

Supplementary Material

Synthesis and characterization of a new ditopic bipyridine-terpyridine bridging ligand using a Suzuki cross-coupling reaction

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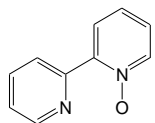
Biomaterials and Medicinal Chemistry Research Centre, Aja University of Medical Sciences, Tehran, Iran

Email: rzi12@uclive.ac.nz

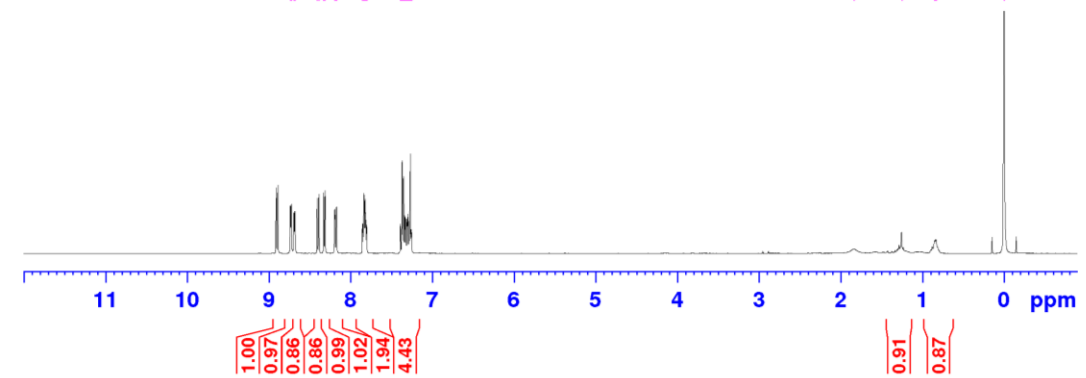
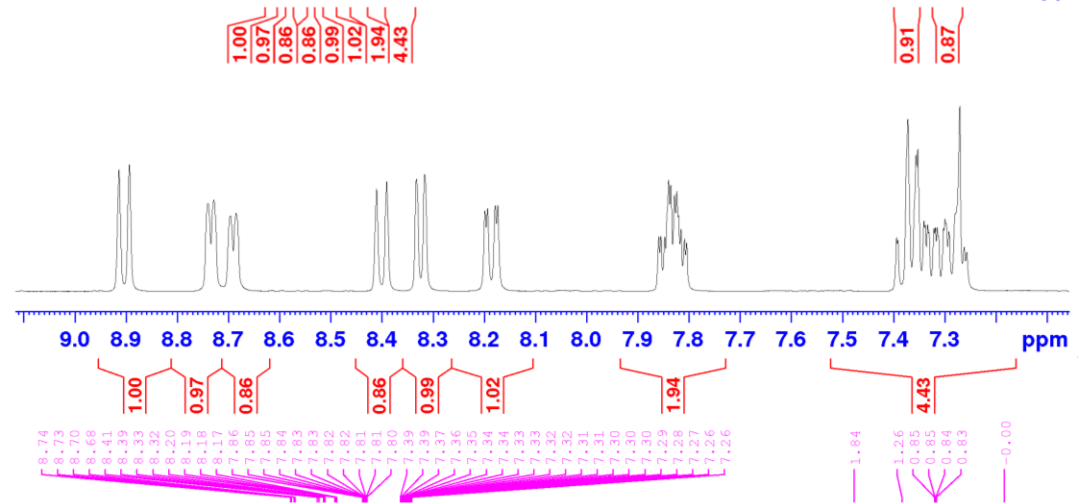
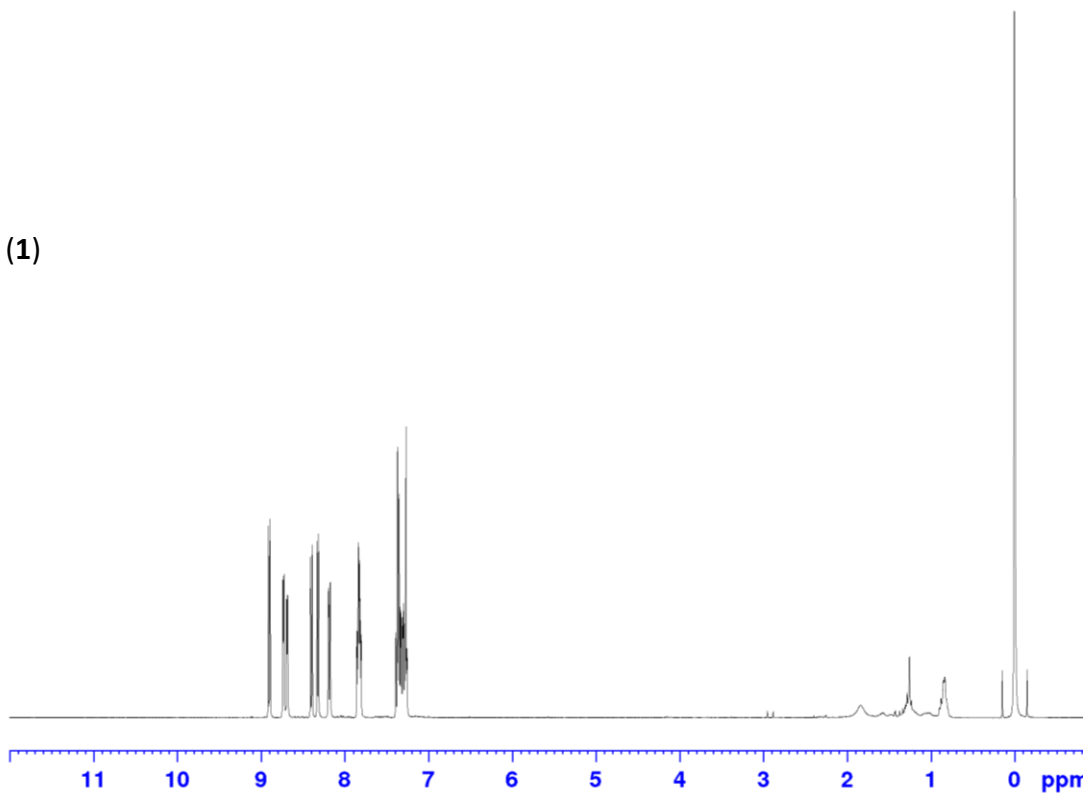
Table of Contents

