ELECTRONIC SUPPLEMENTARY INFORMATION

Adamantane Derivatives of Sulfonamide Molecular Crystals: Structure, Sublimation Thermodynamic Characteristics, Molecular Packing, Hydrogen Bonds Networks

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Table 1ESI. Temperature Dependencies of Saturation Vapor Pressure of the Compounds Studied

1[a]		**2**[b]		**3**[c]		**4**[d]		**6**[e]		**7**[f]	
t [°C]	*P* [Pa]	t [°C]	*P* [Pa]	t [°C]	*P* [Pa]	t [°C]	*P* [Pa]	t [°C]	*P* [Pa]	t [°C]	*P* [Pa]
93.2	$2.58 \cdot 10^{-2}$	90.3	$1.60 \cdot 10^{-2}$	114.3	$4.74 \cdot 10^{-2}$	105.5	$1.10 \cdot 10^{-2}$	90.5	$1.87 \cdot 10^{-2}$	102.0	$4.18 \cdot 10^{-2}$
94.5	$3.04 \cdot 10^{-2}$	94.4	$2.40 \cdot 10^{-2}$	116.4	$5.67 \cdot 10^{-2}$	108.0	$1.50 \cdot 10^{-2}$	94.0	$2.75 \cdot 10^{-2}$	105.0	$5.16 \cdot 10^{-2}$
95.9	$3.50 \cdot 10^{-2}$	98.4	$4.00 \cdot 10^{-2}$	118.6	$7.81 \cdot 10^{-2}$	113.0	$2.40 \cdot 10^{-2}$	96.2	$3.60 \cdot 10^{-2}$	106.5	$6.19 \cdot 10^{-2}$
97.2	$3.93 \cdot 10^{-2}$	101.5	$5.40 \cdot 10^{-2}$	121.5	$1.09 \cdot 10^{-1}$	117.0	$3.30 \cdot 10^{-2}$	98.0	$4.23 \cdot 10^{-2}$	110.0	$8.13 \cdot 10^{-2}$
98.6	$4.75 \cdot 10^{-2}$	104.3	$6.60 \cdot 10^{-2}$	123.1	$1.26 \cdot 10^{-1}$	120.0	$5.20 \cdot 10^{-2}$	100.0	$4.98 \cdot 10^{-2}$	111.0	$9.70 \cdot 10^{-2}$
101.4	$6.08 \cdot 10^{-2}$	107.5	$8.70 \cdot 10^{-2}$	124.8	$1.59 \cdot 10^{-1}$	126.0	$9.00 \cdot 10^{-2}$	102.5	$6.11 \cdot 10^{-2}$	112.0	$1.03 \cdot 10^{-1}$
102.8	$7.32 \cdot 10^{-2}$	111.5	$1.34 \cdot 10^{-1}$	127.1	$2.04 \cdot 10^{-1}$	128.0	$1.07 \cdot 10^{-1}$	105.0	$7.73 \cdot 10^{-2}$	115.5	$1.45 \cdot 10^{-1}$
104.2	$8.38 \cdot 10^{-2}$	115.5	$1.96 \cdot 10^{-1}$	128.2	$2.35 \cdot 10^{-1}$	131.5	$1.22 \cdot 10^{-1}$	108.0	$1.02 \cdot 10^{-1}$	118.0	$1.63 \cdot 10^{-1}$
105.6	$9.06 \cdot 10^{-2}$	119.5	$3.13 \cdot 10^{-1}$	129.4	$2.47 \cdot 10^{-1}$	136.0	$1.89 \cdot 10^{-1}$	110.0	$1.37 \cdot 10^{-1}$	121.0	$2.26 \cdot 10^{-1}$
107.1	$1.06 \cdot 10^{-1}$	124.0	$4.18 \cdot 10^{-1}$	132.4	$3.50 \cdot 10^{-1}$	138.0	$2.35 \cdot 10^{-1}$	112.0	$1.54 \cdot 10^{-1}$	121.5	$2.41 \cdot 10^{-1}$
108.5	$1.27 \cdot 10^{-1}$	128.0	$5.98 \cdot 10^{-1}$	133.9	$4.11 \cdot 10^{-1}$	143.0	$3.64 \cdot 10^{-1}$	114.0	$2.01 \cdot 10^{-1}$	124.0	$2.71 \cdot 10^{-1}$
110.0	$1.51 \cdot 10^{-1}$	132.5	$8.85 \cdot 10^{-1}$	135.6	$5.17 \cdot 10^{-1}$	146.0	$5.18 \cdot 10^{-1}$	116.0	$2.38 \cdot 10^{-1}$	126.0	$3.45 \cdot 10^{-1}$
111.5	$1.73 \cdot 10^{-1}$			137.8	$6.77 \cdot 10^{-1}$	147.5	$5.61 \cdot 10^{-1}$	118.3	$2.84 \cdot 10^{-1}$	128.0	$3.76 \cdot 10^{-1}$
113.0	$1.94 \cdot 10^{-1}$			139.9	$7.63 \cdot 10^{-1}$	153.0	$7.70 \cdot 10^{-1}$				
114.4	$2.27 \cdot 10^{-1}$			142.3	1.01	155.0	$9.89 \cdot 10^{-1}$				
116.0	$2.47 \cdot 10^{-1}$			144.6	1.34	162.0	$15.3 10^{-1}$				
117.5	$2.97 \cdot 10^{-1}$										
119.0	$3.44 \cdot 10^{-1}$										
120.6	$4.02 \cdot 10^{-1}$										

