

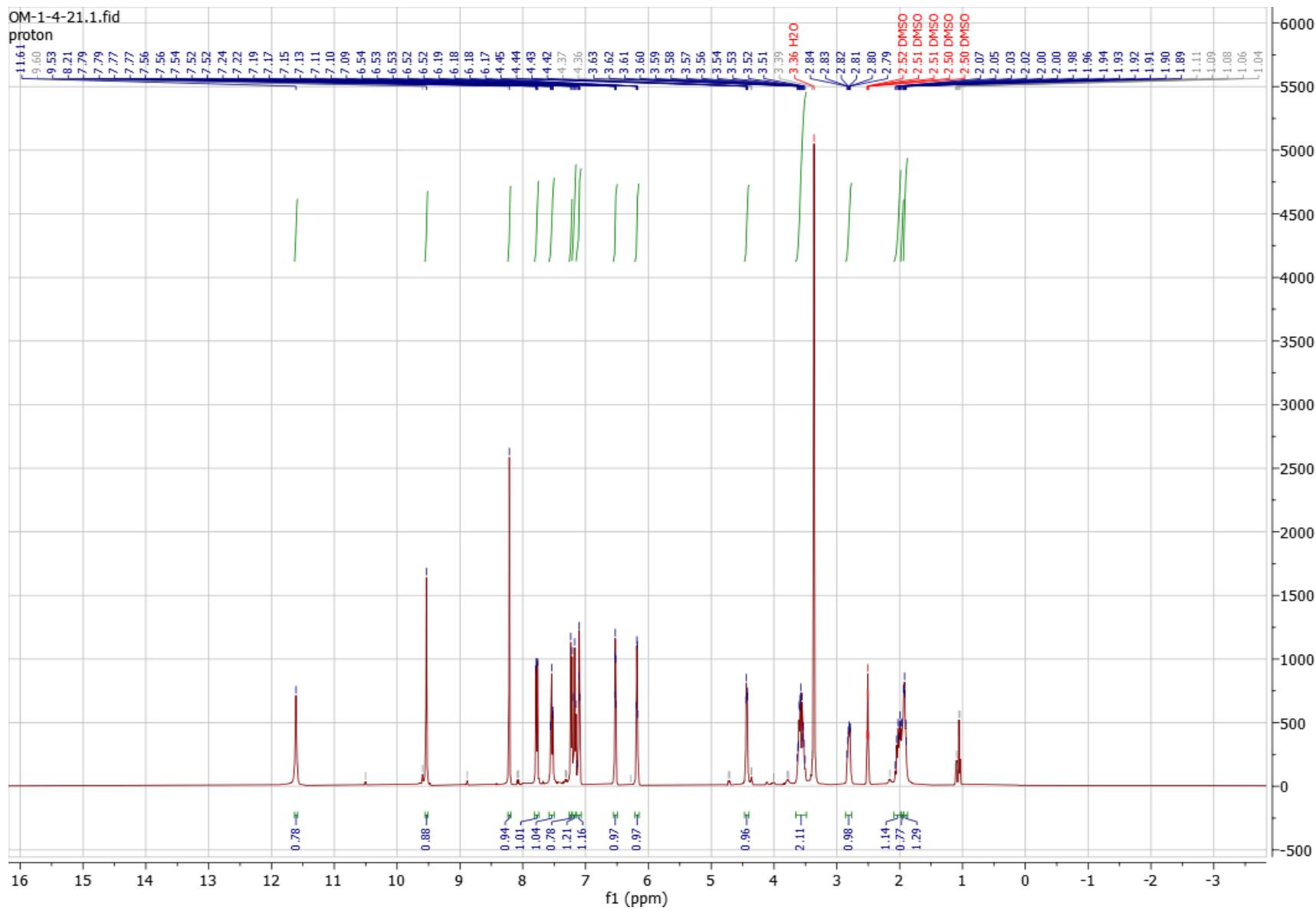
## Supplementary Information

Page Number	Figure
SI1	$^1\text{H}$ NMR spectrum of 4a
SI2	$^{13}\text{C}$ NMR spectrum of 4a
SI3	$^1\text{H}$ NMR spectrum of 4b
SI4	Dept-135 NMR spectrum of 4b
SI5	$^1\text{H}$ NMR spectrum of 4c
SI6	$^{13}\text{C}$ NMR spectrum of 4c
SI7	$^1\text{H}$ NMR spectrum of 4d
SI8	$^{13}\text{C}$ NMR spectrum of 4d
SI9	$^1\text{H}$ NMR spectrum of 4e
SI10	Dept-135 NMR spectrum of 4e
SI11	$^1\text{H}$ NMR spectrum of 4f
SI12	$^{13}\text{C}$ NMR spectrum of 4f
SI13	$^1\text{H}$ NMR spectrum of 4g
SI14	$^{13}\text{C}$ NMR spectrum of 4g
SI15	$^1\text{H}$ NMR spectrum of 4h

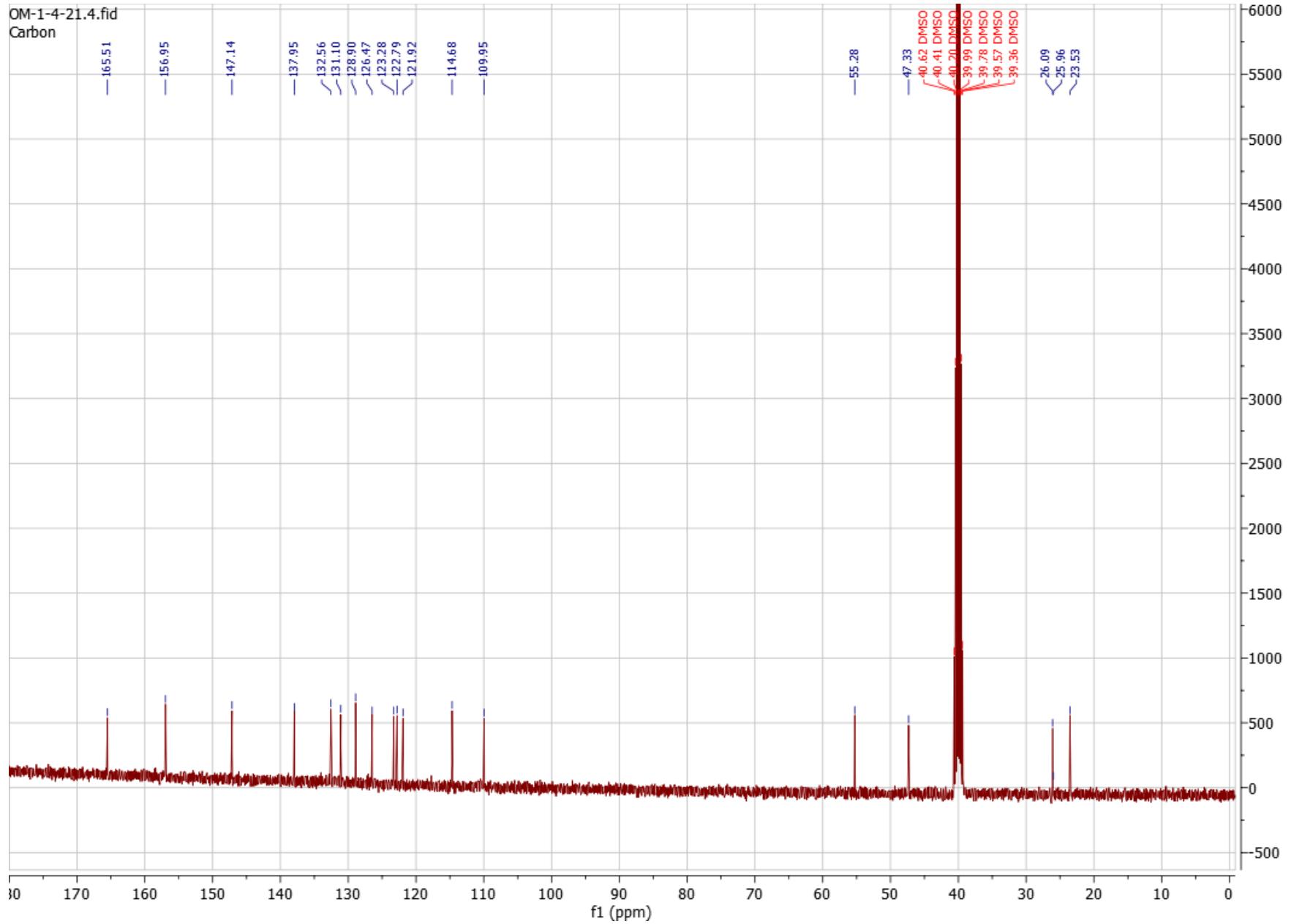
## Supplementary Information

Page Number	Figure
SI16	$^{13}\text{C}$ NMR spectrum of 4h
SI17	$^1\text{H}$ NMR spectrum of 4i
SI18	$^{13}\text{C}$ NMR spectrum of 4i
SI19	$^1\text{H}$ NMR spectrum of 4j
SI20	$^{13}\text{C}$ NMR spectrum of 4j
SI21	$^1\text{H}$ NMR spectrum of 4k
SI22	$^{13}\text{C}$ NMR spectrum of 4k
SI23	$^1\text{H}$ NMR spectrum of 4l
SI24	$^{13}\text{C}$ NMR spectrum of 4l
SI25	$^1\text{H}$ NMR spectrum of 4m
SI26	$^{13}\text{C}$ NMR spectrum of 4m
SI27	$^1\text{H}$ NMR spectrum of 4n
SI28	$^{13}\text{C}$ NMR spectrum of 4n
SI29	$^1\text{H}$ NMR spectrum of 4o
SI30	$^{13}\text{C}$ NMR spectrum of 4o

Page Number	Figure
SI31	<sup>1</sup> H NMR spectrum of 4p
SI32	<sup>13</sup> C NMR spectrum of 4p
SI33	<sup>1</sup> H NMR spectrum of 4q
SI34	<sup>13</sup> C NMR spectrum of 4q
SI35	Dept-135 NMR spectrum of 4q
SI36	Typical MRM chromatograms of <b>4k</b> (top panel) and the IS (below panel) at 0.5 h plasma pharmacokinetic study sample
SI37	Typical MRM chromatograms of <b>4k</b> (top panel) and the IS (below panel) at 0.5 h brain pharmacokinetic study sample
SI38	Typical MRM chromatograms of <b>4k</b> (top panel) and the IS (below panel) at 0.5 h kidney pharmacokinetic study sample
SI39	Typical MRM chromatograms of <b>4k</b> (top panel) and the IS (below panel) at 0.5 h liver pharmacokinetic study sample

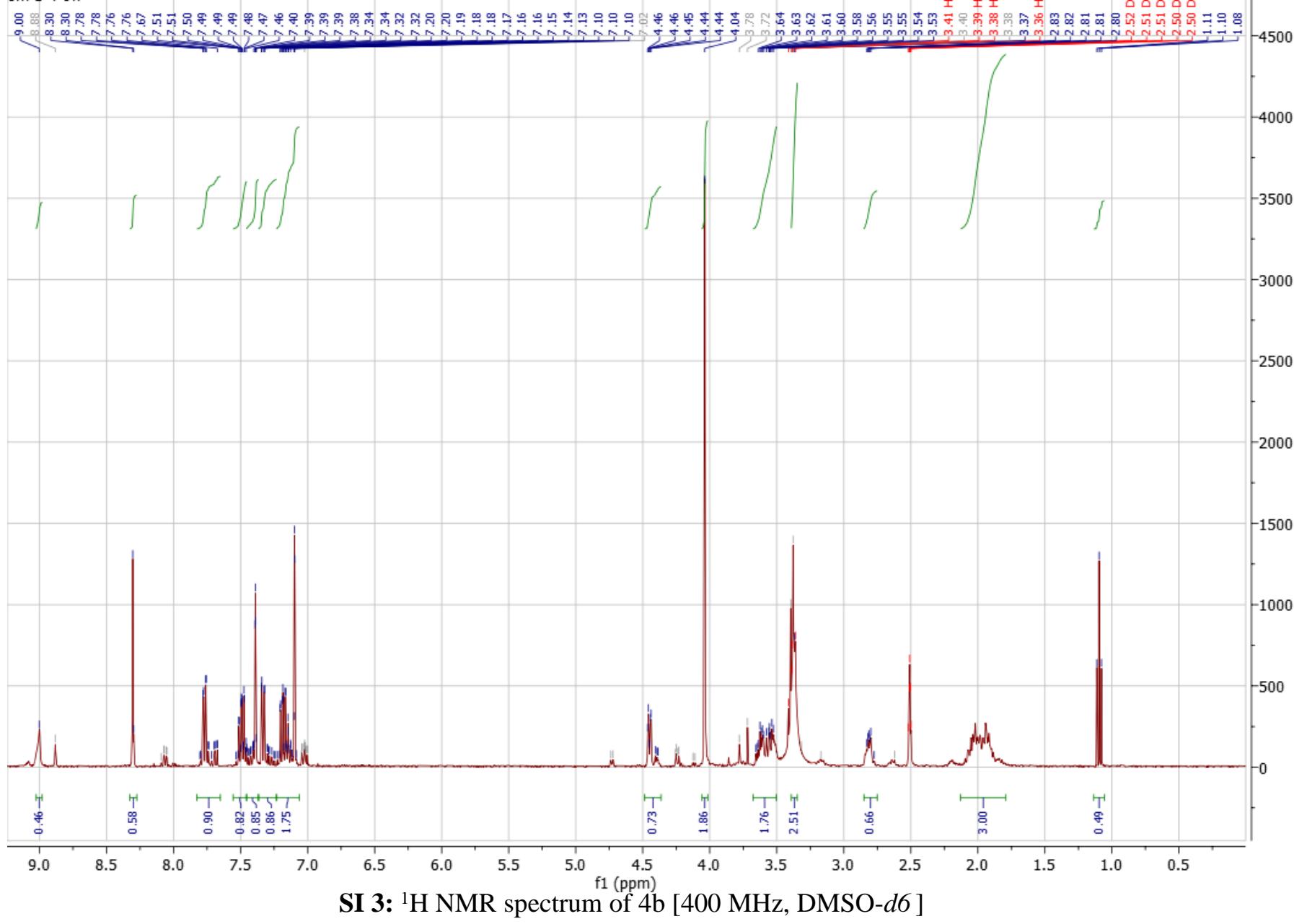


**SI 1:**  $^1\text{H}$  NMR spectrum of 4a [400 MHz, DMSO-*d*<sub>6</sub>]

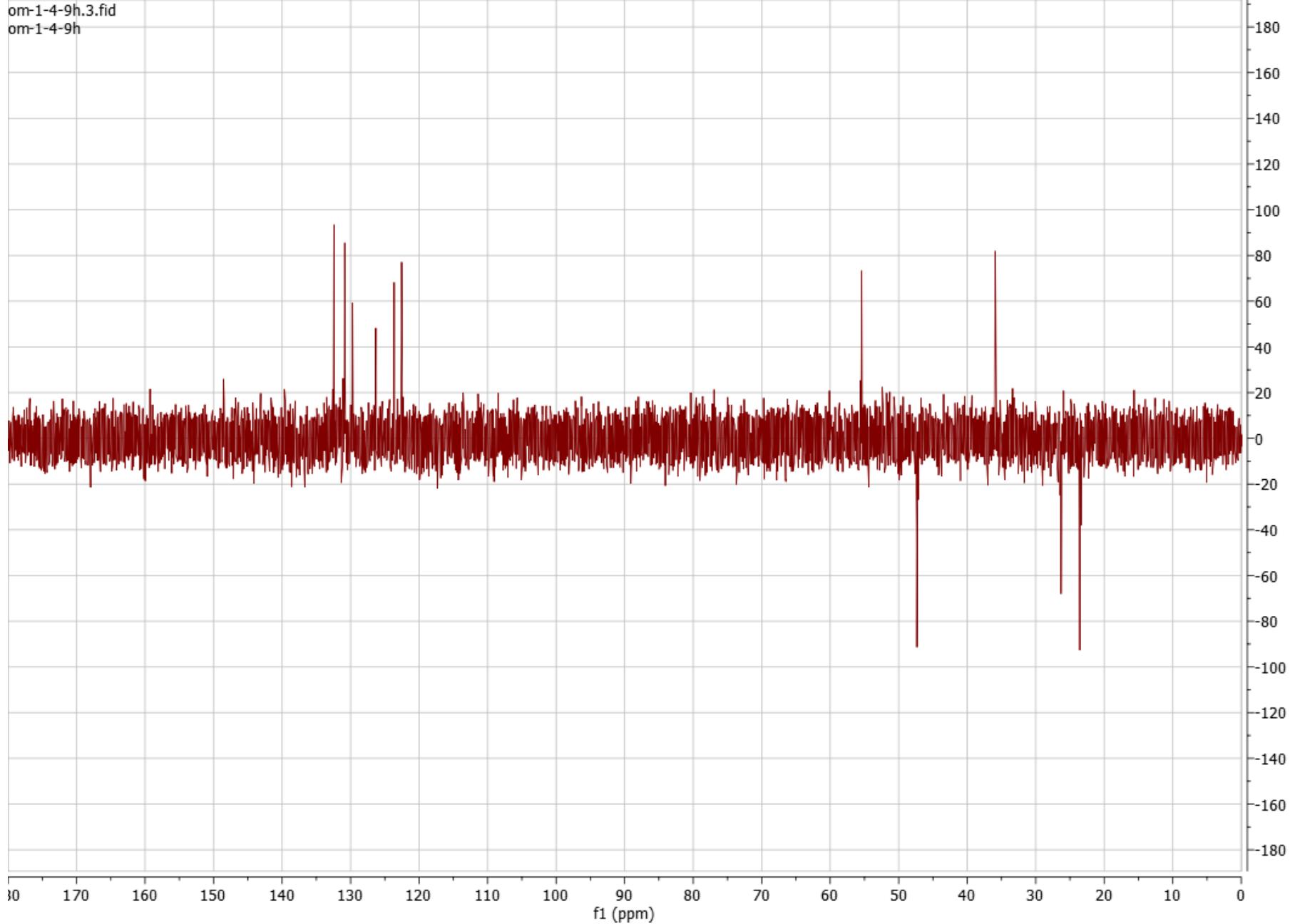


SI 2:  $^{13}\text{C}$  NMR spectrum of 4 a [100 MHz,  $\text{DMSO}-d_6$  ]

