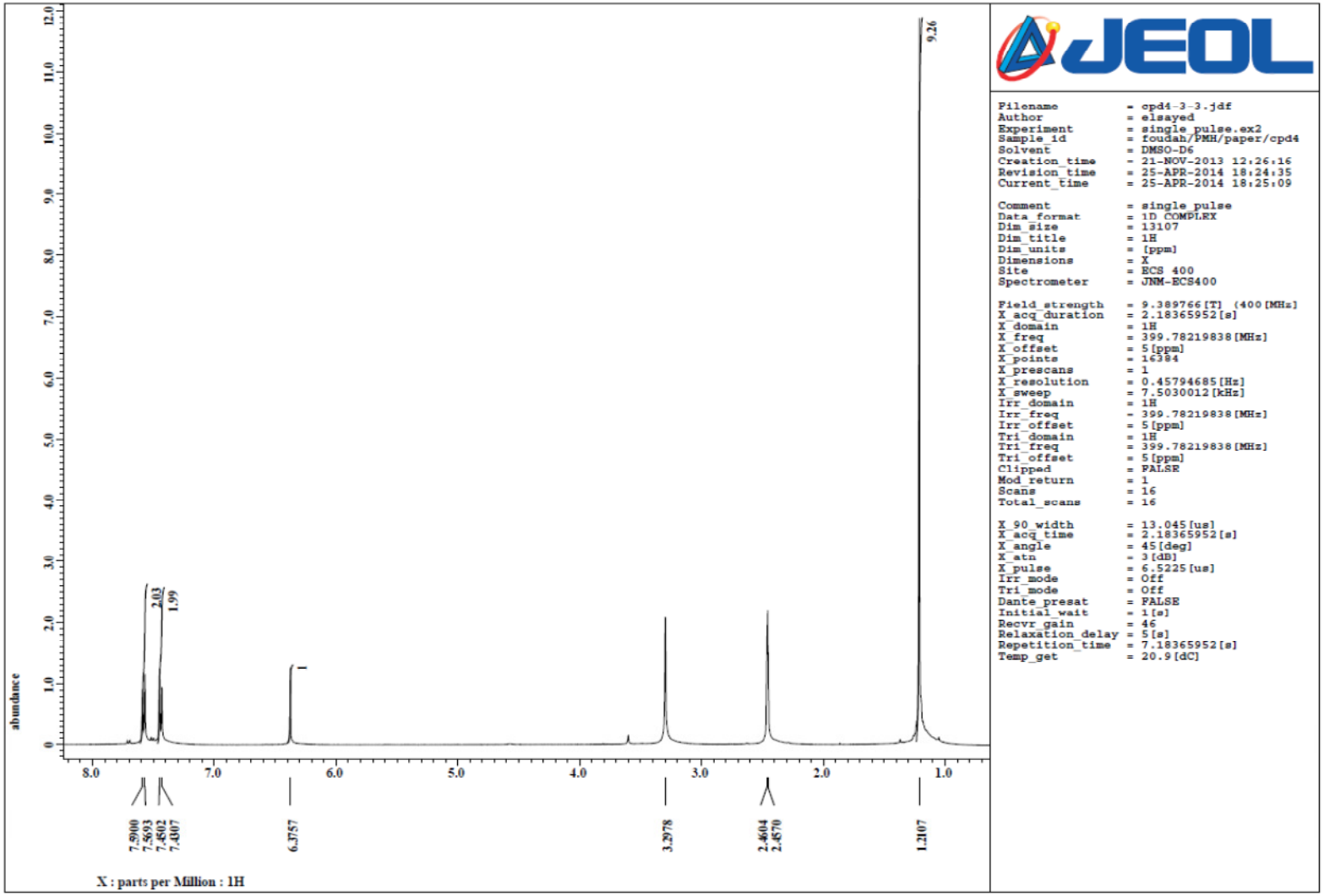

Figure SI5. ^{1}H NMR Spectrum of **5**.

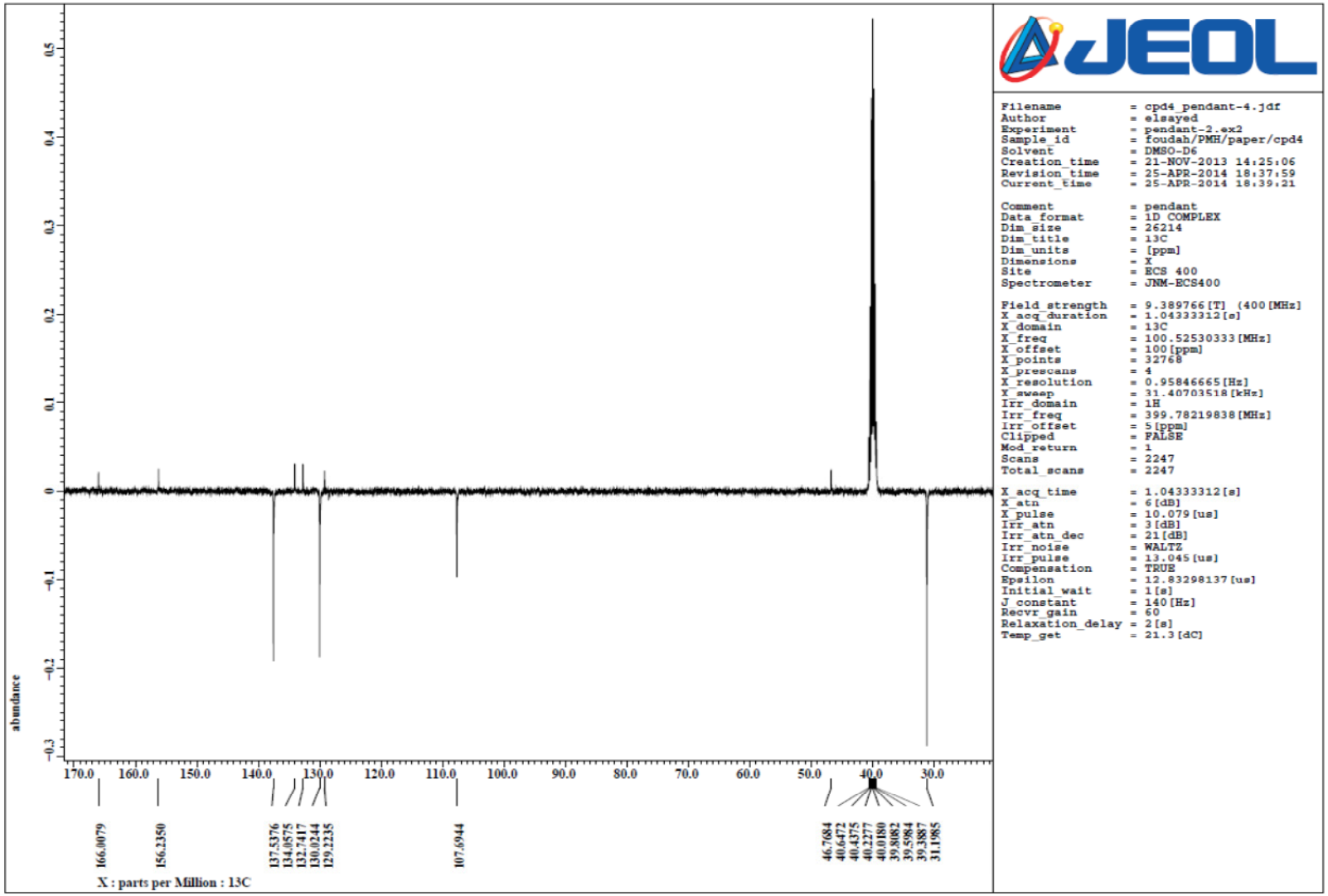

Figure SI6. ^{13}C NMR (PENDANT) Spectrum of **5**.

