

Supporting Information :

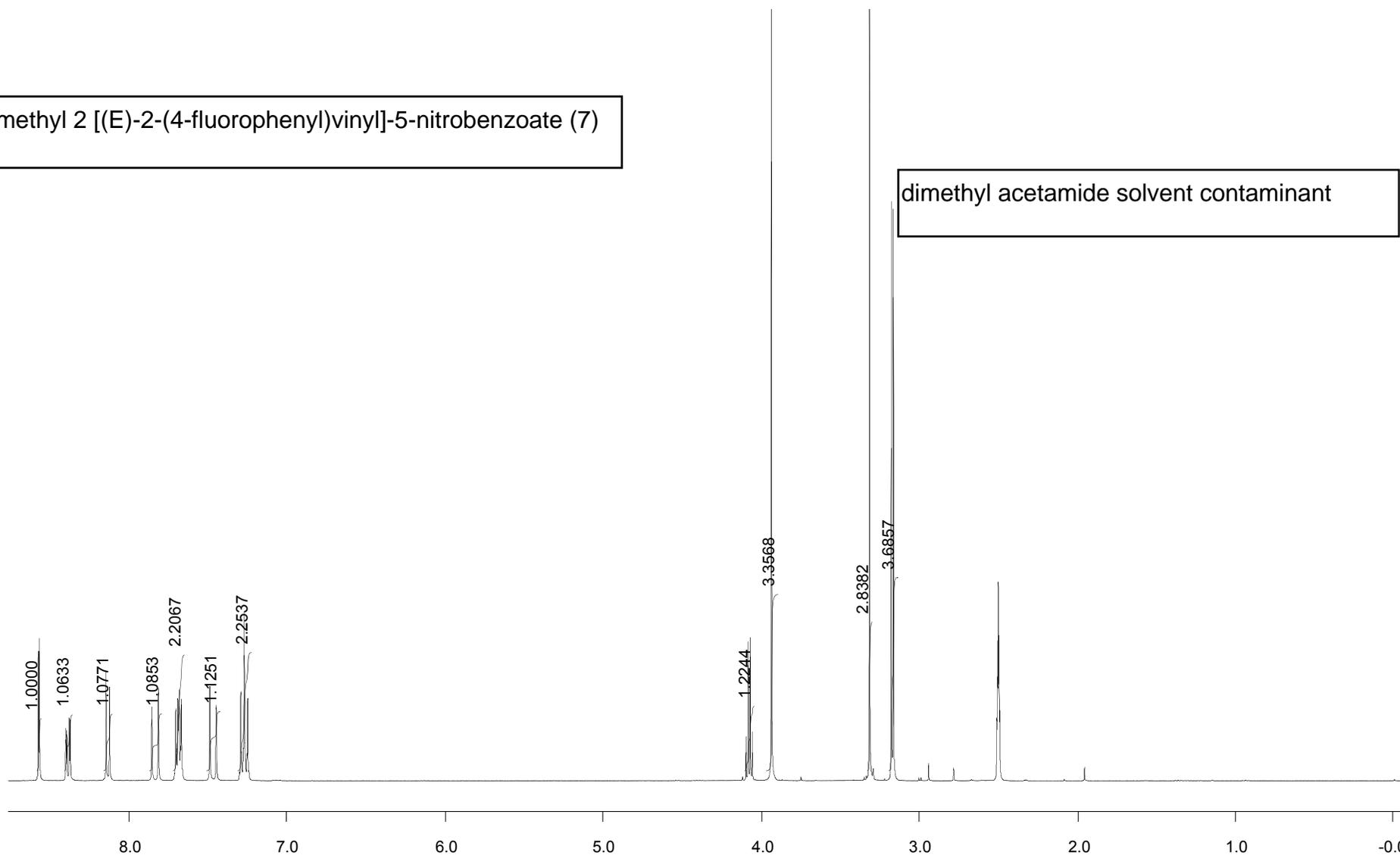
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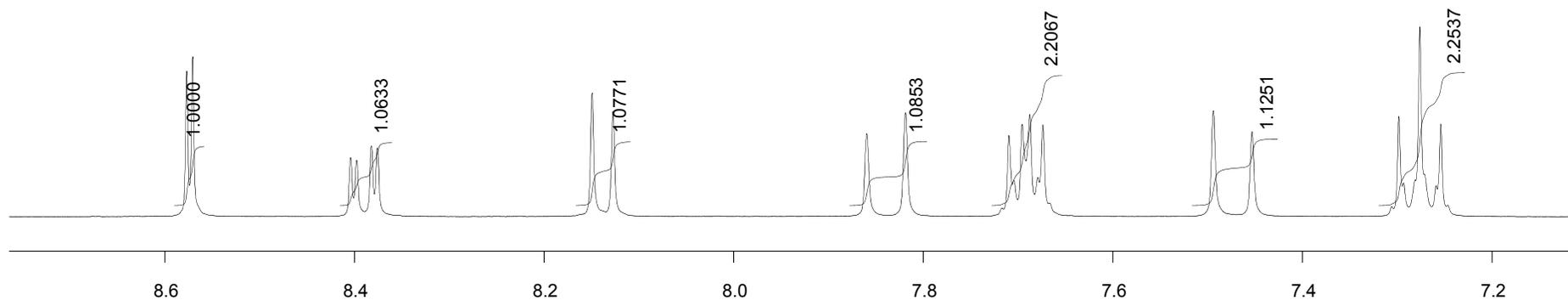
methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)

dimethyl acetamide solvent contaminant



JView Version 0.95 /NMR/chem/nmr/041213023/10/pdata/1/
Joanne Shuffebotham, Stilbene CS03/133A/4, 20.43mg Stilbene
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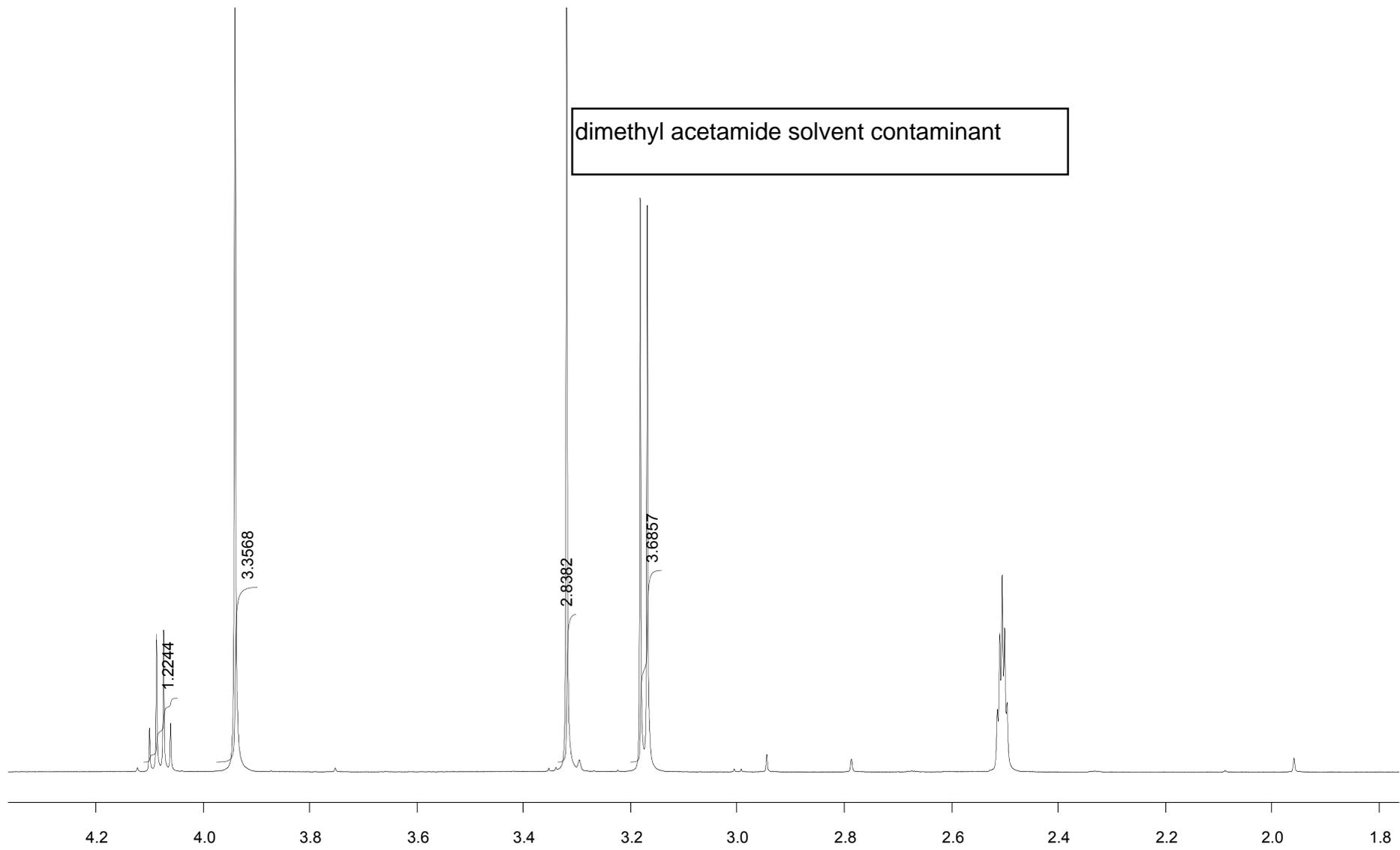
methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)



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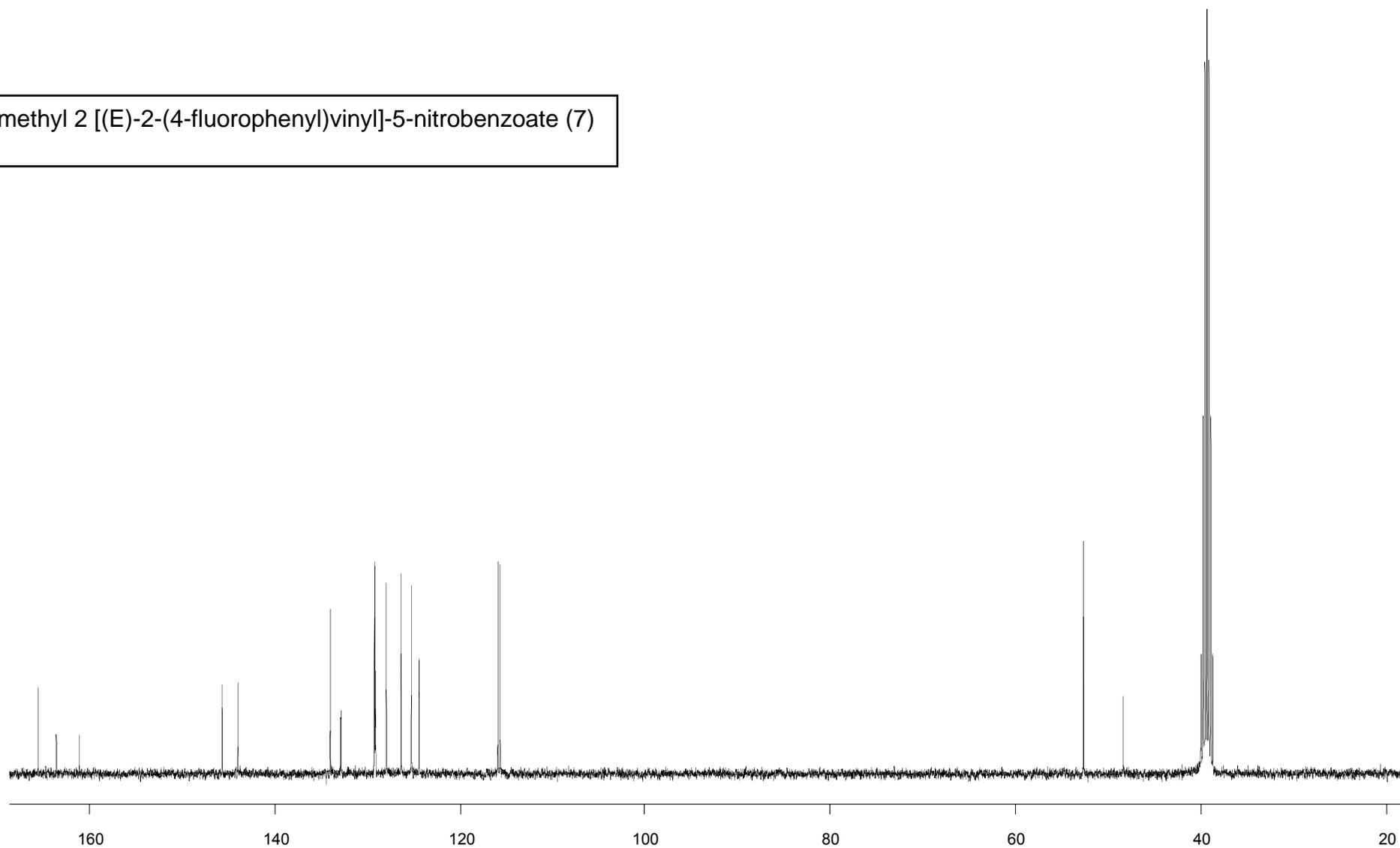
methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)

dimethyl acetamide solvent contaminant



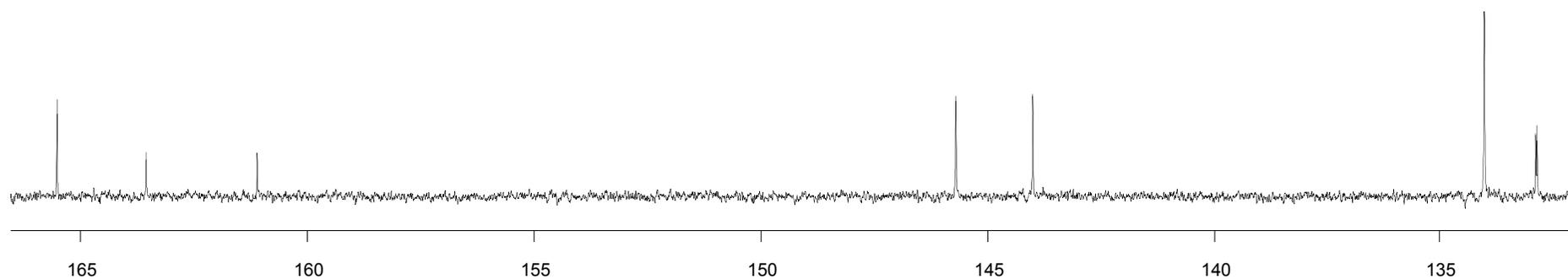
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methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)



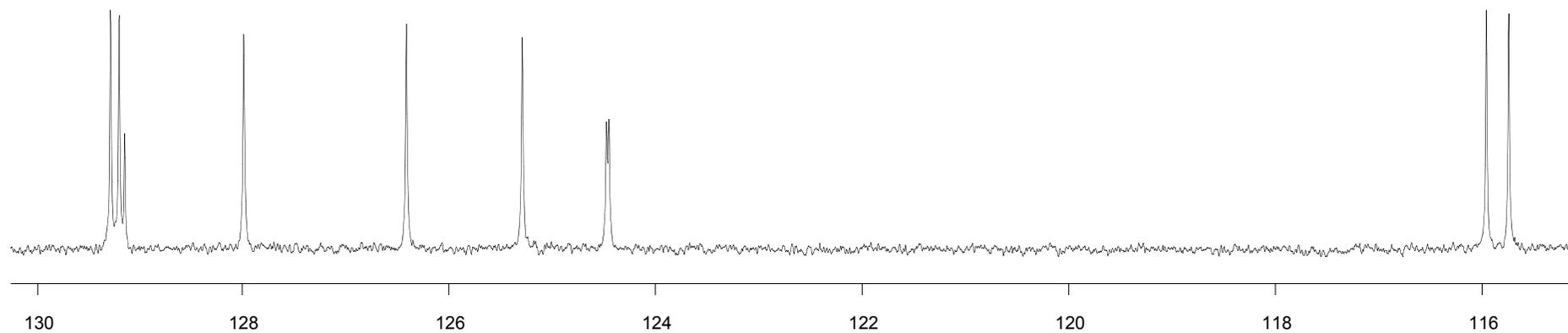
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methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)



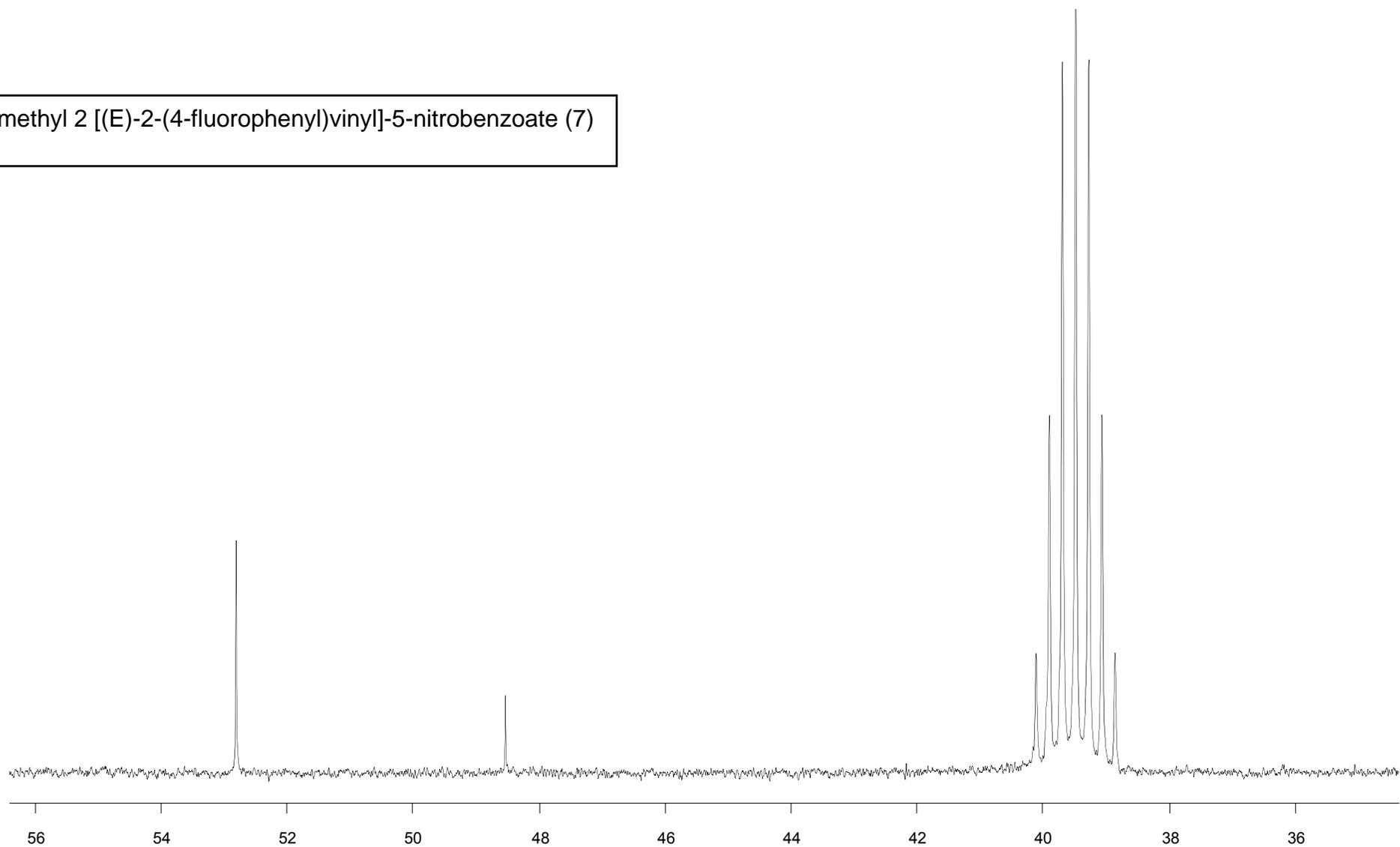
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methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)



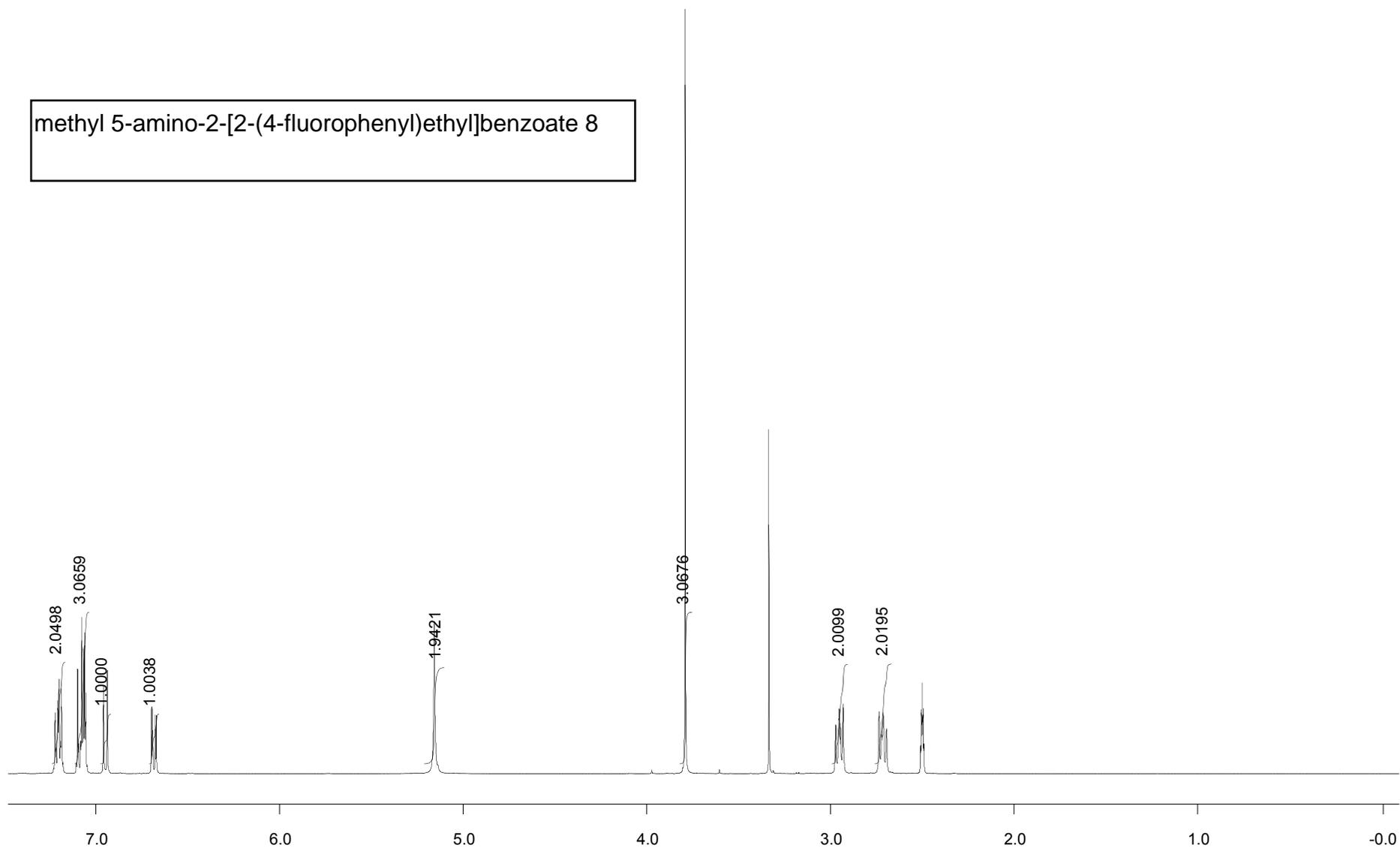
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methyl 2 [(E)-2-(4-fluorophenyl)vinyl]-5-nitrobenzoate (7)



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methyl 5-amino-2-[2-(4-fluorophenyl)ethyl]benzoate 8

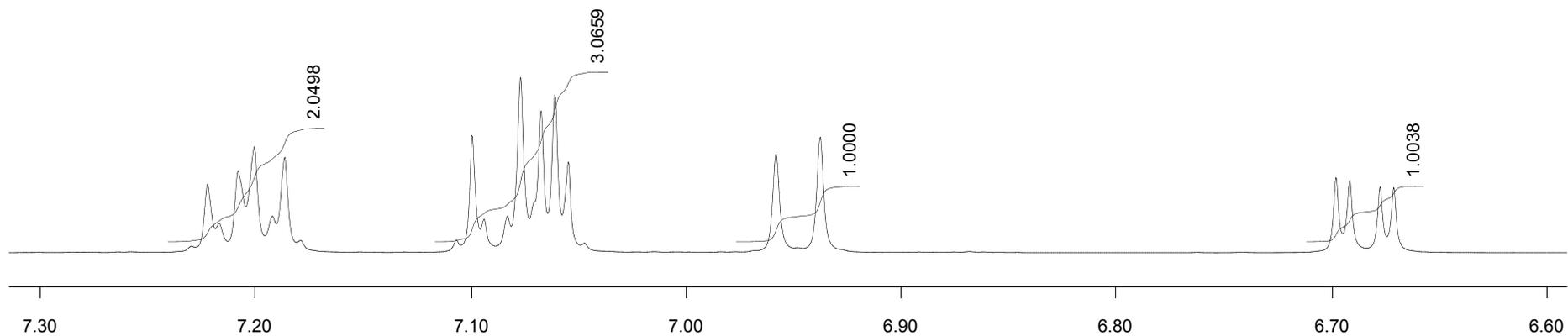


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Victoria Winterbottom, 097868, Sat Amine

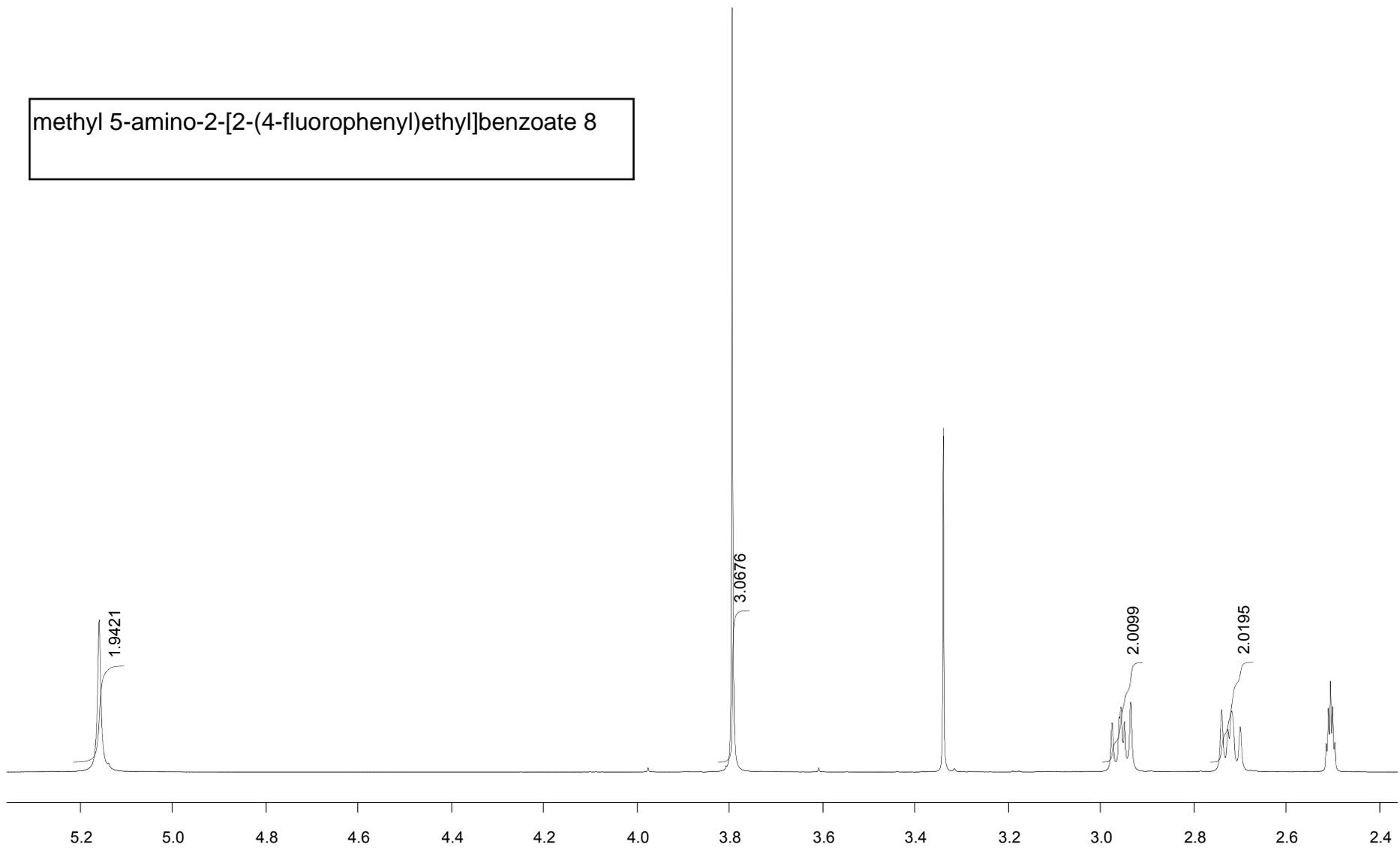
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methyl 5-amino-2-[2-(4-fluorophenyl)ethyl]benzoate 8