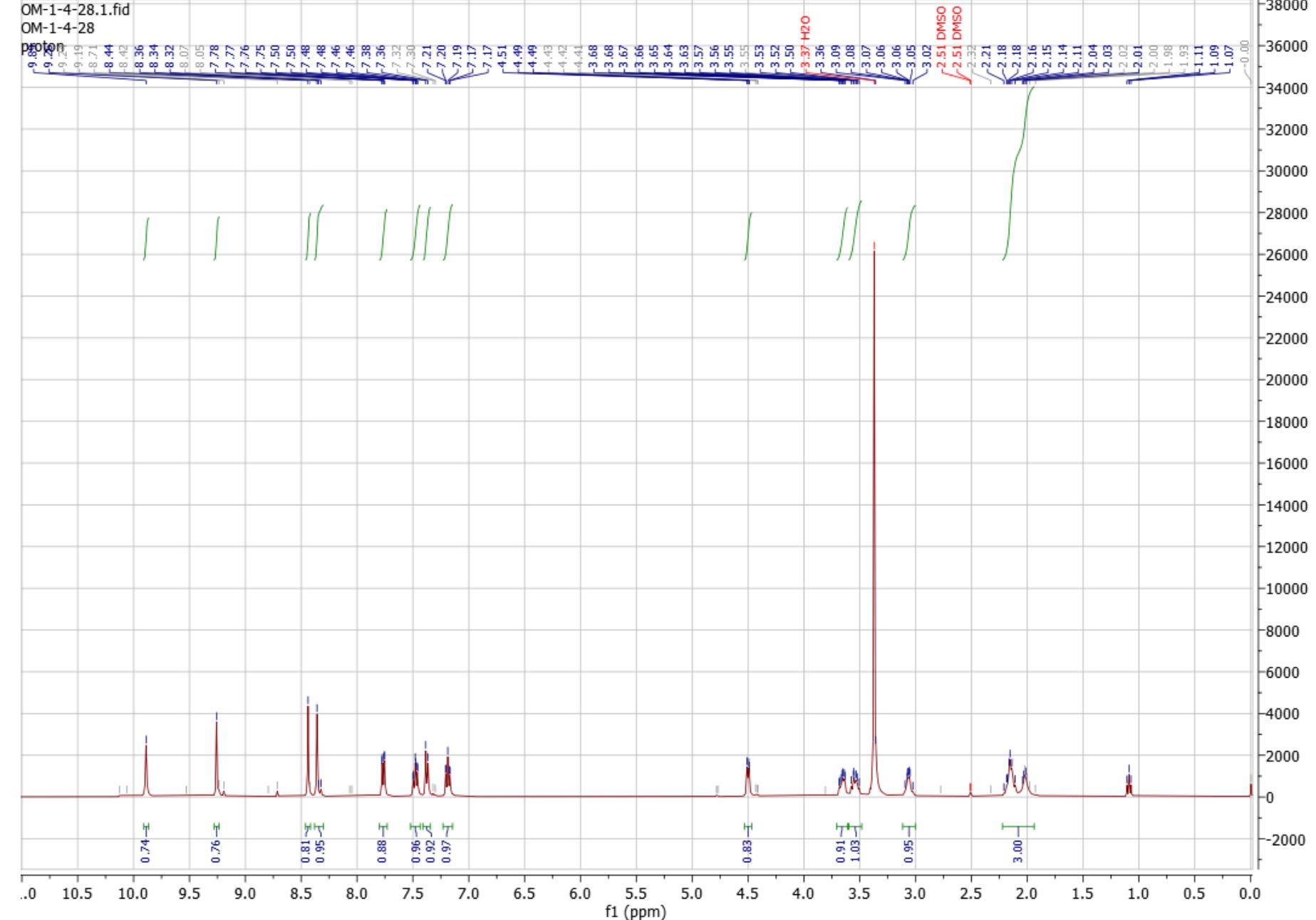
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om-1-4-9h



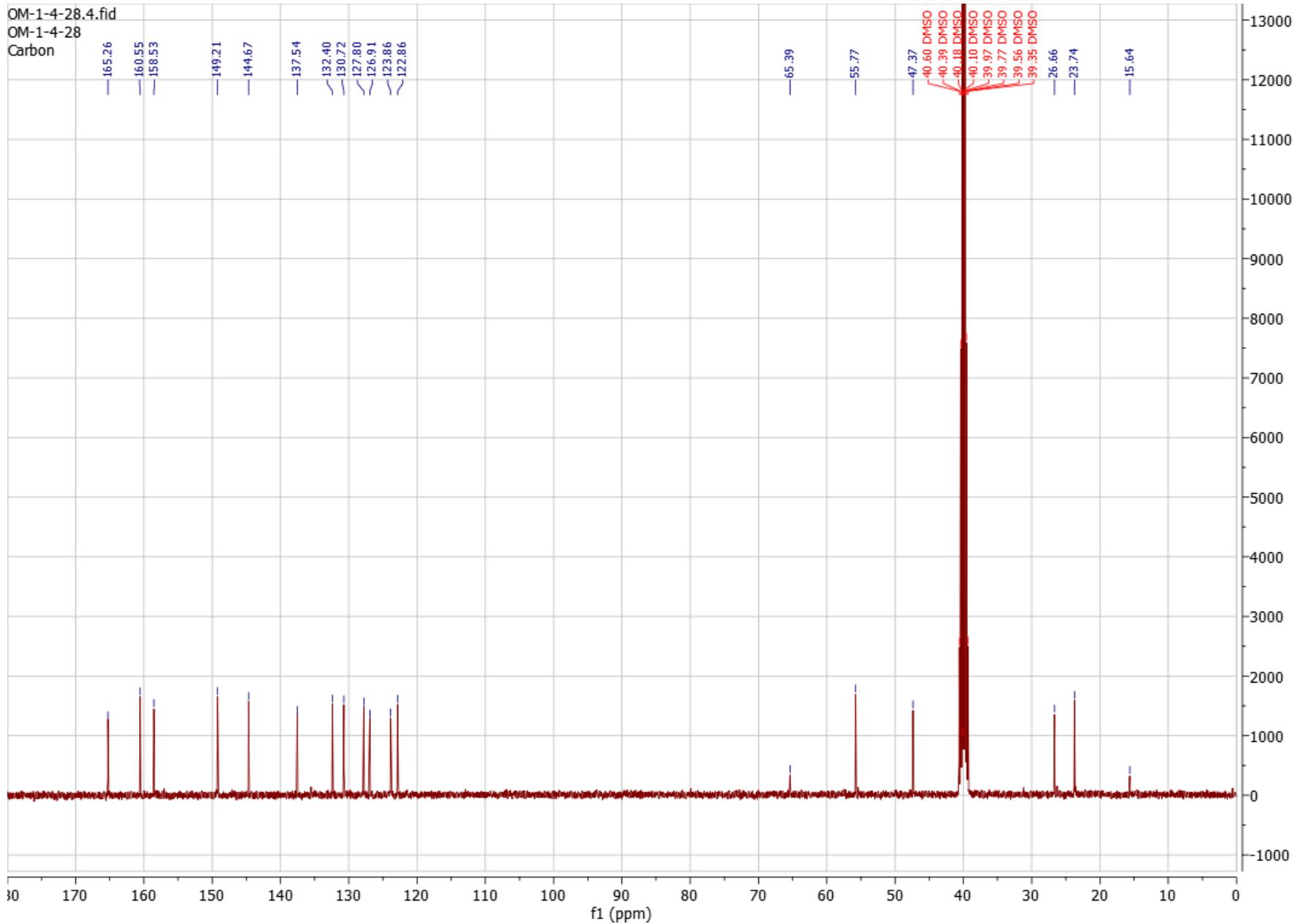
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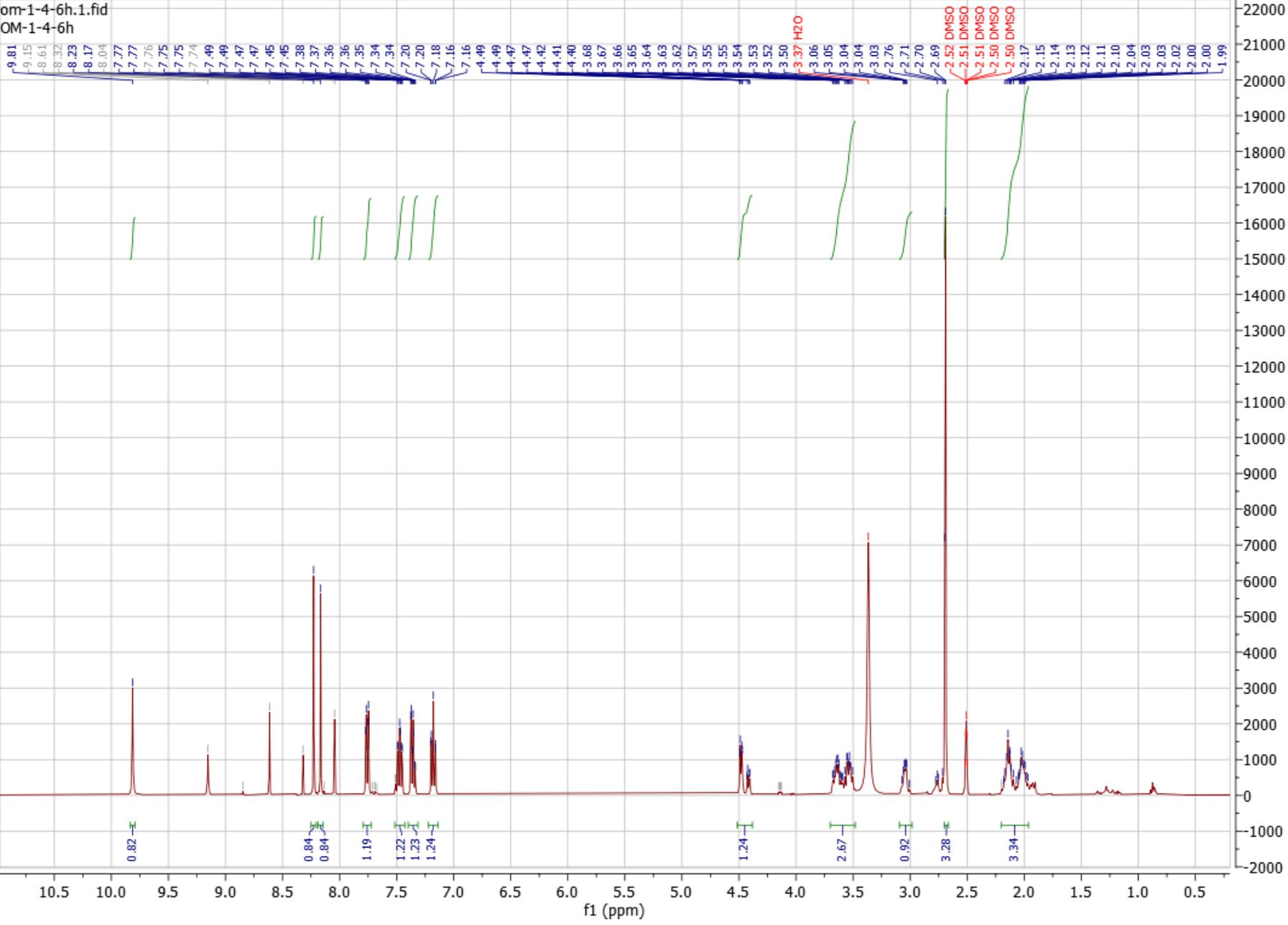
**SI 4:** DEPT-135 spectrum of 4b [100 MHz, DMSO-*d*6 ]



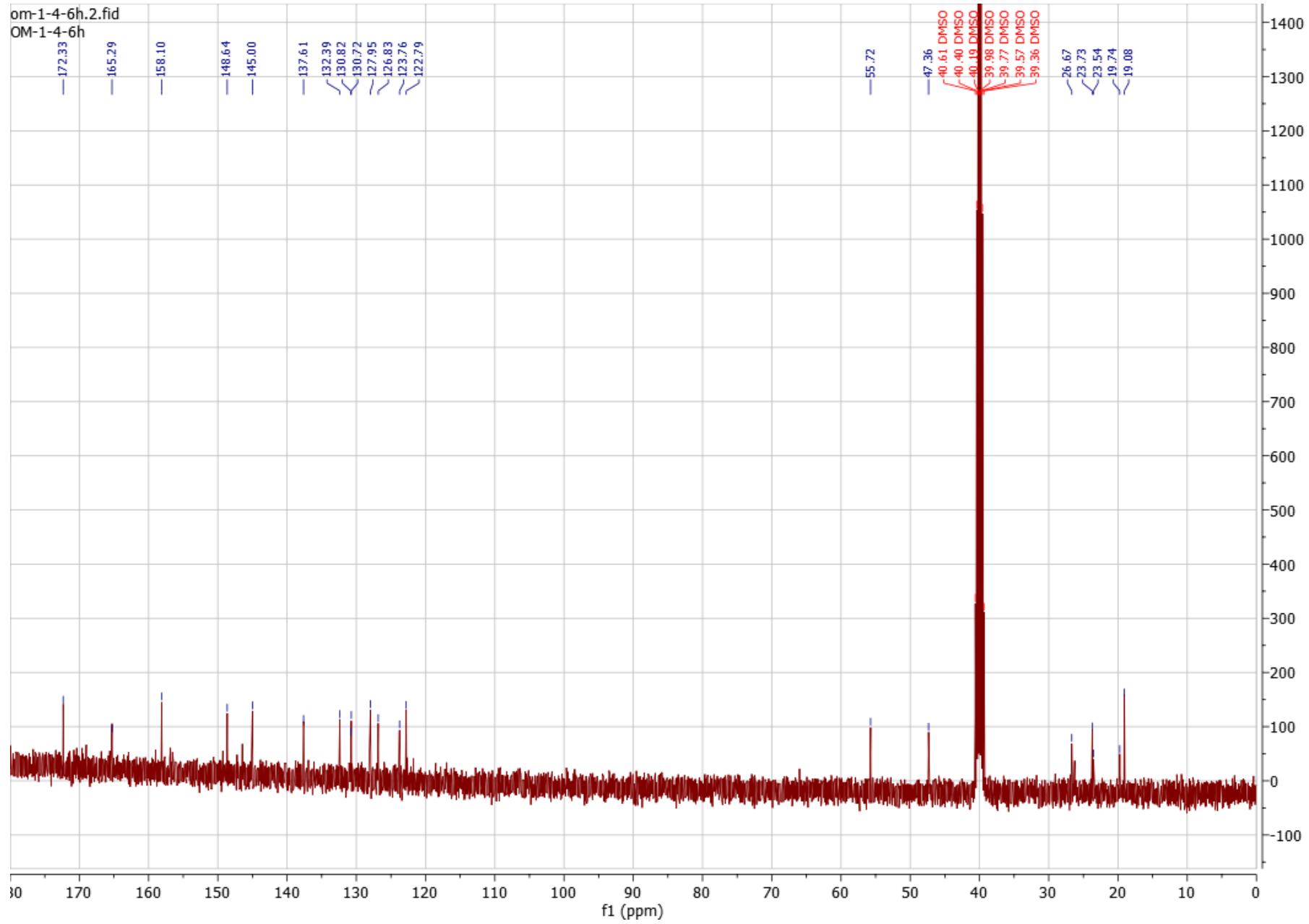
**SI 5:**  $^1\text{H}$  NMR spectrum of 4c [400 MHz, DMSO-*d*6]