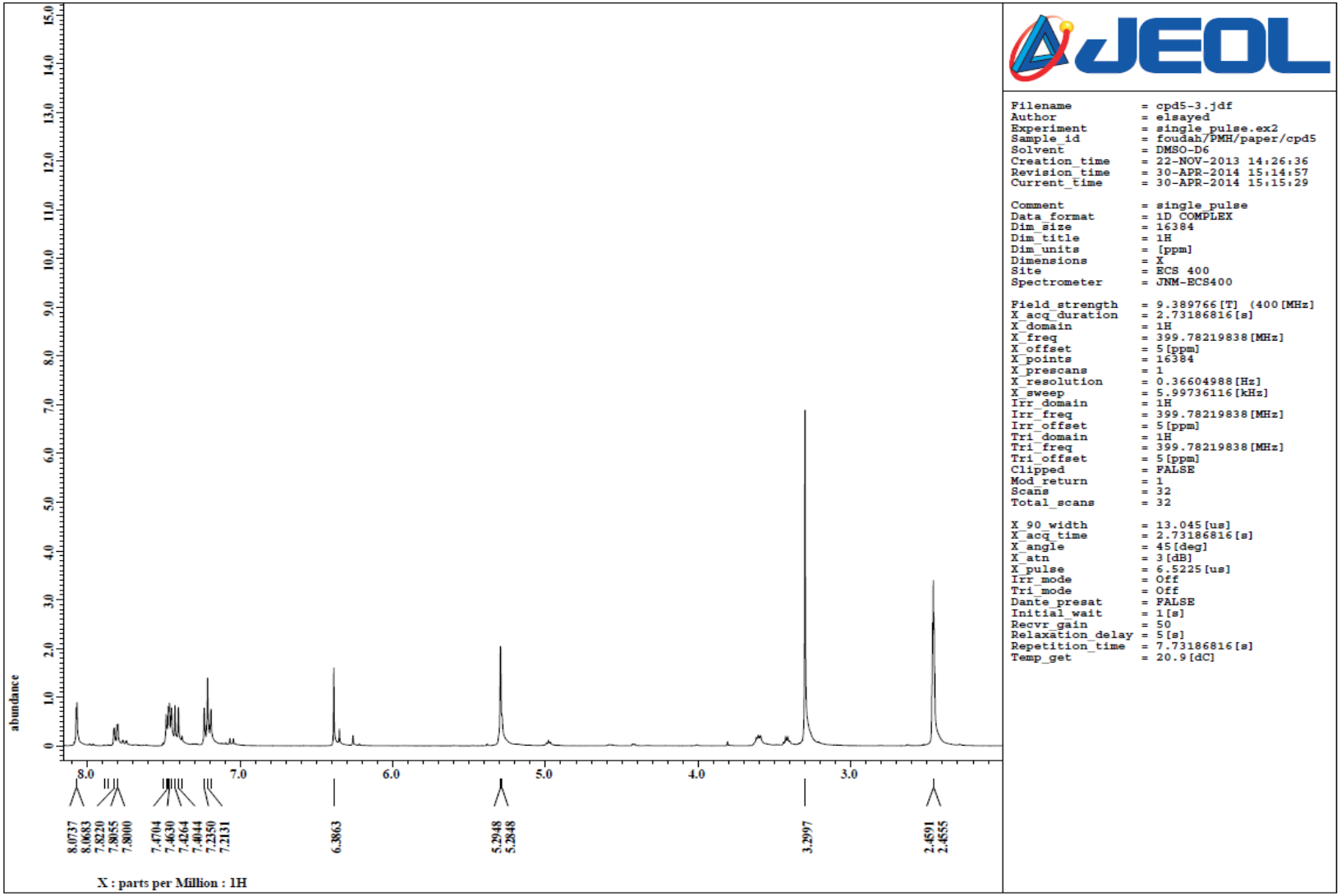

Figure SI7. ^{1}H NMR Spectrum of **6**.

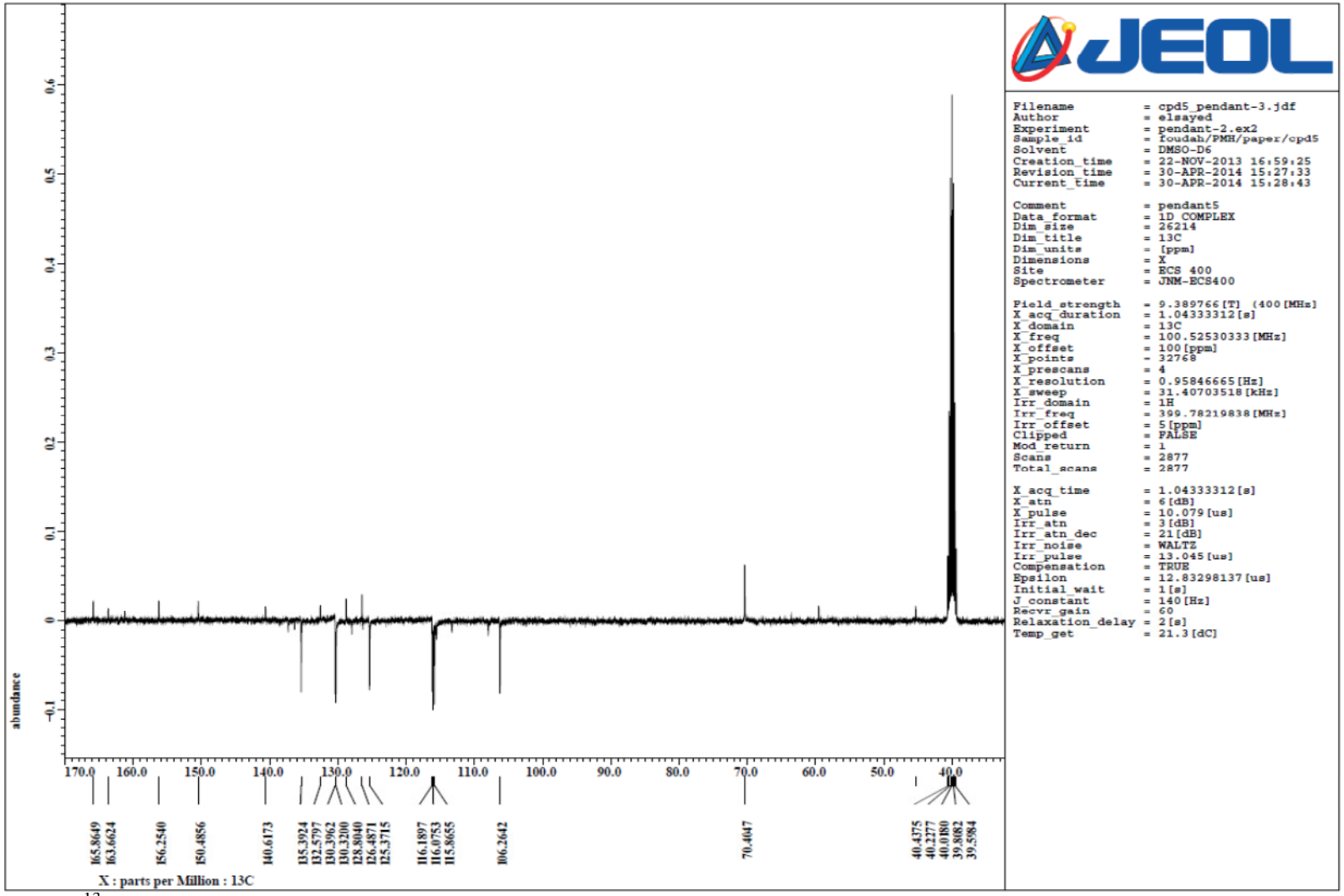

Figure SI8. ^{13}C NMR (PENDANT) Spectrum of **6**.