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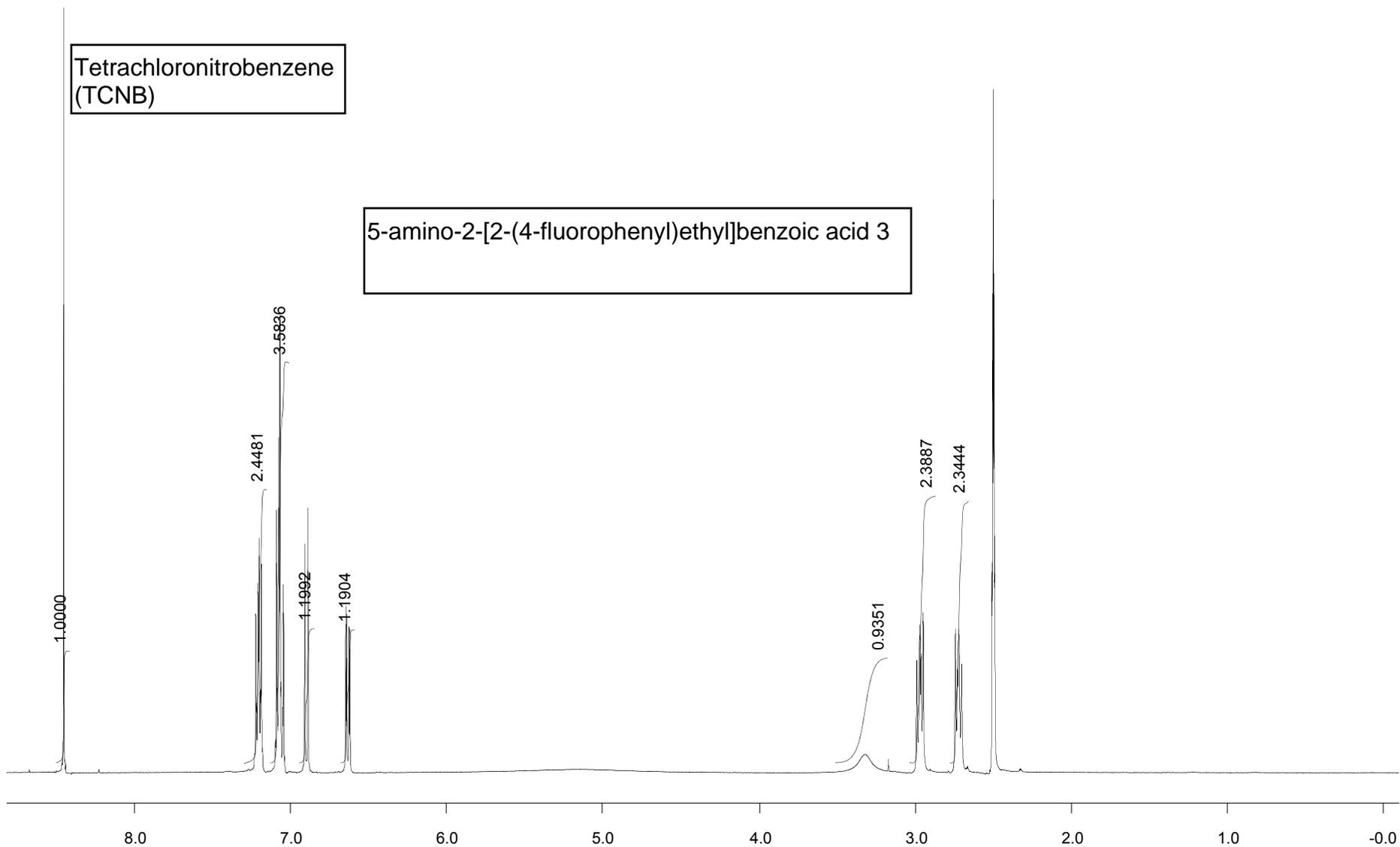
methyl 5-amino-2-[2-(4-fluorophenyl)ethyl]benzoate 8



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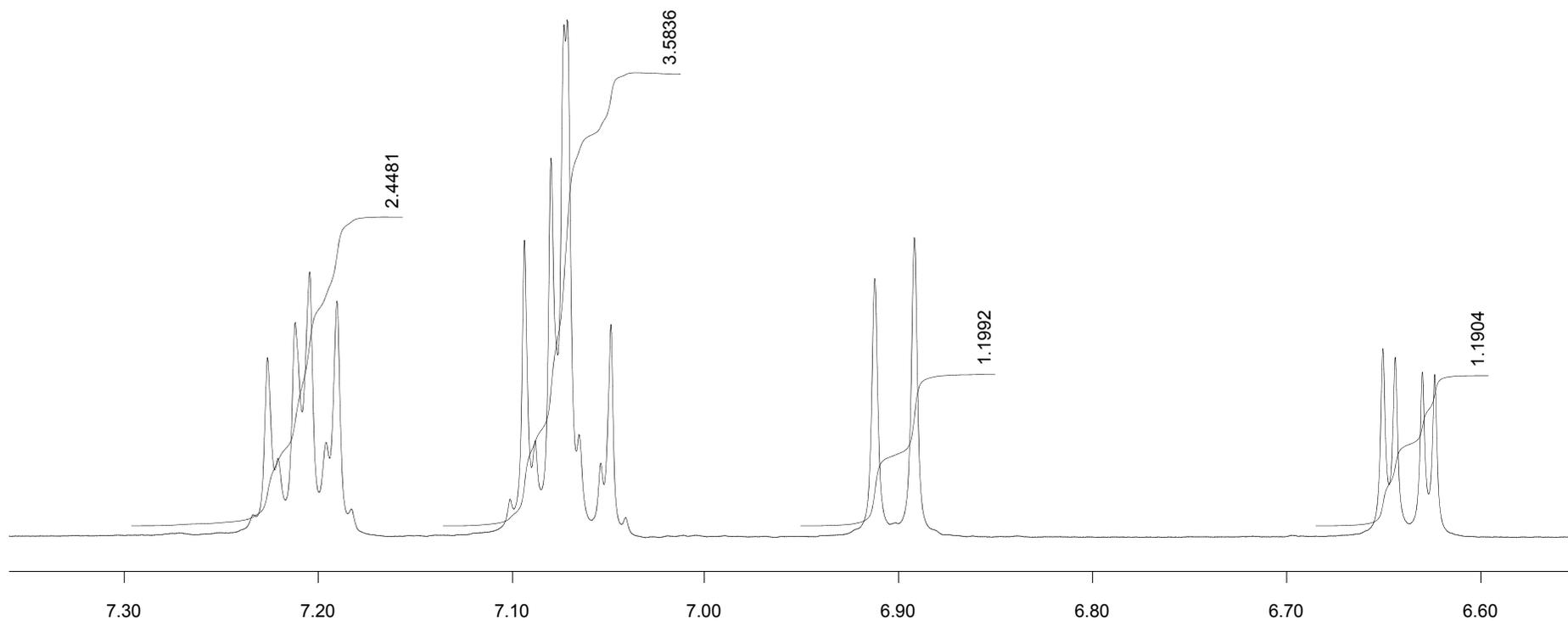
Tetrachloronitrobenzene
(TCNB)

5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



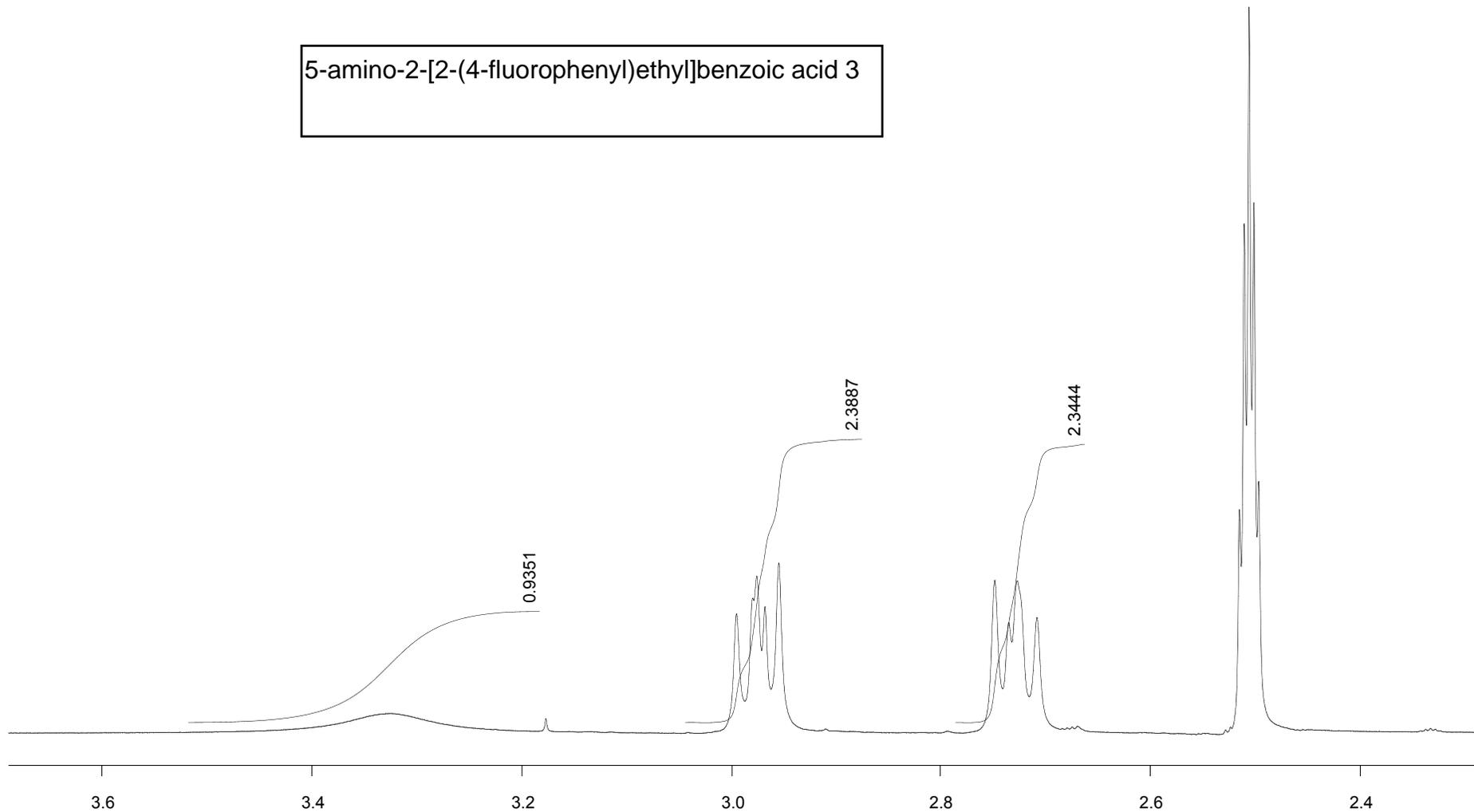
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Printed by RD\M235797 on Mon Jul 16 16:45:12 BST 2007. nucleus: 1H, freq: 400.13 MHz, solvent: DMSO, temperature:300K

5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



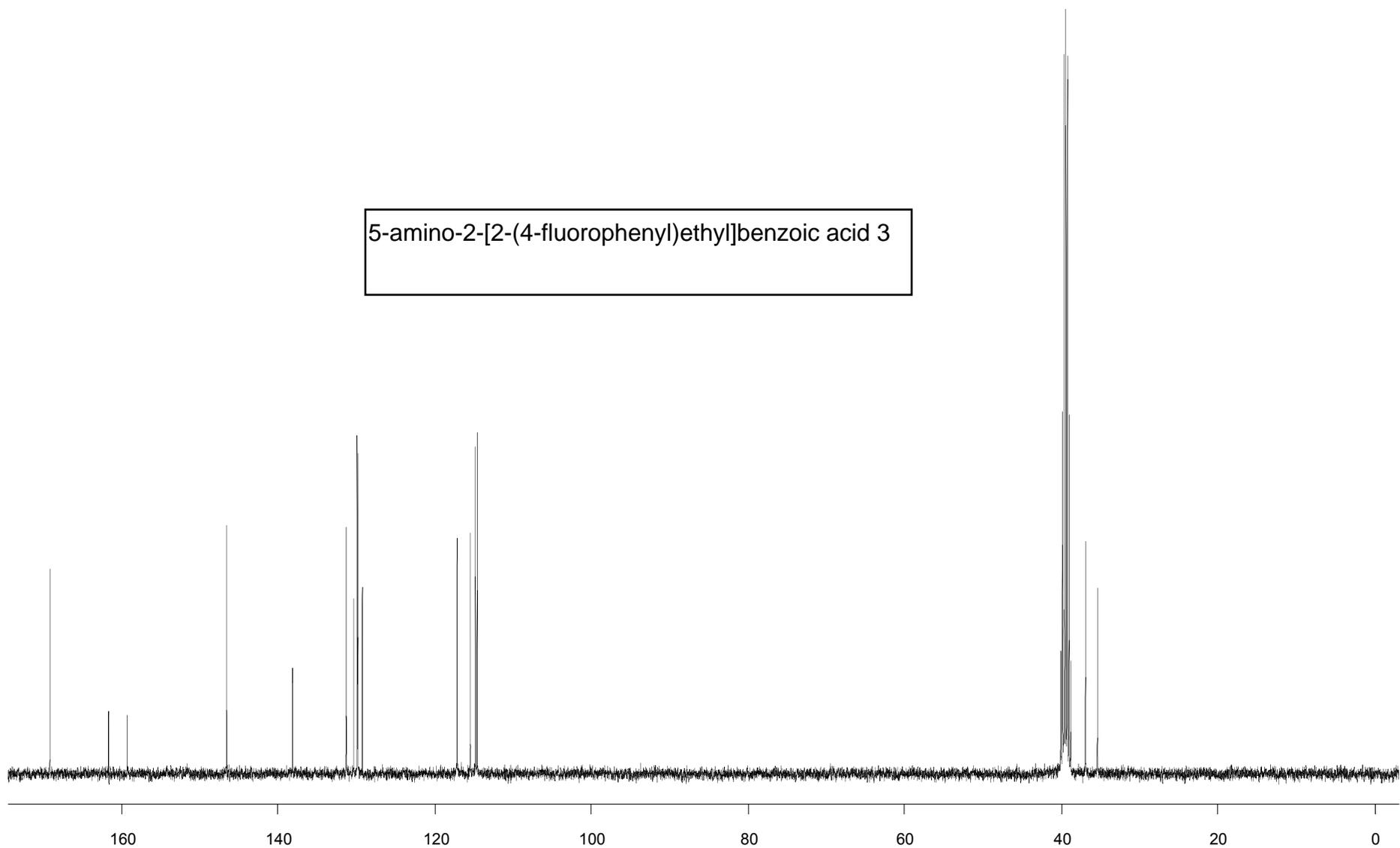
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5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



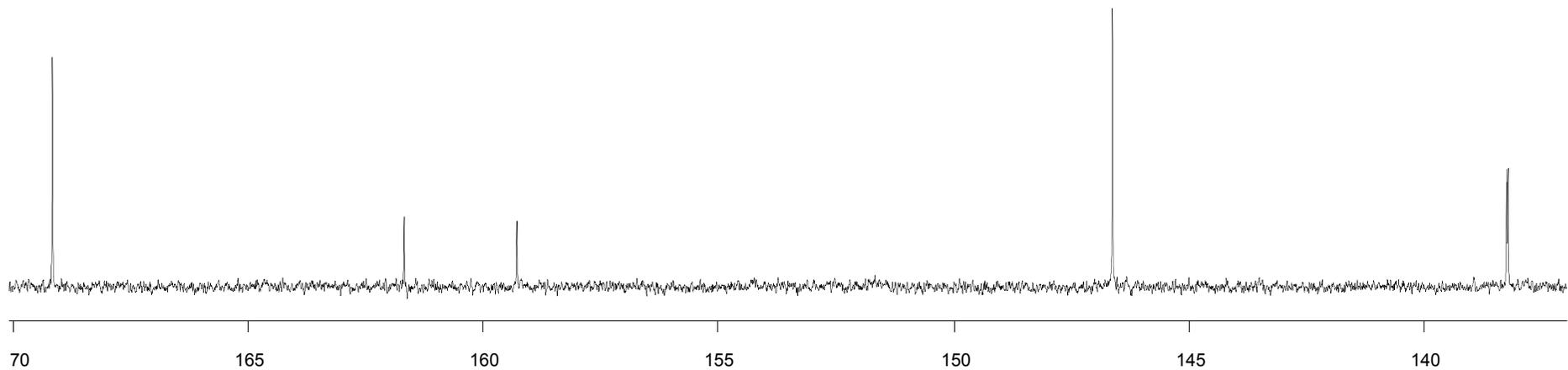
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5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



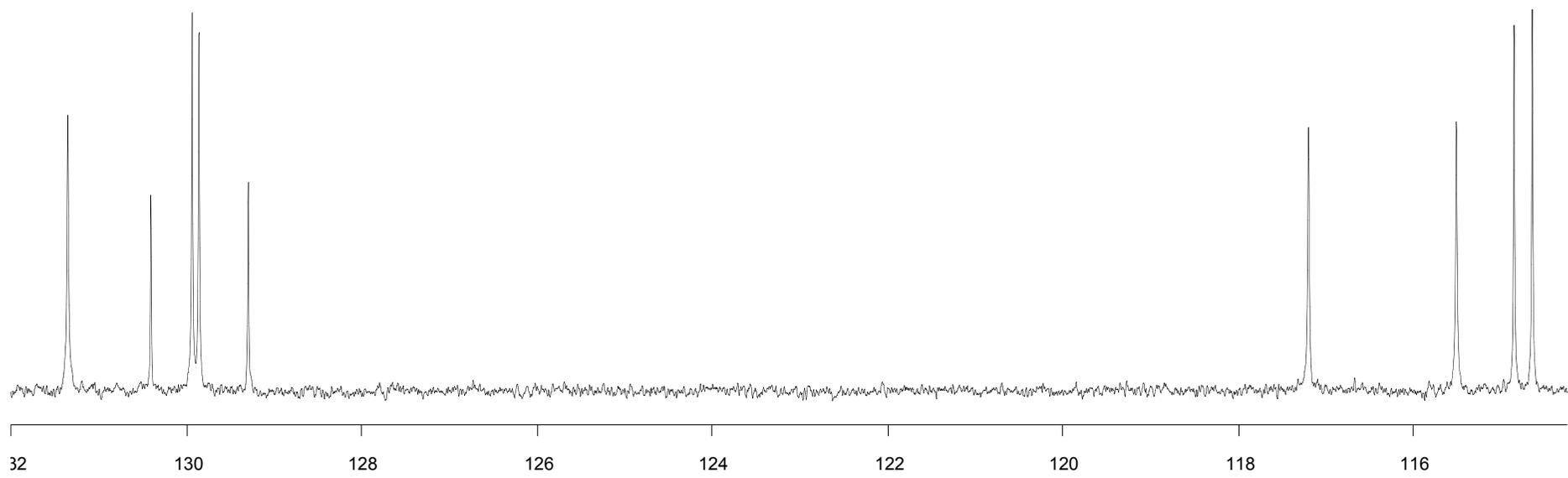
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5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



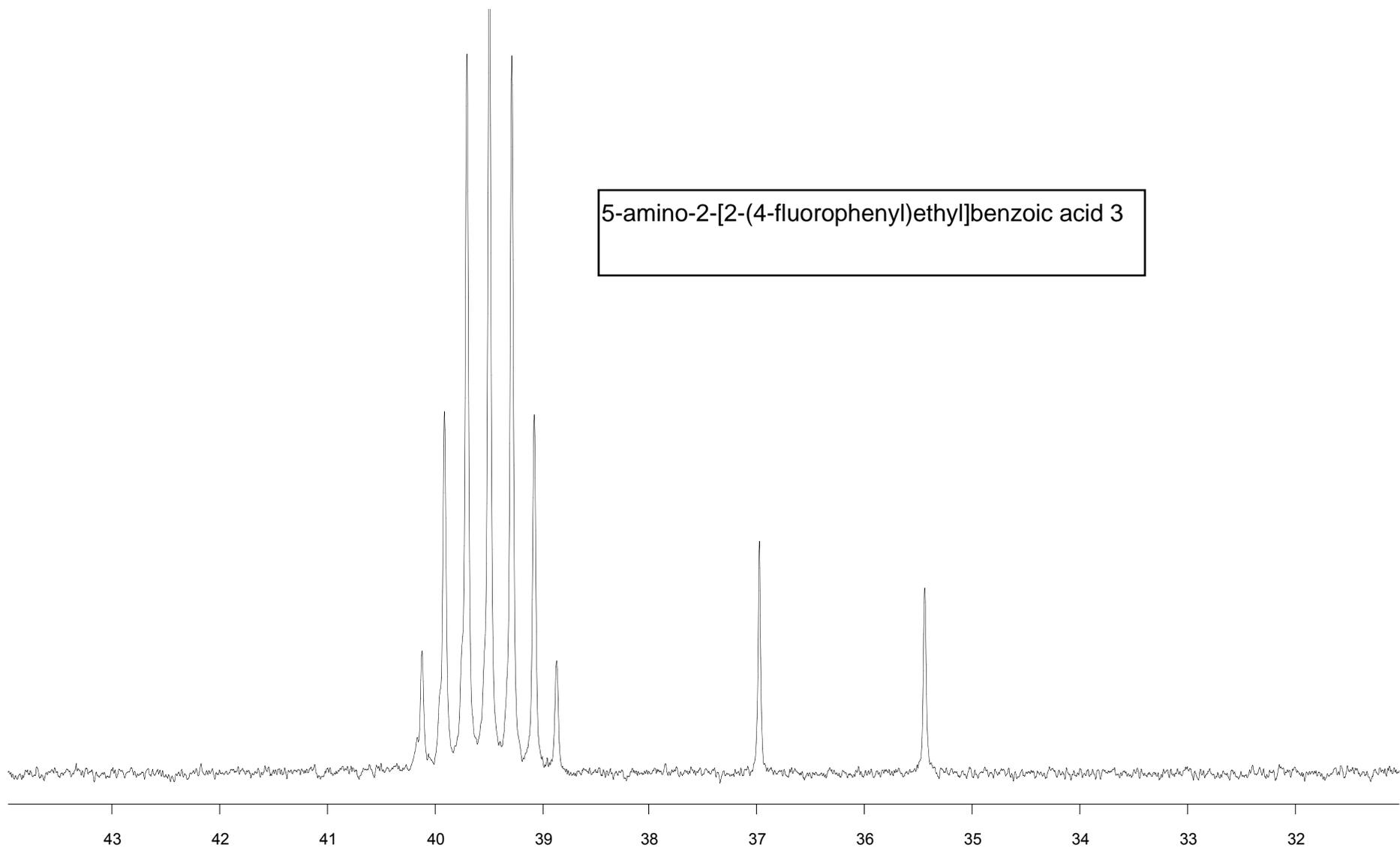
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5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



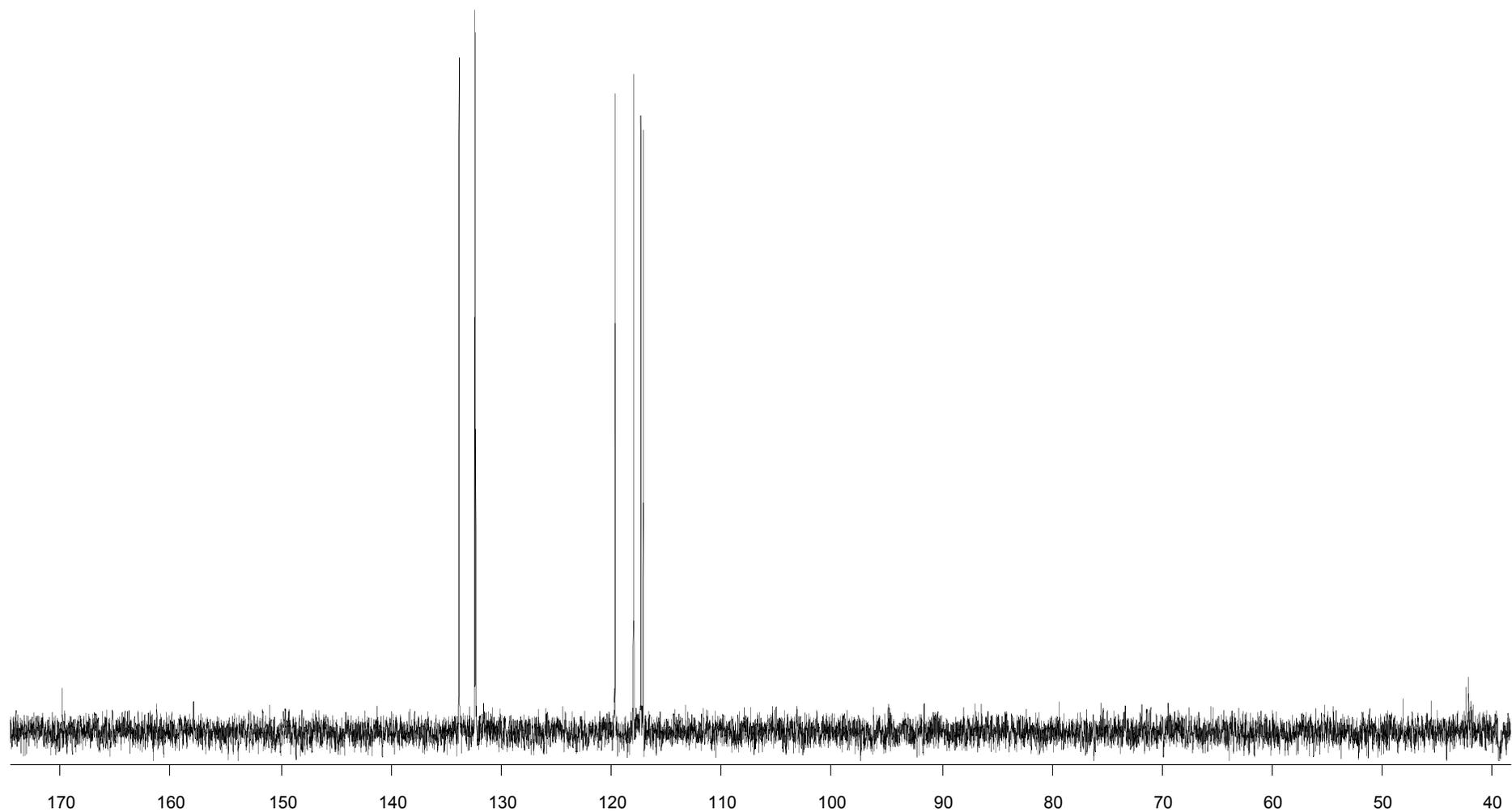
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5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



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13C nmr DEPT_5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3

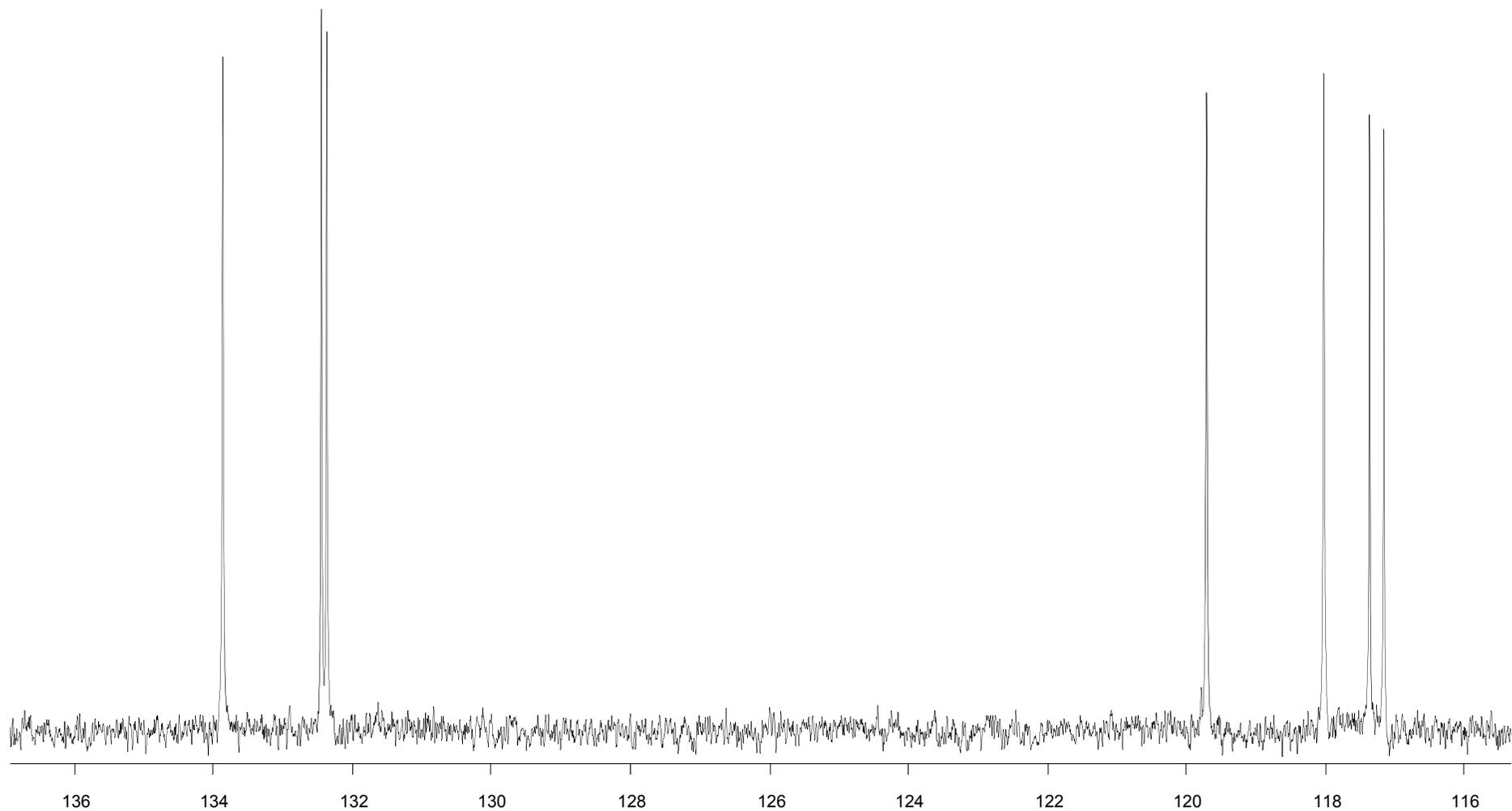


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Lai Chan, 03-klm973-053B, Sat Amine Acid C383_2 Bx U015183