**SI 6:**  $^{13}\text{C}$  NMR spectrum of 4c [400 MHz, DMSO-*d*6 ]

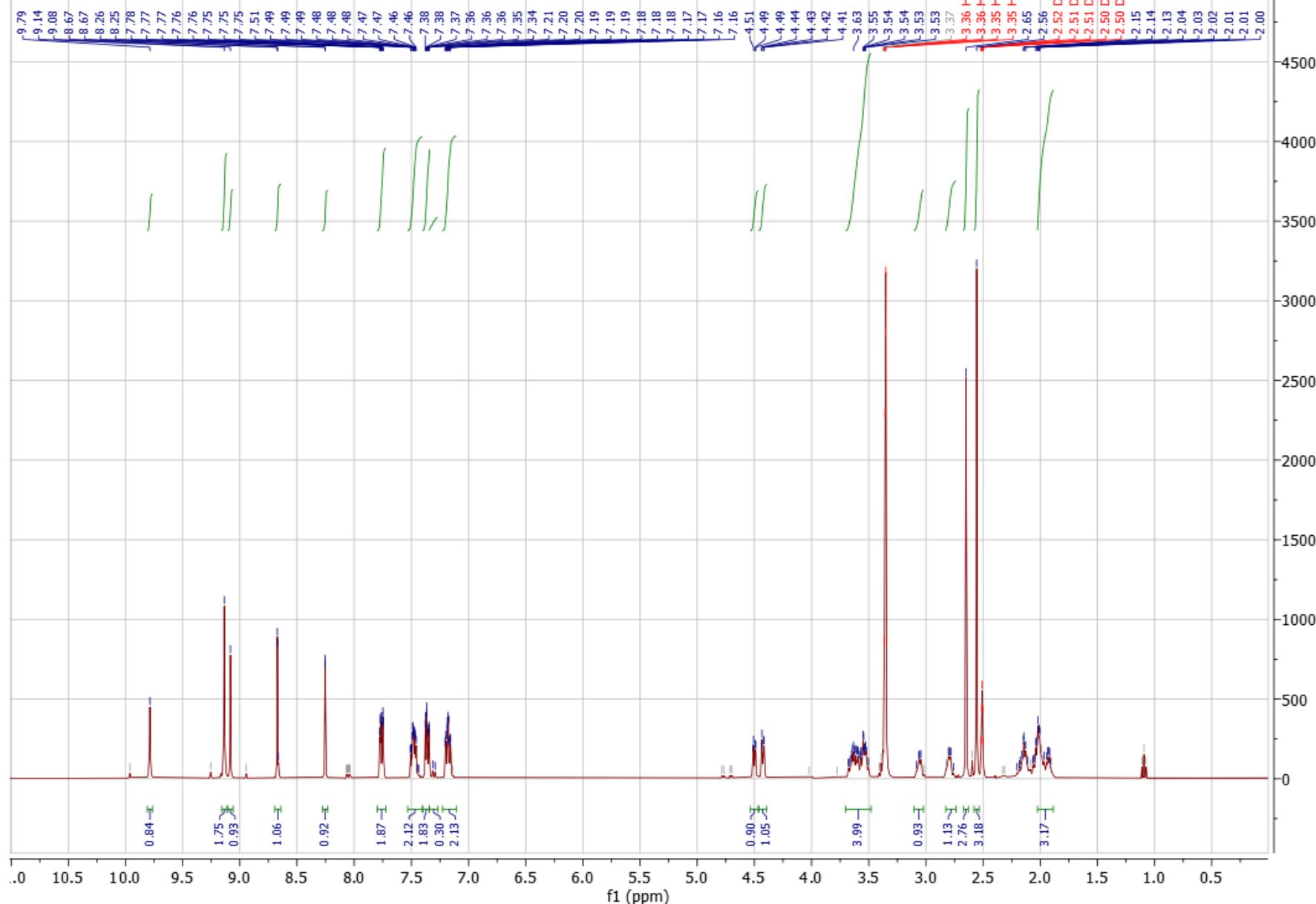


**SI 7:**  $^1\text{H}$  NMR spectrum of 4d [400 MHz, DMSO-*d*6]



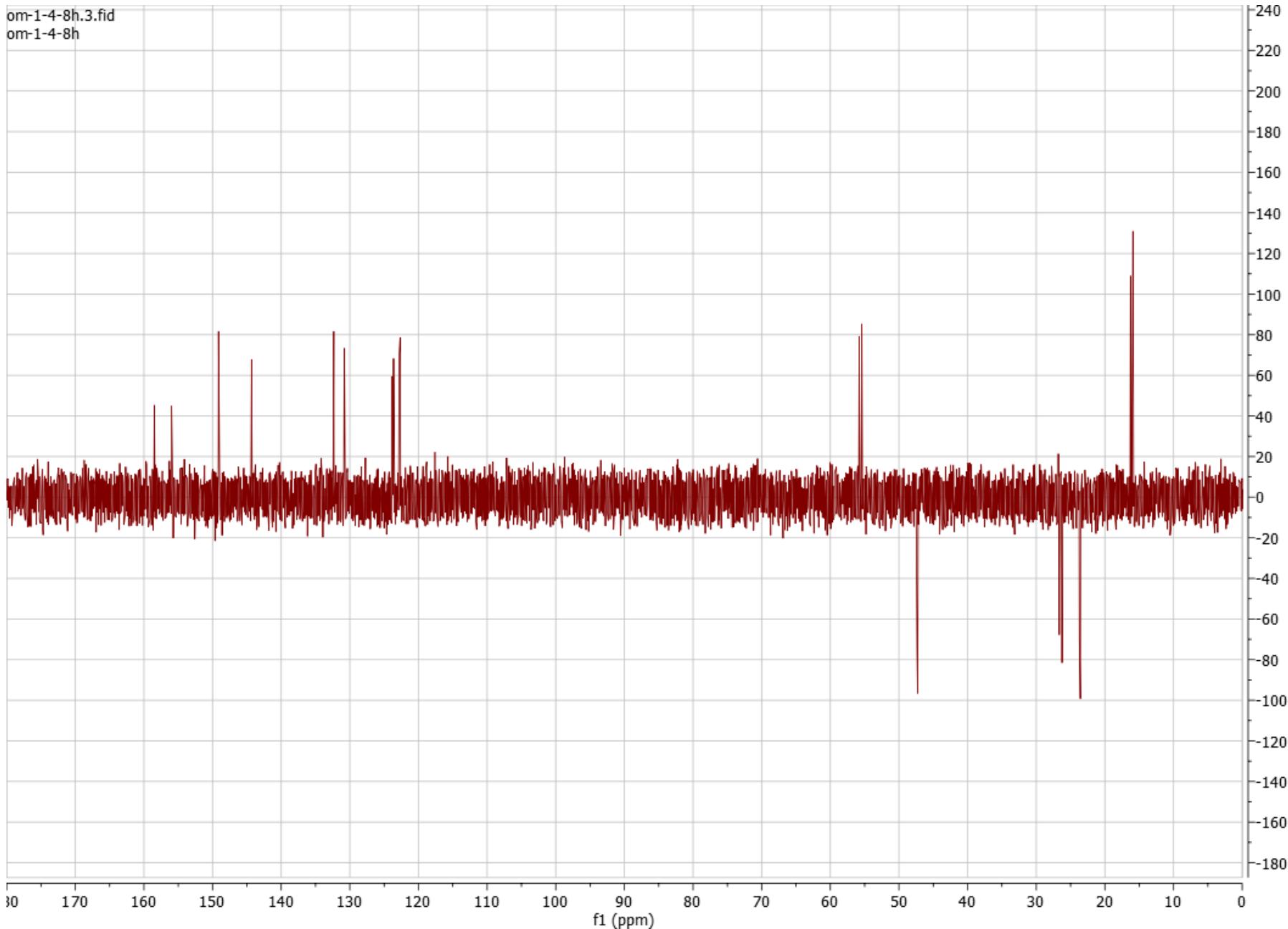
**SI 8:**  $^{13}\text{C}$  NMR spectrum of 4 d [400 MHz,  $\text{DMSO}-d_6$ ]

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om-1-4-8h

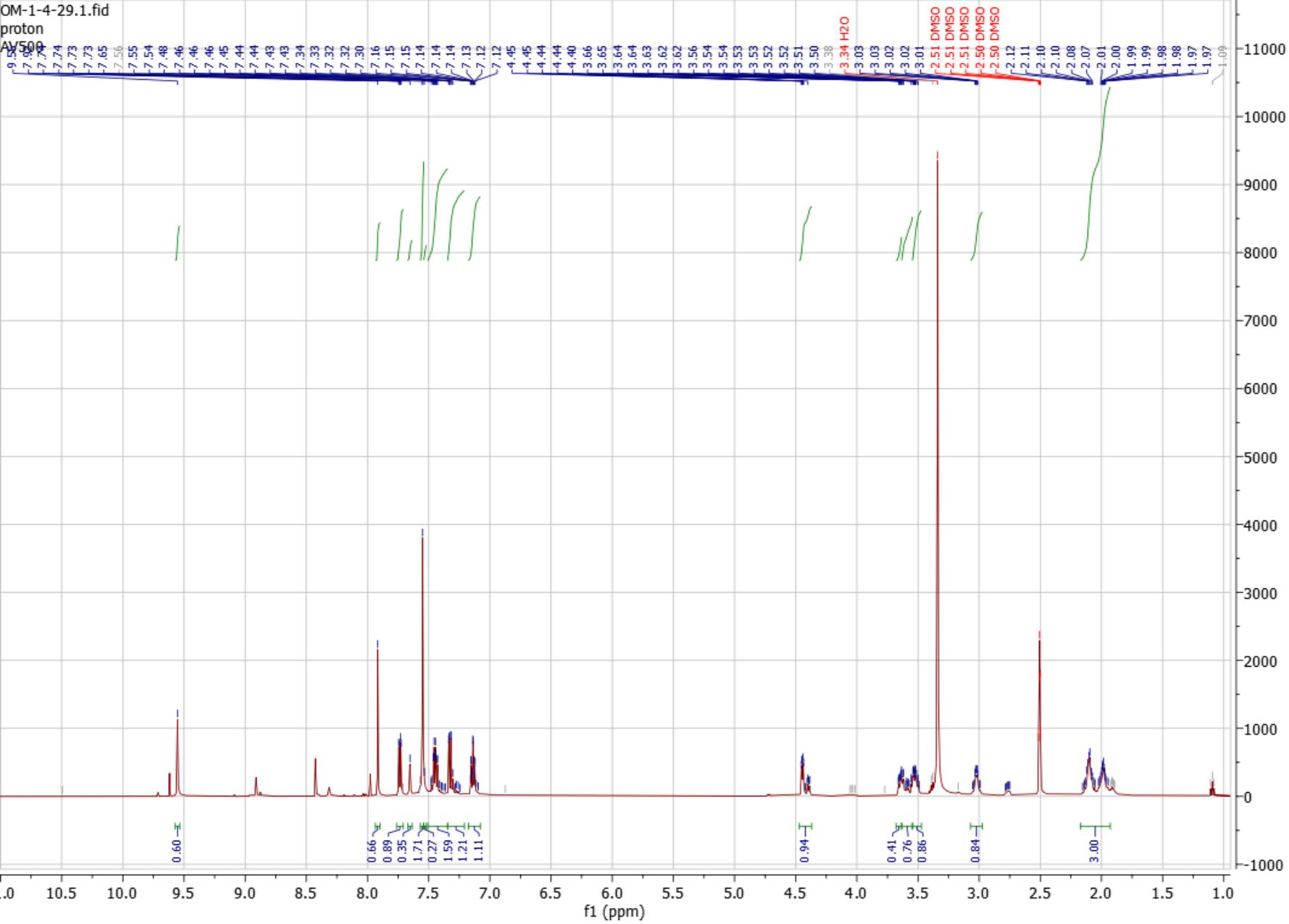


SI 9: <sup>1</sup>H NMR spectrum of 4e [400 MHz, DMSO-*d*6]

om-1-4-8h.3.fid  
om-1-4-8h

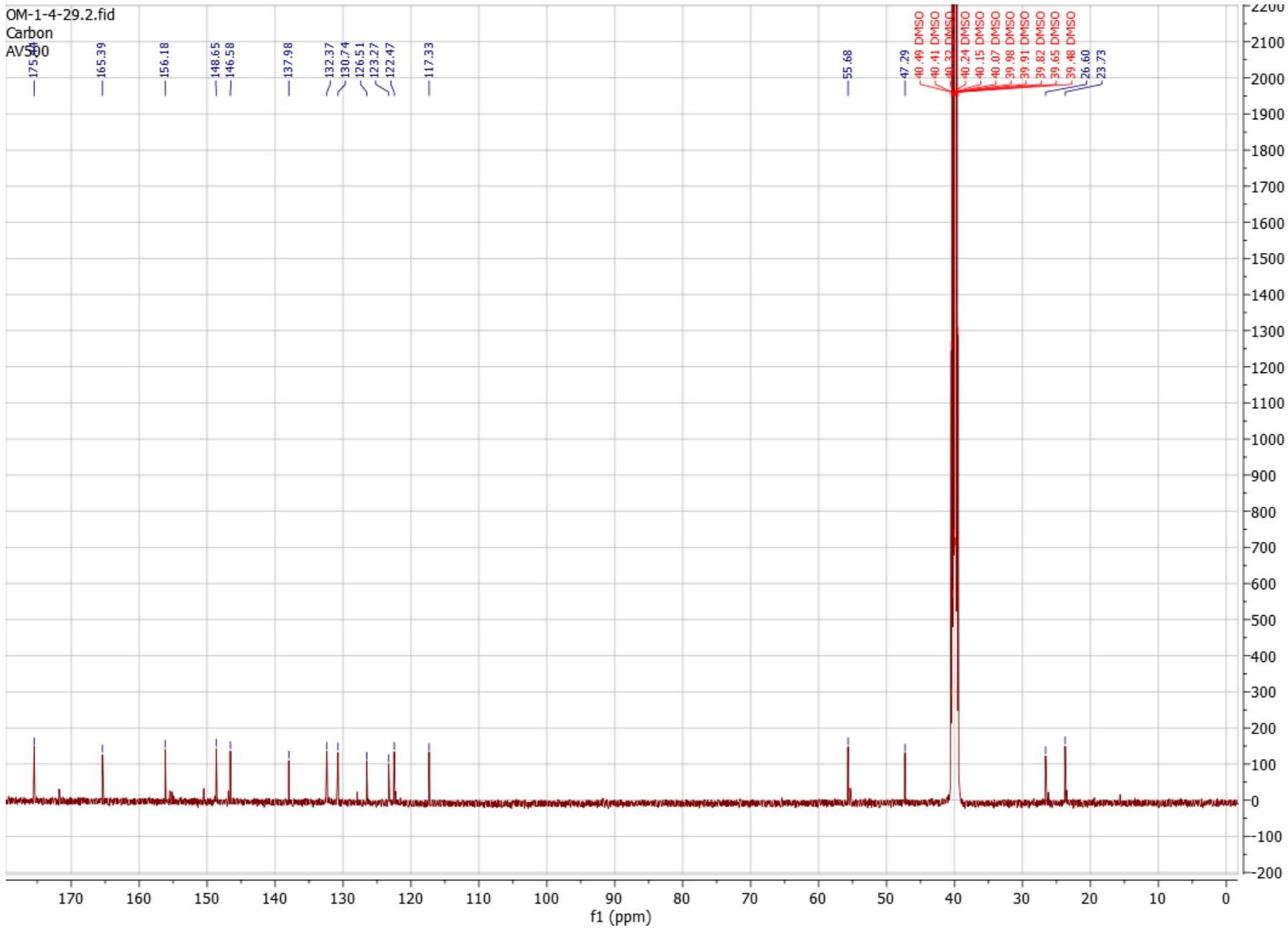


**SI 10:** Dept-135 NMR spectrum of 4 e [100 MHz, DMSO-*d*6]



SI 11: 1H NMR spectrum of 4f [500 MHz, DMSO-*d*6]

OM-1-4-29.2.fid  
Carbon  
AV500



SI 12:  $^{13}\text{C}$  NMR spectrum of 4f [125 MHz,  $\text{DMSO}-d_6$ ]



**SI 13:**  $^1\text{H}$  NMR spectrum of 4g [500 MHz, DMSO-*d*6]

OM-1-4-26.2.fid

Carbon

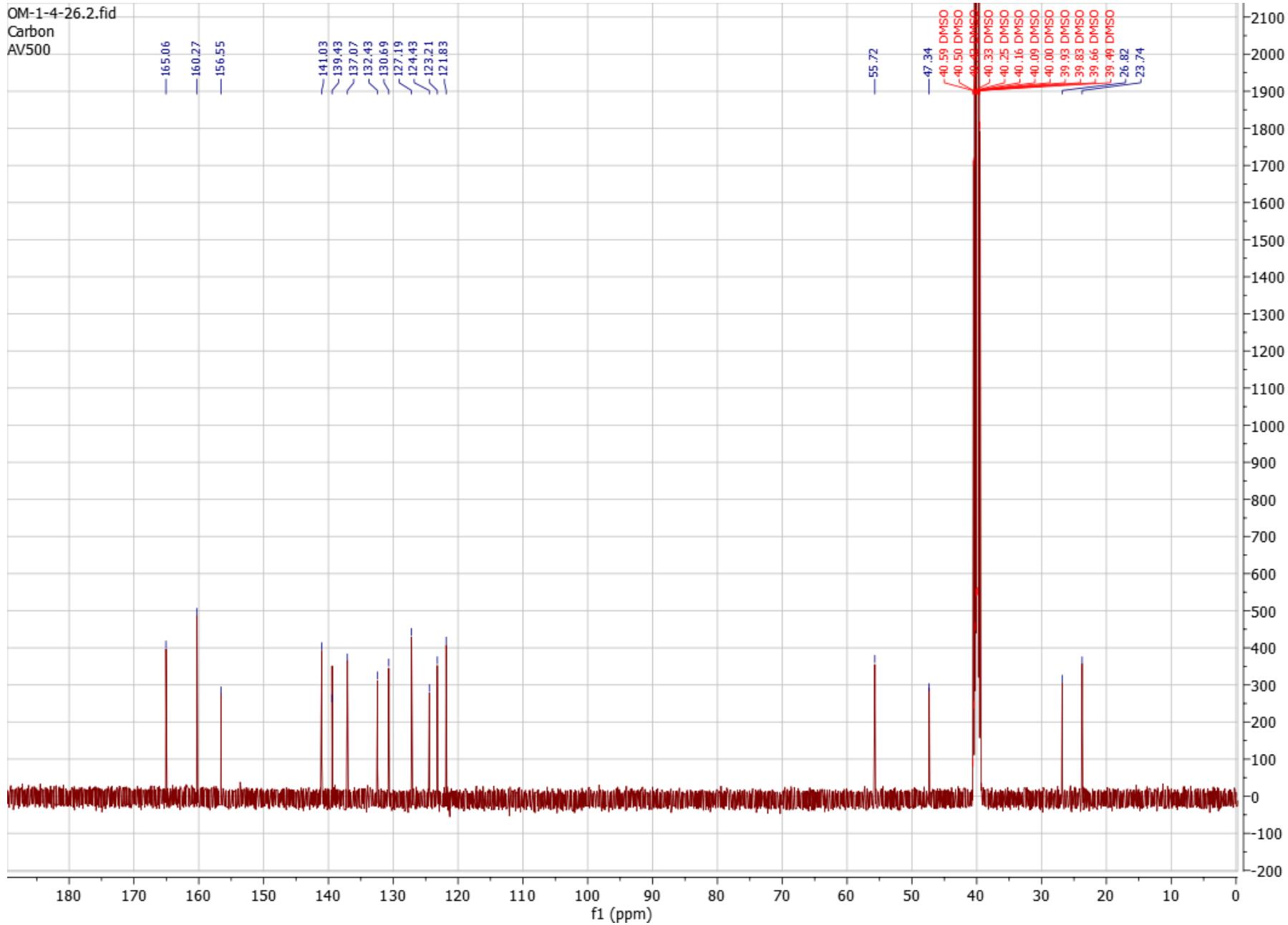
AV500

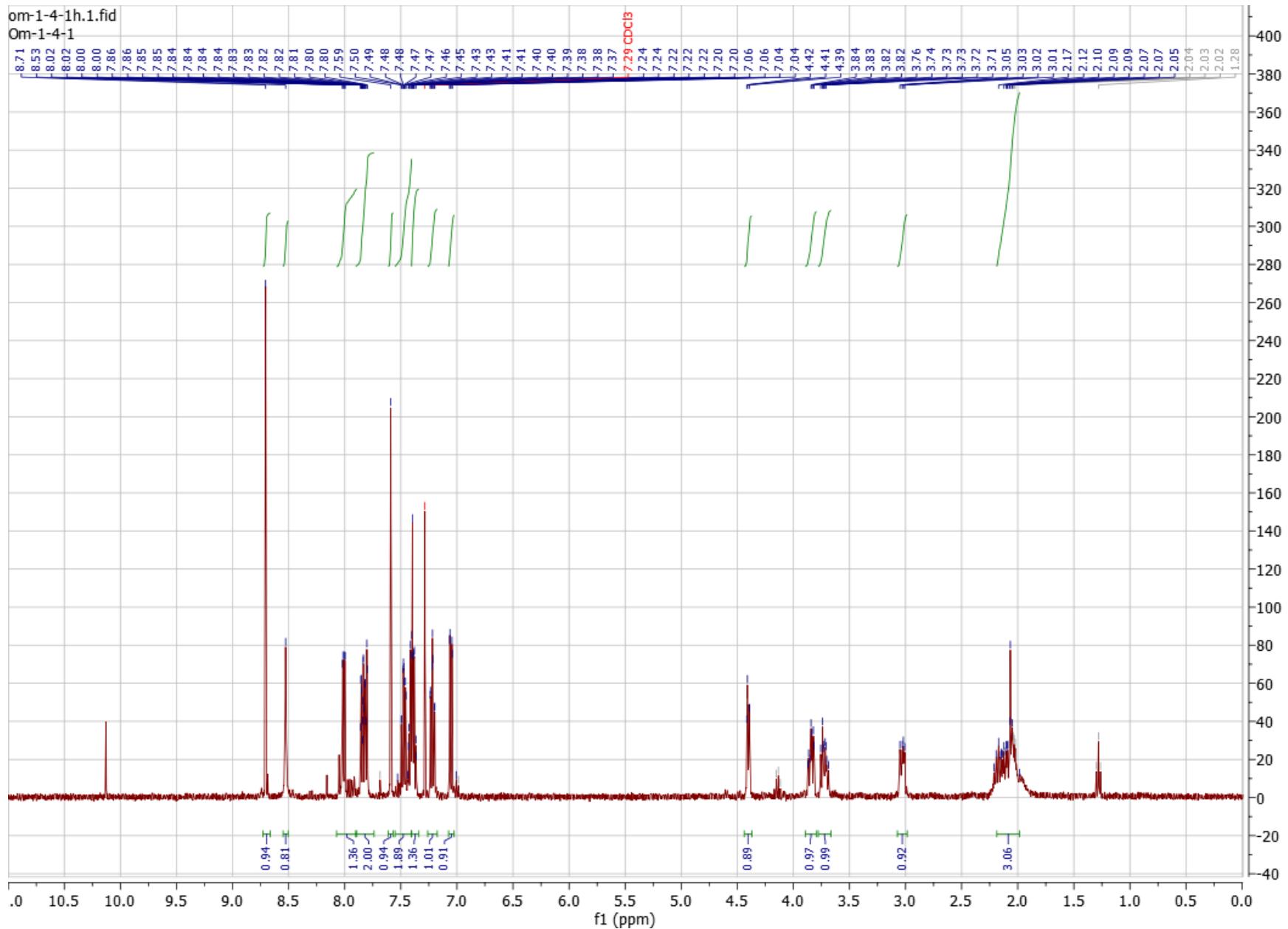
— 165.06  
— 160.27  
— 156.55

— 141.03  
— 139.43  
— 137.07  
— 132.43  
— 130.69  
— 127.19  
— 124.43  
— 123.21  
— 121.83

