

## Expedited Selection of NMR Chiral Solvating Agents for Determination of Enantiopurity

Lu Yang\*<sup>†</sup>, Thomas Wenzel\*<sup>††</sup>, R. Thomas Williamson<sup>†</sup>, Melodie Christensen<sup>†</sup>, Wes Schafer<sup>†</sup>, Christopher J. Welch\*<sup>†</sup>

### Supporting Information:

SI 1. NMR spectra (500 MHz, CDCl<sub>3</sub>) of all screening results showing full enantiodifferentiation. (S4-S58).

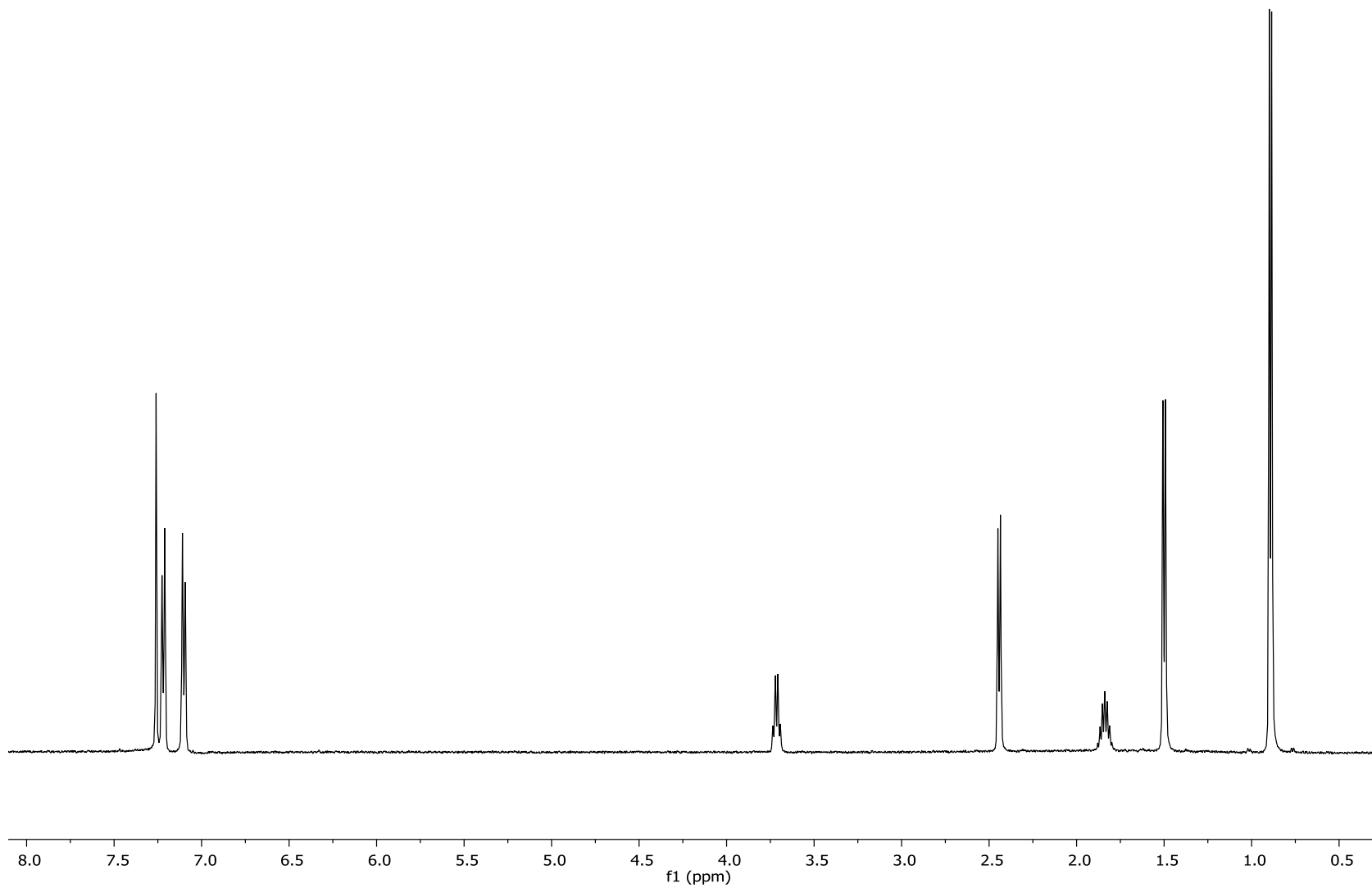
SI 2. A summary of HTE screening results (xlsx)

S4      A (1)  
S5      A (1) – C (13)  
S6      A (1) – C (22)  
S7      A (2)  
S8      A (2) – C (13)  
S9      A (2) – C (22)  
S10     A (3)  
S11     A (3) – C (11)  
S12     A (3) – C (13)  
S13     A (3) – C (28)  
S14     A (4)  
S15     A (4) – C (11)  
S16     A (4) – C (13)  
S17     A (5)  
S18     A (5) – C (8)  
S19     A (5) – C (9)  
S20     A (5) – C (17)  
S21     A (5) – C (25)  
S22     A (5) – C (32)

S23 A (6)  
S24 A (6) – C (5)  
S25 A (6) – C (25)  
S26 A (7)  
S27 A (7) – C (28)  
S28 A (8)  
S29 A (8) – C (30)  
S30 A (8) – C (32)  
S31 A (9)  
S32 A (9) – C (28)  
S33 A (10)  
S34 A (10) – C (32)  
S35 A (13)  
S36 A (13) – C (30)  
S37 A (14)  
S38 A (14) – C (13)  
S39 A (14) – C (21)  
S40 A (14) – C (22)  
S41 A (14) – C (25)  
S42 A (14) – C (28)  
S43 A (14) – C (32)  
S44 A (15)  
S45 A (15) – C (18)  
S46 A (16)  
S47 A (16) – C (7)

- S48 A (16) – C (8)
- S49 A (16) – C (13)
- S50 A (16) – C (22)
- S51 A (16) – C (28)
- S52 A (2) – C (32) <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>).
- S53 A (17)
- S54 A (17) 1D Pure Shift
- S55 A (17) – C (25)
- S56 A (17) – C (25) 1D Pure Shift
- S57 A (17) – C (25) <sup>1</sup>H-<sup>1</sup>H COSY spectrum (500 MHz, CDCl<sub>3</sub>).
- S58 A (17) – C (25) 2D ROESY spectrum (500 MHz, CDCl<sub>3</sub>).

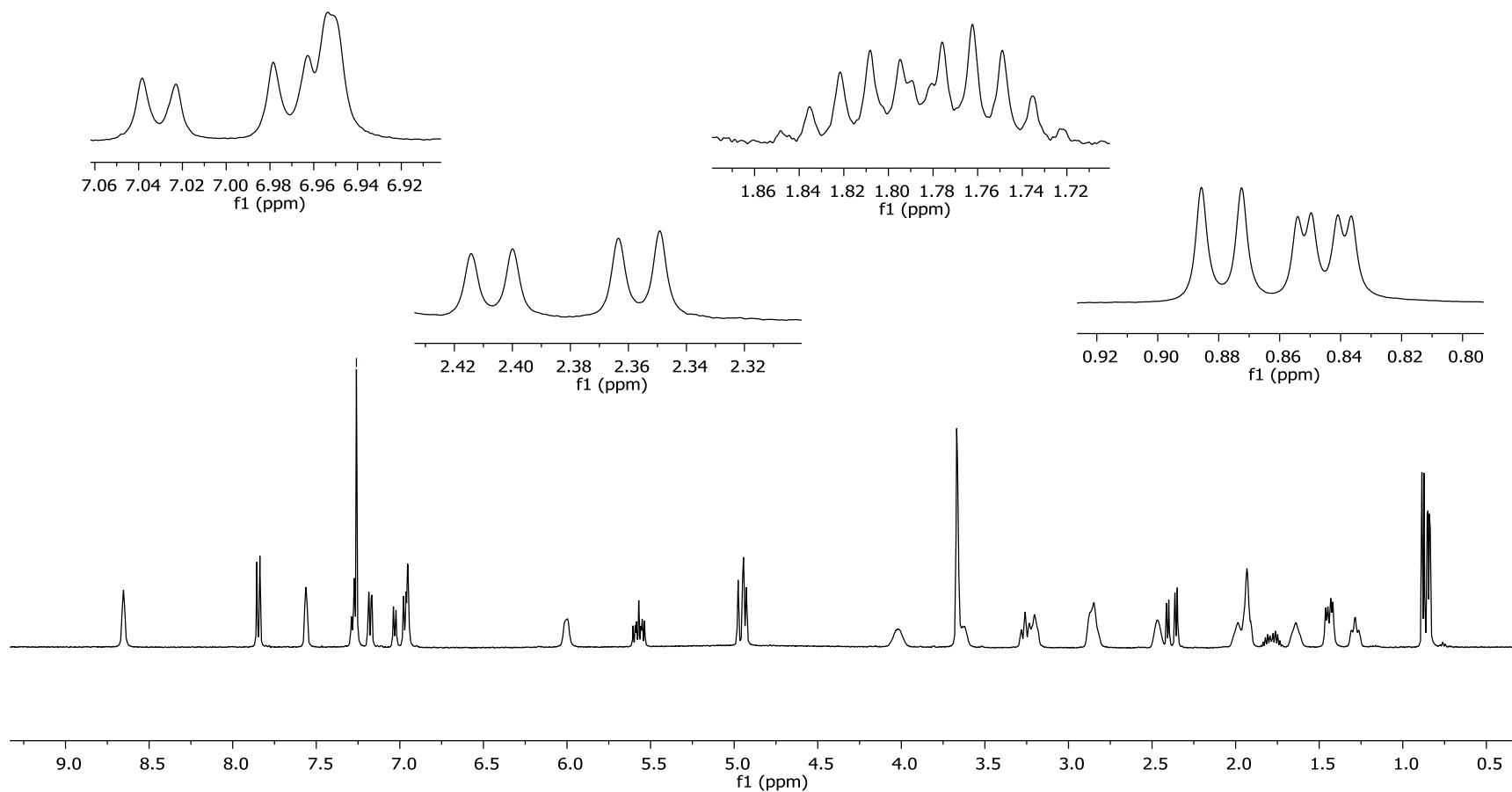
A1



S4

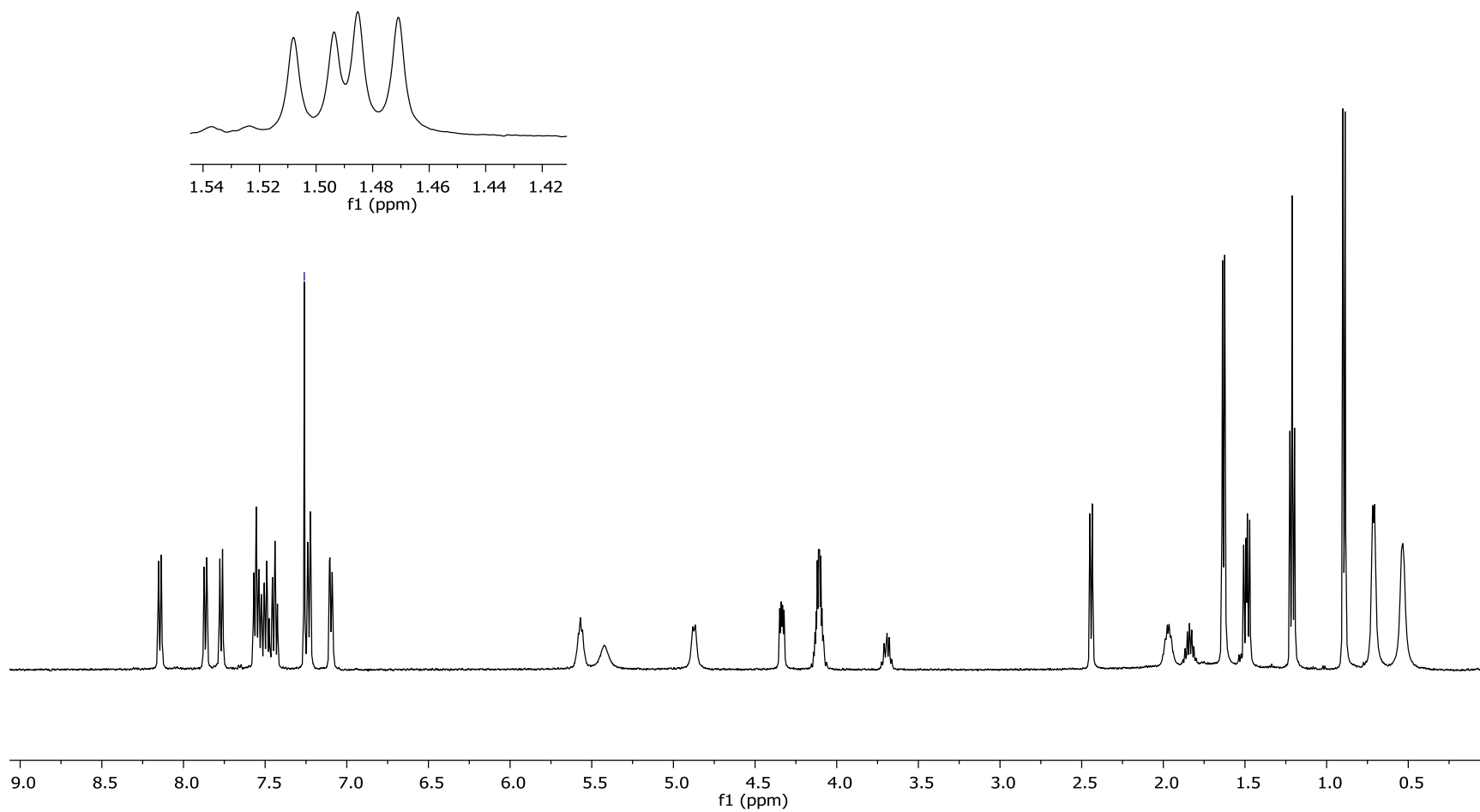
A1-C13

7.26



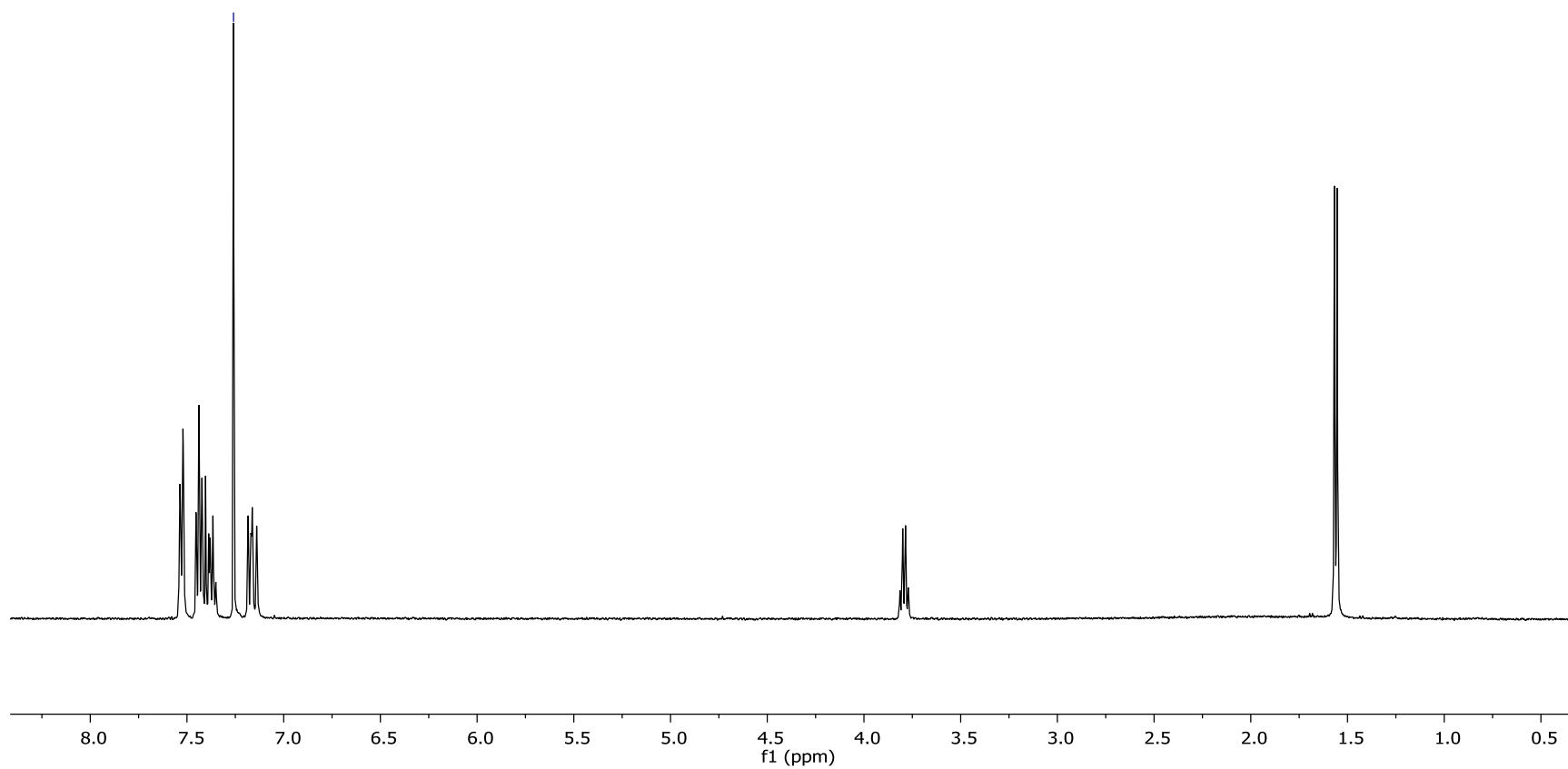
A1-C22

7.26



A2

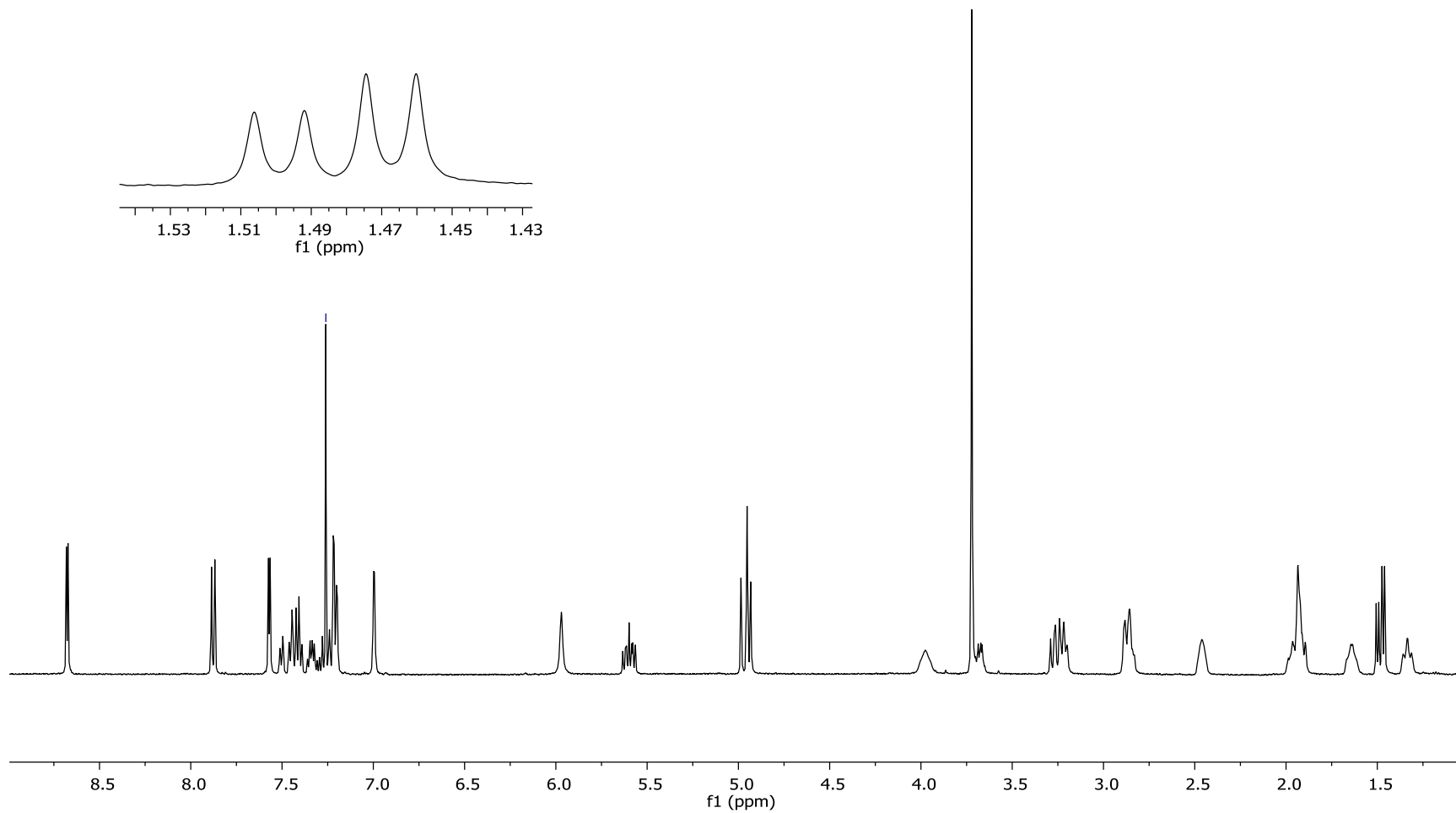
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S7