Printed by m235797 on Mon Jul 16 16:55:51 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

13C nmr DEPT_5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3



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Lai Chan, 03-klm973-053B, Sat Amine Acid C383_2 Bx U015183
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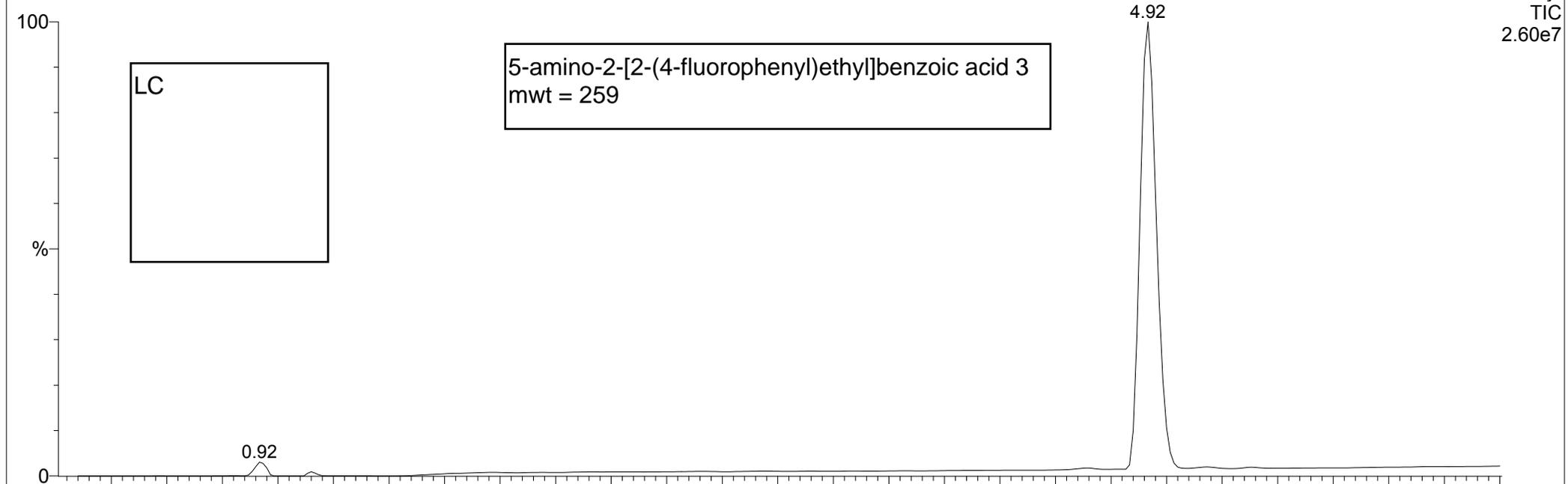
Sat Amine Acid

LaiChan252-1

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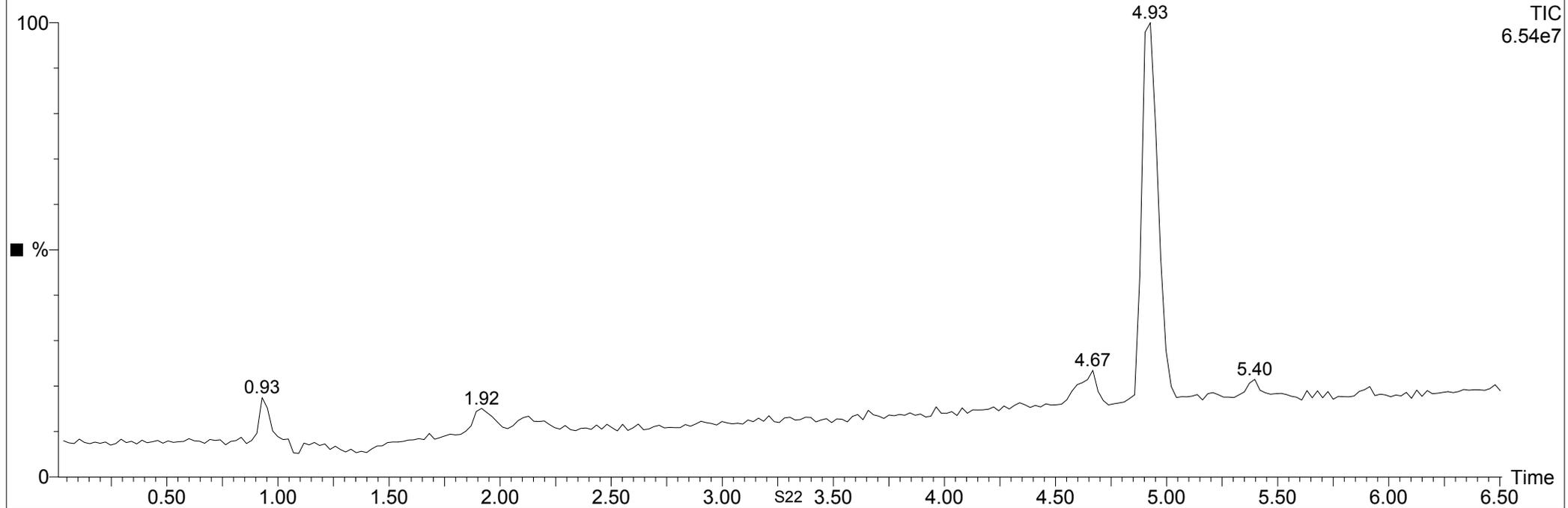
5-amino-2-[2-(4-fluorophenyl)ethyl]benzoic acid 3
mwt = 259

LC



LaiChan252-1

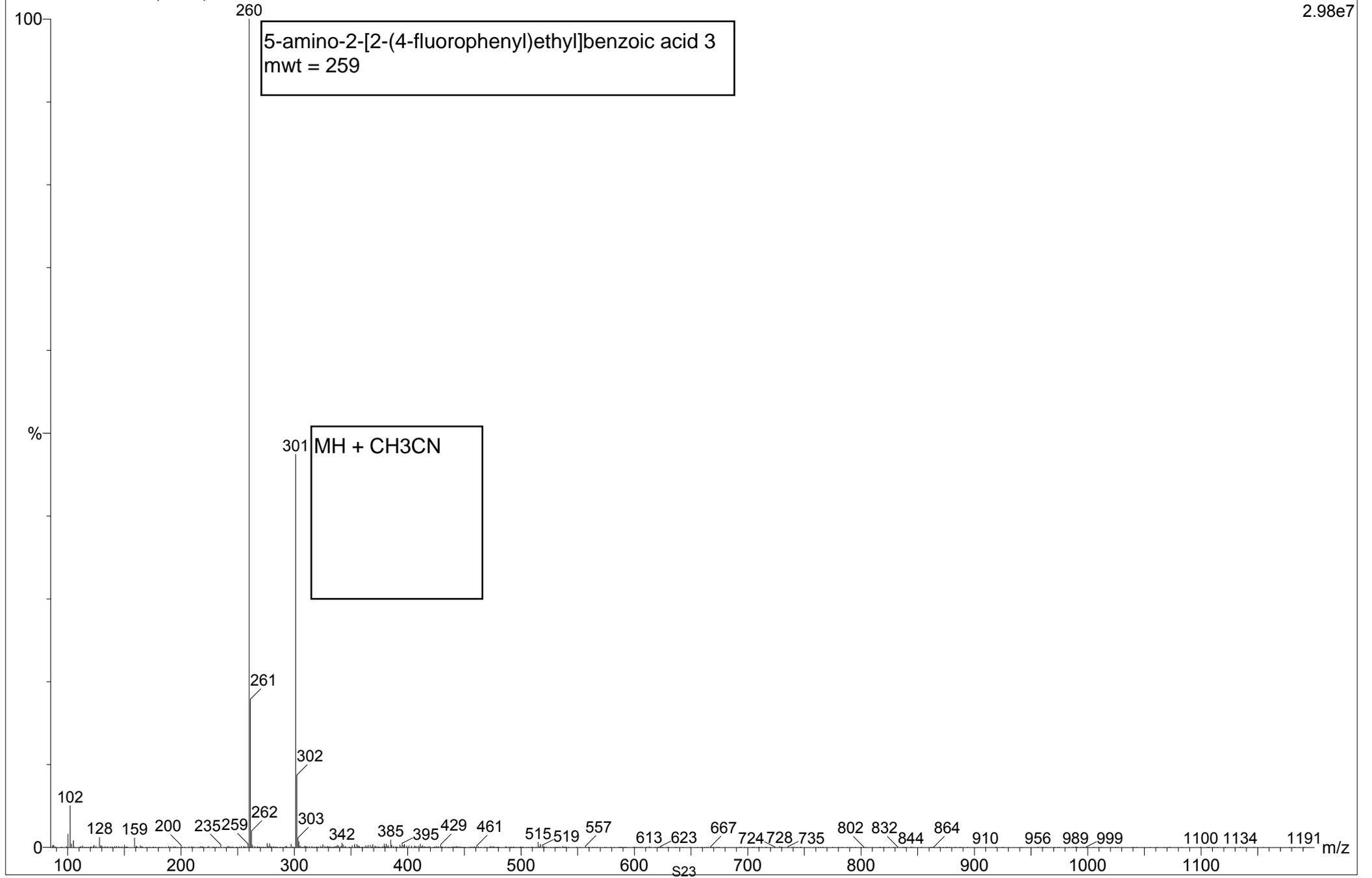
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TIC
6.54e7



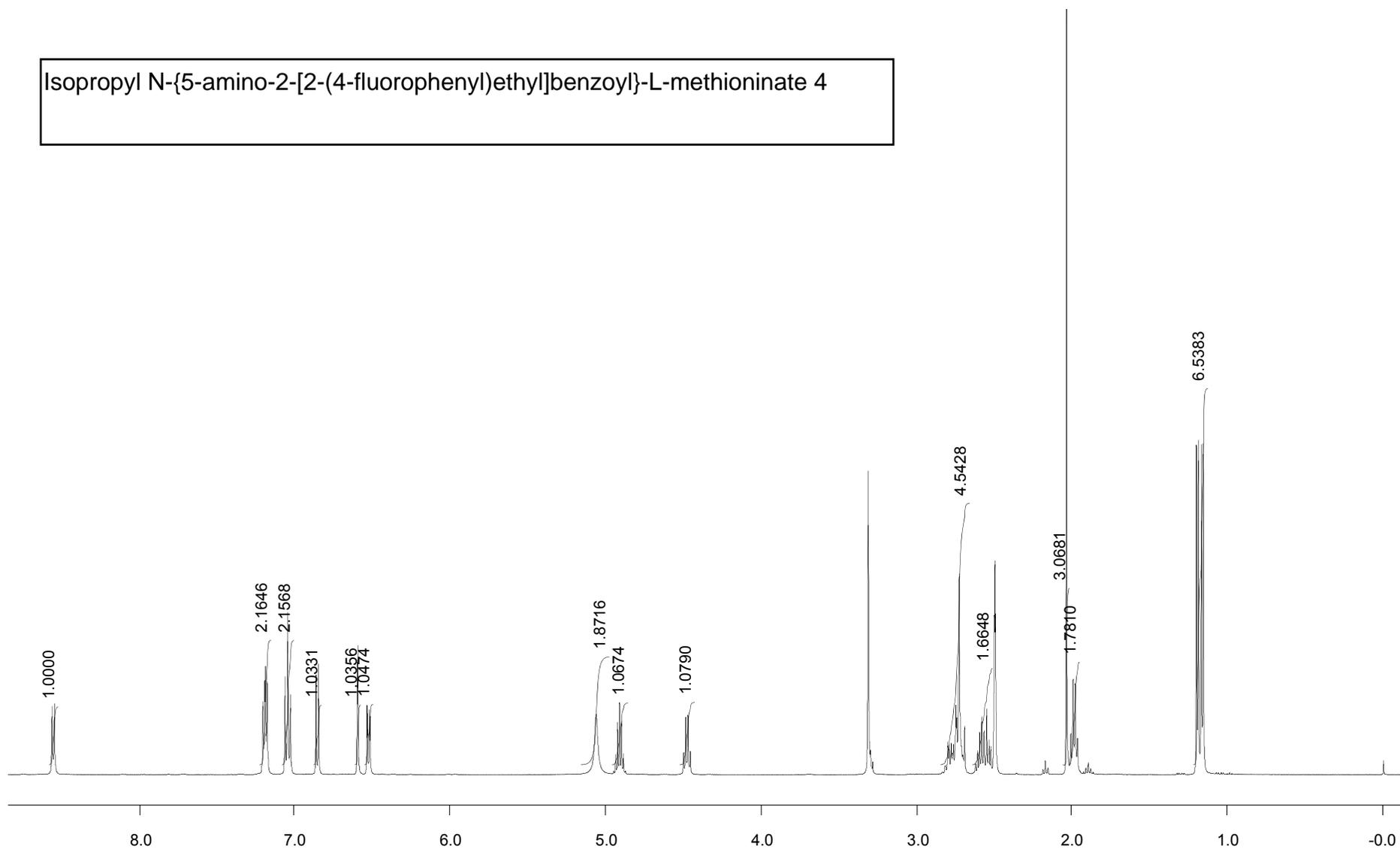
Sat Amine Acid

LaiChan252-1 210 (4.927)

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Isopropyl N-{5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methioninate 4

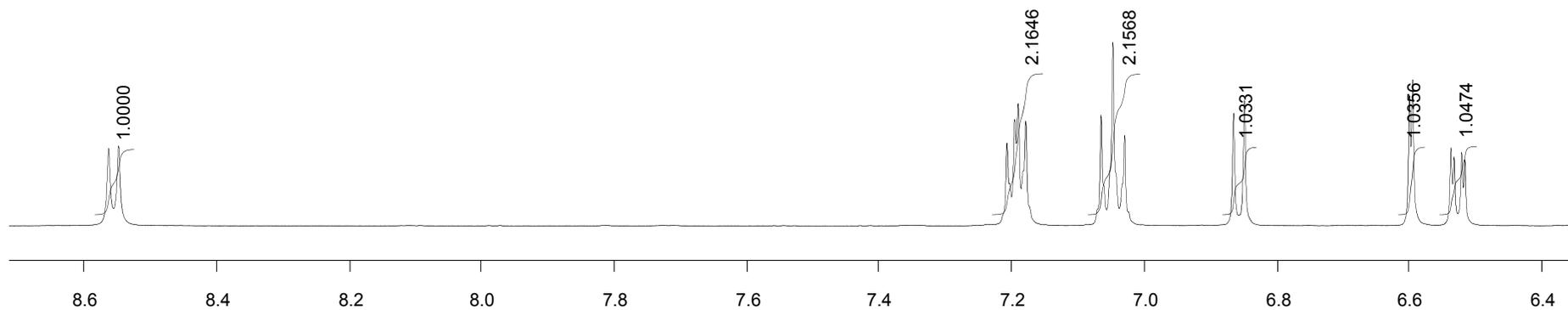


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Isopropyl N-{5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methioninate 4

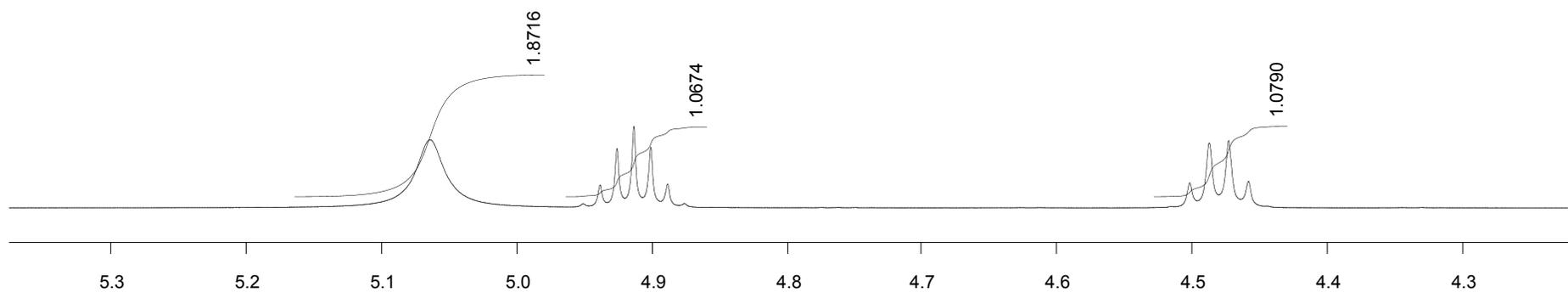


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Lai Chan, 03-klm973-053, C407_2 Met Sat Amine

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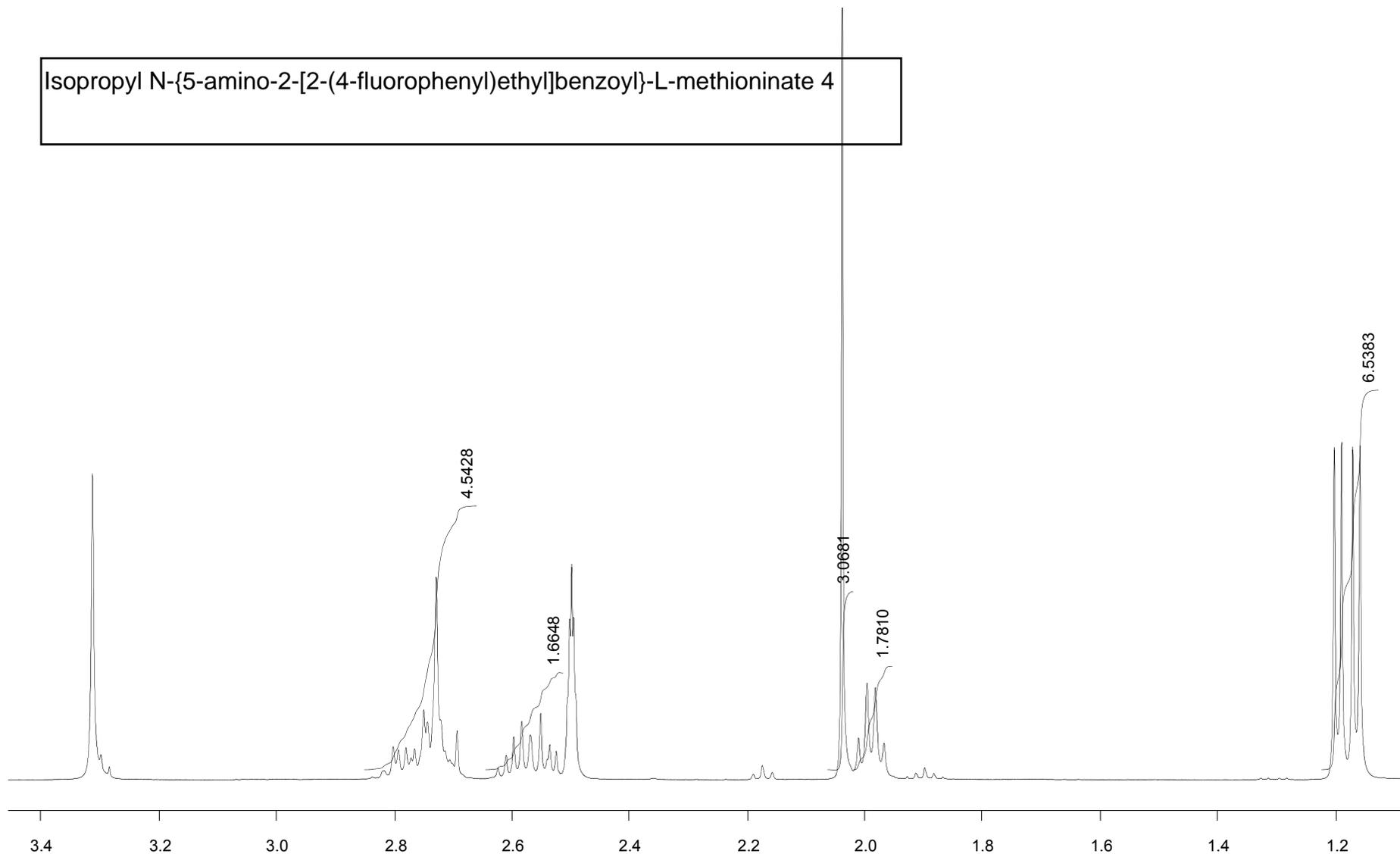


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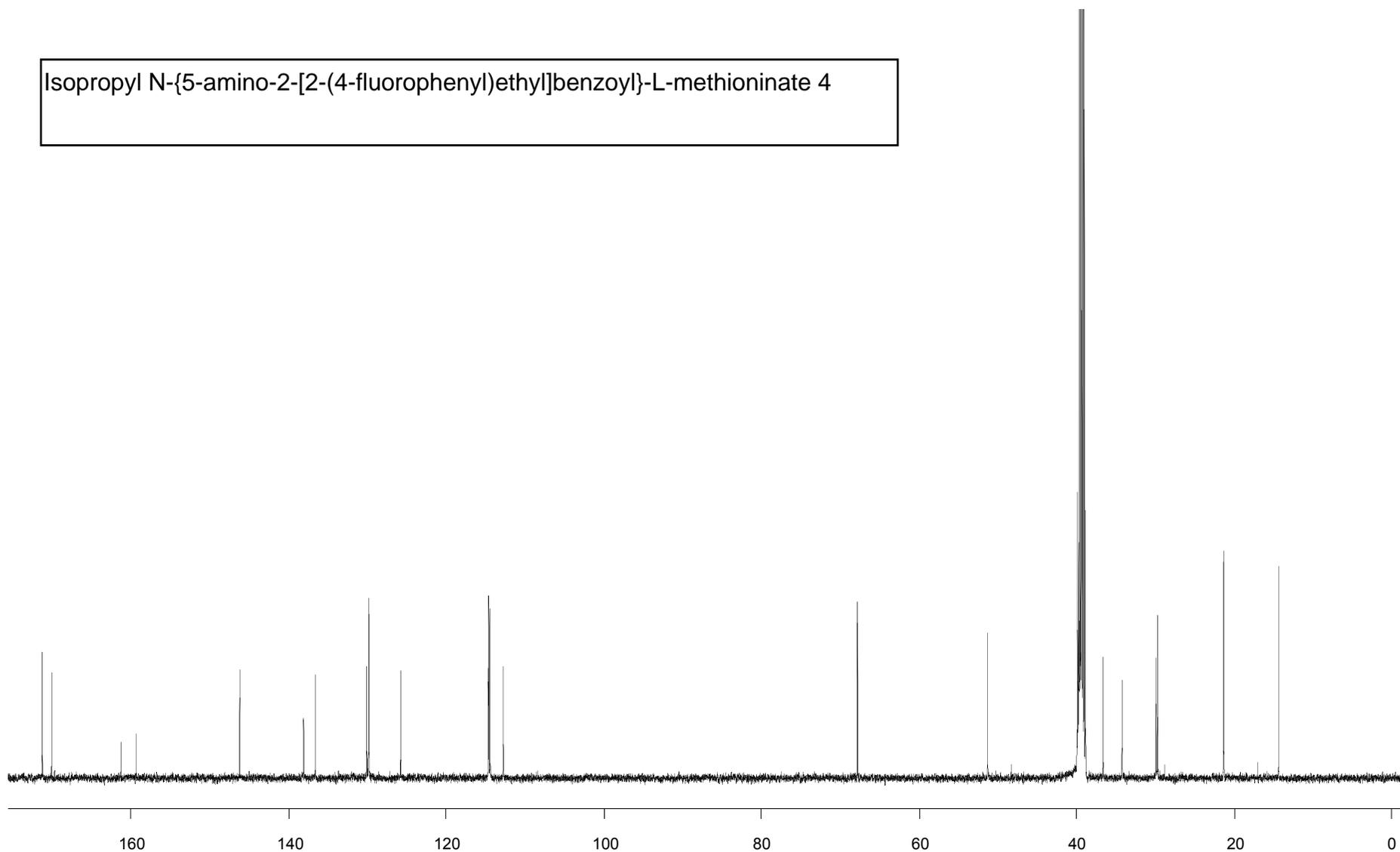


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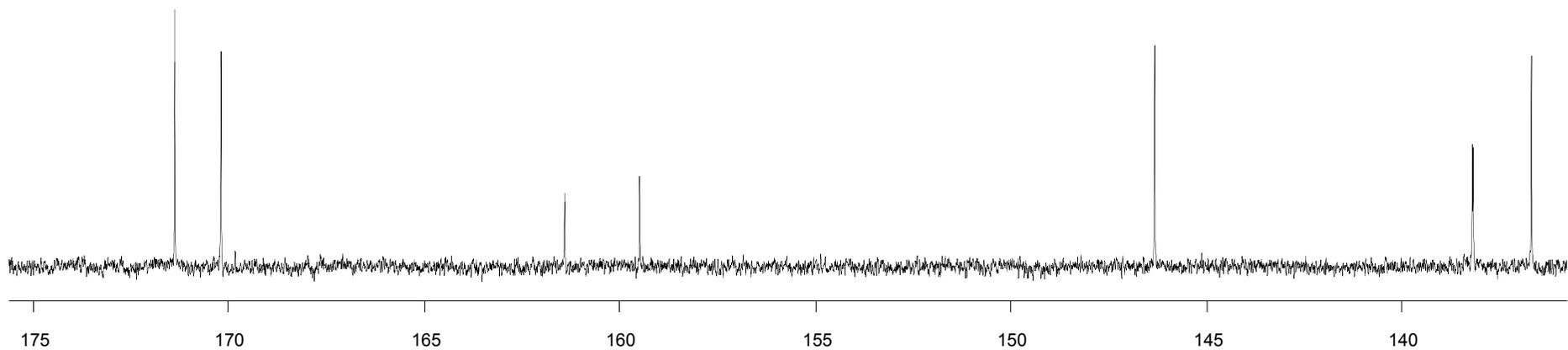


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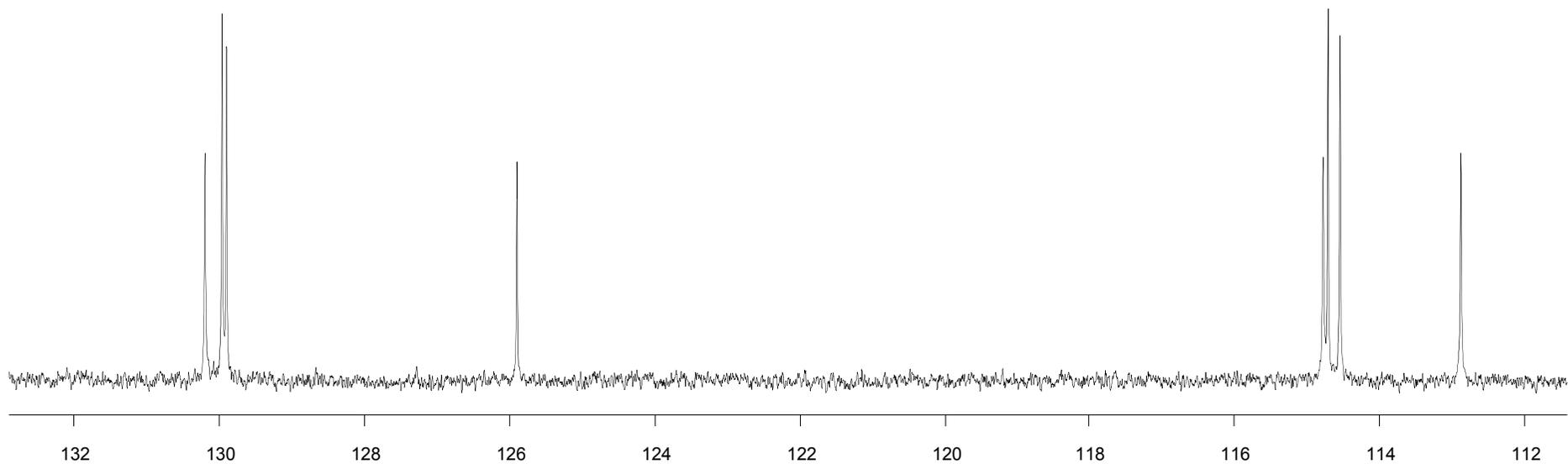


