

SUPPORTING INFORMATION

Manuscript title: Efficient one-pot two catalyst system in the construction of 2-substituted benzimidazoles: synthesis of Benzimidazo[1,2-c]quinazolines

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^b*Boehringer Ingelheim Pharma GmbH & Co. KG, Birkendorfer Strasse 65, 88397 Biberach an der Riss, Germany*

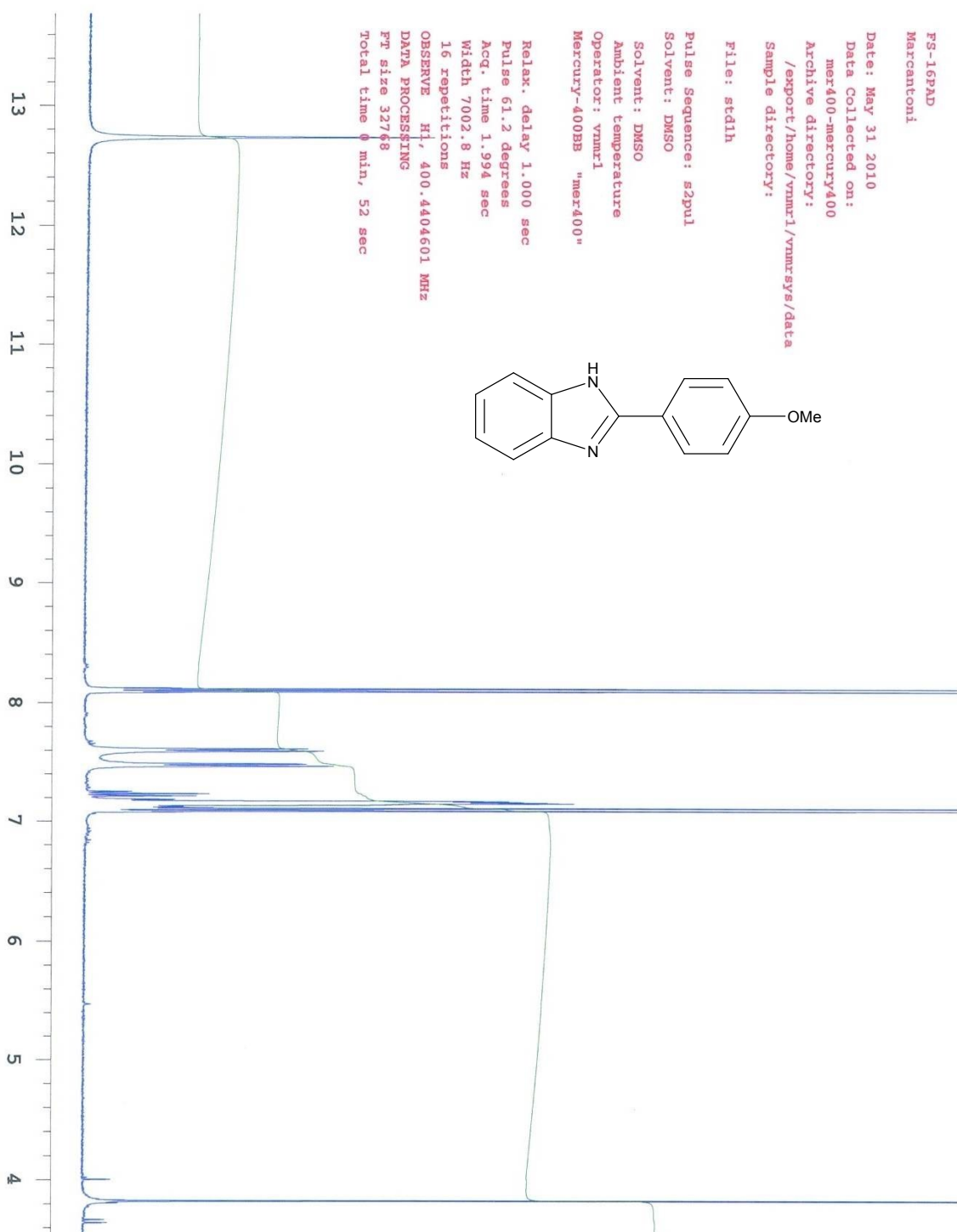
^c*BI Research Italia S.a.s. of BI IT S.r.l., Via Lorenzini 8, I-20139 Milano, Italy.*

E-mail: enrico.marcantoni@unicam.it

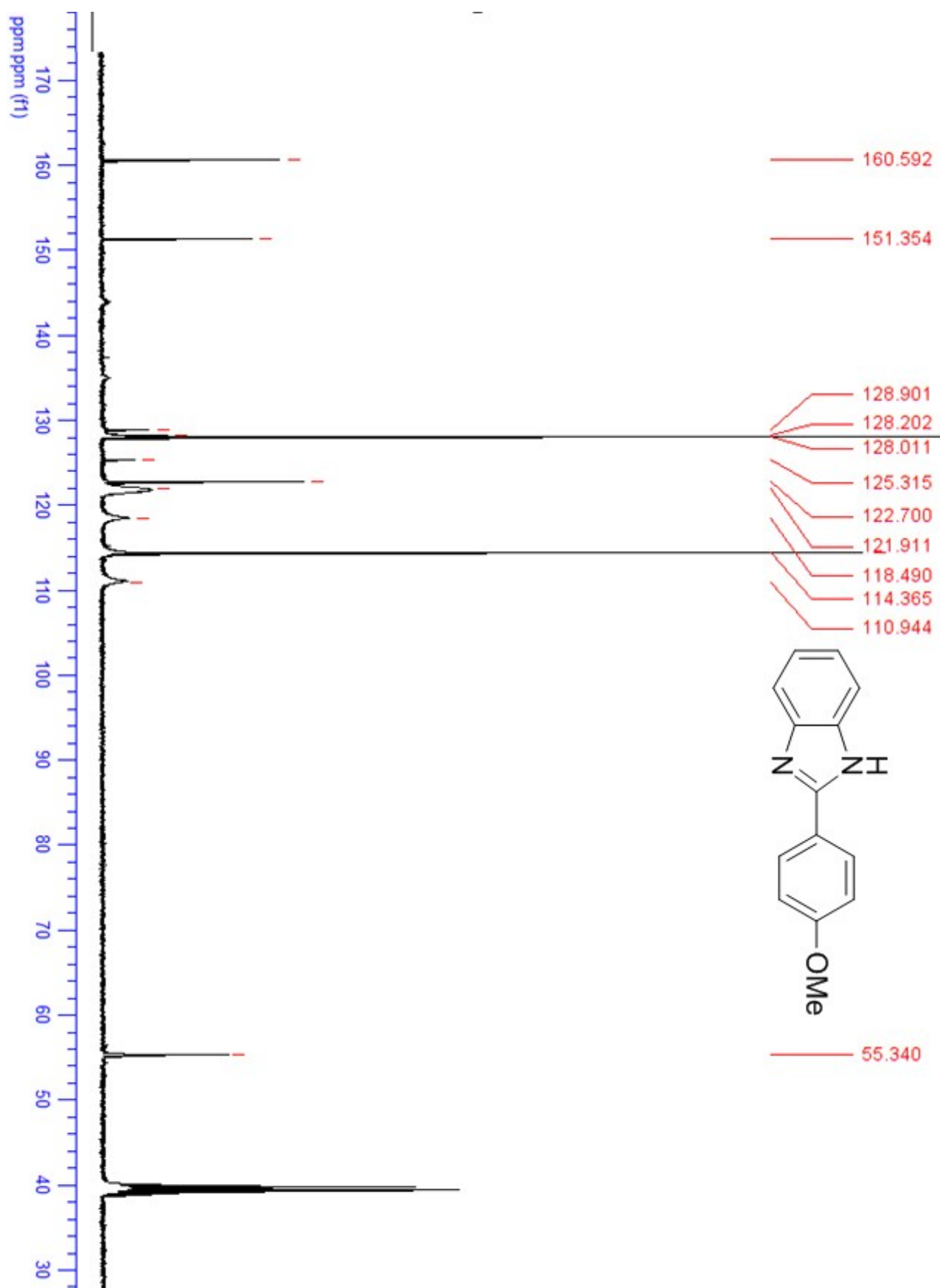
Table of Contents

Copy of ¹ H-NMR, ¹³ C-NMR, EI-MS, ESI-MS spectra	S1-S40
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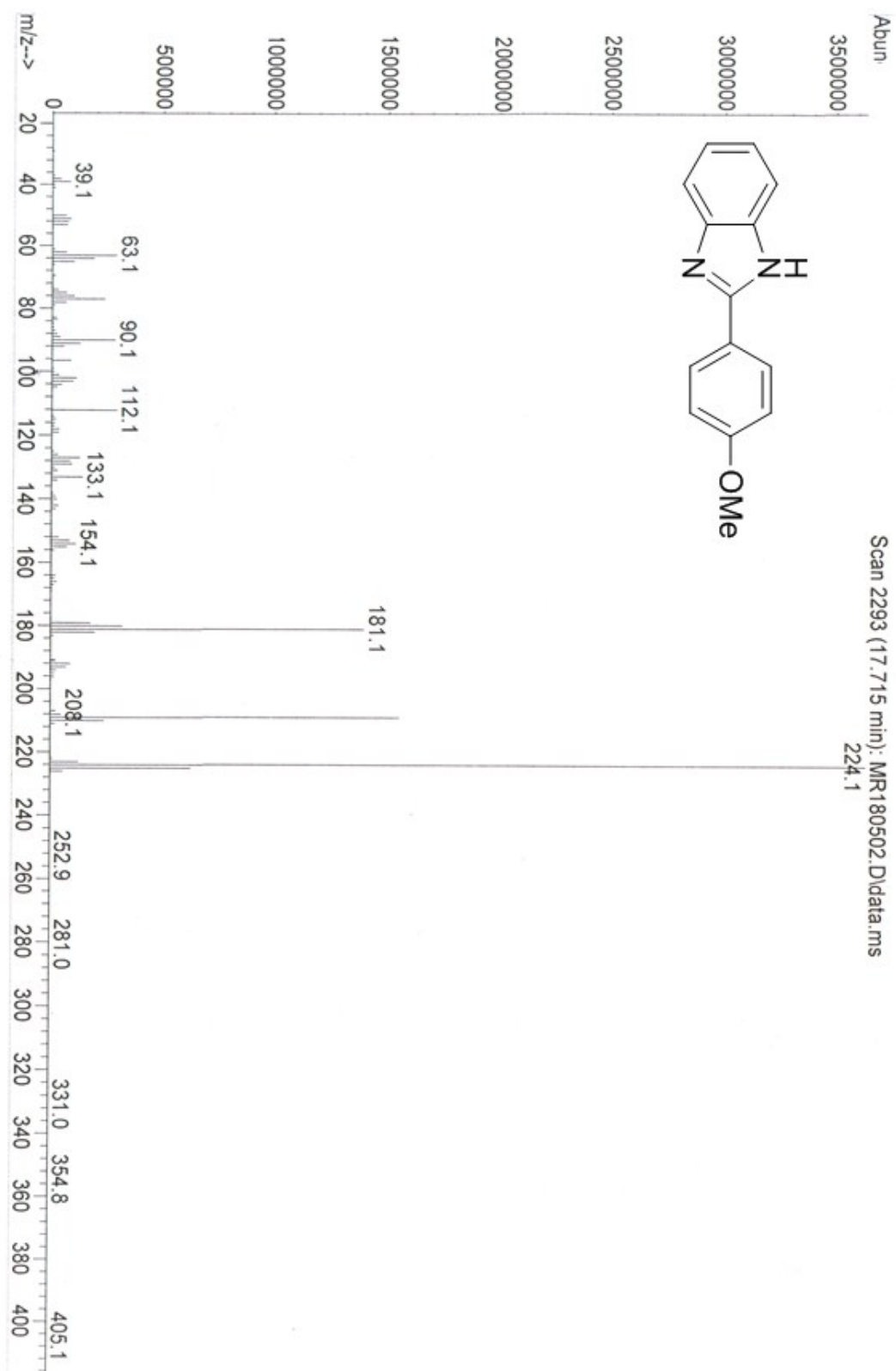
Compound **3a** ($^1\text{H-NMR}$, DMSO-d_6)



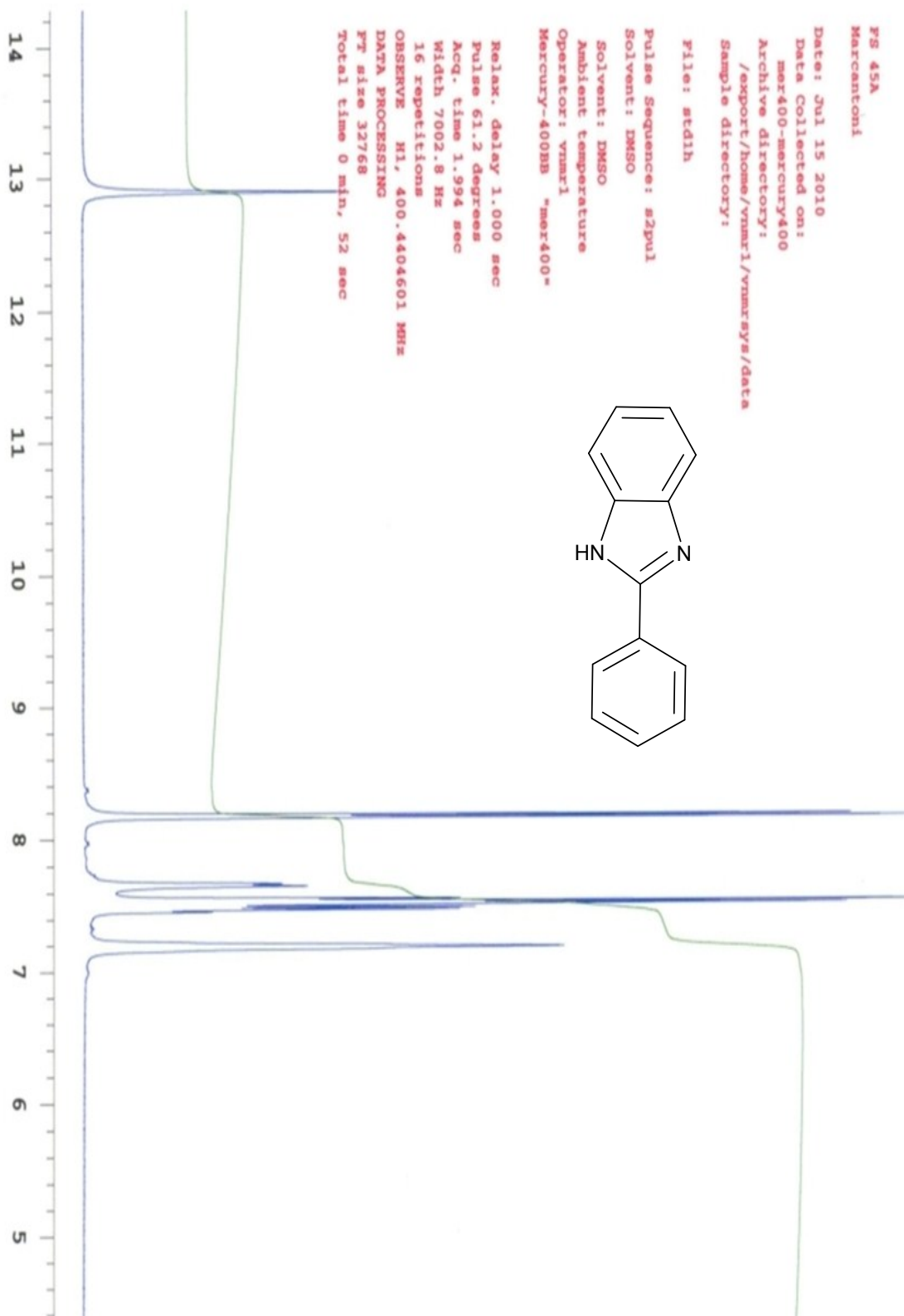
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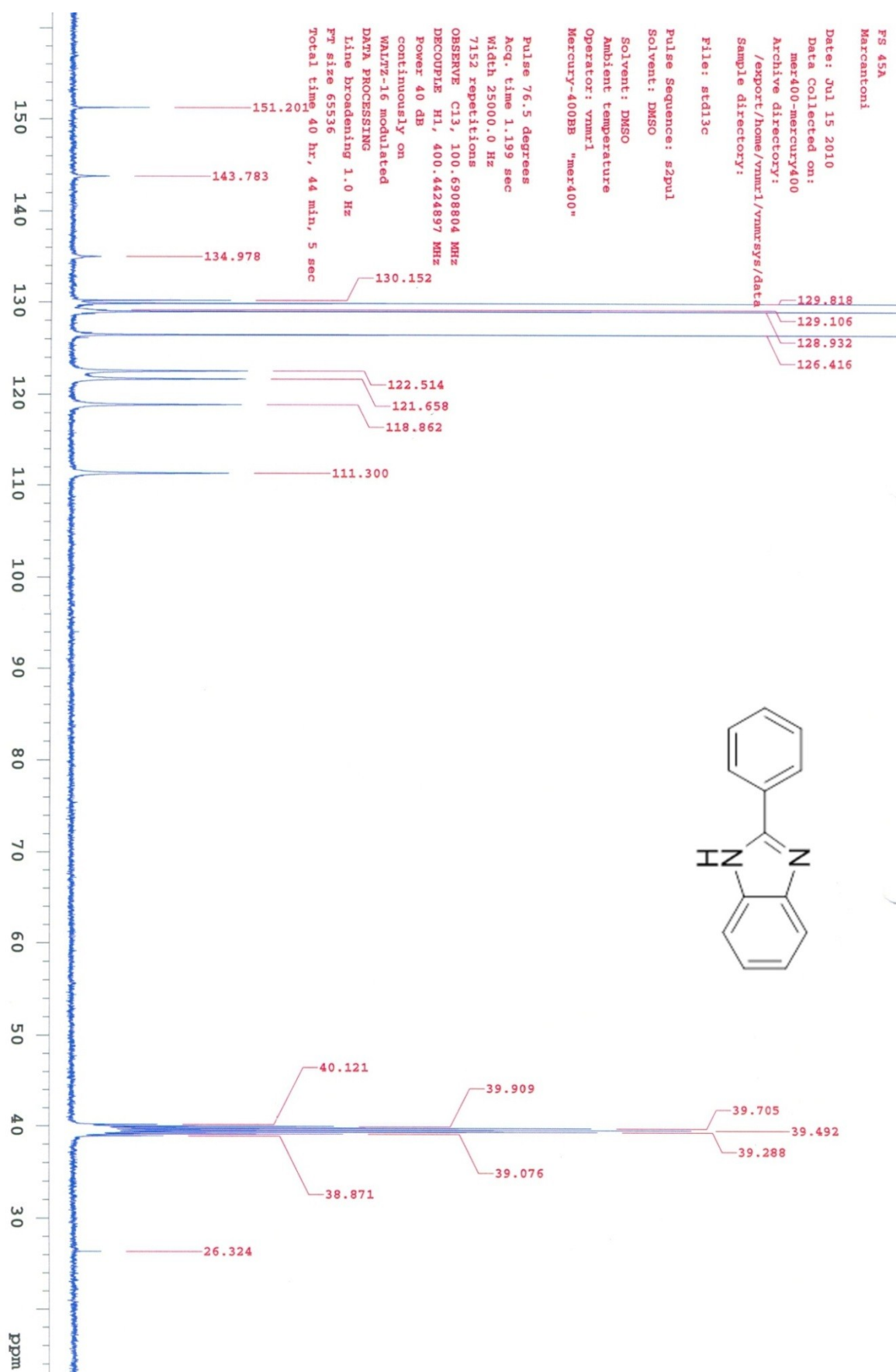
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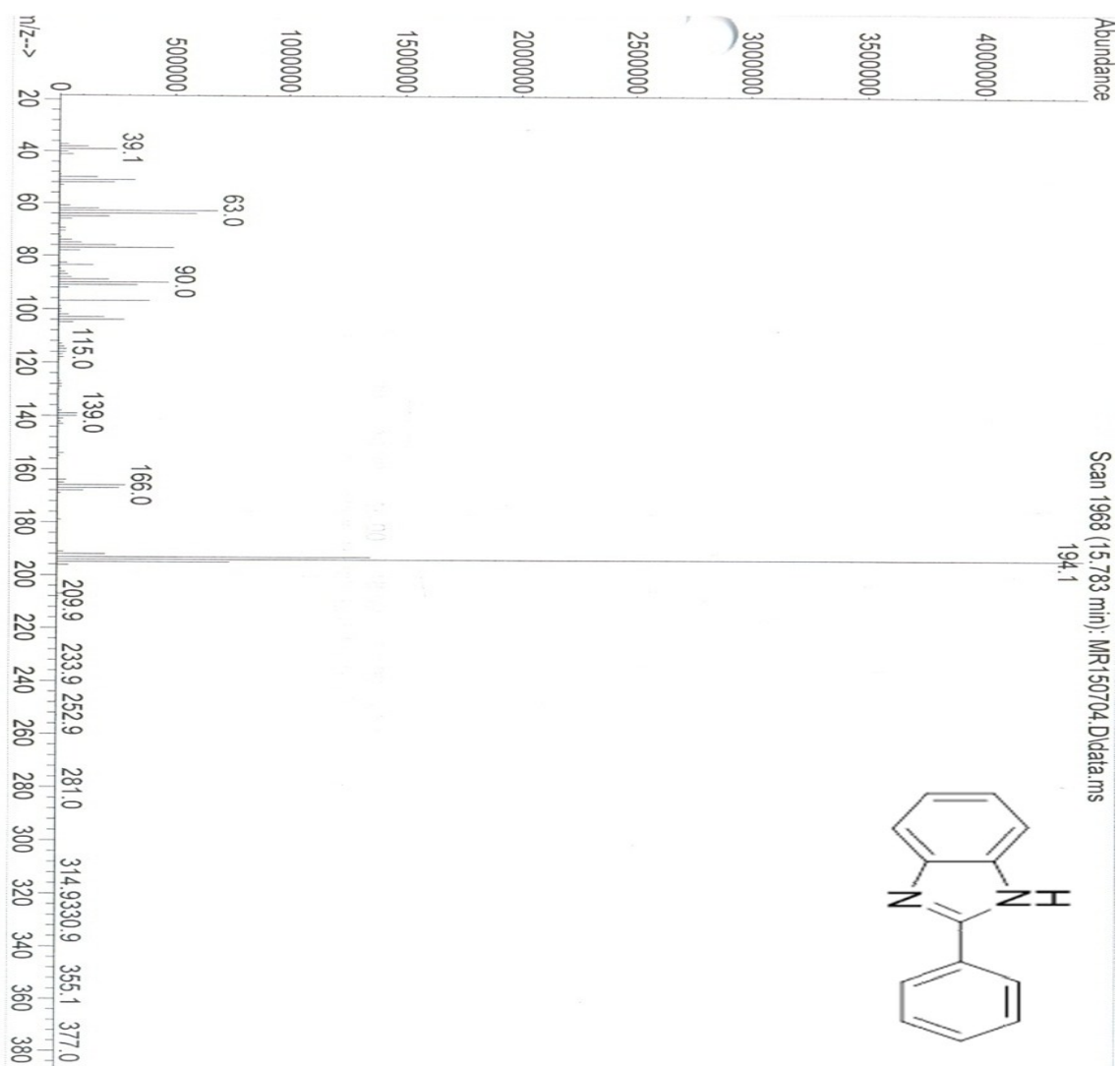
Compound **3b** ($^1\text{H-NMR}$, DMSO-d_6)