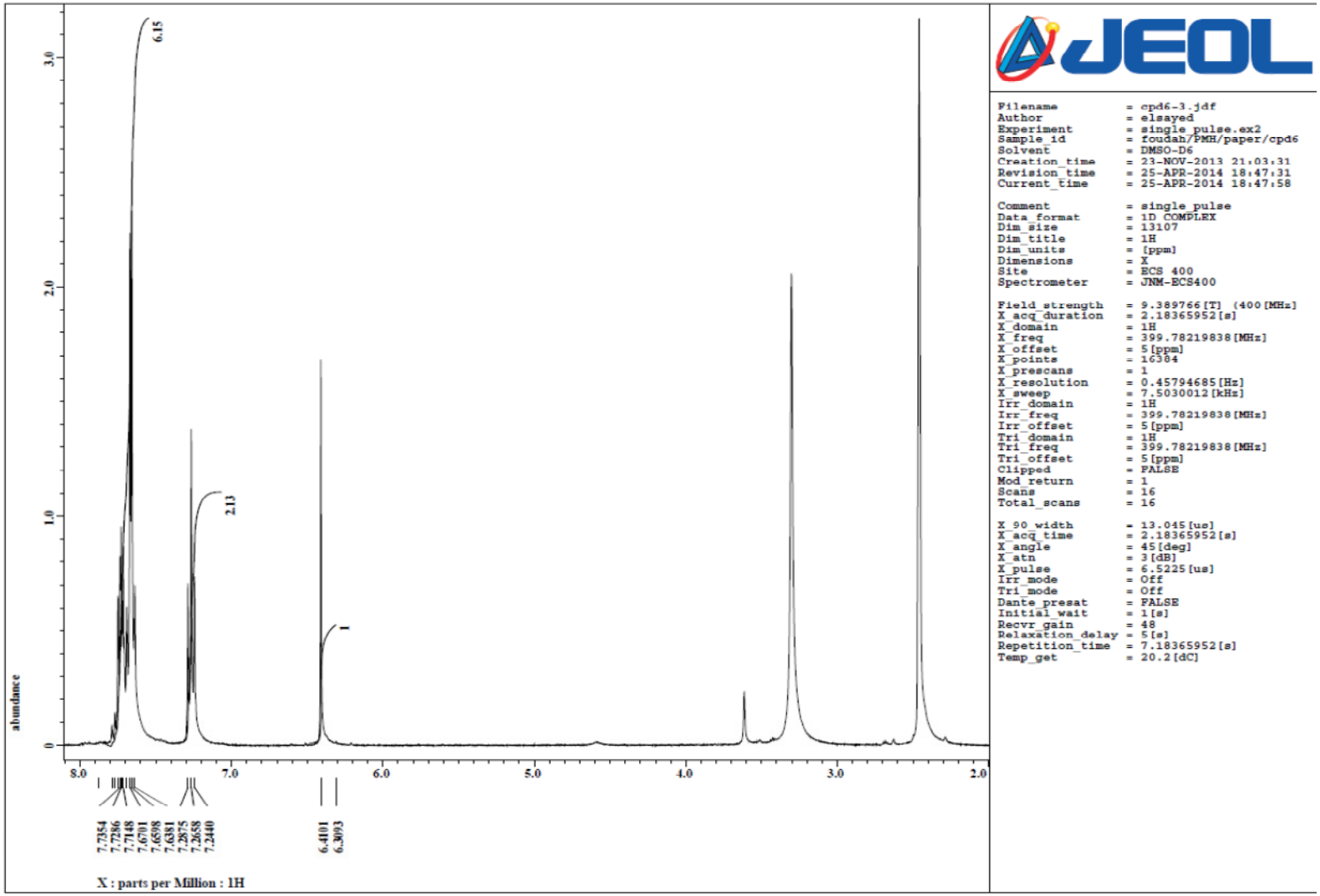

Figure SI9. [1]H NMR Spectrum of **7**.

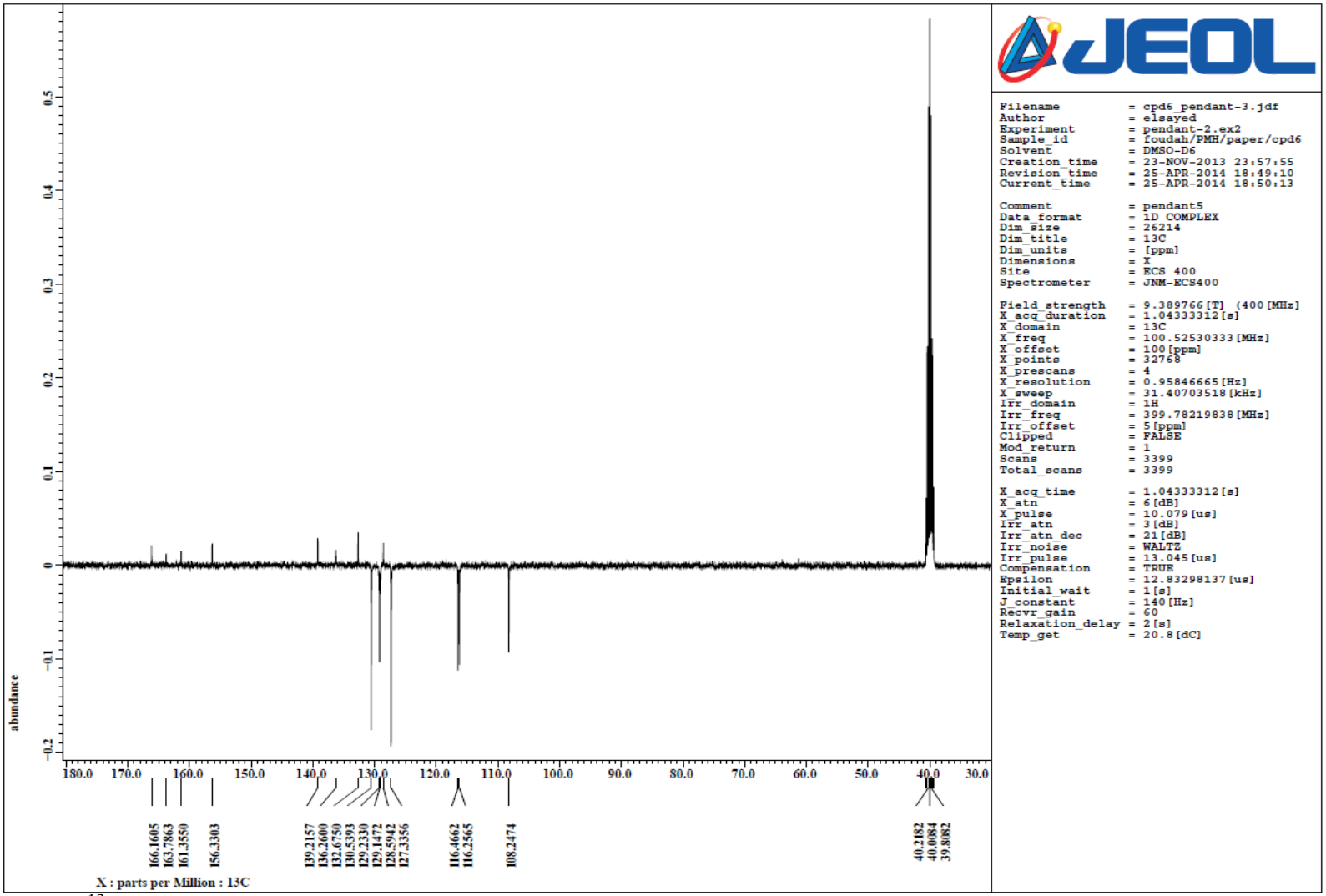

Figure SI10. ^{13}C NMR (PENDANT) Spectrum of **7**.

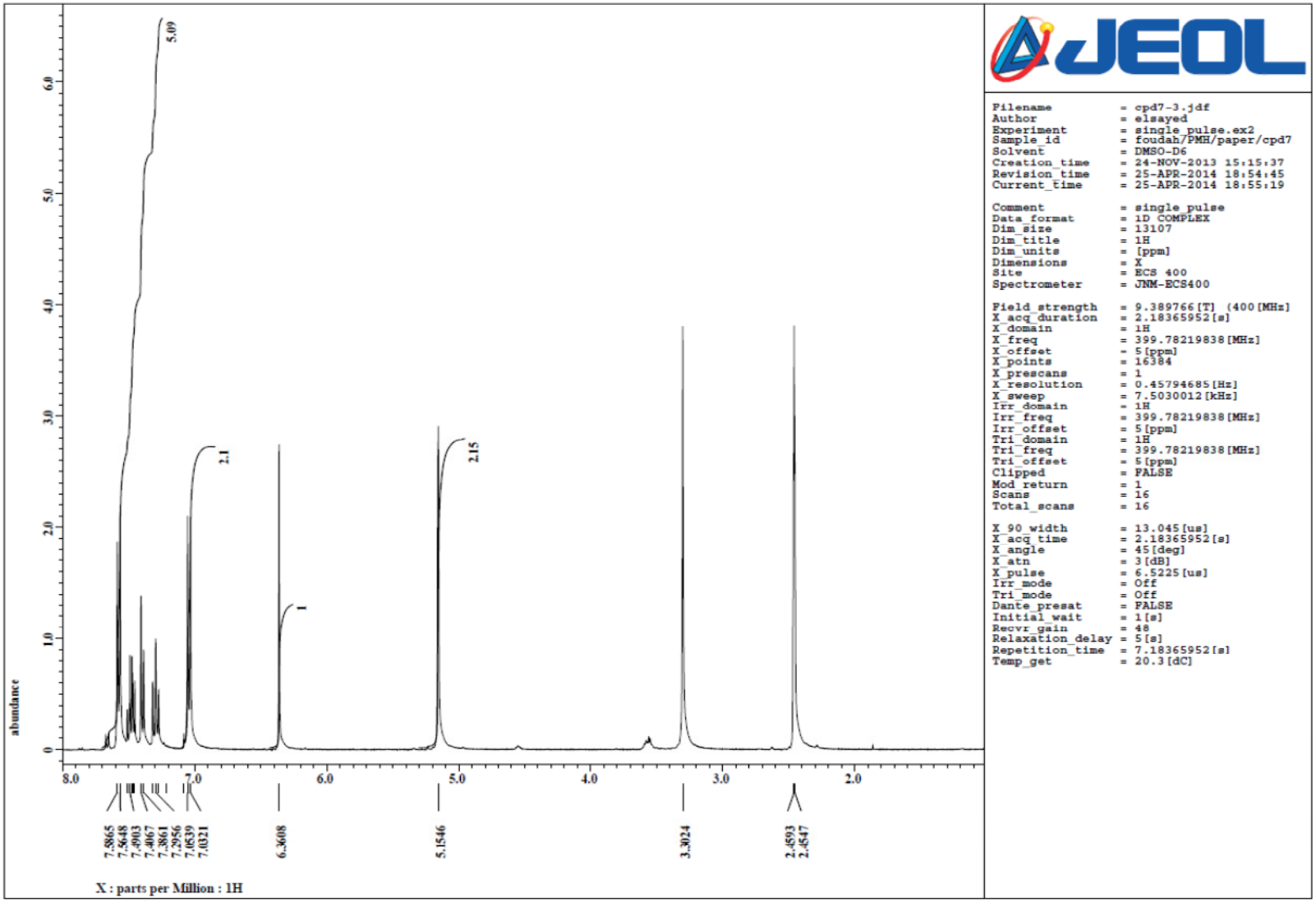

Figure SI11. ^{1}H NMR Spectrum of **8**.