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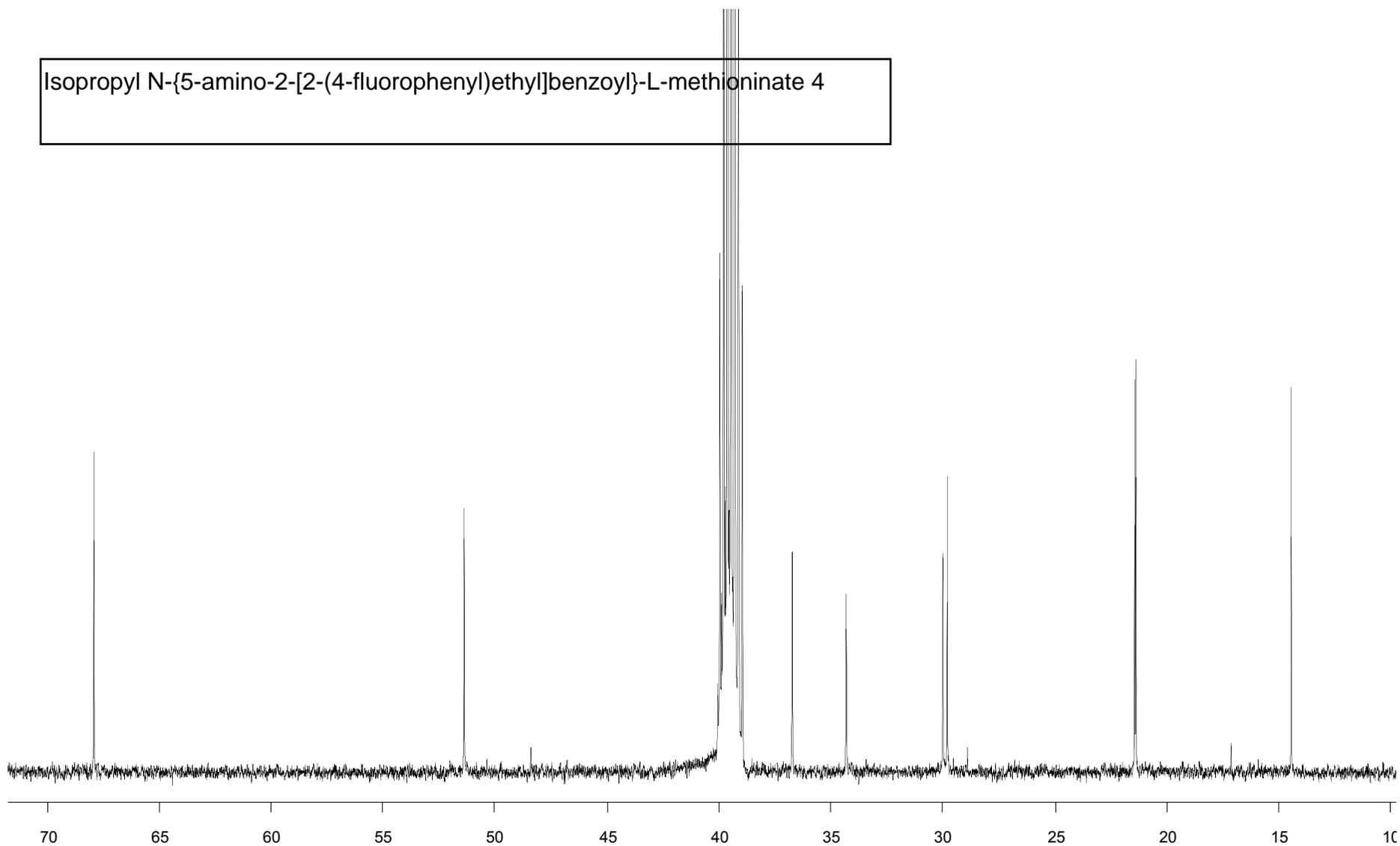


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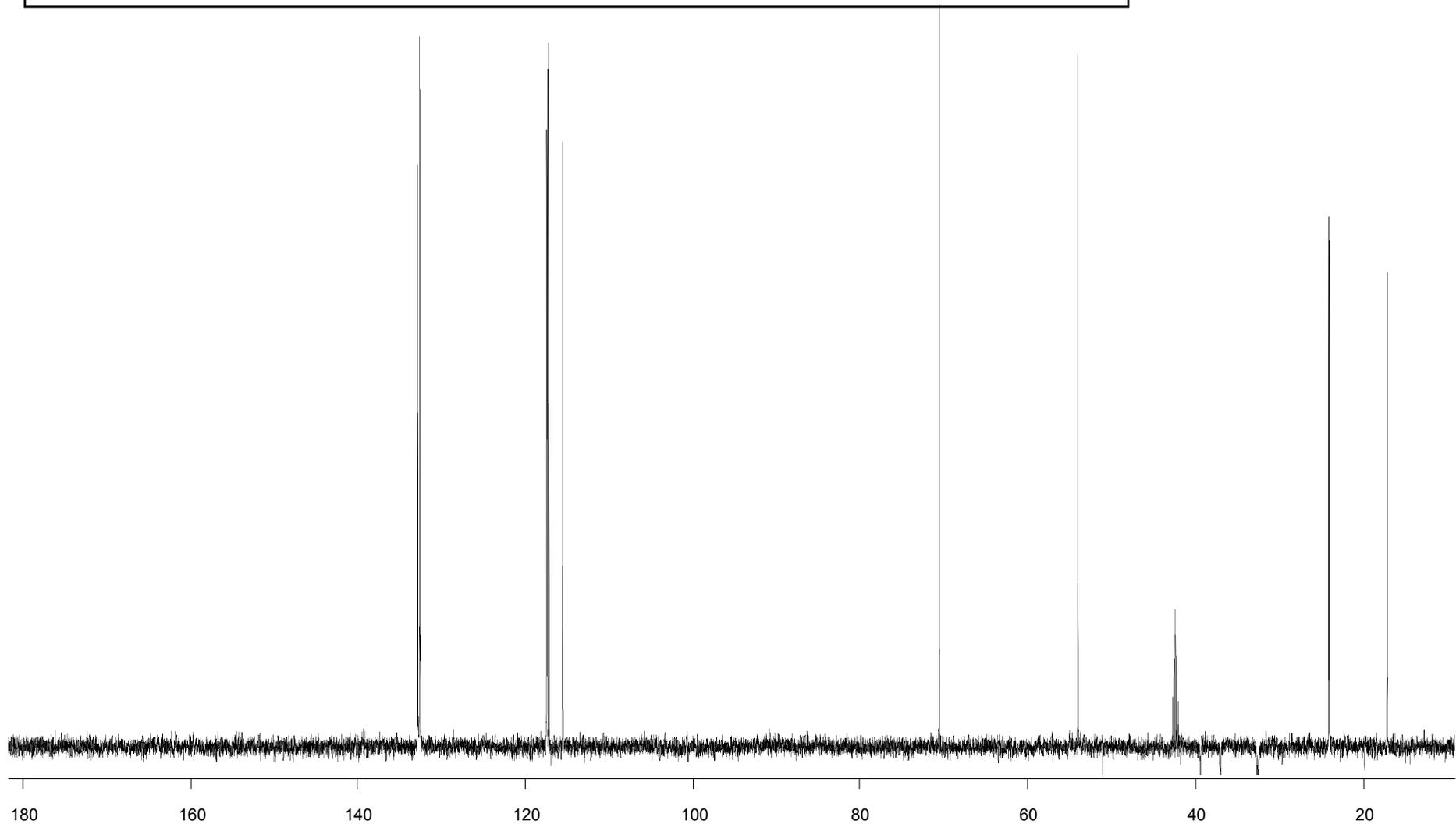


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Lai Chan, 03-klm973-053, C407_2 Met Sat Amine

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13C DEPT nmr_Isopropyl N-{5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methioninate 4

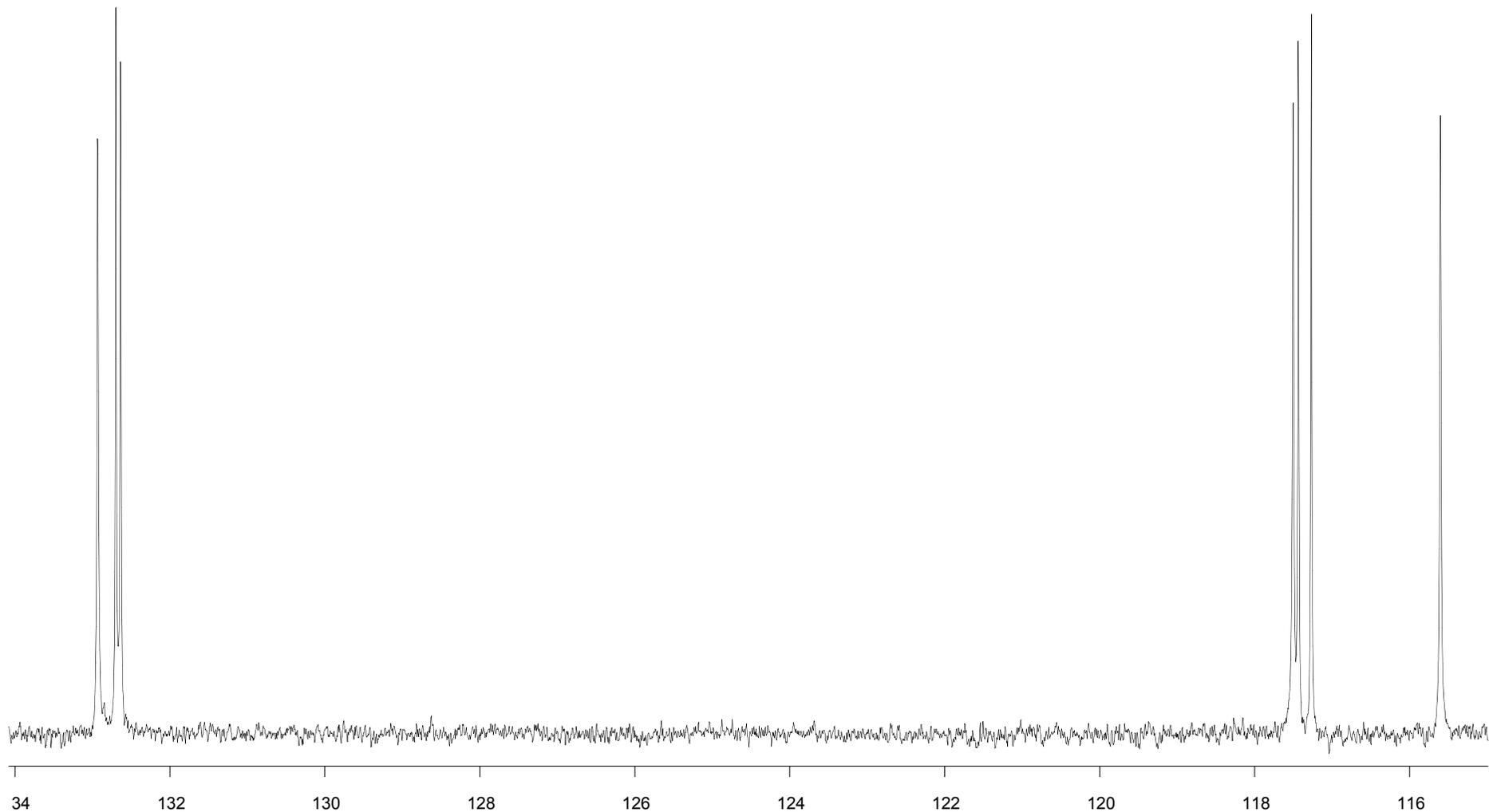


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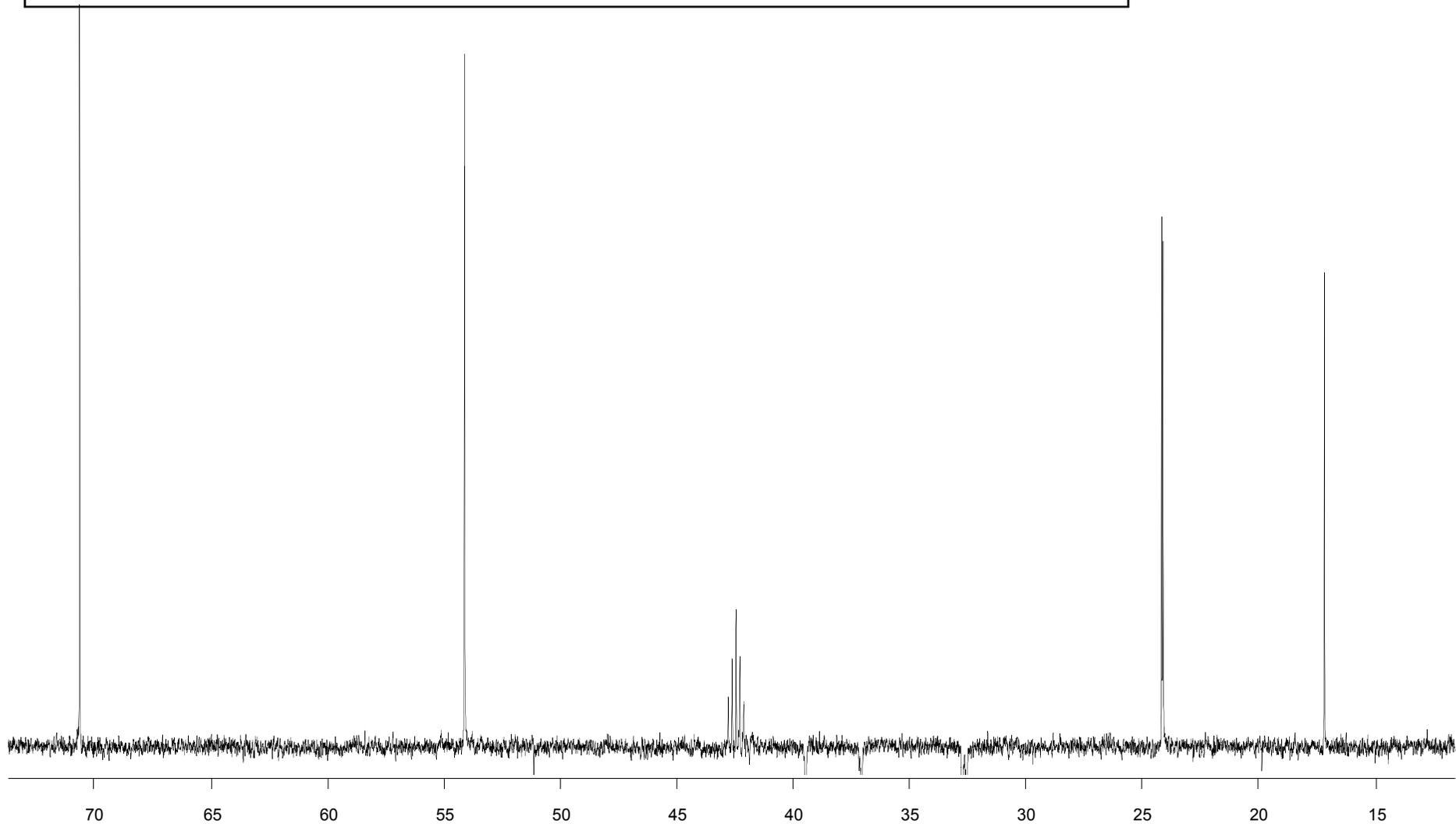


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13C DEPT nmr_Isopropyl N-{5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methioninate 4



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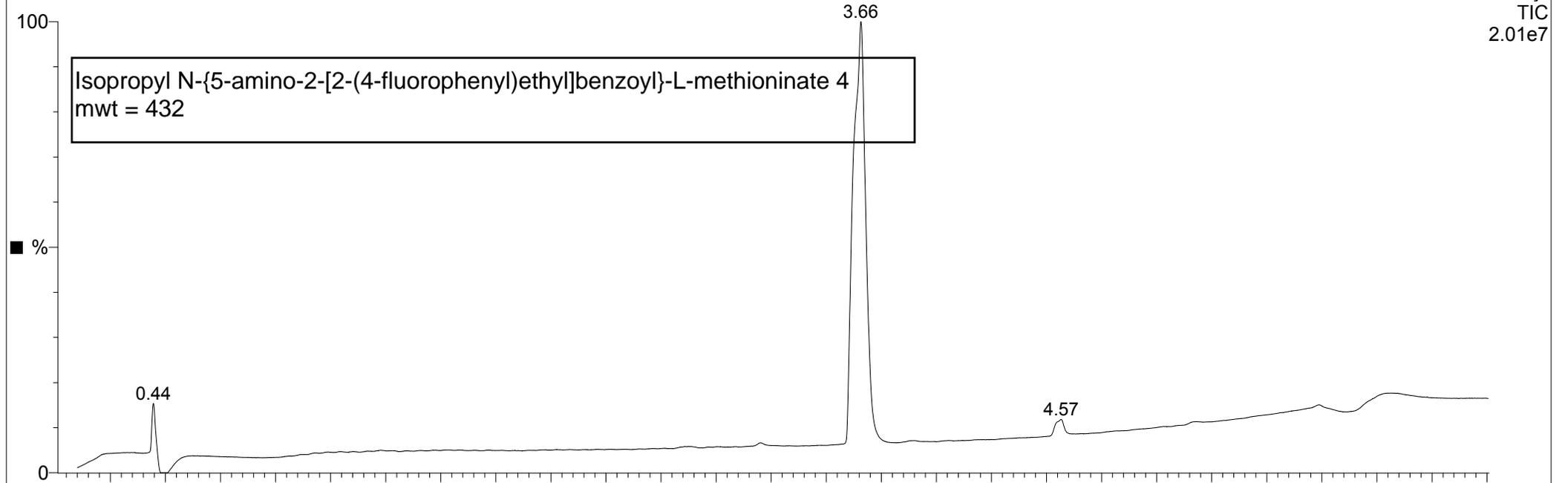
Lai Chan, 03-klm973-053, C407_2 Met Sat Amine

Printed by m235797 on Mon Jul 16 17:26:03 BST 2007. nucleus: 13C, freq: 125.76 MHz, solvent: DMSO, temperature:300K

Met Sat Amine

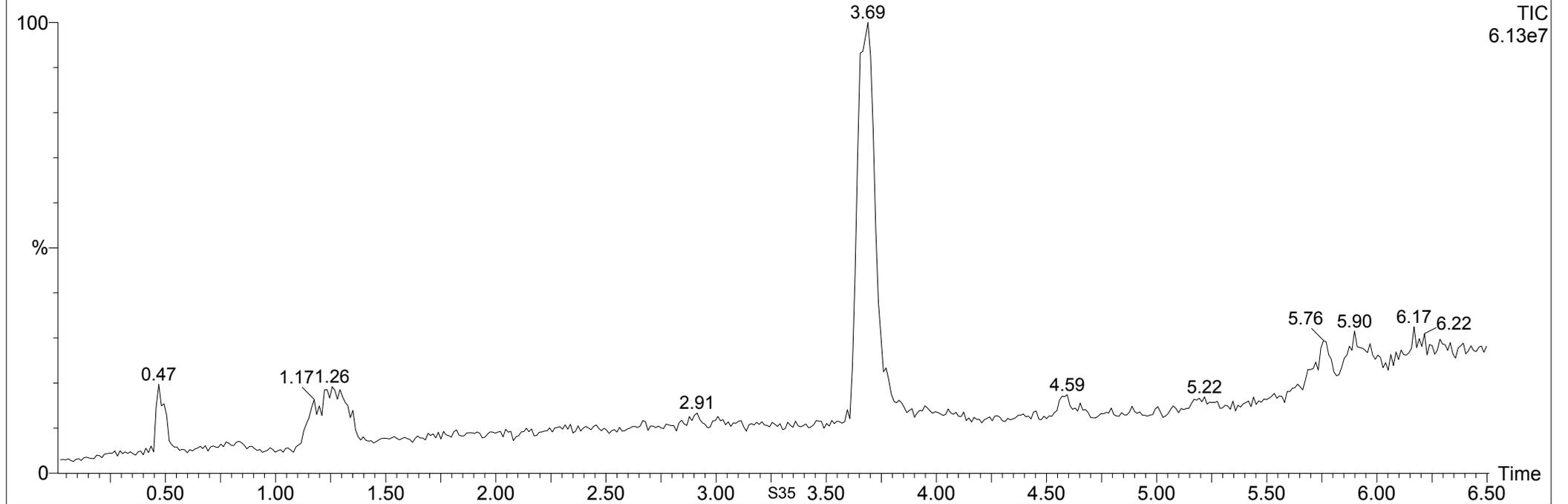
LaiChan247-1

2: Diode Array
TIC
2.01e7



LaiChan247-1

1: Scan ES+
TIC
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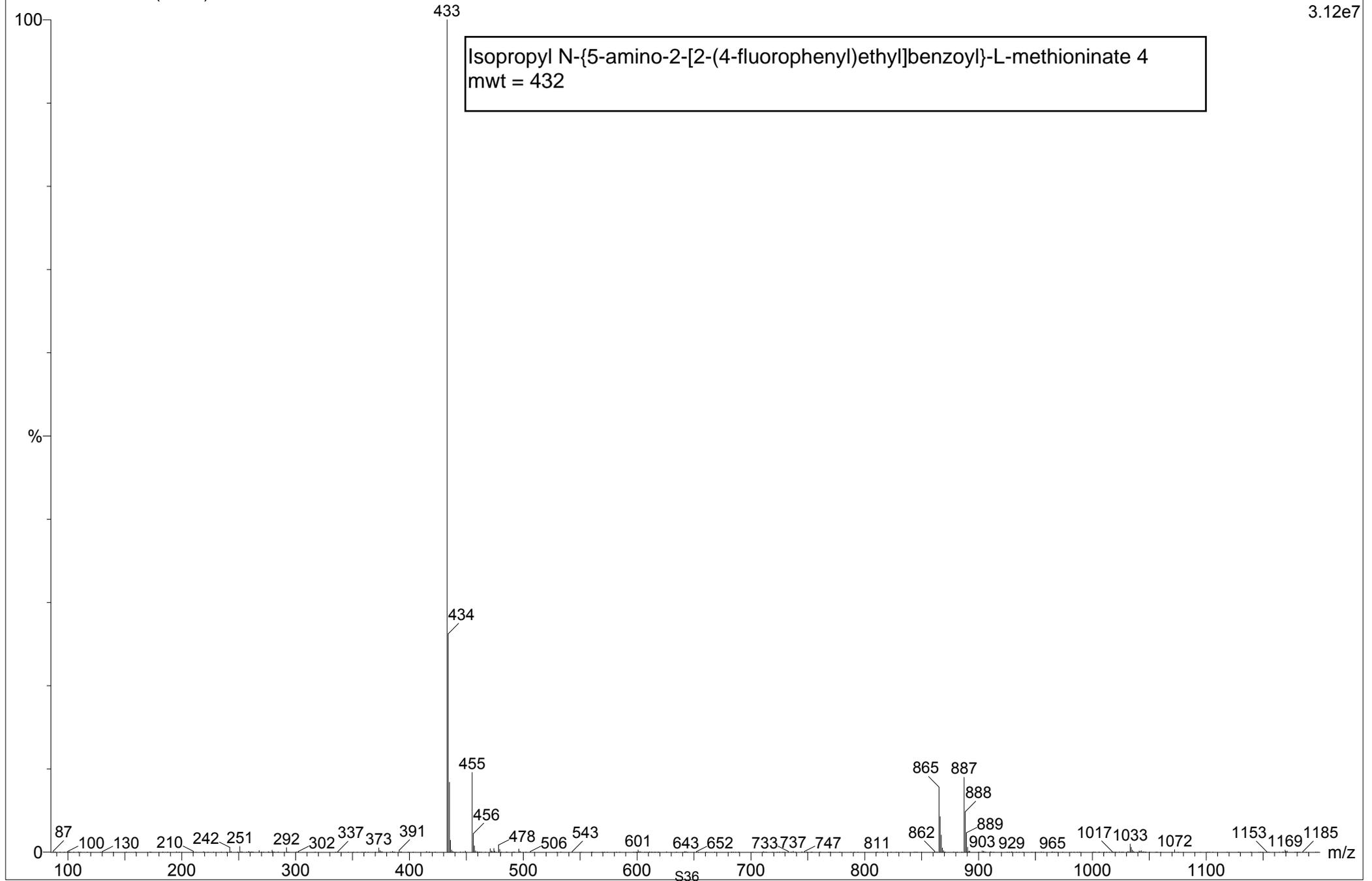


Met Sat Amine

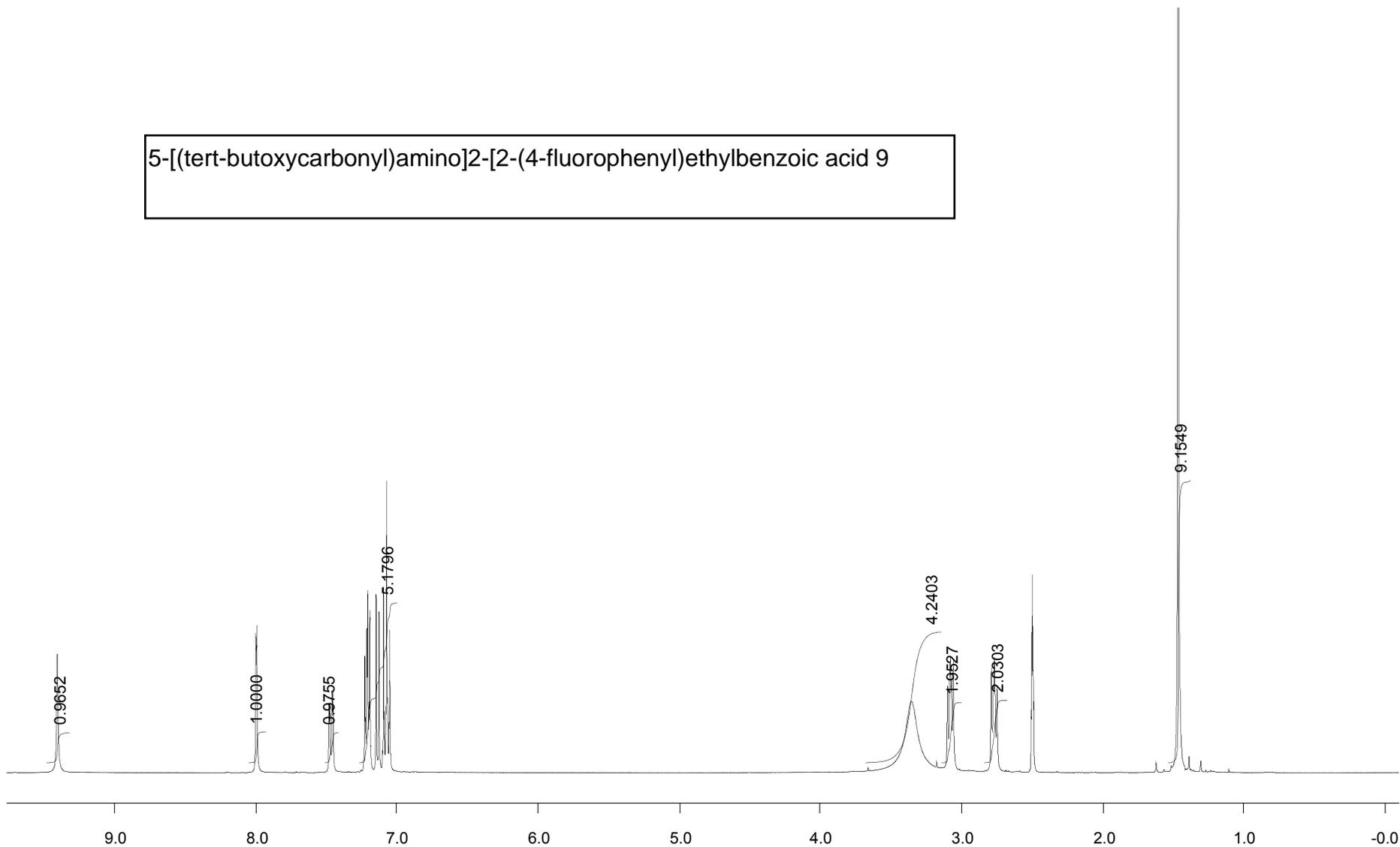
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Isopropyl N-{5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methioninate 4
mwt = 432



5-[(tert-butoxycarbonyl)amino]2-[2-(4-fluorophenyl)ethyl]benzoic acid 9

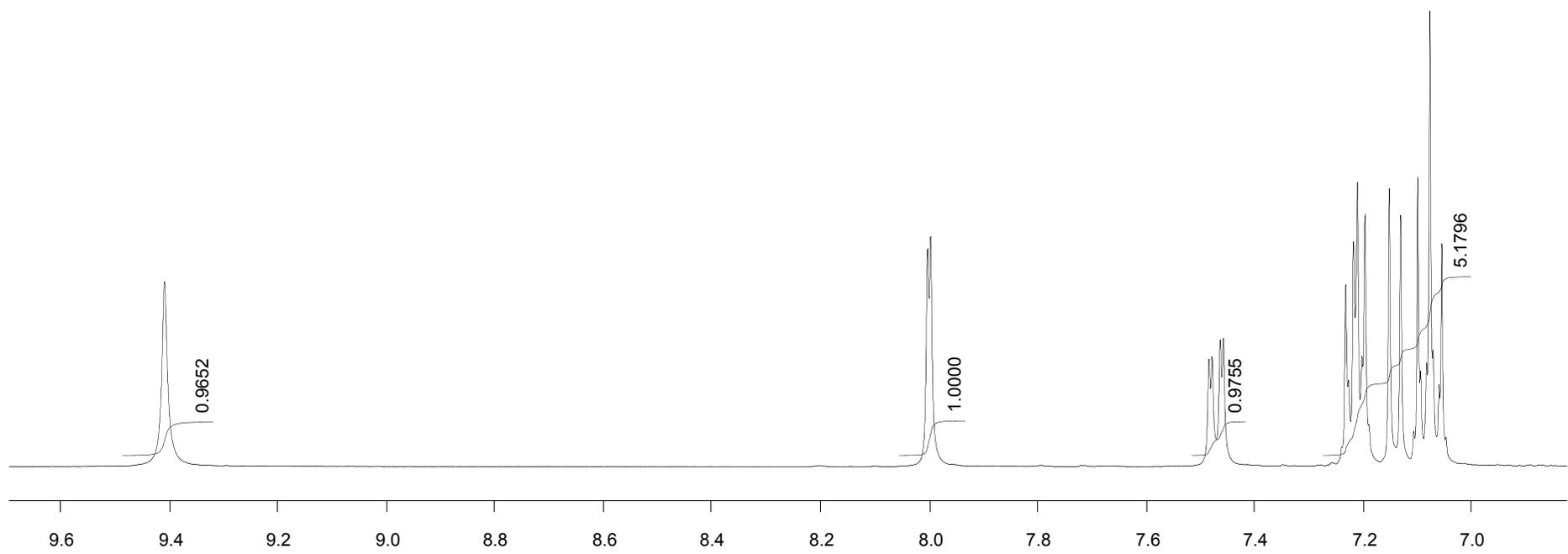


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Dawn Sievwright, 01-KWDN841-44, Em Williams