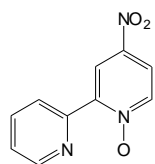
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|---|----|
| 1. Information | S2 |
| 2. ^1H and ^{13}C NMR spectra and LC-Mass spectra of compounds (1)-(9) and ligand (I) | S3 |

Unless otherwise mentioned, all ^1H and ^{13}C NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometer with tetramethylsilane (TMS) as internal standard. Chemical shifts (δ) are reported in parts per million (ppm) downfield of TMS. An agilent LC/MS-6410 Triple Quadruple mass spectrometer interfaced with electrospray ionization (ESI) ion source was used.

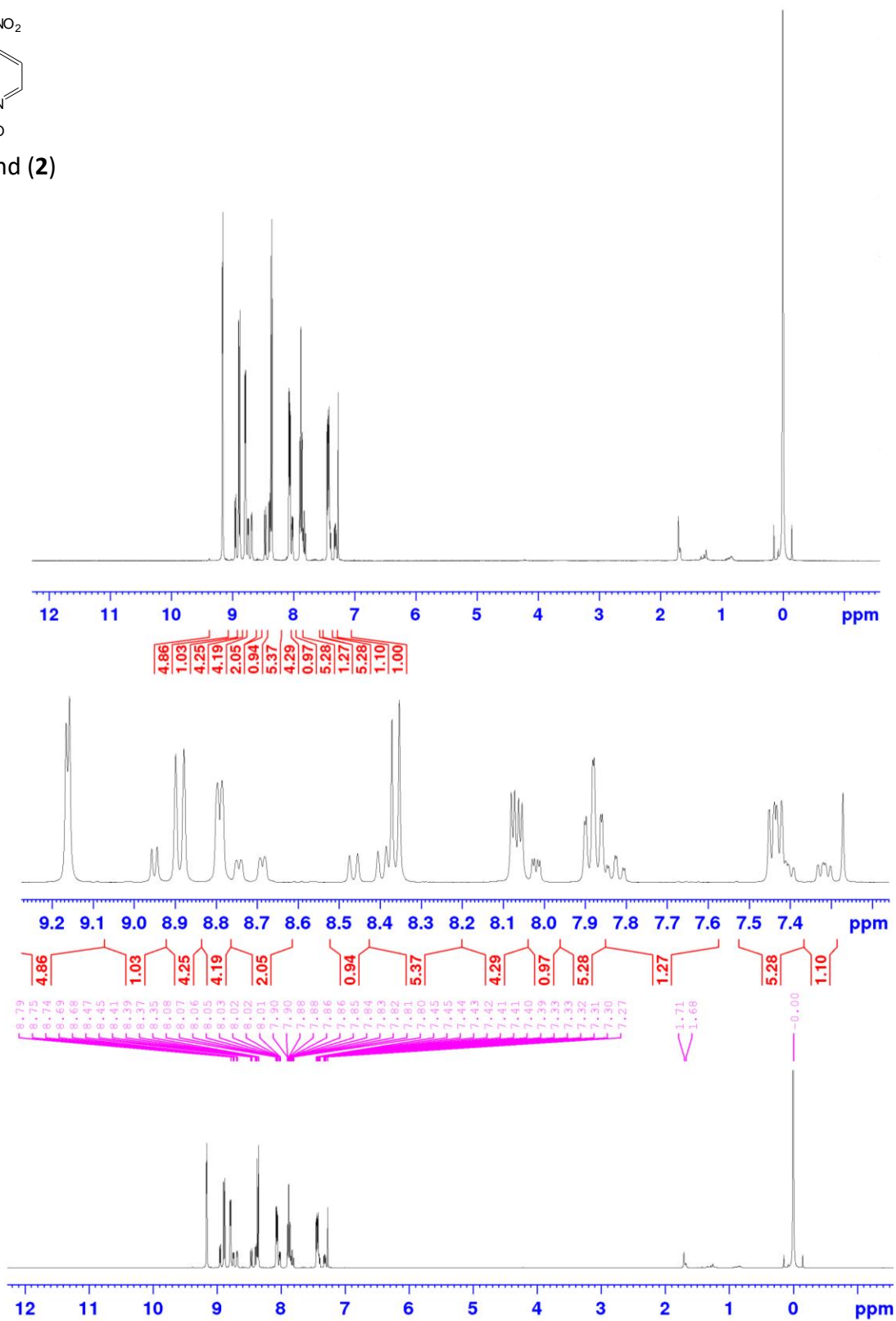


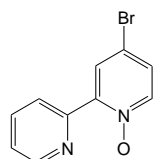
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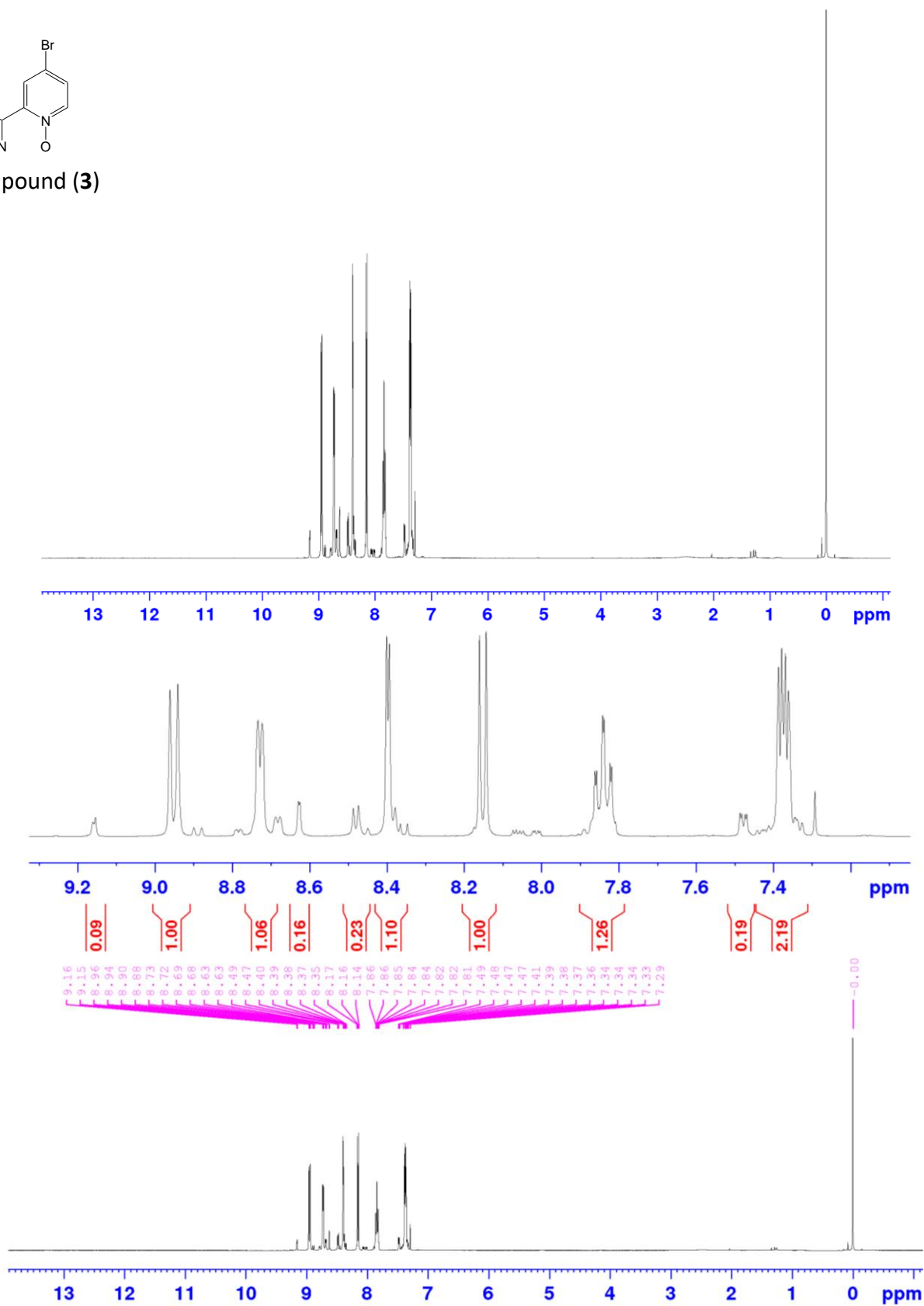