A2-C13

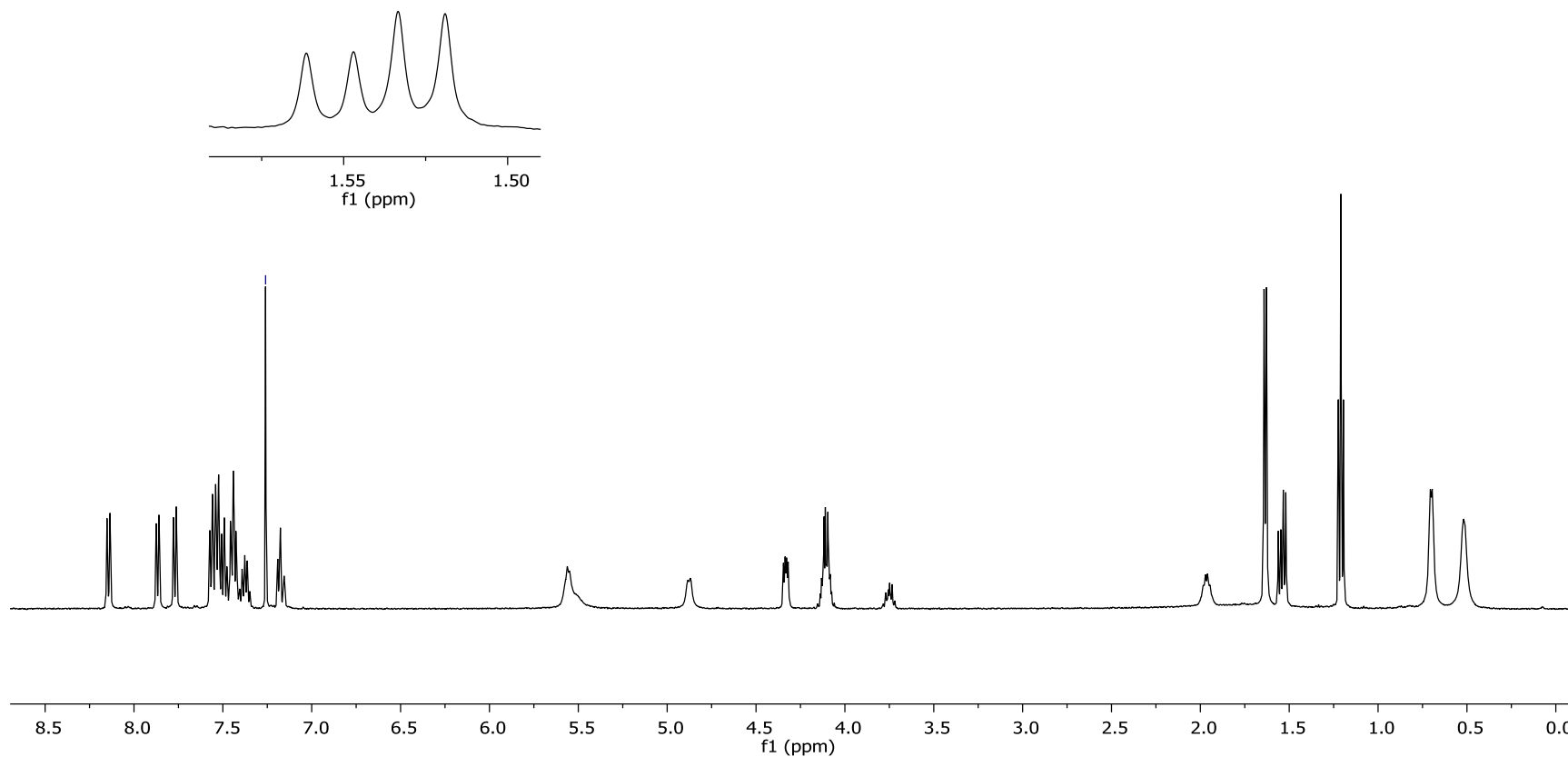
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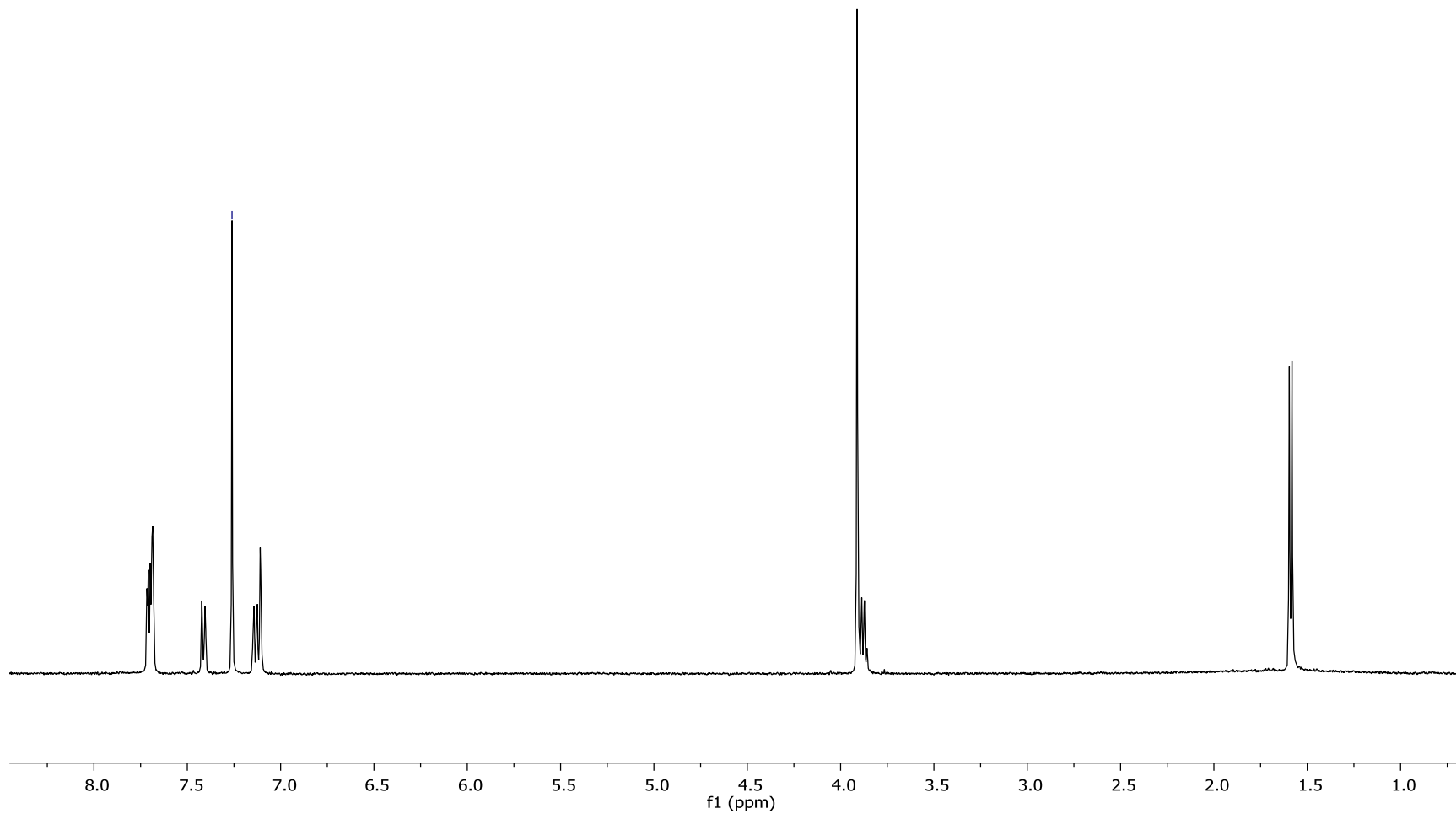
A2-C22

7.26



A3

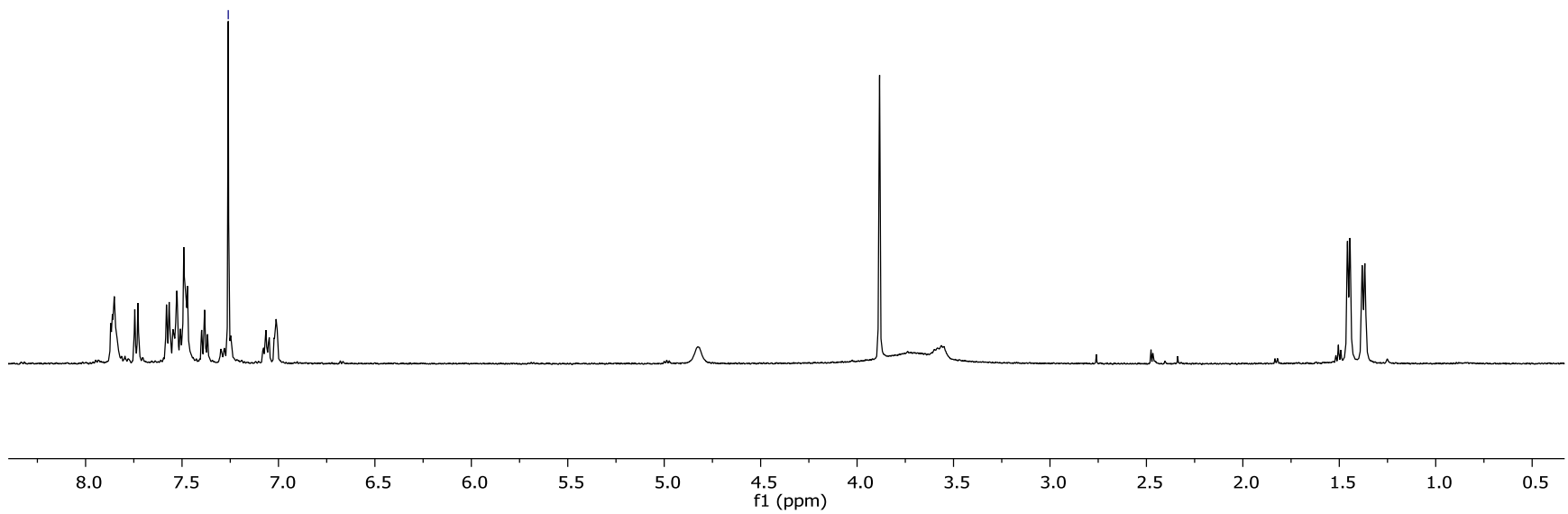
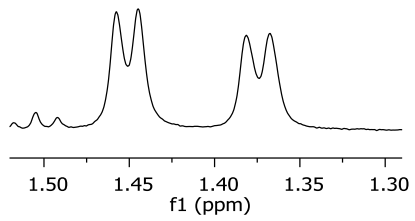
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S10

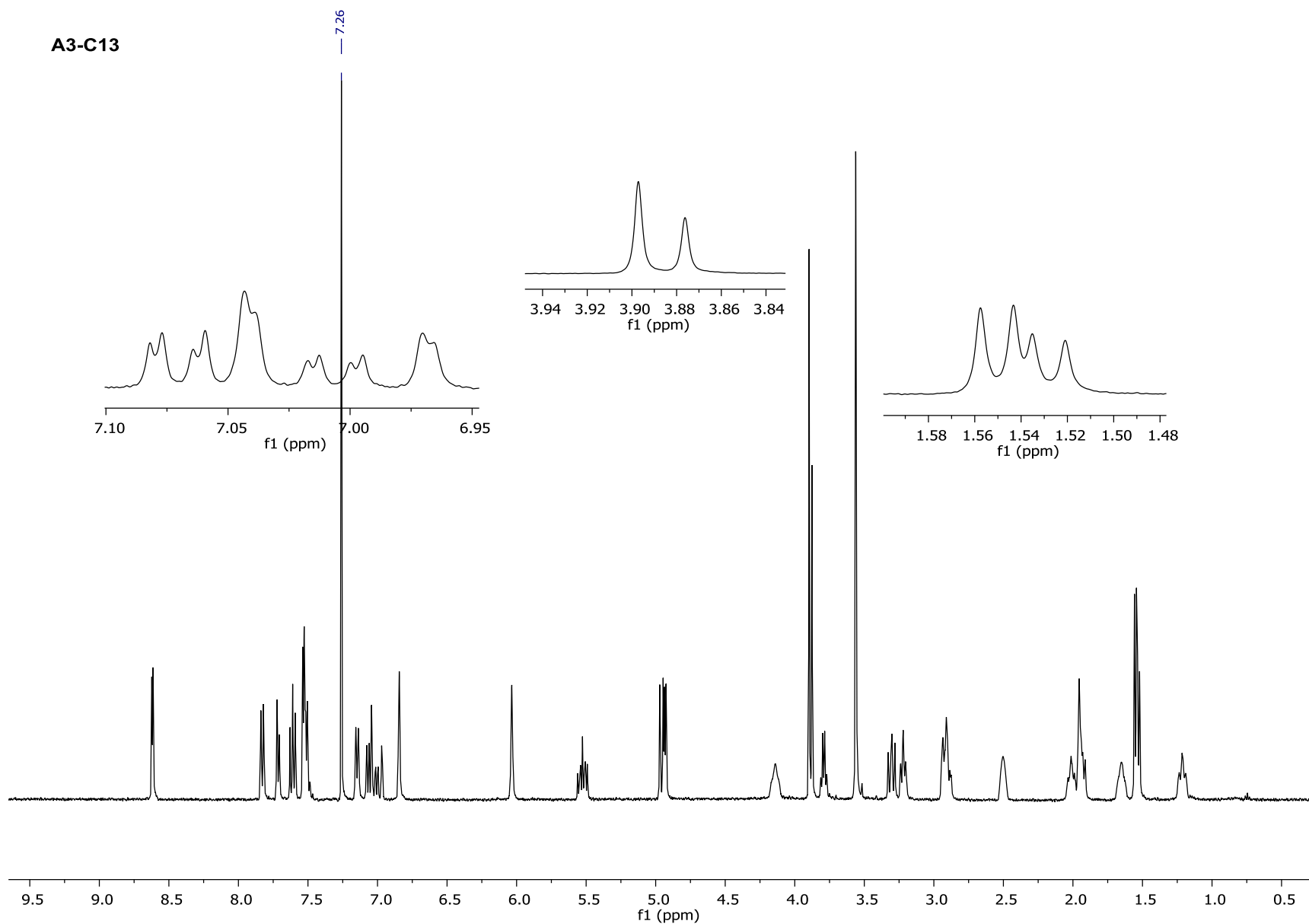
A3-C11

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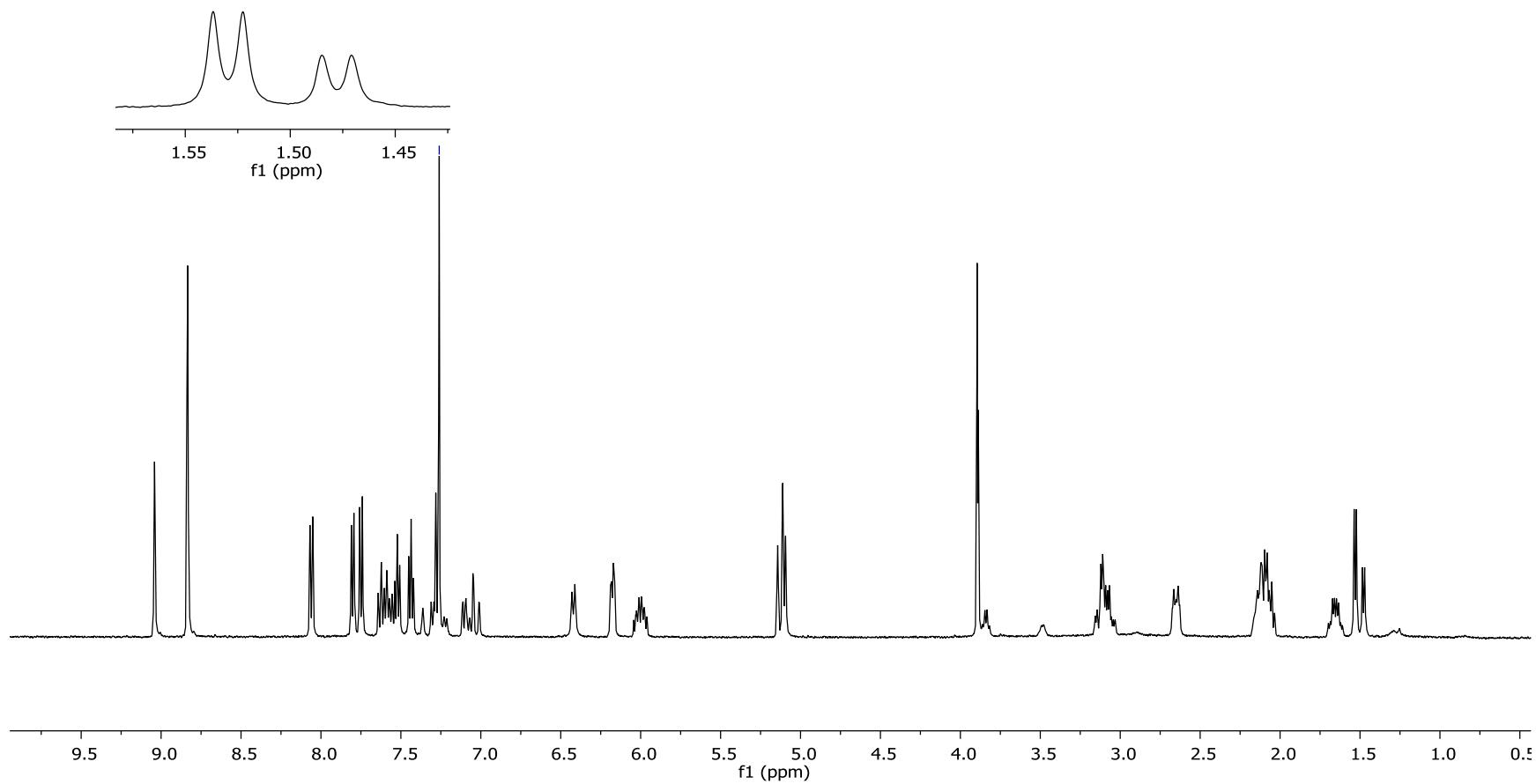
S11

A3-C13



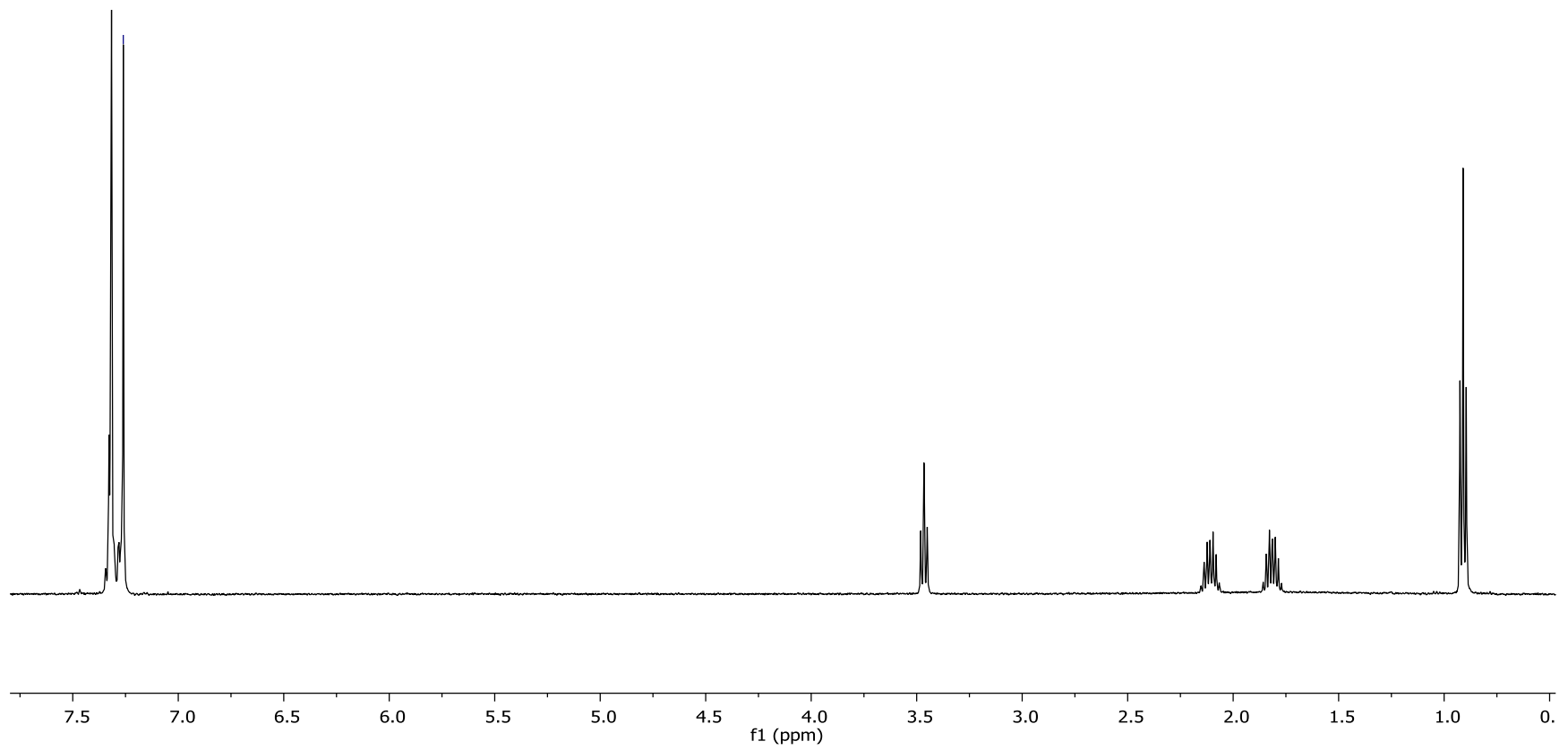
A3-C28

7.26



A4

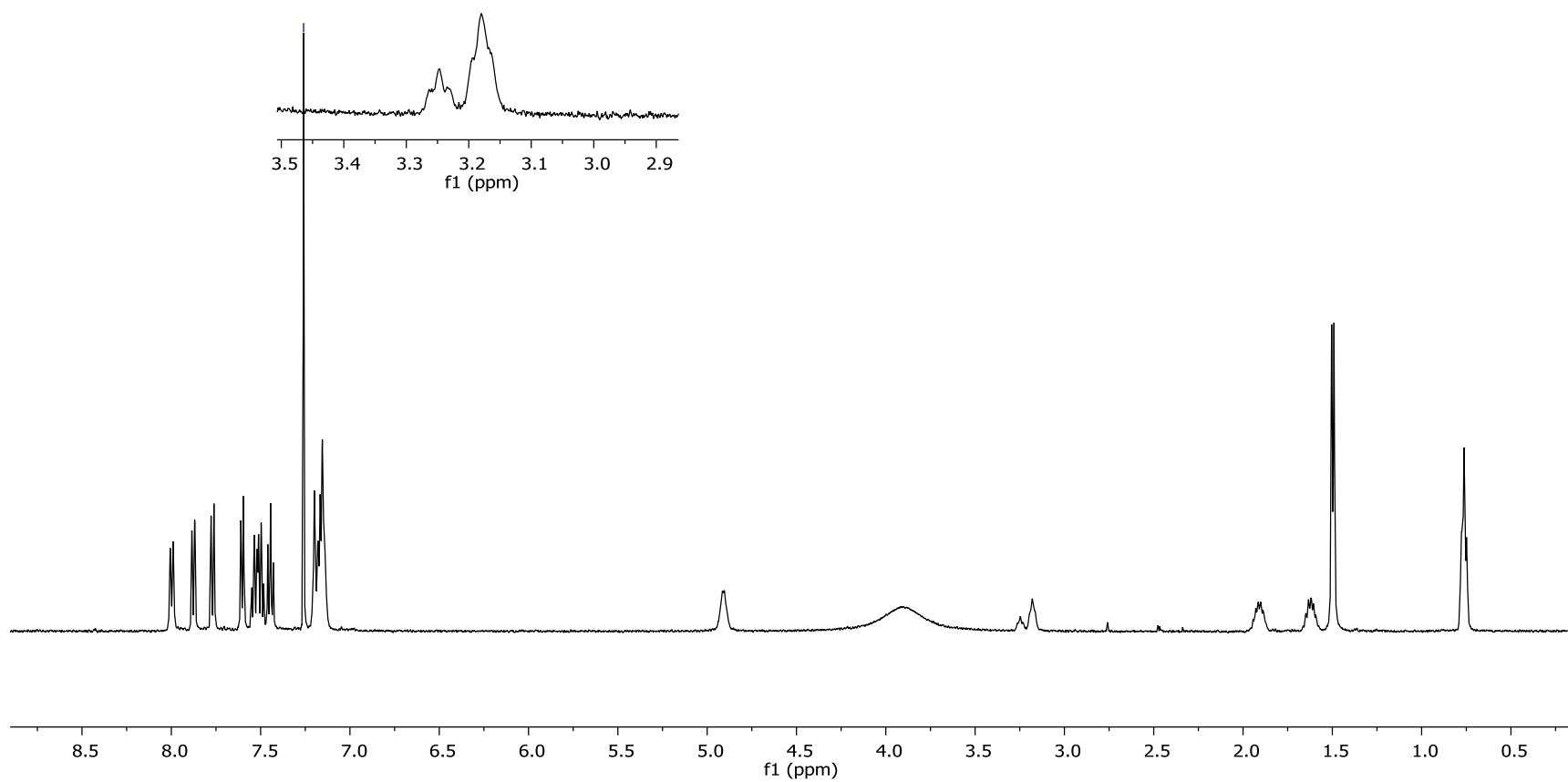
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S14