[a] $\ln(P[\mathrm{Pa}]) = (35.5 \pm 0.3) - (14322 \pm 98)/T$; $\sigma = 2.5 \cdot 10^{-2}$; r = 0.9997; F = 21370; n=19
[b] $\ln(P[\mathrm{Pa}]) = (34.4 \pm 0.4) - (14012 \pm 149)/T$; $\sigma = 4.5 \cdot 10^{-2}$; r = 0.9993; F = 8836; n=12
[c] $\ln(P[\mathrm{Pa}]) = (42.9 \pm 0.4) - (17808 \pm 151)/T$; $\sigma = 3.4 \cdot 10^{-2}$; r = 0.9996; F = 13902; n=16
[d] $\ln(P[\mathrm{Pa}]) = (33.7 \pm 0.4) - (14449 \pm 171)/T$; $\sigma = 7.0 \cdot 10^{-2}$; r = 0.9989; F = 7149; n=16
[e] $\ln(P[\mathrm{Pa}]) = (34.2 \pm 0.5) - (13875 \pm 193)/T$; $\sigma = 4.17 \cdot 10^{-2}$; r = 0.9986; F = 5182; n=13
[f] $\ln(P[\mathrm{Pa}]) = (31.7 \pm 0.6) - (13089 \pm 217)/T$; $\sigma = 4.19 \cdot 10^{-2}$; r = 0.9987; F = 3641; n=13

Table 2ESI. Thermodynamic Characteristics of Sublimation and Fusion Processes of Adamantane Derivatives Selected from Literature

Compound	CAS	ΔG_{sub}^{298} [kJ·mol^{-1}]	ΔH_{sub}^{298} [kJ·mol^{-1}]	T_m [K]	ΔH_{fus}^{T} [kJ·mol^{-1}]	Method[a]	Ref
2,2-di-NO_2-adamantane	88381-75-3	38.2	96.4 ± 1.4	491.2 ± 0.2	5.1 ± 0.2	Transpiration	[1]
Adamantan-2-one (phase I)	700-58-3	27.2	66.3 ± 0.8	557.6± 0.2	11.8 ± 0.2	K-E	[2]
1-NO_2-Adamantane	7575-82-8	29.5	63.6 ± 1.0	432.2 ± 0.2	4.2 ± 0.4	Transpiration	[1]
2-NO_2-Adamantane	54564-31-7	36.1	58 ± 2.3	441.7 ± 0.5	4.2 ± 0.2	Transpiration	[1]
Adamantane	281-23-2	21.4 ± 0.4	59.1 ± 0.2	534.3 ± 0.1	14.0 ± 0.3	SM	[3]
2-CN-2-NO_2-Adamantane	128478-71-7	26.9	70.0 ± 1.9	462.2	-	Transpiration	[1]
1-CN-Adamantane	23074-42-2	30.9	67.2 ± 0.8	459 ± 1	-	K-E	[4]
1-Me-Adamantane	768-91-2	-	67.8 ± 1.3	377.2	-	BG	[5]
2-Me-Adamantane	700-56-1	-	68.2 ± 1.2	418.2	-	BG	[5]
1-Adamantyl methyl ketone	1660-04-4	27.4	84.2 ± 0.6	328 ± 1	-	K-E	[6]
2,2-di-Me-Adamantane	19740-34-2	-	73.6 ± 1.3	422.2	-	BG	[5]
1,3-di-Me-Adamantane	702-79-4	-	67.8 ± 1.3	-	-	Ebulliometry	[5]
N,N-dimethyl-1-Adamantylcarboxamide	1502-00-7	37.9	97.5 ± 0.3	350 ± 1	-	K-E	[7]
1,3,5-tri-Me-Adamantane	707-35-7	-	77.8	295.15	-	BG	[5]
1,1-di-Adamantyl ketone	38256-01-8	53.3	109.0 ± 1.8	-	-		[6]
1-Adamantylfluorodiphenylmethane	154393-25-6	57.4	125.9 ± 1.3	405.2 ± 0.2	-	Transpiration	[8]
2-Cl-Adamantane	7346-41-0	24.2	61.5 ± 0.9	467.4 ± 0.2	-	K-E	[9]
1-OH-Adamantane	768-95-6	31.9	85 ± 1	554 ± 2	-	K-E	[10]
2-OH-2-Me-Adamantane	702-98-7	31.8	91.3 ± 0.8	490 ± 1	-	K-E	[10]
1-Br-Adamantane (I)	768-90-1	24.7	63.2 ± 2.1	392	-	K-E	[11]
1-Br-Adamantane (II)	768-90-1	25	71.6 ± 1.1	-	-	K-E	[11]
1-NH_2-Adamantane	768-94-5	22.5	61.7 ± 0.6	-	-	Transpiration	[12]
1-COOH-Adamantane	828-51-3	-	98.7 ± 4.5	447.2 ± 0.2	16.2 ± 0.4	DSC	[13]

[a] K-E – Knudsen-Effusion; SM – Static Manometer; BG - Bourdon gauge;