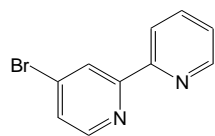
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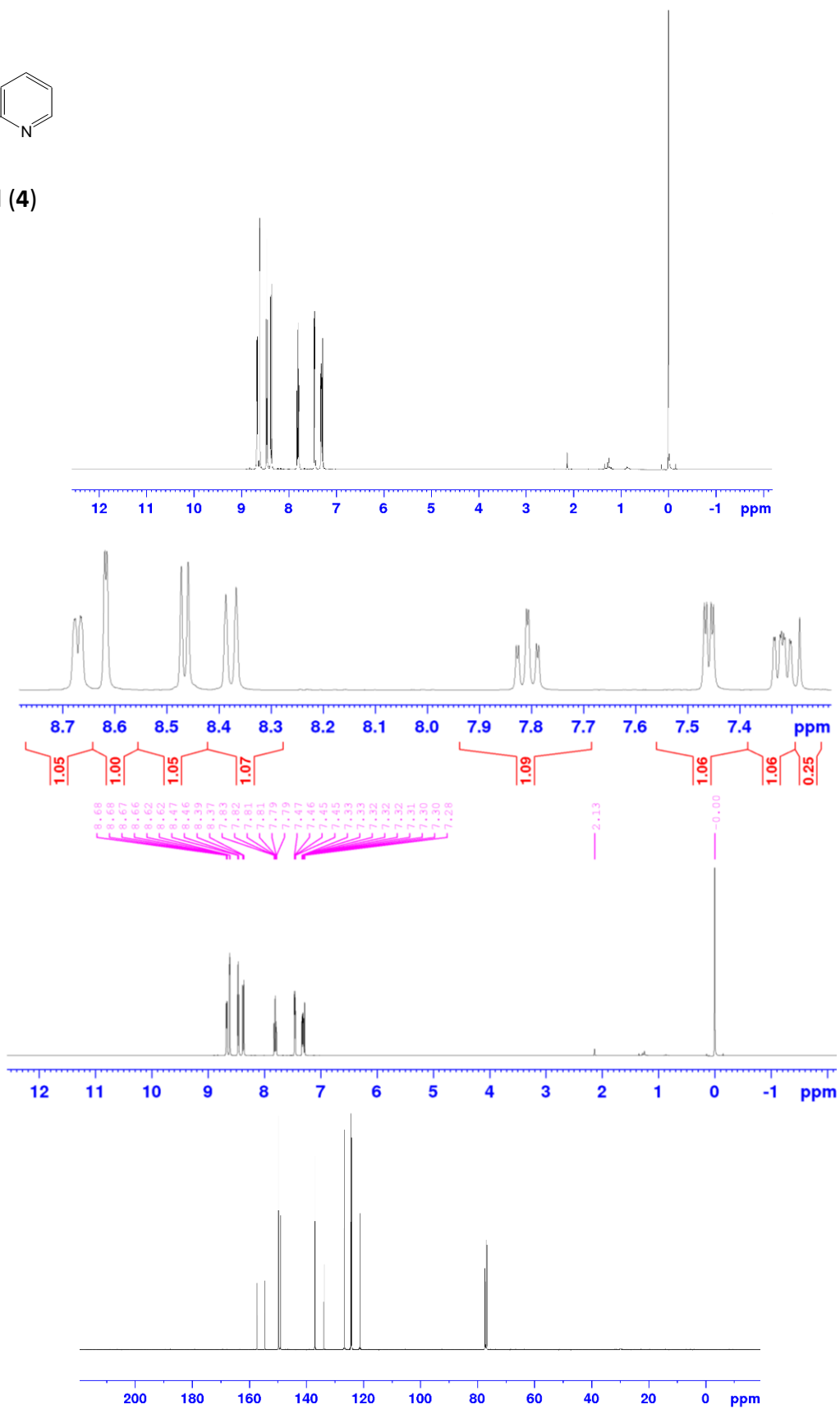