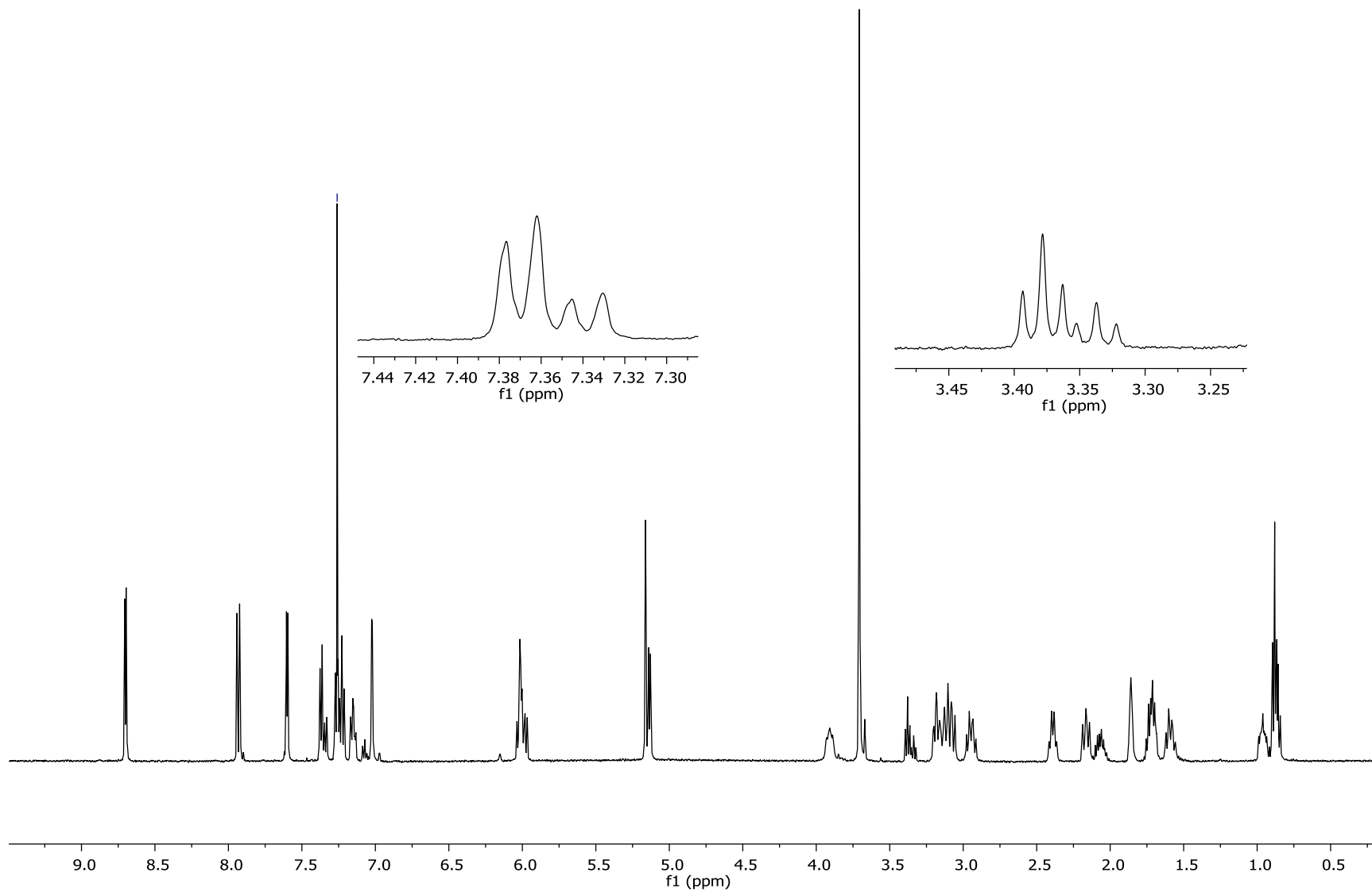
A4-C11

7.26



A4-C13

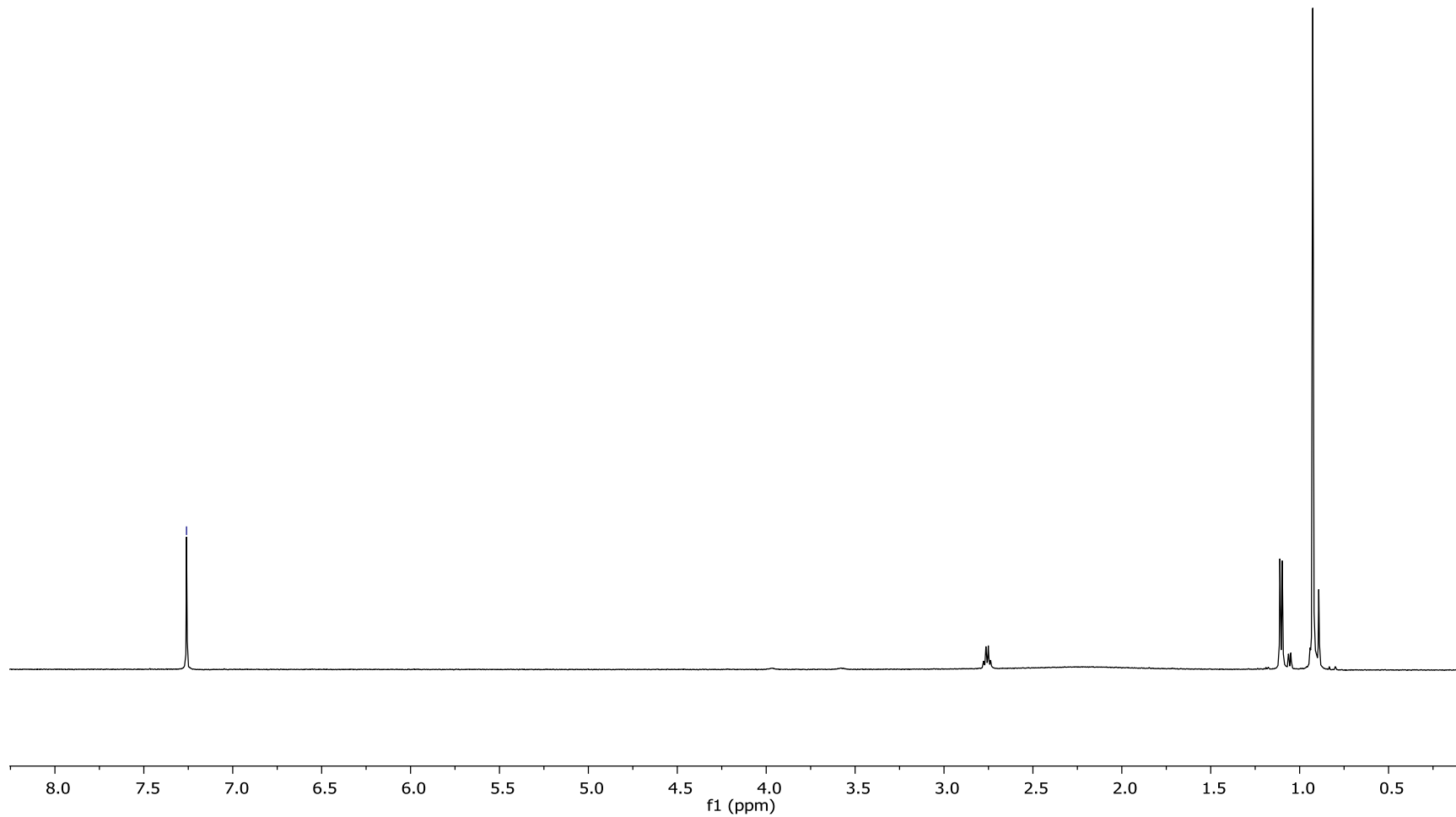
7.36





A5

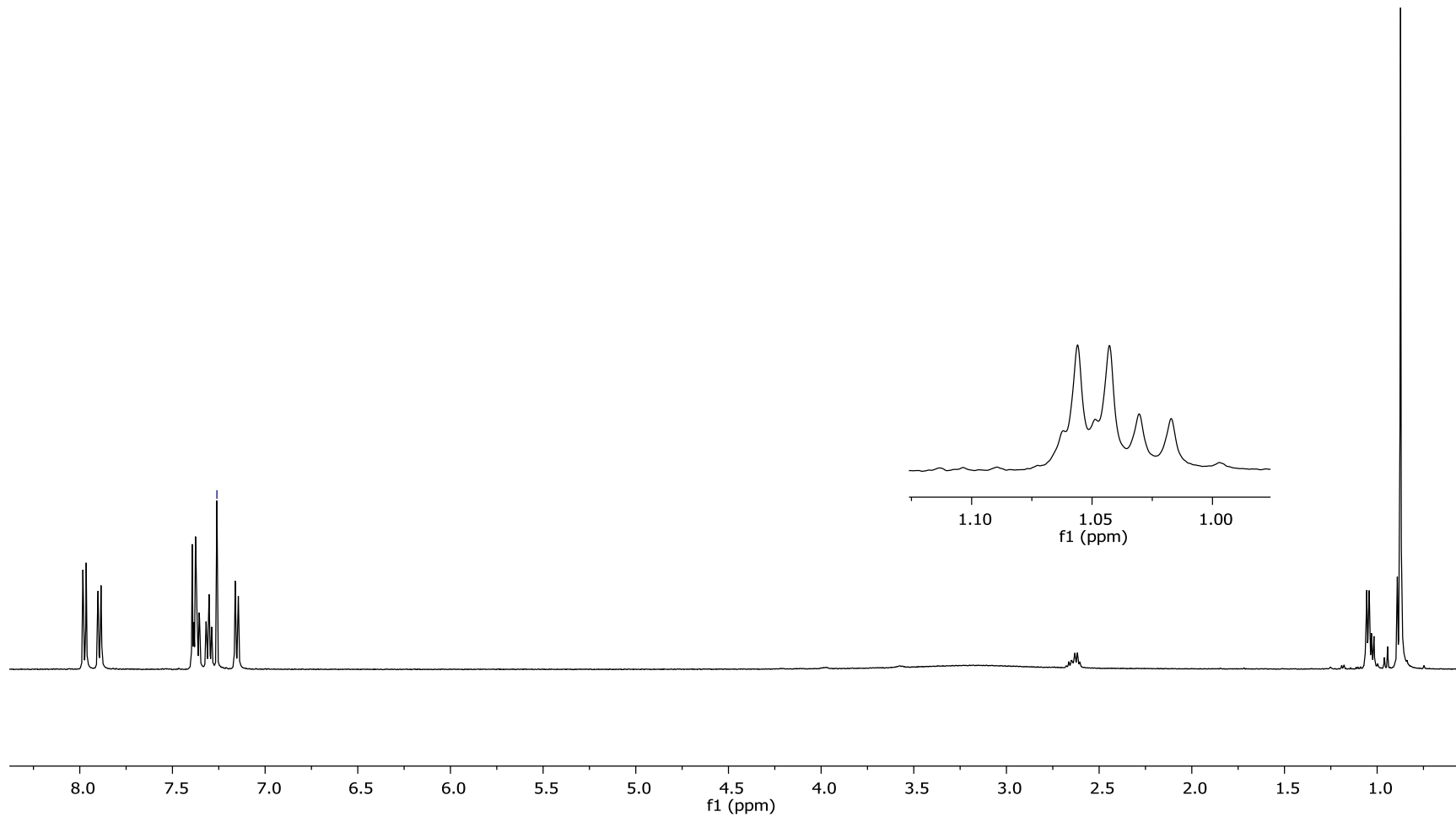
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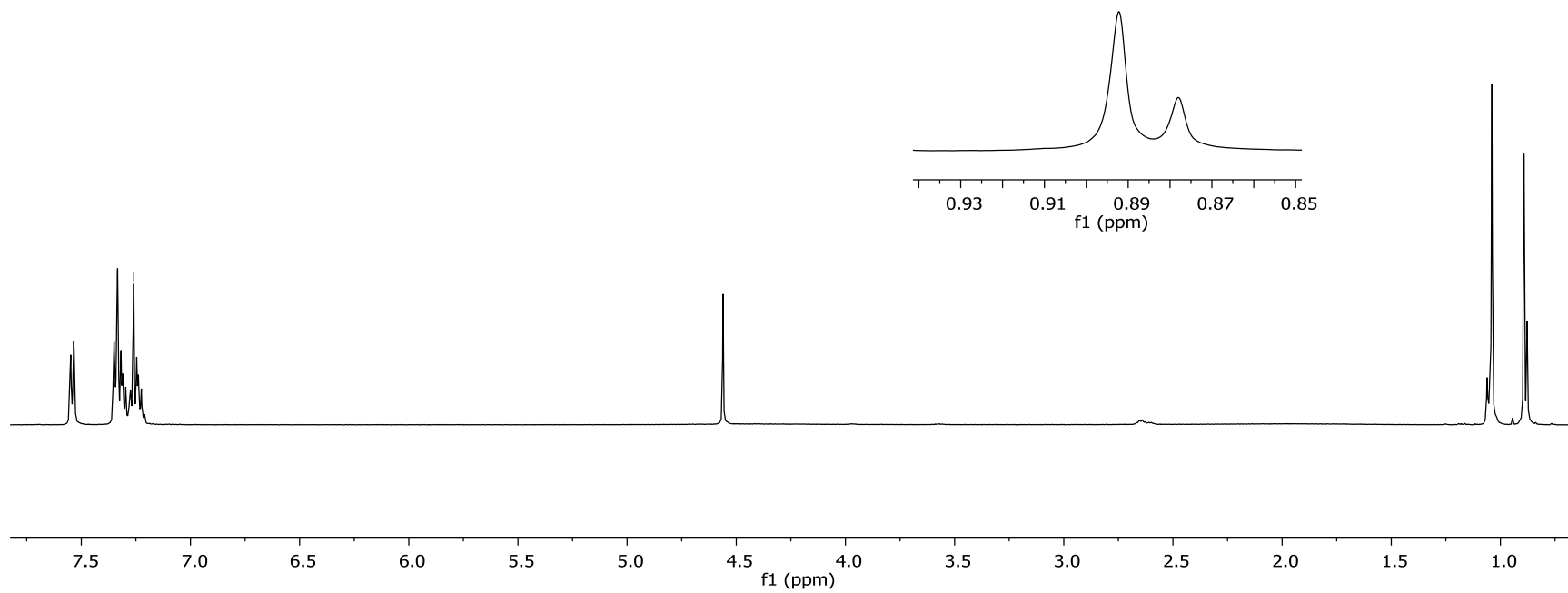
S17

A5-C8

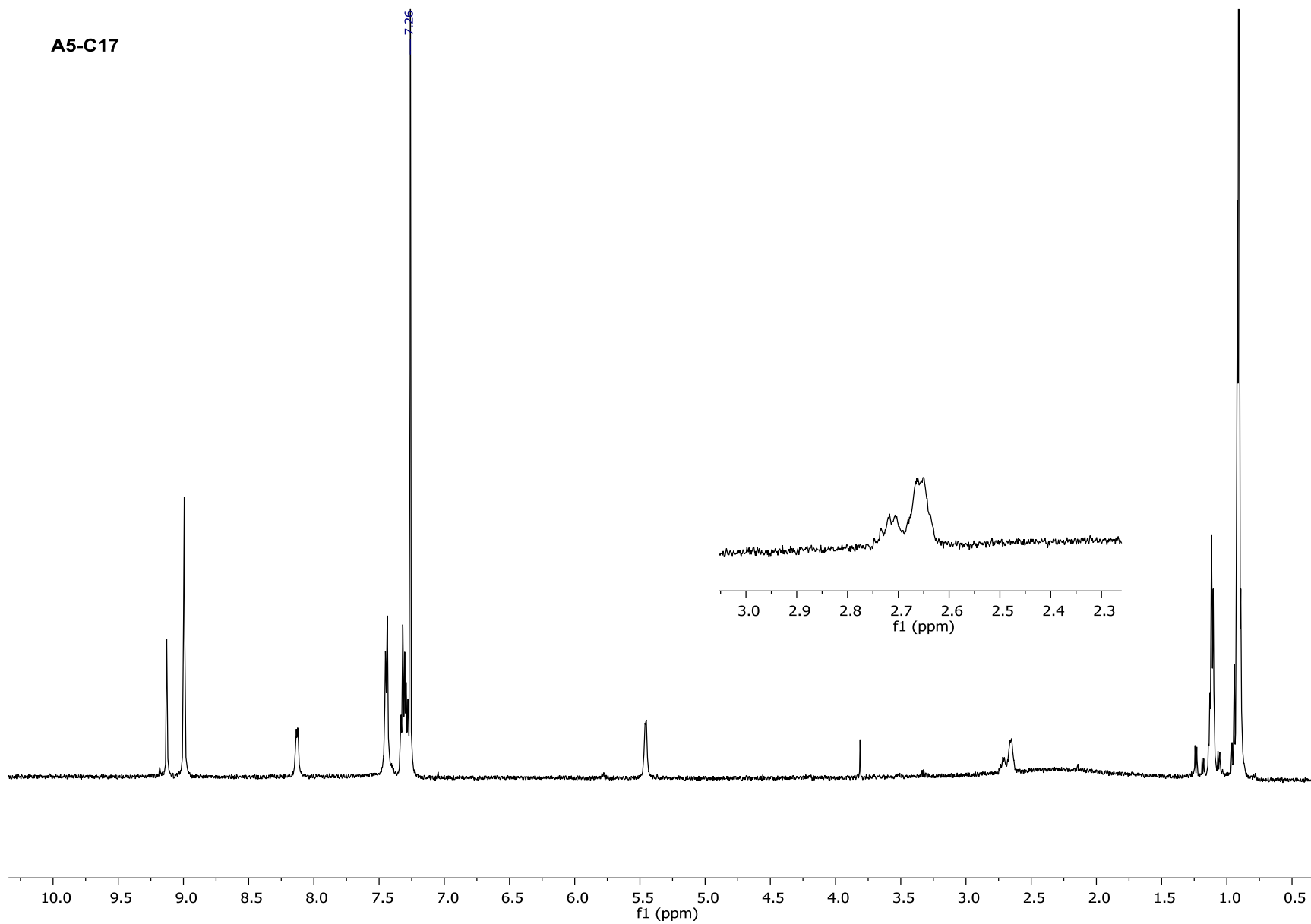
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A5-C9 | 7.26