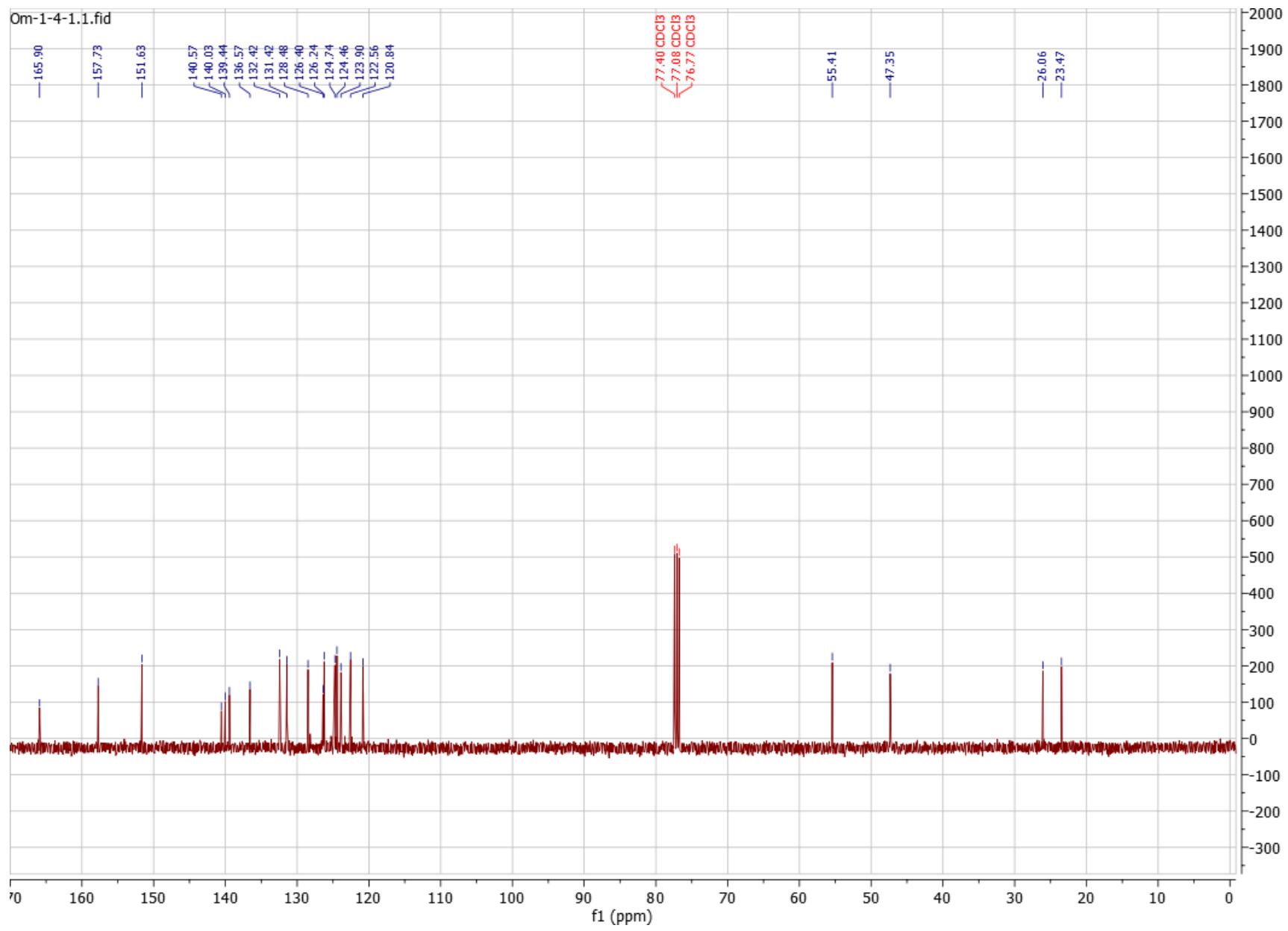
— 55.72

— 47.34  
— 40.59 DMSO  
— 40.50 DMSO  
— 40.42 DMSO  
— 40.33 DMSO  
— 40.25 DMSO  
— 40.16 DMSO  
— 40.09 DMSO  
— 40.00 DMSO  
— 39.93 DMSO  
— 39.83 DMSO  
— 39.49 DMSO  
— 26.82  
— 23.74

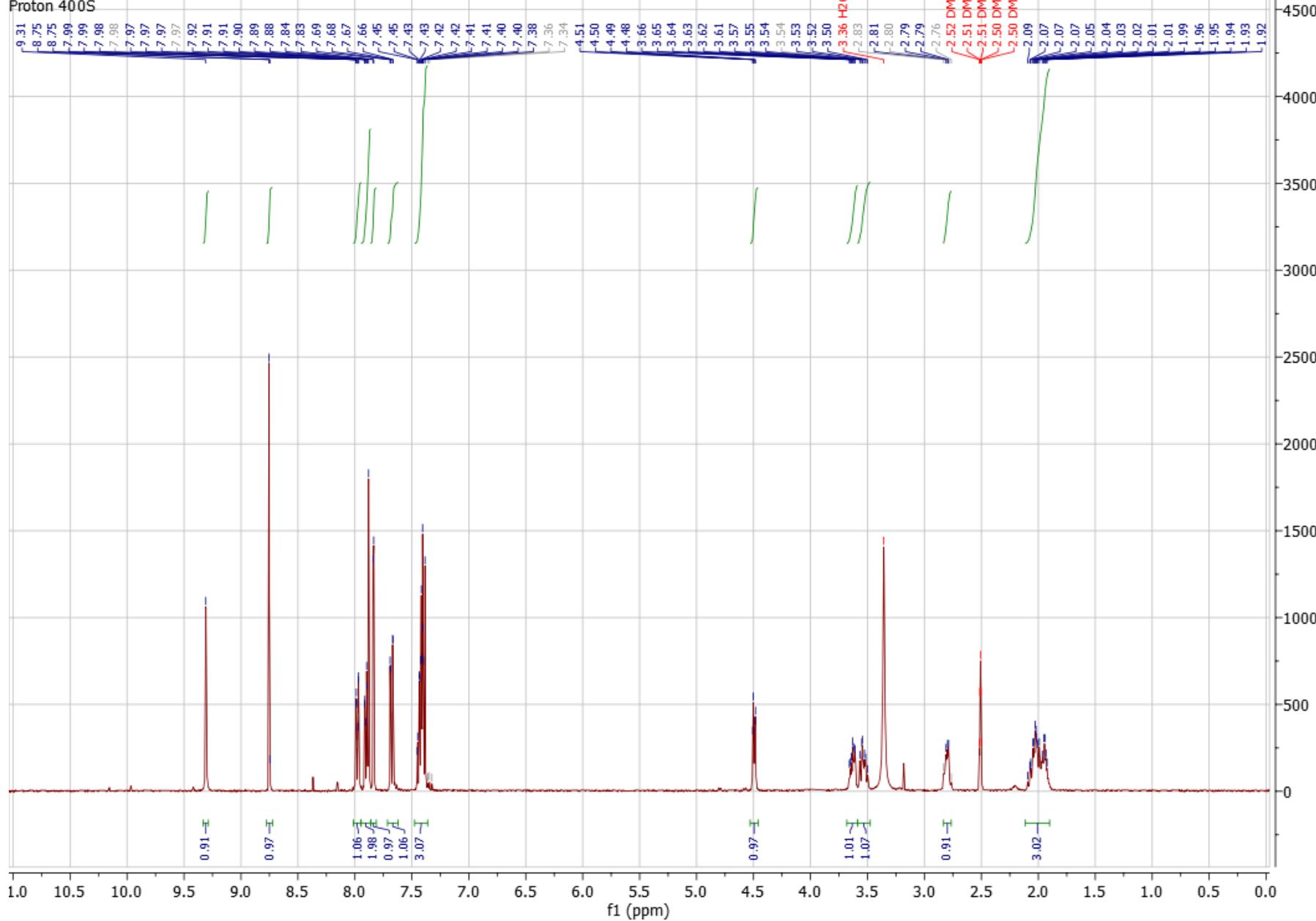
SI 14:  $^{13}\text{C}$  NMR spectrum of 4g [125 MHz, DMSO-*d*6]

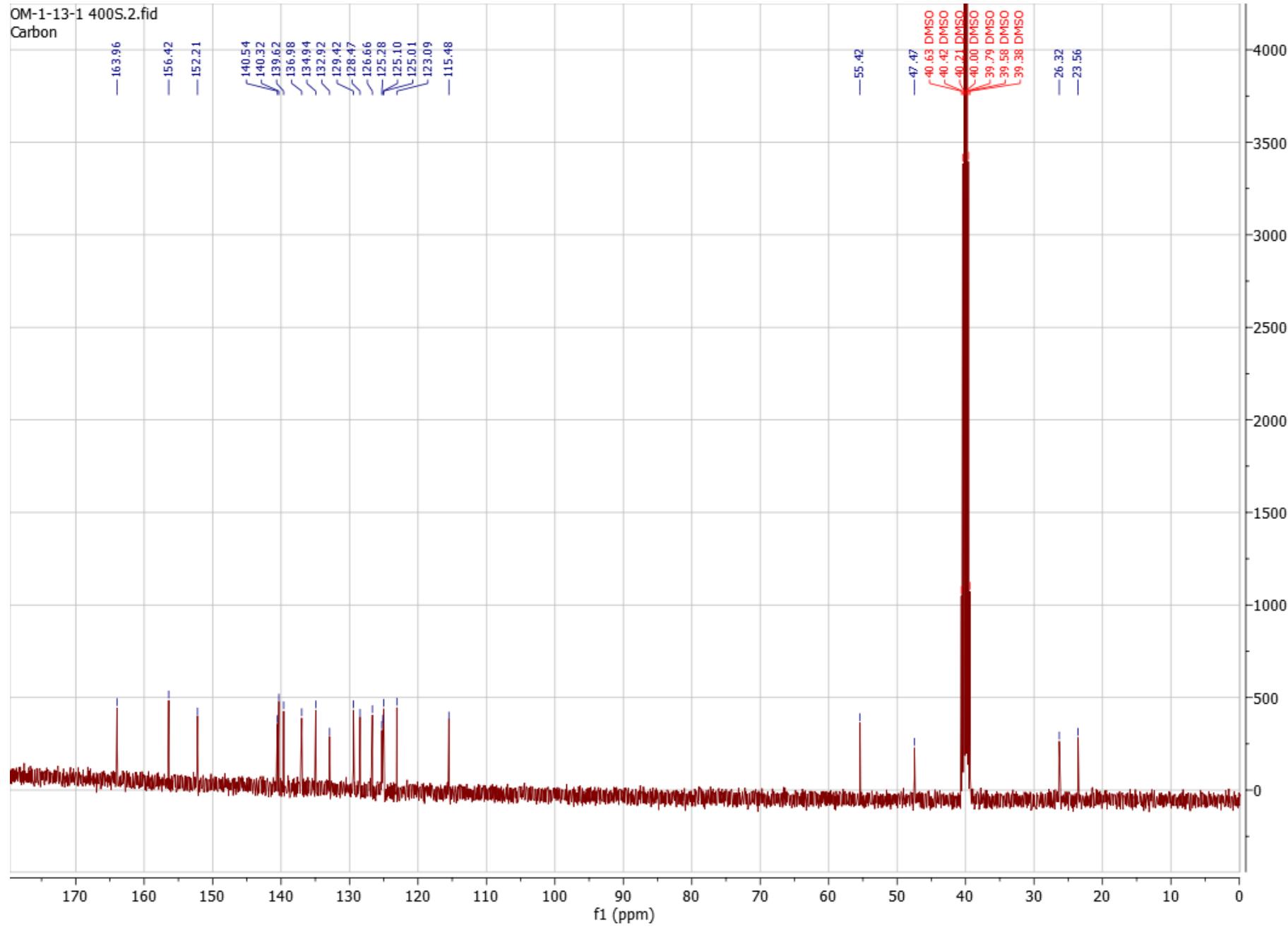


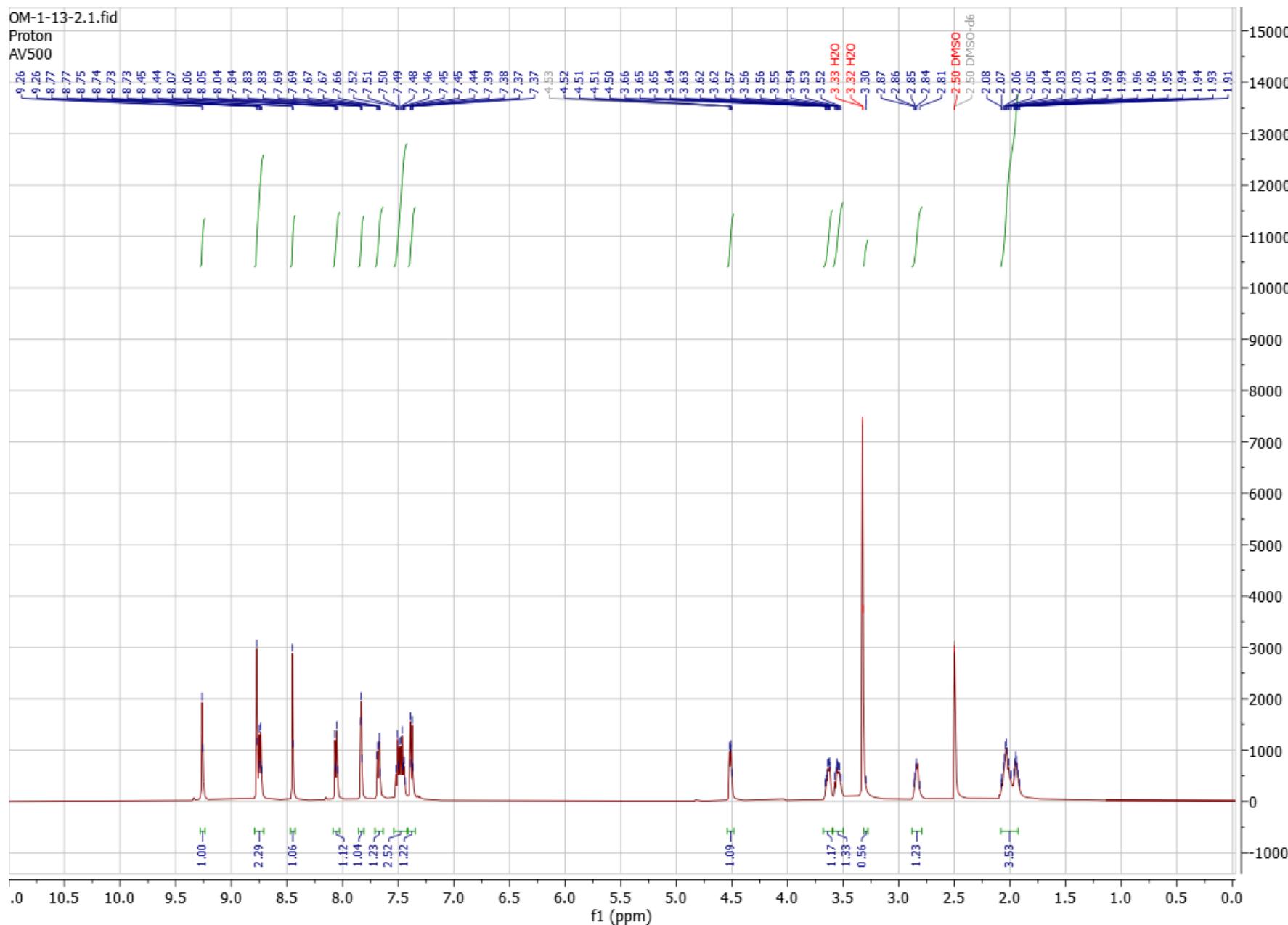
**SI 15:**  $^1\text{H}$  NMR spectrum of 4h [400 MHz,  $\text{CDCl}_3\text{-}d$ ]