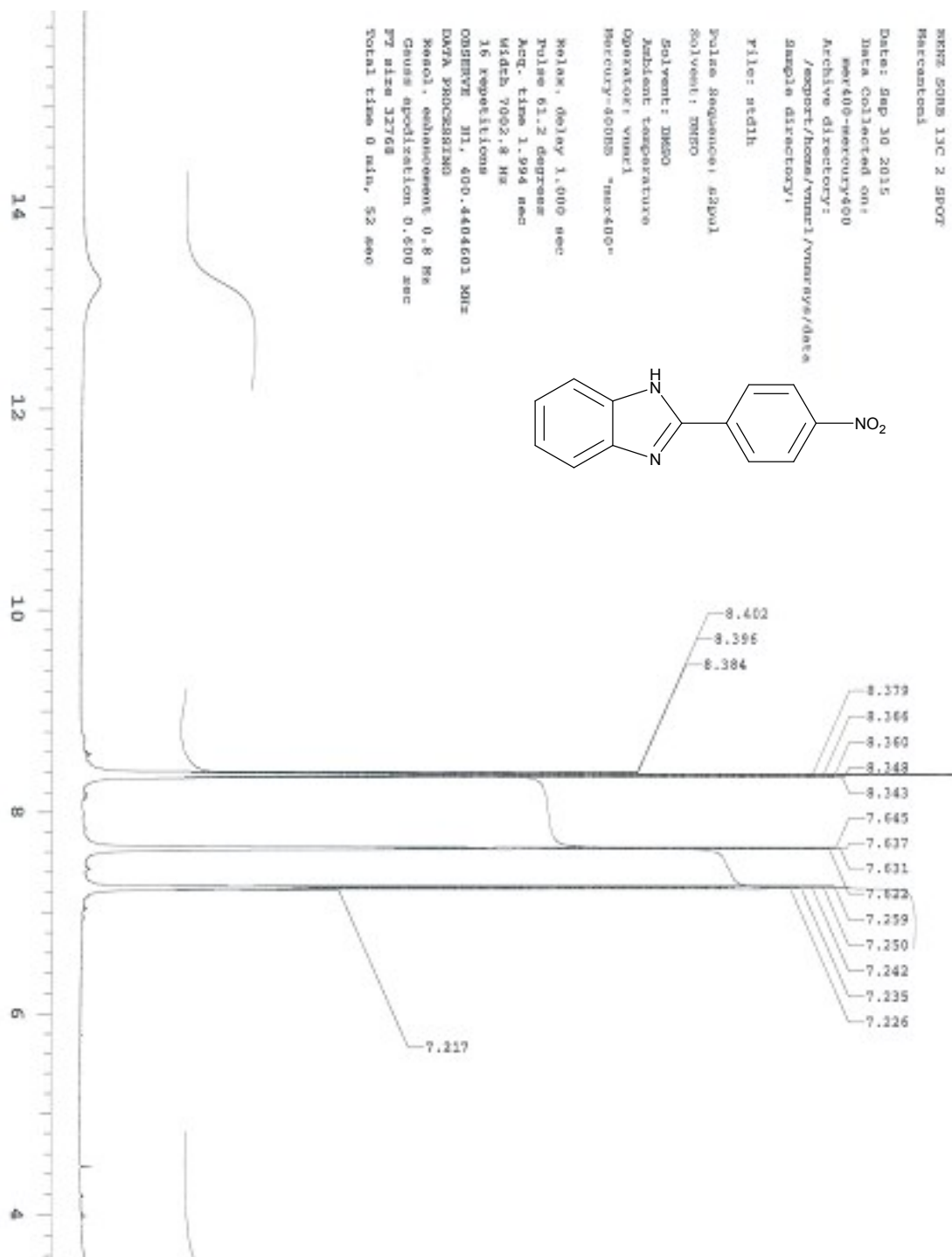


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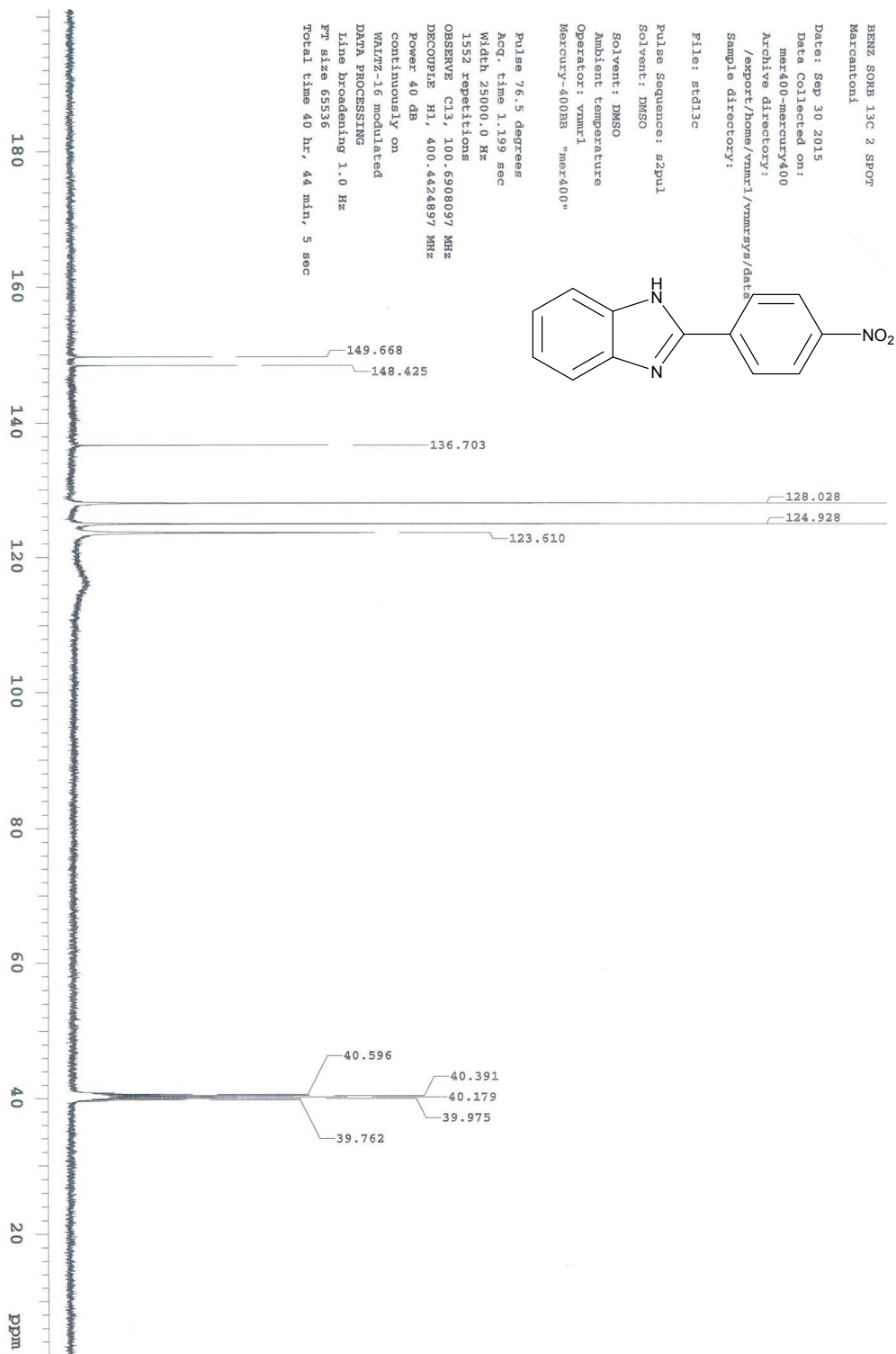


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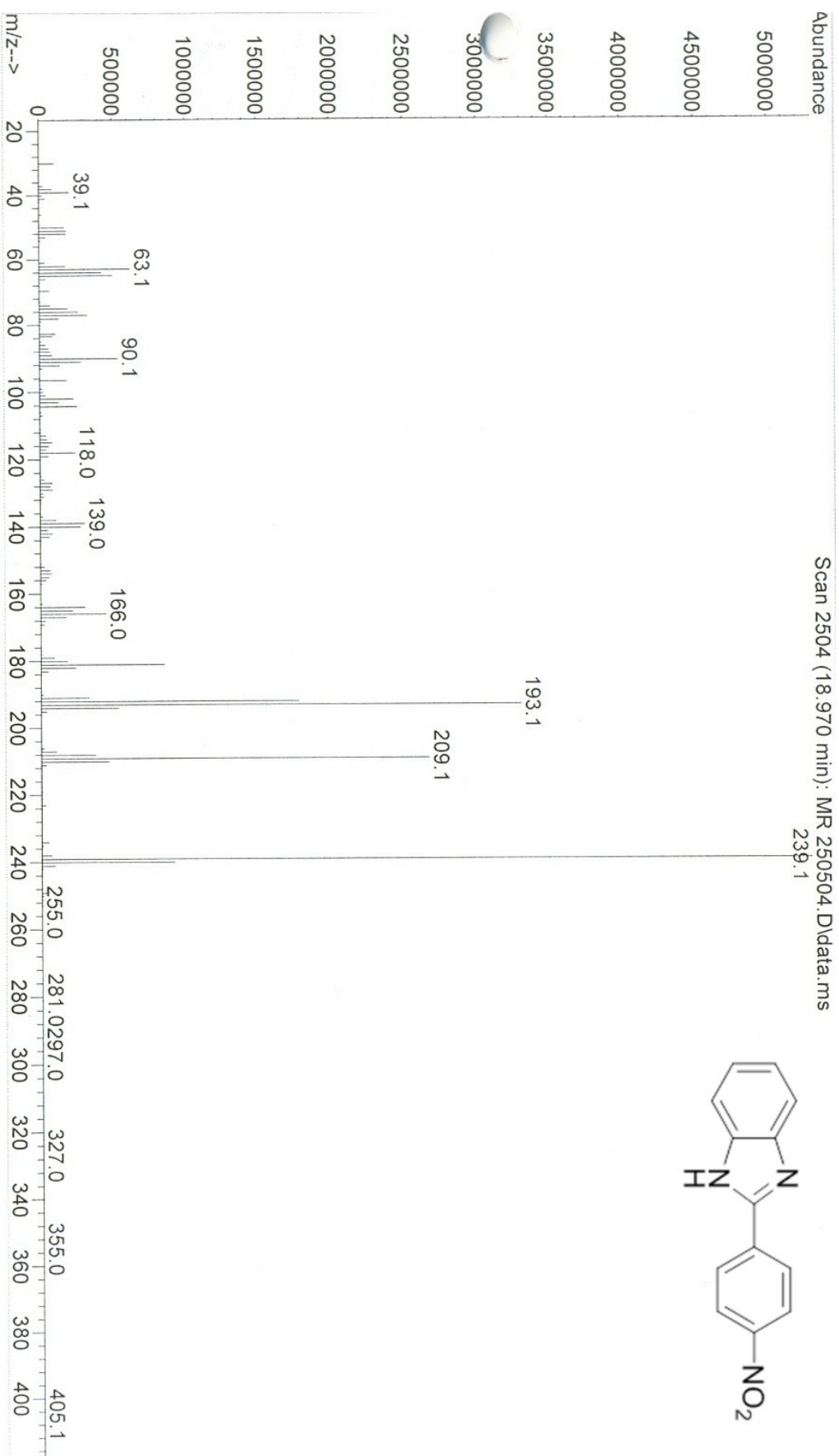


S8
Compound **3c** (^{13}C -NMR, DMSO- d_6)