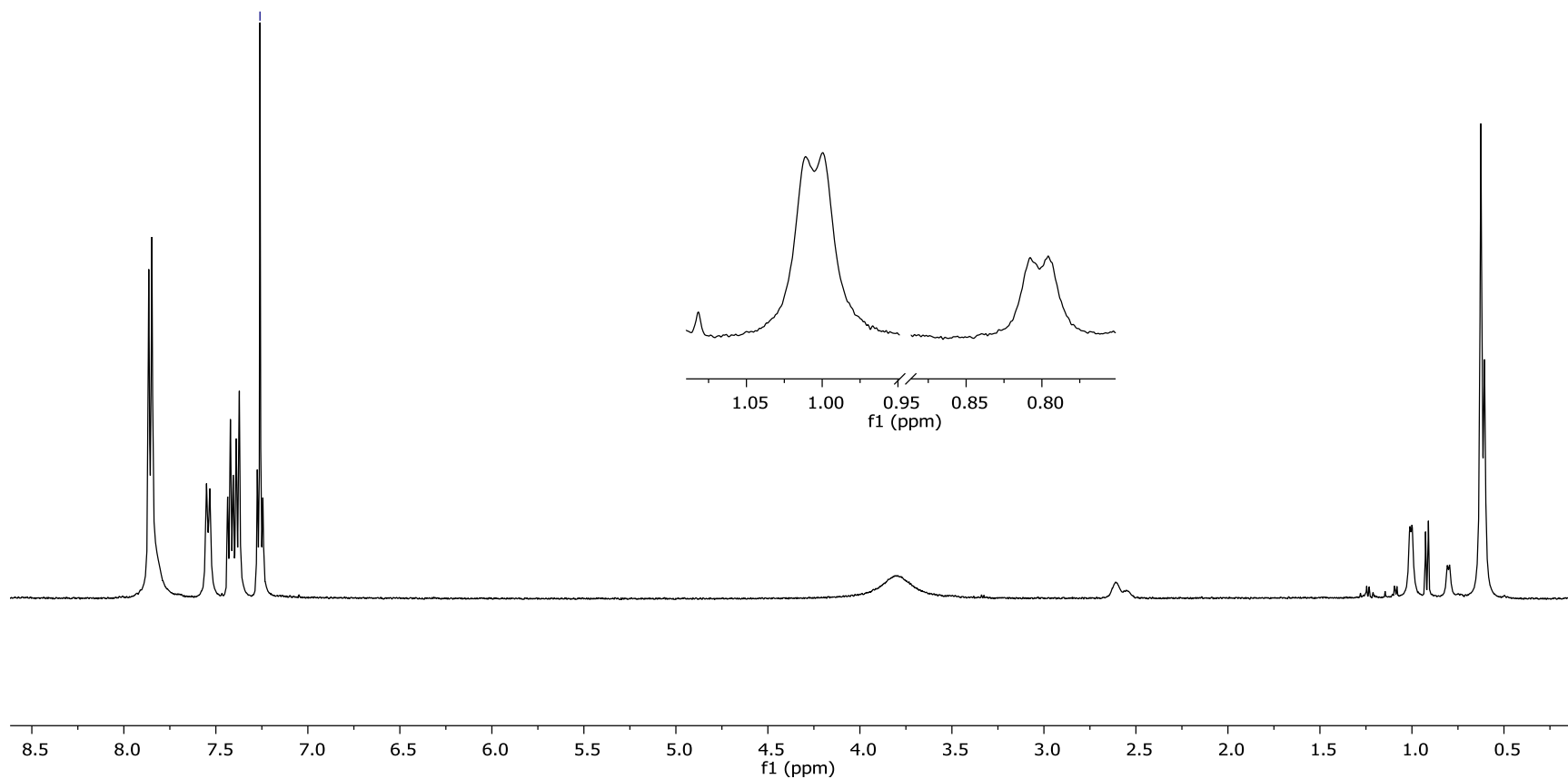


A5-C17

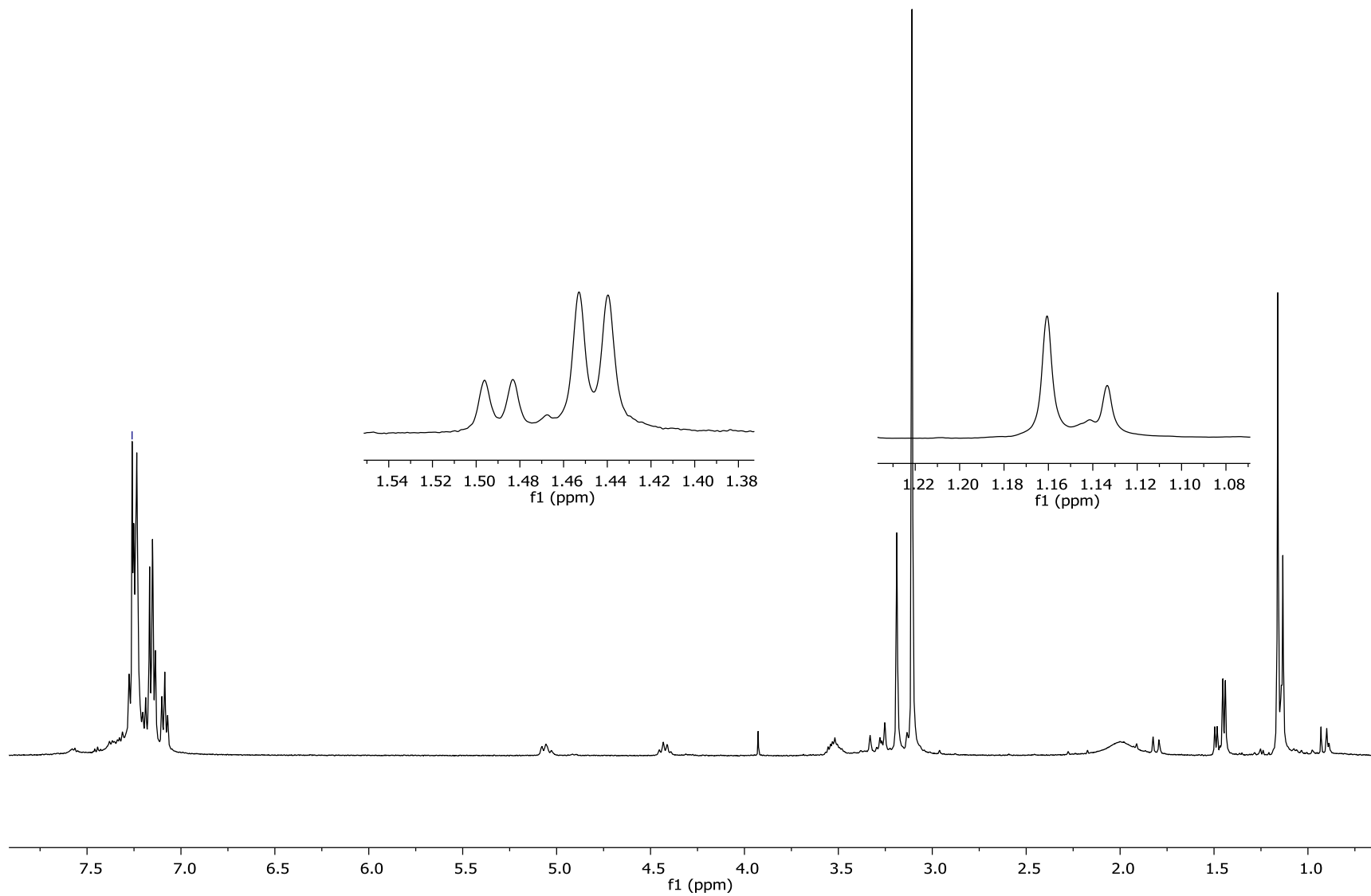


A5-C25

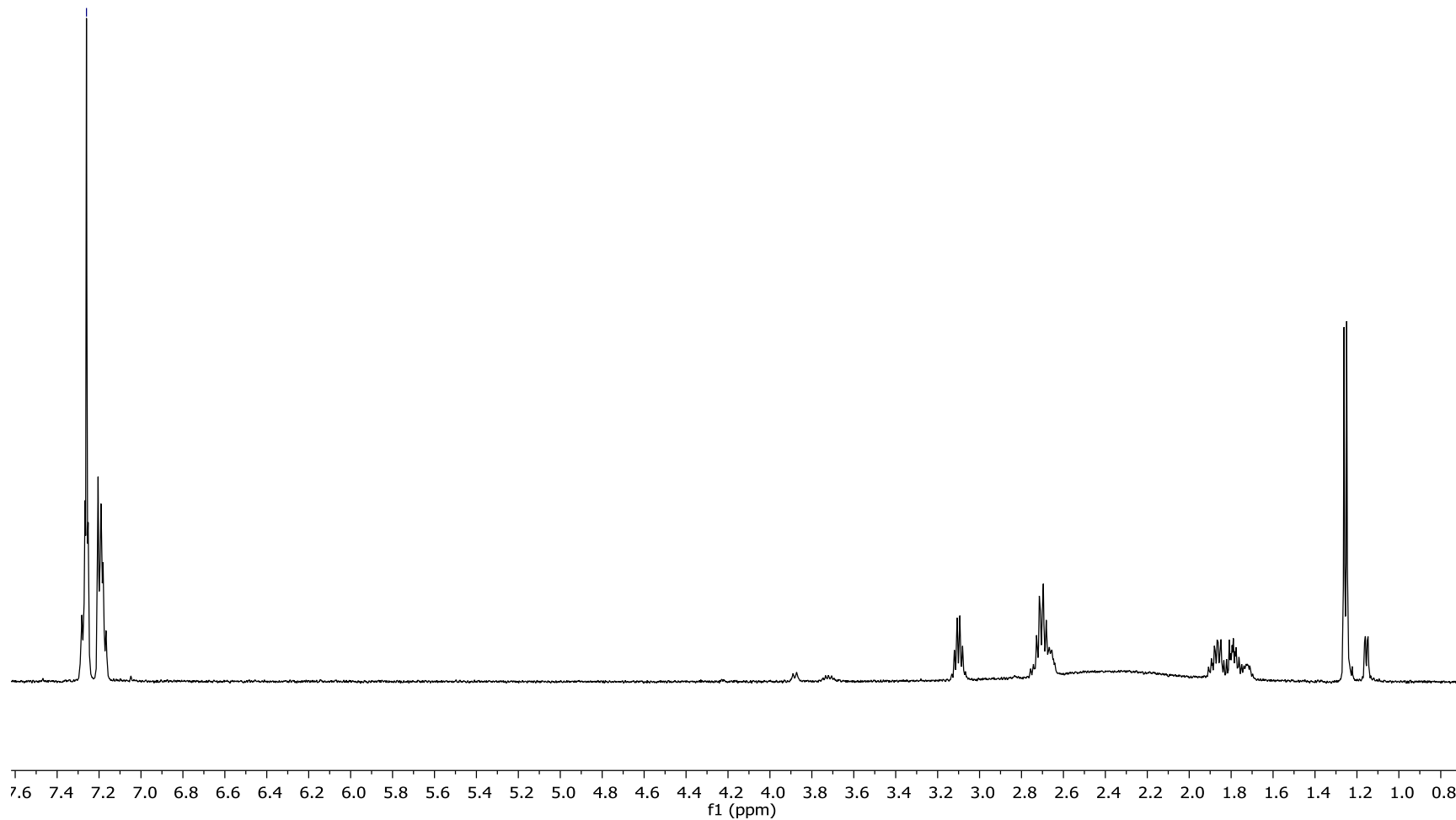
7.26



A5-C32 | 7.26

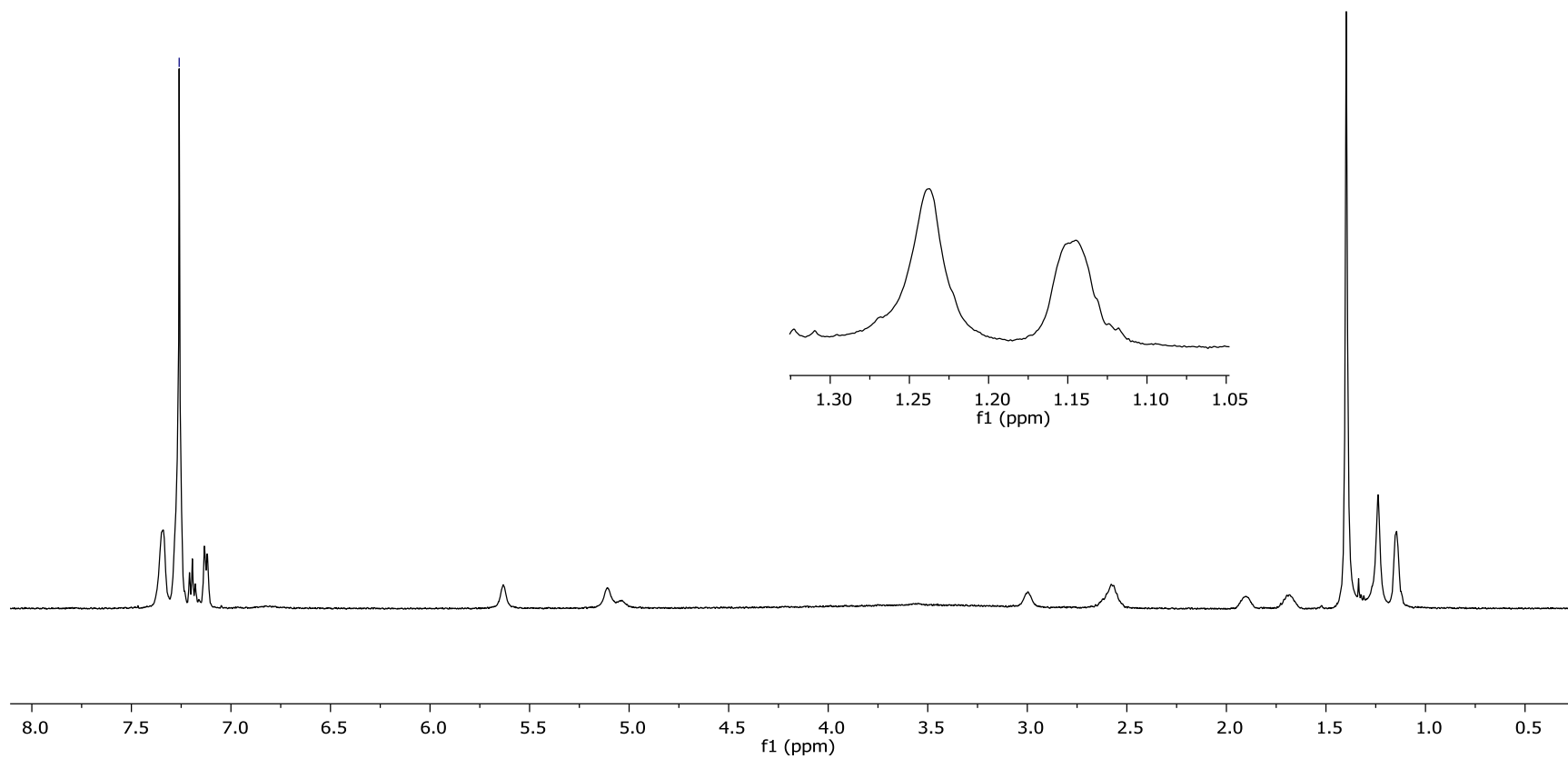


A6  
7.26



A6-C5

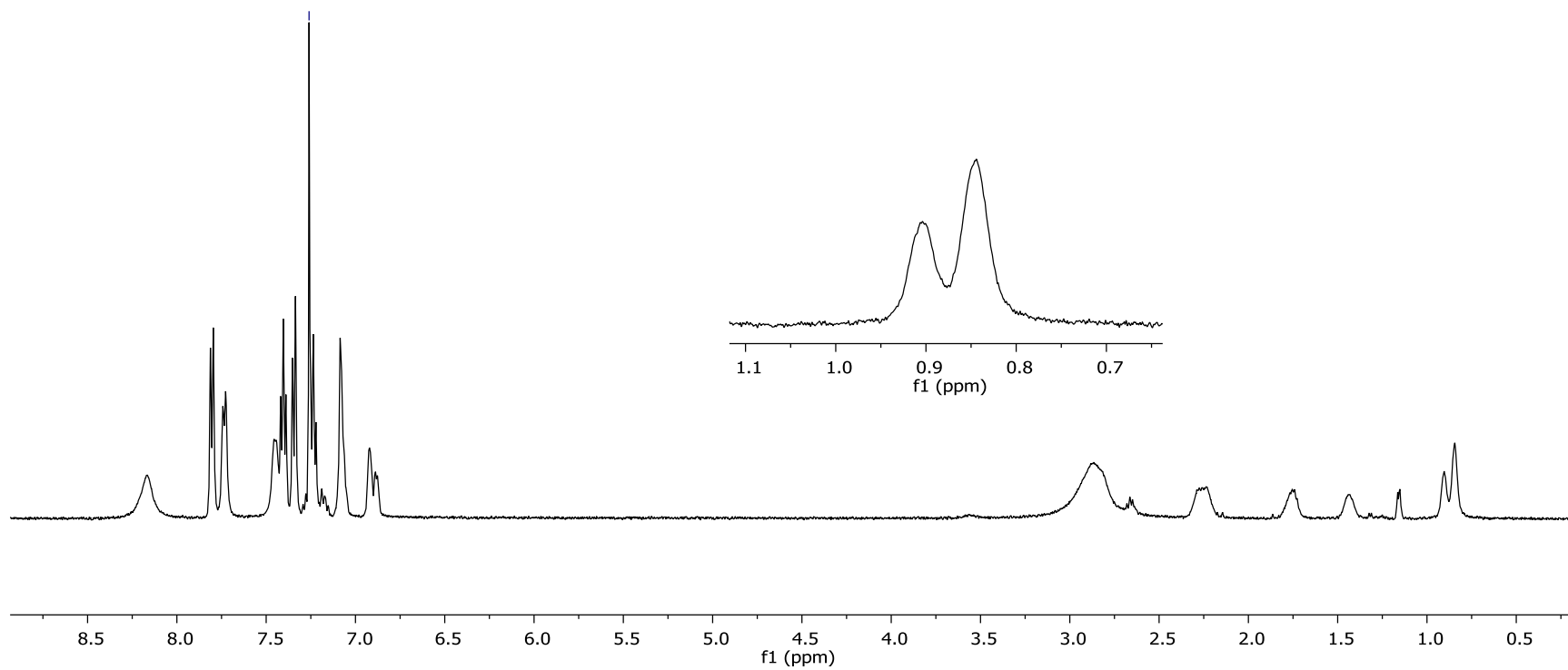
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A6-C25

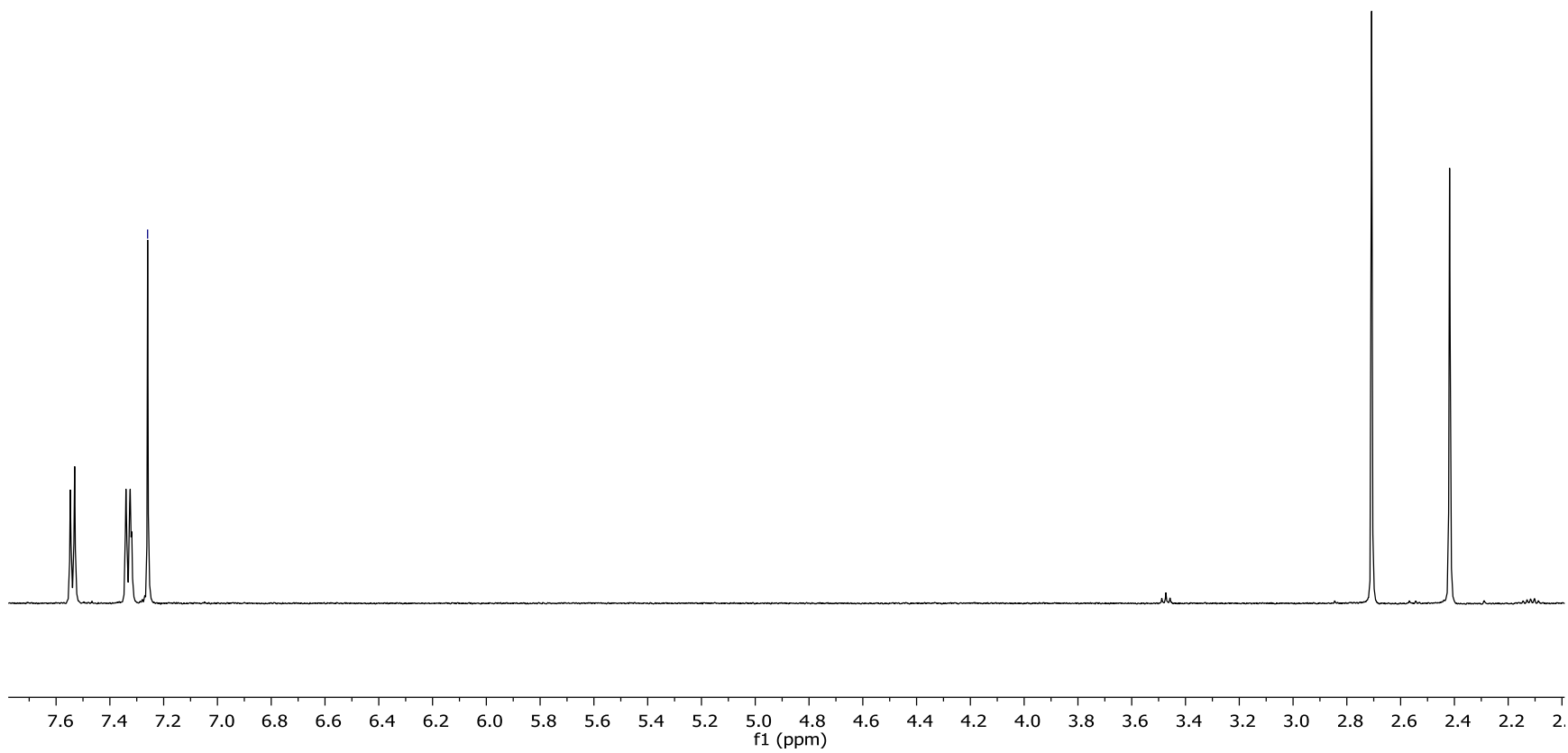
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S25