**SI 16:**  $^{13}\text{C}$  NMR spectrum of 4h [100 MHz,  $\text{CDCl}_3\text{-}d$ ]

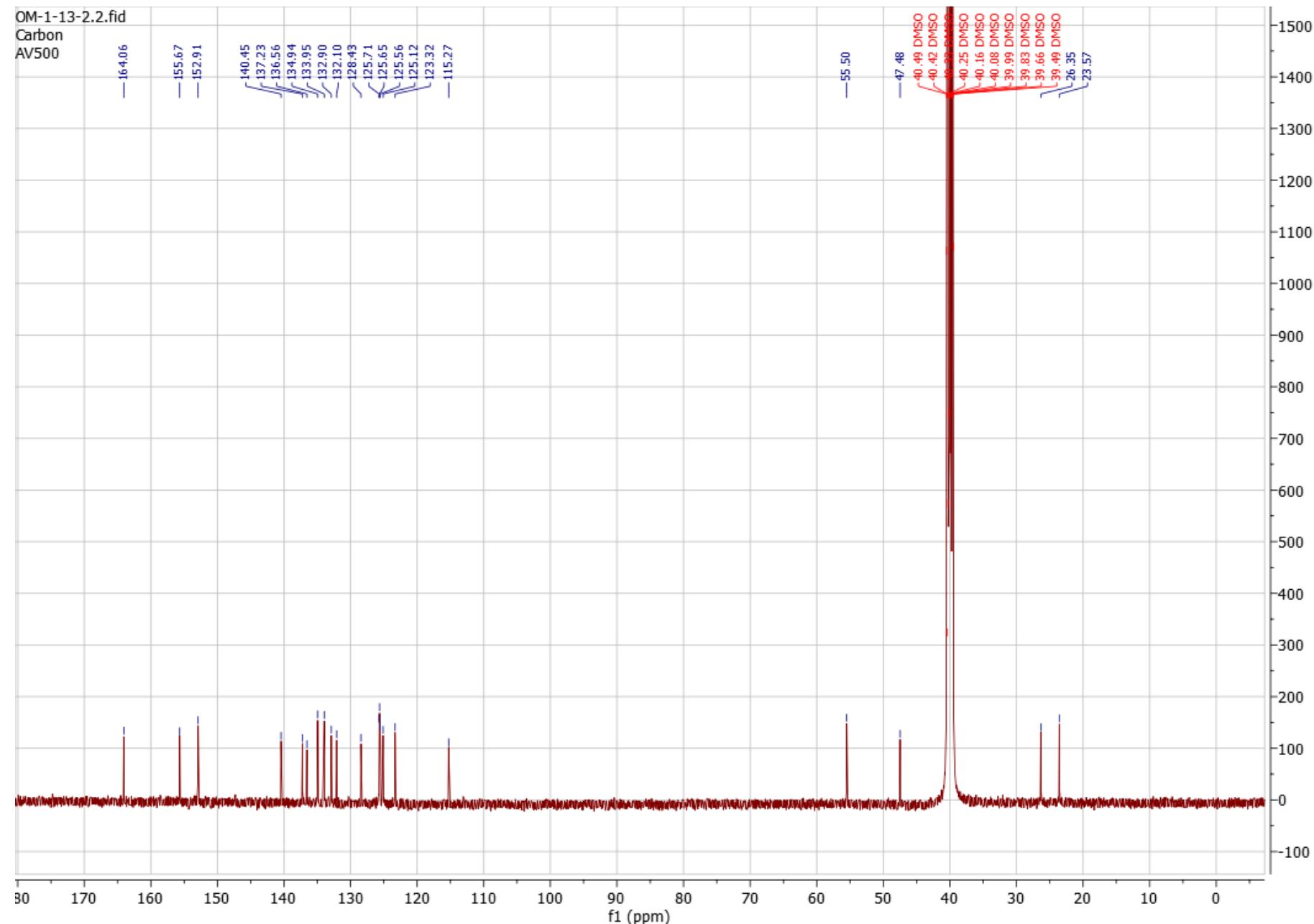
SI 17:  $^1\text{H}$  NMR spectrum of 4i [400 MHz,  $\text{DMSO}-d_6$ ]

SI 18:  $^{13}\text{C}$  NMR spectrum of 4i [400 MHz,  $\text{DMSO}-d_6$ ]

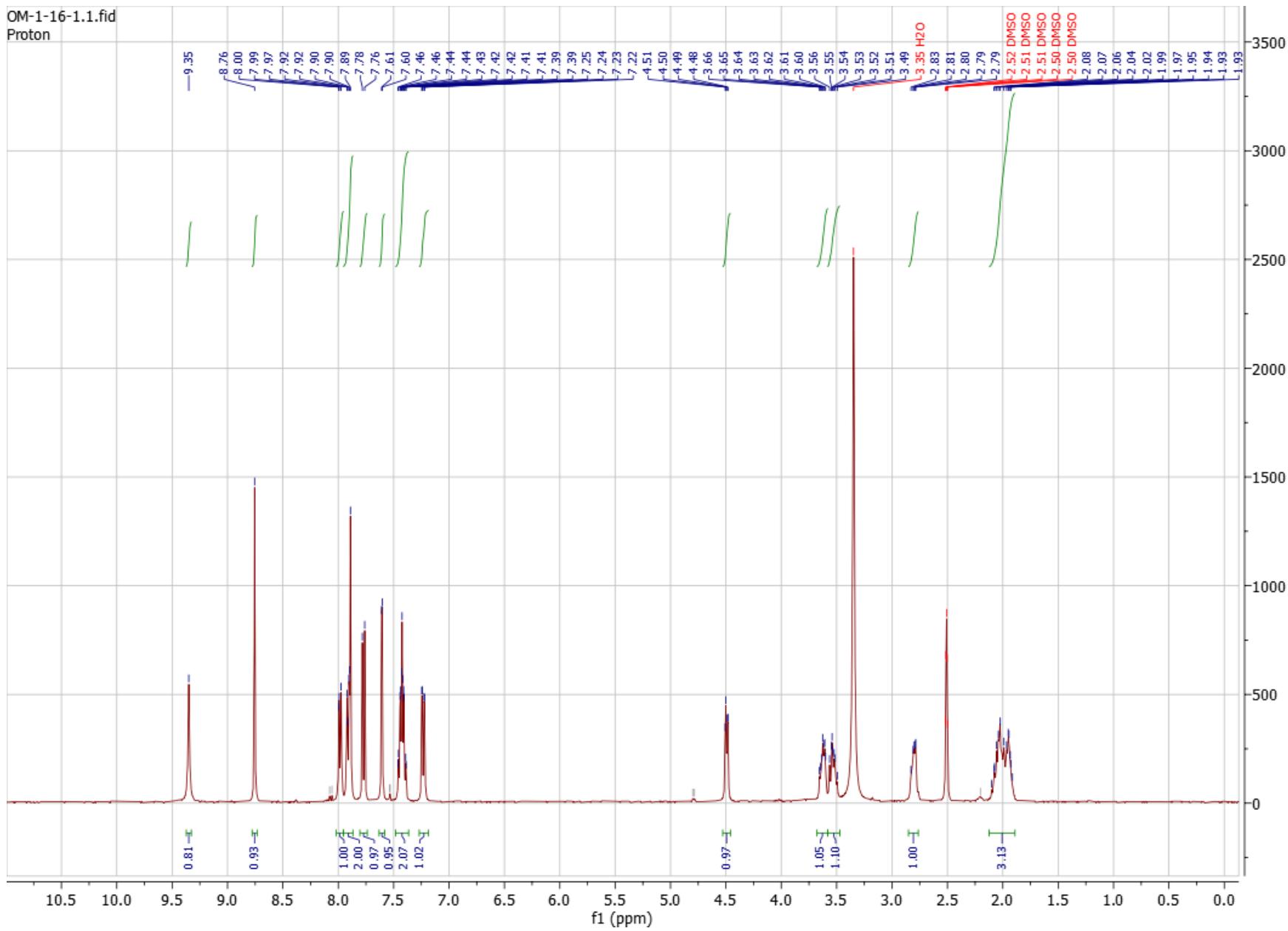


**SI 19:**  $^1\text{H}$  NMR spectrum of 4j [500 MHz, DMSO-*d*6]

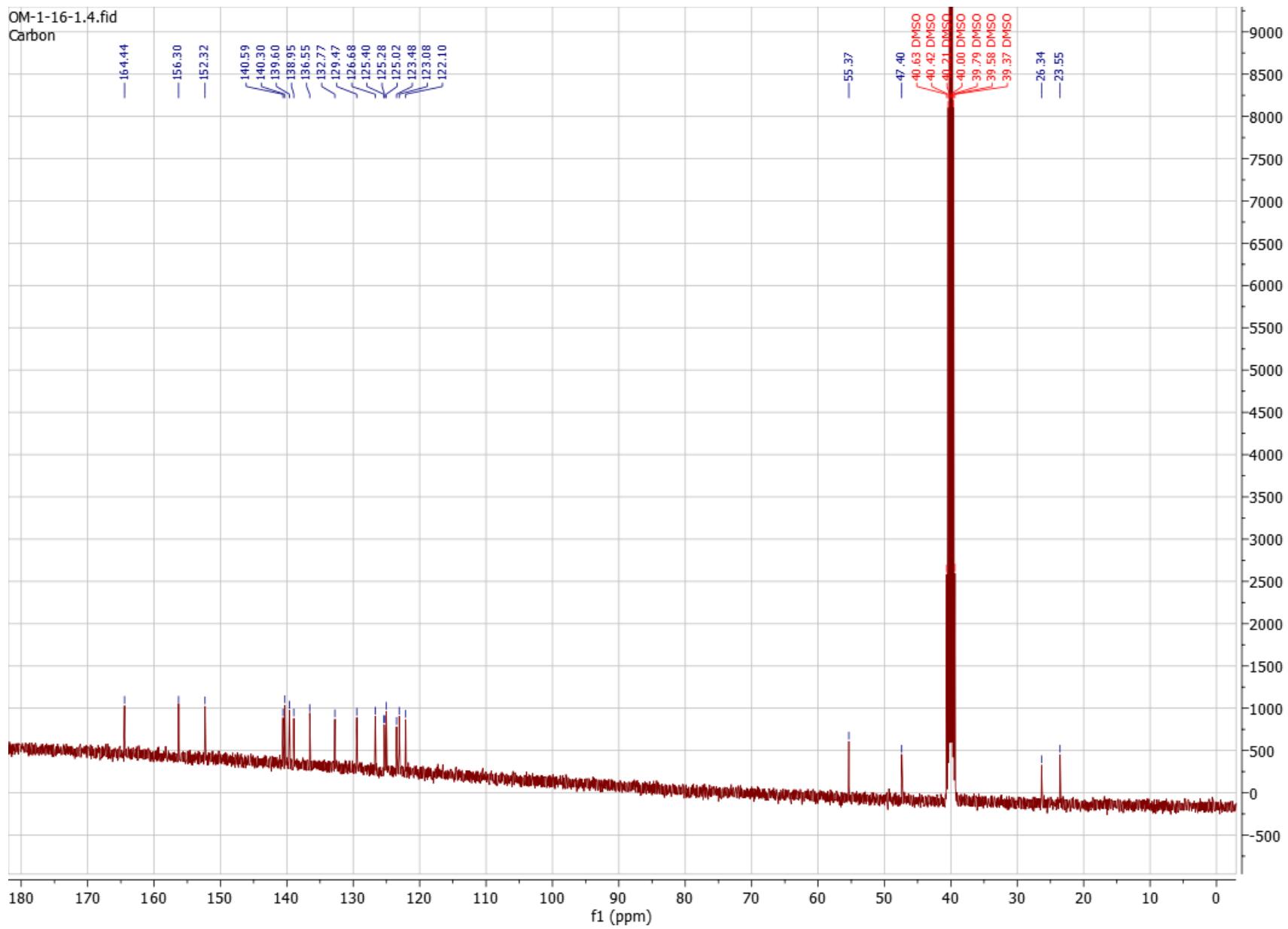
OM-1-13-2.2.fid  
Carbon  
AV500



SI20:  $^{13}\text{C}$  NMR spectrum of 4j [125 MHz,  $\text{DMSO}-d_6$



**SI21:**  $^1\text{H}$  NMR spectrum of 4k [400 MHz, DMSO-*d*6]

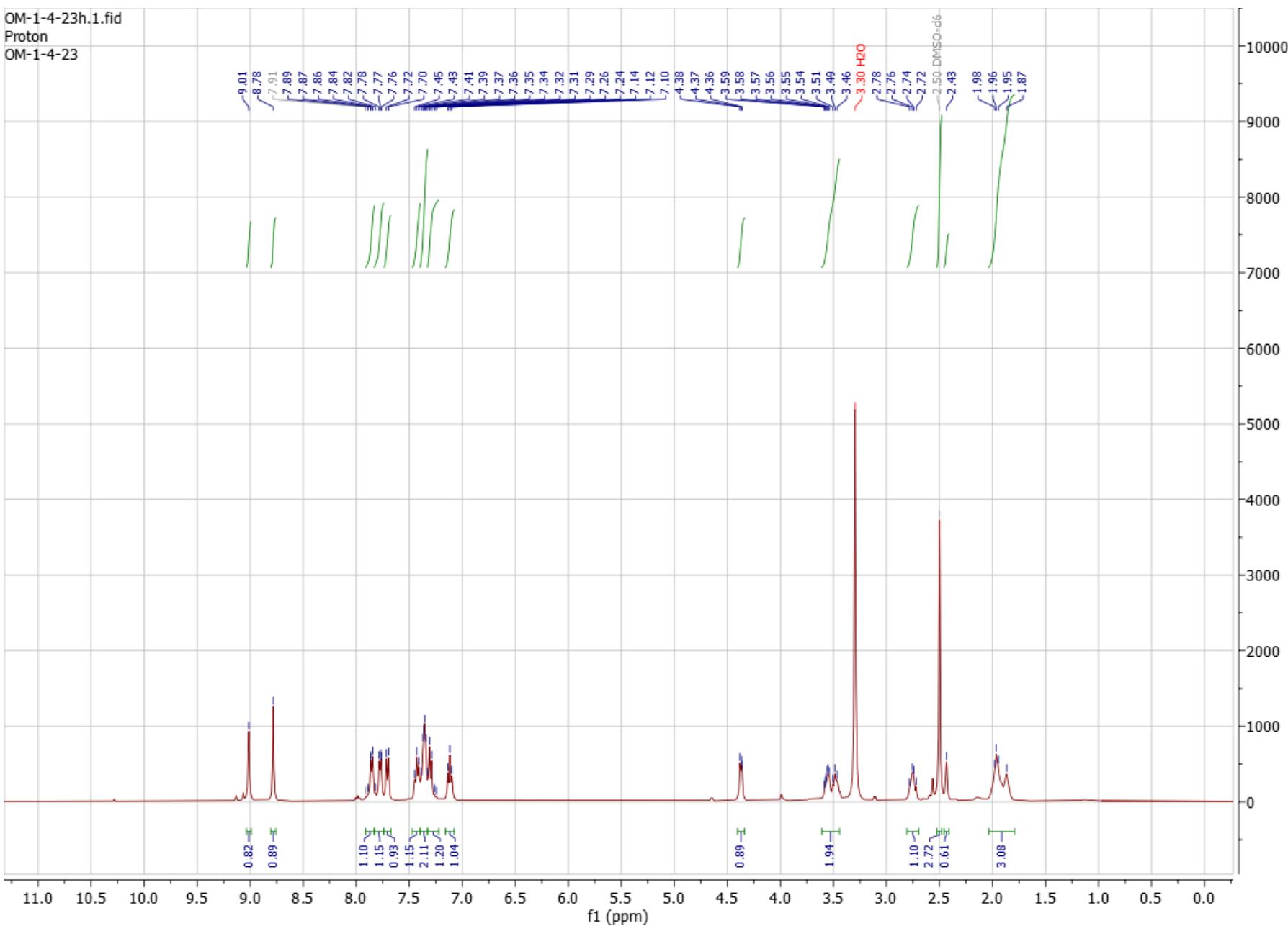


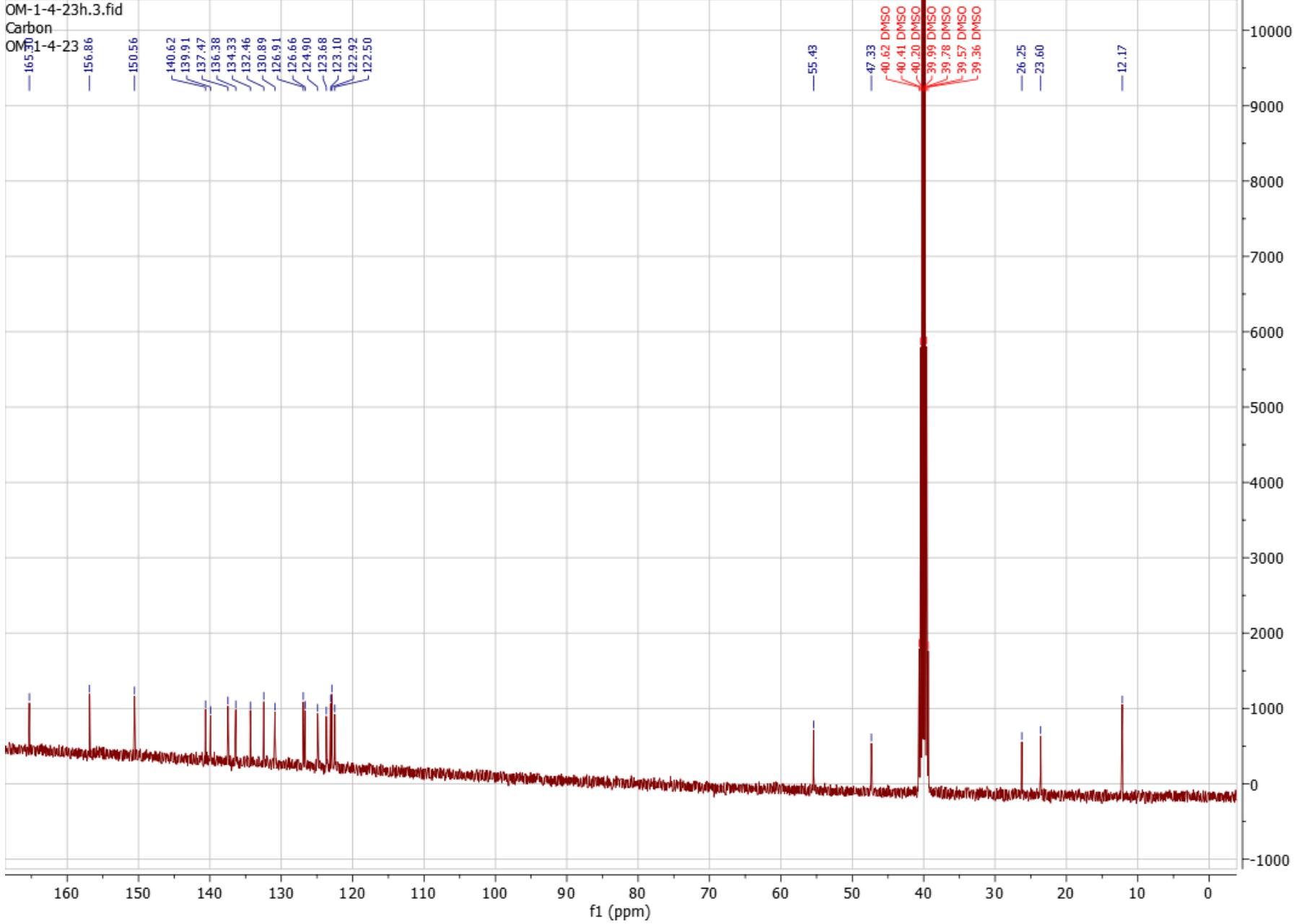
**SI22:**  $^{13}\text{C}$  NMR spectrum of 4k [100 MHz,  $\text{DMSO}-d_6$ ]