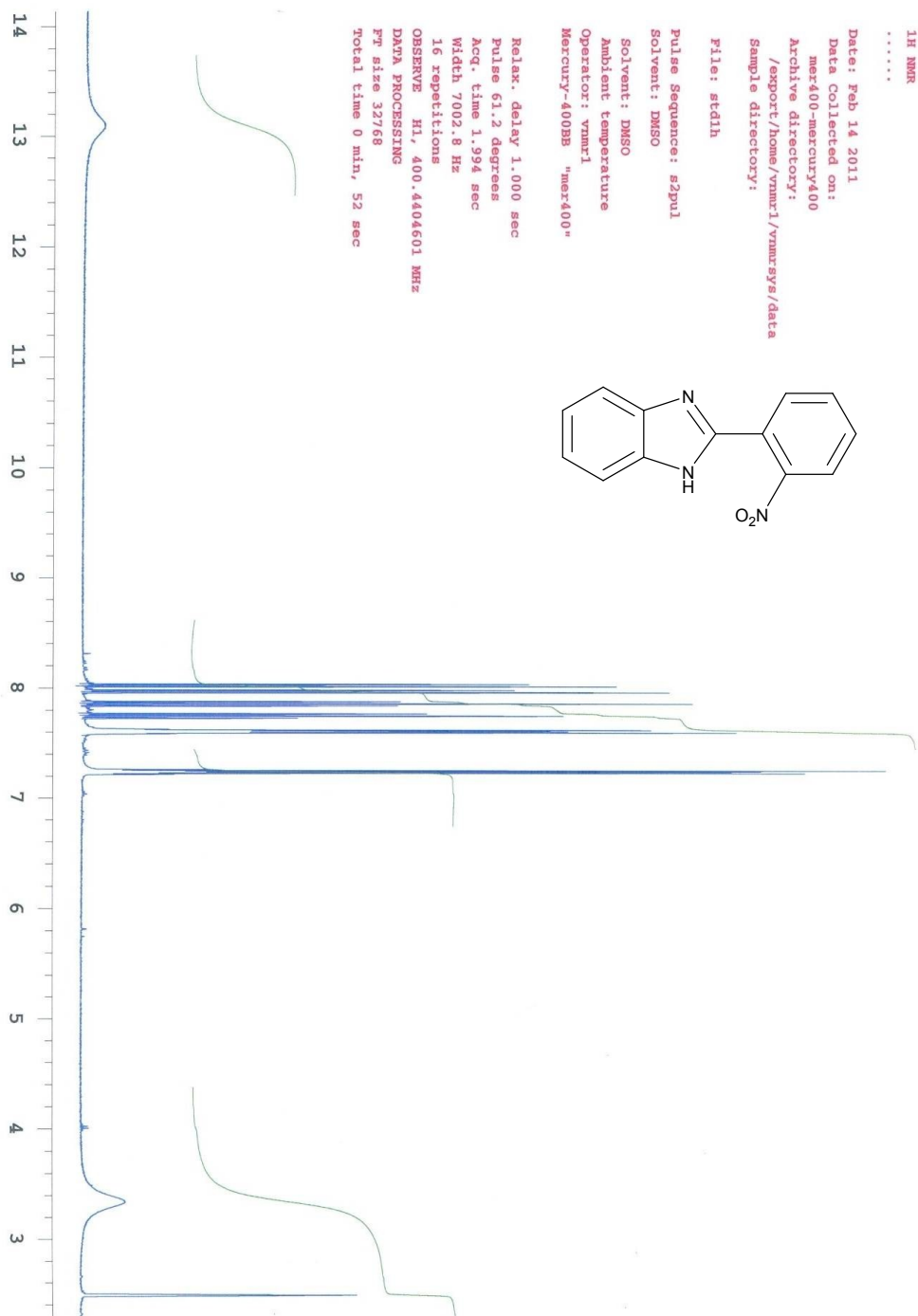


S9

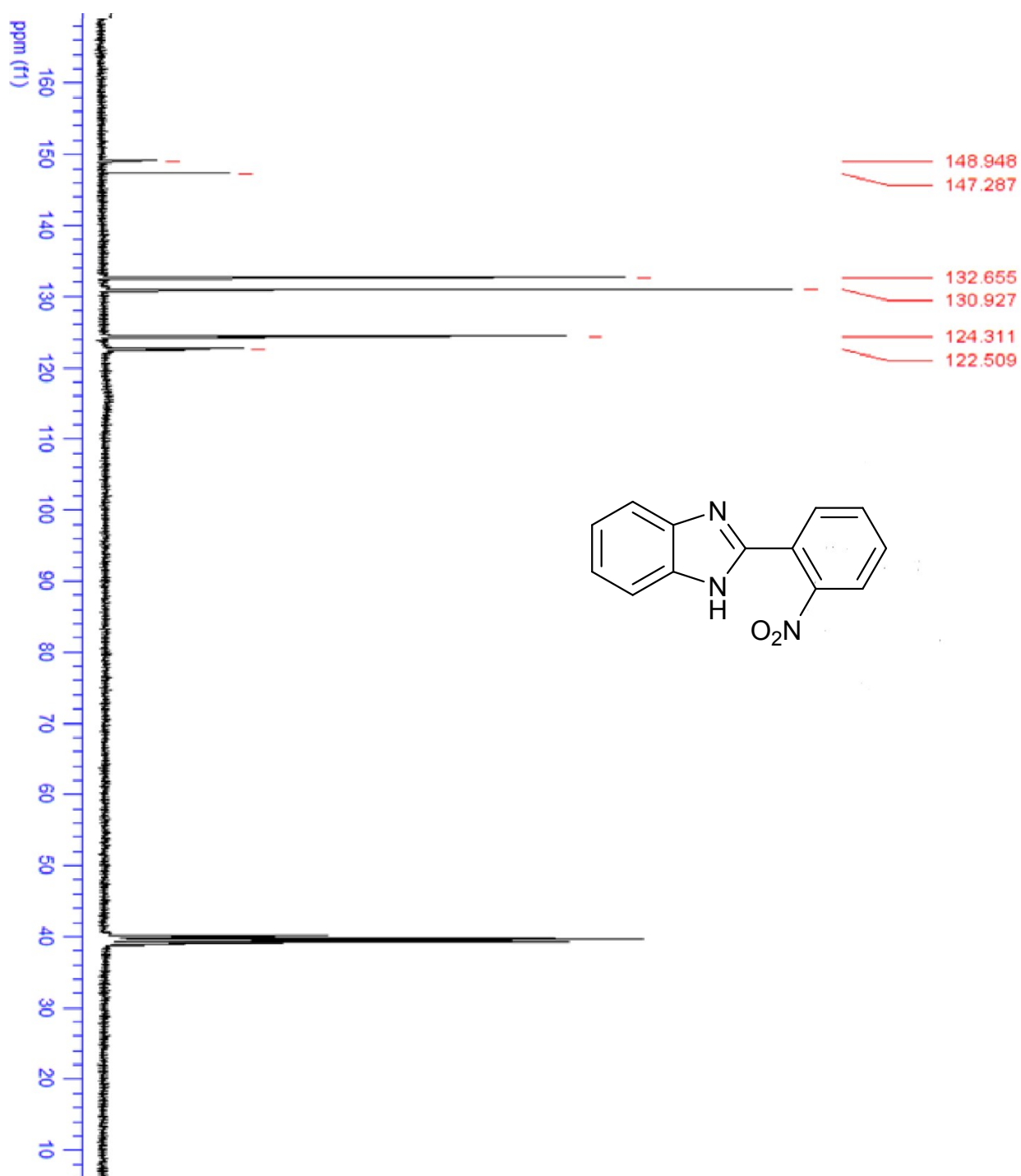
Compound **3c** (EI-MS)



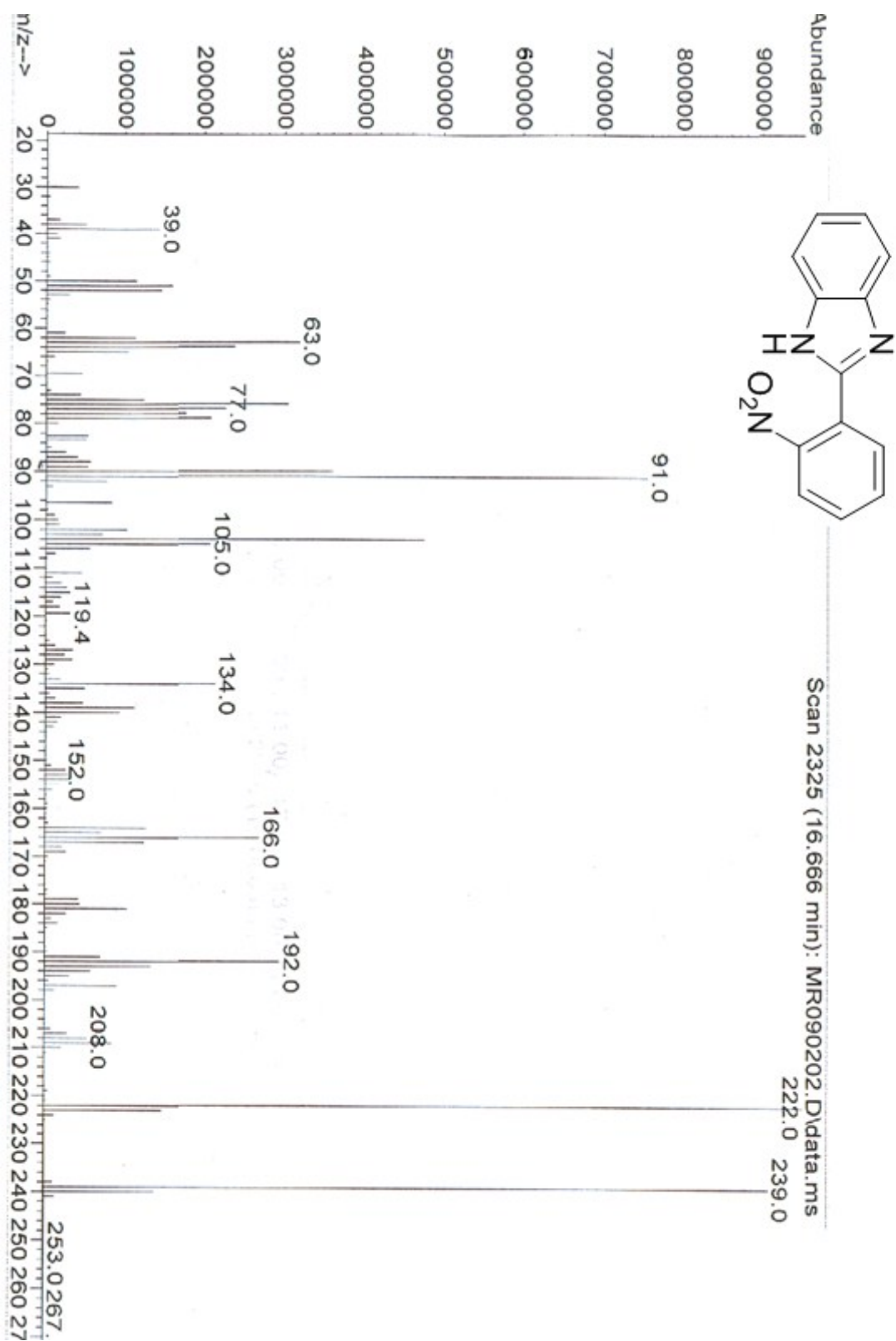
Compound **3d** (^1H -NMR, DMSO- d_6)



Compound **3d** (^{13}C -NMR, DMSO- d_6)



S12
Compound **3d** (EI-MS)



FS-41A
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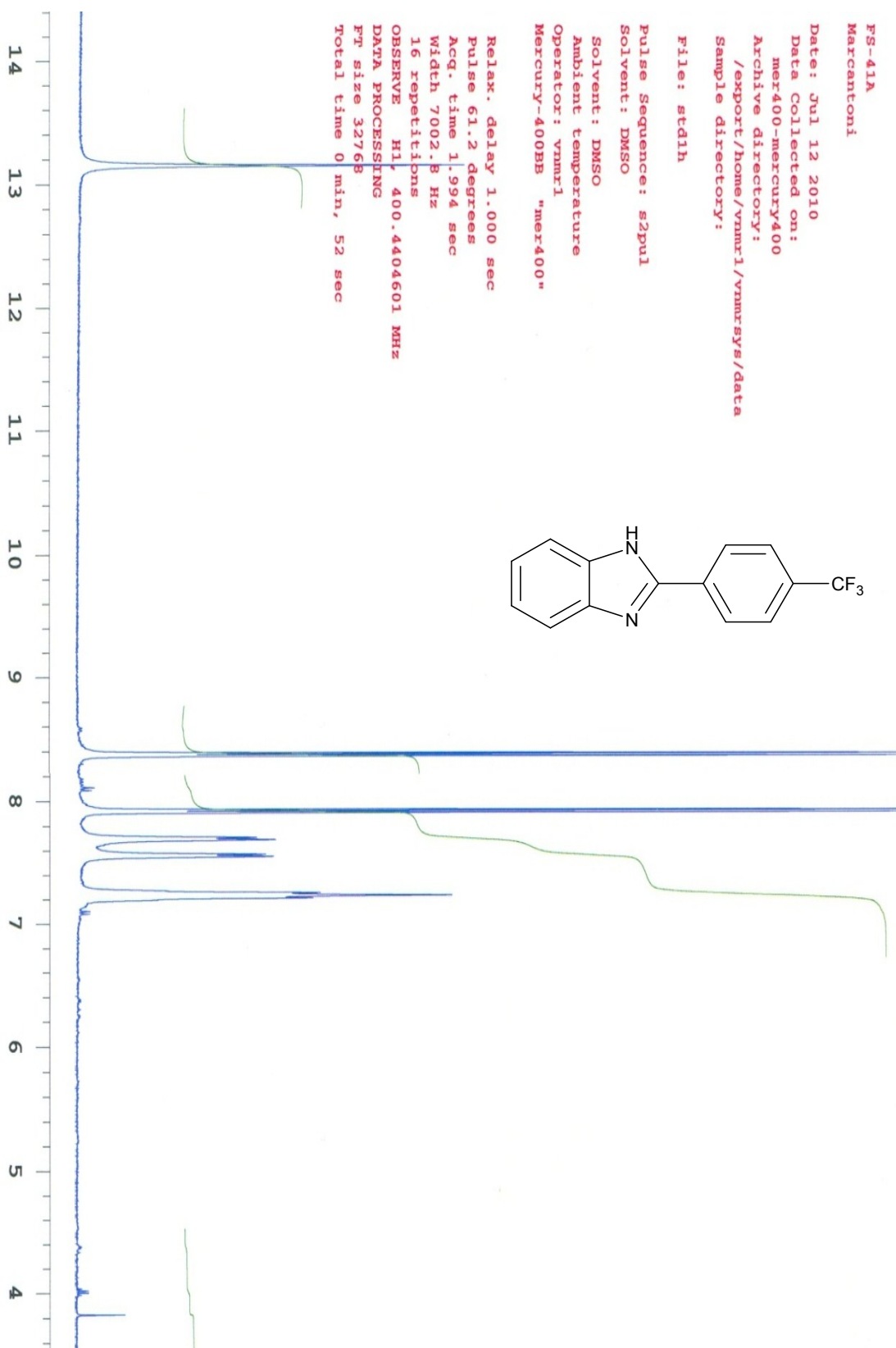
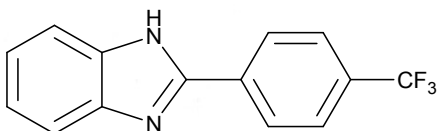
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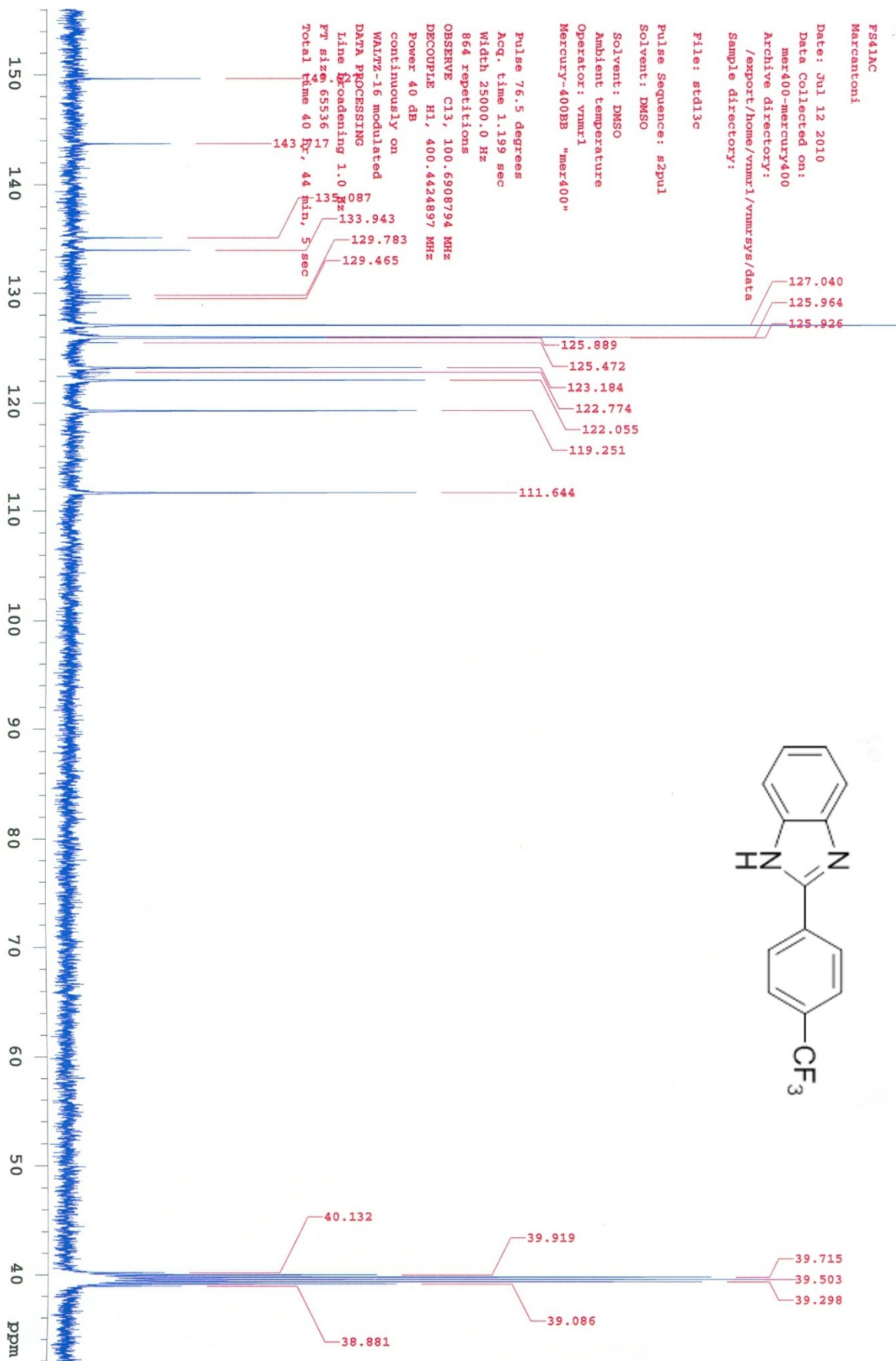
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Solvent: DMSO

Solvent: DMSO
Ambient temperature
Operator: vnmr1
Mercury-400BB "mer400"