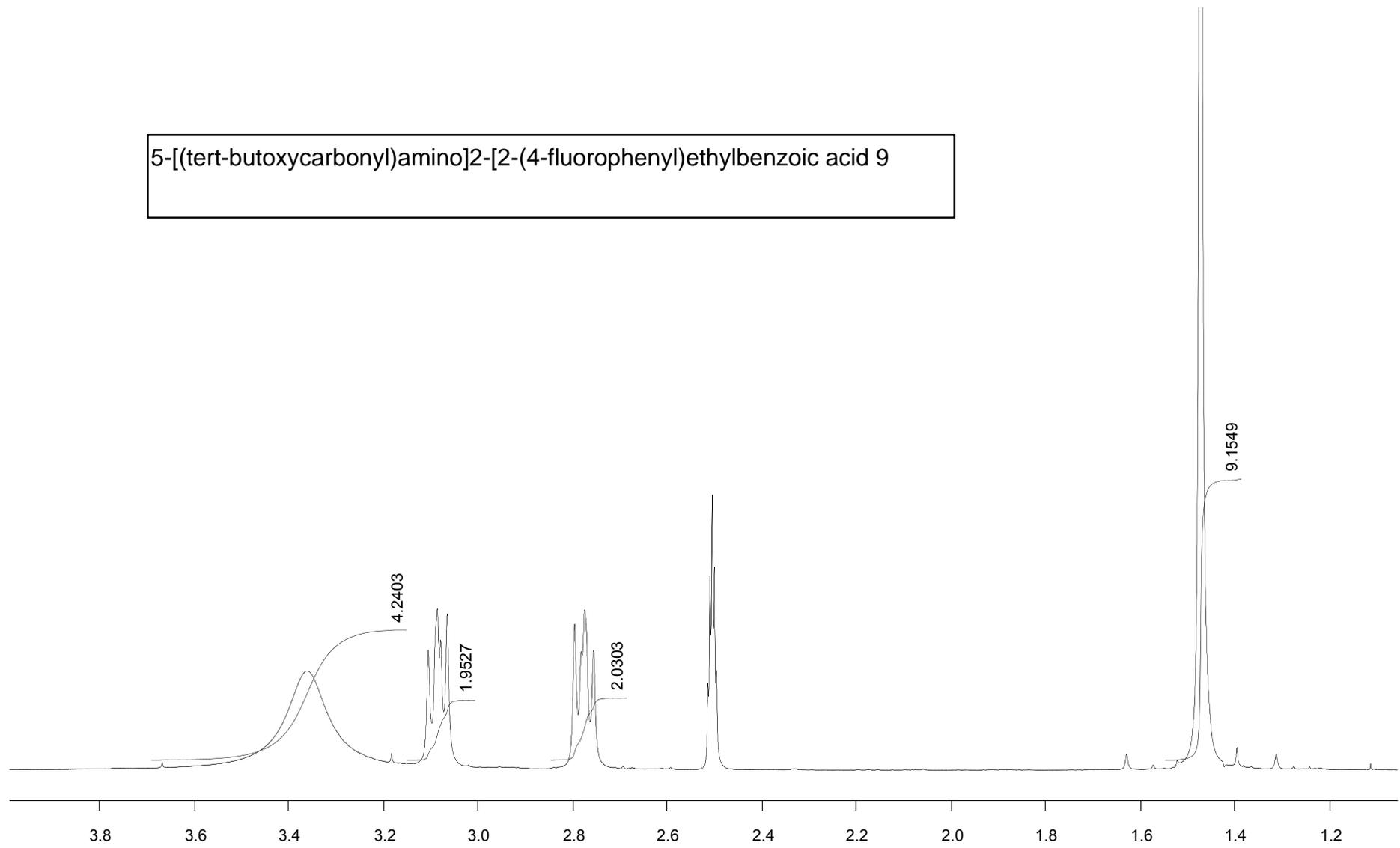
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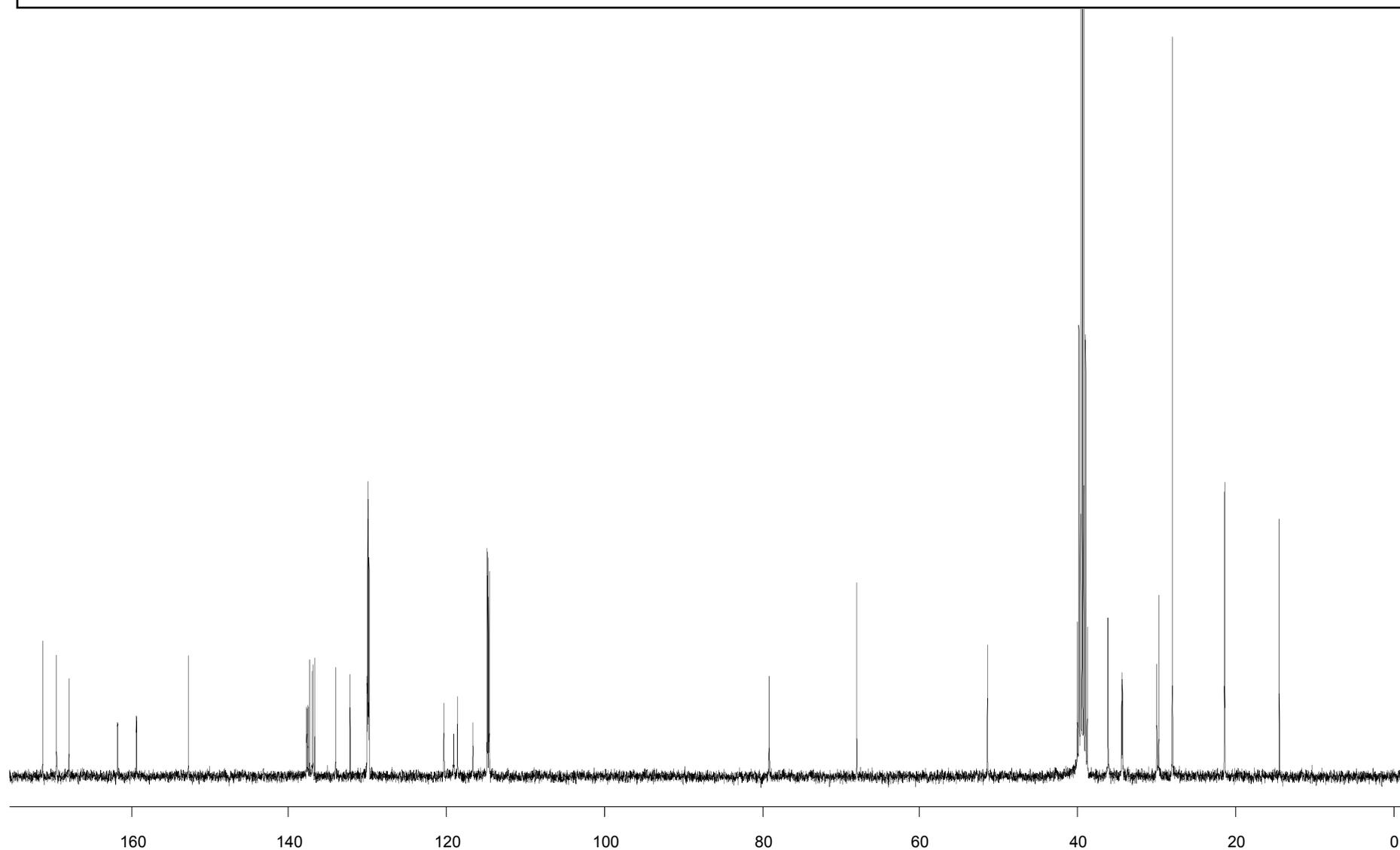
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Dawn Sievwright, 01-KWDN841-44, Em Williams
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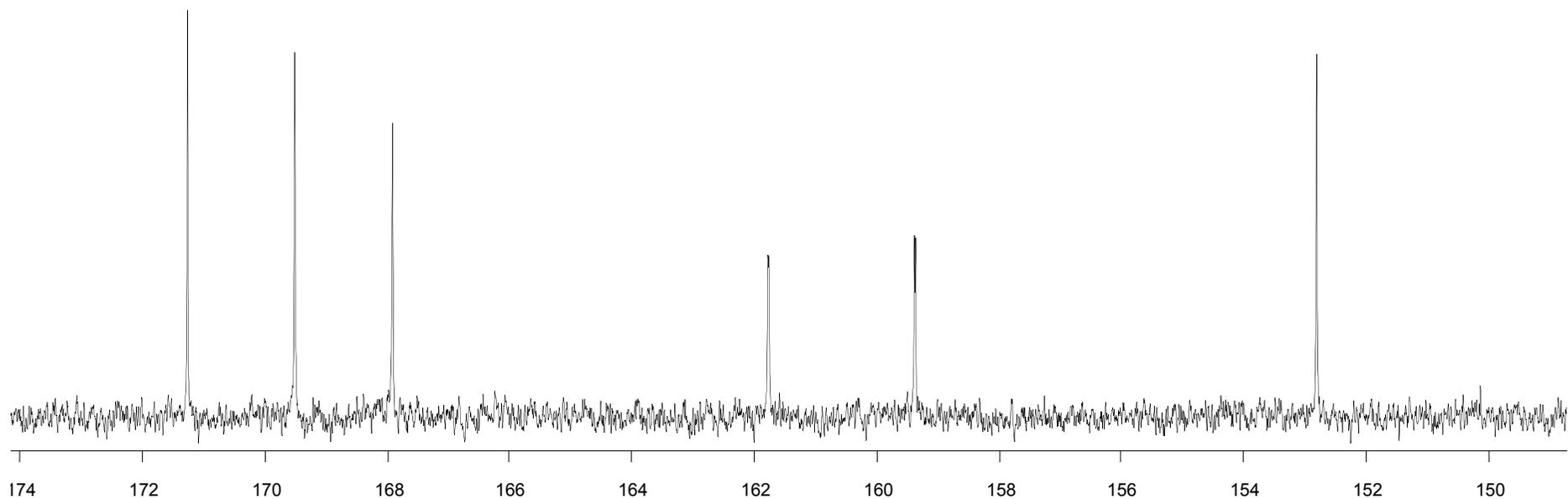
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Dawn Sievwright, 01-KWDN841-44, Em Williams
Printed by RD\M235797 on Mon Jul 16 17:46:38 BST 2007. nucleus: 1H, freq: 400.13 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-({5-[tert-butoxycarbonyl]amino}-2-(4-fluorophenyl)ethyl]benzoyl}amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinininate 10



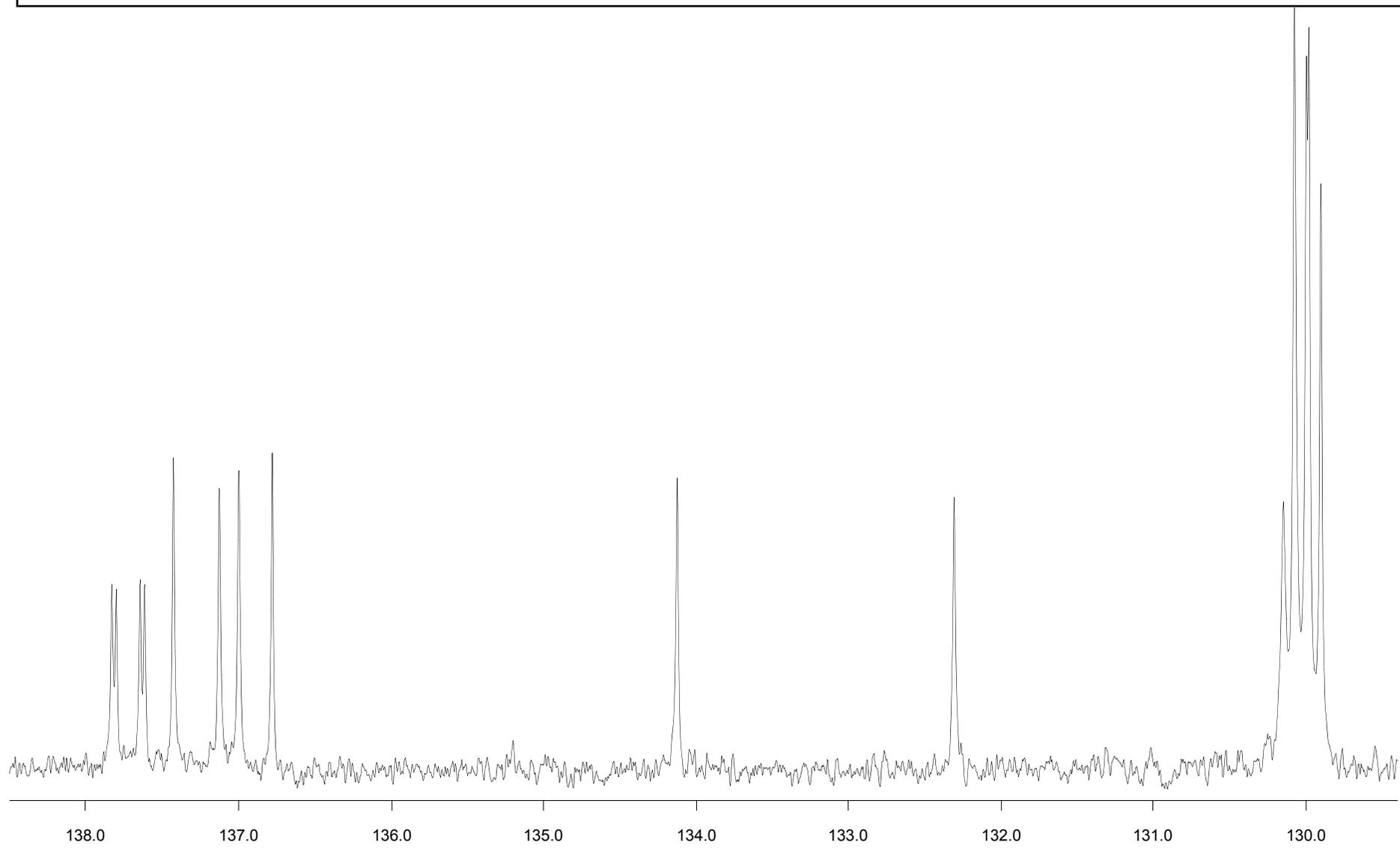
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Em Williams, 01-kwdn841-48C, AZD3409 BOC SAD CROP1
Printed by m235797 on Mon Jul 16 18:08:04 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

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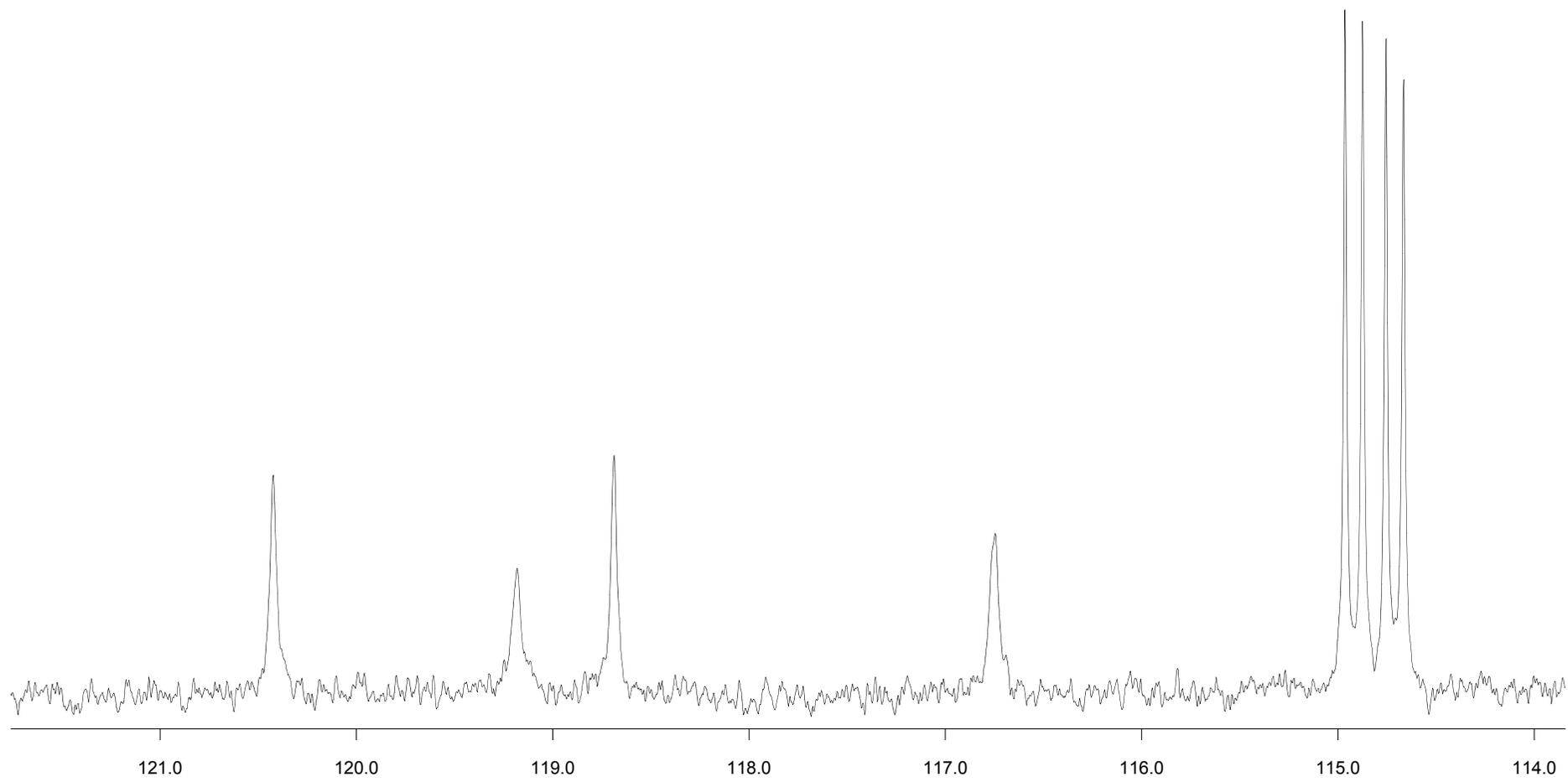
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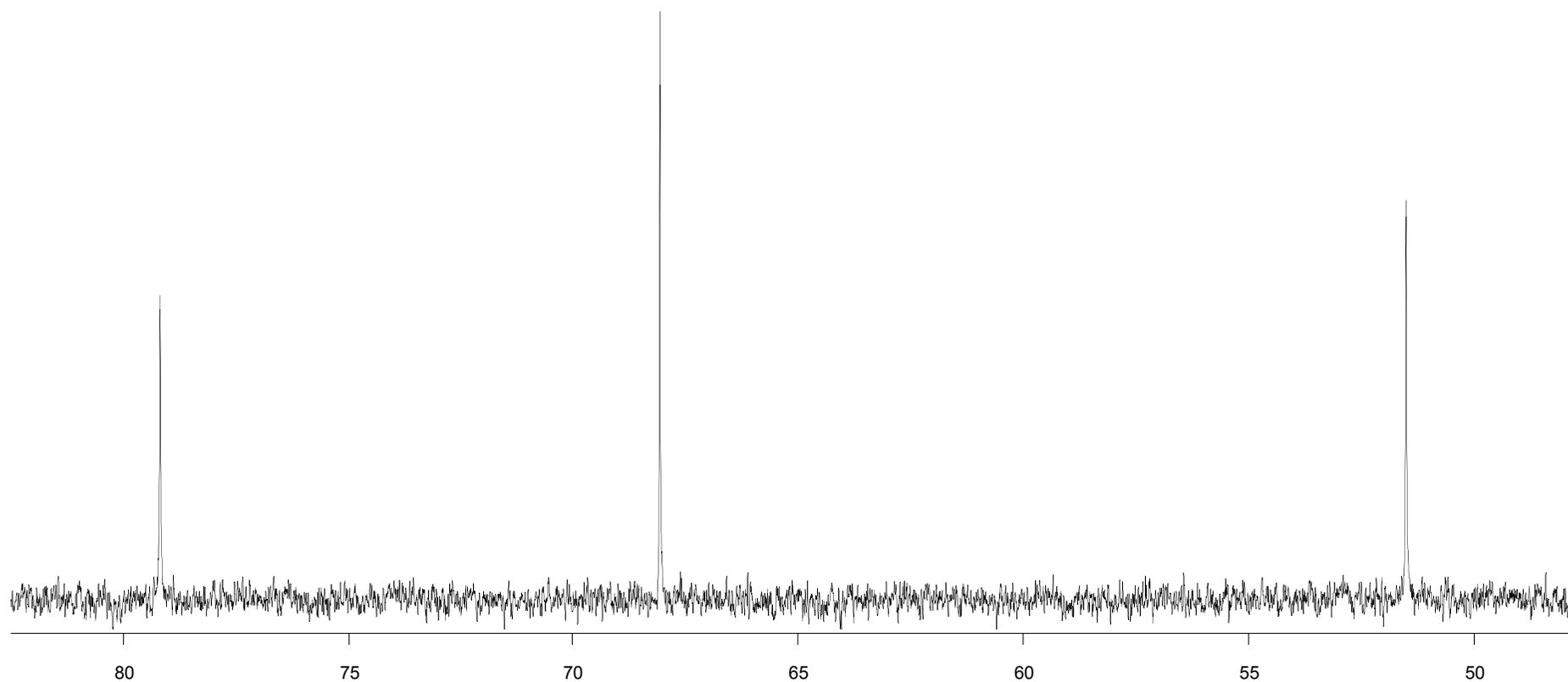
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Em Williams, 01-kwdn841-48C, AZD3409 BOC SAD CROP1
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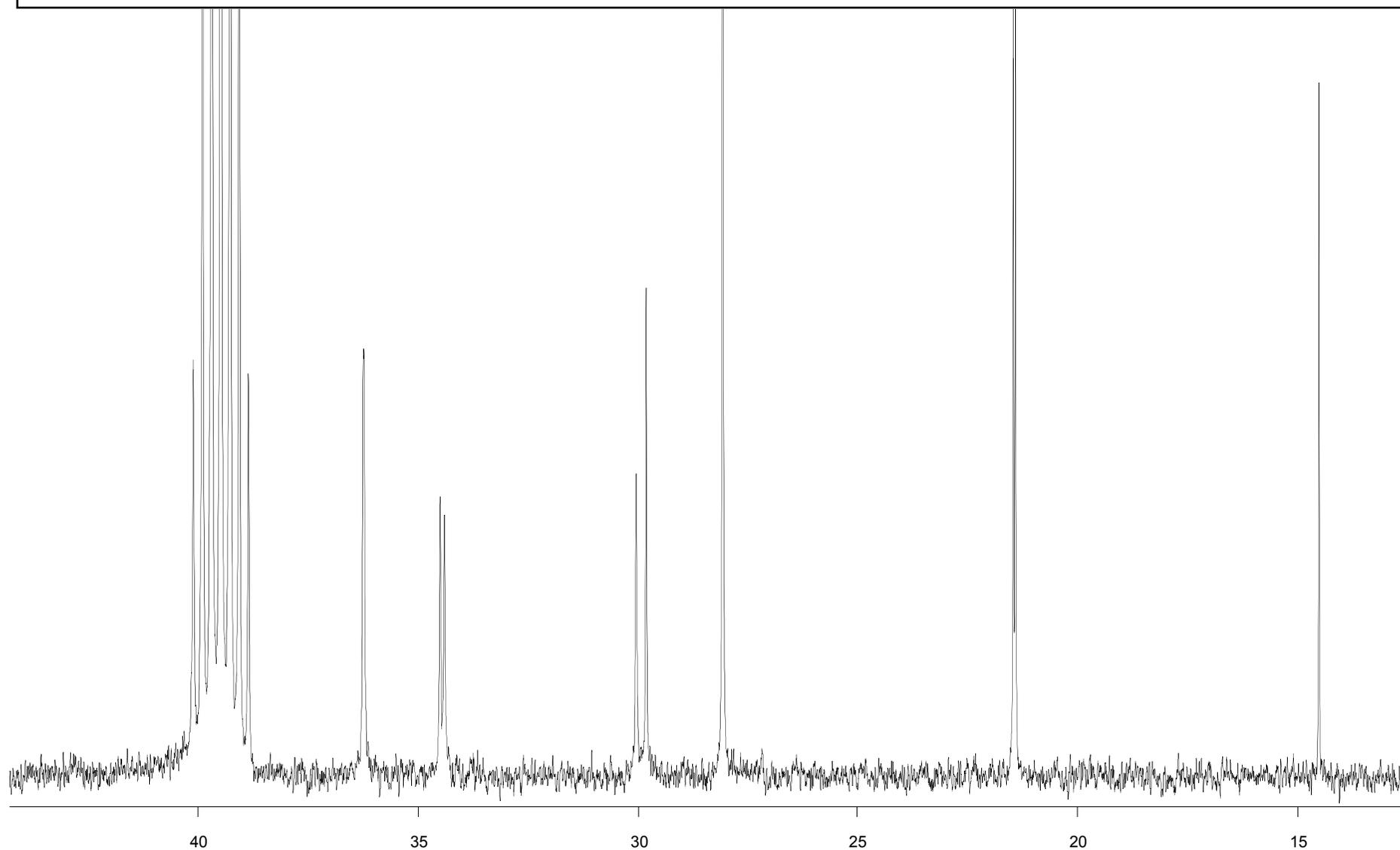
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Printed by m235797 on Mon Jul 16 18:09:49 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-({5-[tert-butoxycarbonyl]amino}-2-(4-fluorophenyl)ethyl]benzoyl}amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininatate 10



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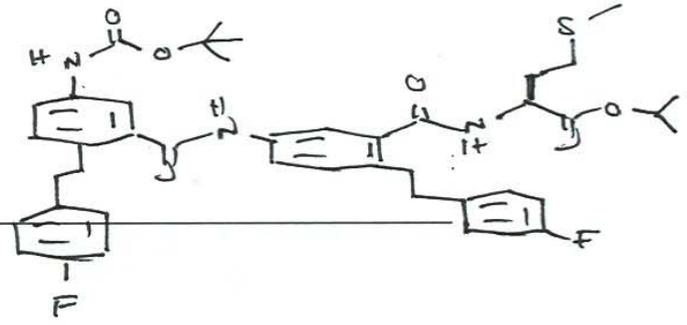
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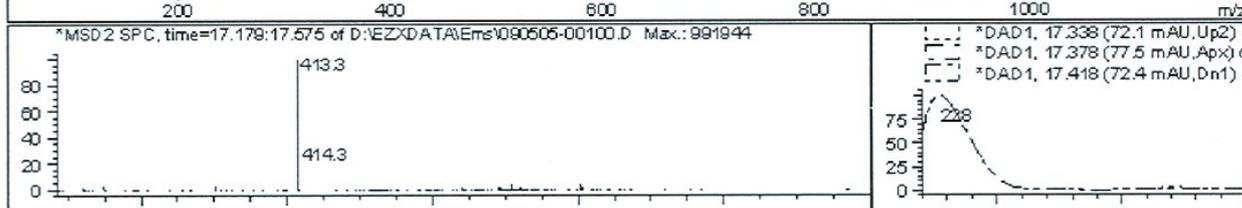
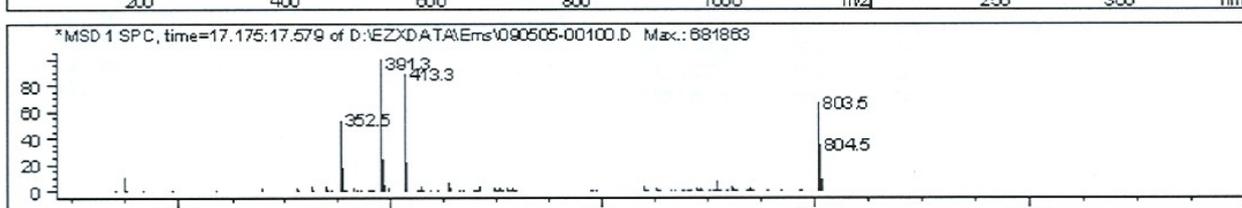
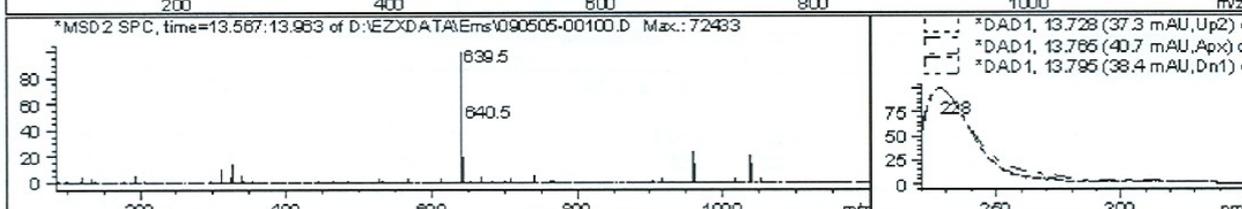
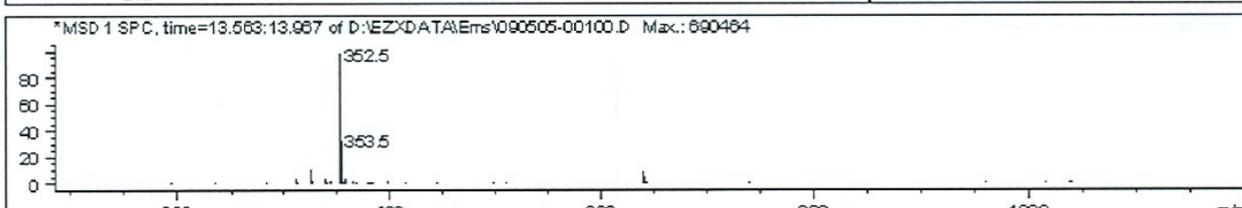
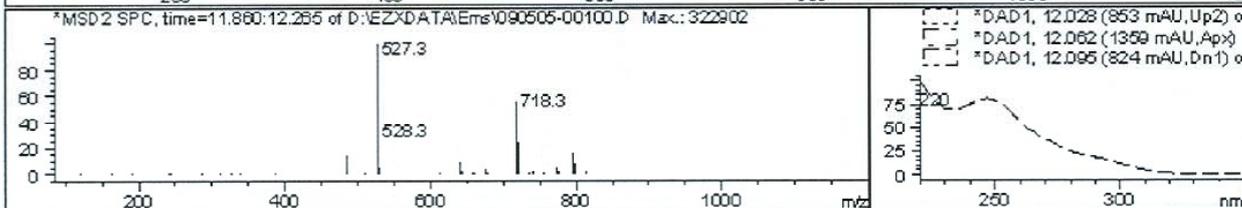
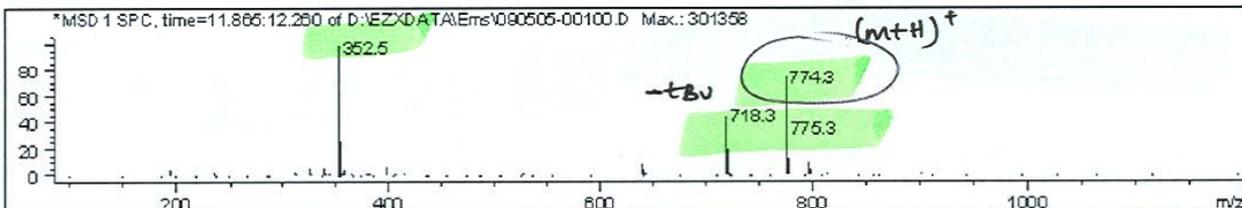
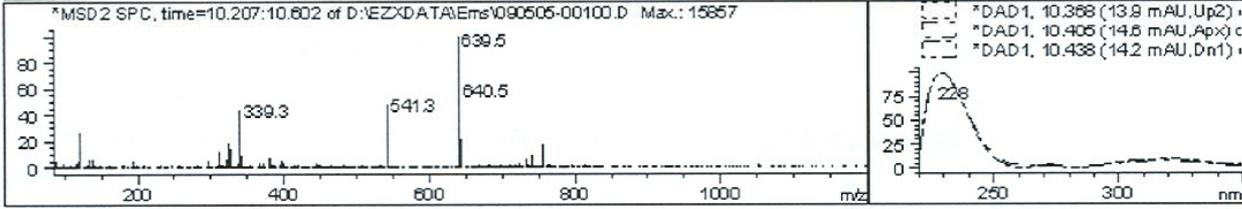
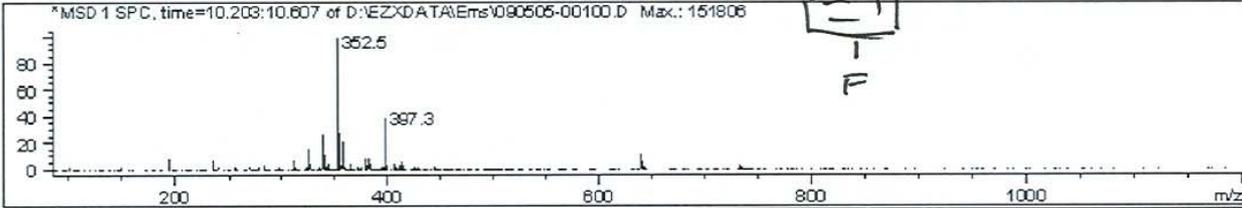
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Em Williams, 01-kwdn841-48C, AZD3409 BOC SAD CROP1
Printed by m235797 on Mon Jul 16 18:10:42 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl
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 -fluorophenyl)ethyl]benzoyl}-L-methininat
 (10)