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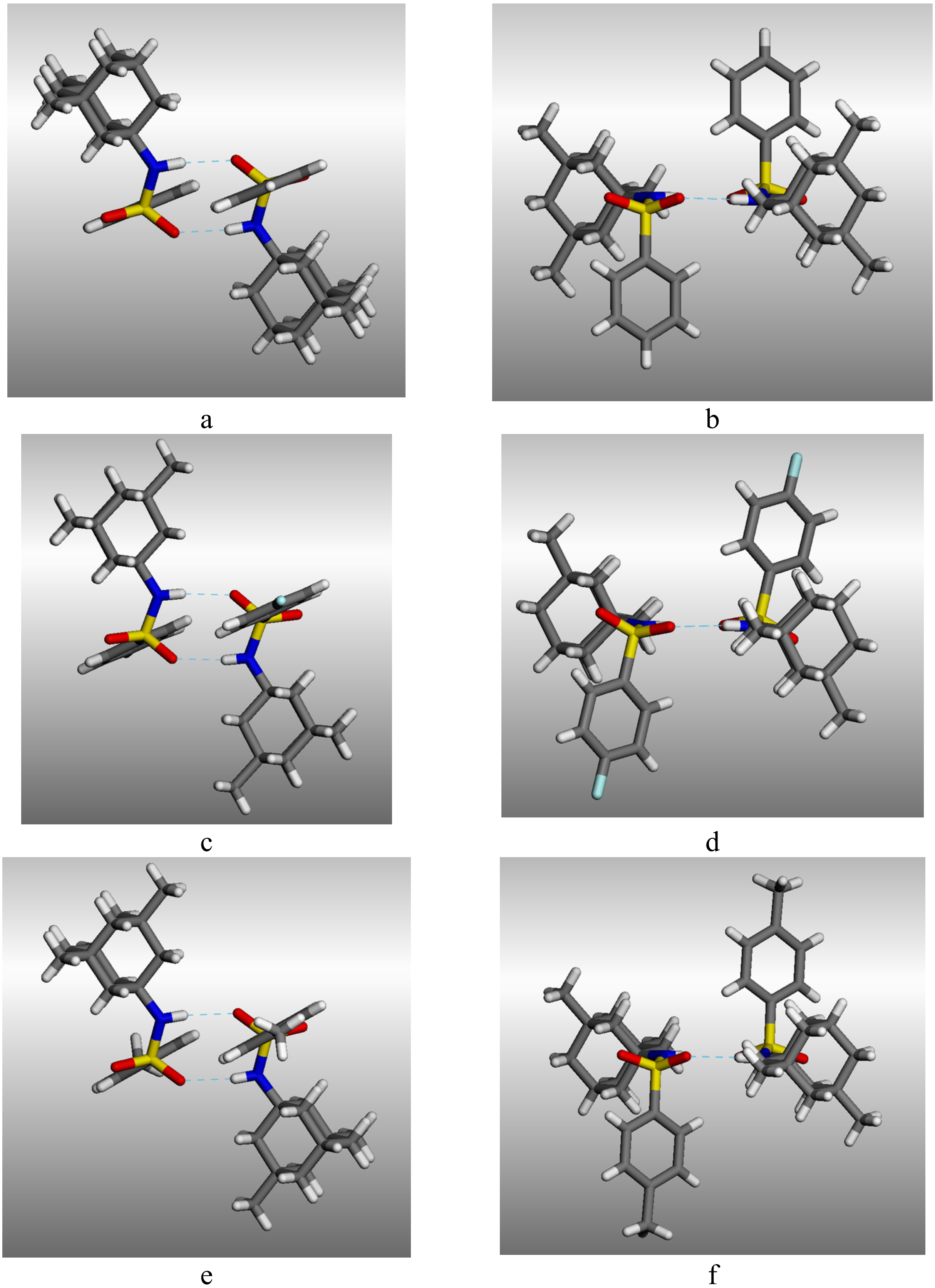

Fig. 1ESI. Dimers projections in two perpendicular planes for compounds **5** (a, b), **6** (c, d), **7** (e, f).