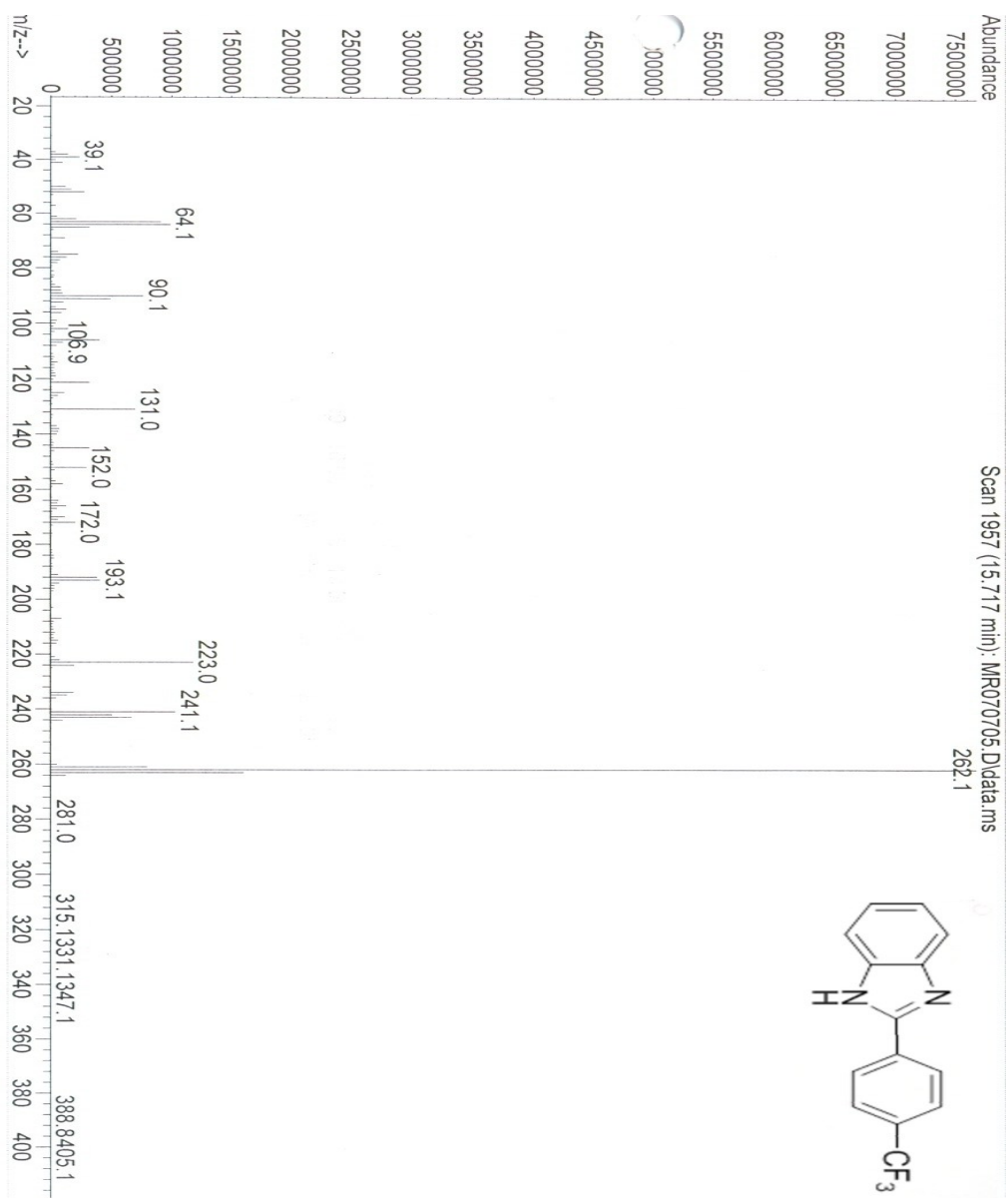
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16 repetitions
OBSERVE H1, 400.4404601 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 52 sec



S14
Compound **3e** (^{13}C -NMR, DMSO- d_6)



S15
Compound 3e (EI-MS)



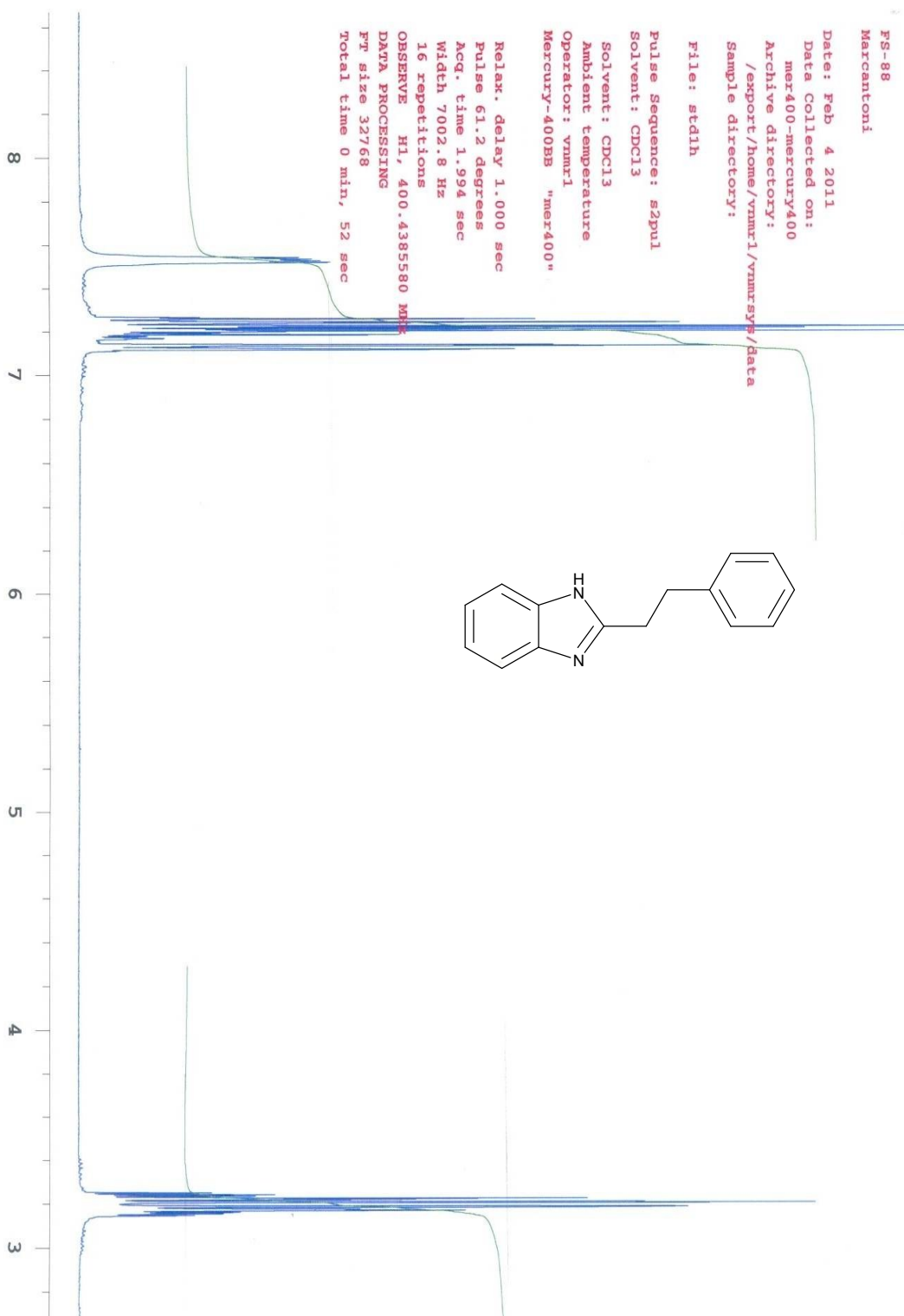
FS-88
Marcantoni

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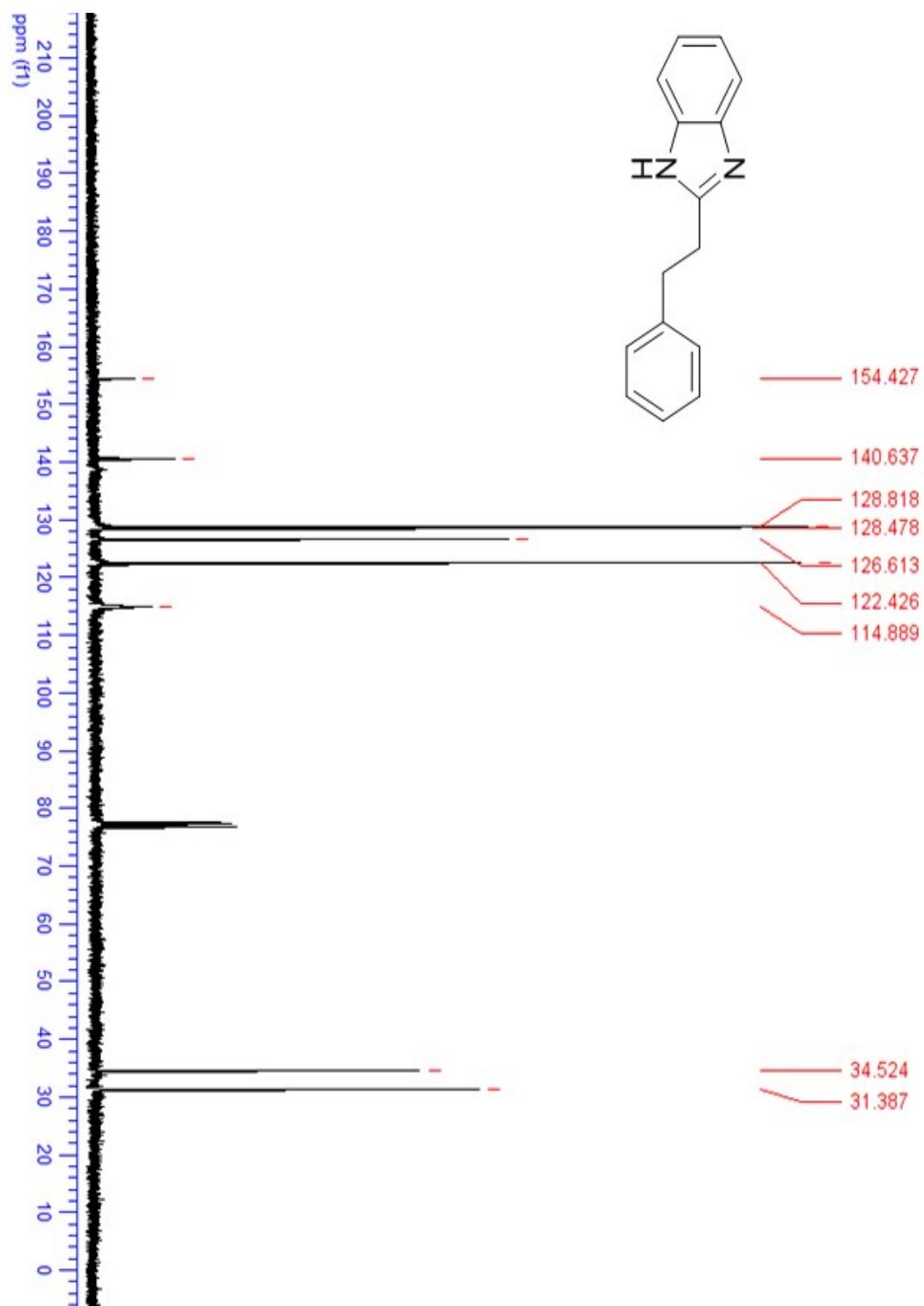
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Solvent: CDCl3
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Mercury-400BB "mer400"

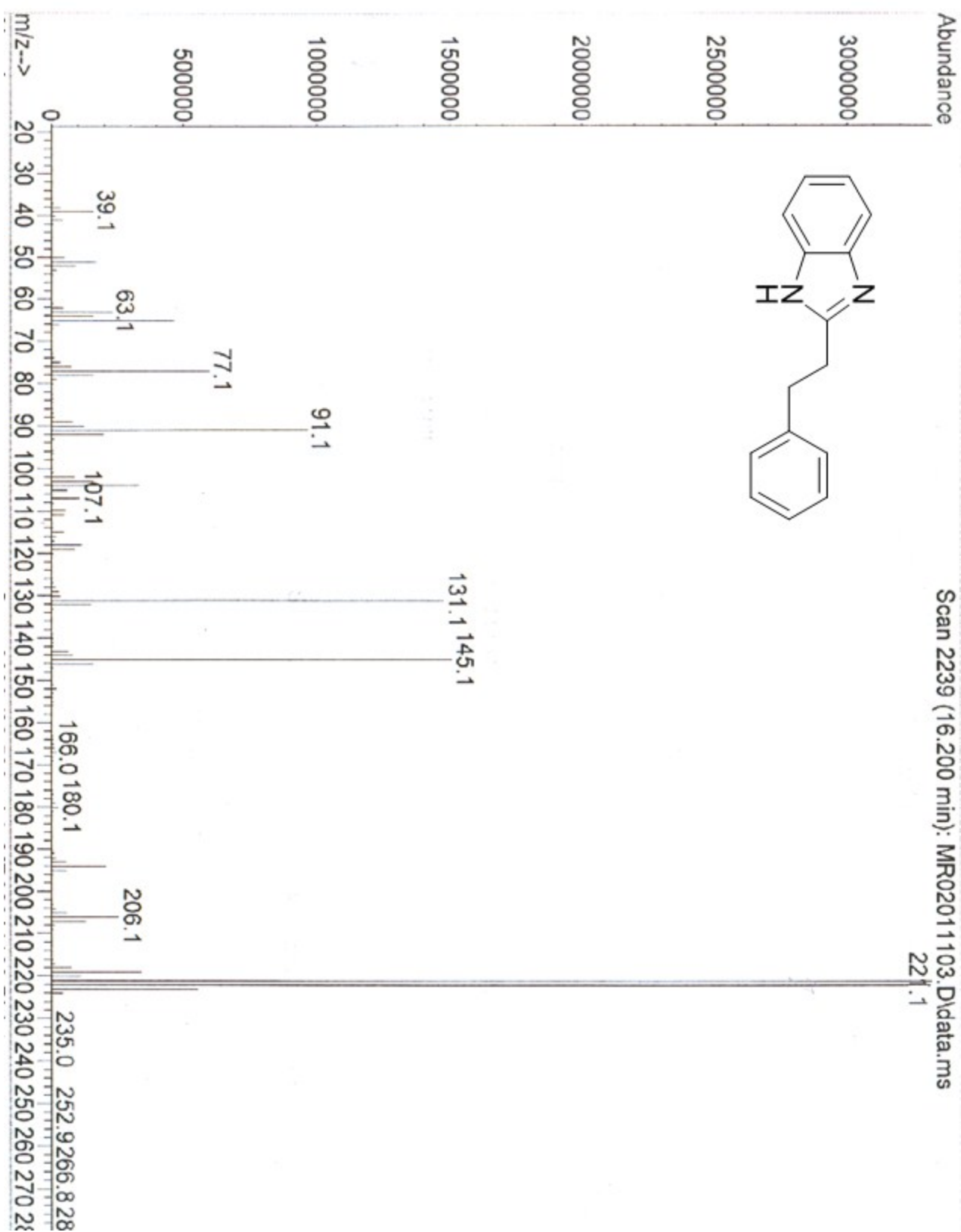
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DATA PROCESSING
F1 size 32768
Total time 0 min, 52 sec



S17
Compound **3f** (^{13}C -NMR, CDCl_3)



S18
Compound **3f** (EI-MS)



S19
Compound **3g** ($^1\text{H-NMR}$, CDCl_3)

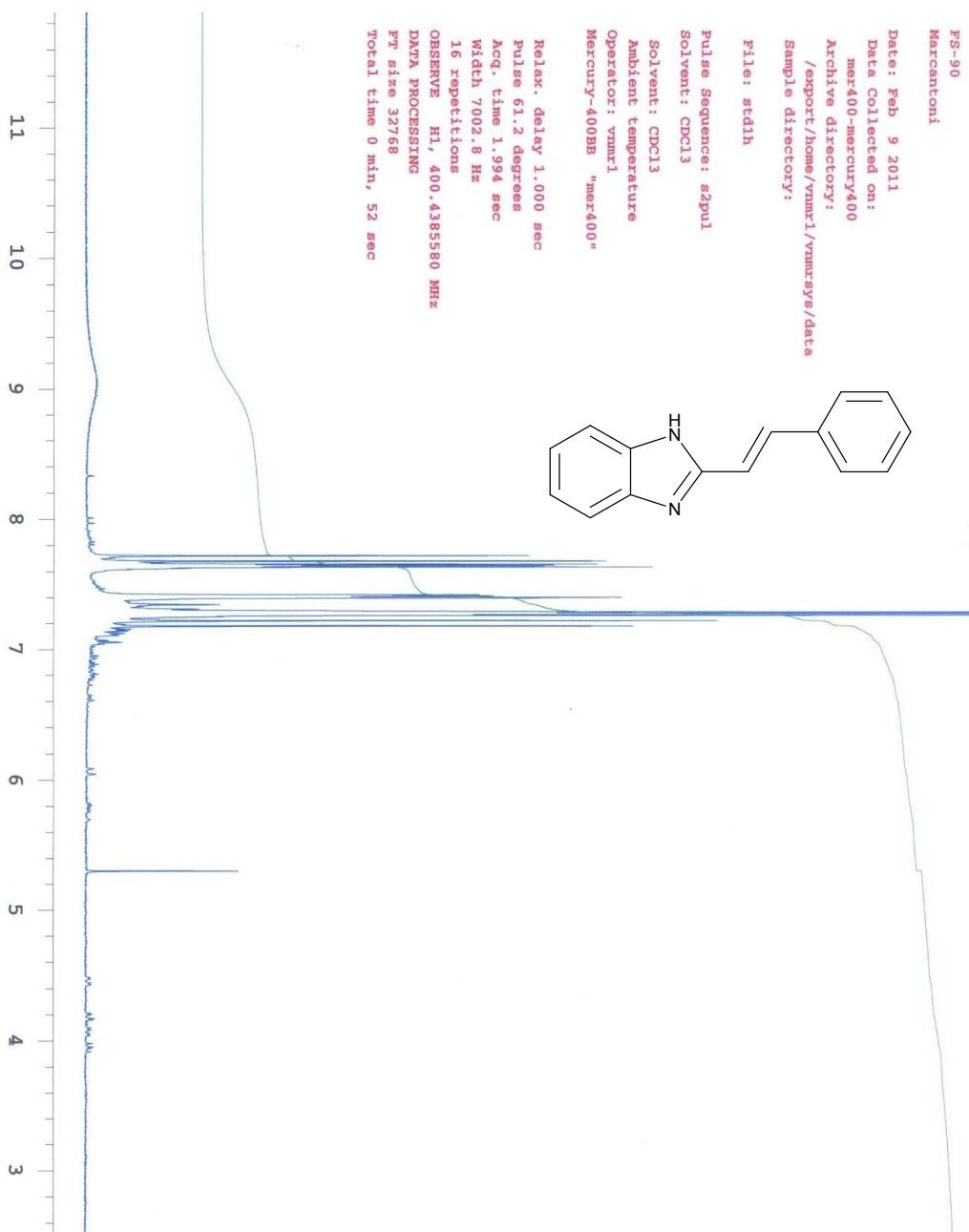
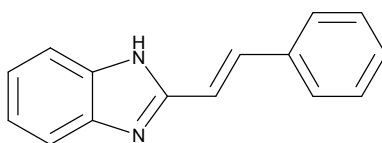
FS-90
Marcantonio