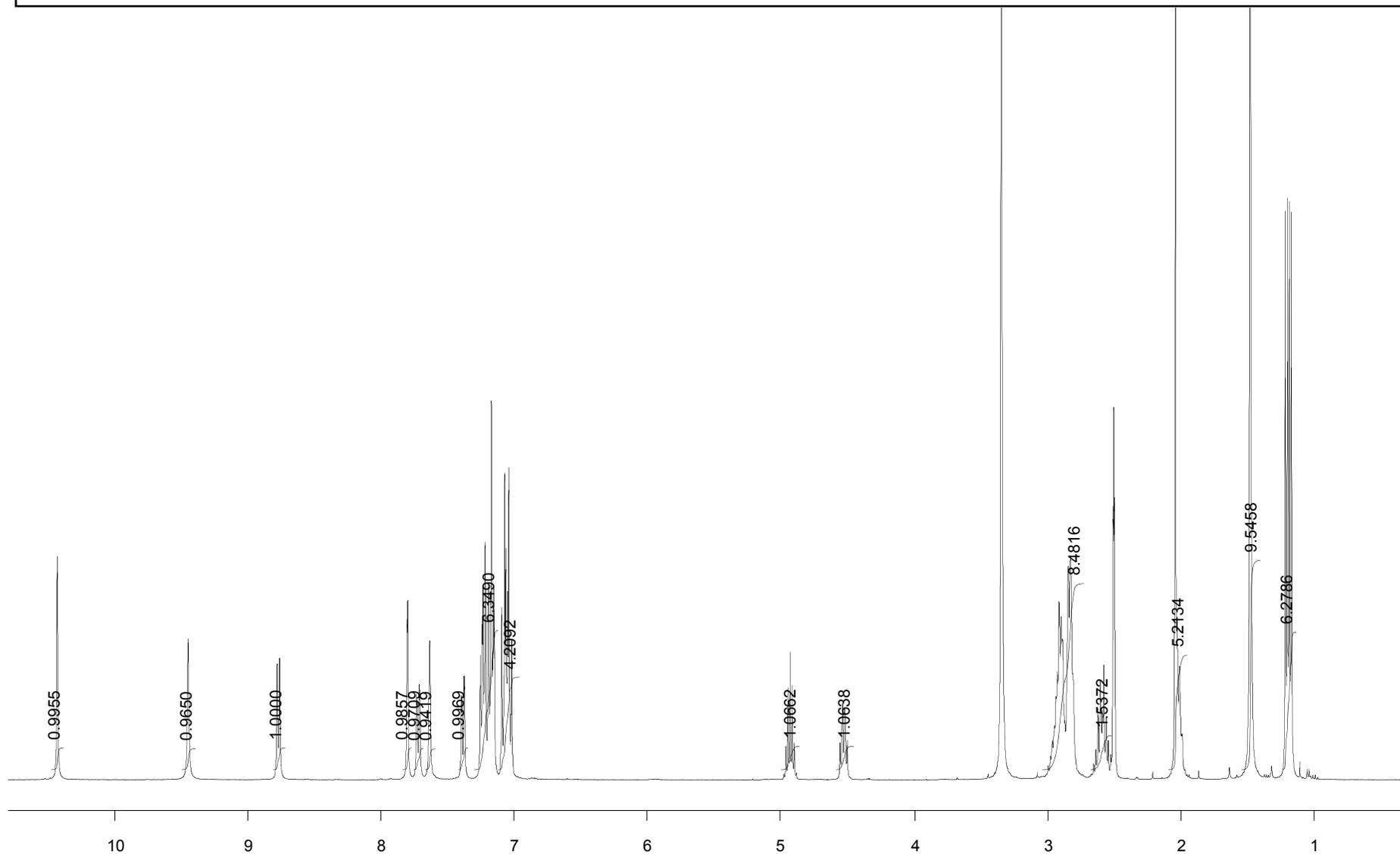
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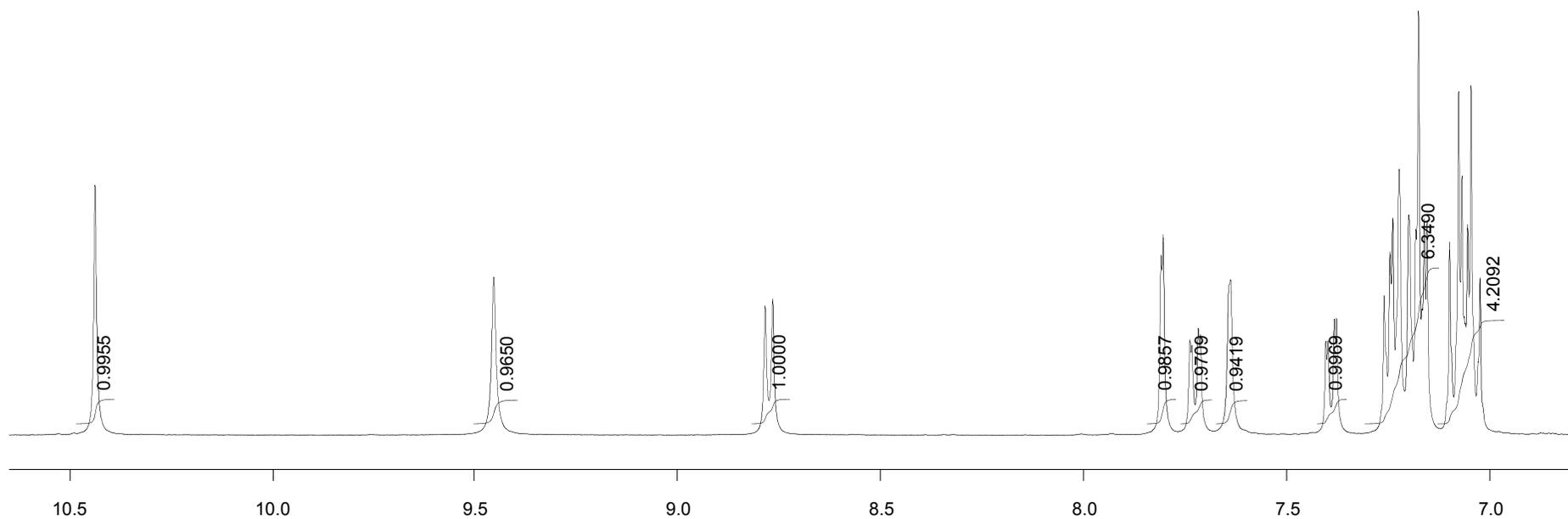


Isopropyl N-{5-((5-[tert-butoxycarbonyl]amino)-2-(4-fluorophenyl)ethyl)benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininatate 10



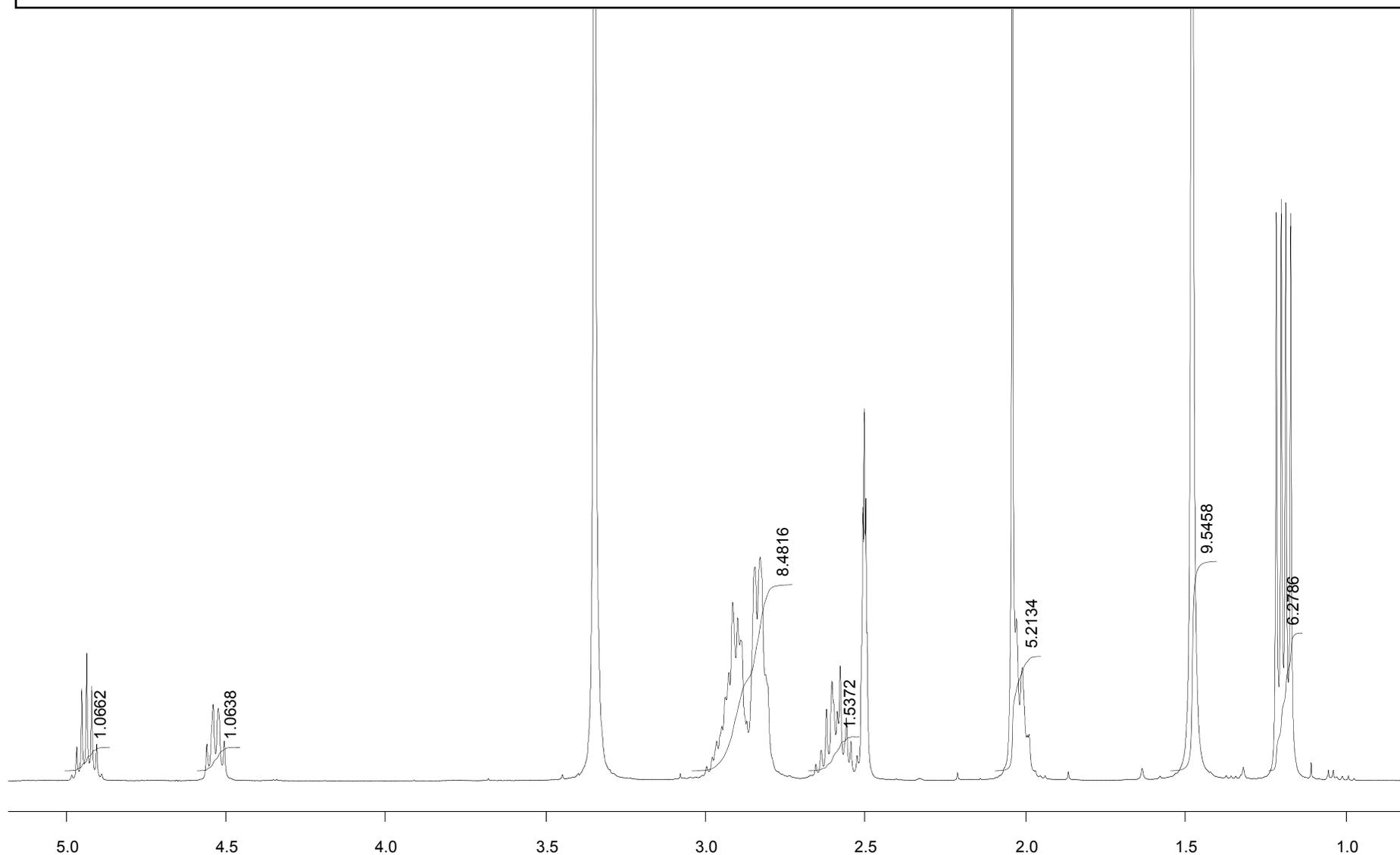
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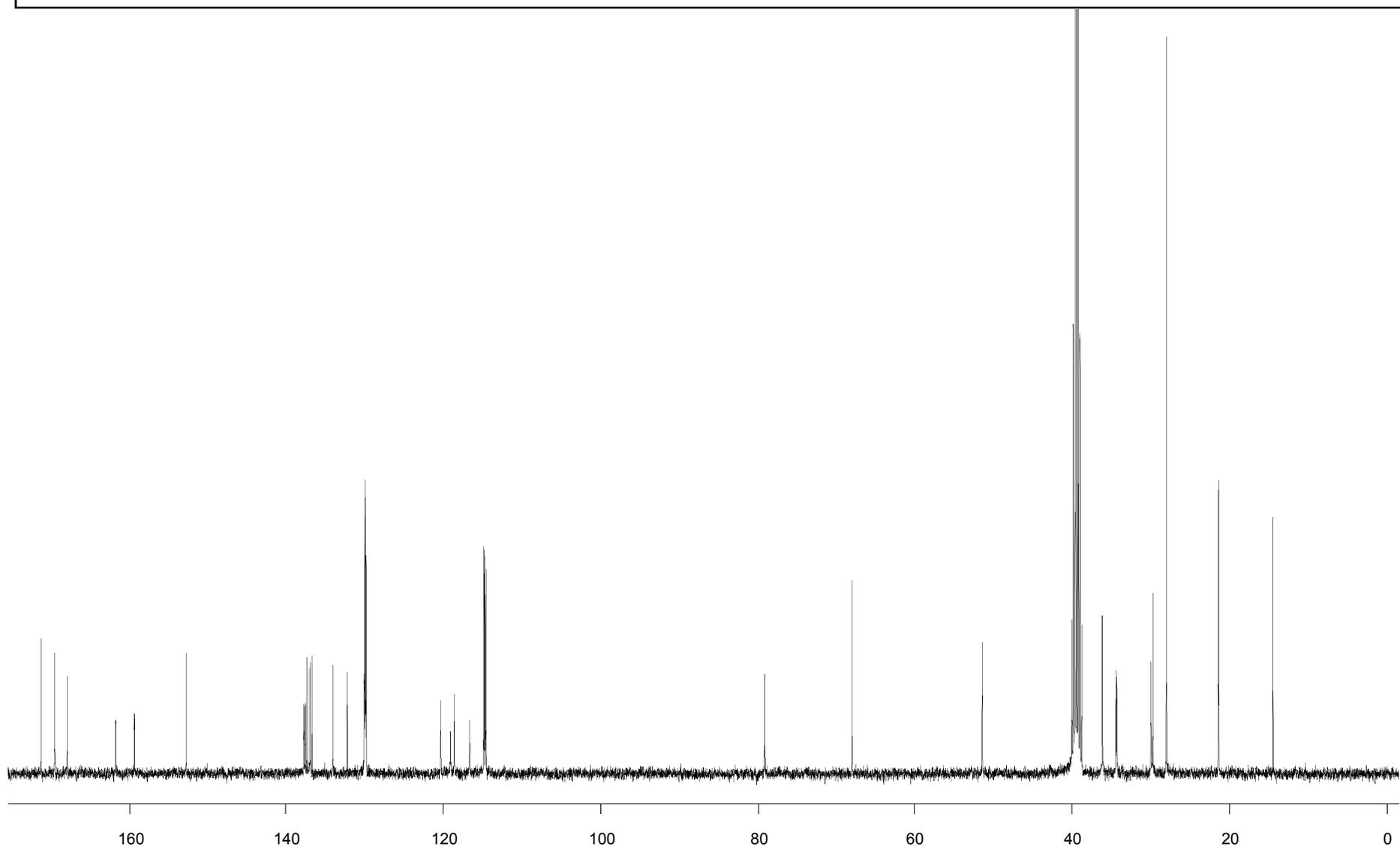
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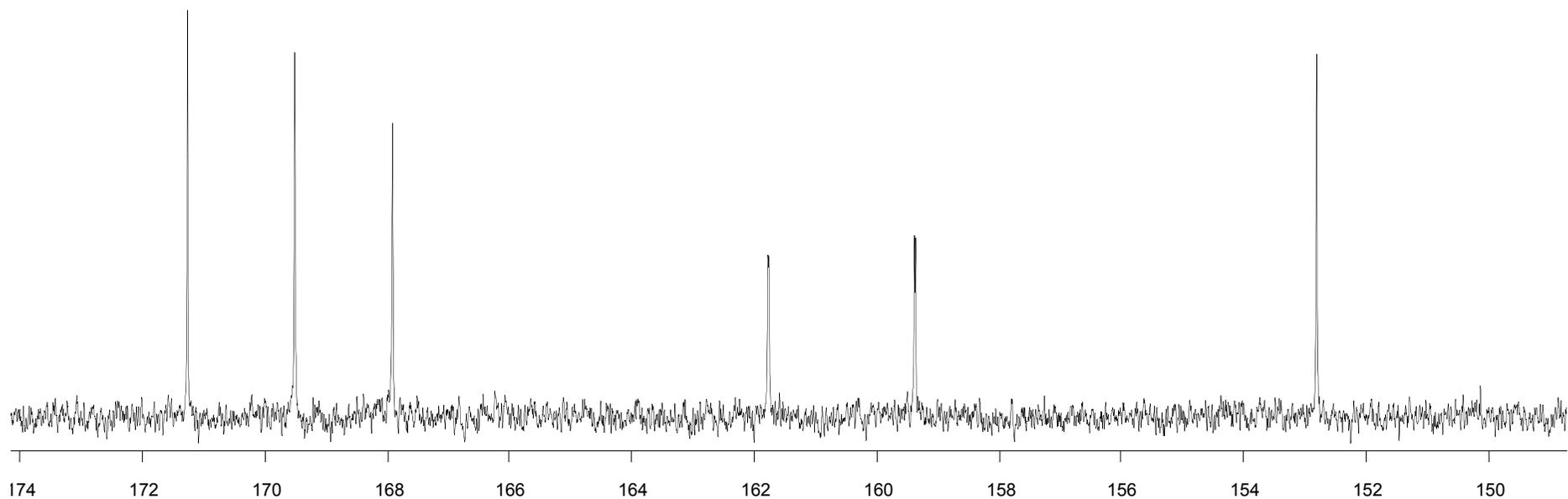
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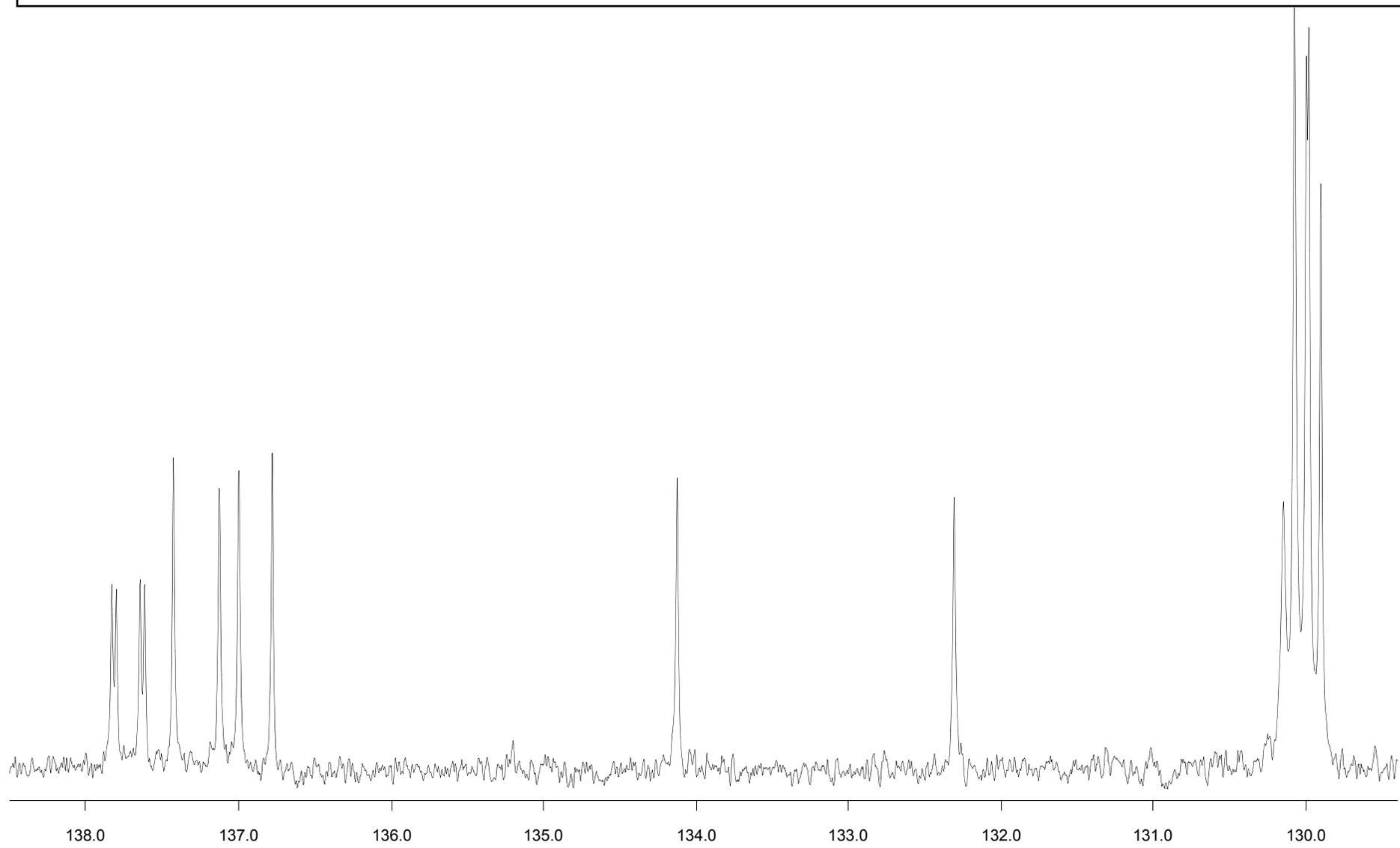
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Em Williams, 01-kwdn841-48C, AZD3409 BOC SAD CROP1
Printed by m235797 on Mon Jul 16 18:08:04 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-({5-[tert-butoxycarbonyl]amino}-2-(4-fluorophenyl)ethyl]benzoyl}amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinininate 10