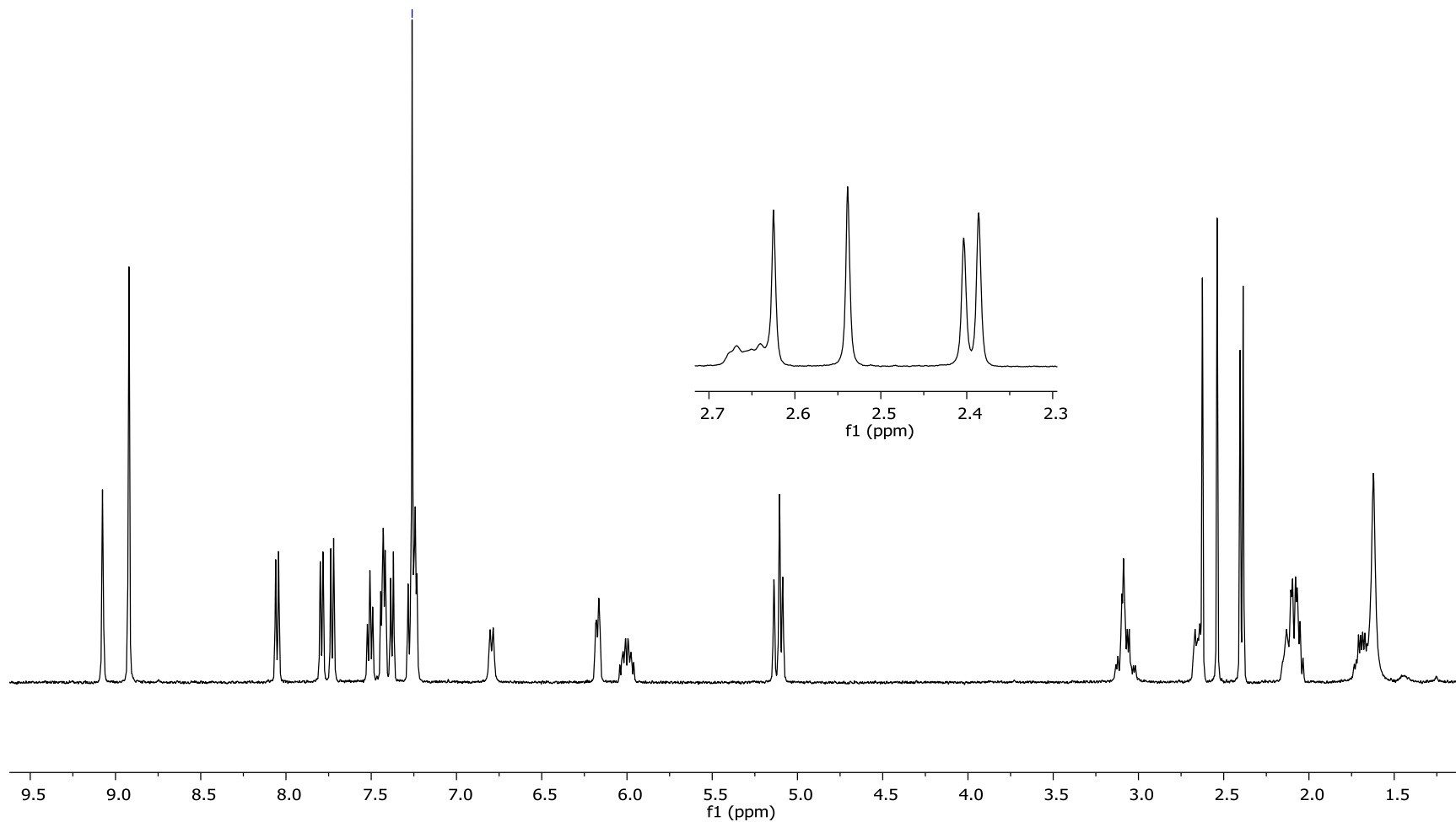
A7

7.26



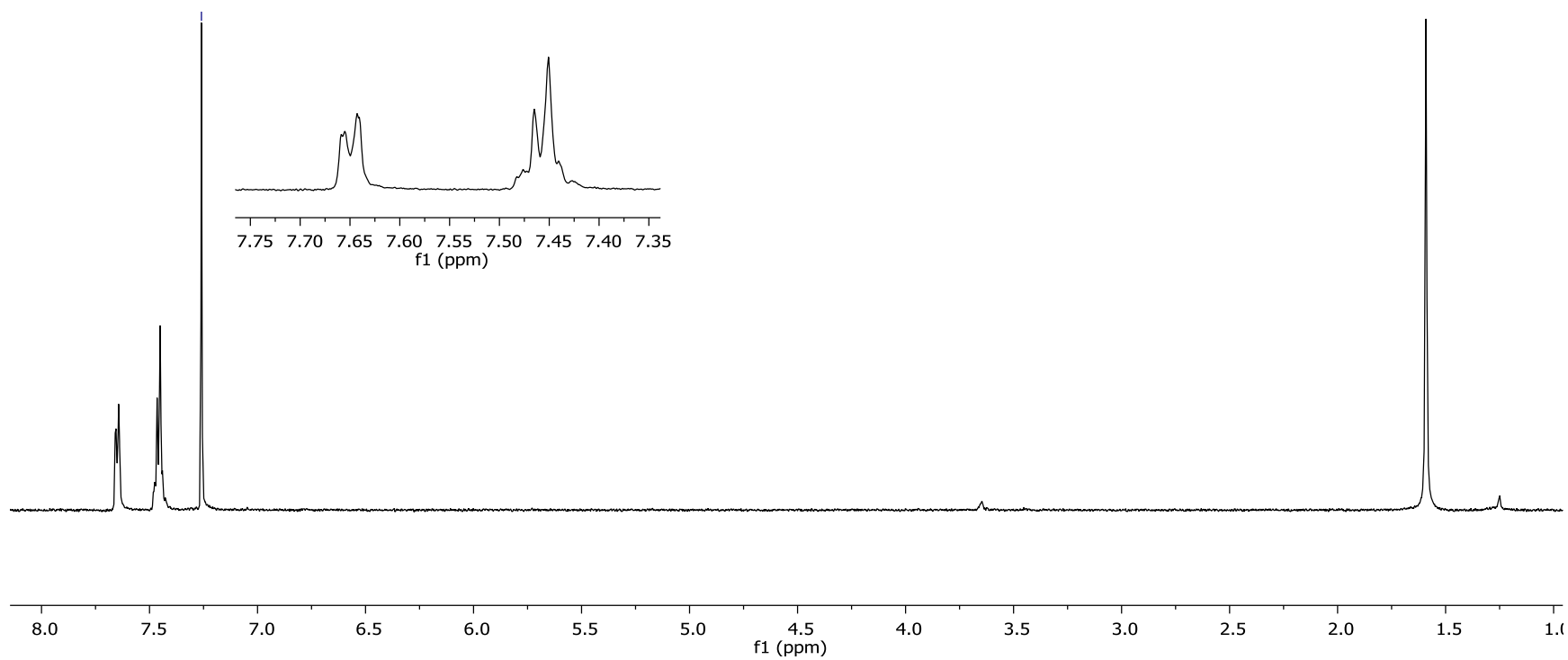
A7-C28

7.26



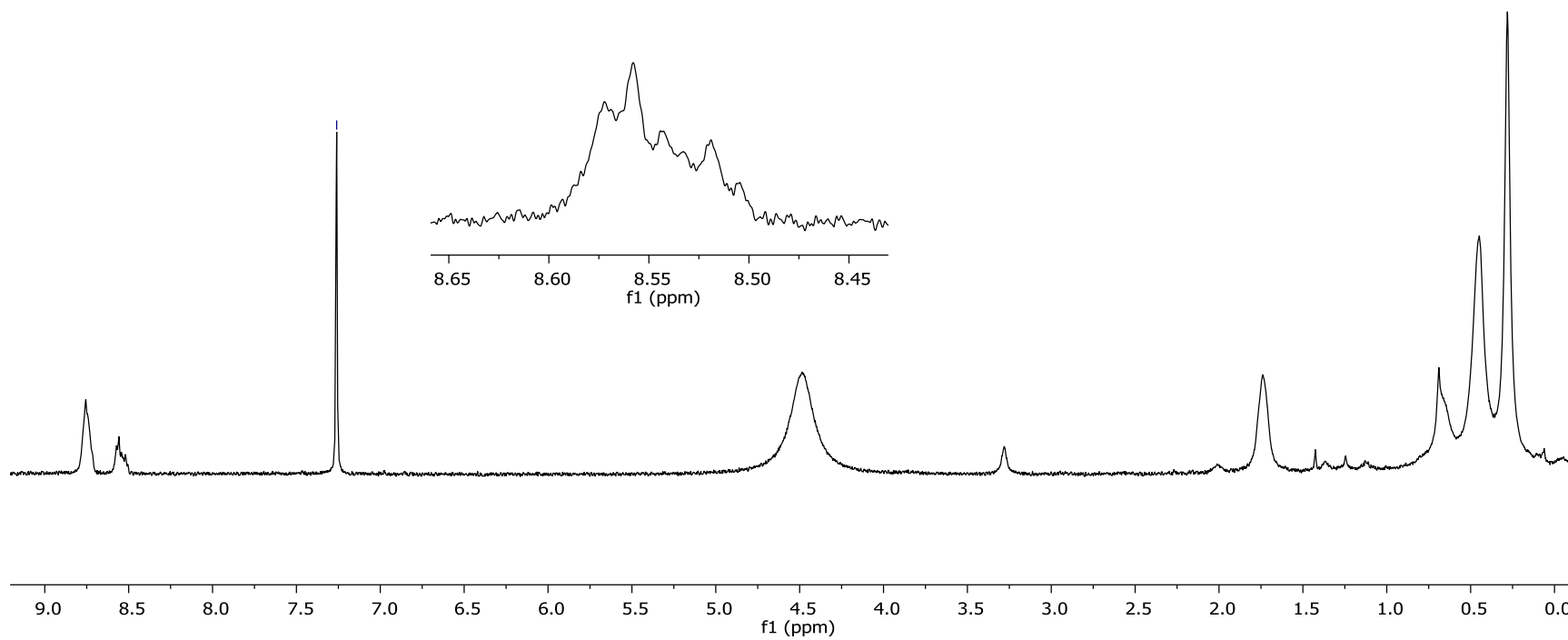
A8

7.26



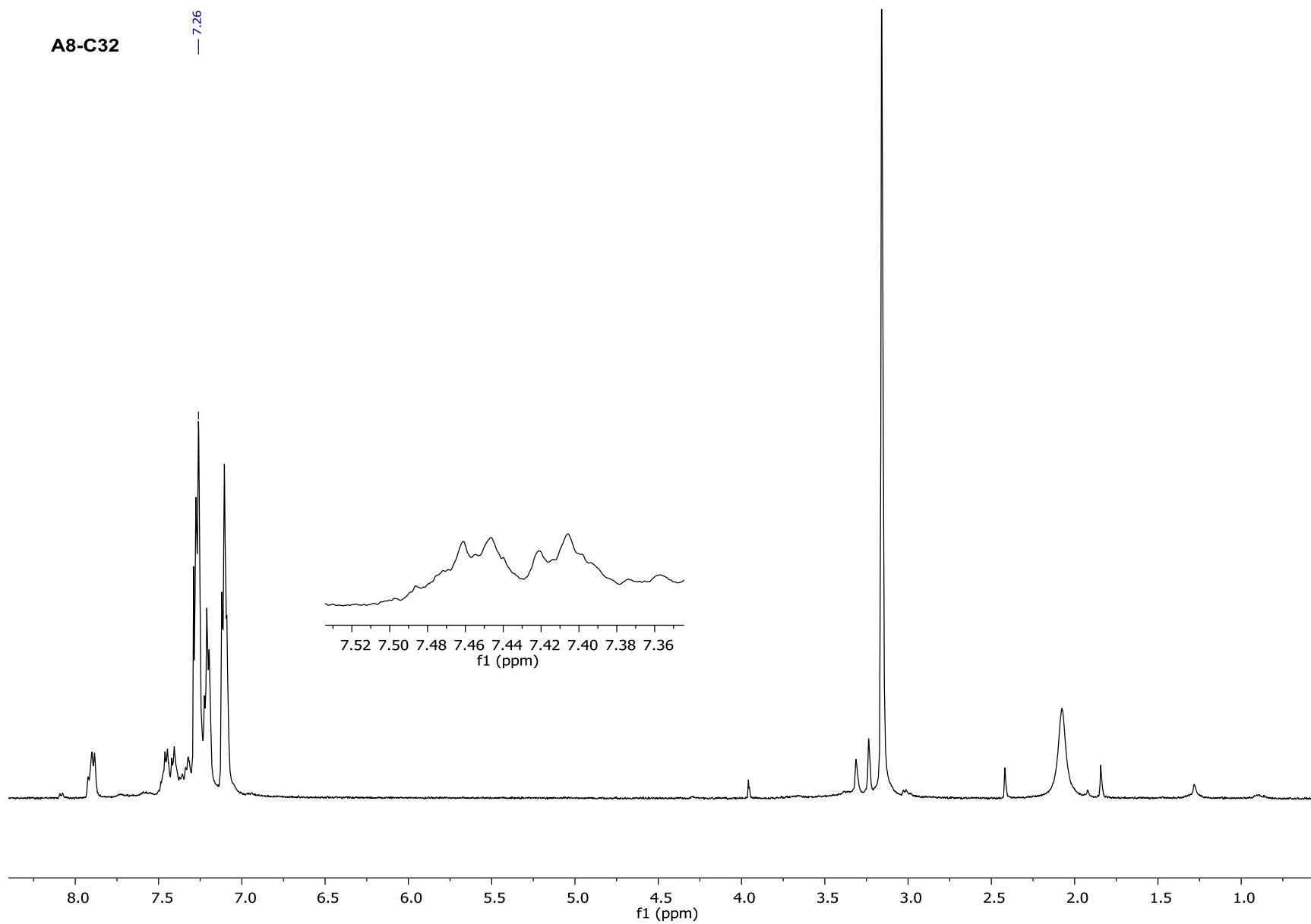
A8-C30

7.26



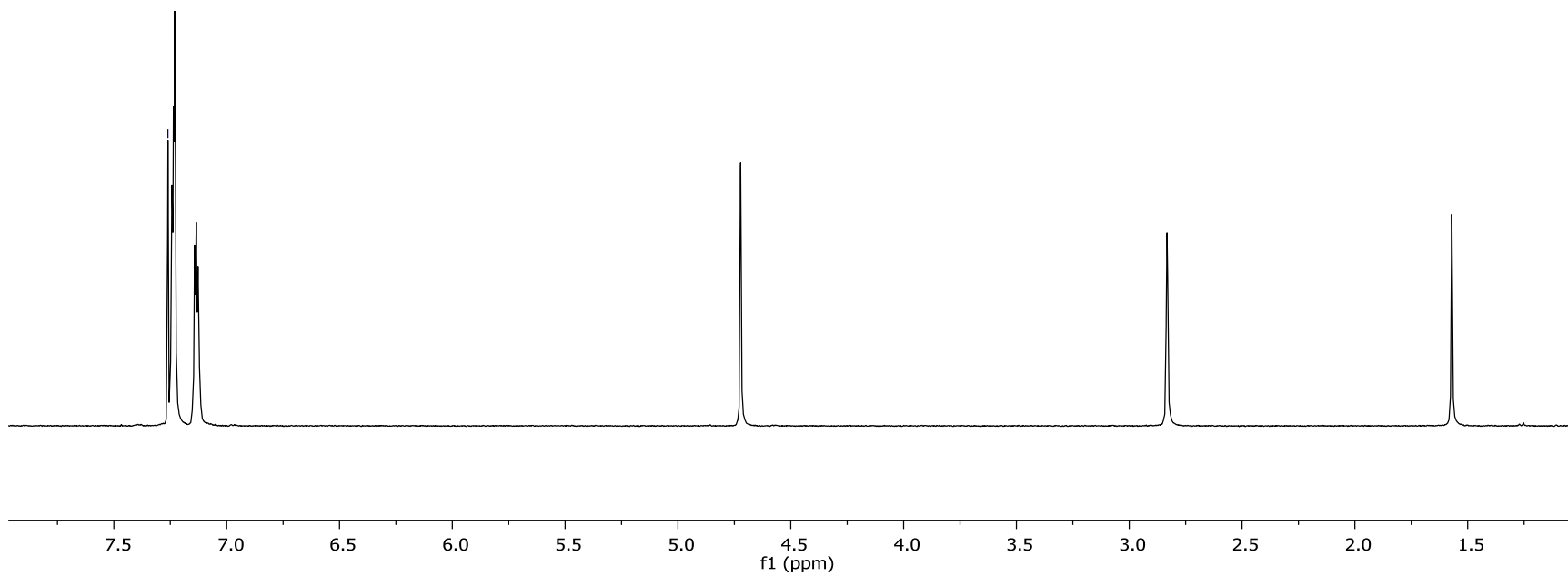
A8-C32

7.26



A9

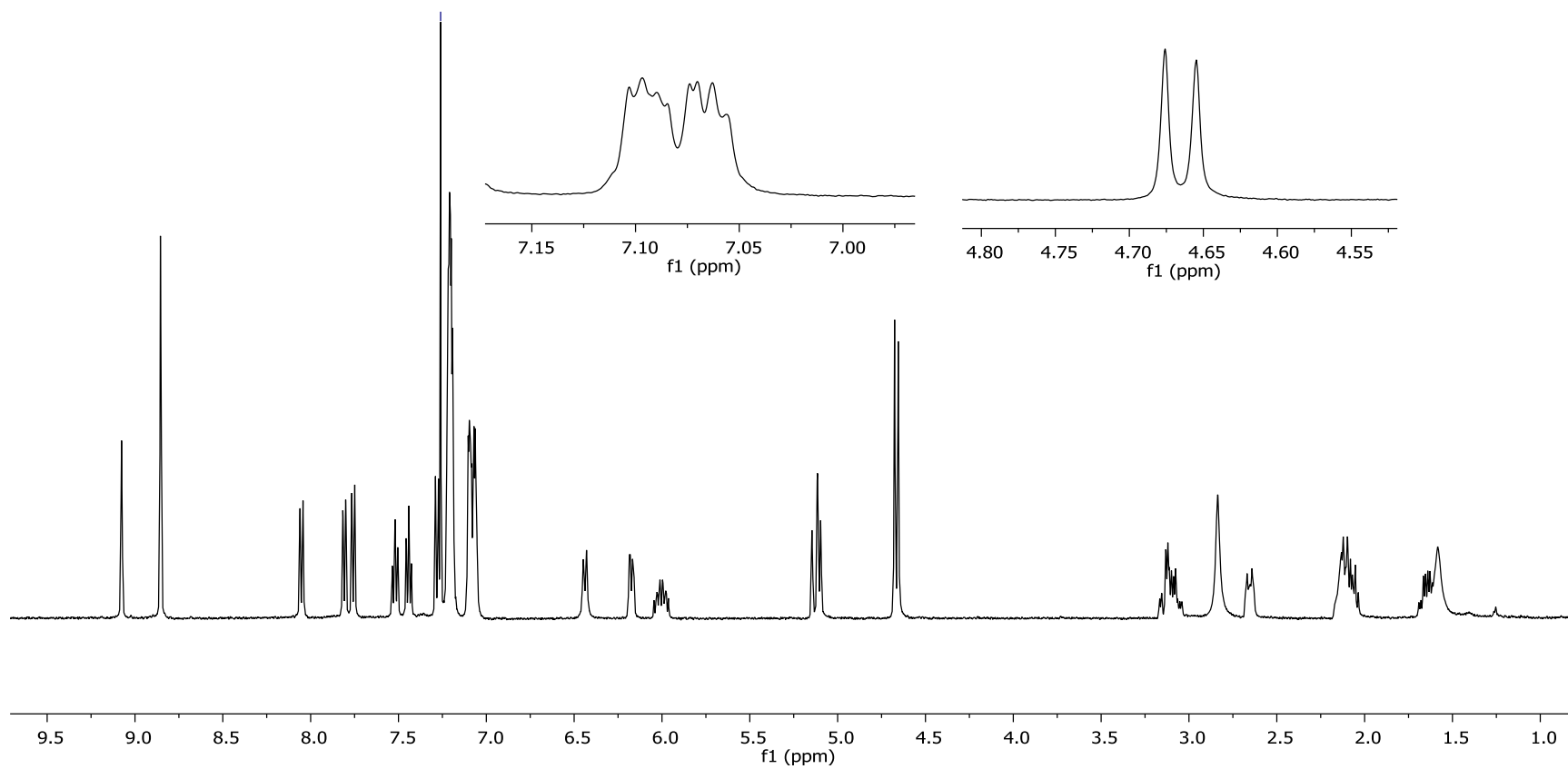
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S31

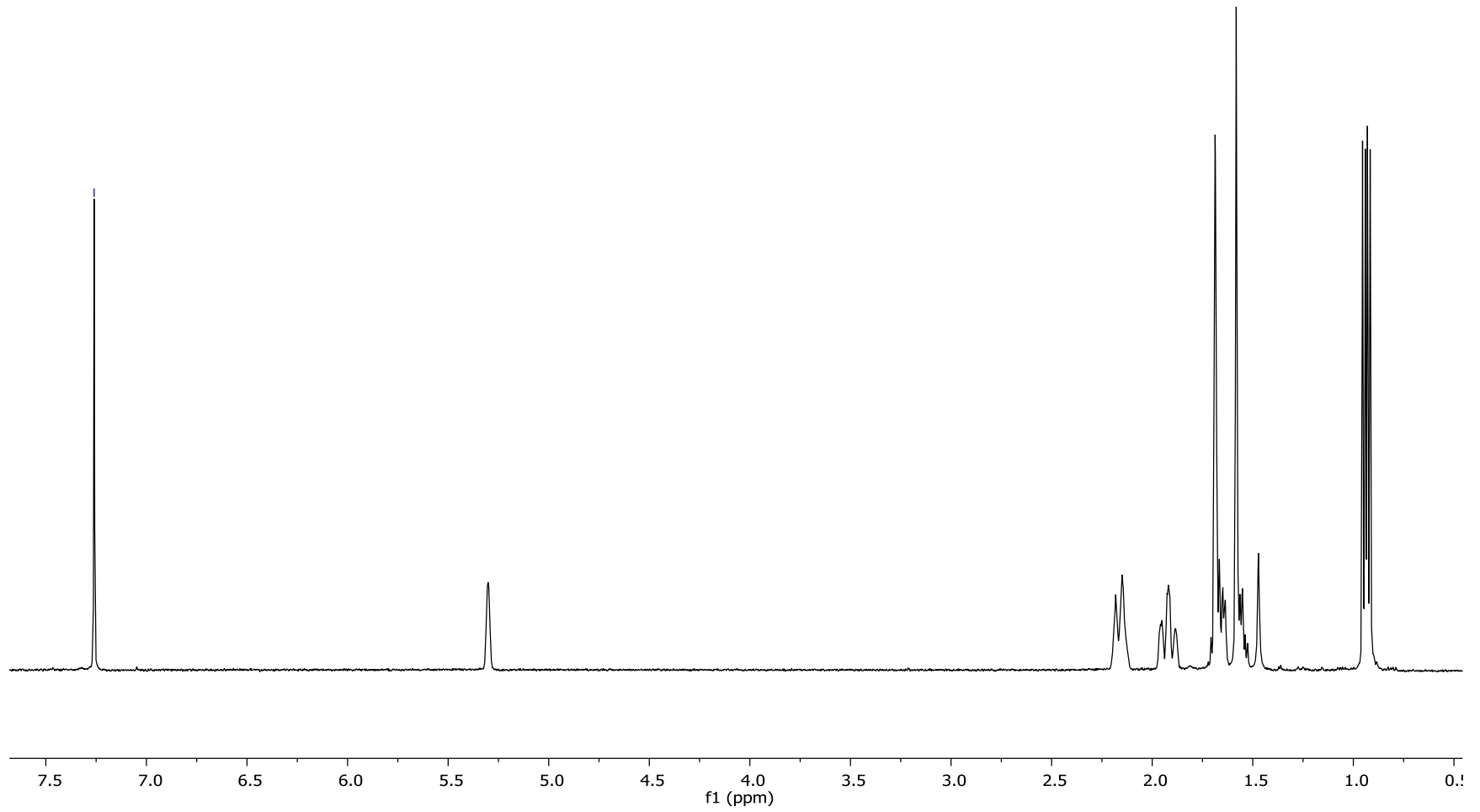
A9-C28

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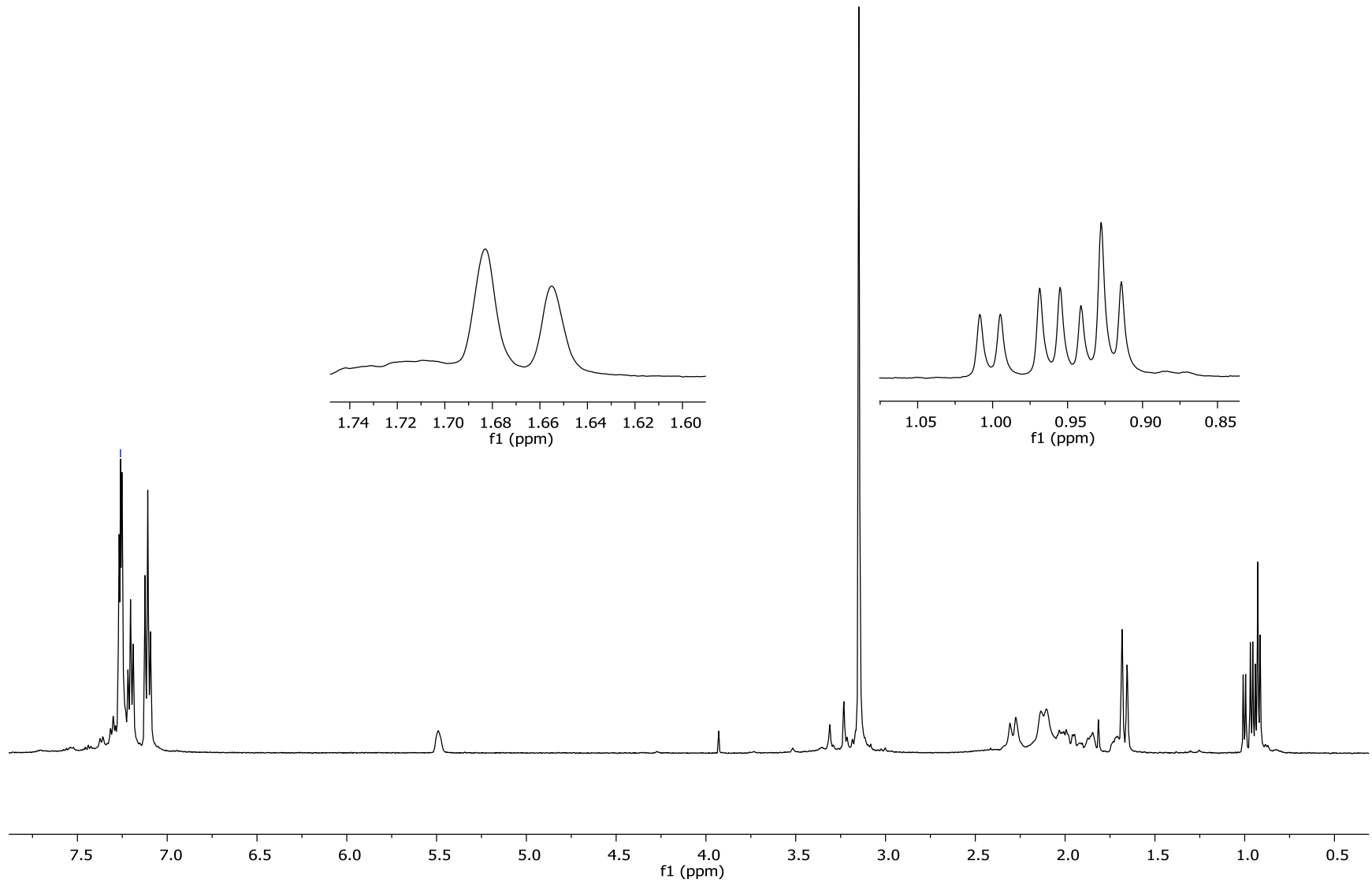