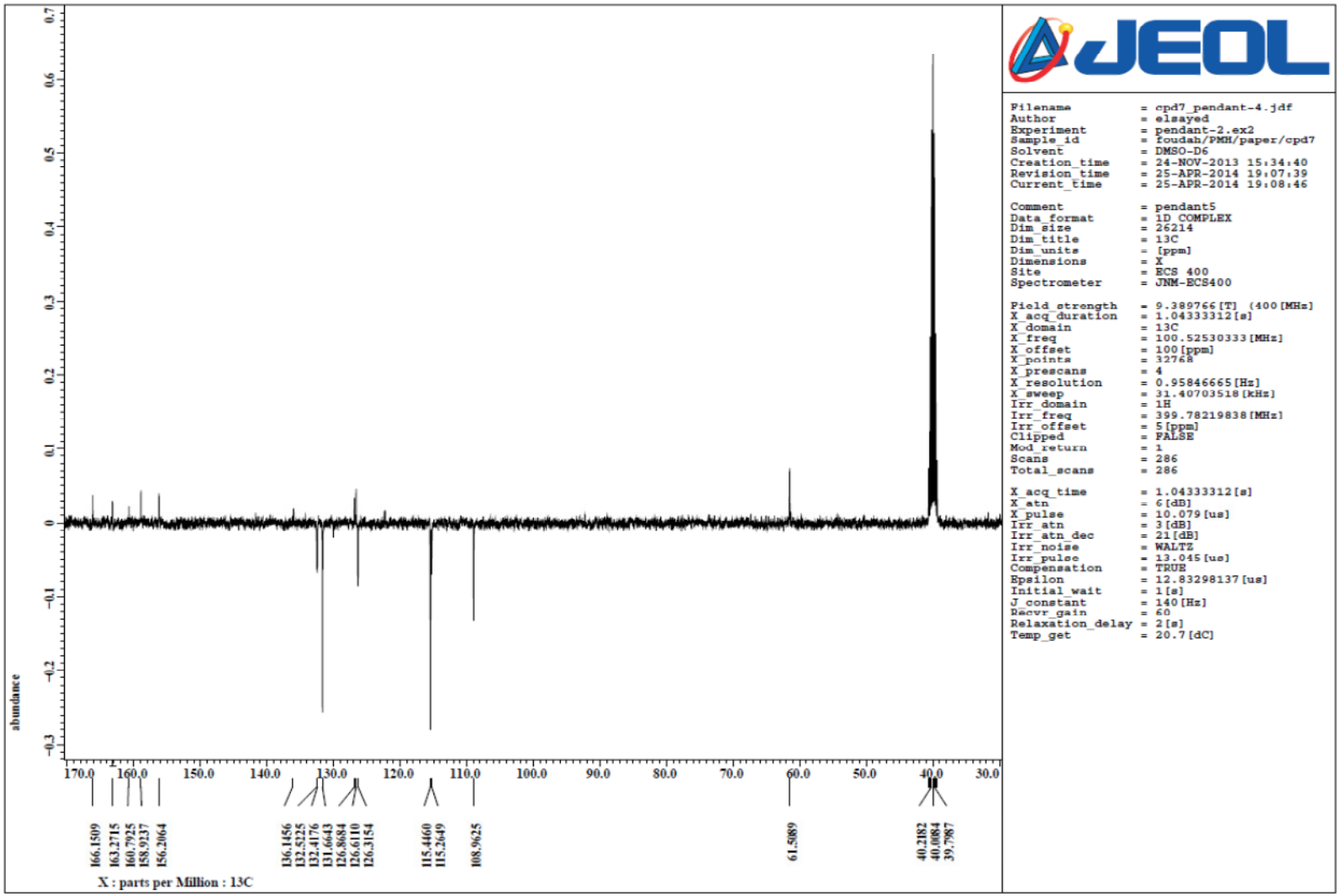

Figure SI12. ^{13}C NMR (PENDANT) Spectrum of **8**.

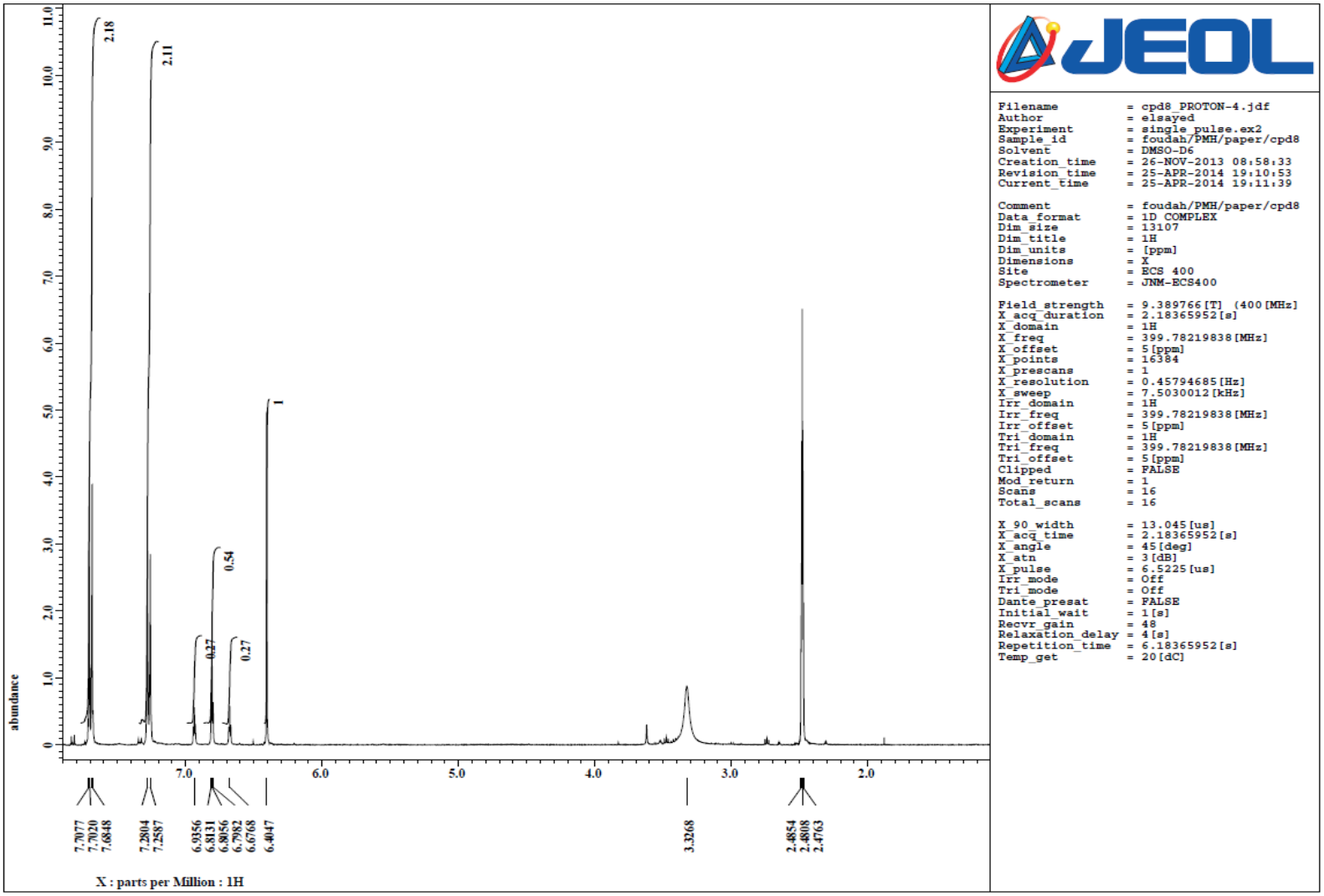

Figure SI13. ^{1}H NMR Spectrum of **9**.