OM-1-4-23h.1.fid

Proton

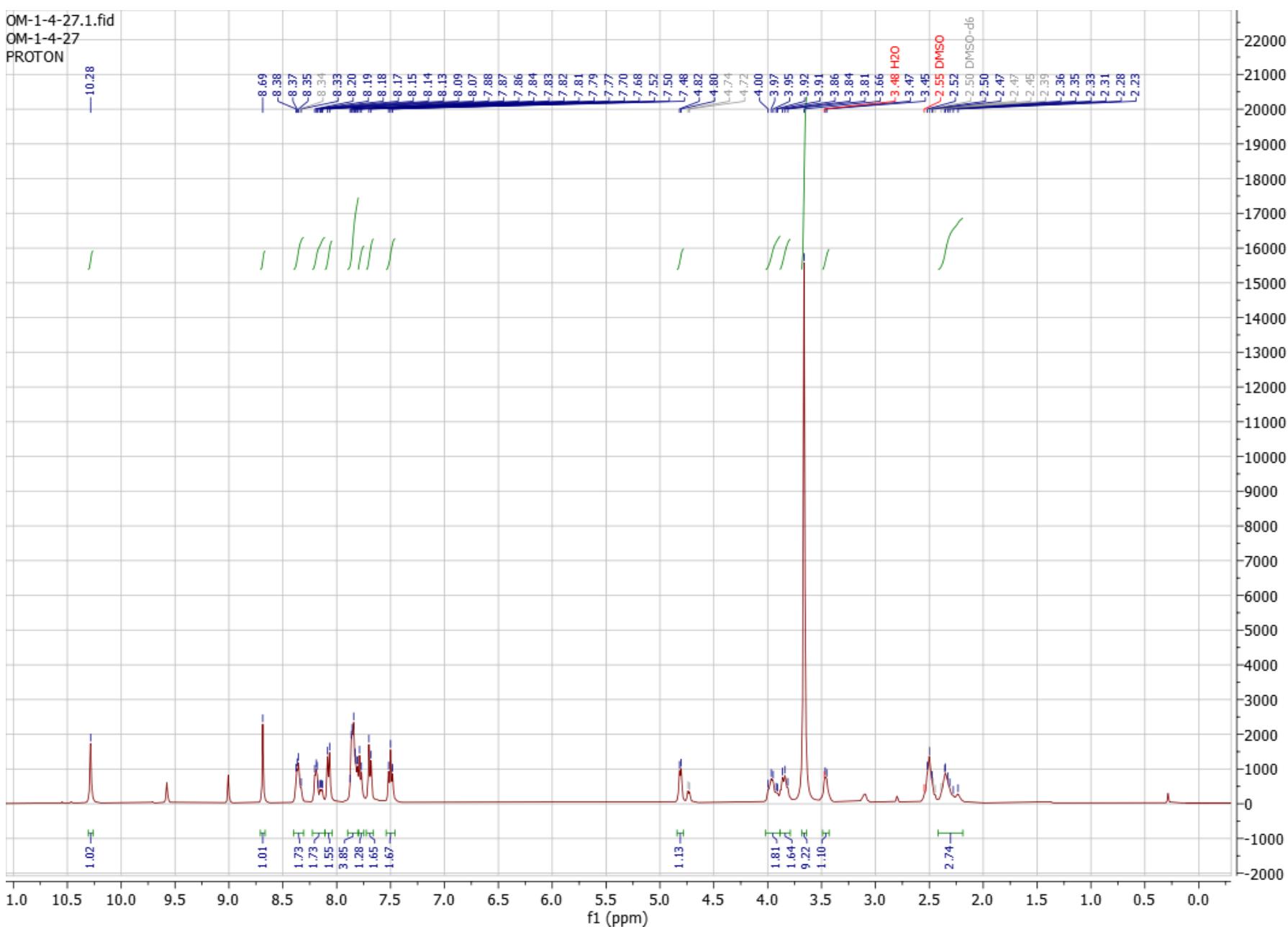
OM-1-4-23

SI23:  $^1\text{H}$  NMR spectrum of 41 [400 MHz, DMSO- $d_6$ ]

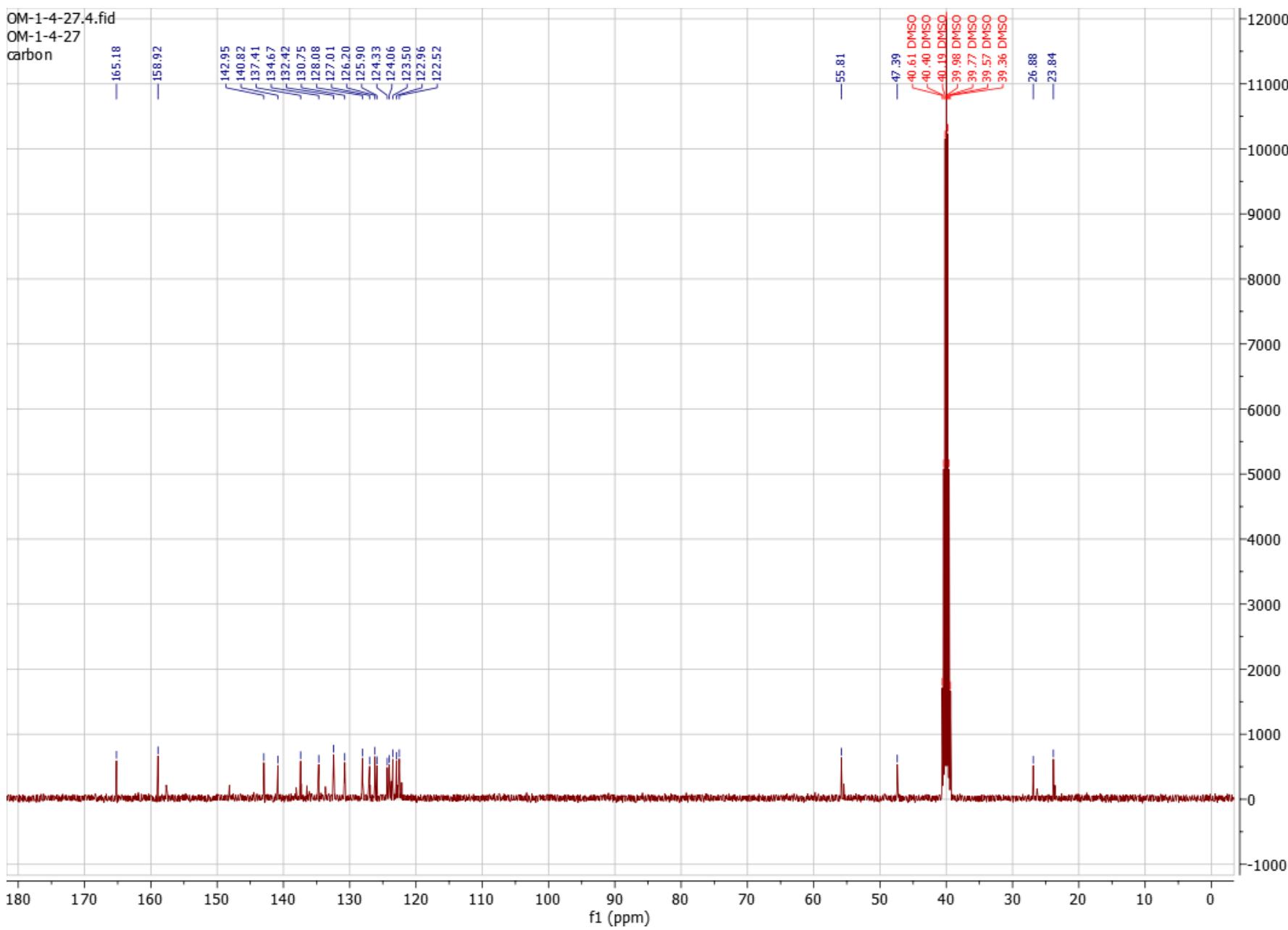


SI24:  $^{13}\text{C}$  NMR spectrum of 41 [100 MHz,  $\text{DMSO}-d_6$ ]

OM-1-4-27.1.fid  
OM-1-4-27  
PROTON

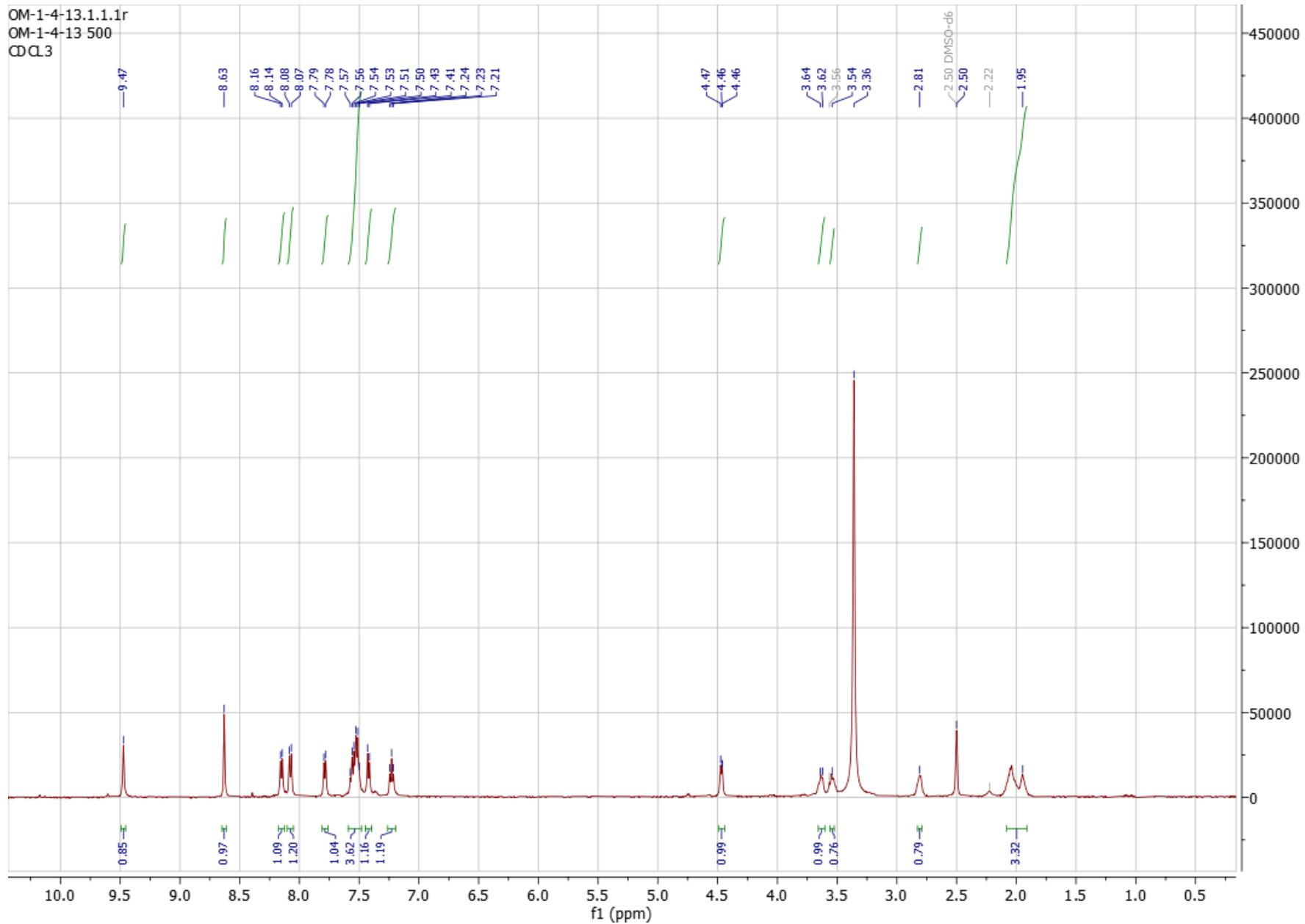


SI25:  $^1\text{H}$  NMR spectrum of 4m [400 MHz, DMSO-*d*6]



**SI26:**  $^{13}\text{C}$  NMR spectrum of 4m [100 MHz,  $\text{DMSO}-d_6$ ]

OM-1-4-13.1.1.1r  
OM-1-4-13 500  
CDCl<sub>3</sub>



SI27: <sup>1</sup>H NMR spectrum of 4n [500 MHz, DMSO-*d*6]

OM-1-4-13.2.fid  
OM-1-4-13 500  
CDCl<sub>3</sub>

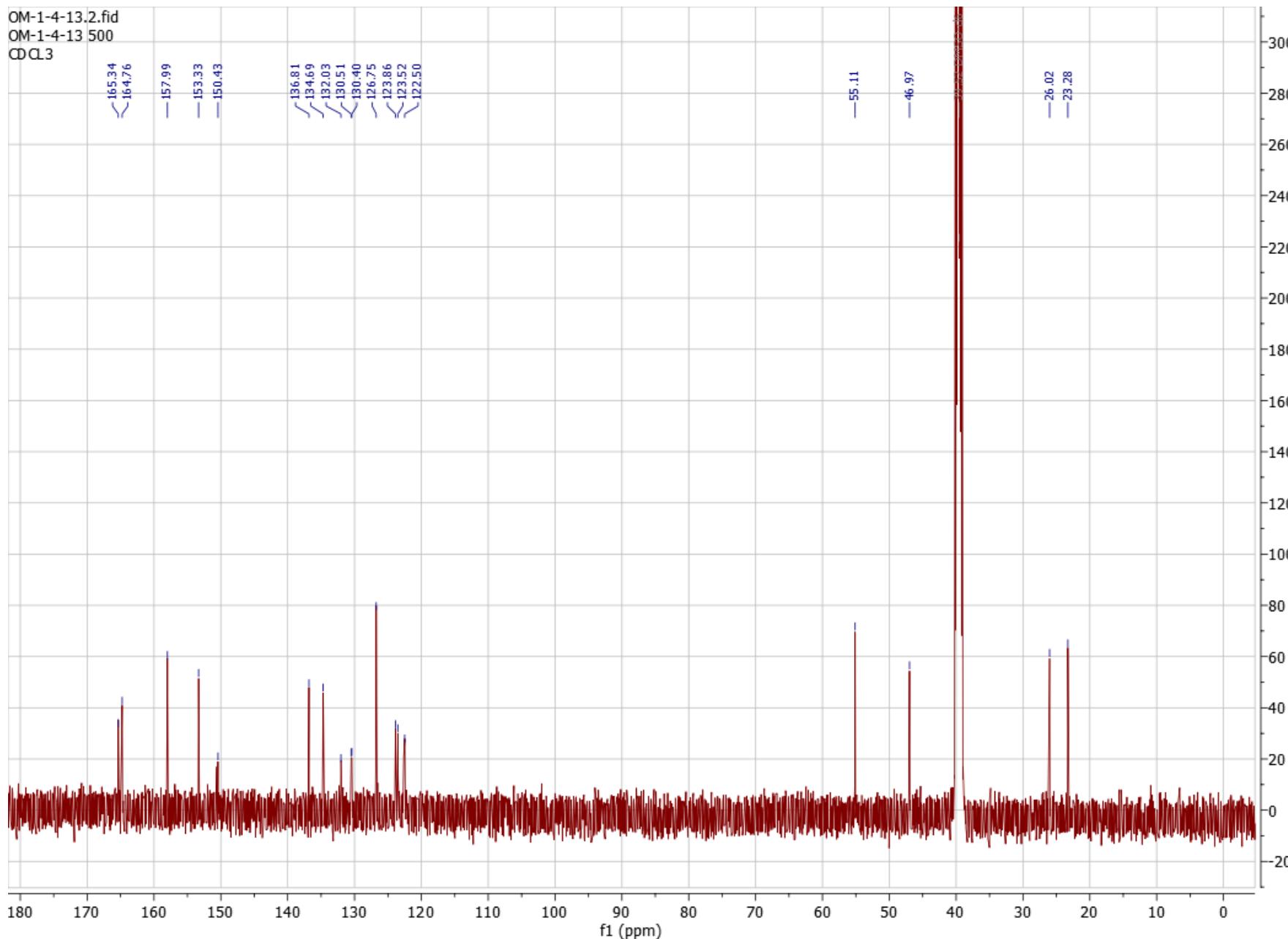
— 165.34  
— 164.76  
— 157.99  
— 153.33  
— 150.43

✓ 136.81  
✓ 134.69  
✓ 132.03  
✓ 130.51  
✓ 130.40  
— 126.75  
— 123.86  
✓ 123.52  
✓ 122.50