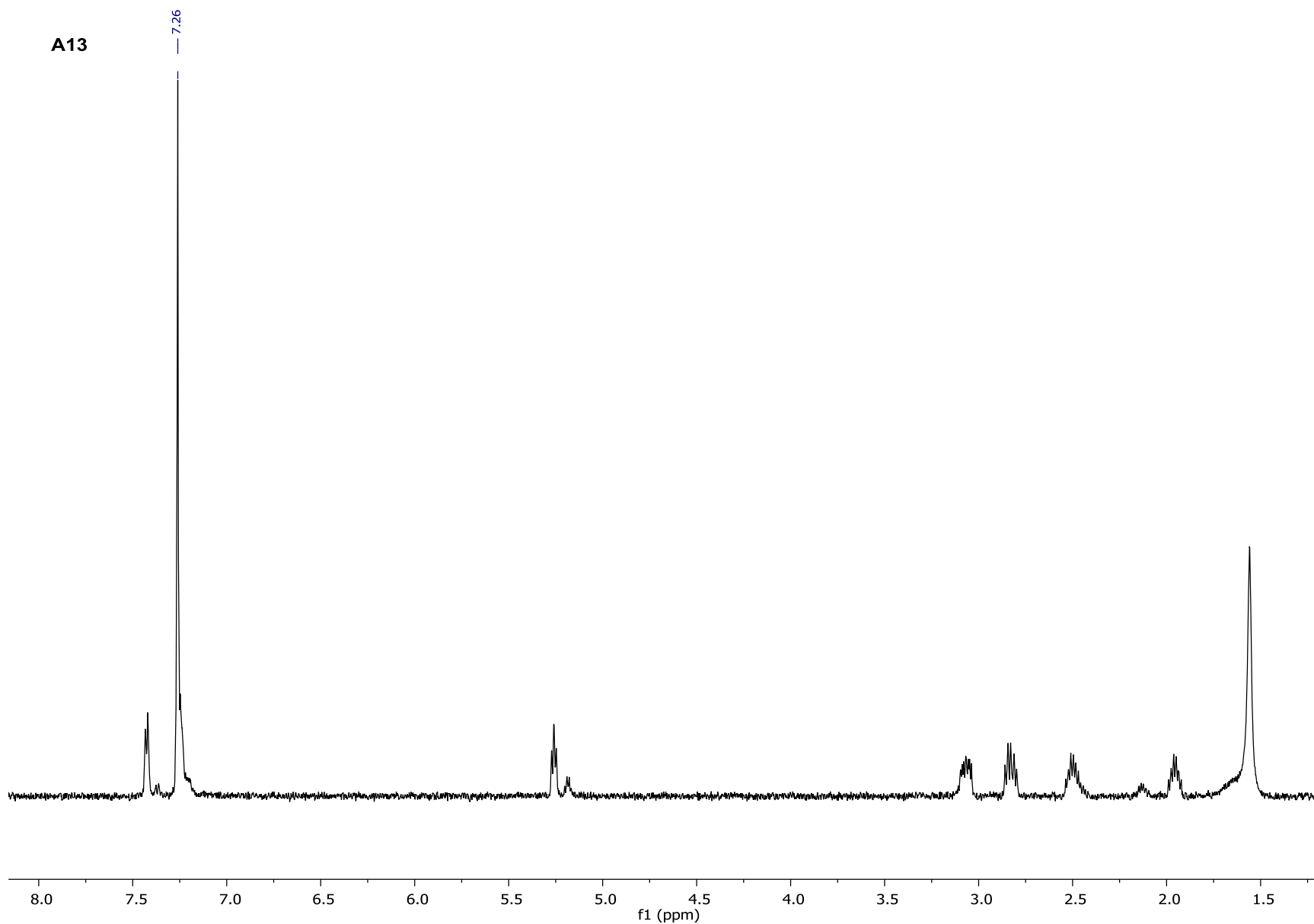
A10  
7.26



S33

A10-C32  
7.26

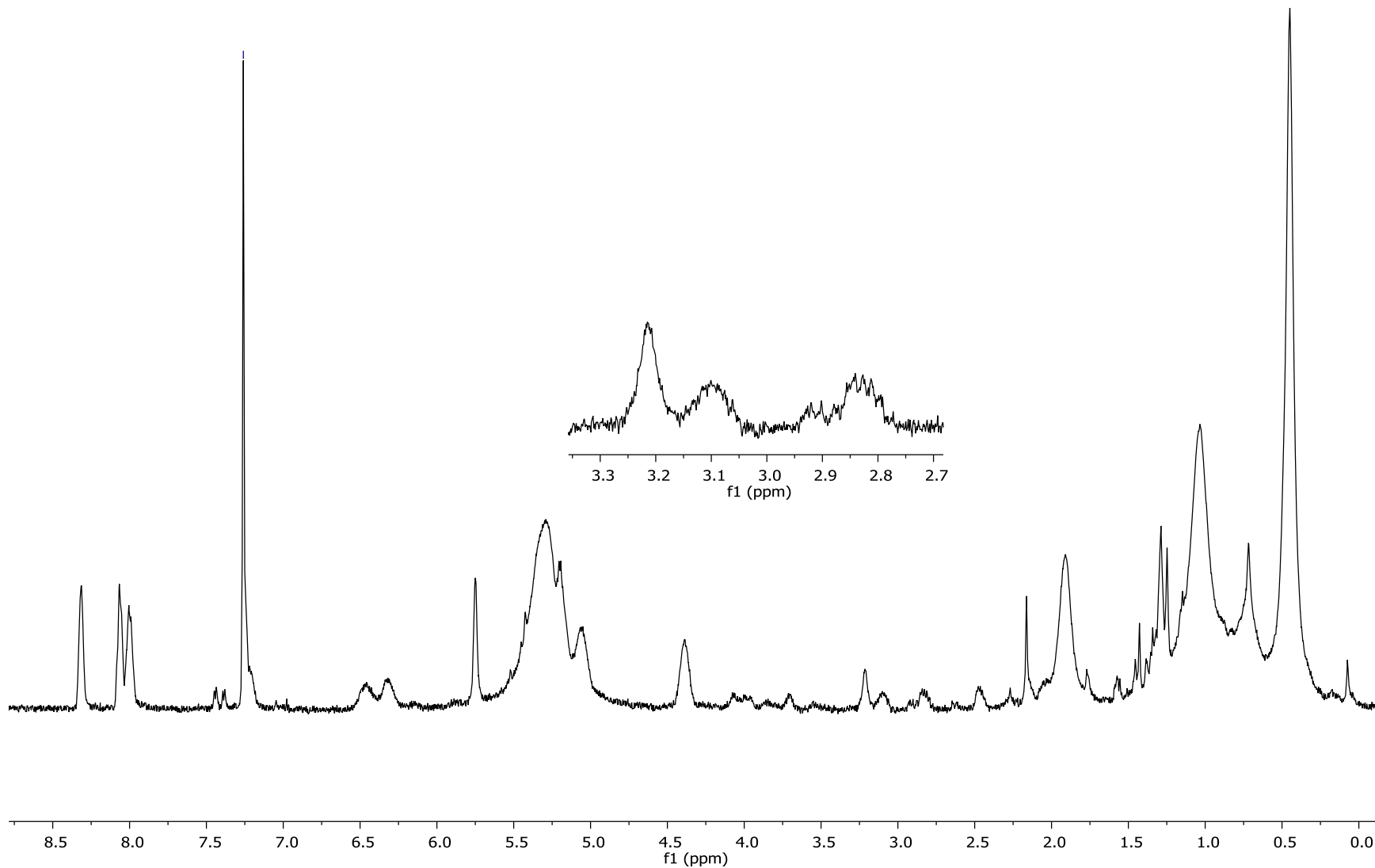




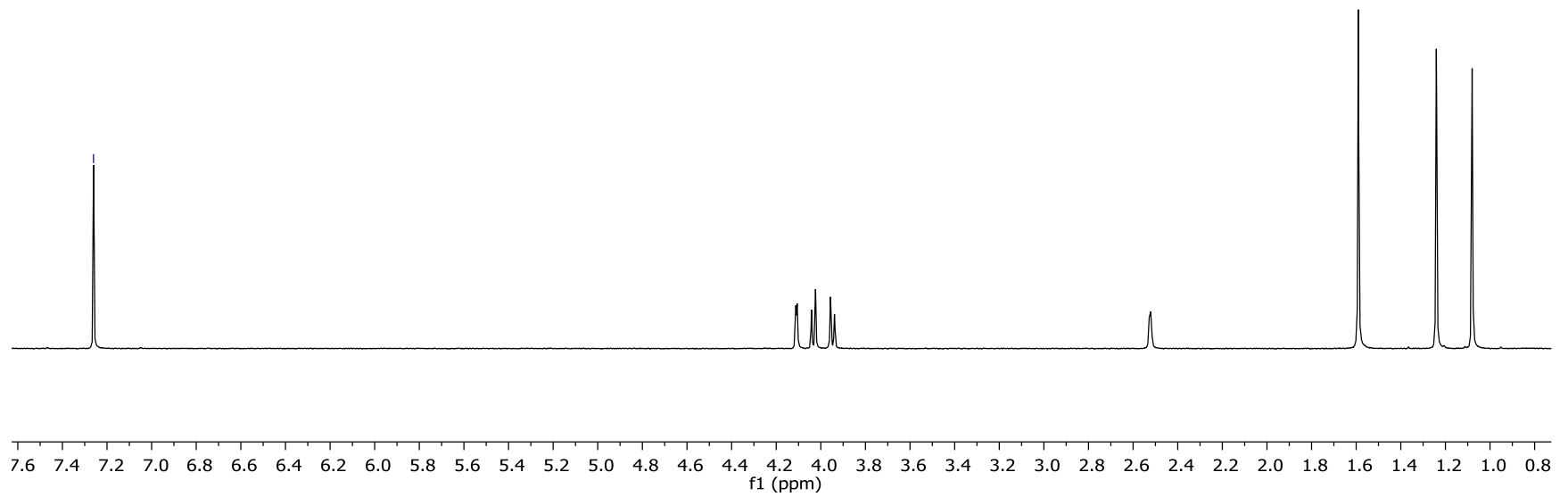
S35

A13-C30

7.26



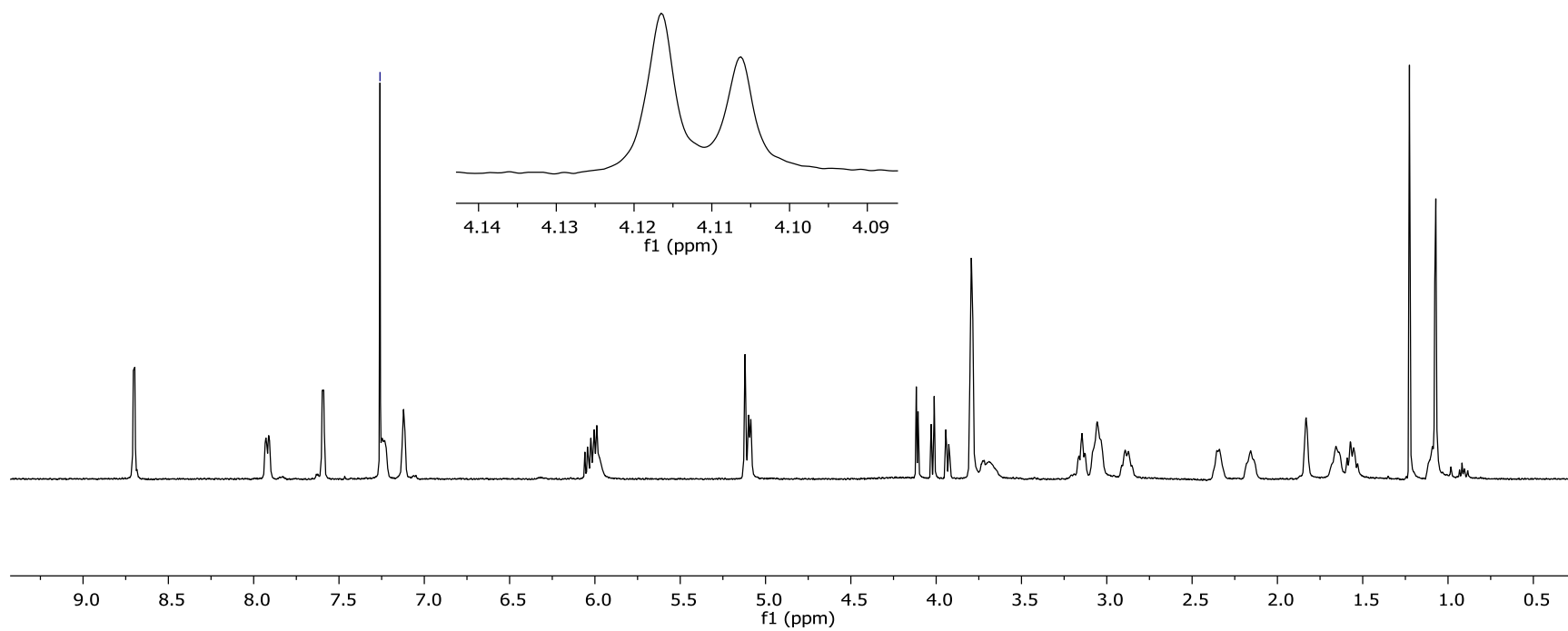
A14  
7.26



S37

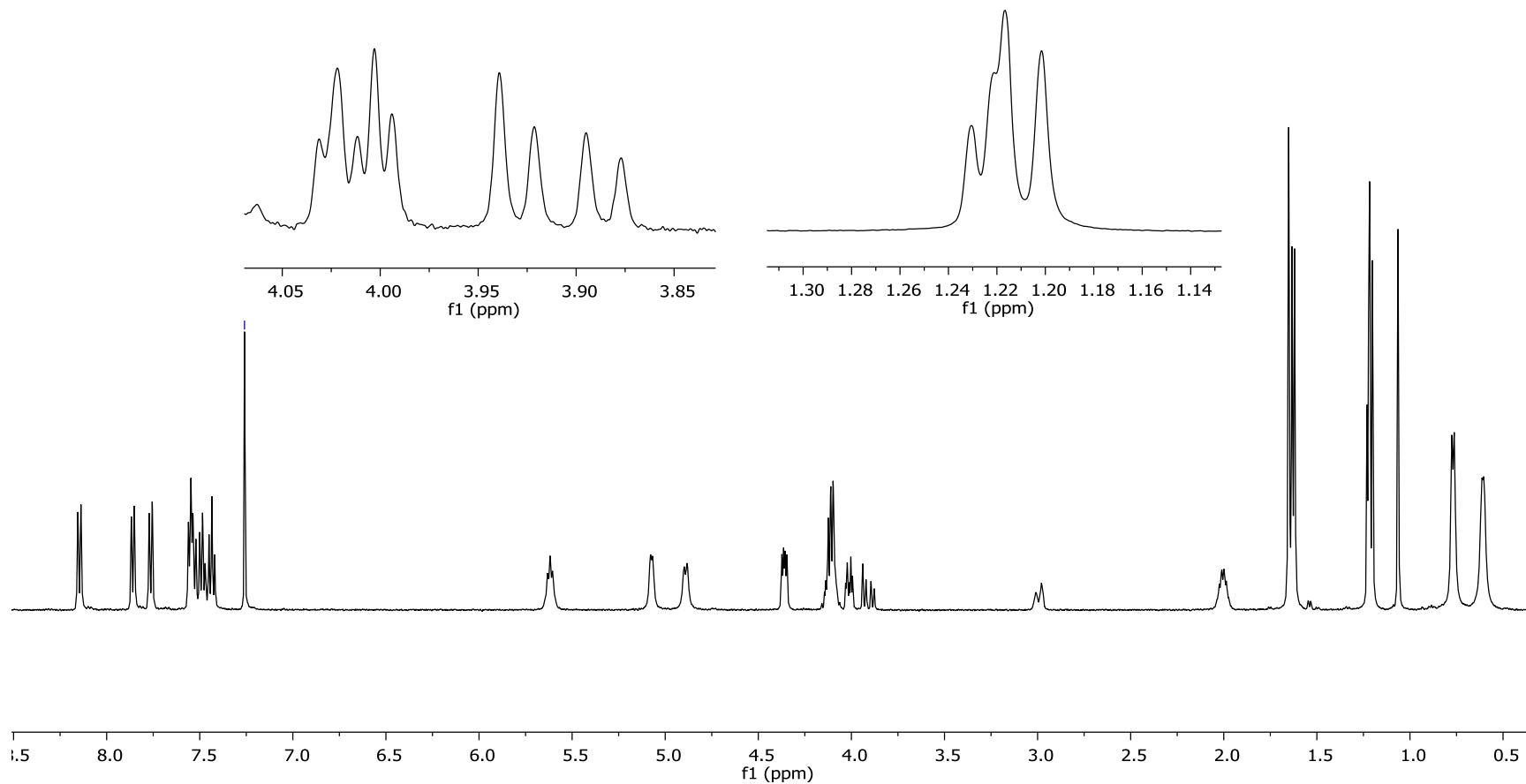
A14-C13

7.26



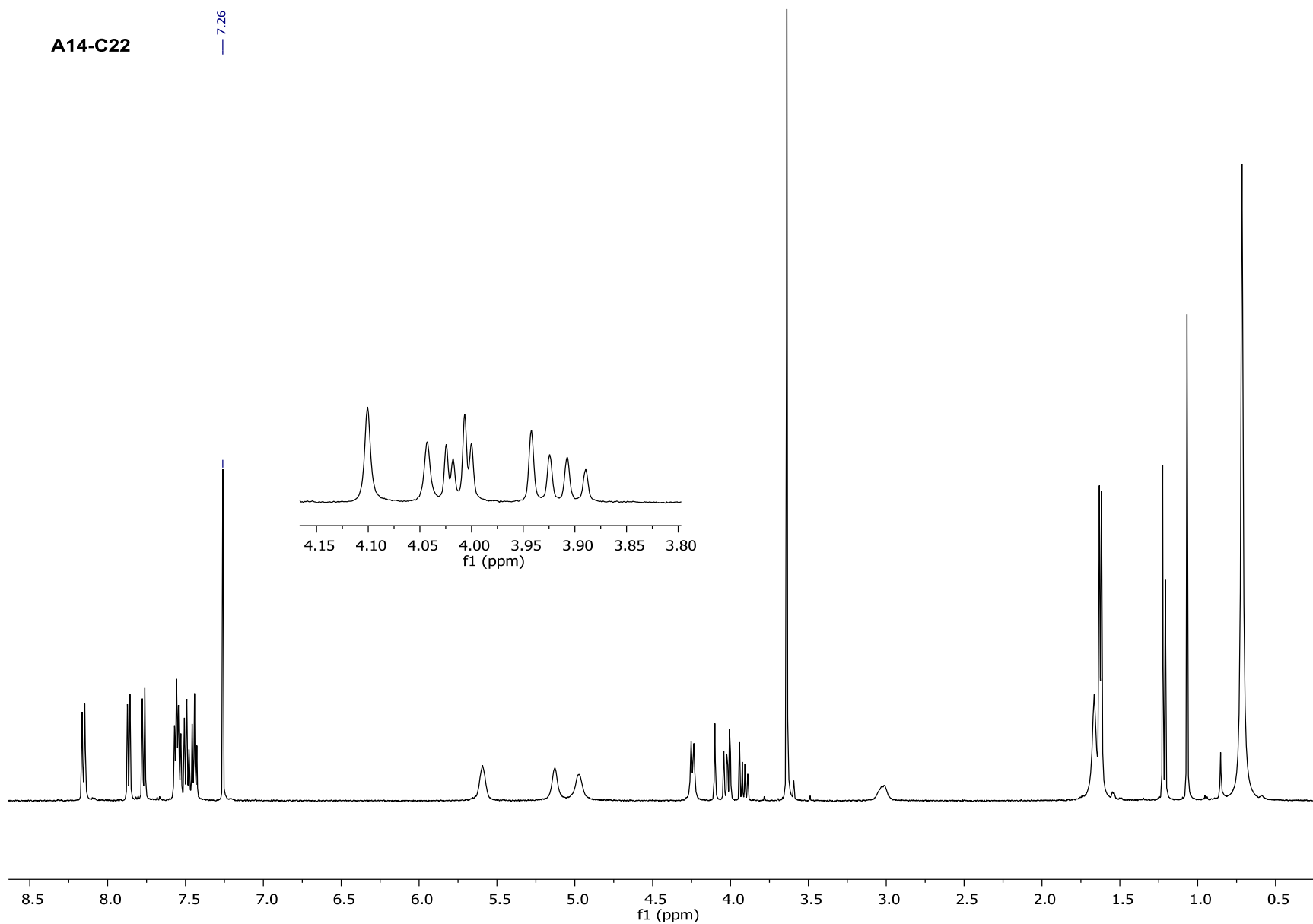
A14-C21

7.26



A14-C22

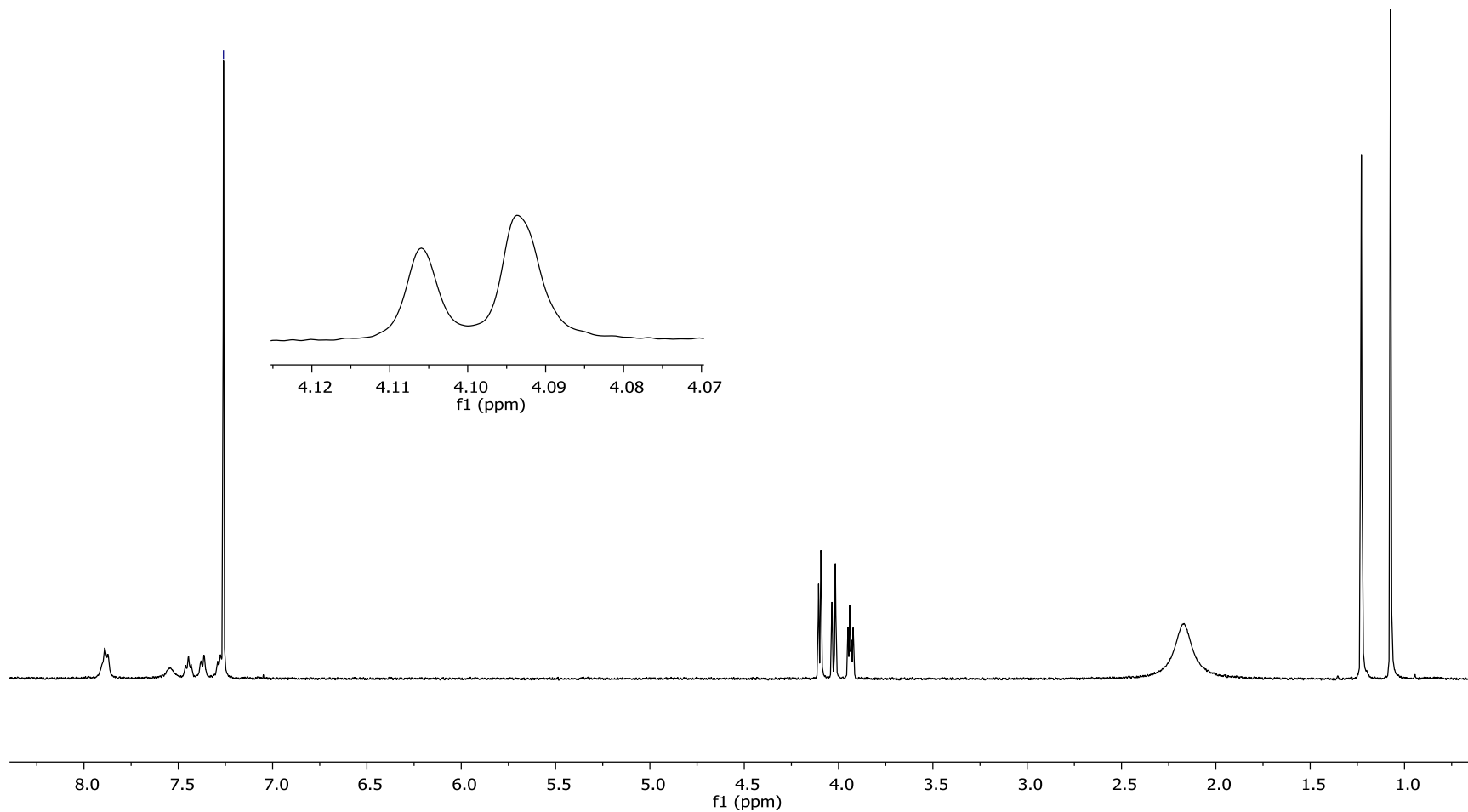
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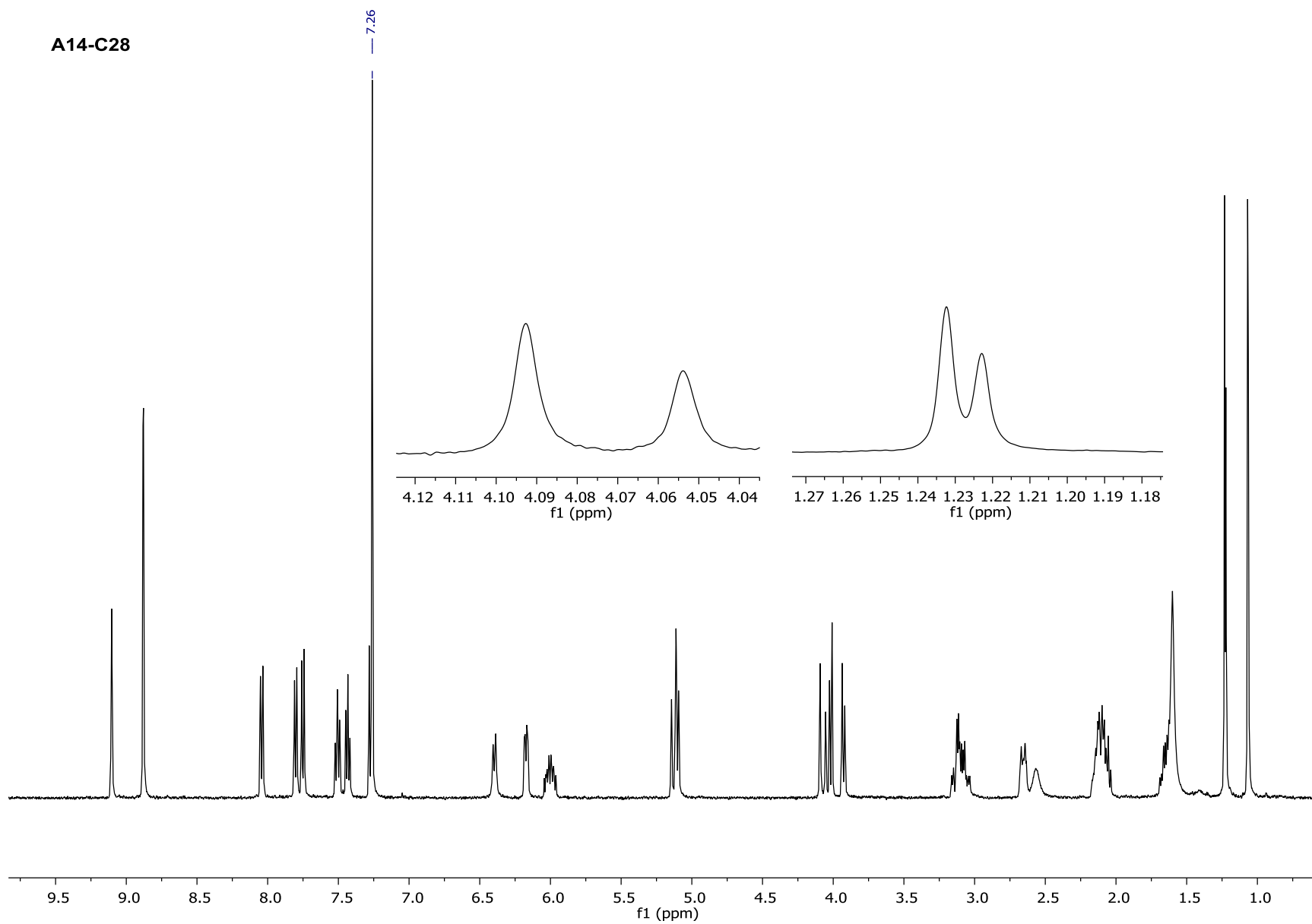