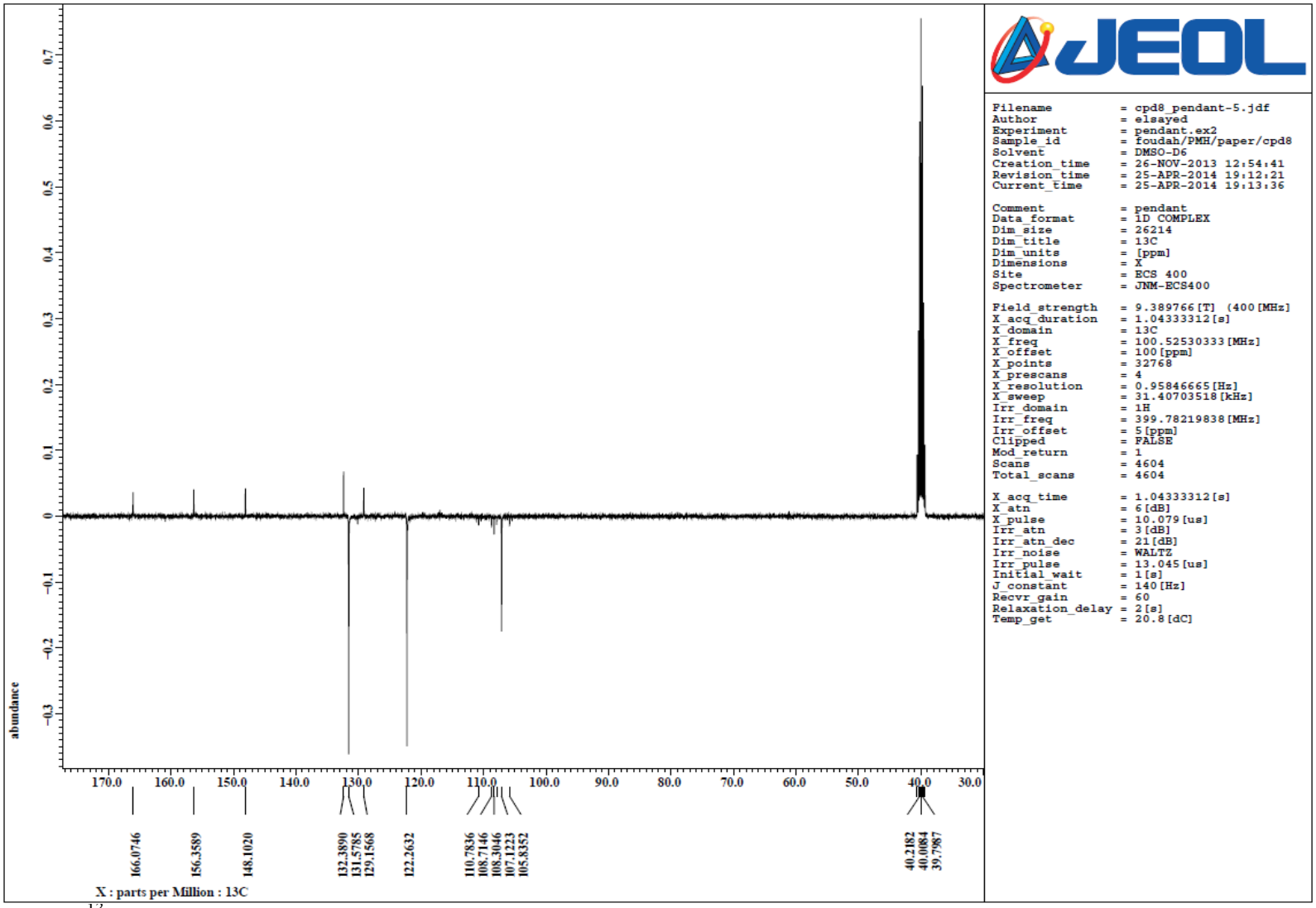

Figure SI14. ^{13}C NMR (PENDANT) Spectrum of **9**.

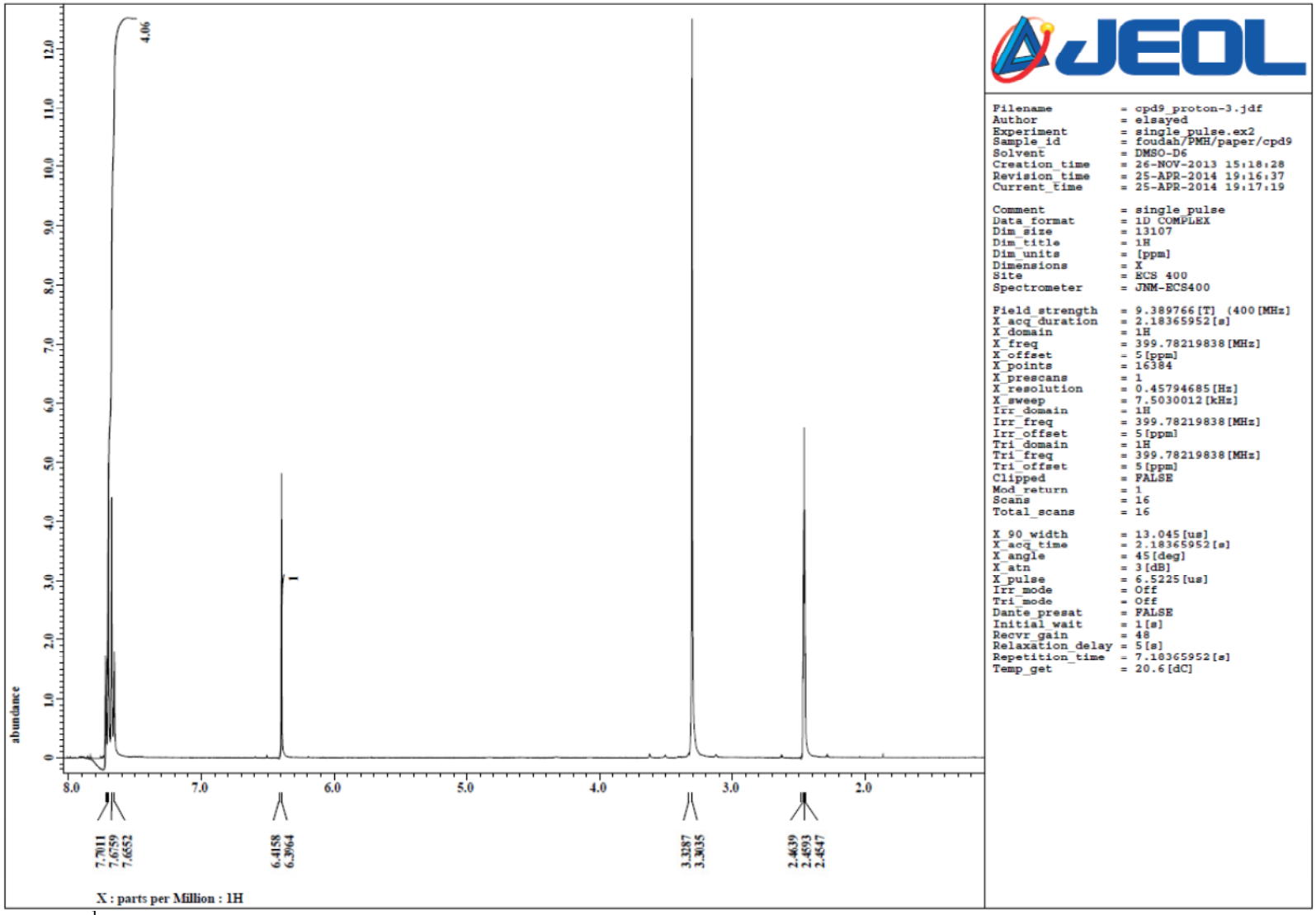

Figure SI15. ^{1}H NMR Spectrum of **10**.