Date: Feb 9 2011
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Sample directory:

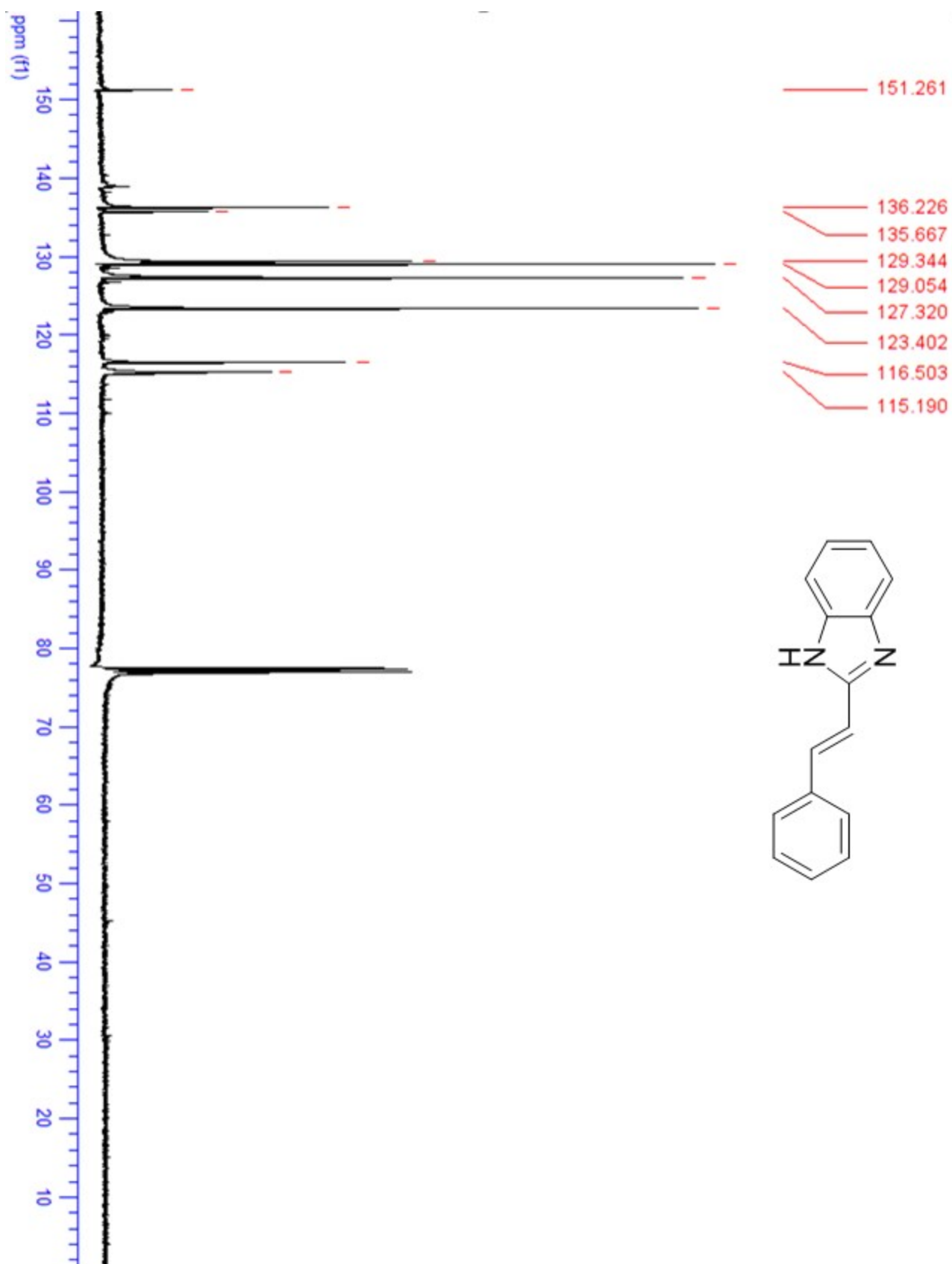
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Solvent: CDCl3
Solvent: CDCl3
Ambient temperature
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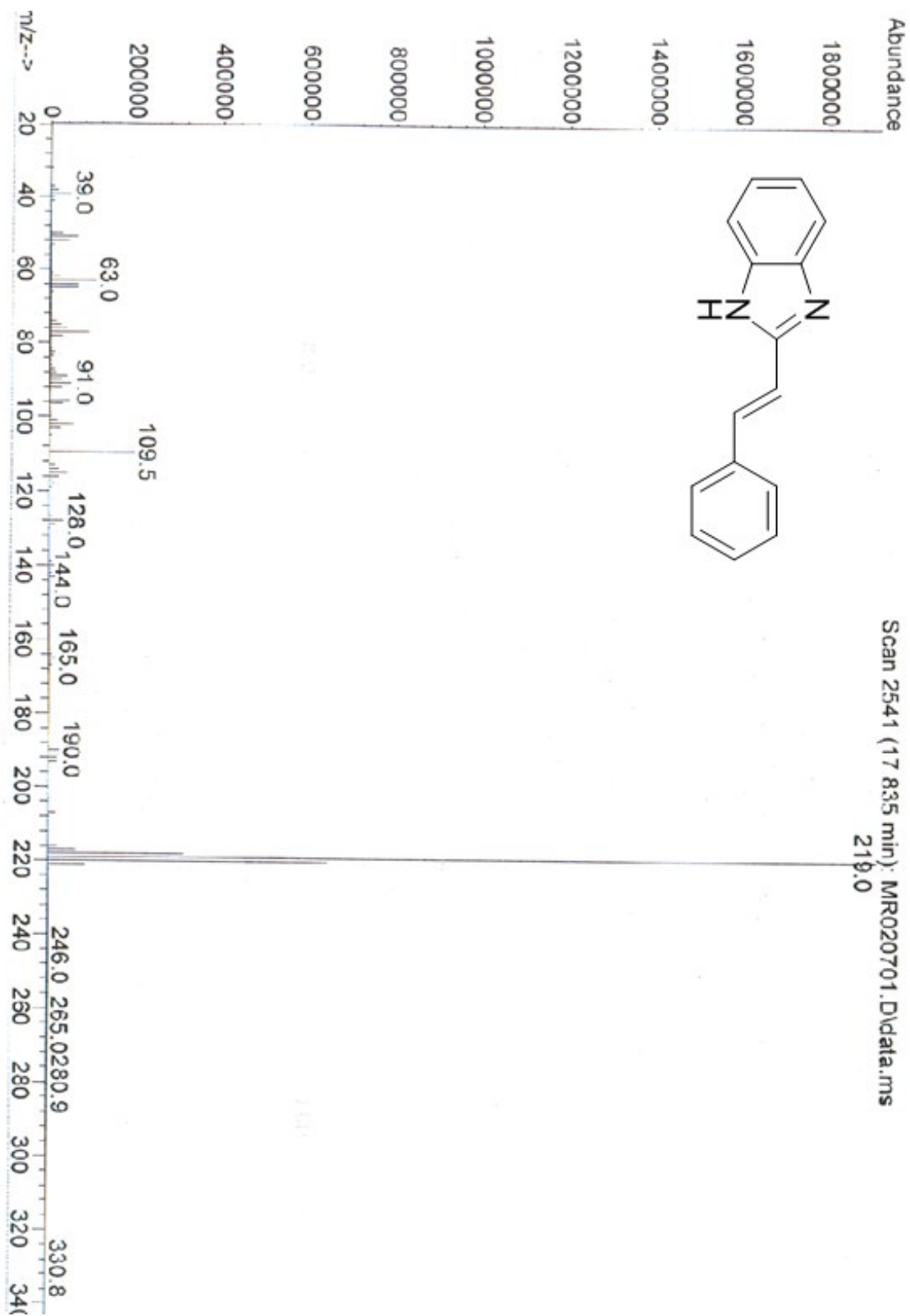
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DATA PROCESSING
FT size 32768
Total time 0 min, 52 sec



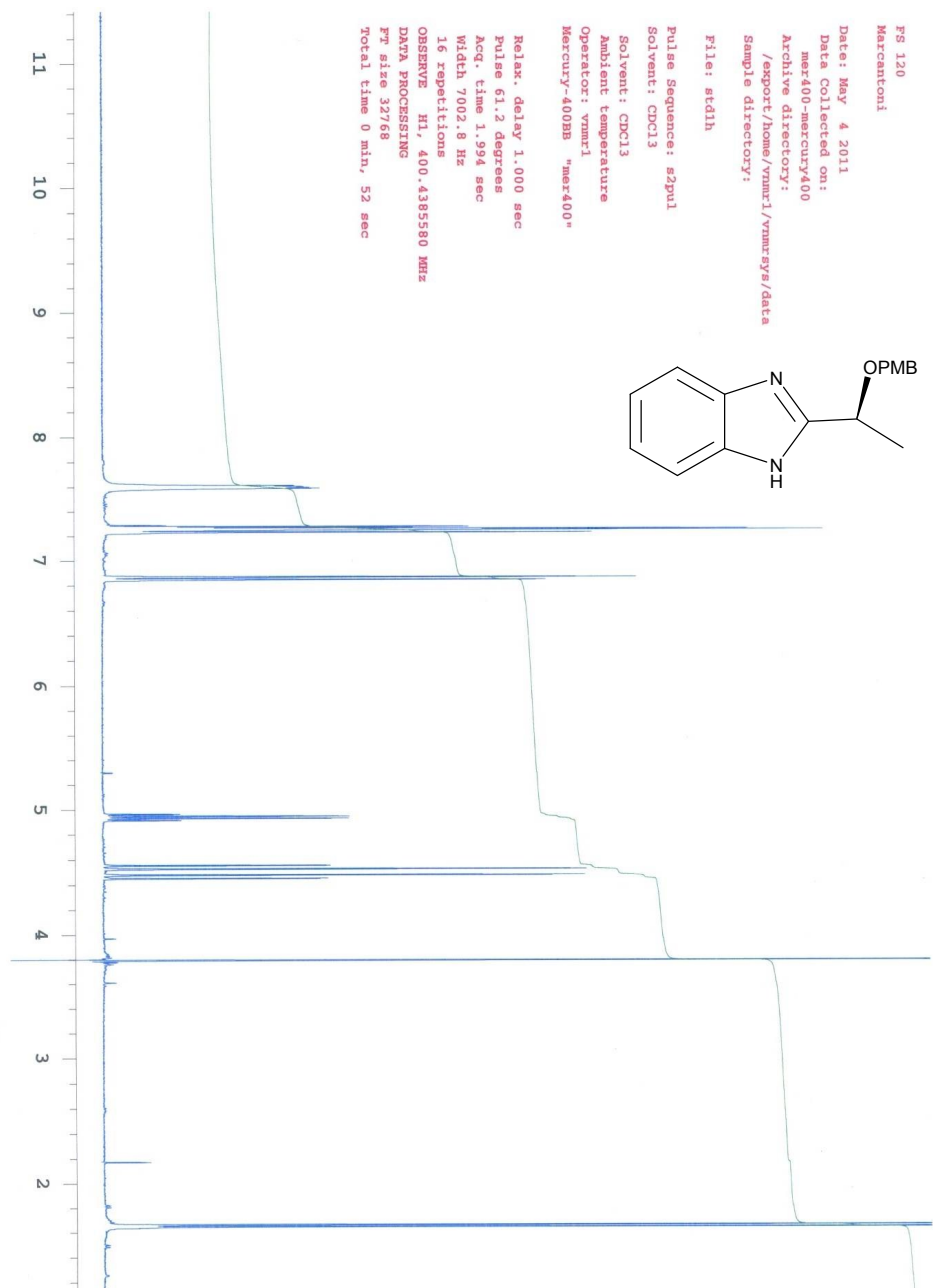
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Compound **3g** (¹³C-NMR, CDCl₃)



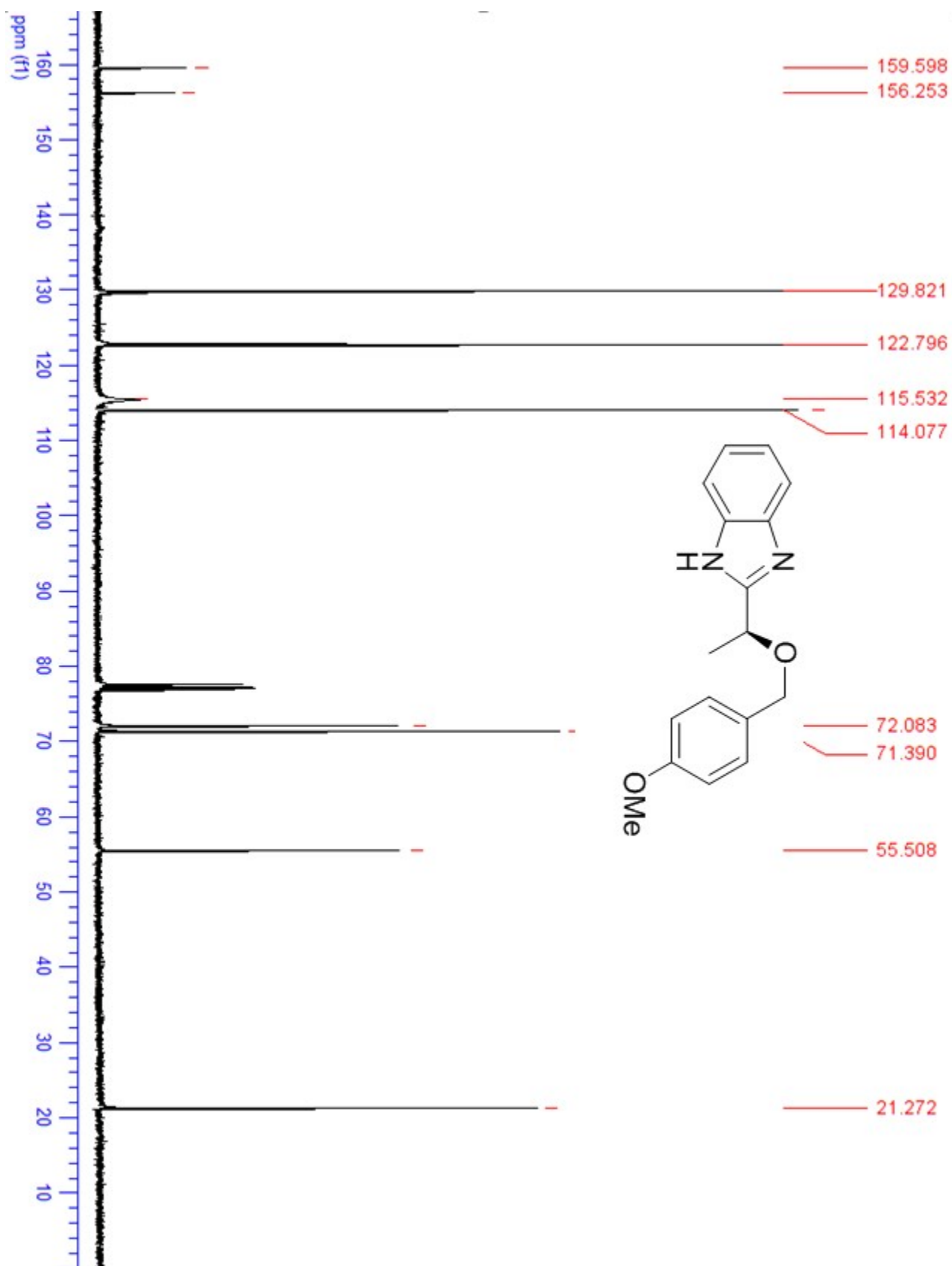
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Compound **3g** (EI-MS)

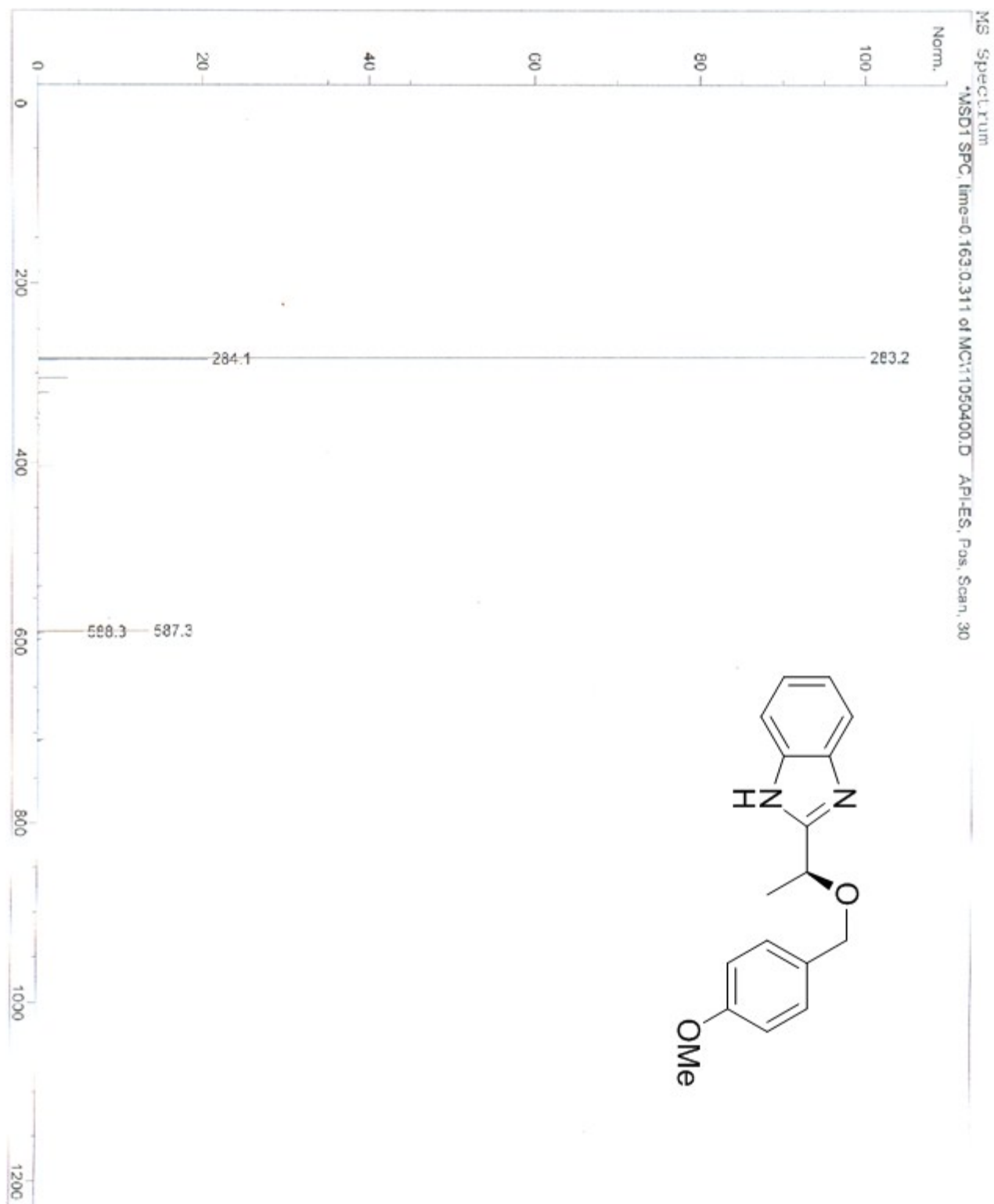


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Compound **3h** ($^1\text{H-NMR}$, CDCl_3)