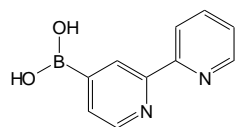
Compound (3)





Compound (4)





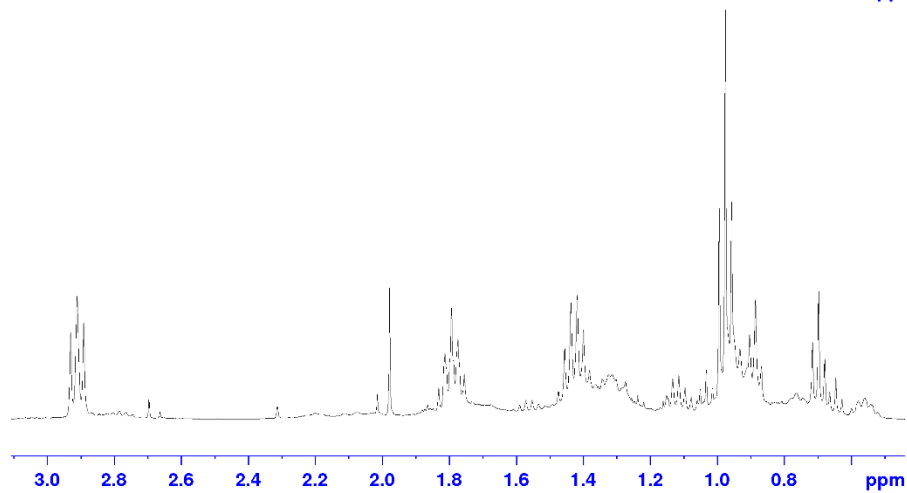
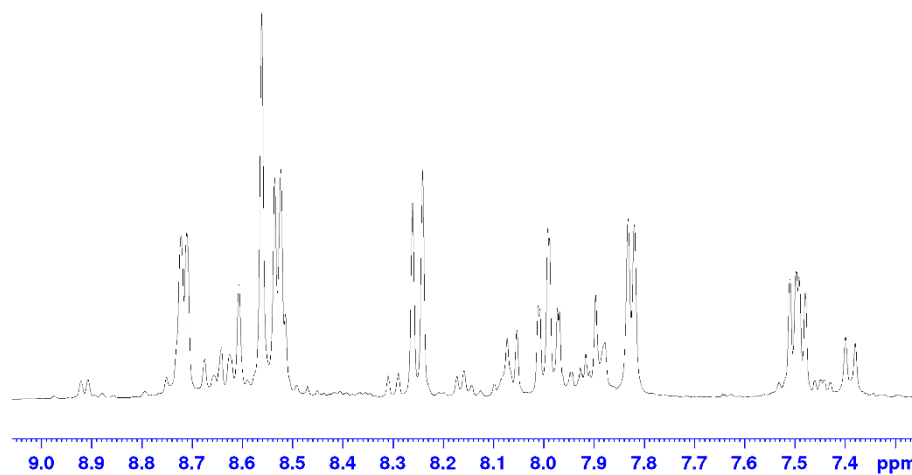
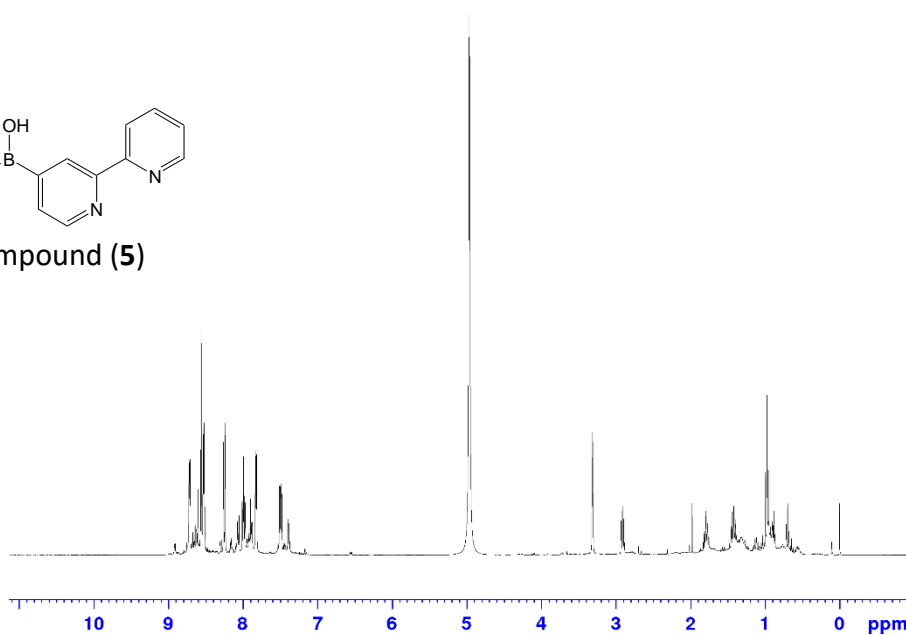
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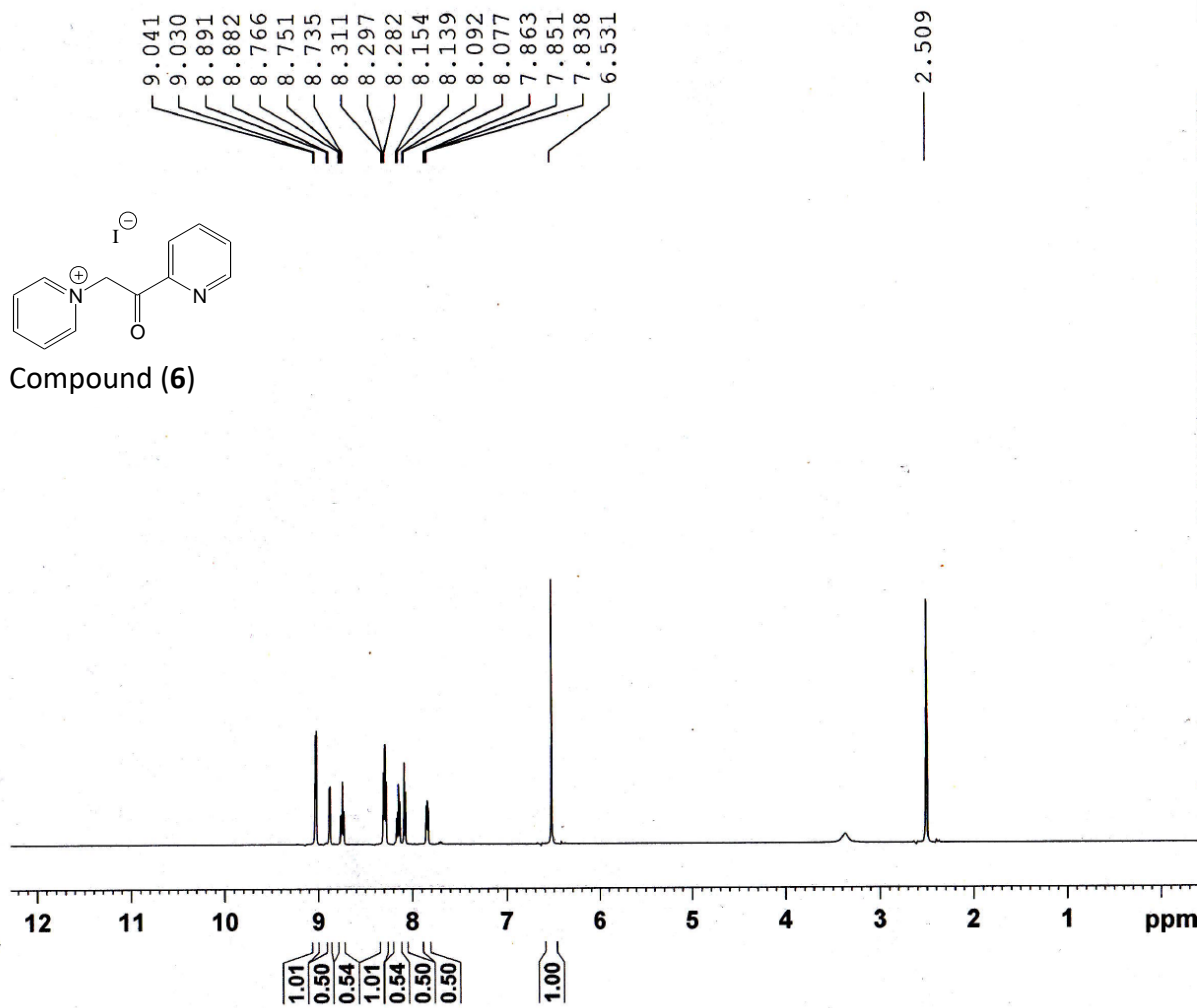
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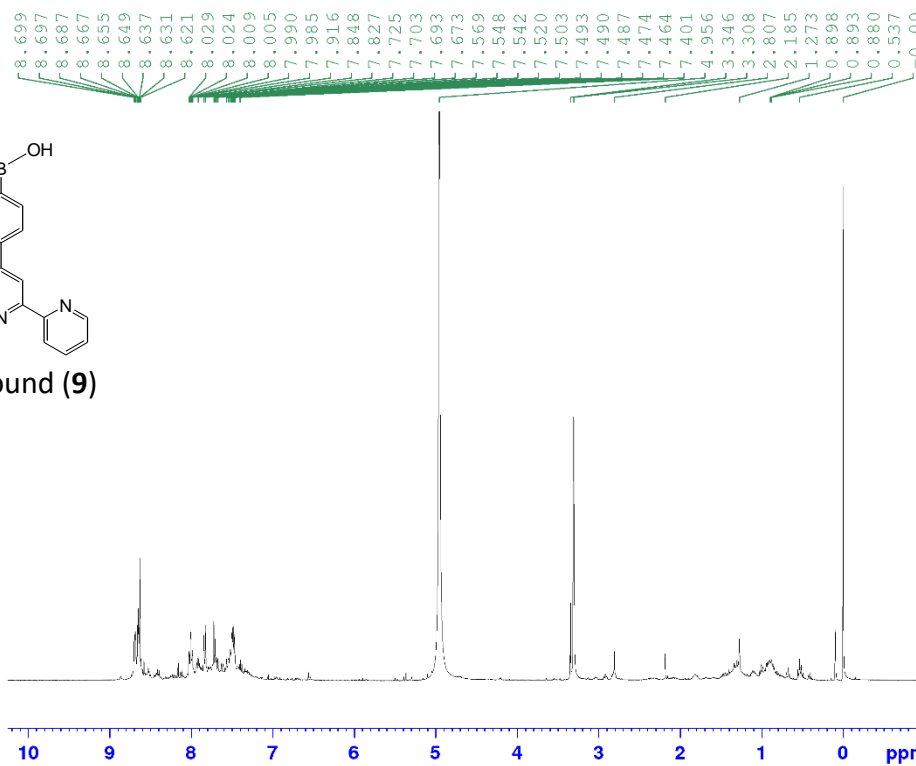
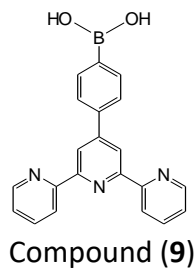
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DS       2
SWE      8012.820 Hz
FIDRES   0.244532 Hz
AQ        4.0894465 sec
RG        103.76
DW        62.400 usec
DE        6.50 usec
TE        292.1 K
D1        1.00000000 sec
TDO       1
SFO1     400.2024712 MHz
NUC1      1H
P1        14.00 usec
PL1       13.00000000 W