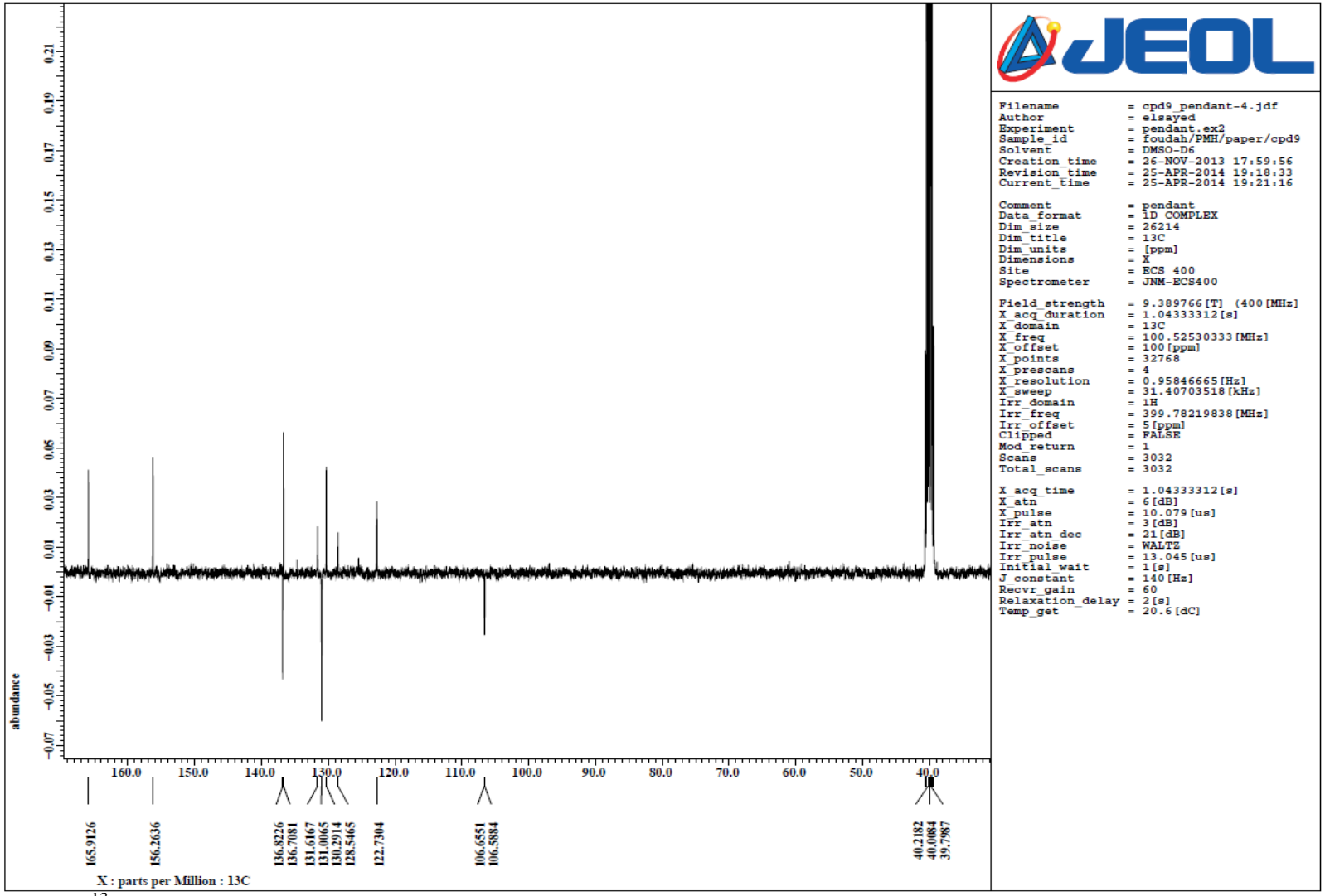

Figure SI16. ^{13}C NMR (PENDANT) Spectrum of **10**.

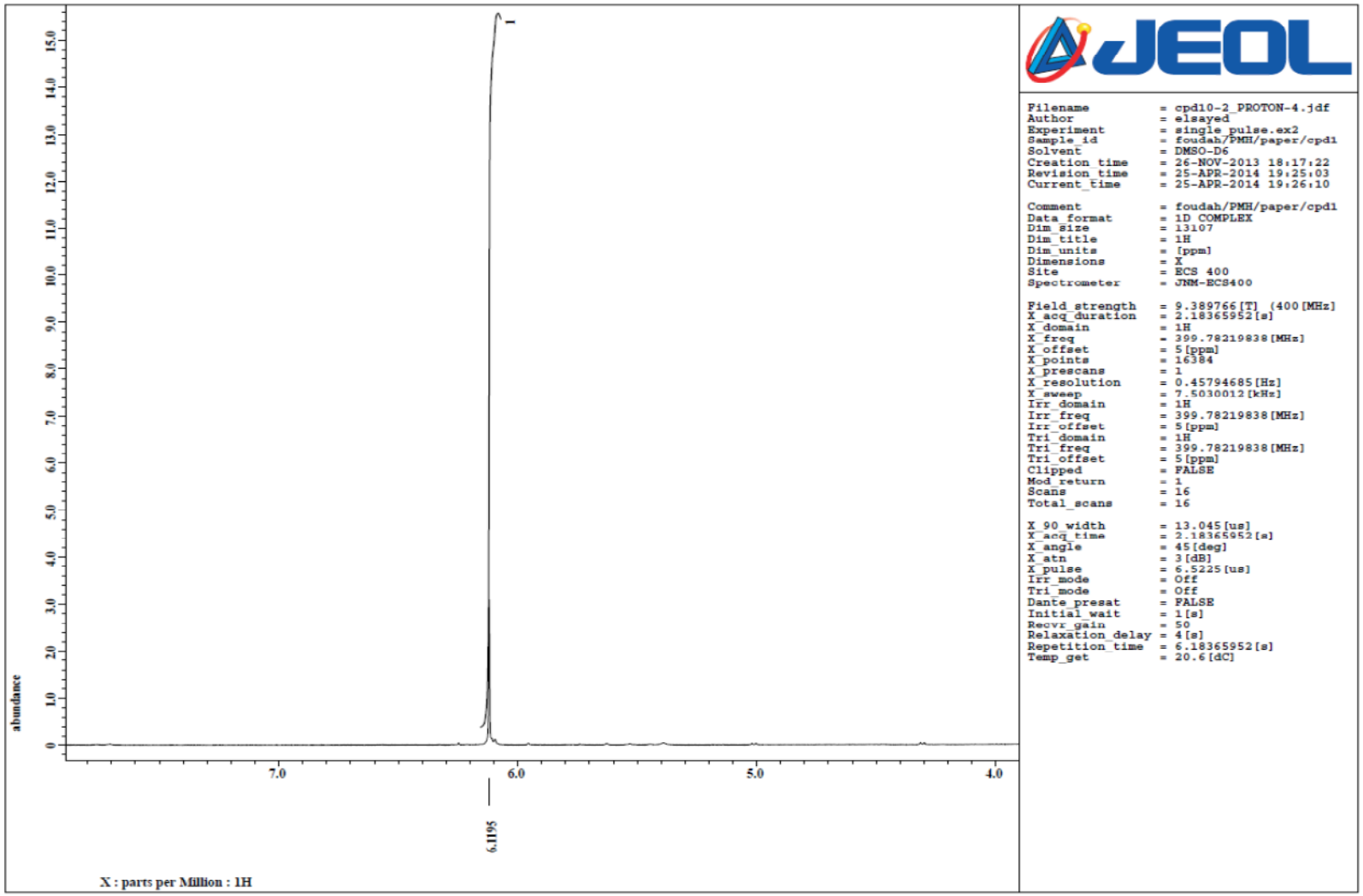

Figure SI17. ^{1}H NMR Spectrum of **11**.