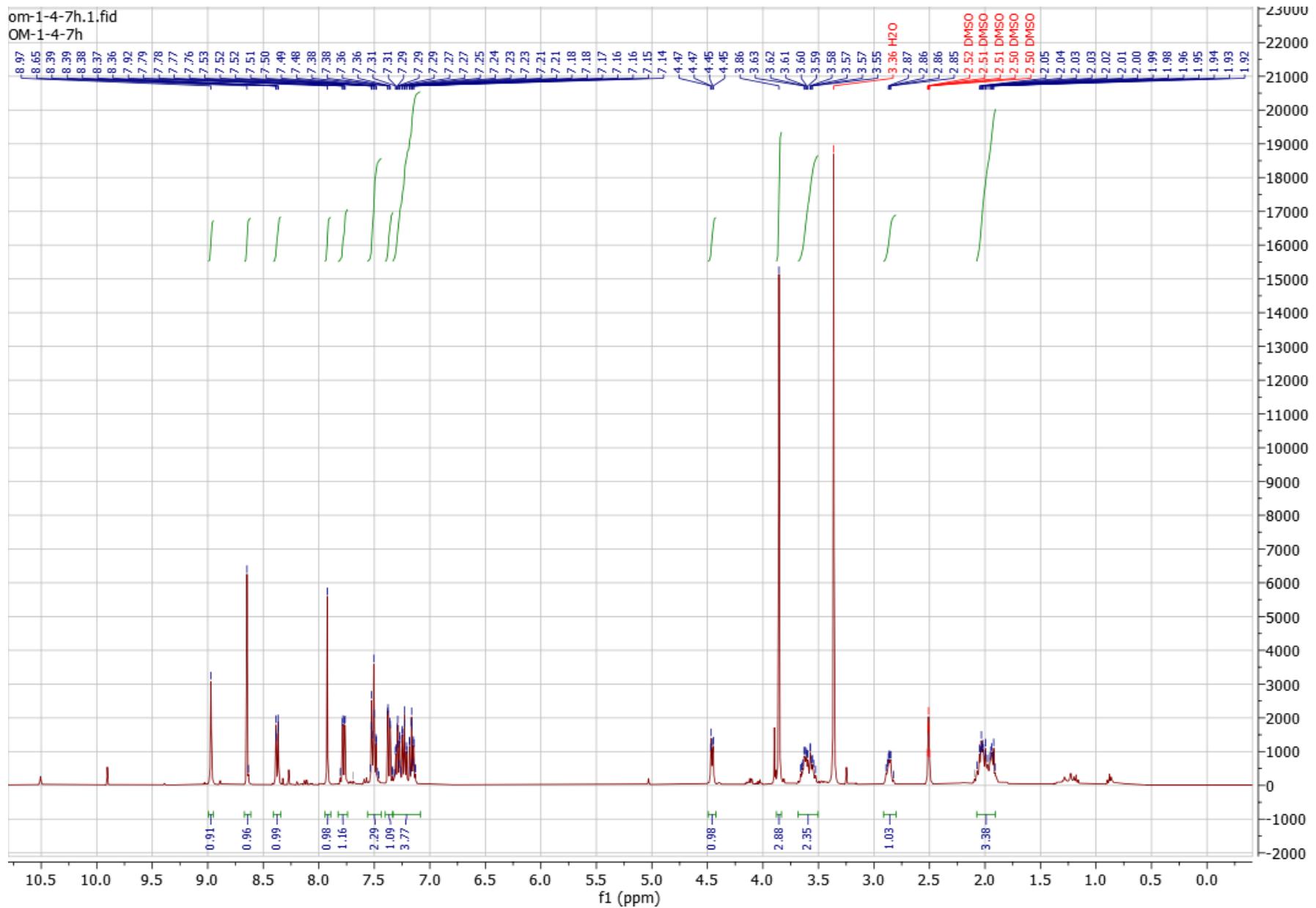
— 55.11

— 46.97

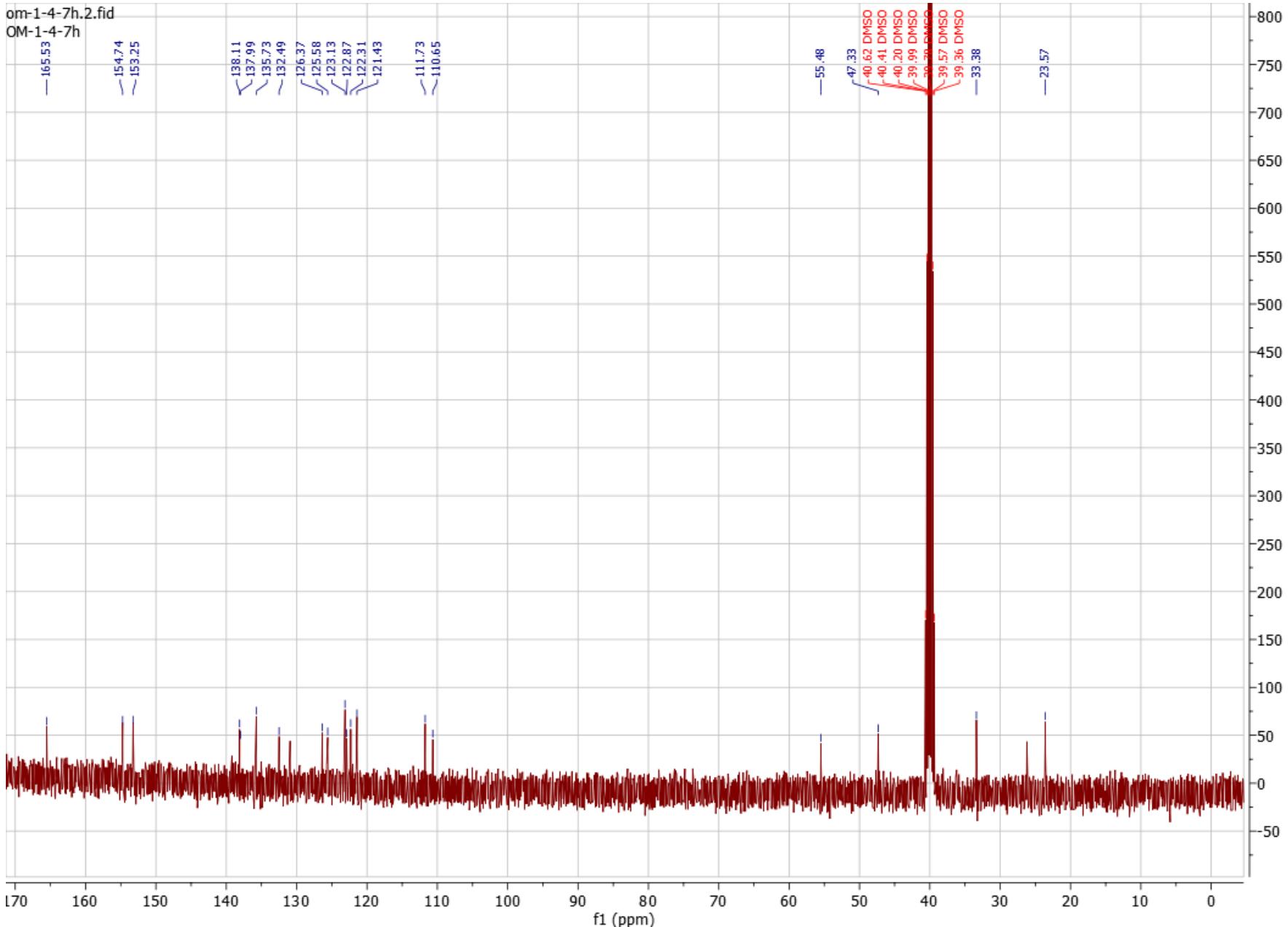
— 26.02  
— 23.28



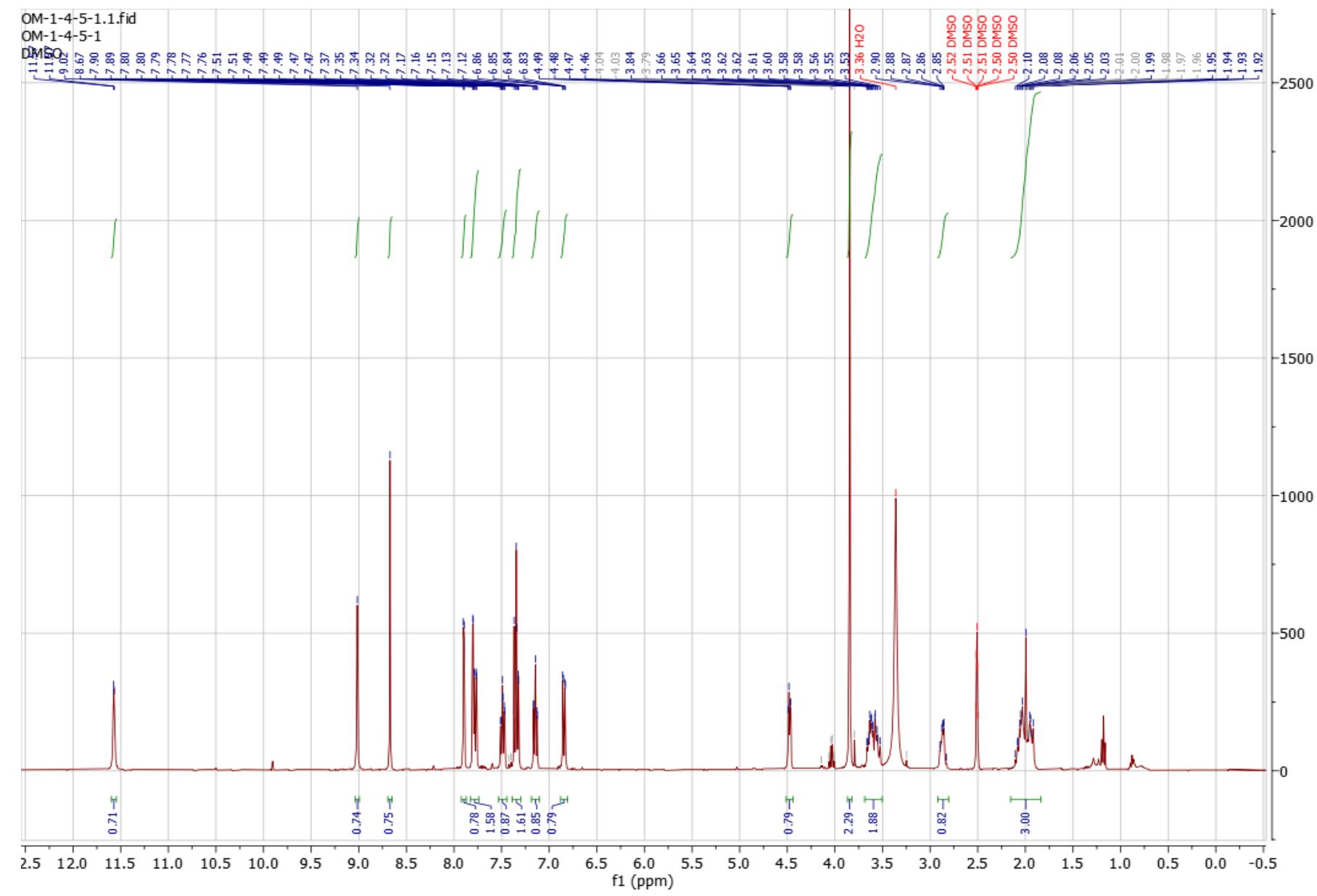
SI28: <sup>13</sup>C NMR spectrum of 4n [125 MHz, DMSO-*d*6]



**SI29:**  $^1\text{H}$  NMR spectrum of 4o [400 MHz, DMSO-*d*6]

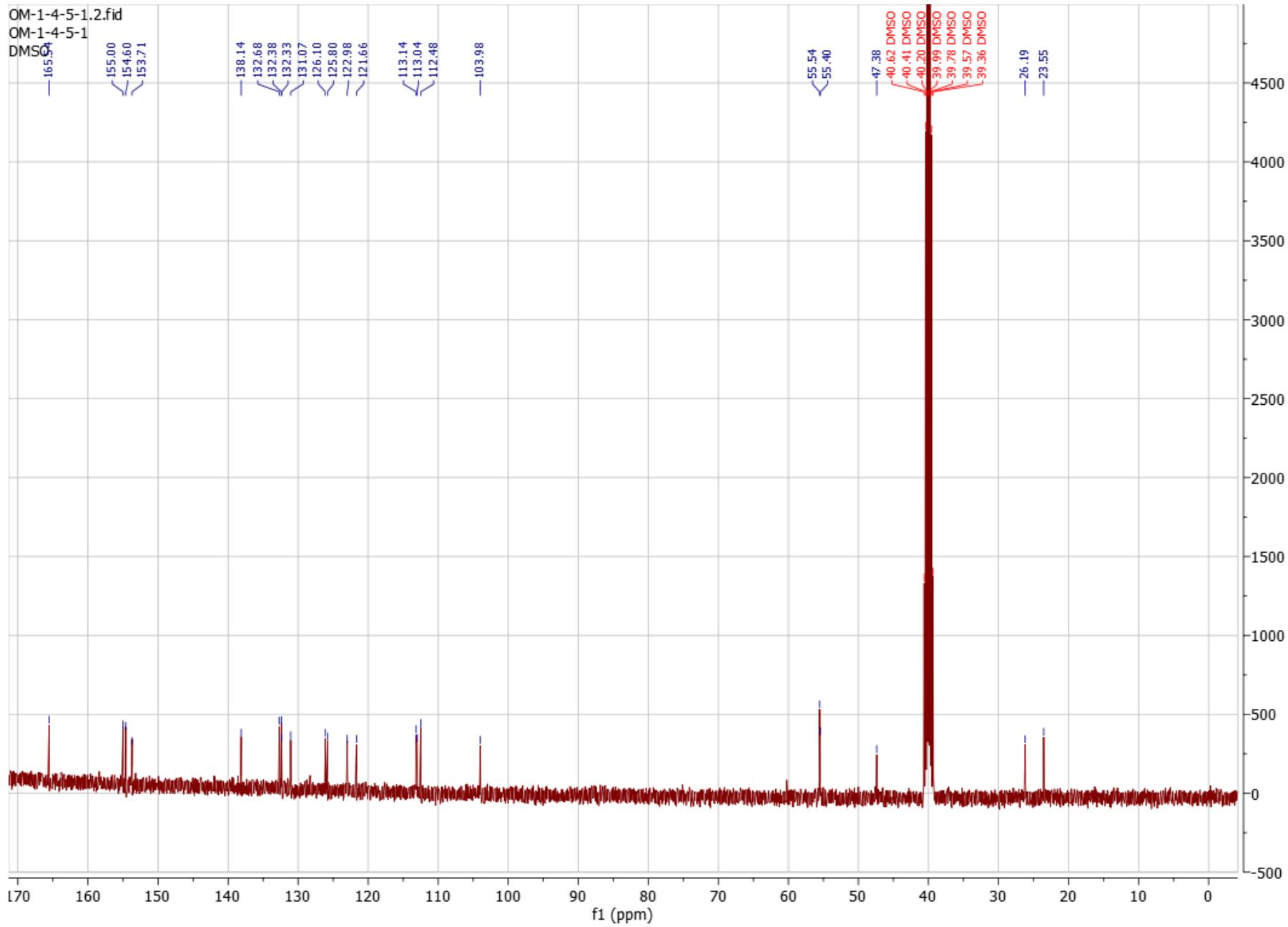


SI30:  $^{13}\text{C}$  NMR spectrum of 4o [100 MHz,  $\text{DMSO}-d_6$ ]



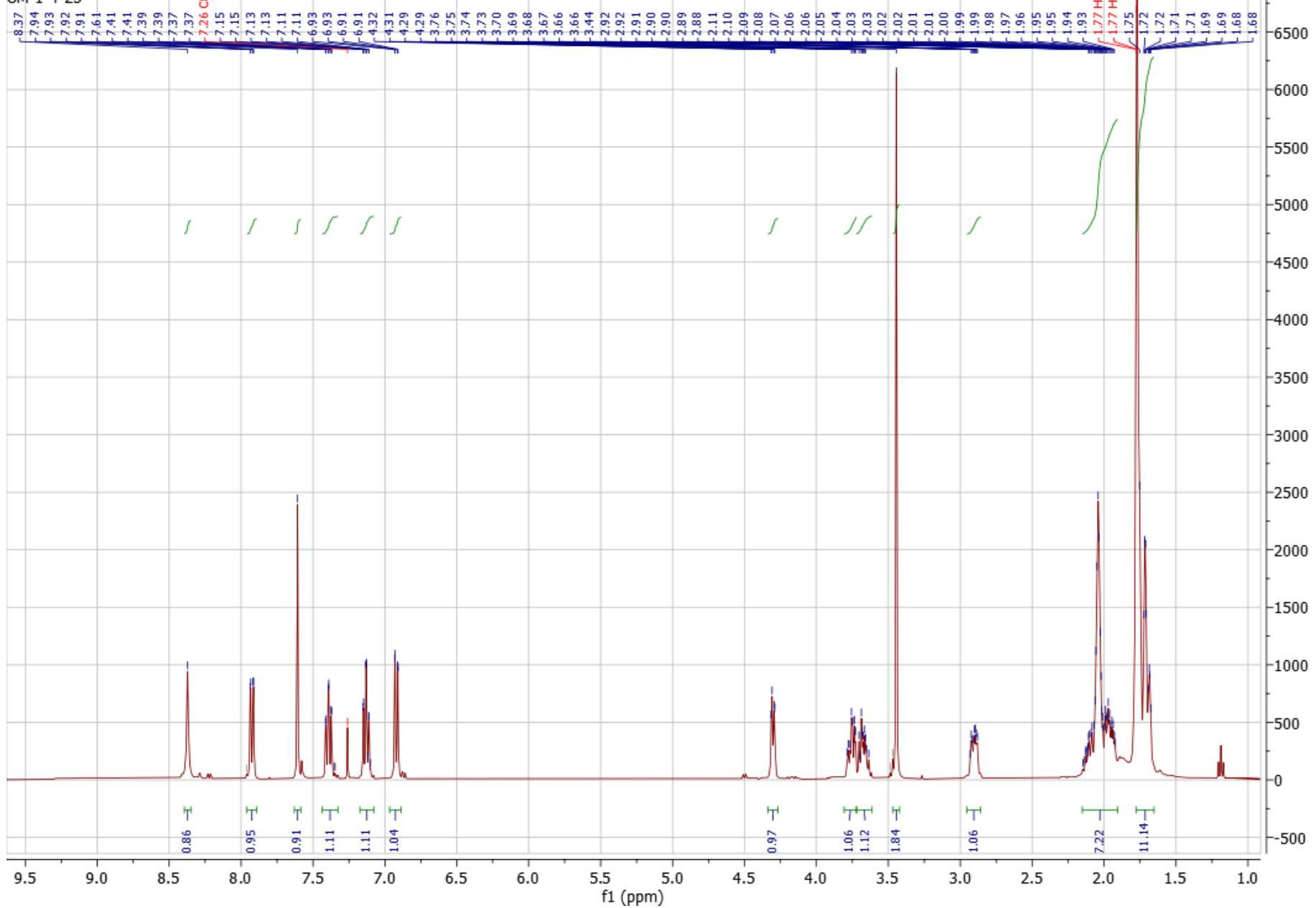
**SI31:**  $^1\text{H}$  NMR spectrum of 4p [400 MHz, DMSO-*d*6]

OM-1-4-5-1.2.fid  
OM-1-4-5-1  
DMSO



SI32:  $^{13}\text{C}$  NMR spectrum of 4p [100 MHz, DMSO-*d*6]

OM-1-4-25.1.fid  
OM-1-4-25



SI33:  $^1\text{H}$  NMR spectrum of 4q [400 MHz,  $\text{DMSO}-d_6$ ]

OM-1-4-25.4.fid  
OM-1-4-25

-168.99  
-166.11

-157.01

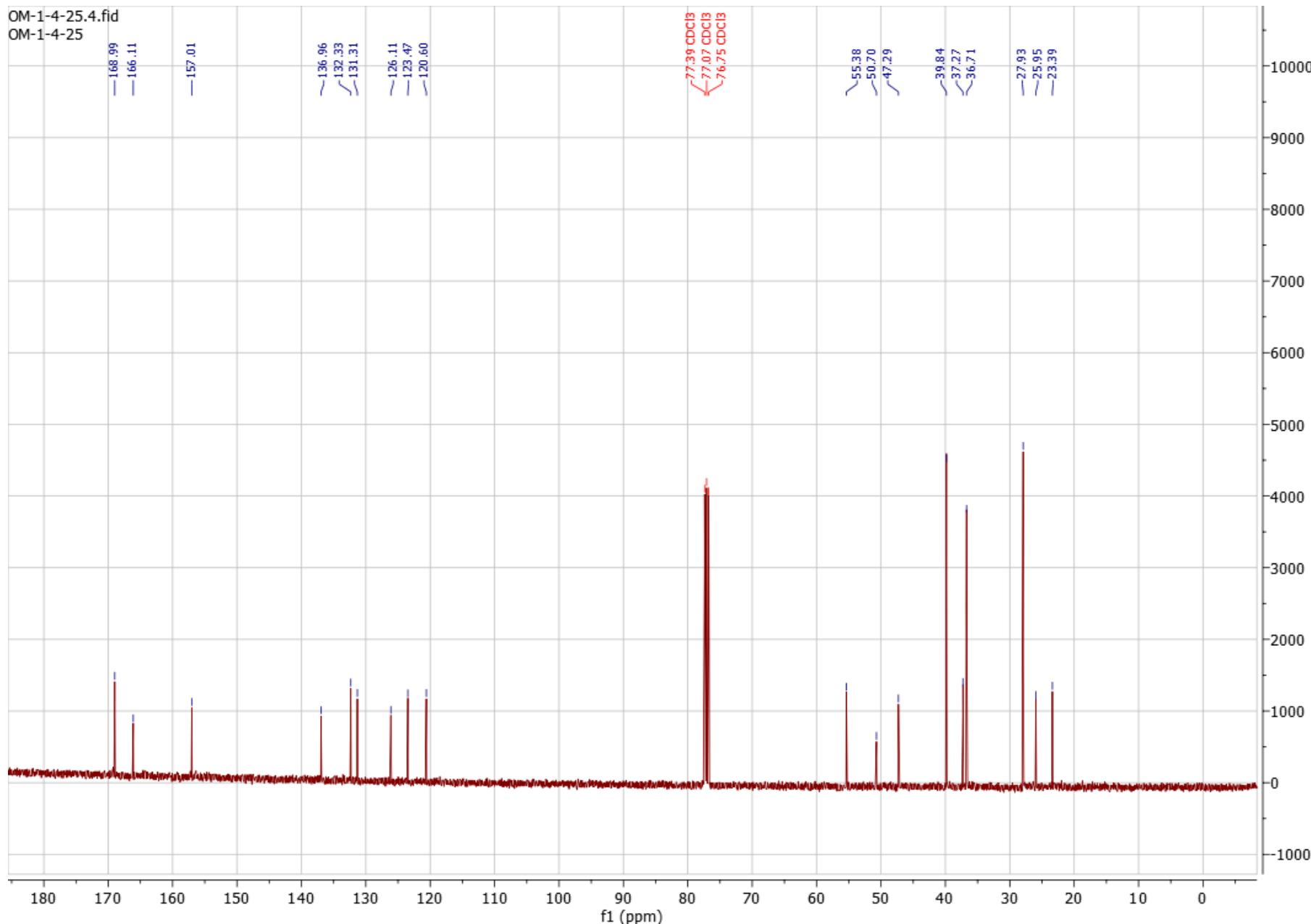
~136.96  
132.33  
131.31  
-126.11  
-123.47  
-120.60