A14-C25

7.26

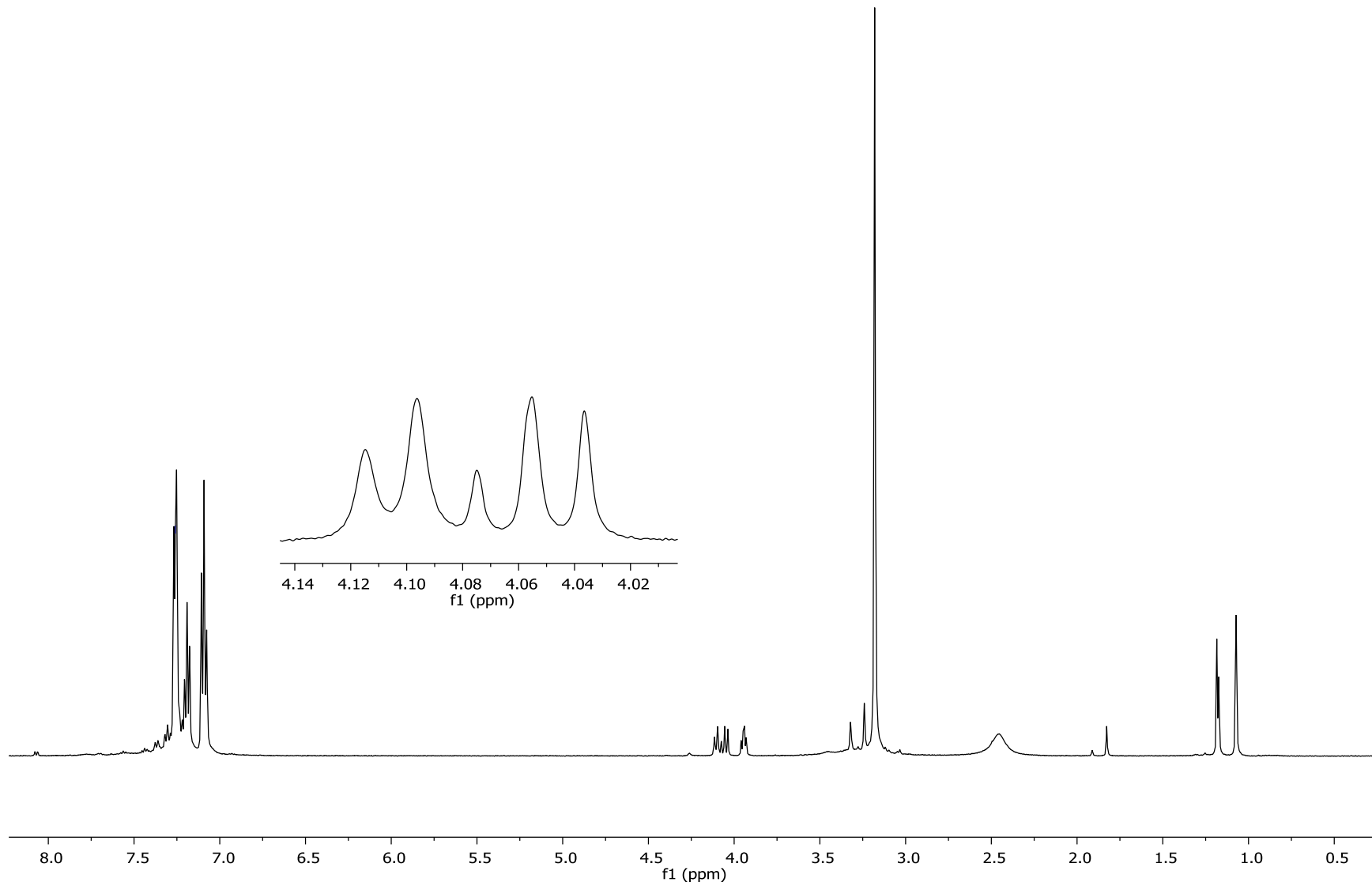


A14-C28



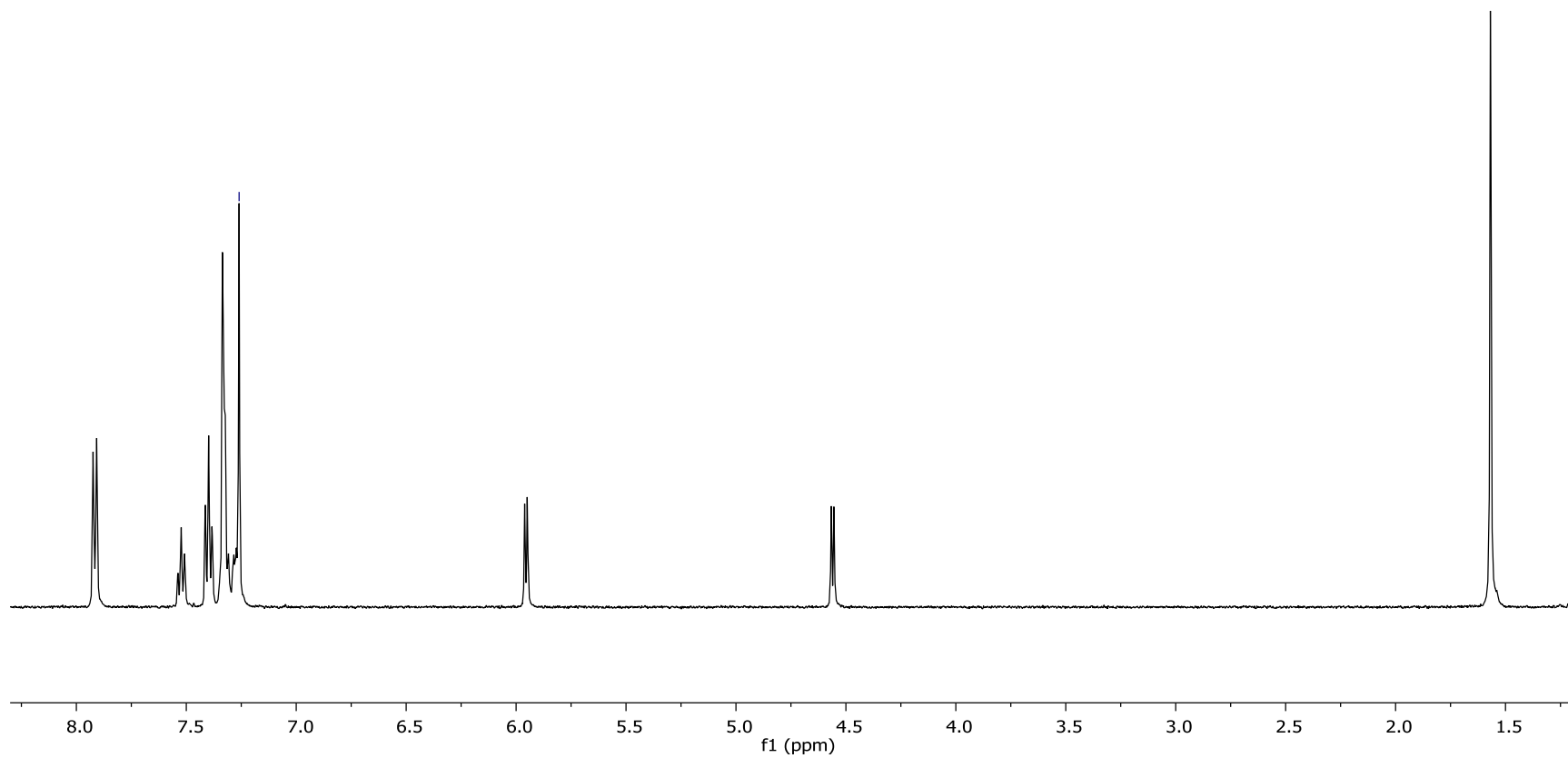
A14-C32

7.26



A15

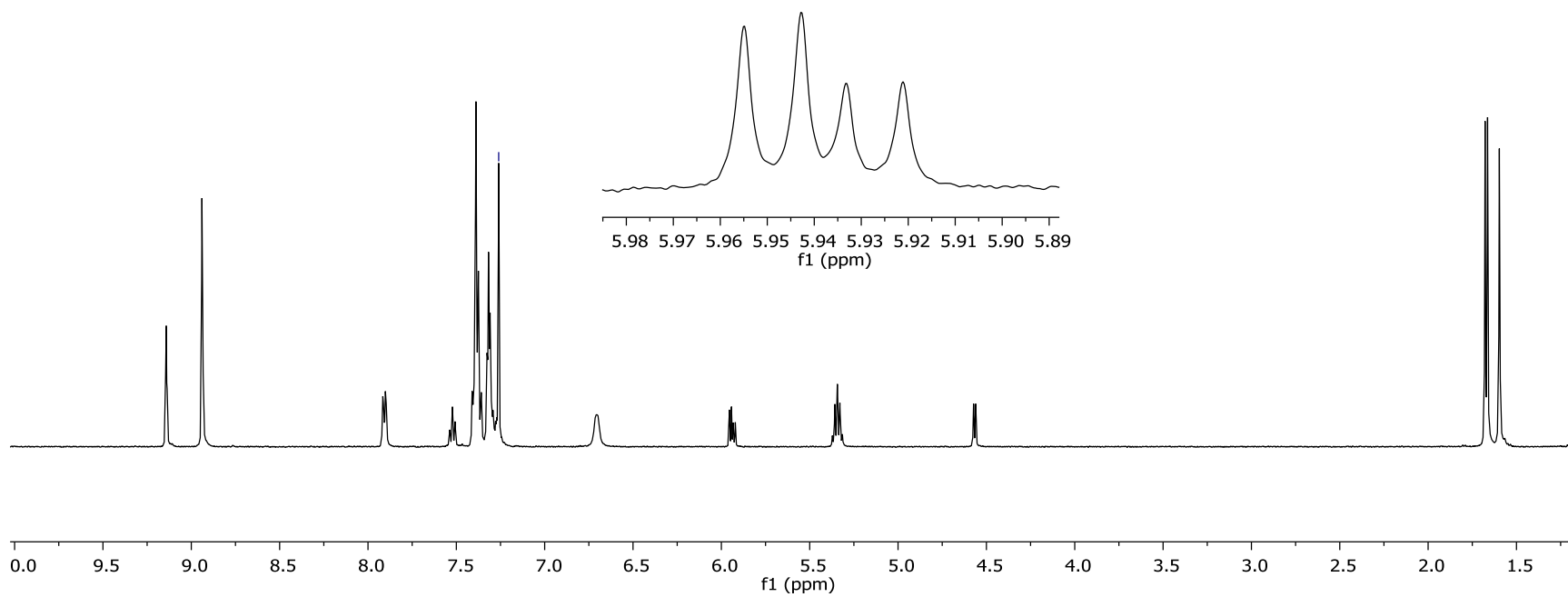
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S44

A15-C18

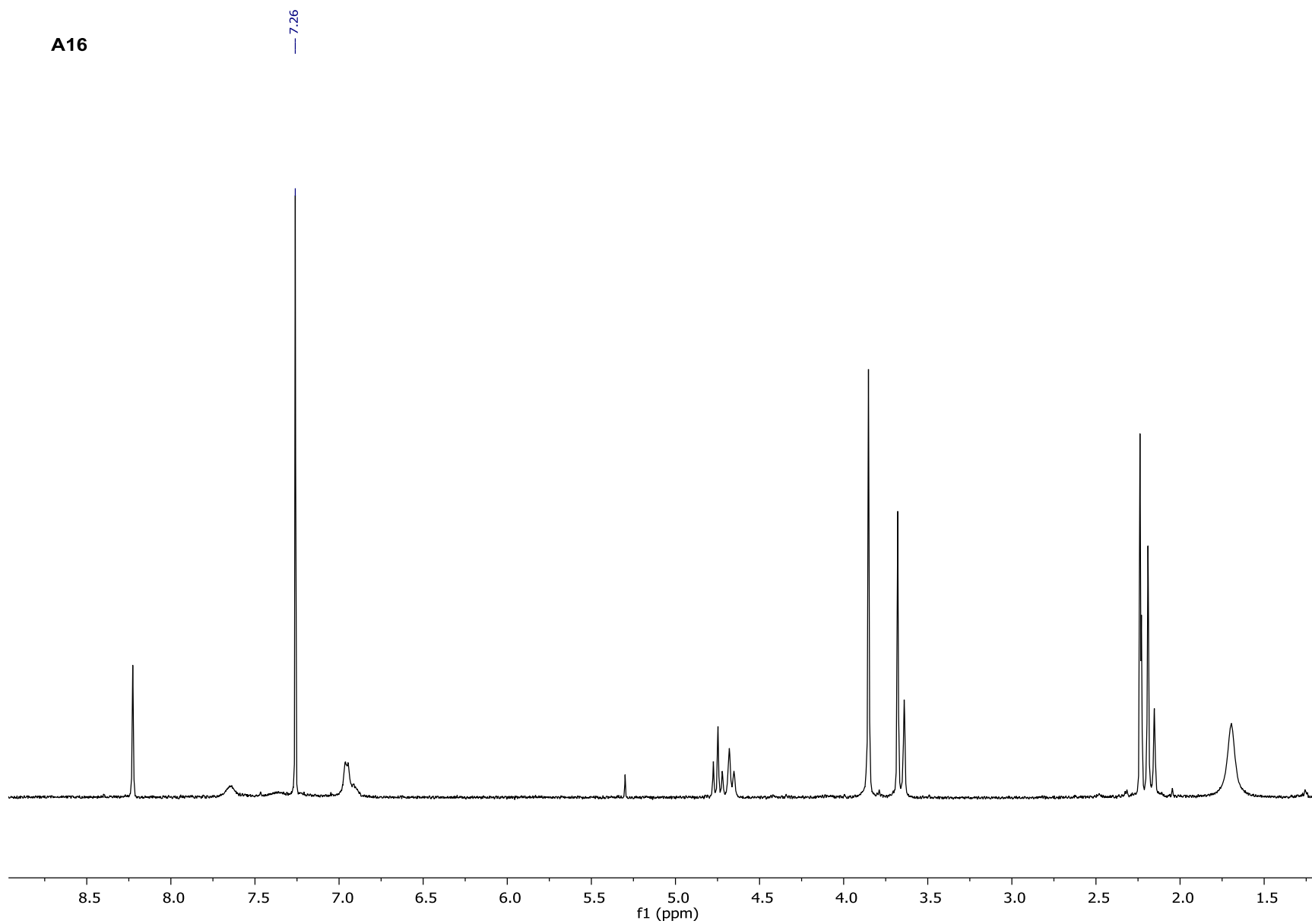
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S45

A16

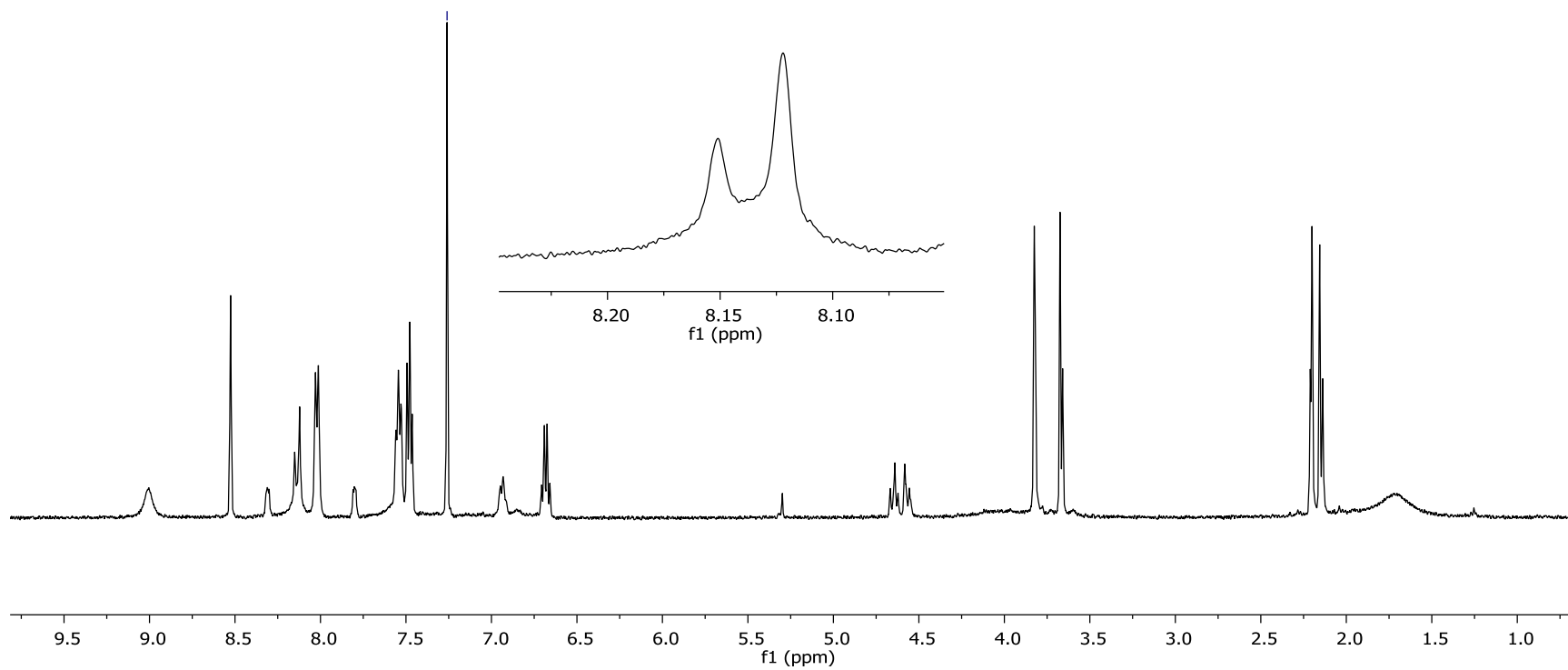
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S46