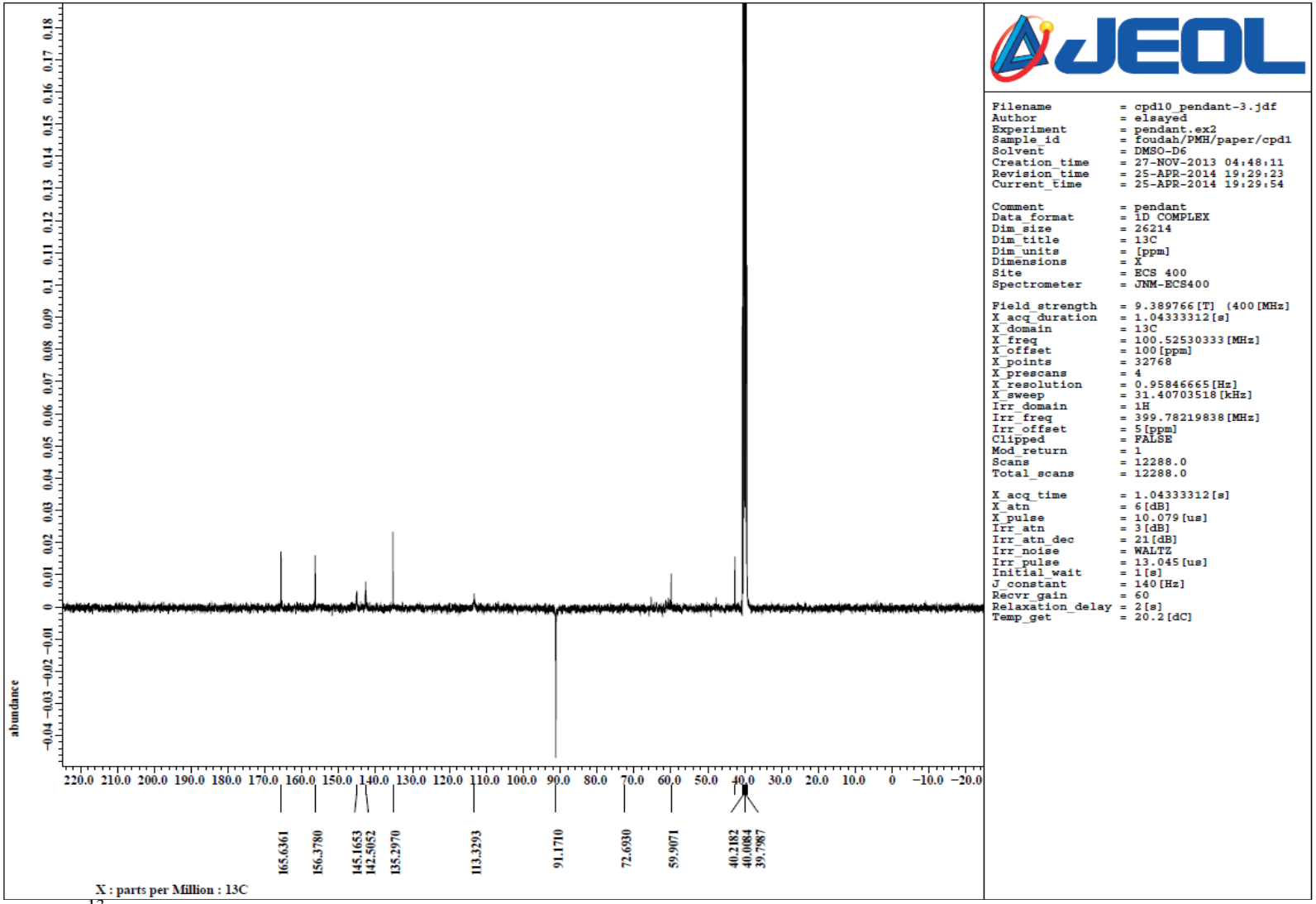

Figure SI18. ^{13}C NMR (PENDANT) Spectrum of **11**.

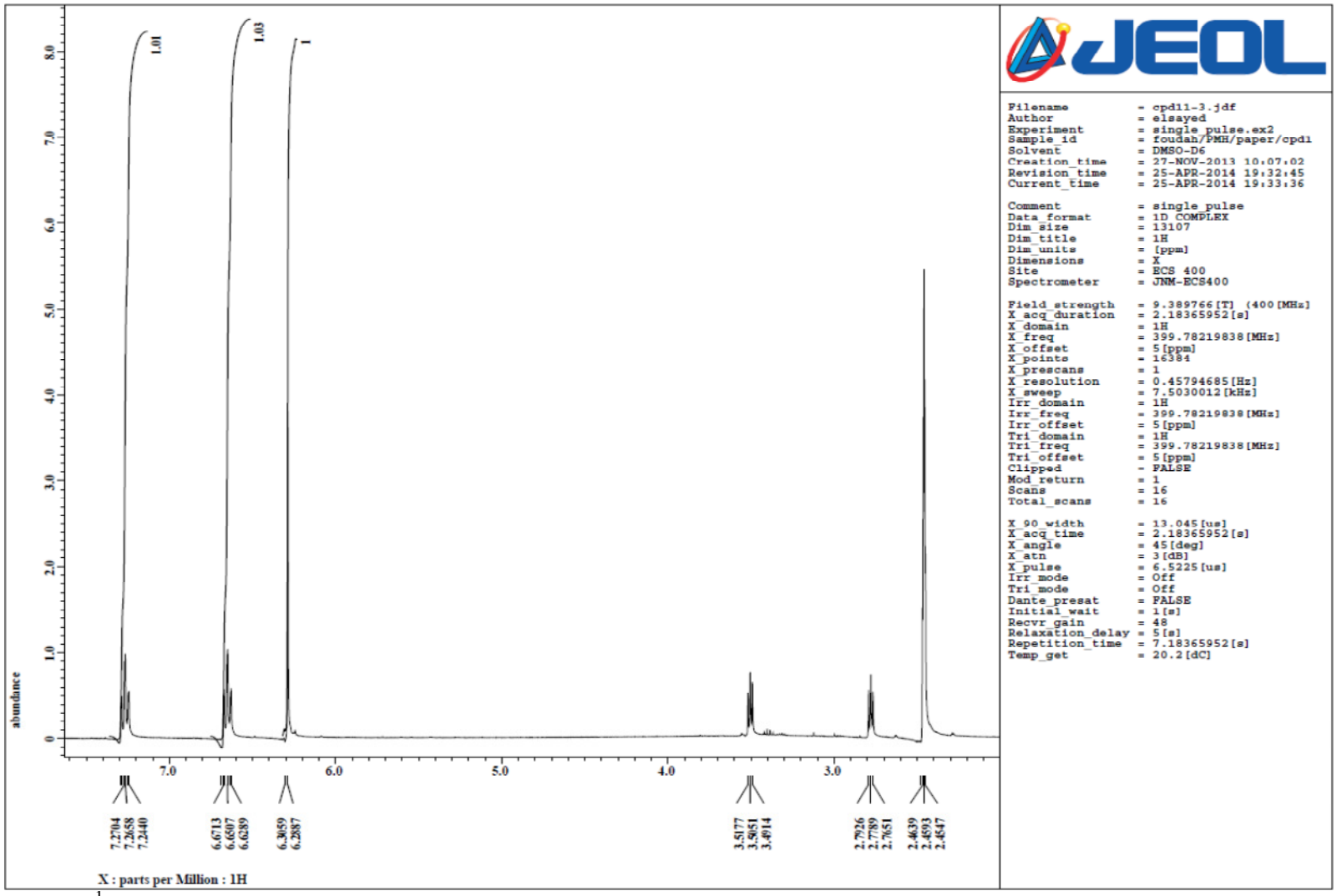

Figure SI19. ^{1}H NMR Spectrum of **12**.

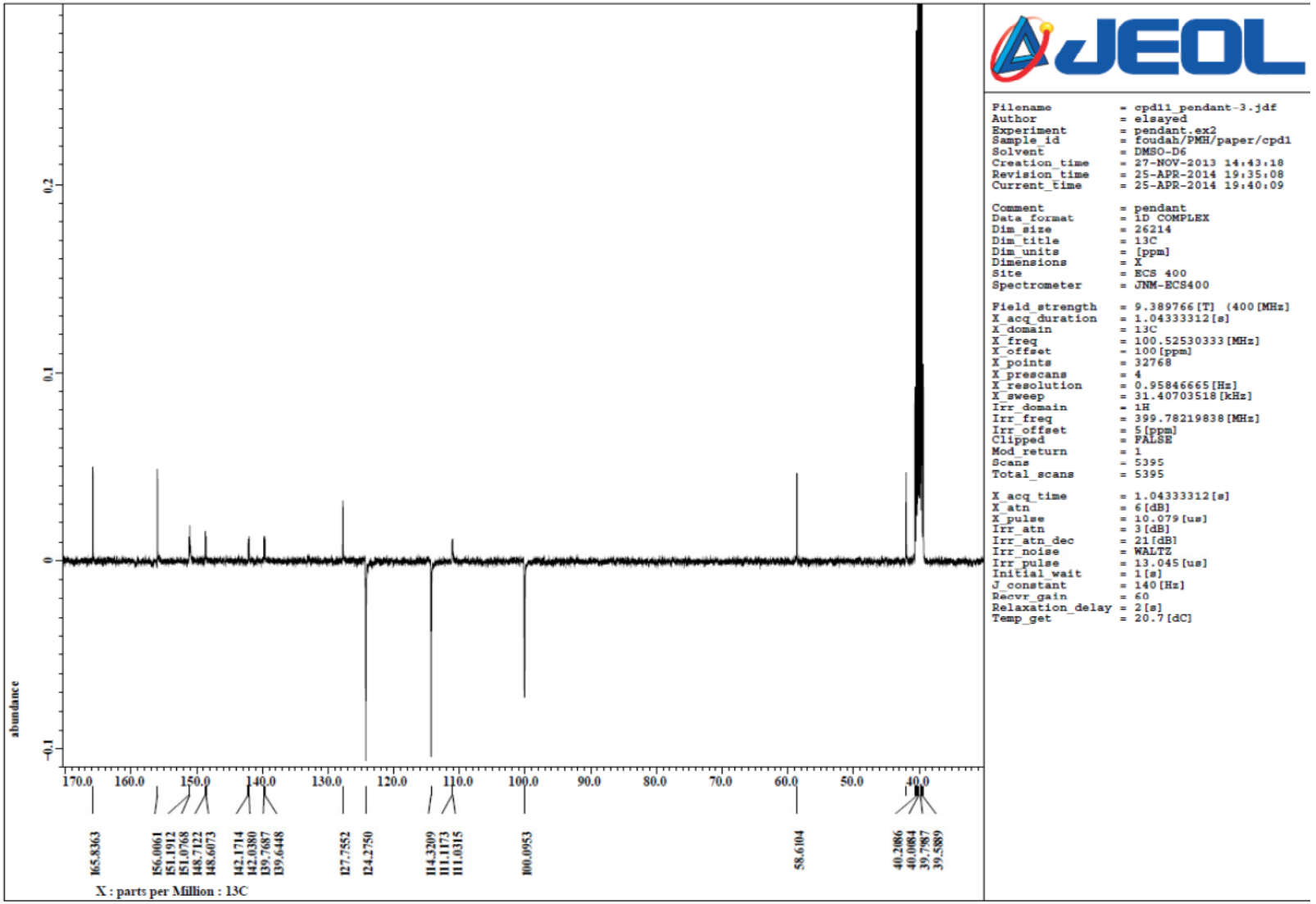

Figure SI20. ^{13}C NMR (PENDANT) Spectrum of **12**.