77.39 CDCl<sub>3</sub>  
77.07 CDCl<sub>3</sub>  
76.75 CDCl<sub>3</sub>

55.38  
50.70  
47.29

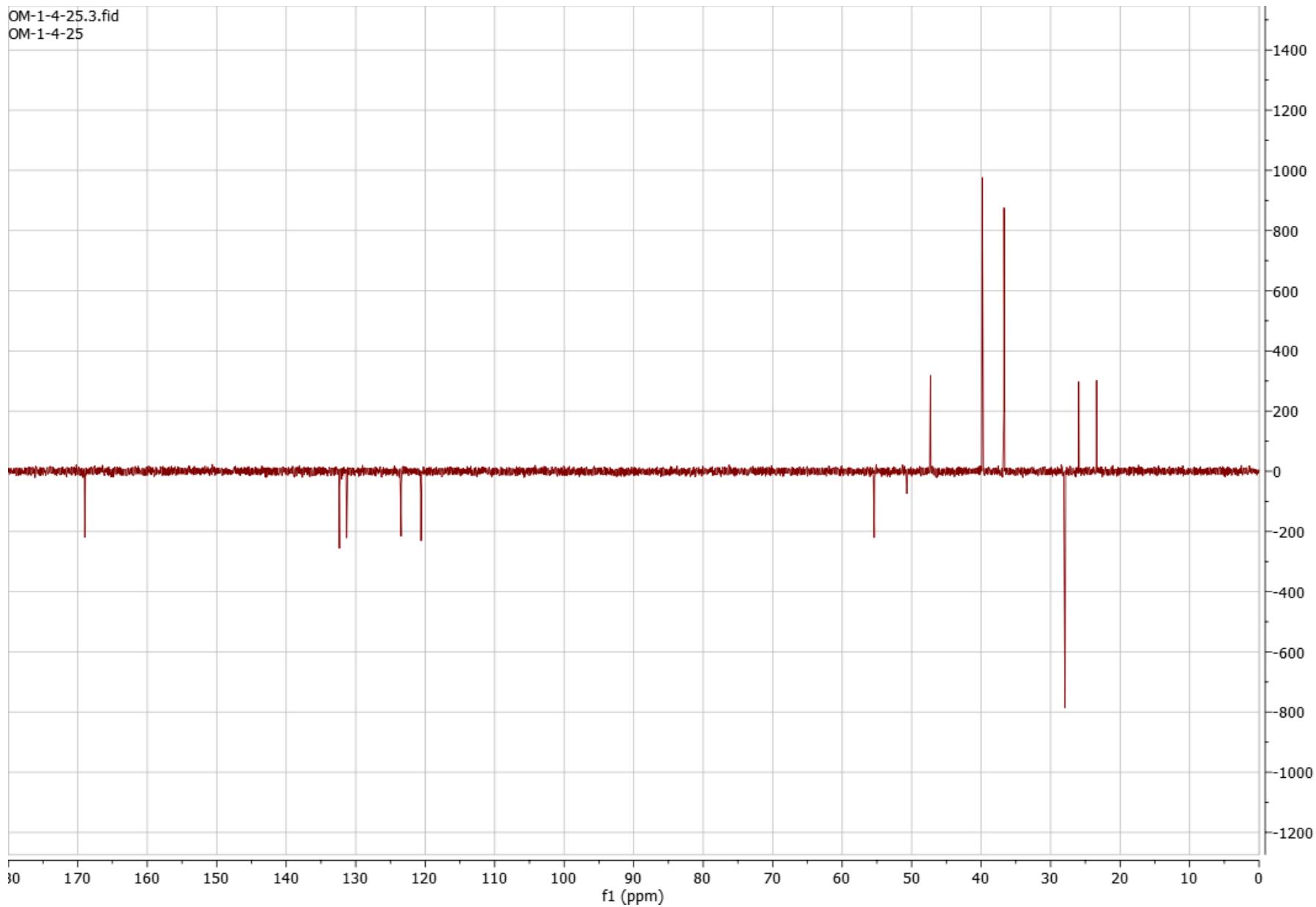
39.84  
37.27  
36.71

-27.93  
-25.95  
-23.39

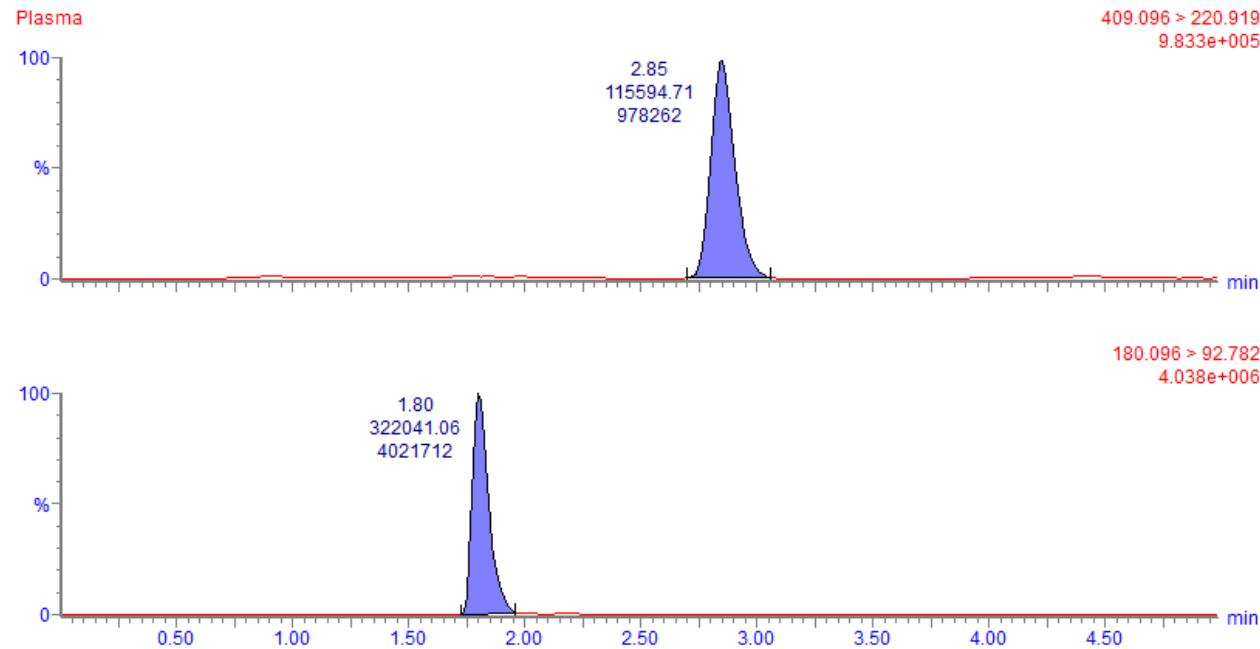


SI34: <sup>13</sup>C NMR spectrum of 4q [100 MHz, DMSO-*d*6]

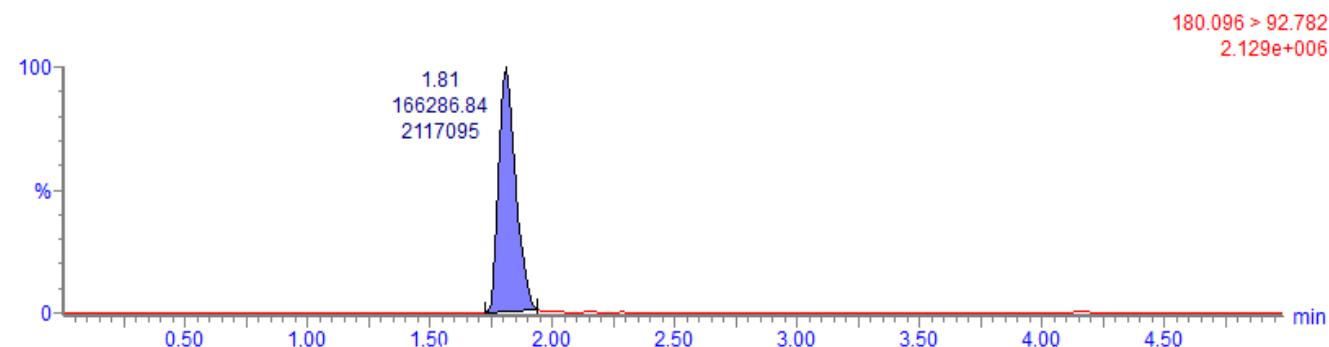
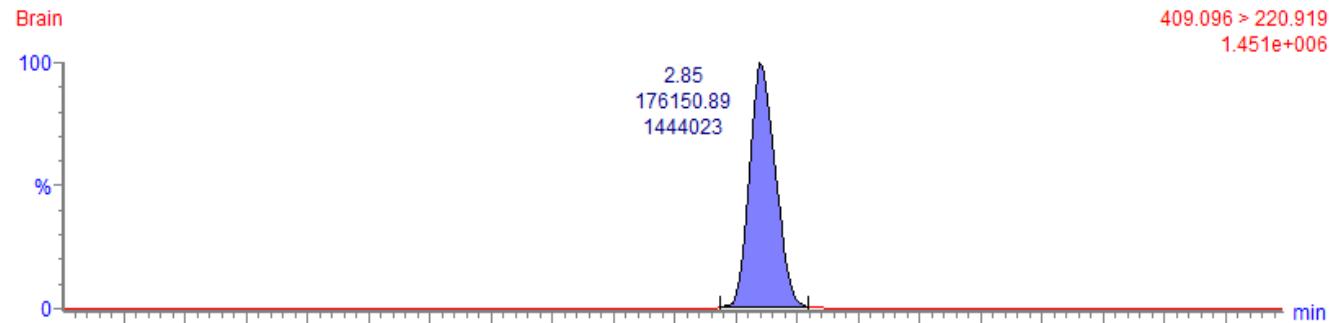
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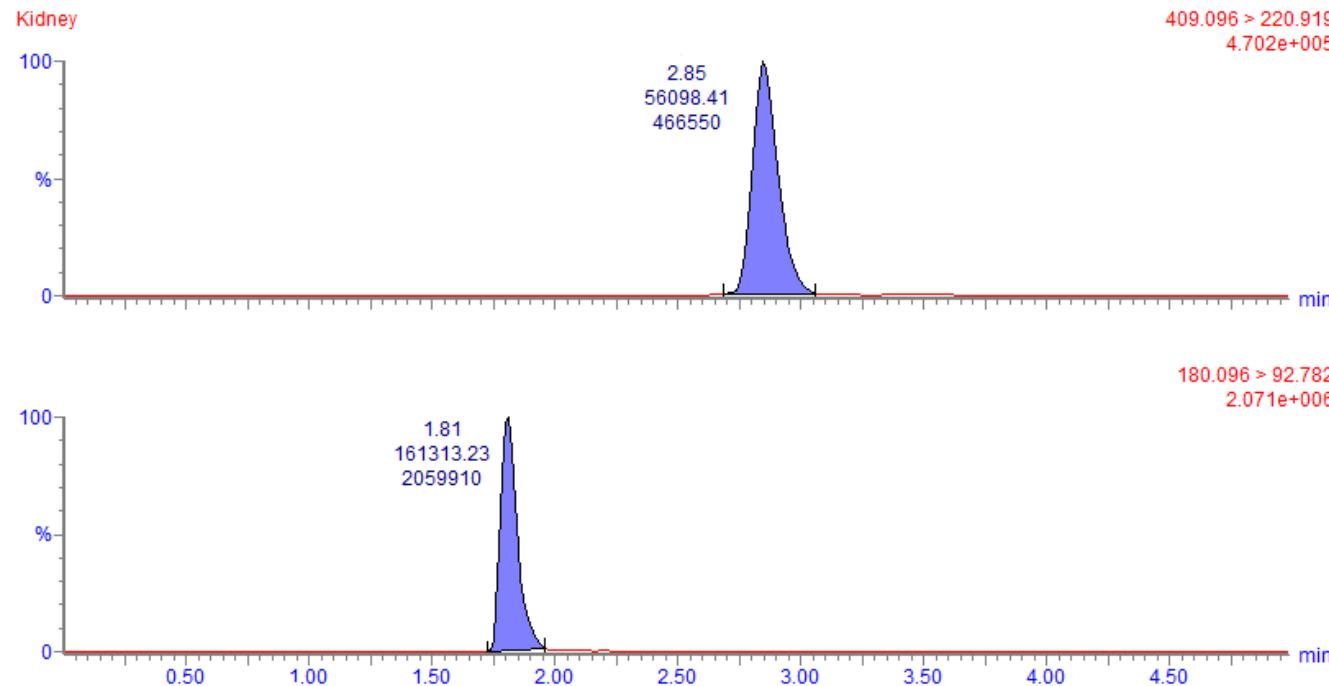
**SI35:** Dept-135 spectrum of 4q [100 MHz, DMSO-*d*6]



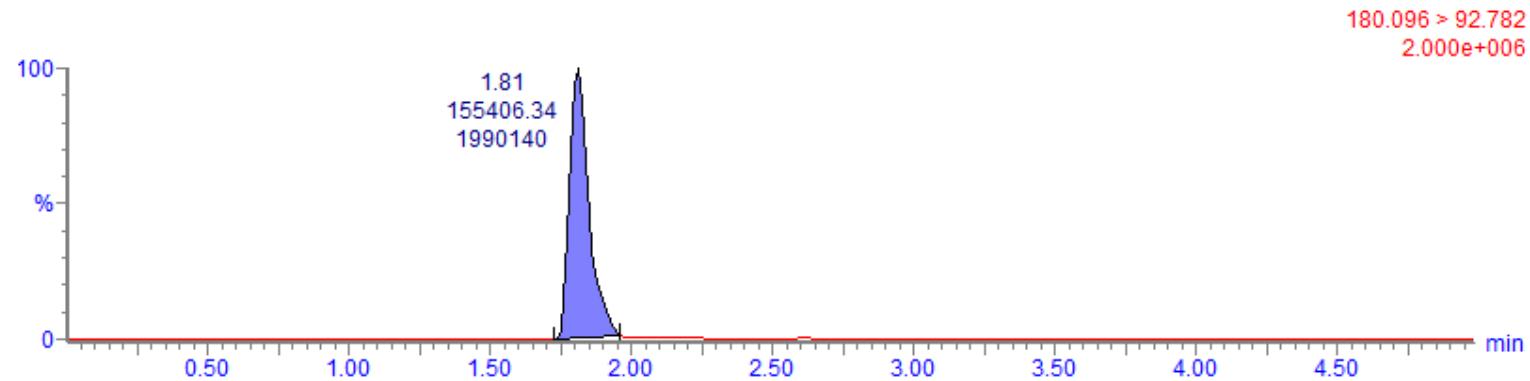
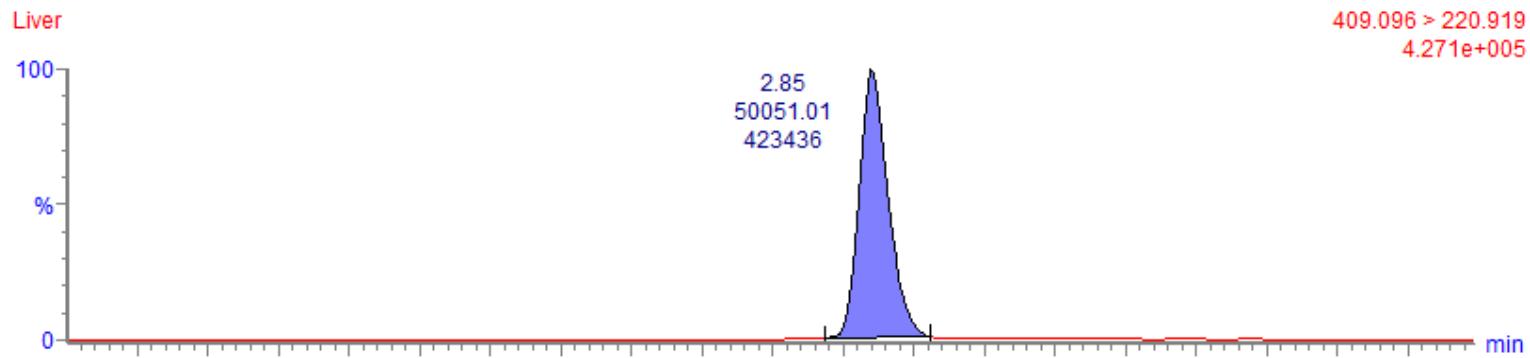
**SI36:** Typical MRM chromatograms of **4k** (top panel) and the IS (below panel) at 0.5 h plasma pharmacokinetic study sample



**SI37:** Typical MRM chromatograms of **4k** (top panel) and the IS (below panel) at 0.5 h brain pharmacokinetic study sample



**SI38:** Typical MRM chromatograms of **4k** (top panel) and the IS (below panel) at 0.5 h kidney pharmacokinetic study sample



**SI39:** Typical MRM chromatograms of **4k** (top panel) and the IS (below panel) at 0.5 h liver pharmacokinetic study sample