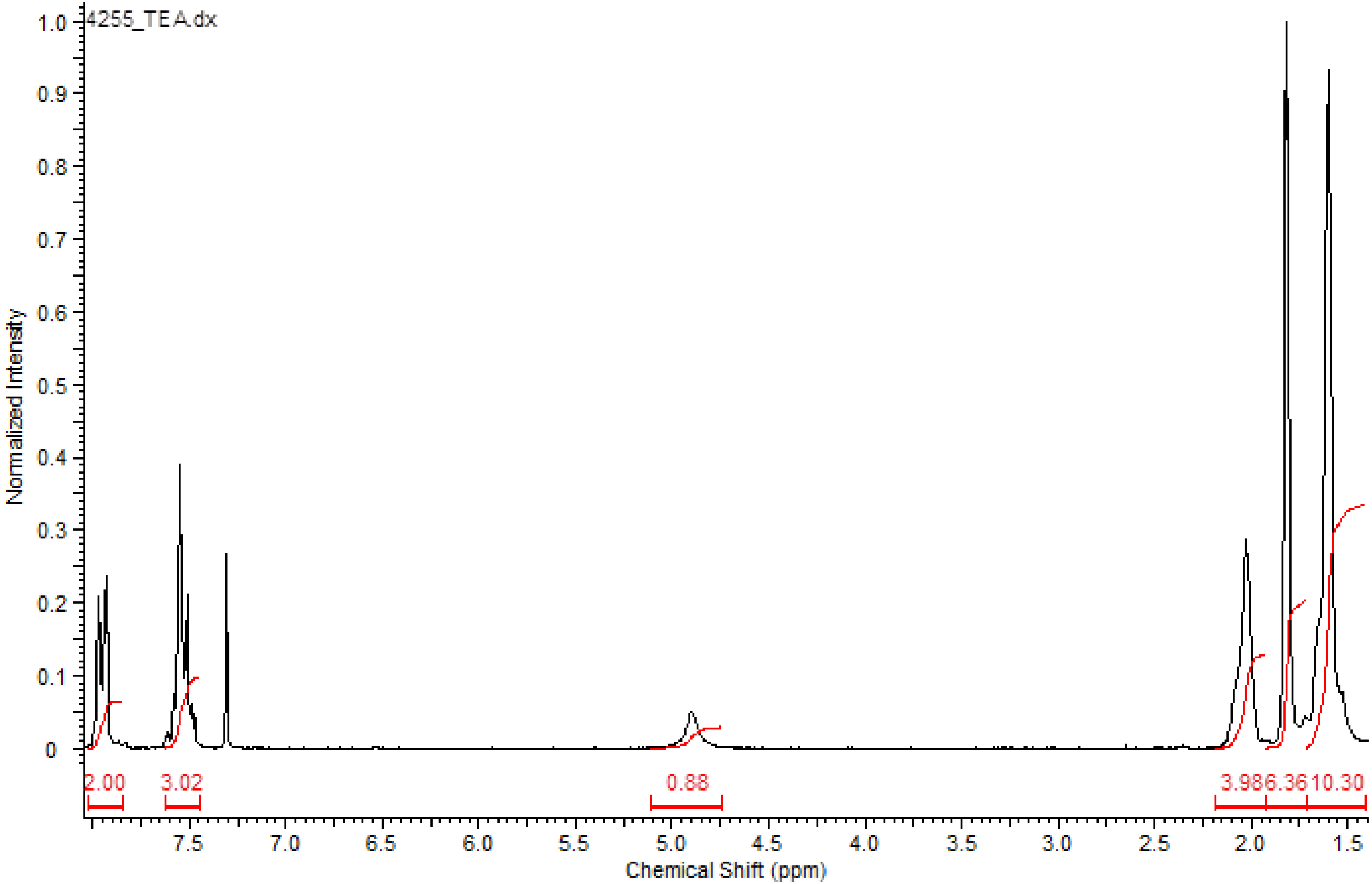

Fig. 2ESI. ^{1}H NMR spectrum of compound (**1**) in $CDCl_3$

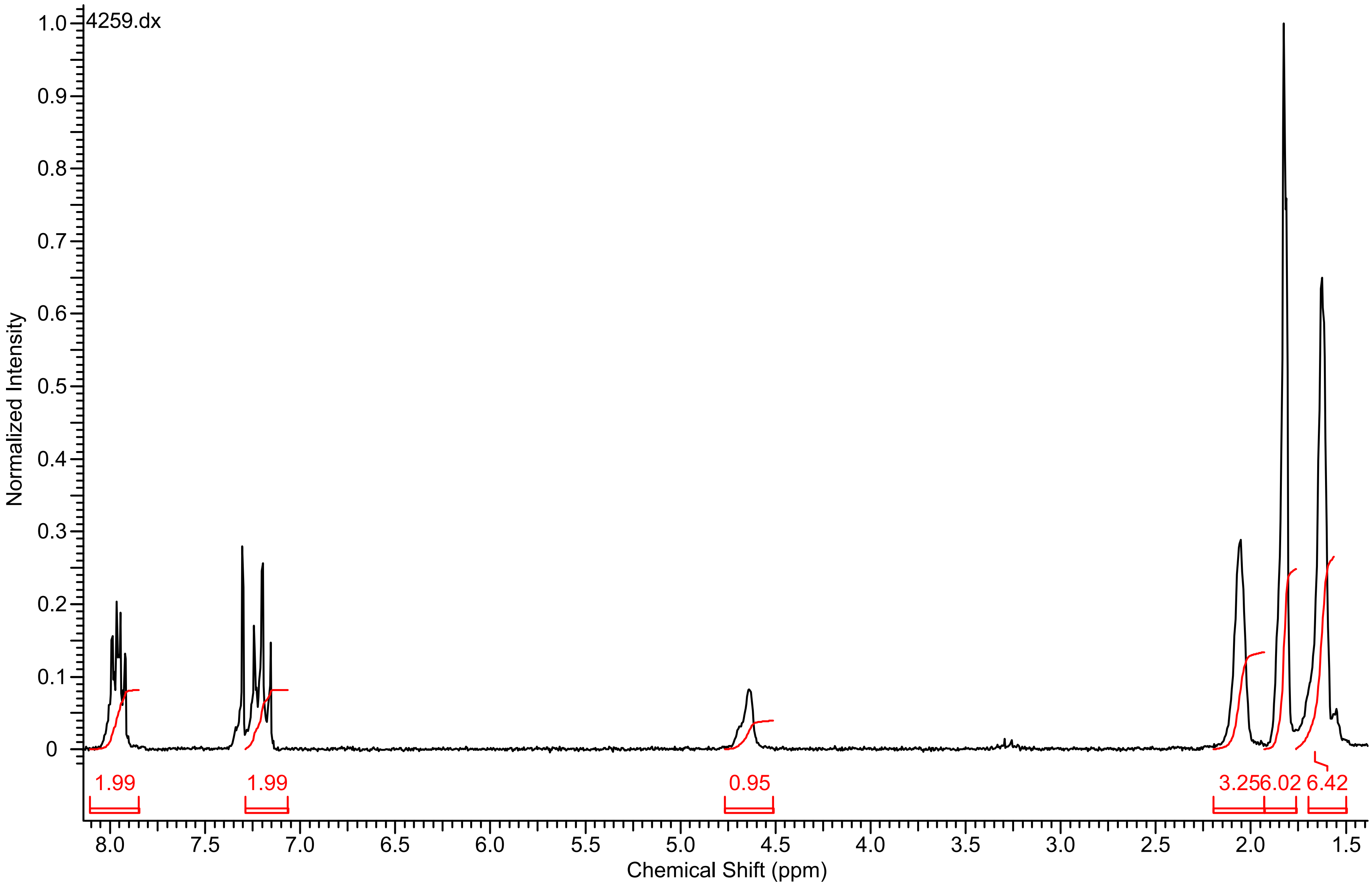