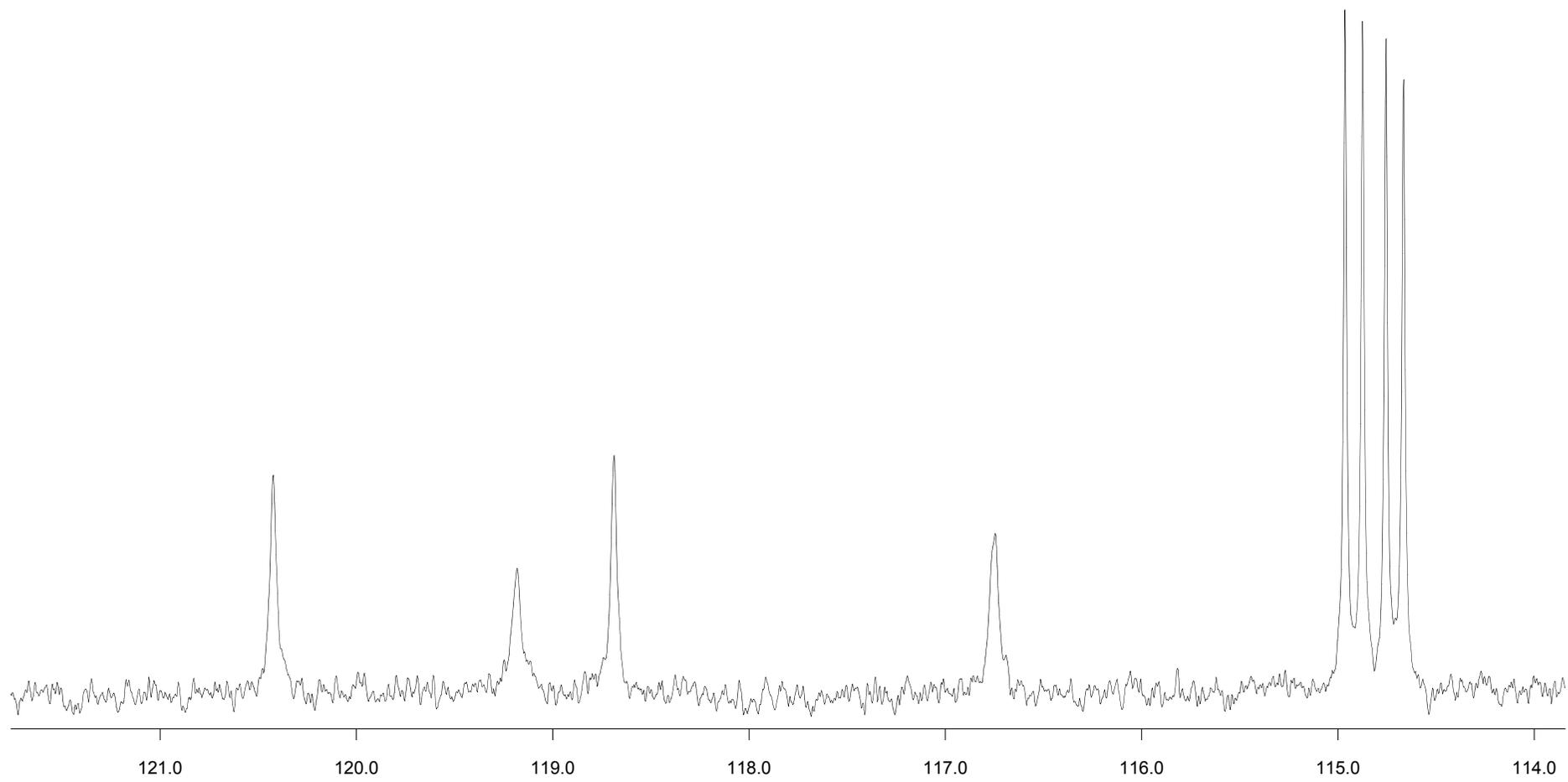
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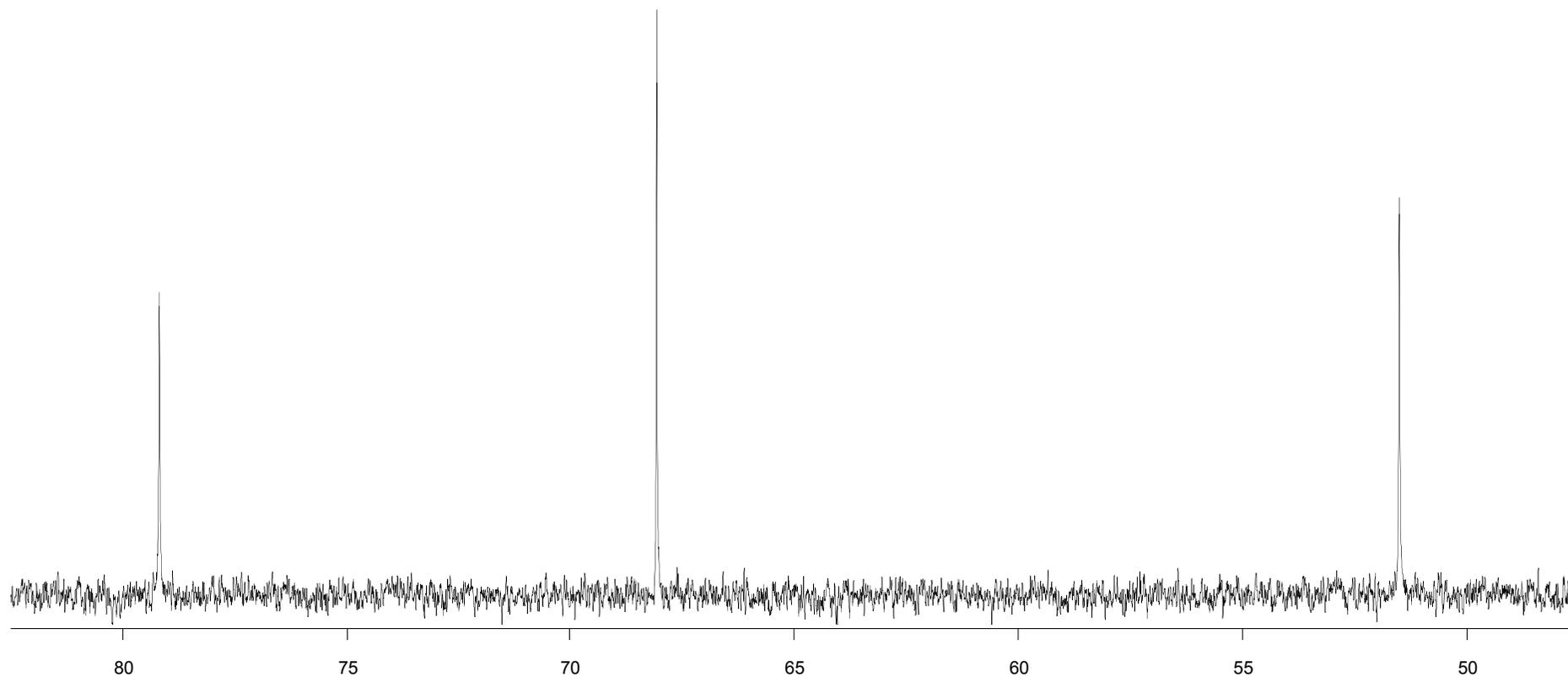
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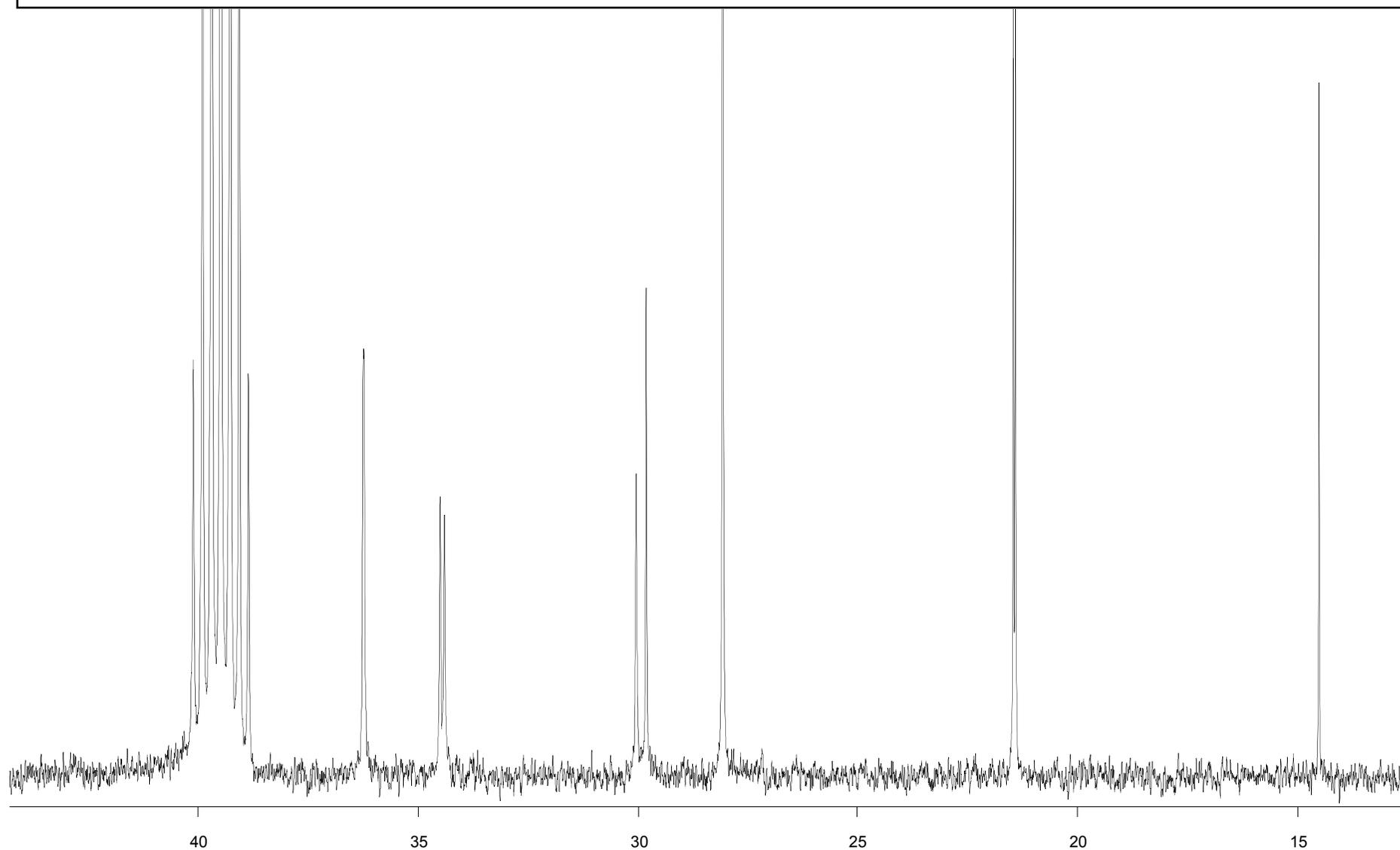
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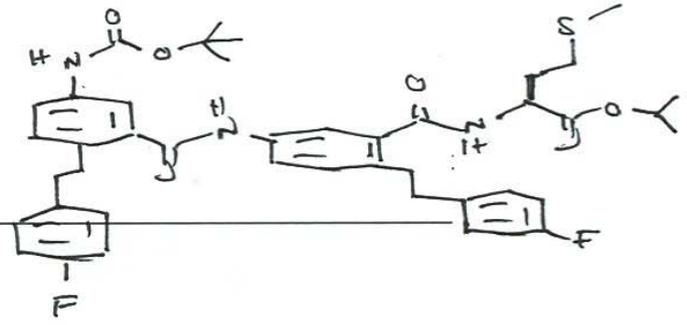
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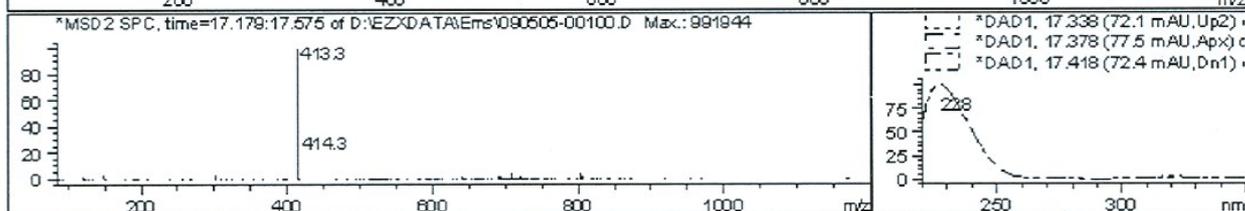
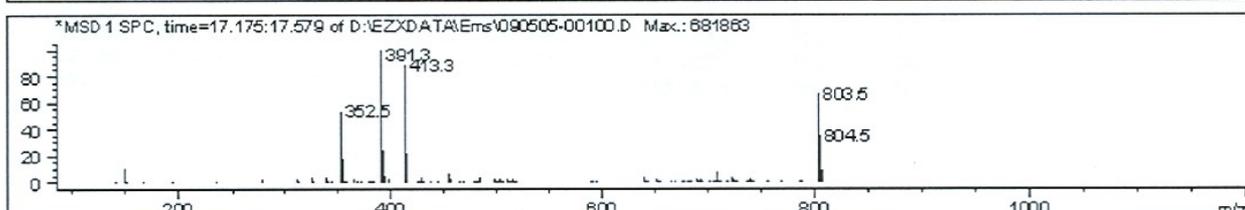
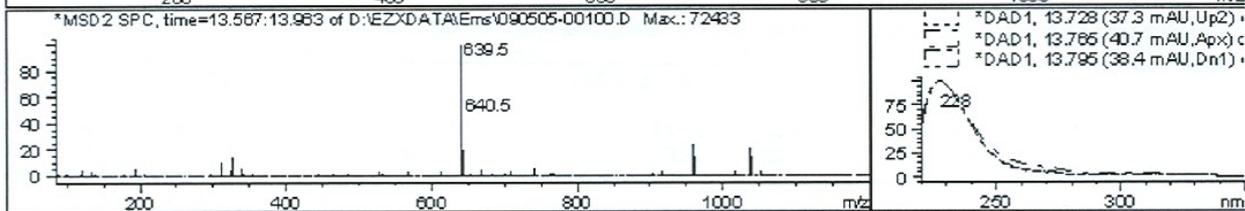
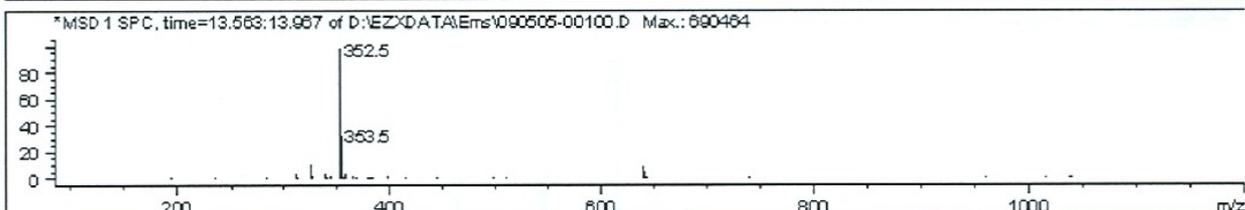
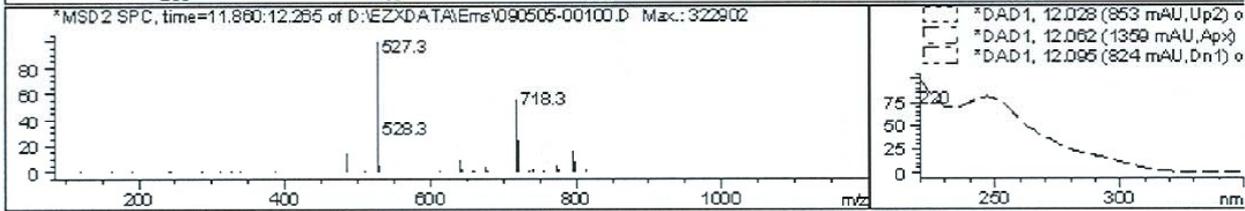
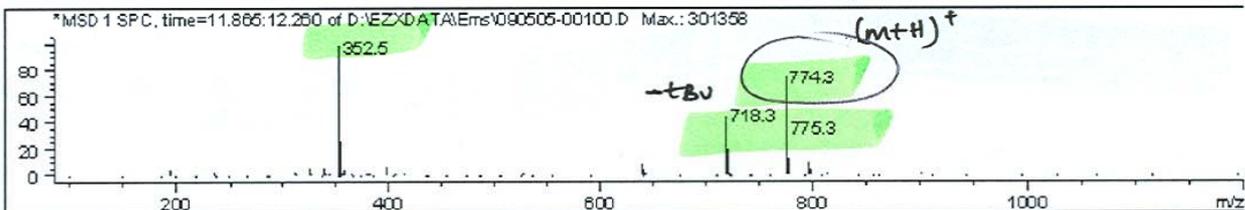
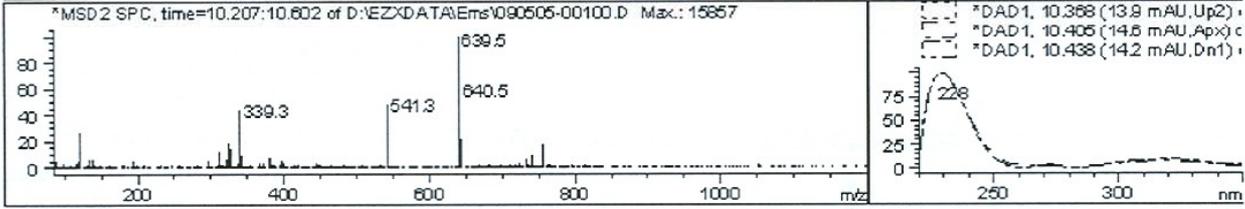
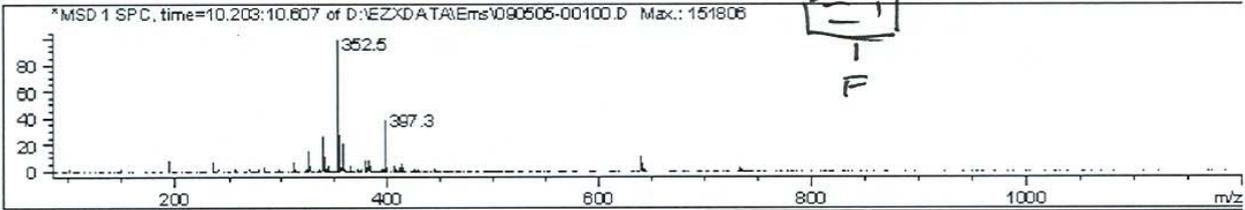
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Em Williams, 01-kwdn841-48C, AZD3409 BOC SAD CROP1
Printed by m235797 on Mon Jul 16 18:10:42 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl
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 -fluorophenyl)ethyl]benzoyl}-L-methininat
 (10)

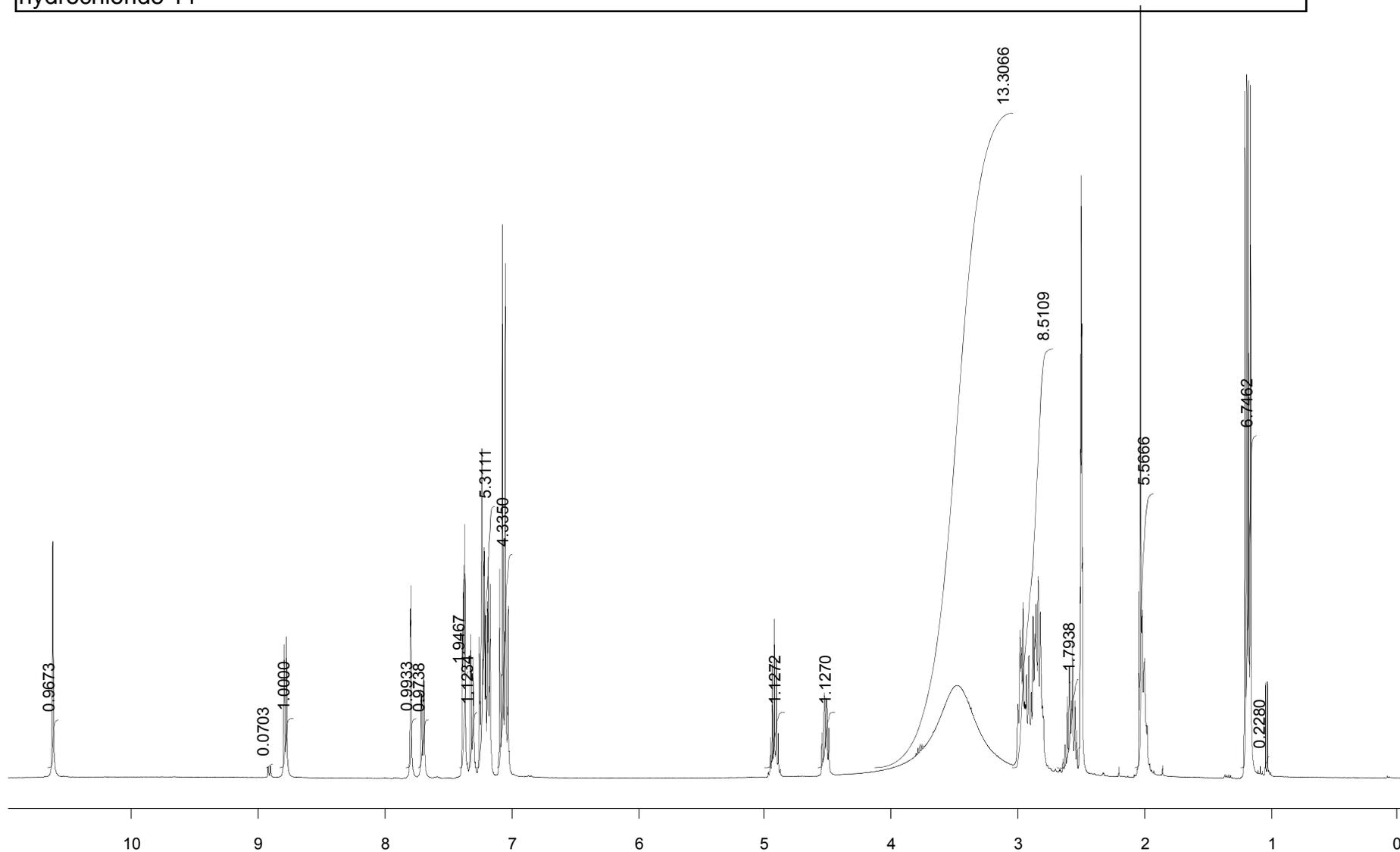
Boc SaD mol = 773.9



Data File D:\EZXDATA\Ems\090505-00100.D
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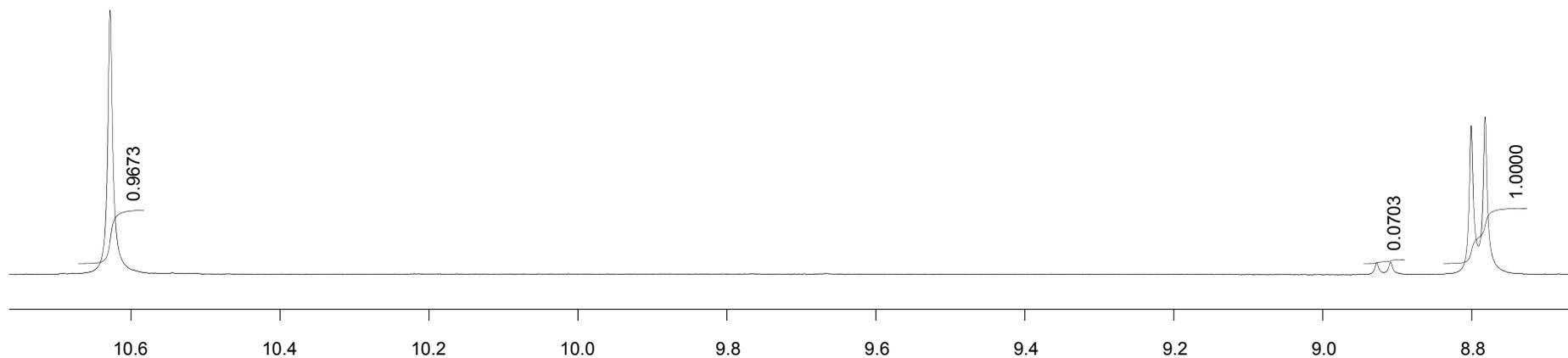


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

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hydrochloride 11

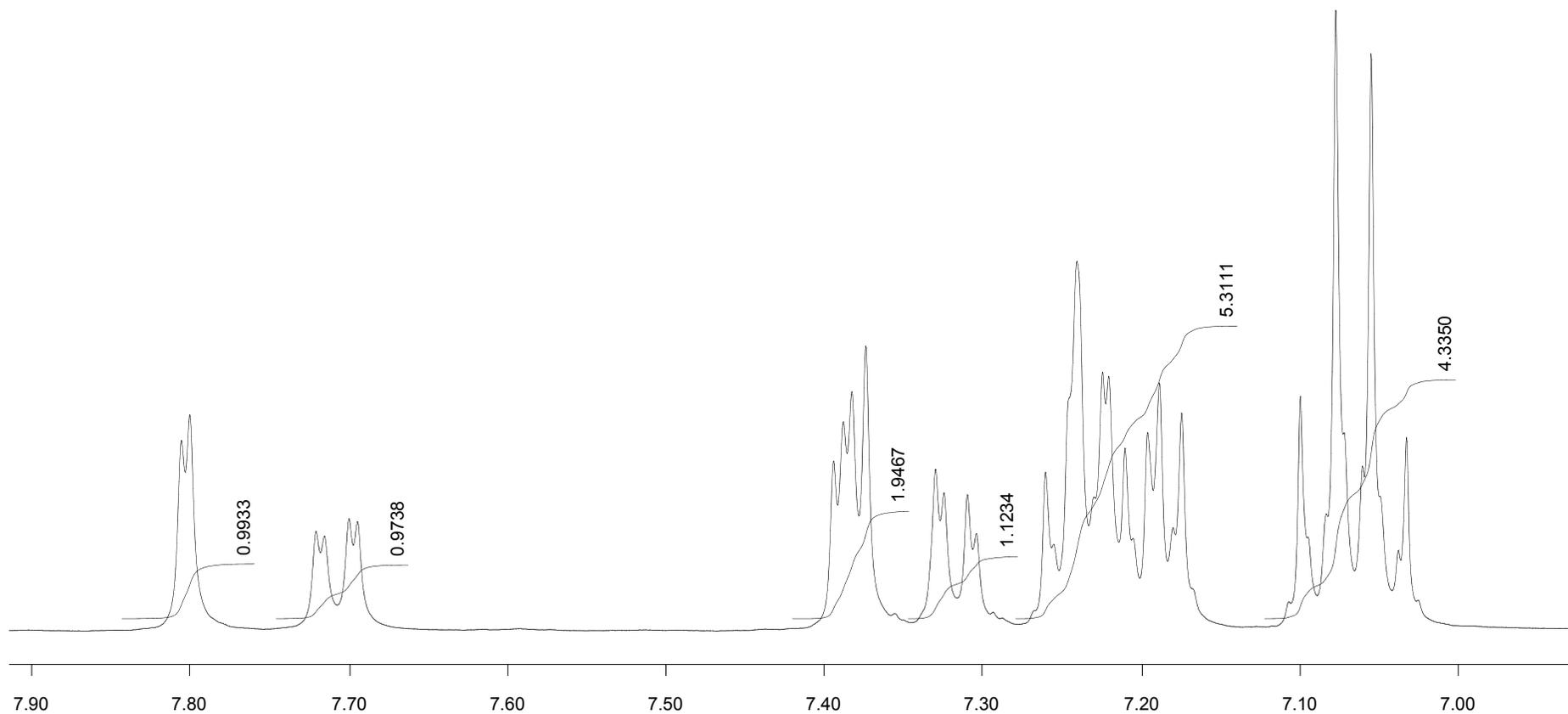


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

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Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininat
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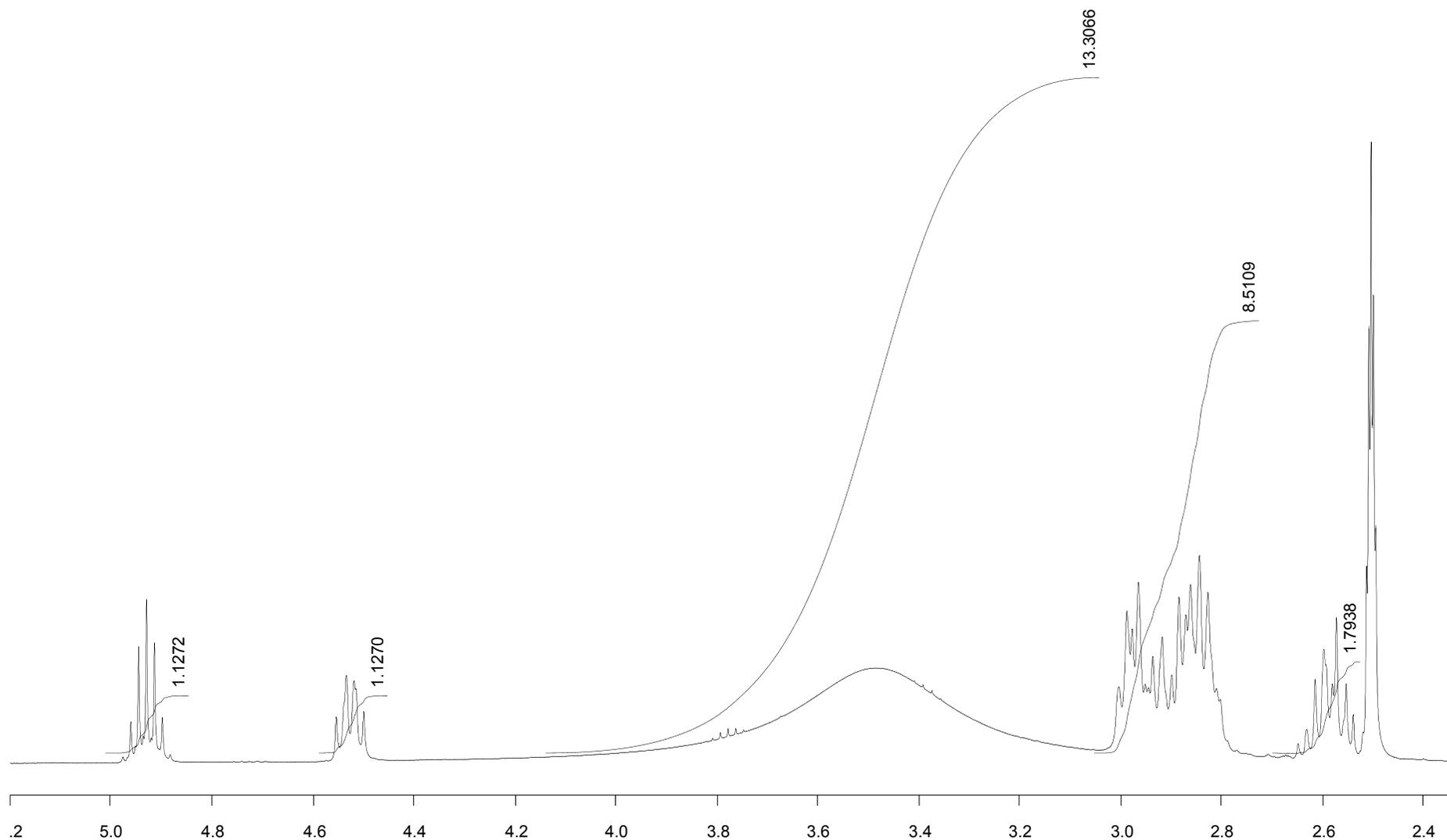


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

Printed by RD\M235797 on Mon Jul 16 18:42:15 BST 2007. nucleus: 1H, freq: 400.13 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininiate hydrochloride 11

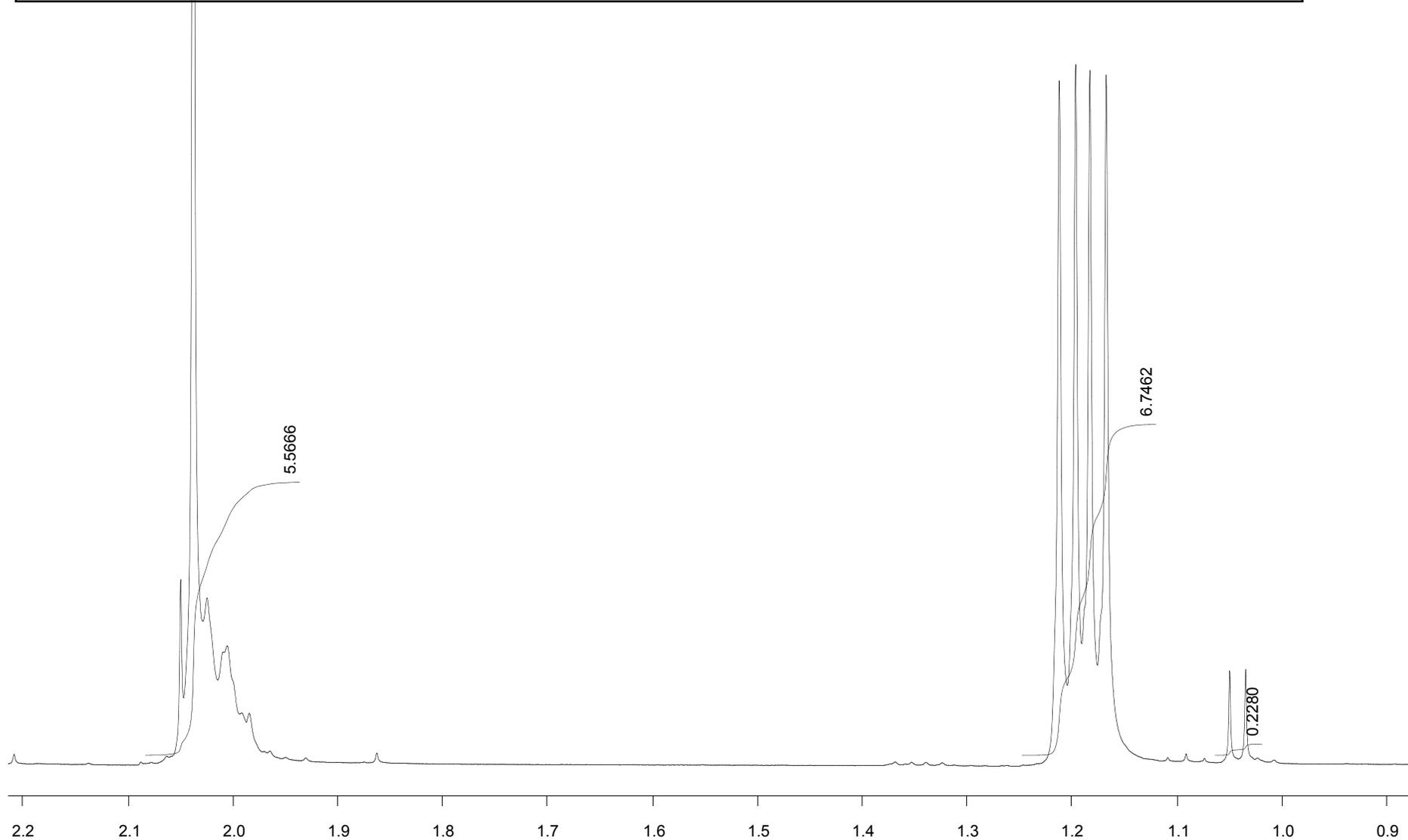


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

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Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininat
hydrochloride 11