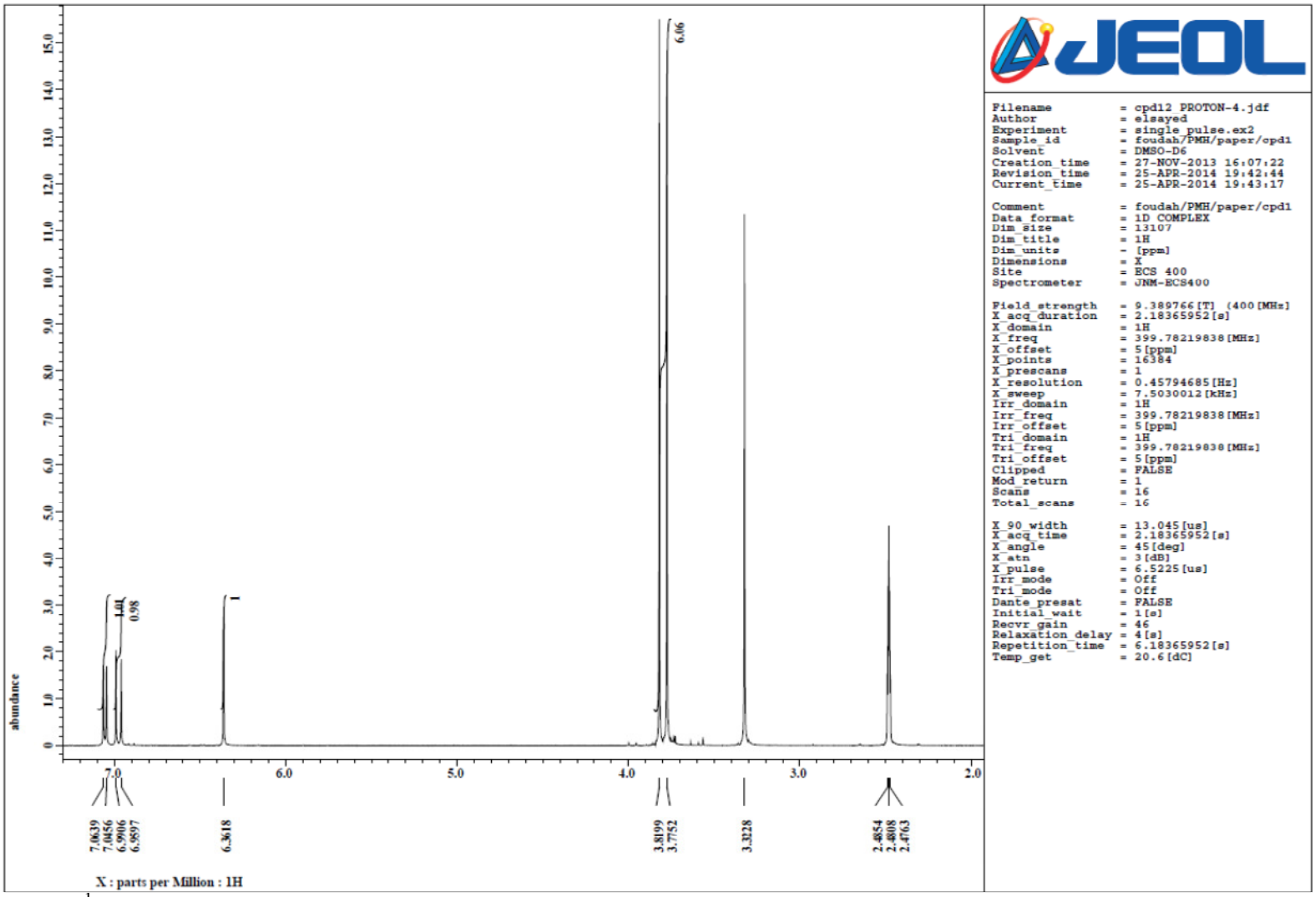

Figure SI21. [1]H NMR Spectrum of **13**.

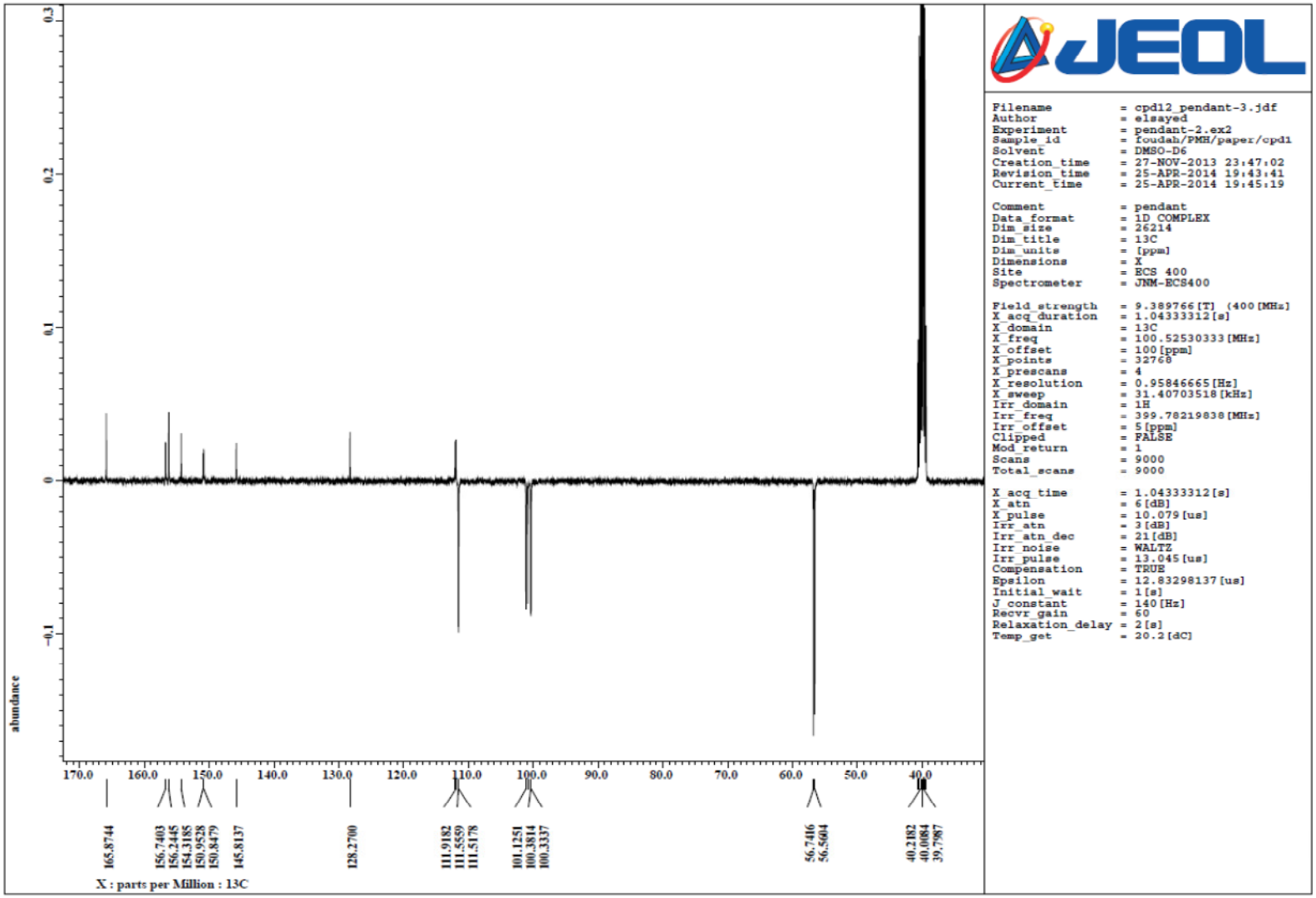

Figure SI22. ^{13}C NMR (PENDANT) Spectrum of **13**.