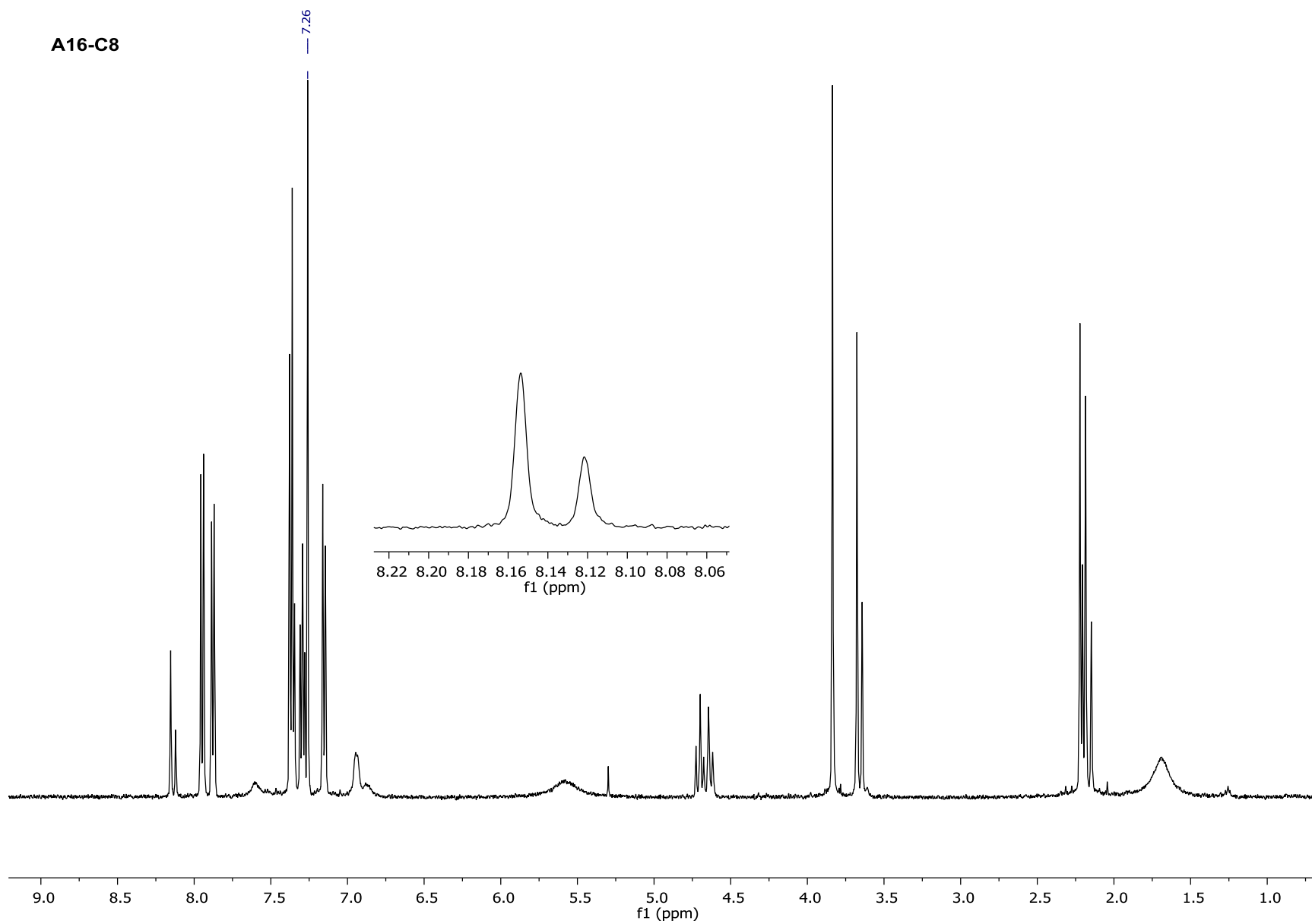
A16-C7

7.26



S47

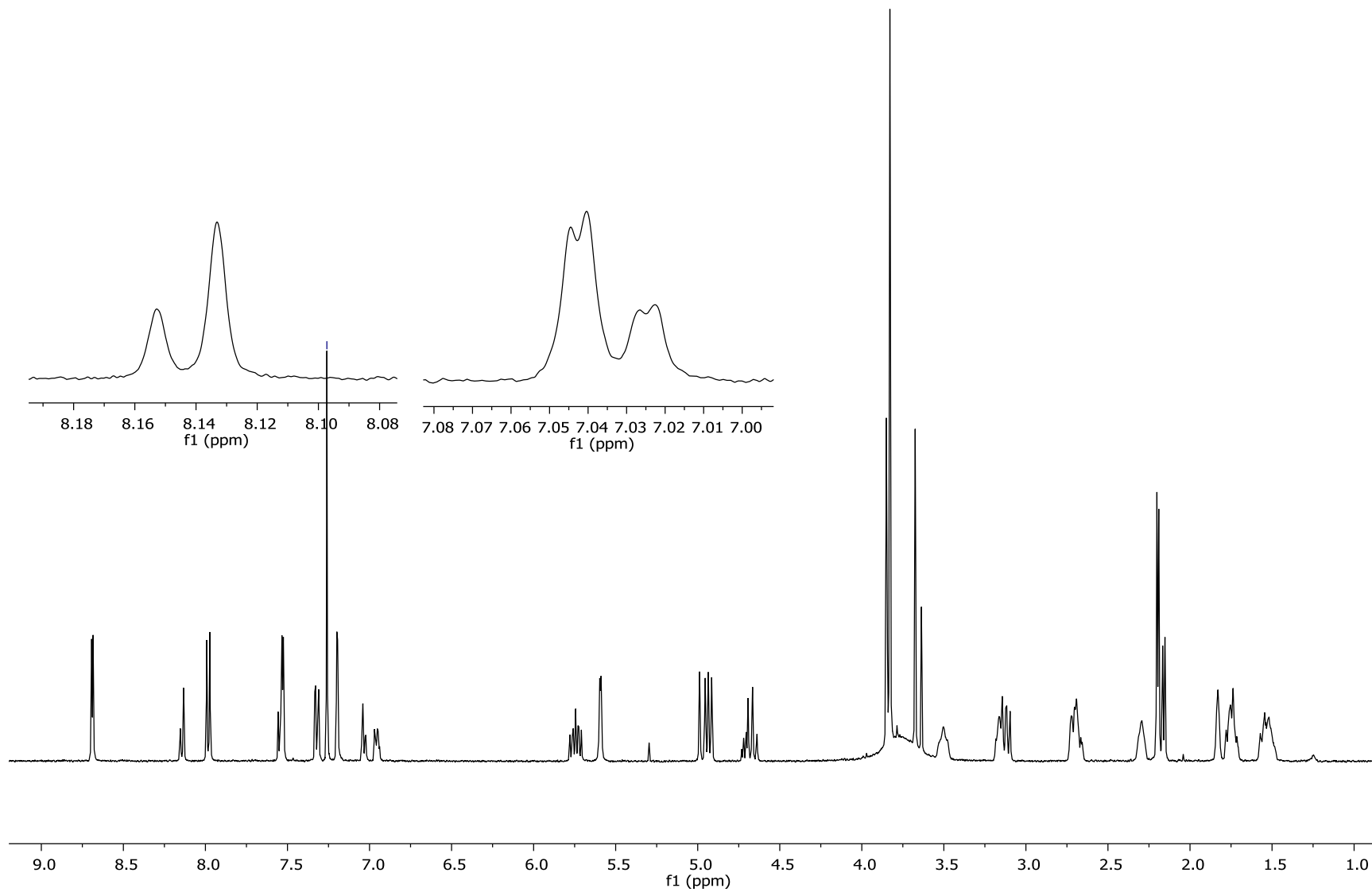
A16-C8





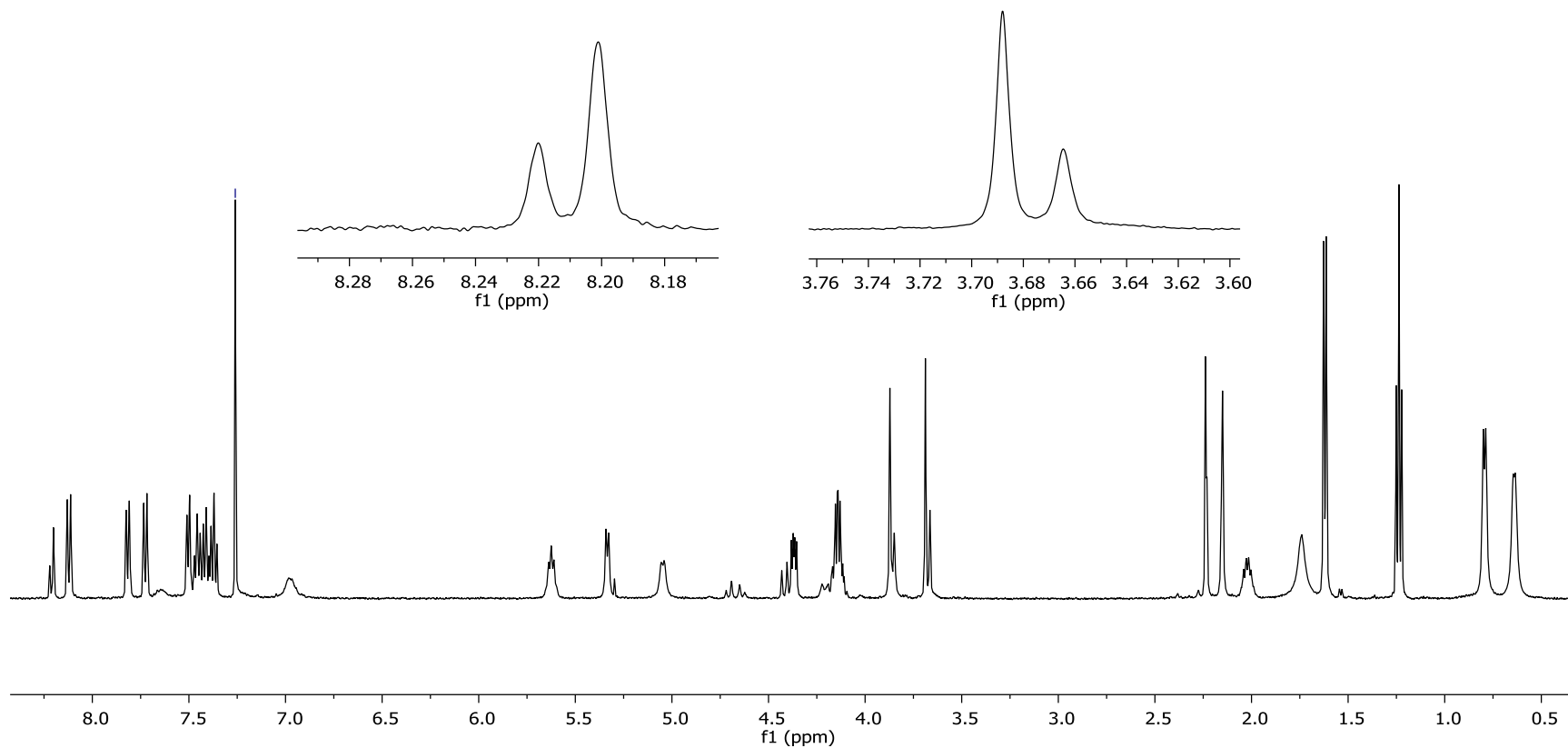
A16-C13

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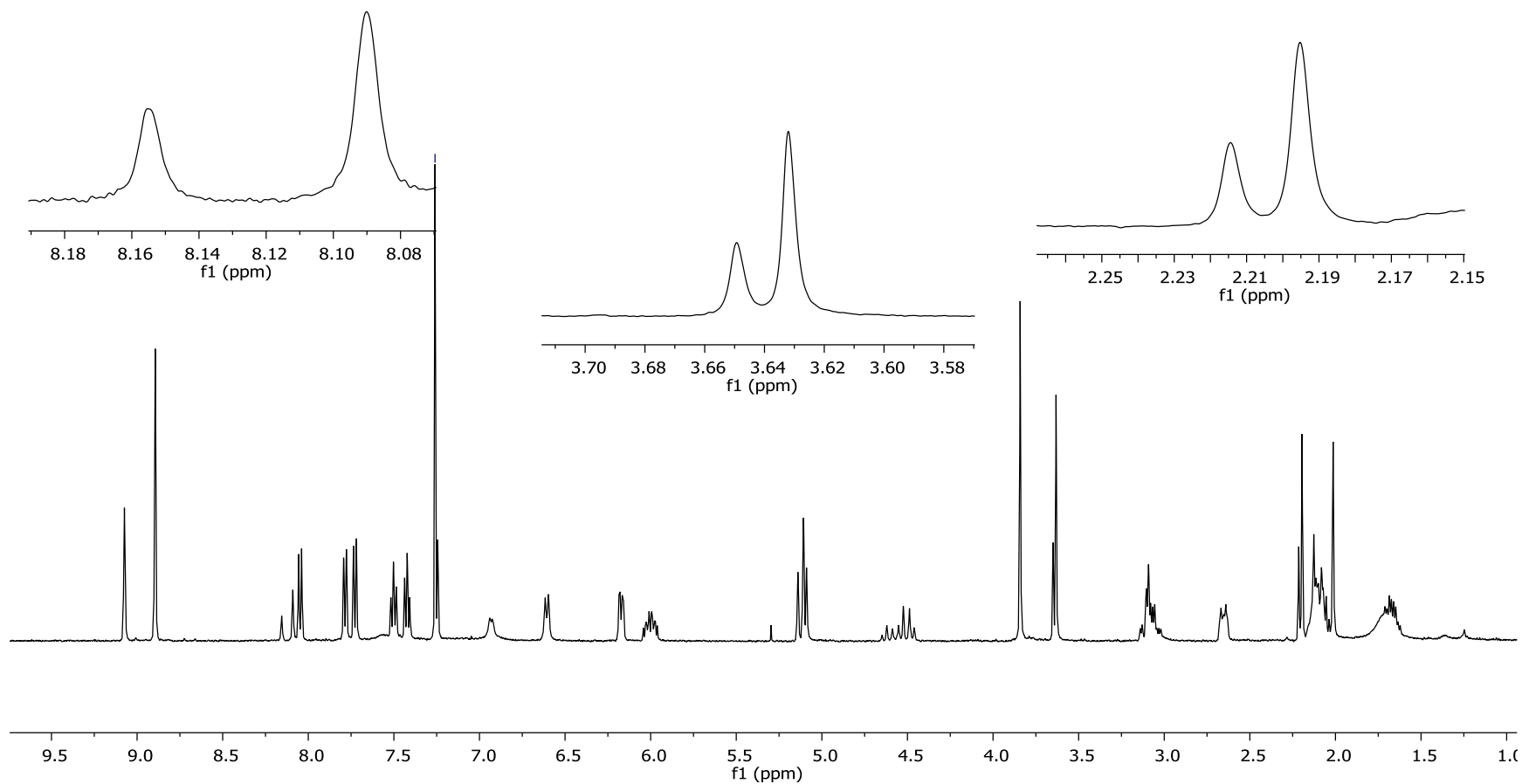
A16-C22

7.26

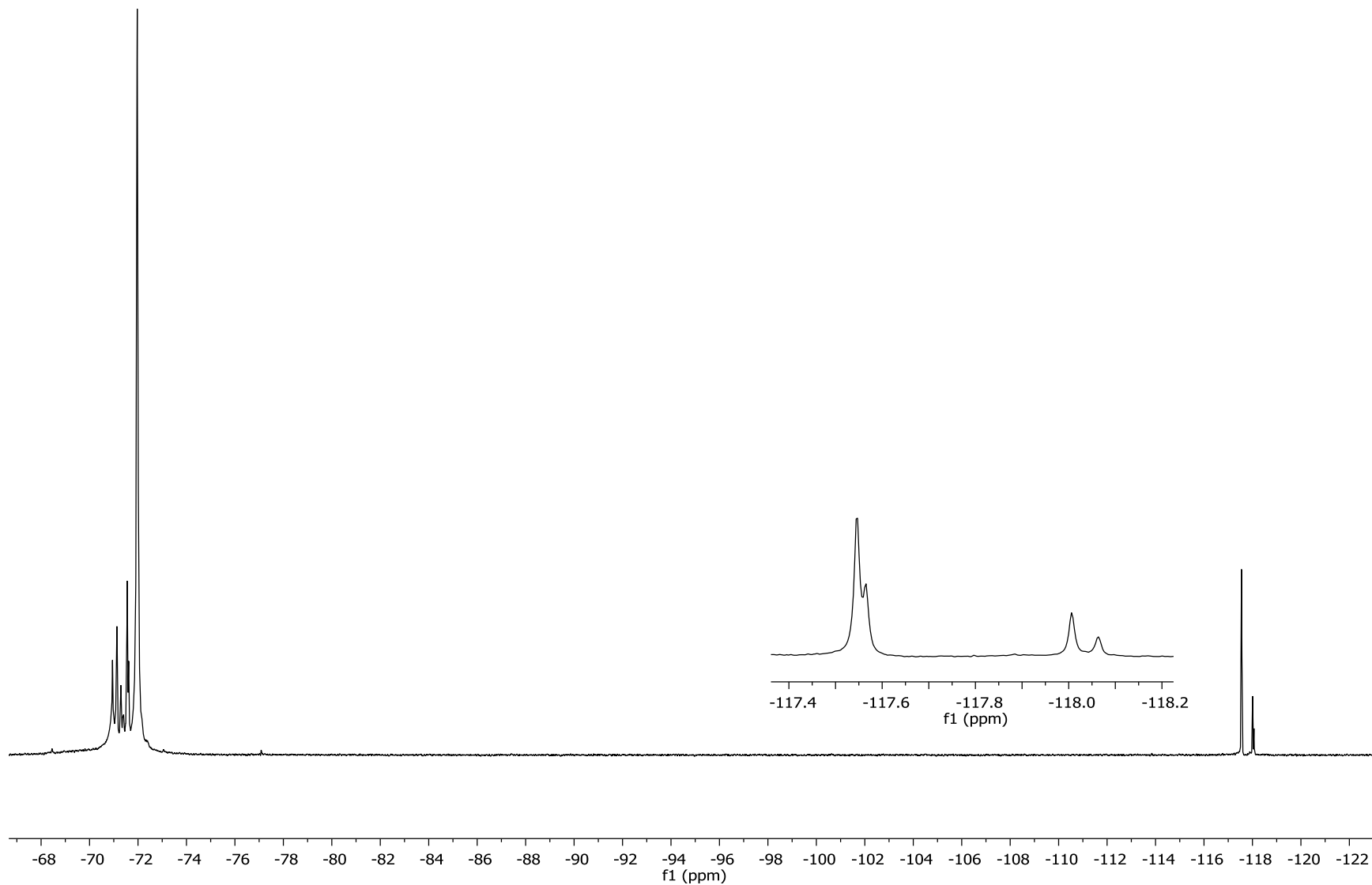


A16-C28

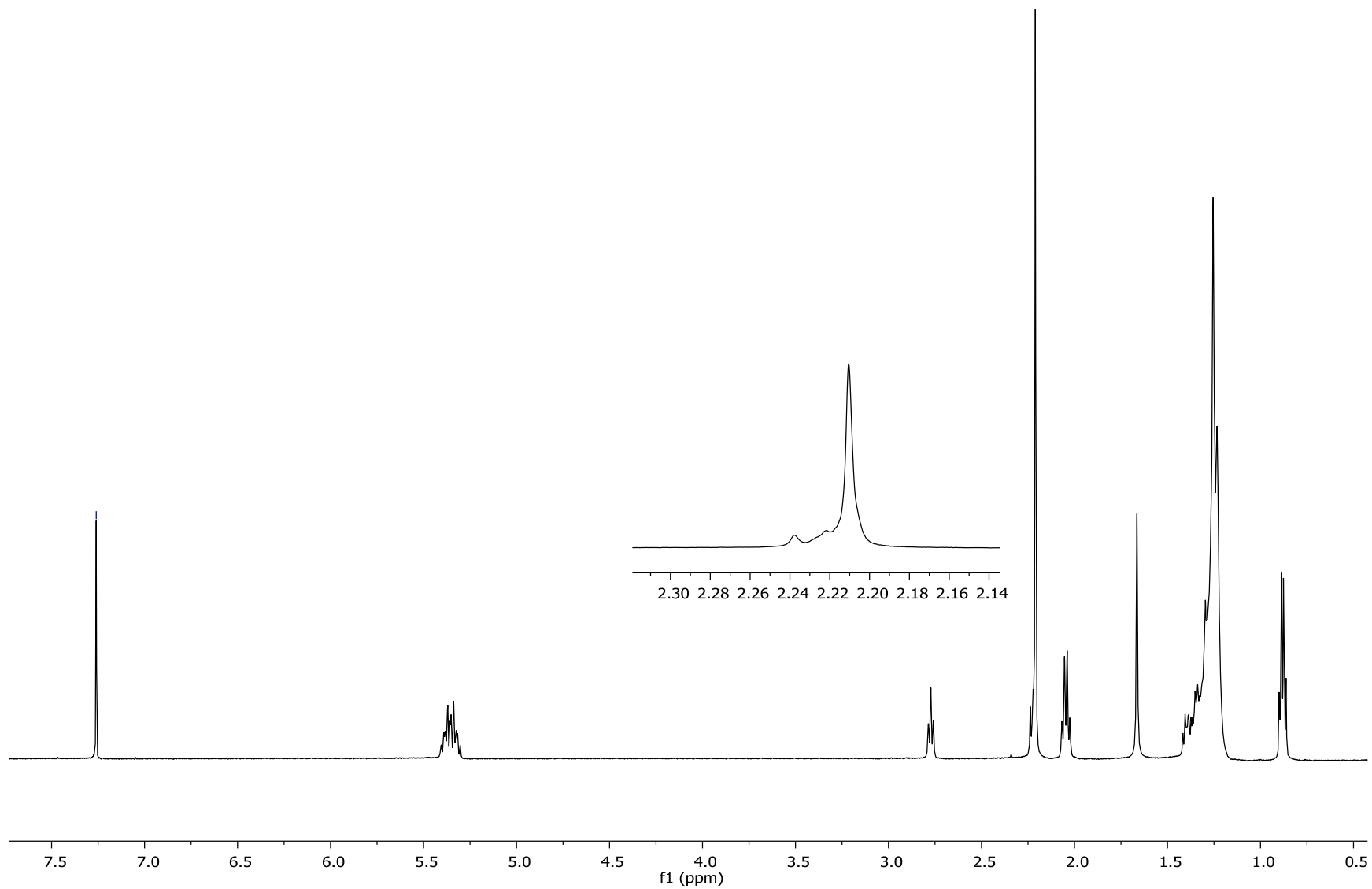
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A2-C32 19F NMR (471 MHz, CDCl3)

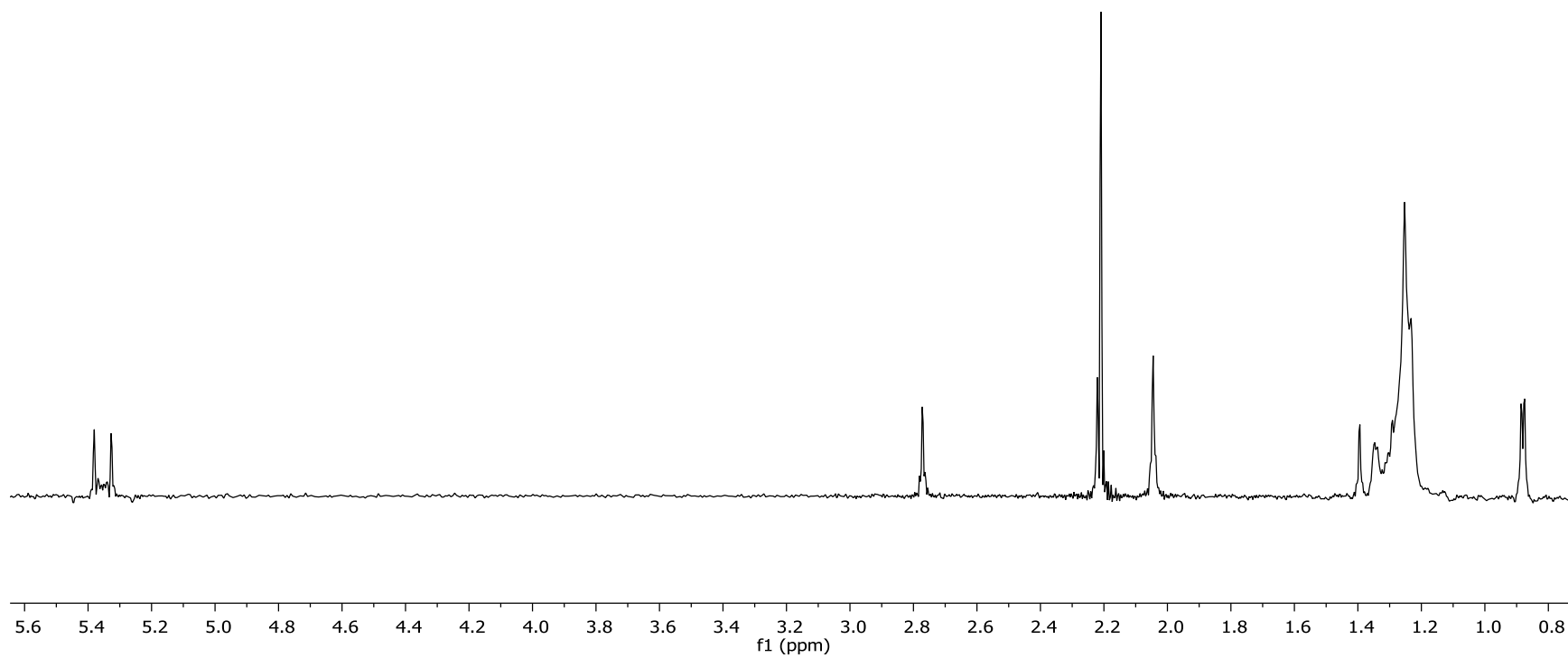


A17 | 7.26

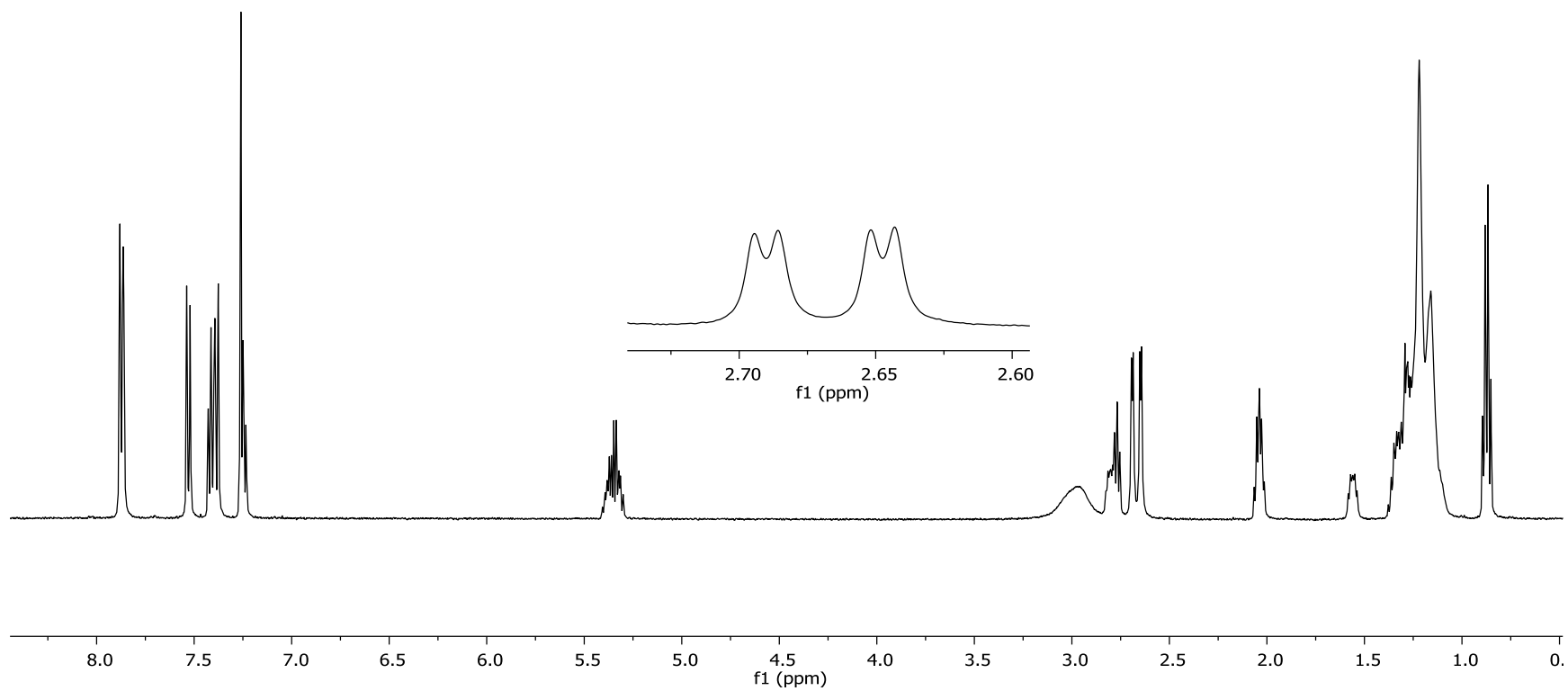


S53

A17 1D Pure Shift



A17-C25



S55

A17-C25 1D Pure Shift