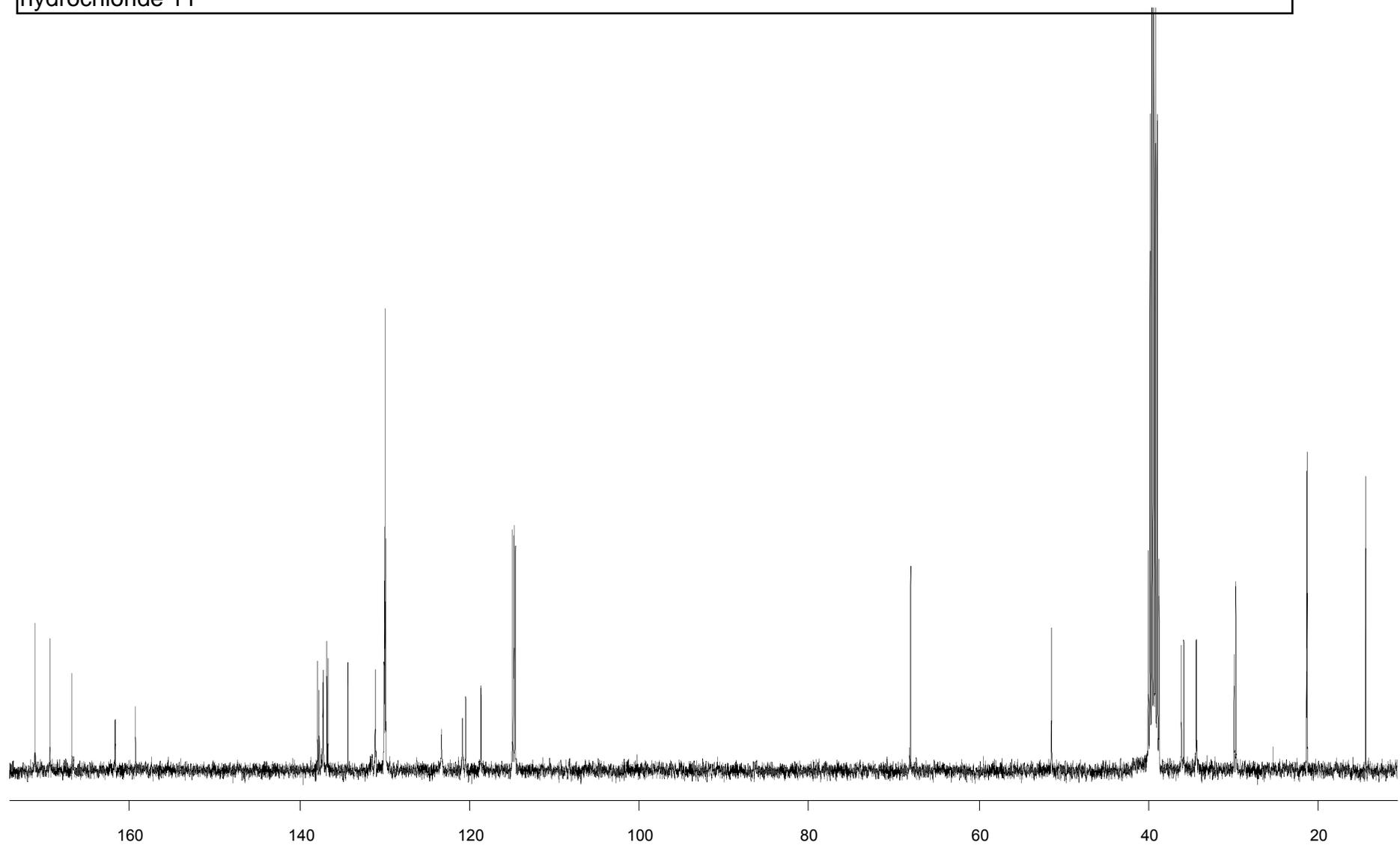


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

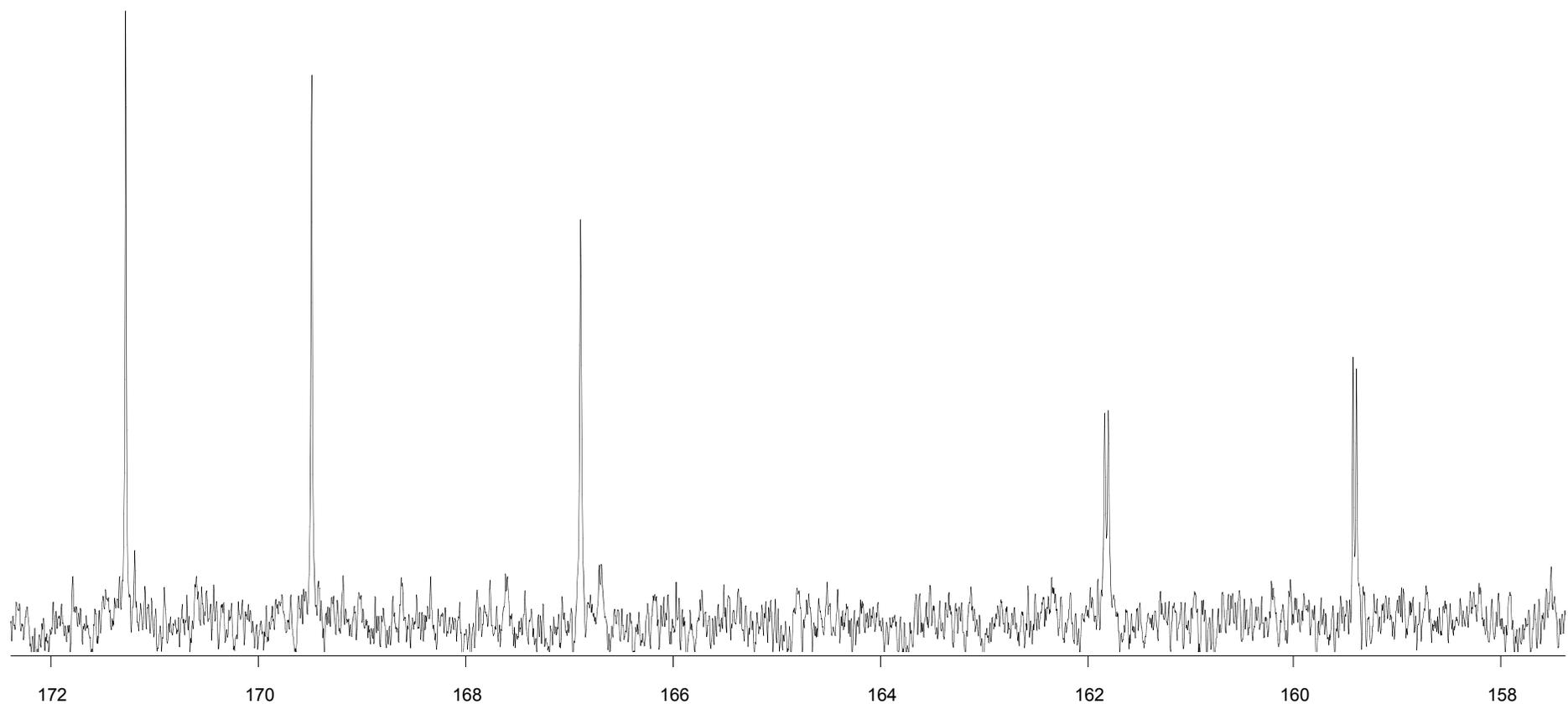
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hydrochloride 11



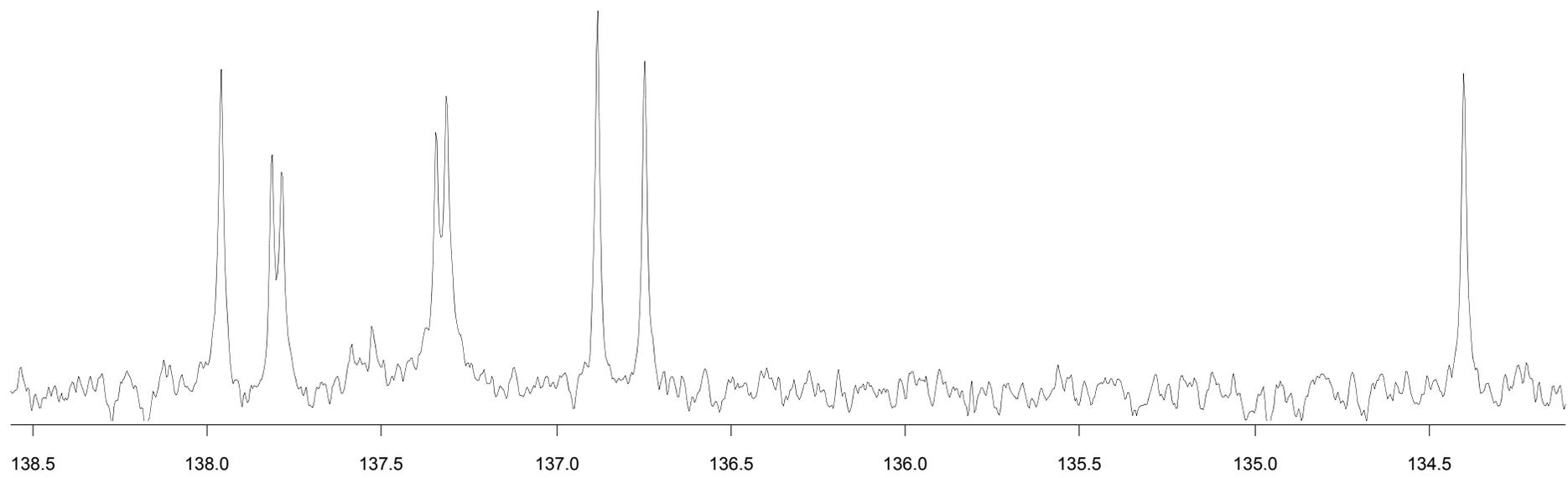
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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:45:17 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

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hydrochloride 11



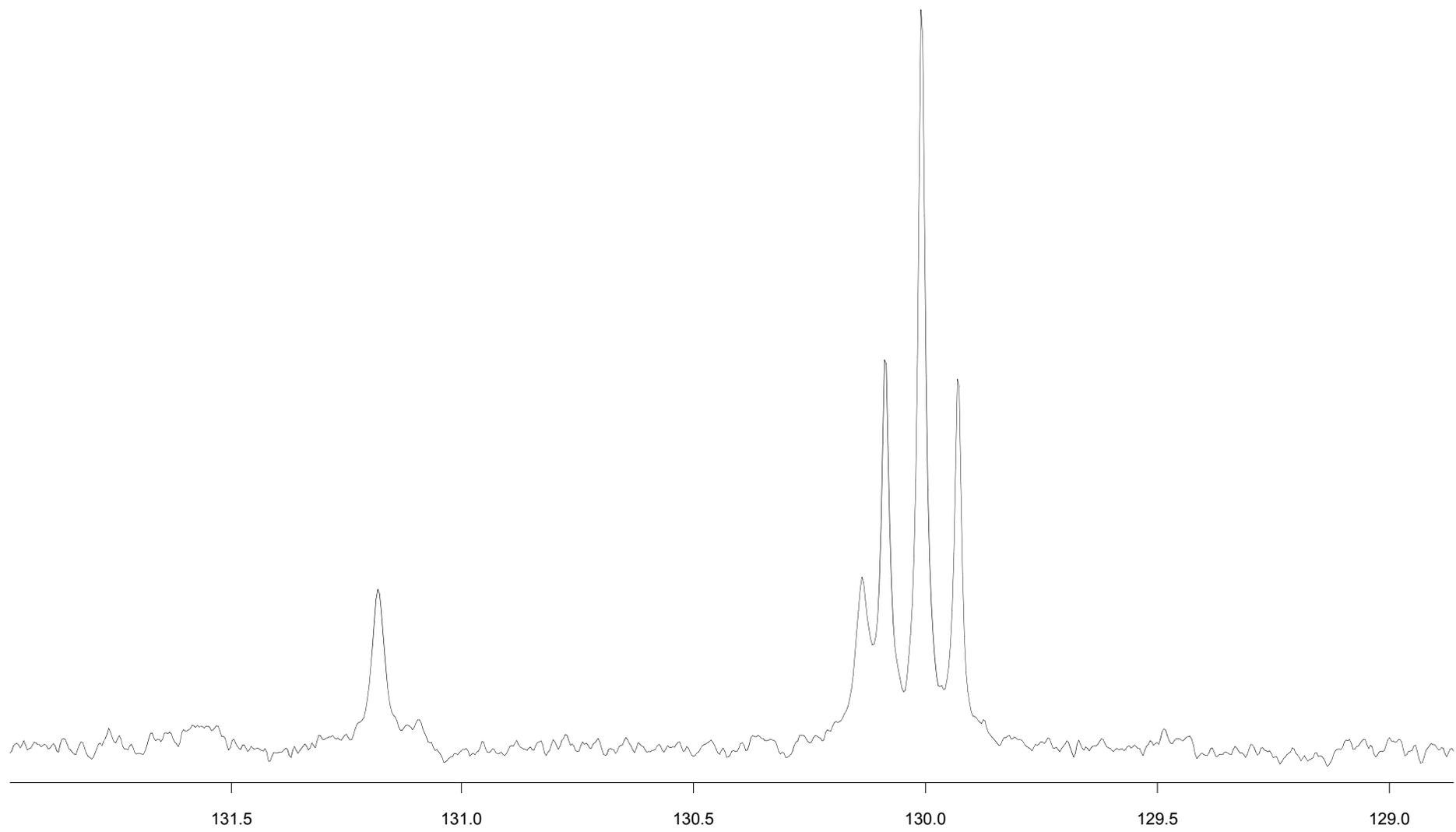
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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:46:10 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininatate hydrochloride 11



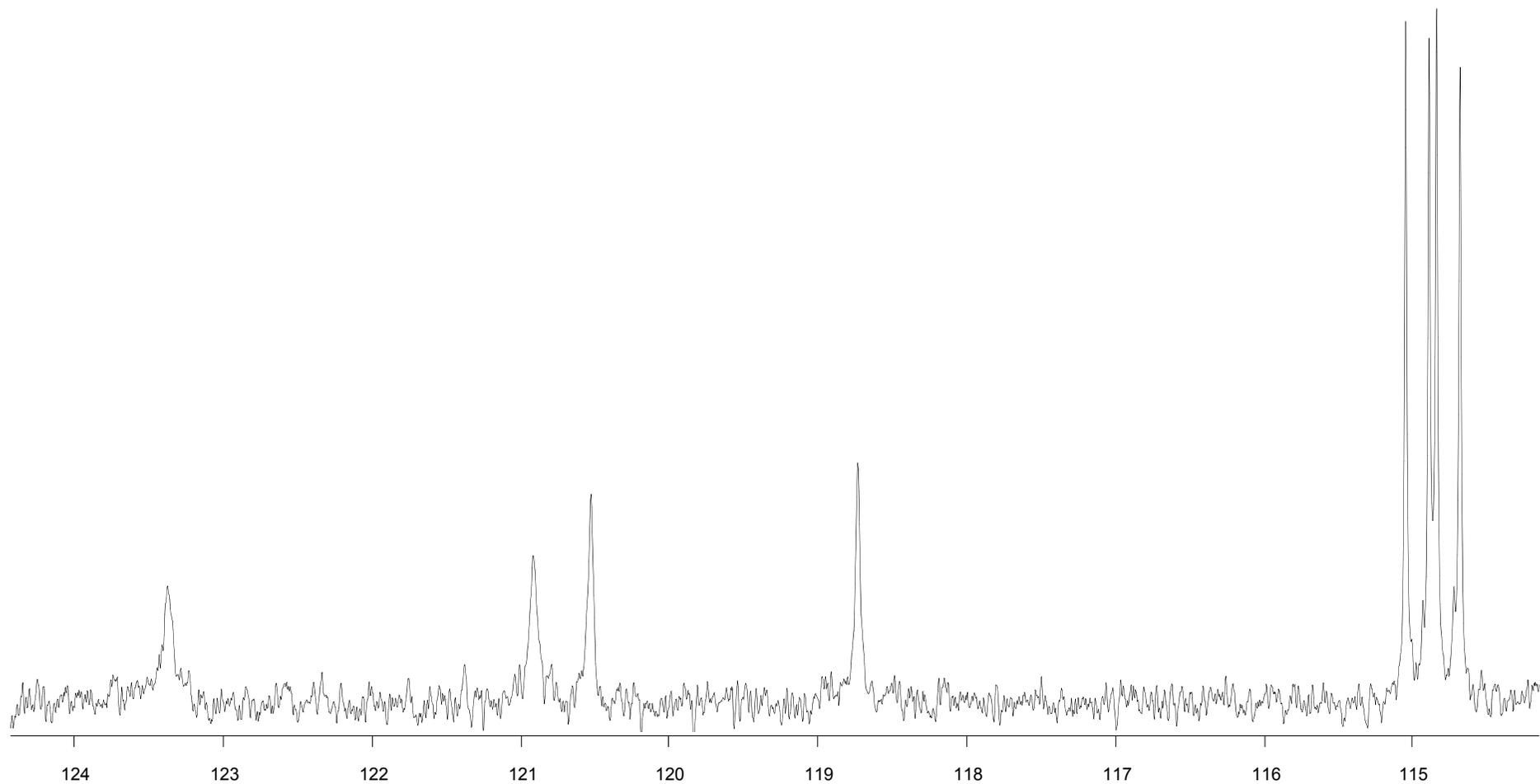
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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:47:26 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinate hydrochloride 11



JView Version 0.95 /NMR/pdd/nmr/050519018/11/pdata/1/
Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:48:02 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinate hydrochloride 11

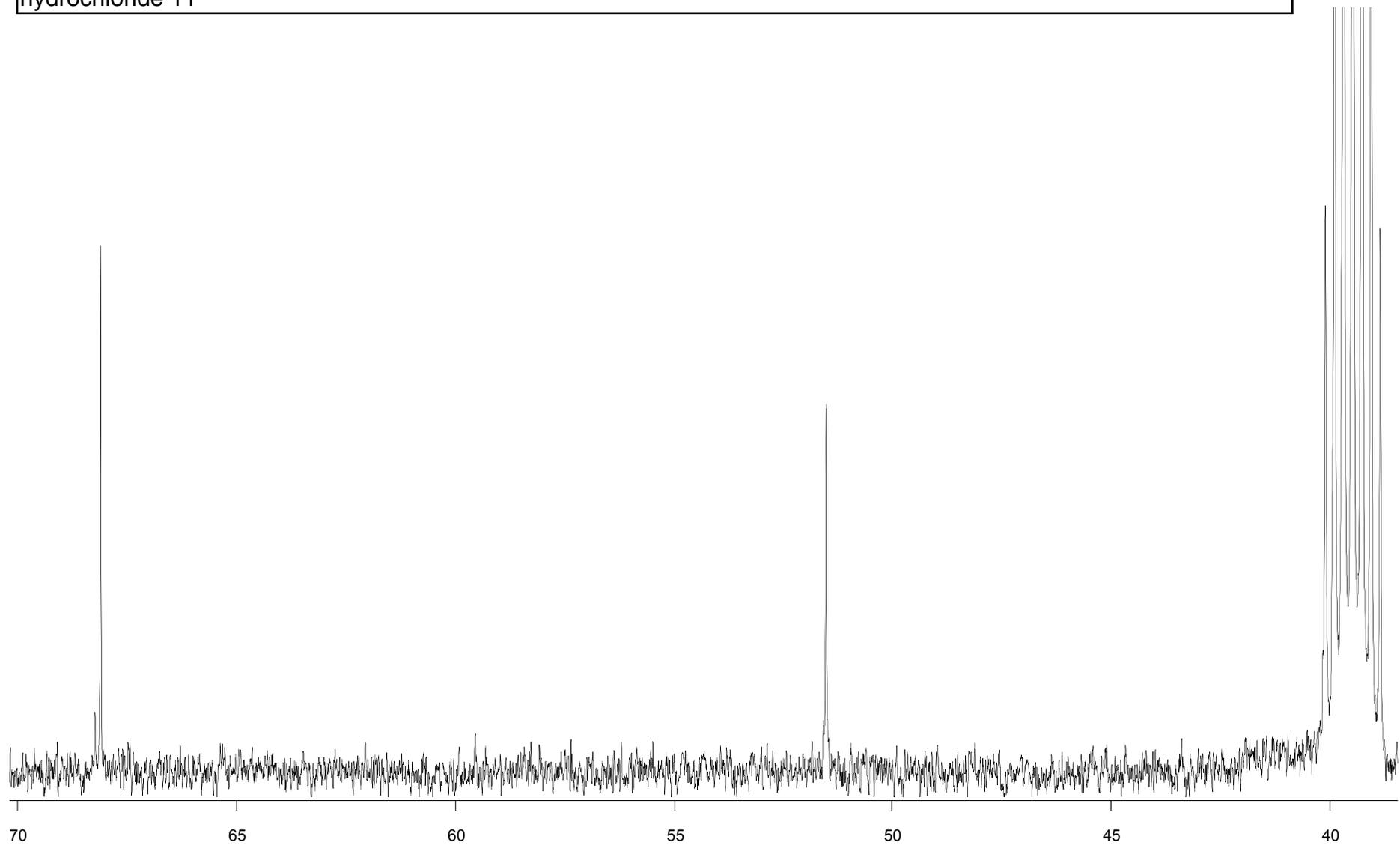


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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

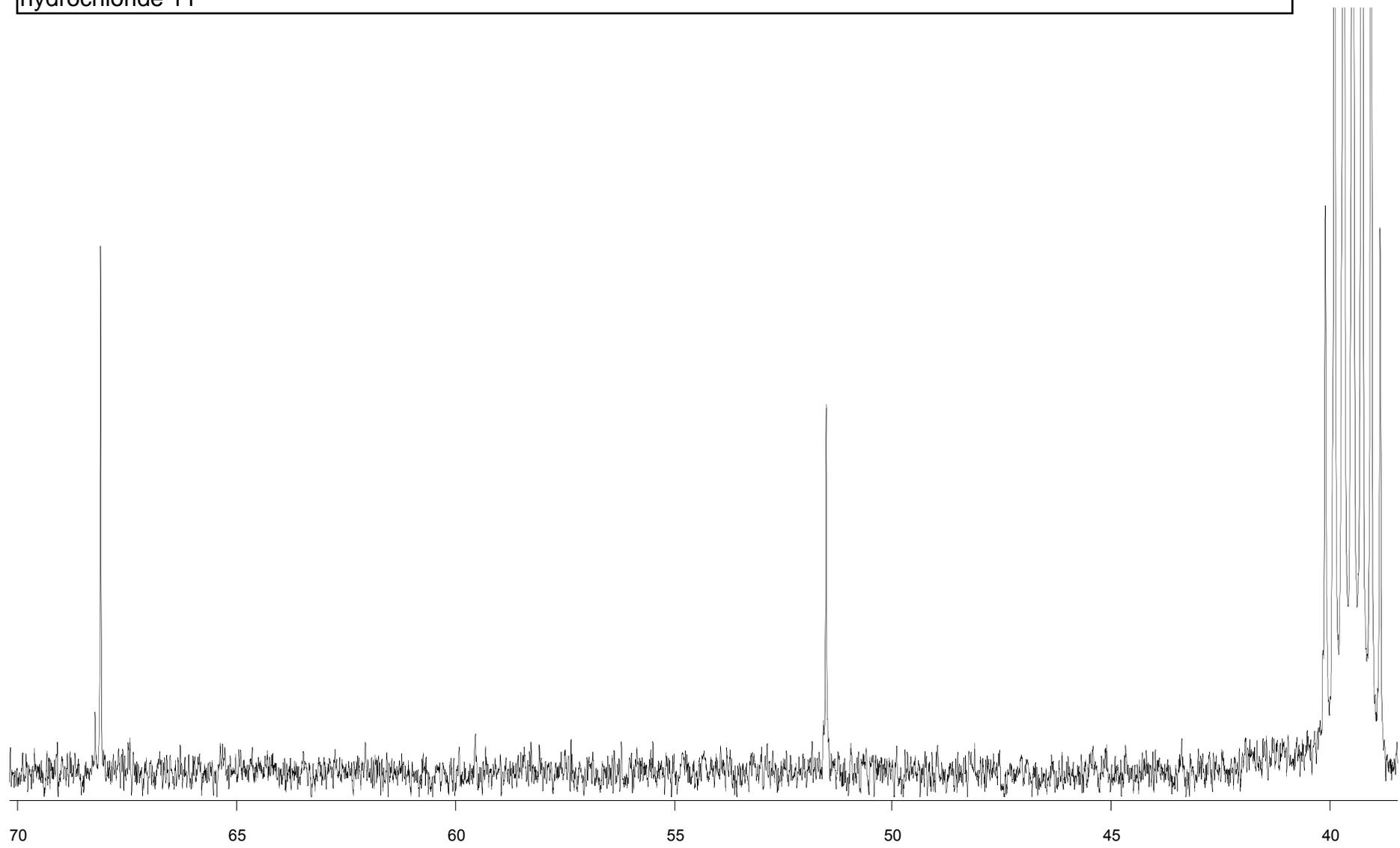
Printed by m235797 on Mon Jul 16 18:48:26 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-({5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinate hydrochloride 11



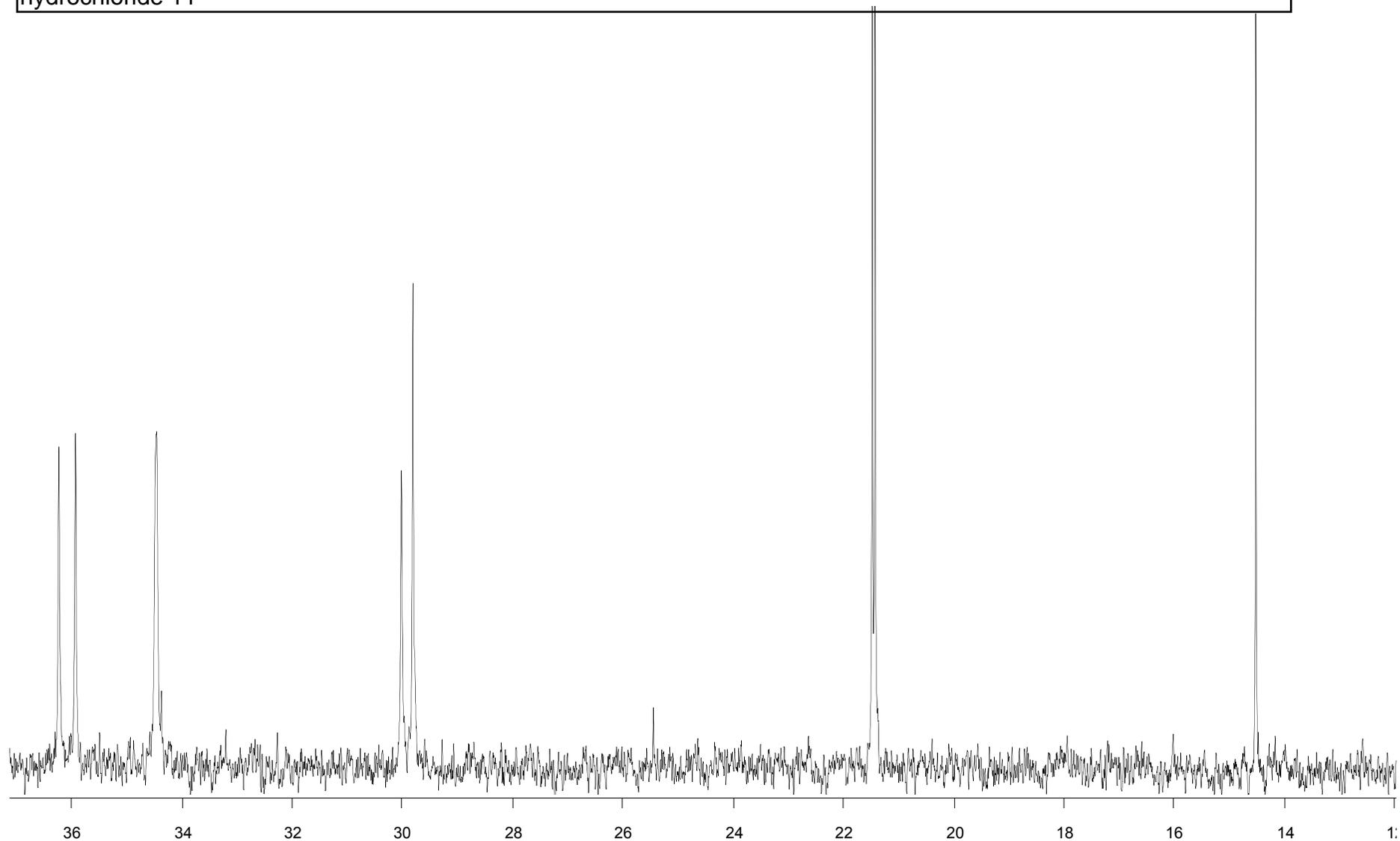
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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:49:54 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-({5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl}amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methinate hydrochloride 11



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Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl
Printed by m235797 on Mon Jul 16 18:49:54 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K

Isopropyl N-{5-((5-amino-2-[2-(4-fluorophenyl)ethyl]benzoyl)amino)-2-[2-(4-fluorophenyl)ethyl]benzoyl}-L-methininat
hydrochloride 11



JView Version 0.95 /NMR/pdd/nmr/050519018/11/pdata/1/

Em Williams, 01-kwdn841-49A, AZD3409 SAD.HCl

Printed by m235797 on Mon Jul 16 18:49:25 BST 2007. nucleus: 13C, freq: 100.61 MHz, solvent: DMSO, temperature:300K