Fig. 3ESI. ^{1}H NMR spectrum of compound (**2**) in $CDCl_3$

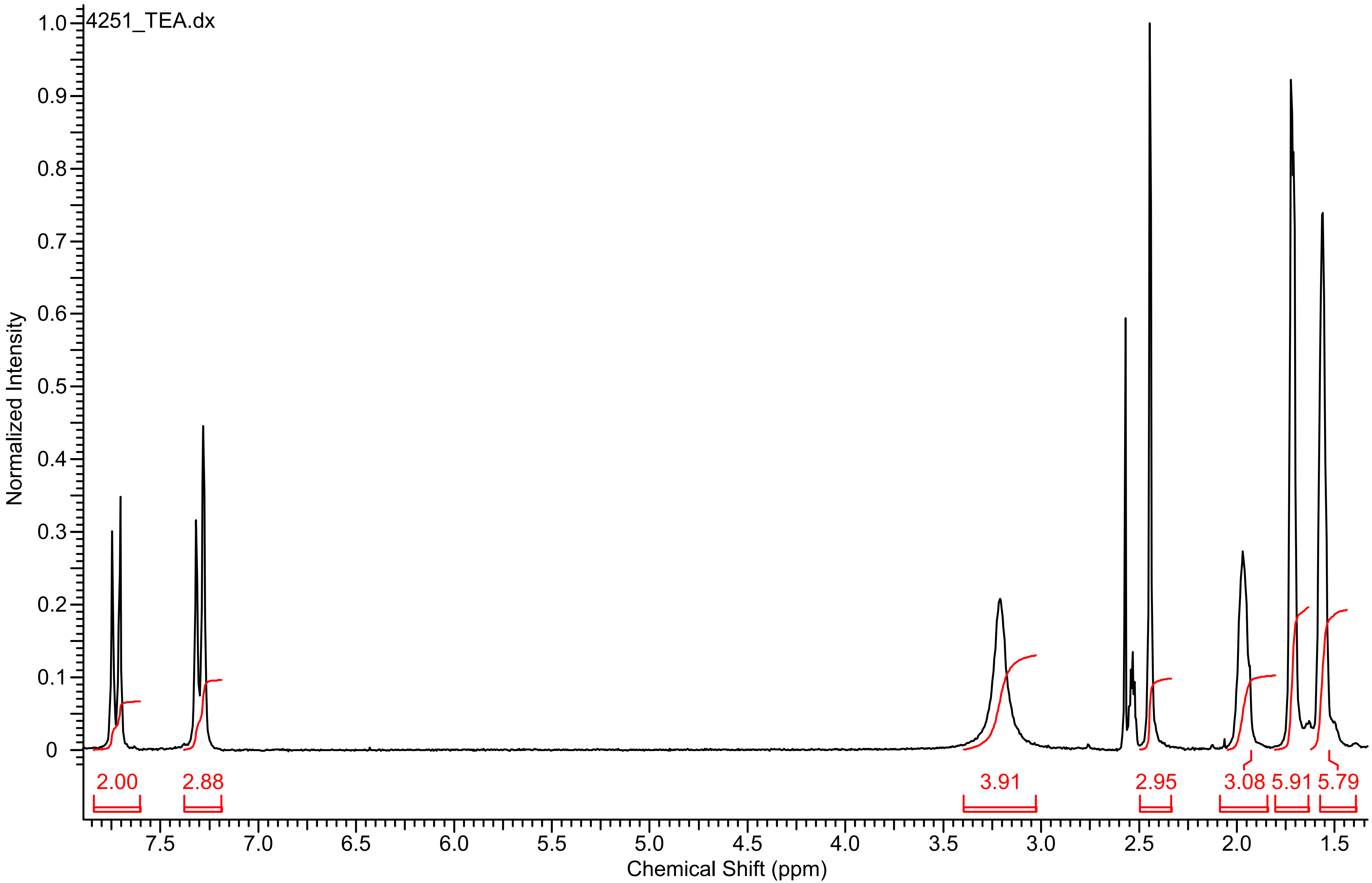

Fig. 4ESI. [1]H NMR spectrum of compound (**3**) in DMSO

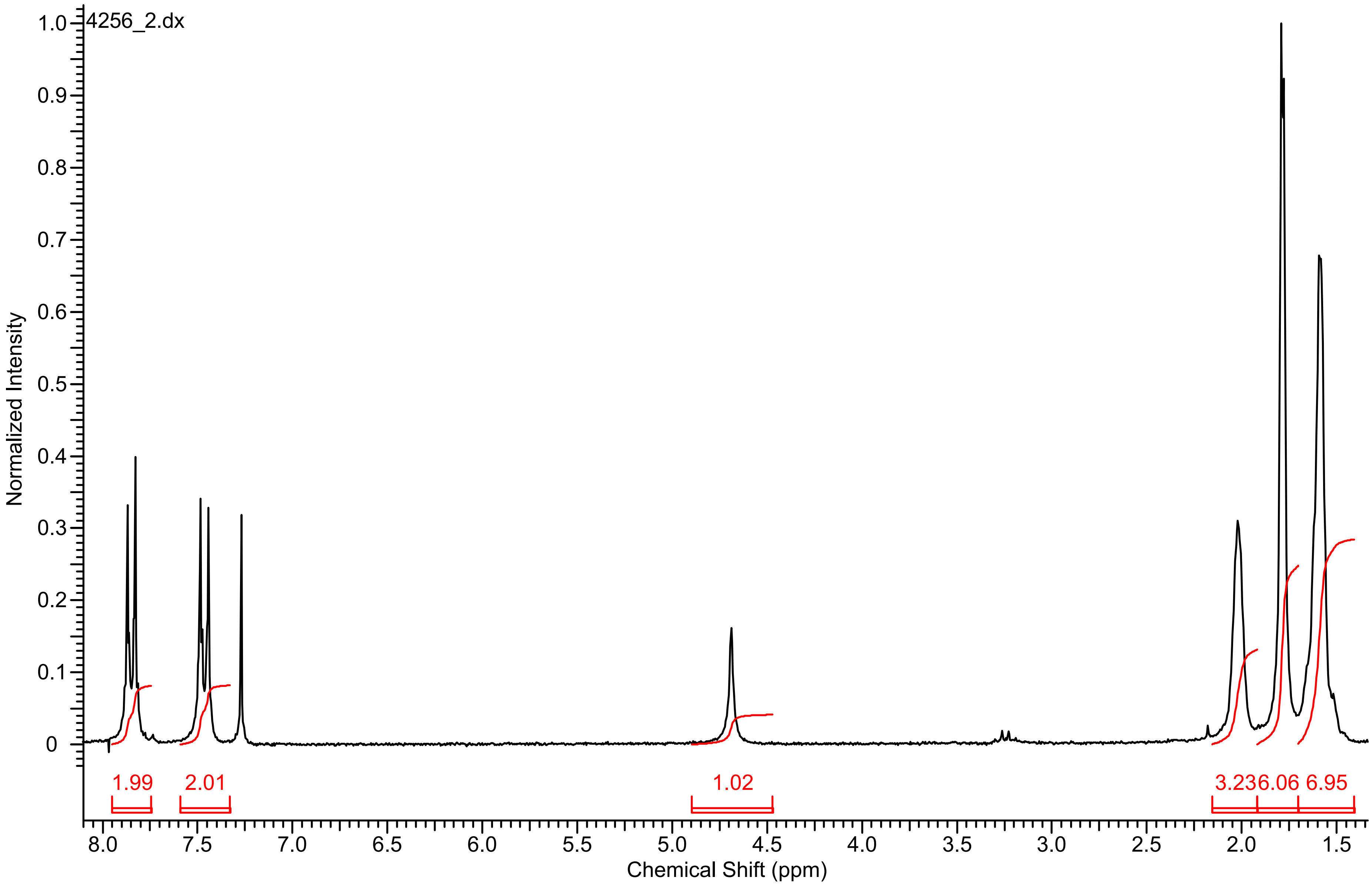