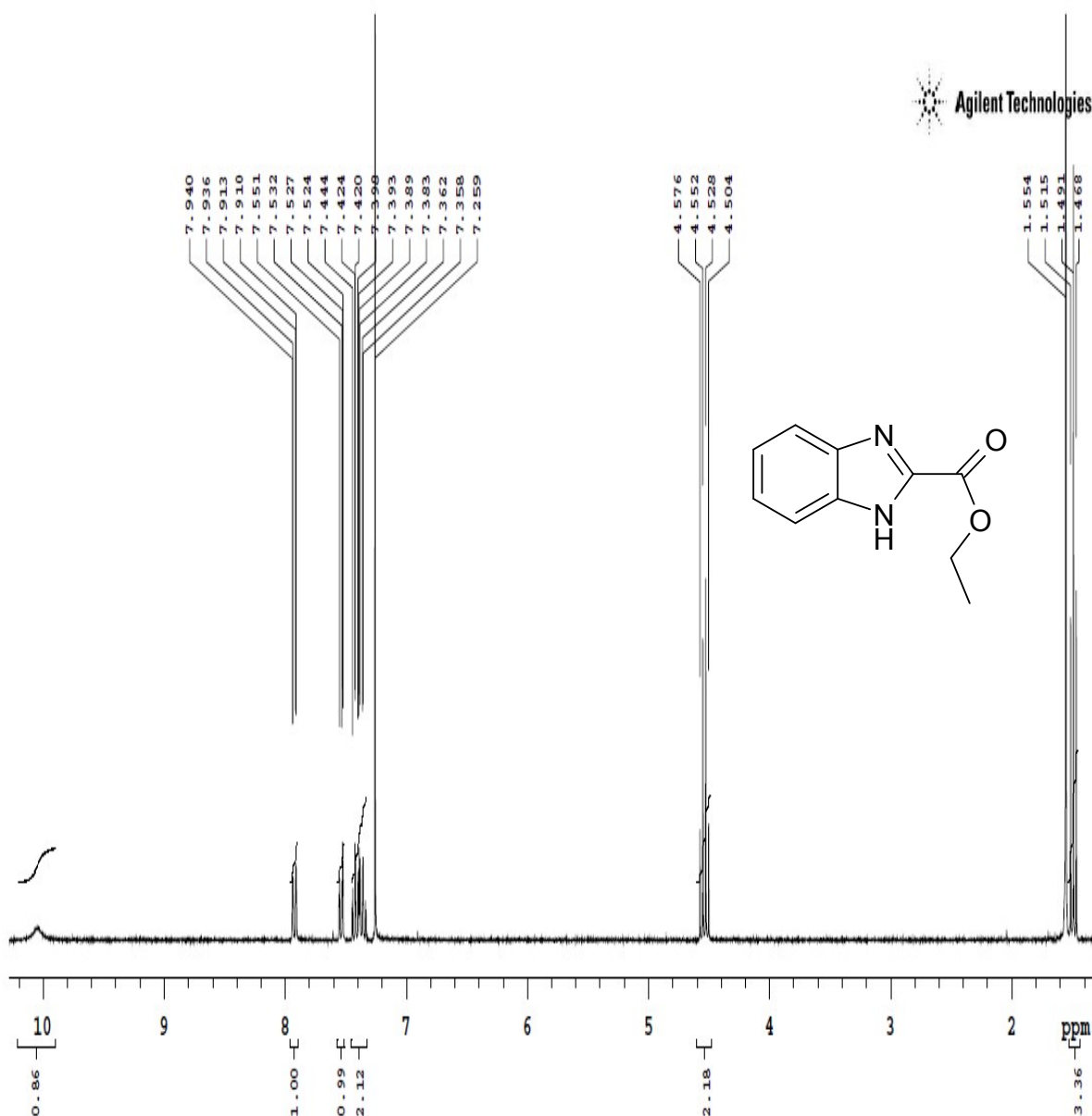


S23
Compound **3h** (^{13}C -NMR, CDCl_3)



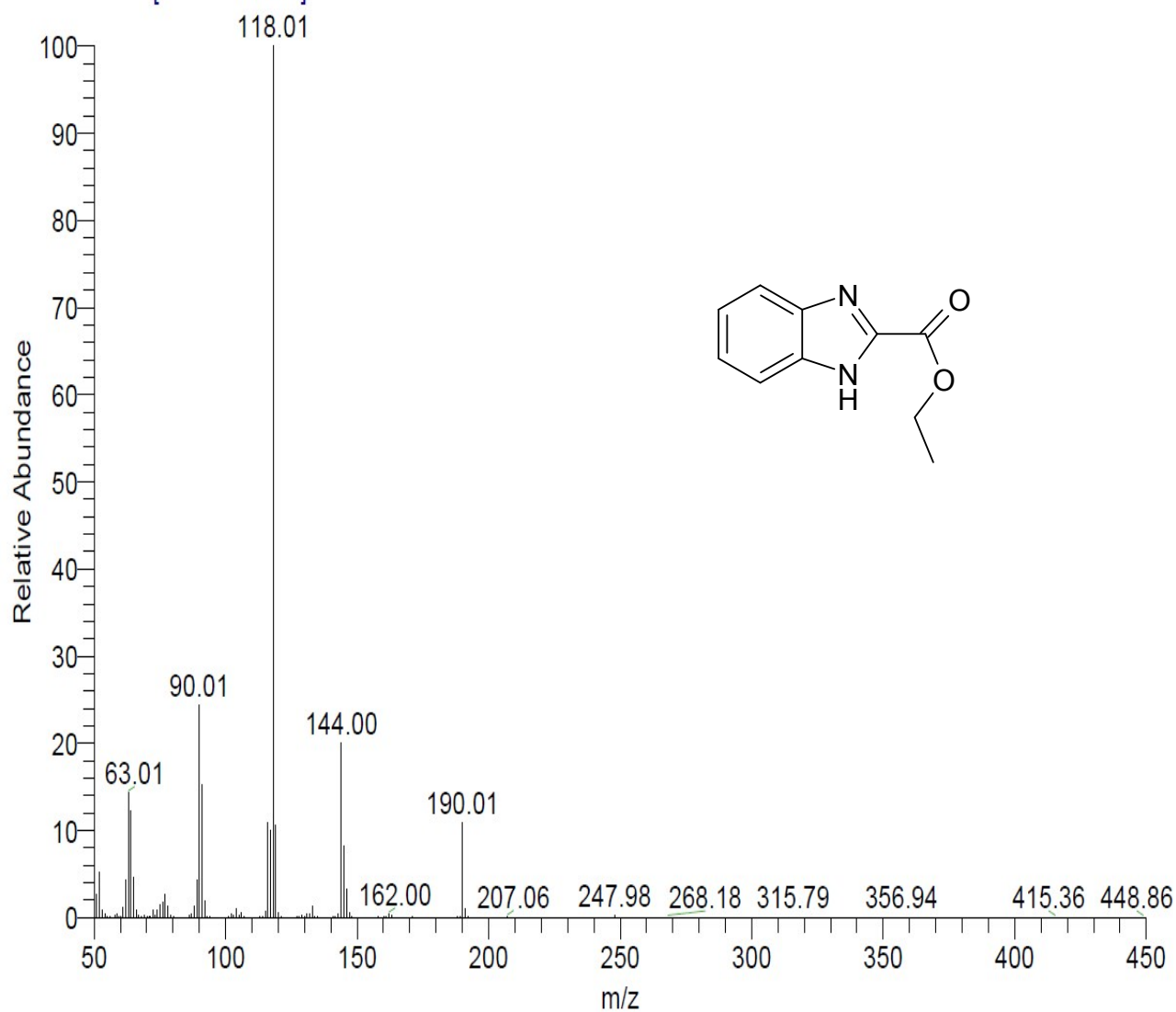


S25
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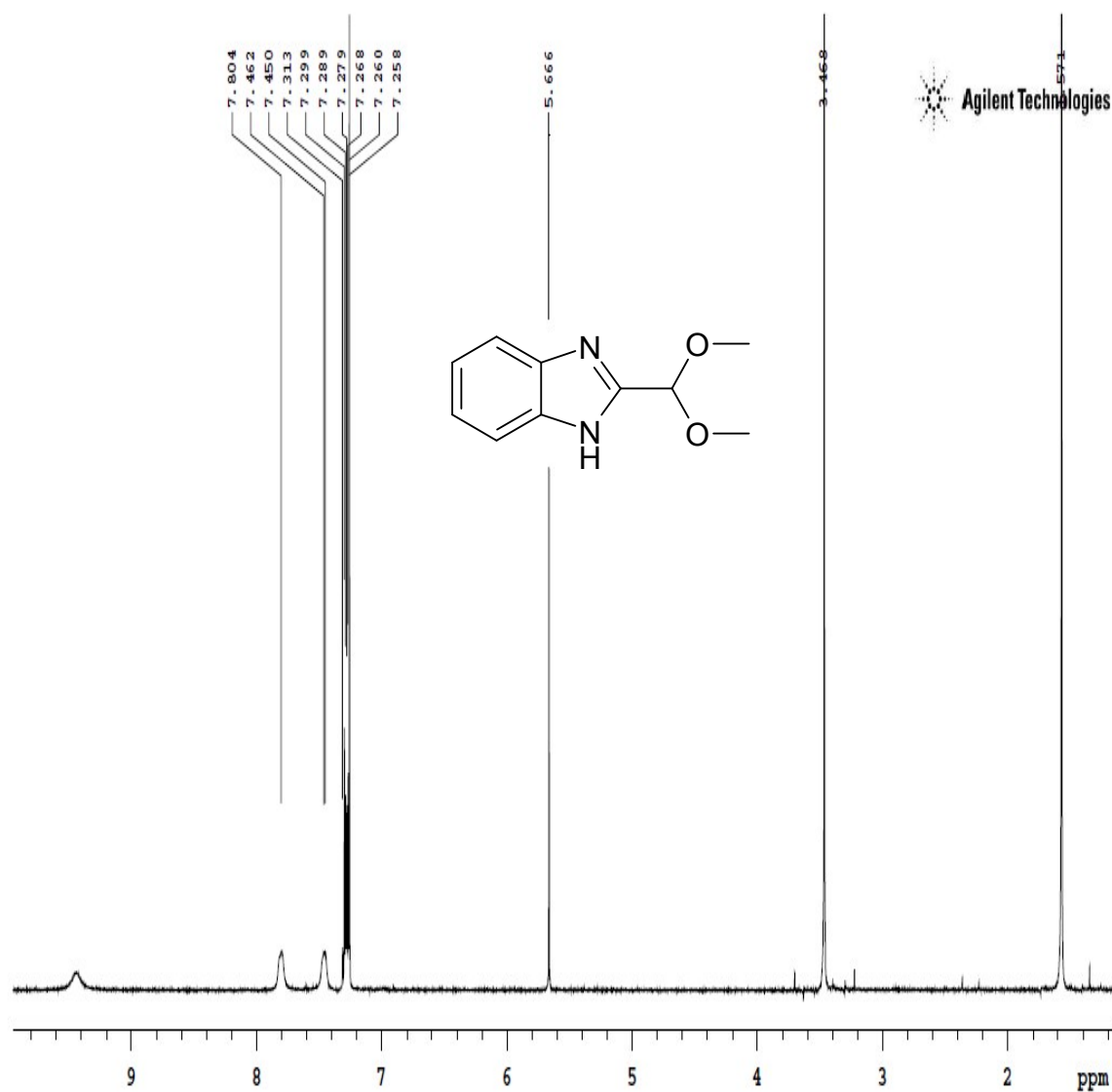


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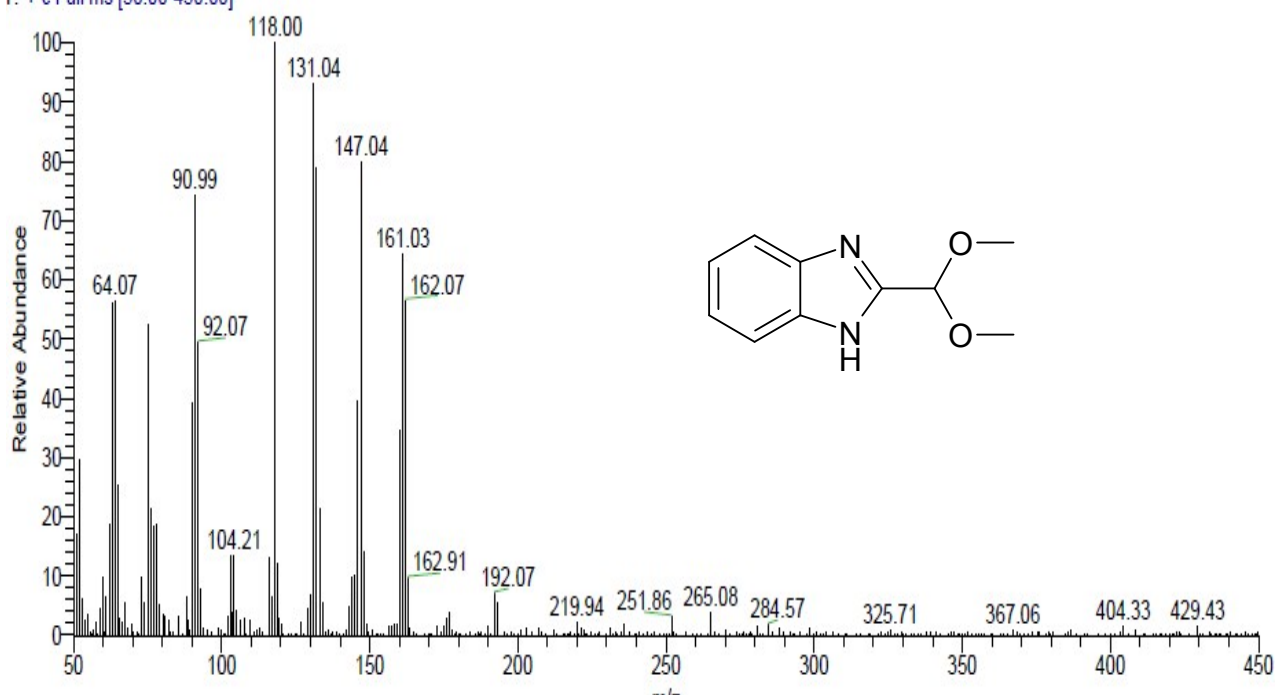


S27
Compound **3j** (^1H -NMR, CDCl_3)



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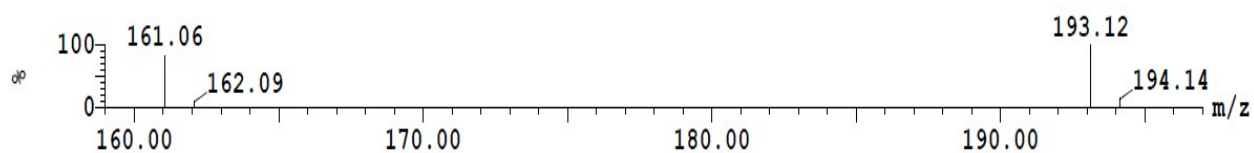


Peak ID Compound Time Mass Found

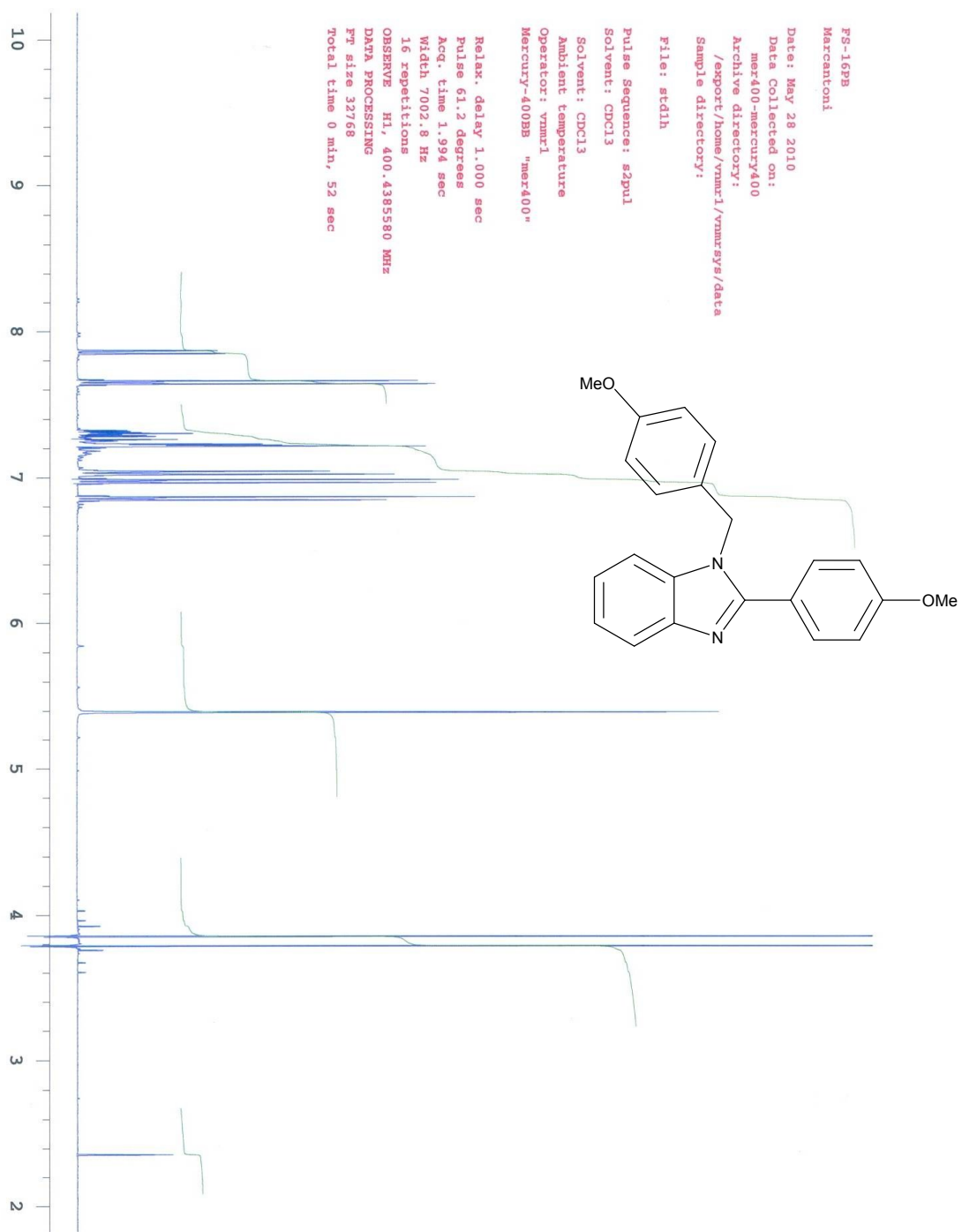
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SAMPLE: 1:41 Combine (80:82-(76:77+88:89))