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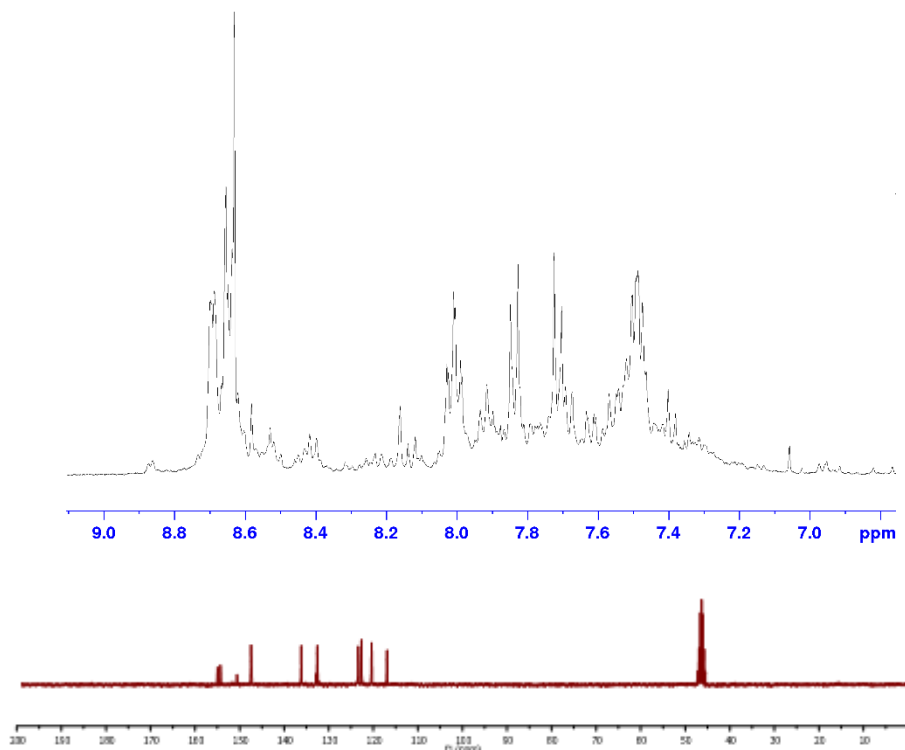