Fig. 5ESI. ^{1}H NMR spectrum of compound (**4**) in $CDCl_3$

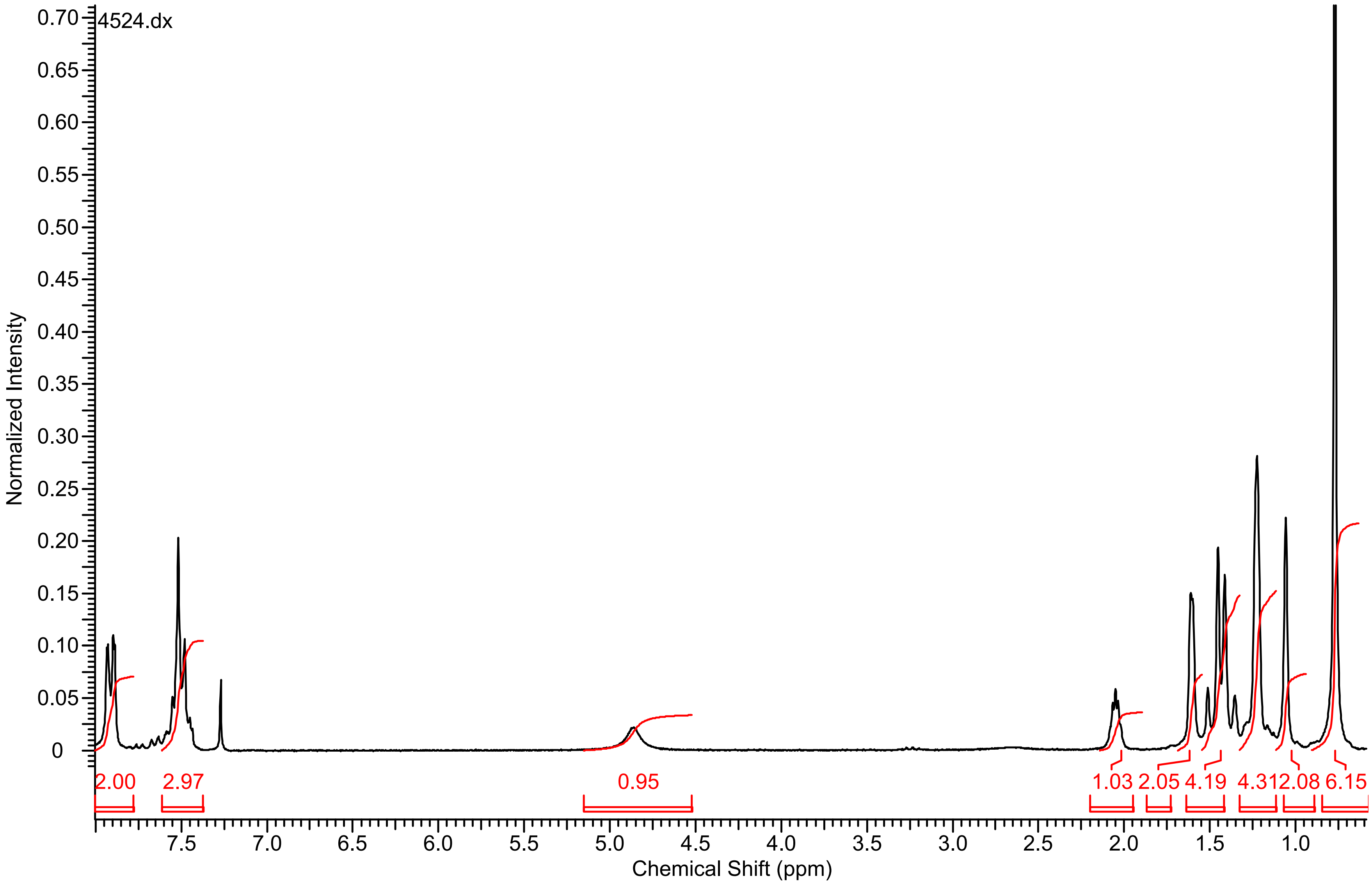

Fig. 6ESI. ^{1}H NMR spectrum of compound (**5**) in $CDCl_3$