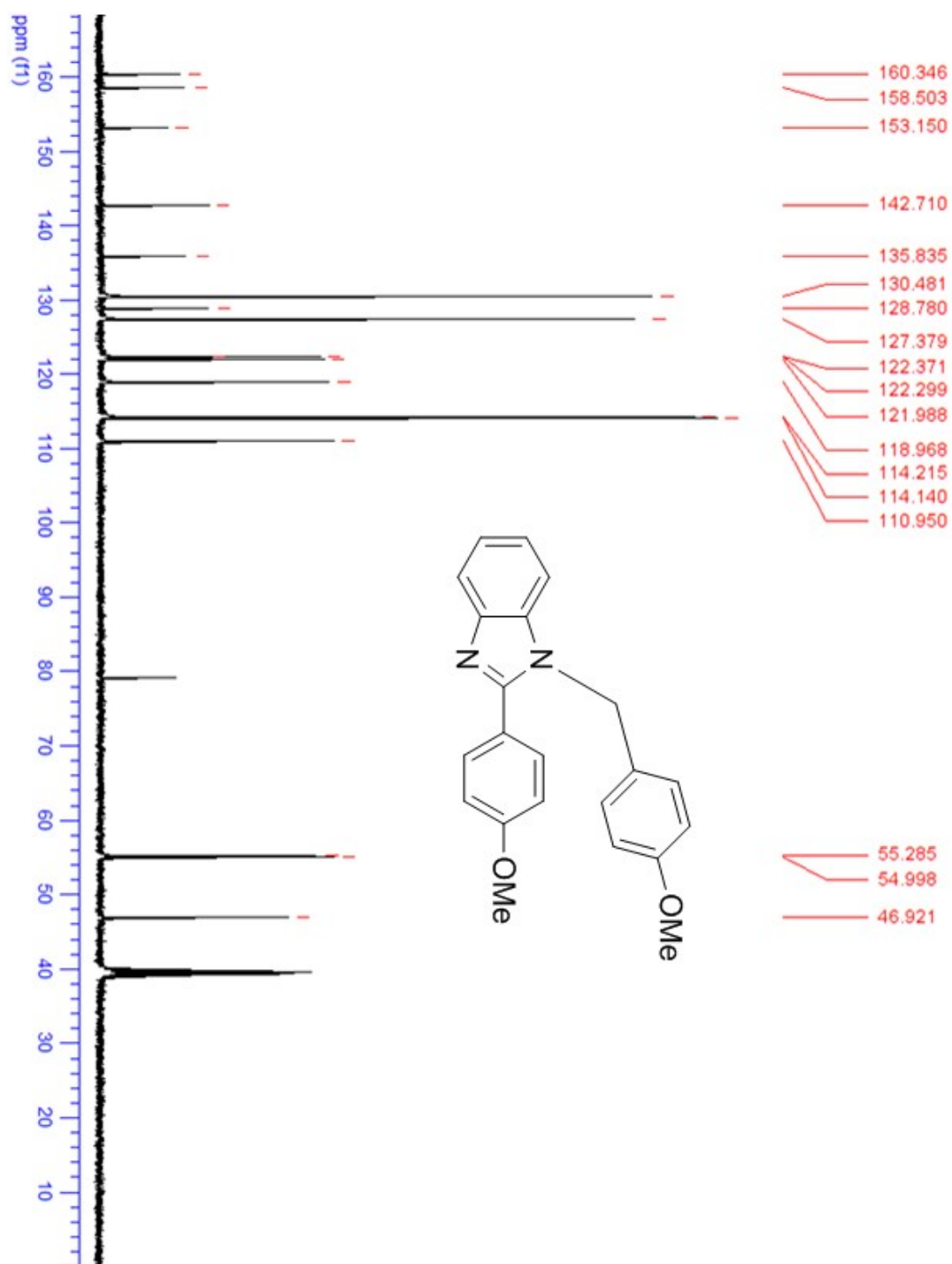
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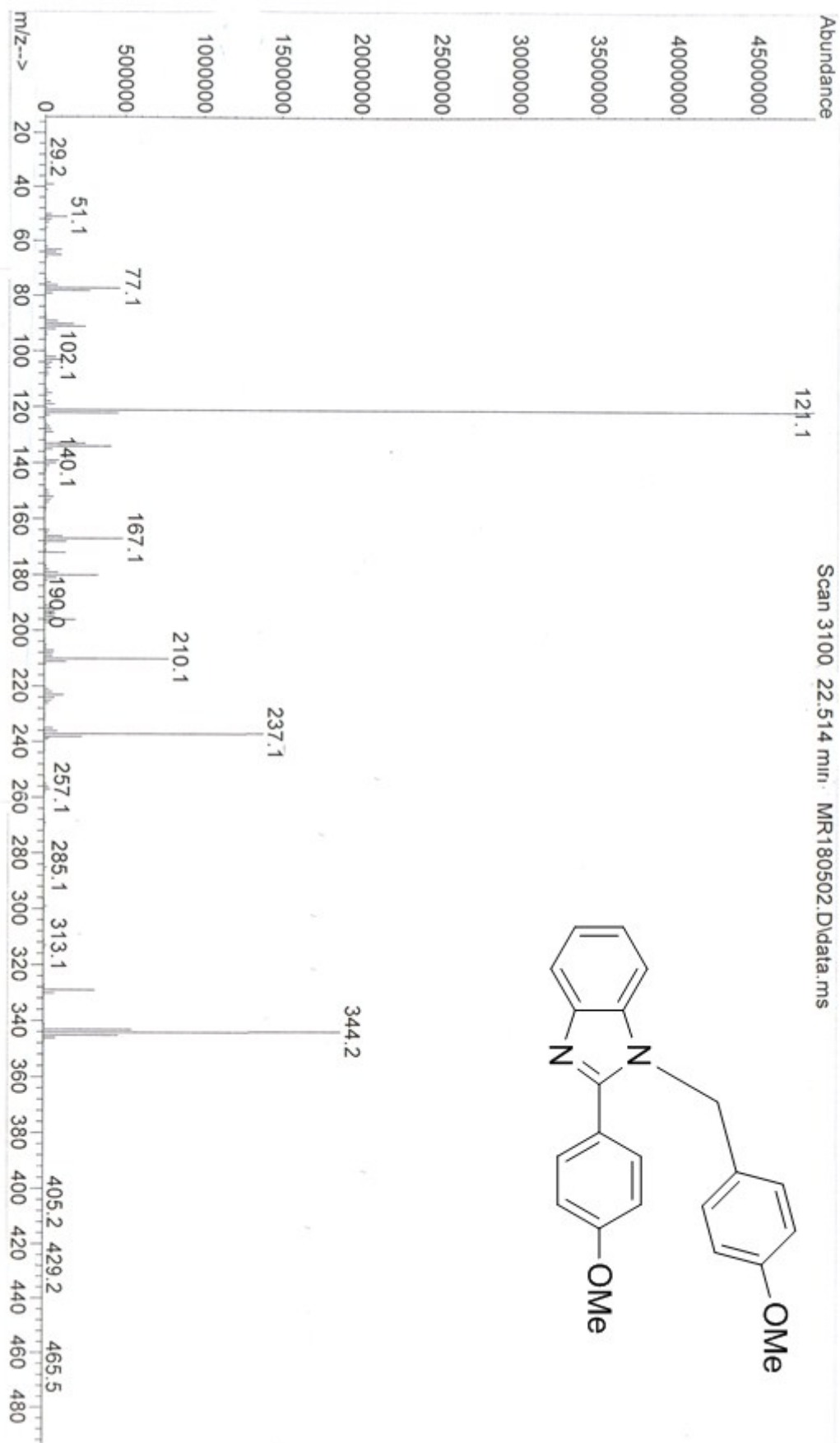


S29
Compound **4a** ($^1\text{H-NMR}$, CDCl_3)

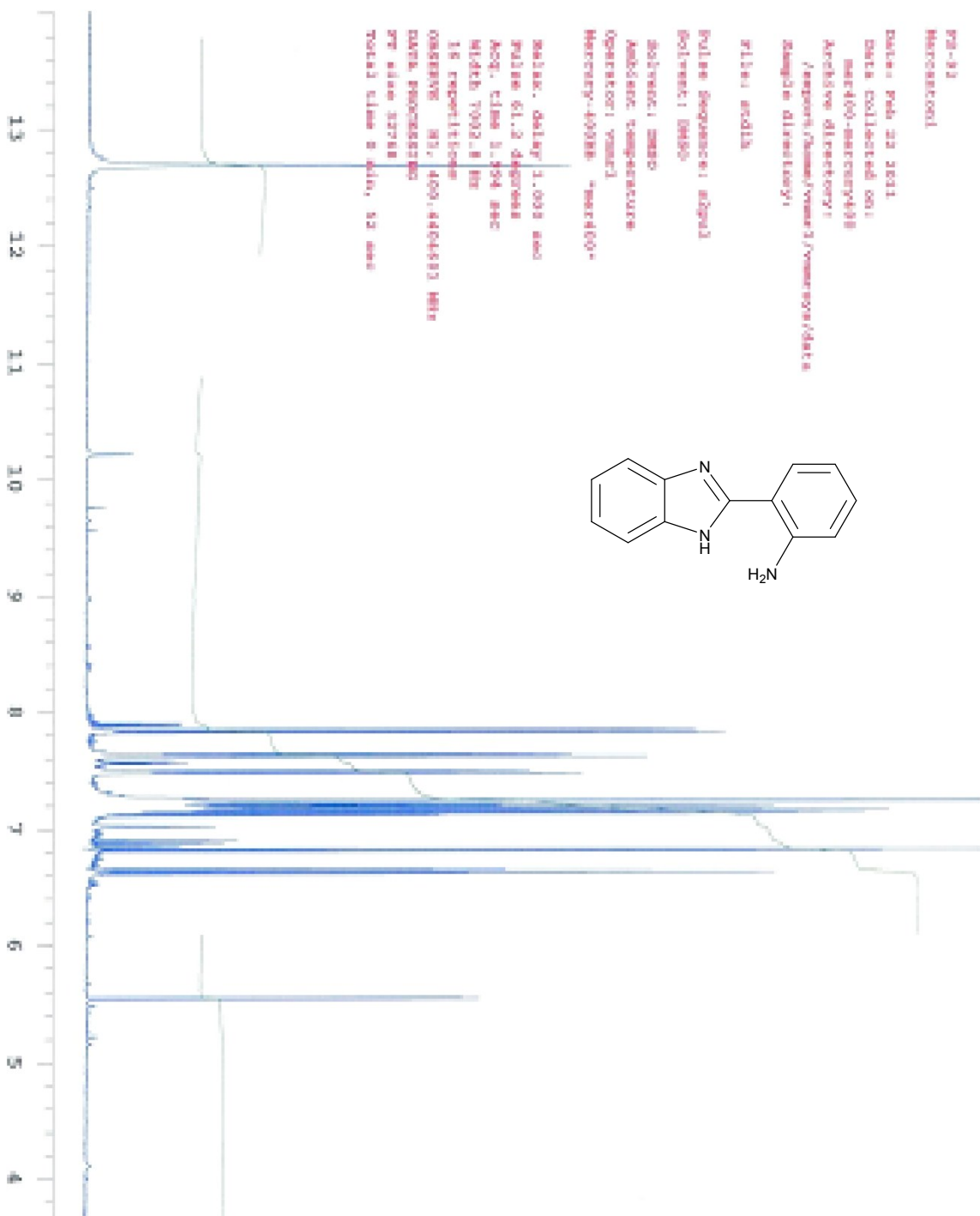


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 Compound **4a** (^{13}C -NMR, DMSO- d_6)