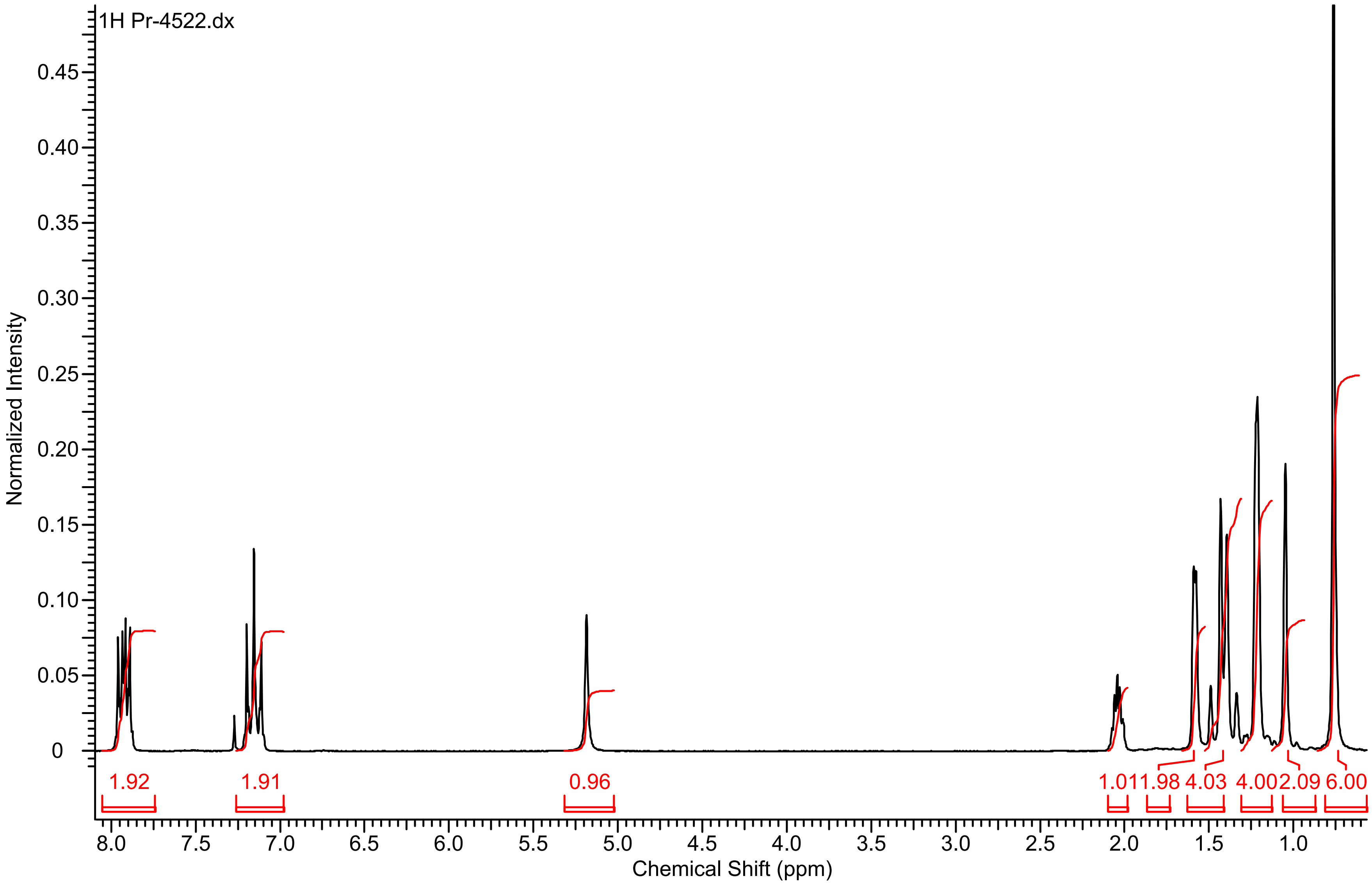

Fig. 7ESI. [1]H NMR spectrum of compound (**6**) in $CDCl_3$

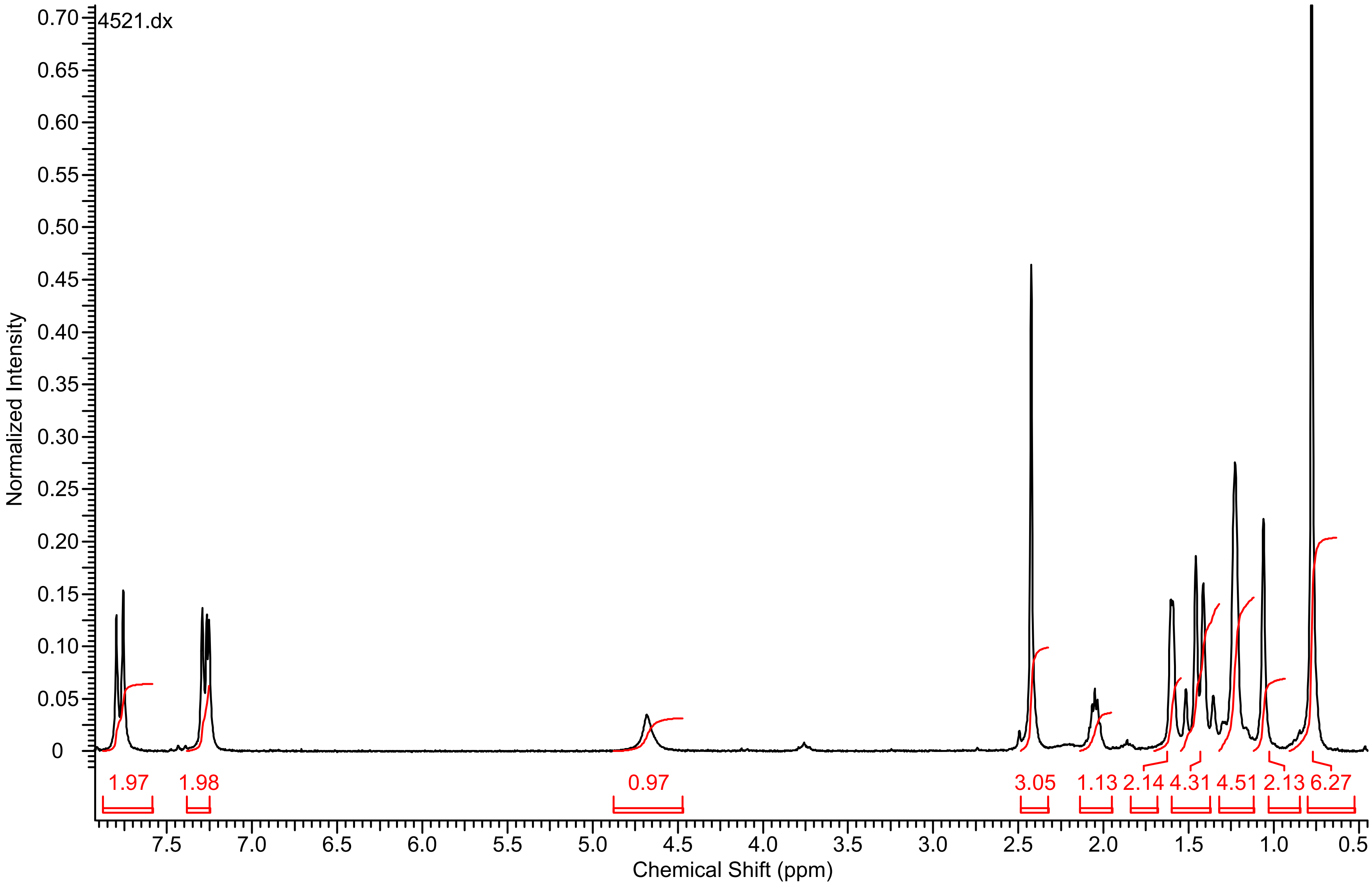

Fig. 8ESI. ^{1}H NMR spectrum of compound (**7**) in $CDCl_3$

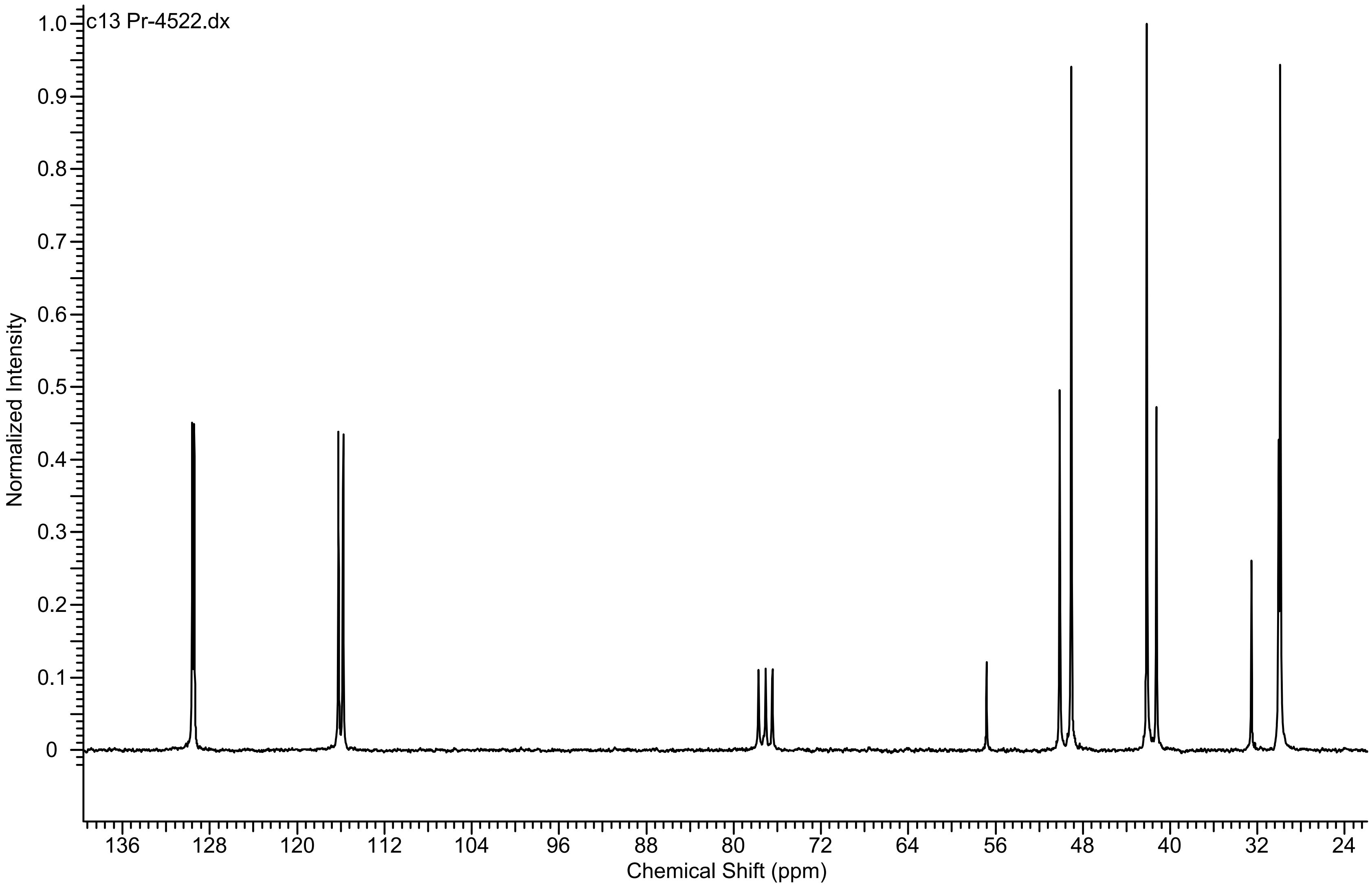

Fig. 9ESI. ^{13}C NMR spectrum of compound (**6**) in $CDCl_3$