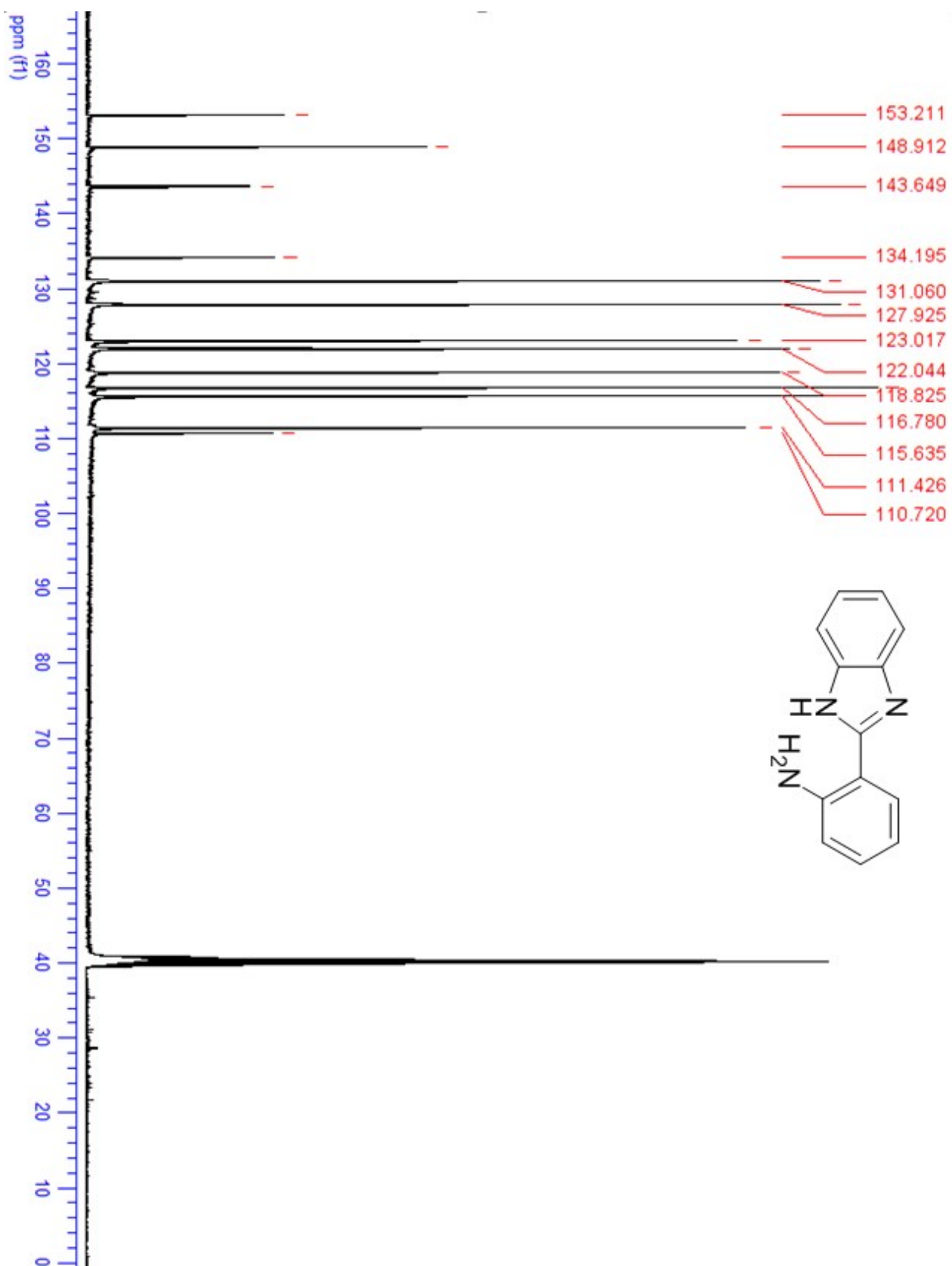


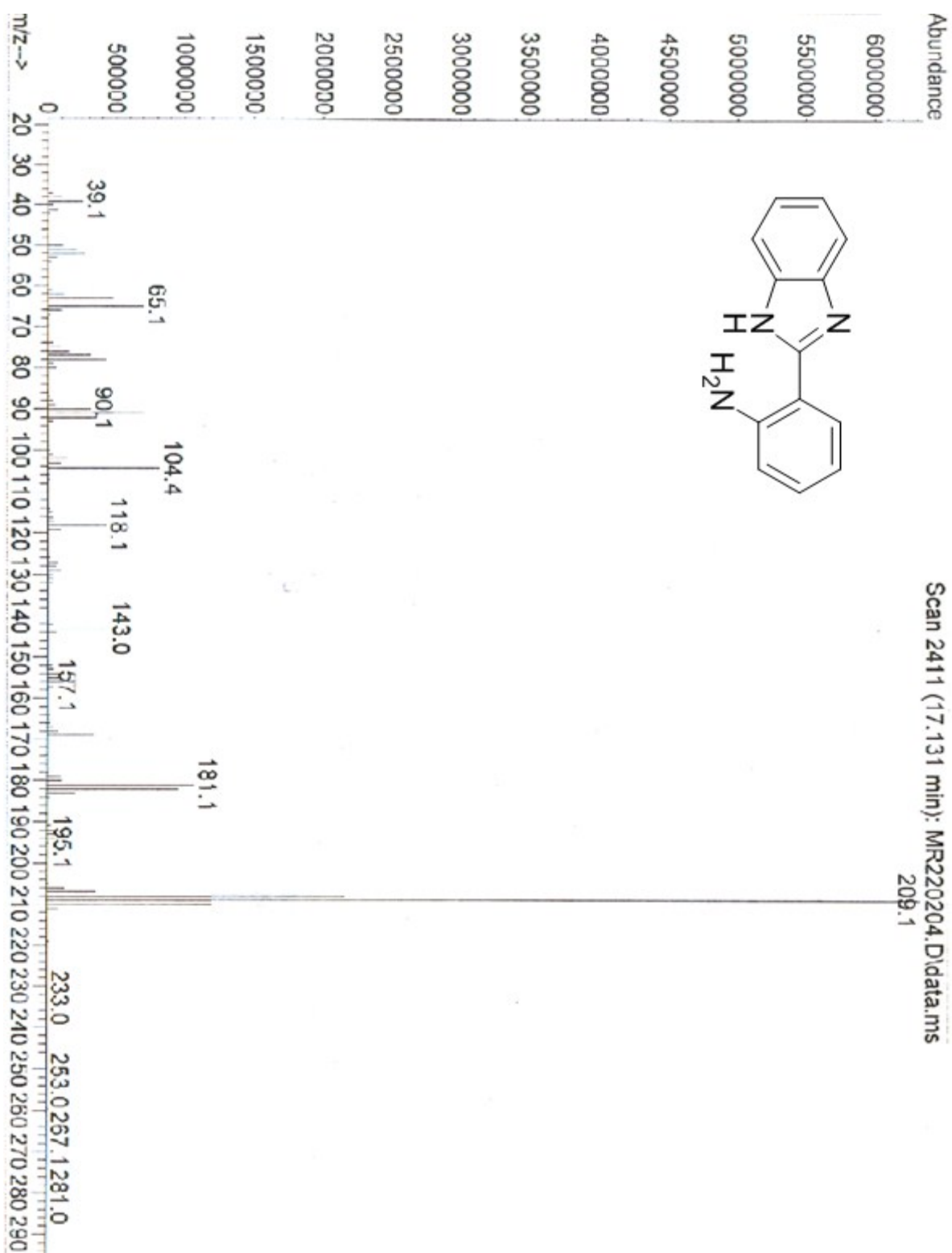


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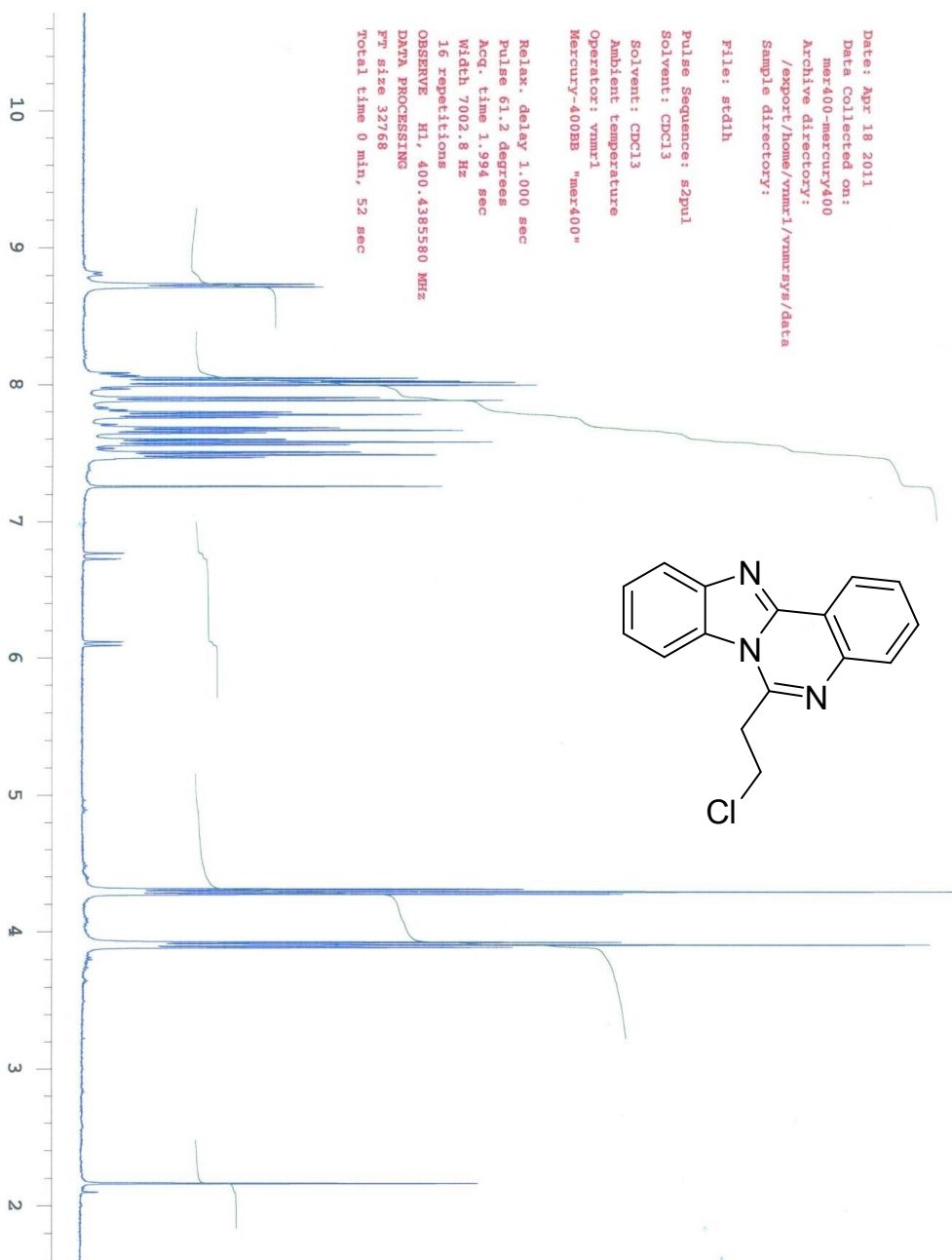


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 Compound 9 (^{13}C -NMR, DMSO-d_6)

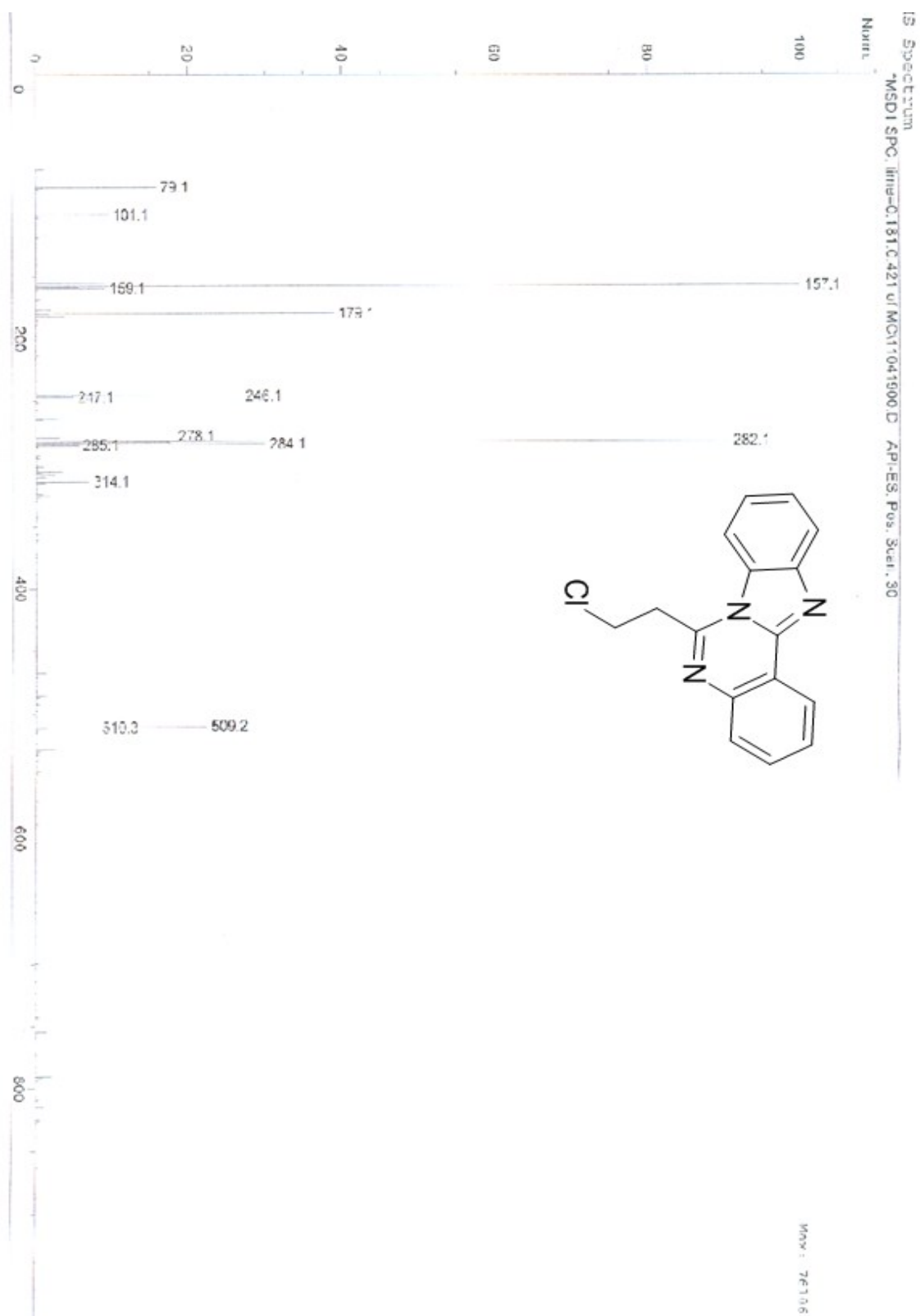




S35
Compound **10** (^1H -NMR, CDCl_3)



S36
Compound **10** (ESI-MS)



S37
Compound **11** (^1H -NMR, CD_3OD)

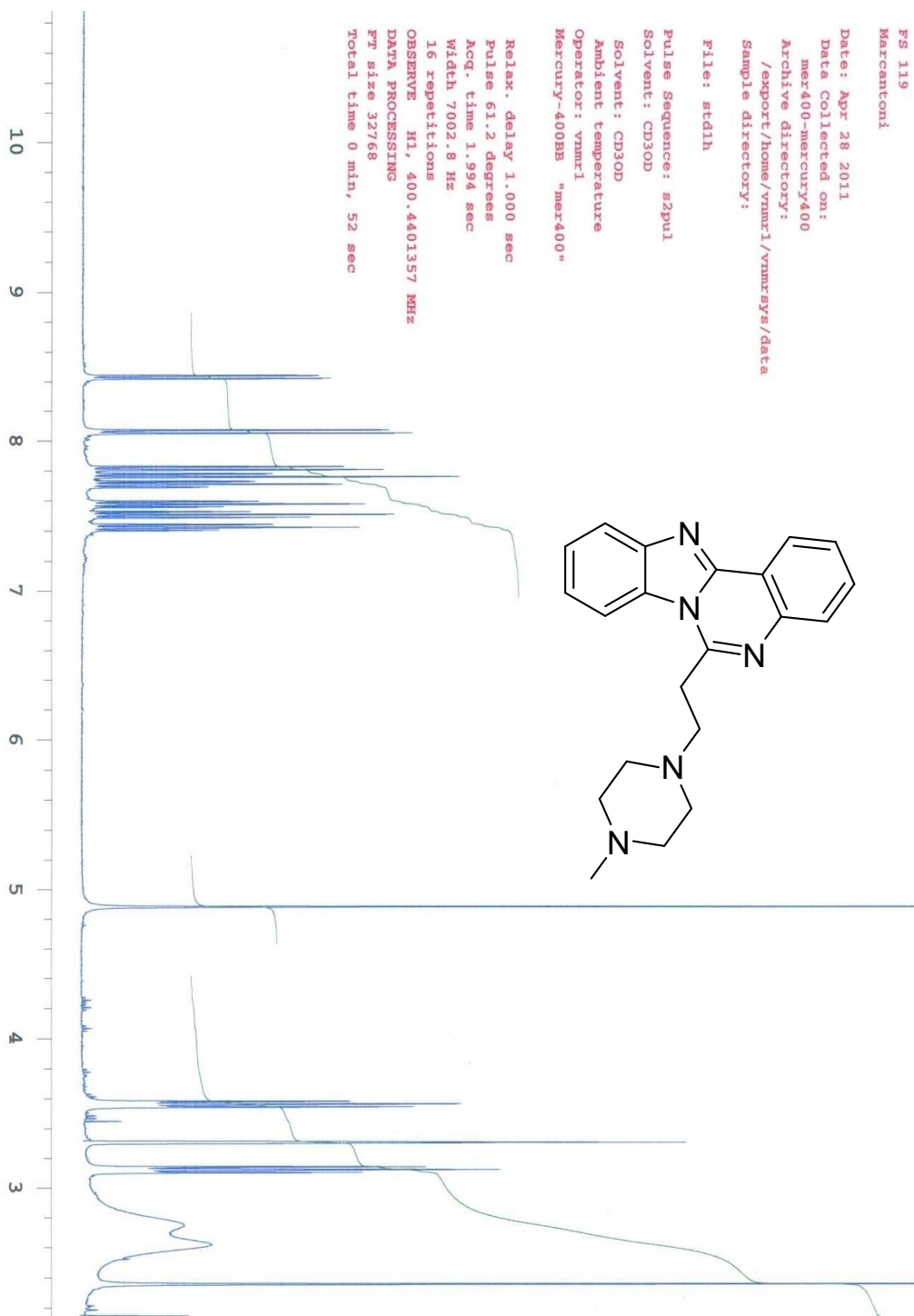
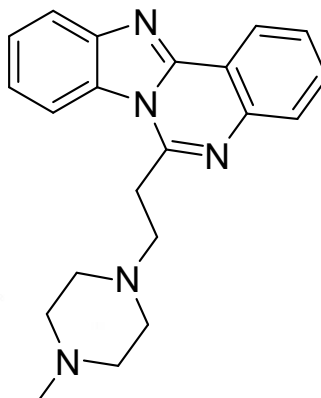
FS 119
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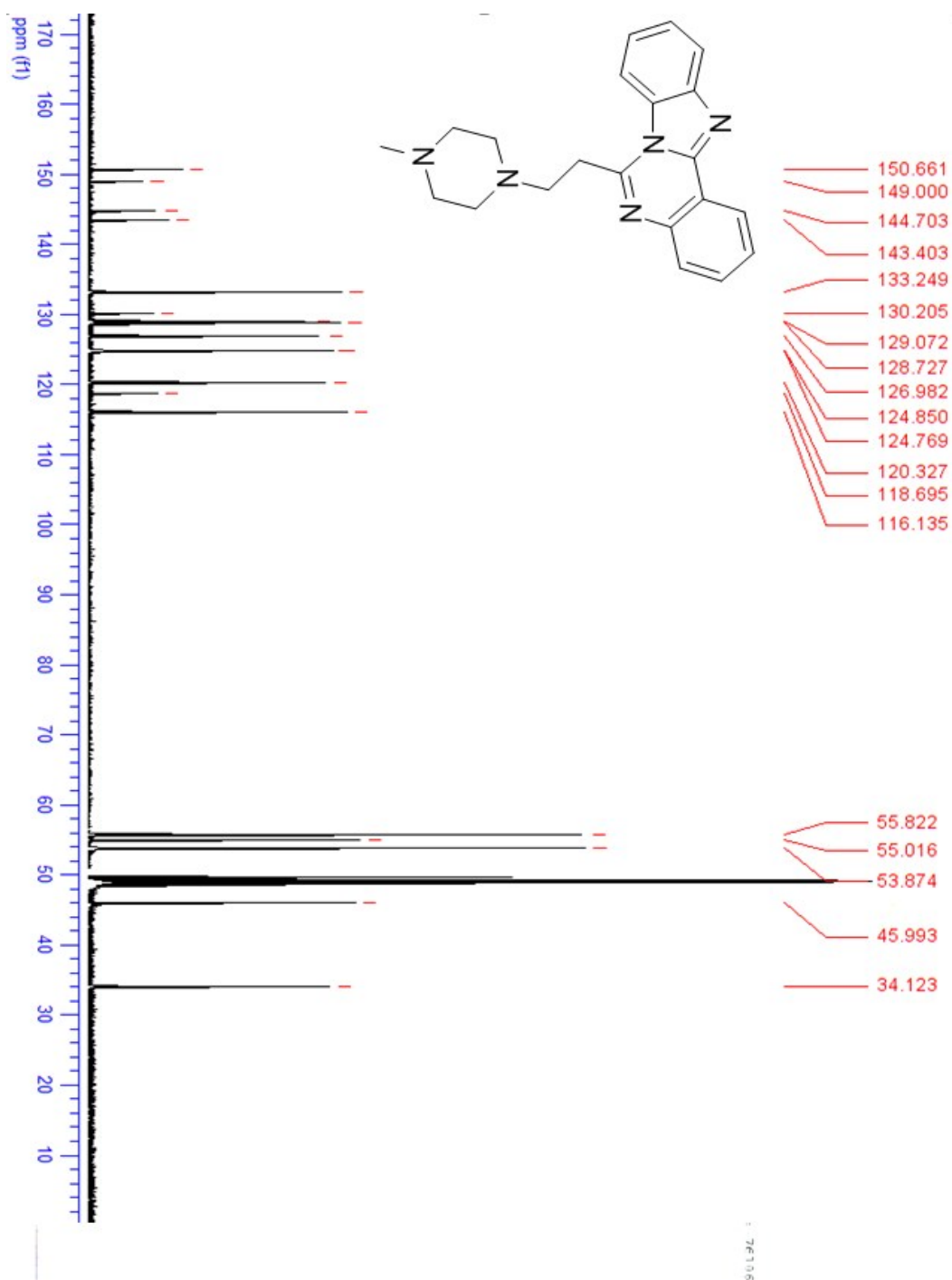
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Sample directory:

File: std1h

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Solvent: CD3OD
Ambient temperature
Operator: vnmr1
Mercury-400BB "mer400"

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Pulse 61.2 degrees
Acq. time 1.994 sec
Width 7002.8 Hz
16 repetitions
OBSERVE H1, 400.4401357 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 52 sec





S39
Compound 11 (ESI-MS)