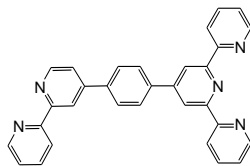


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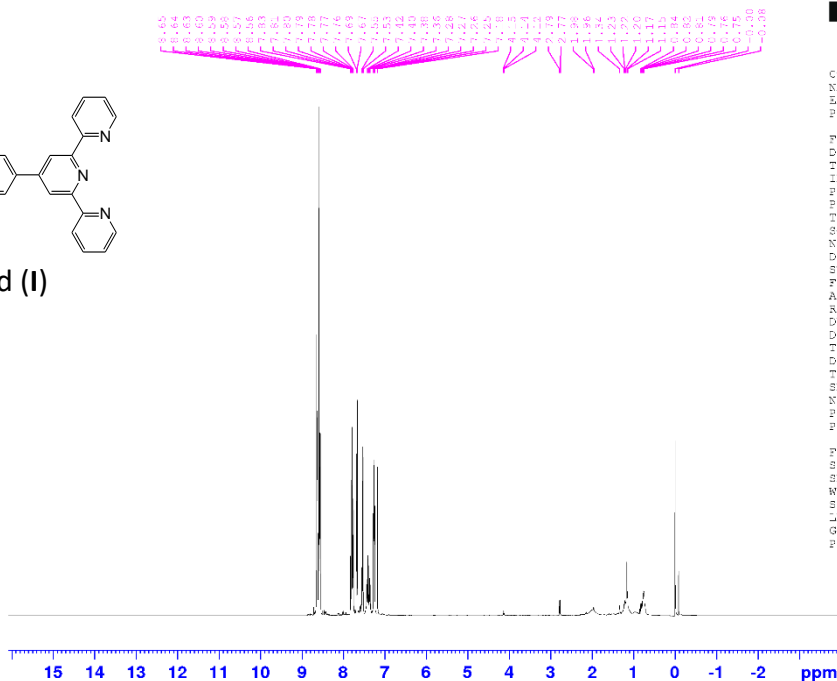
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 DI 1.0000000 sec
 IDO 1
 SFOL 400.2024712 MHz
 NUCL 1H
 PI 14.00 usec
 PLW 13.0000000 W

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Compound (I)

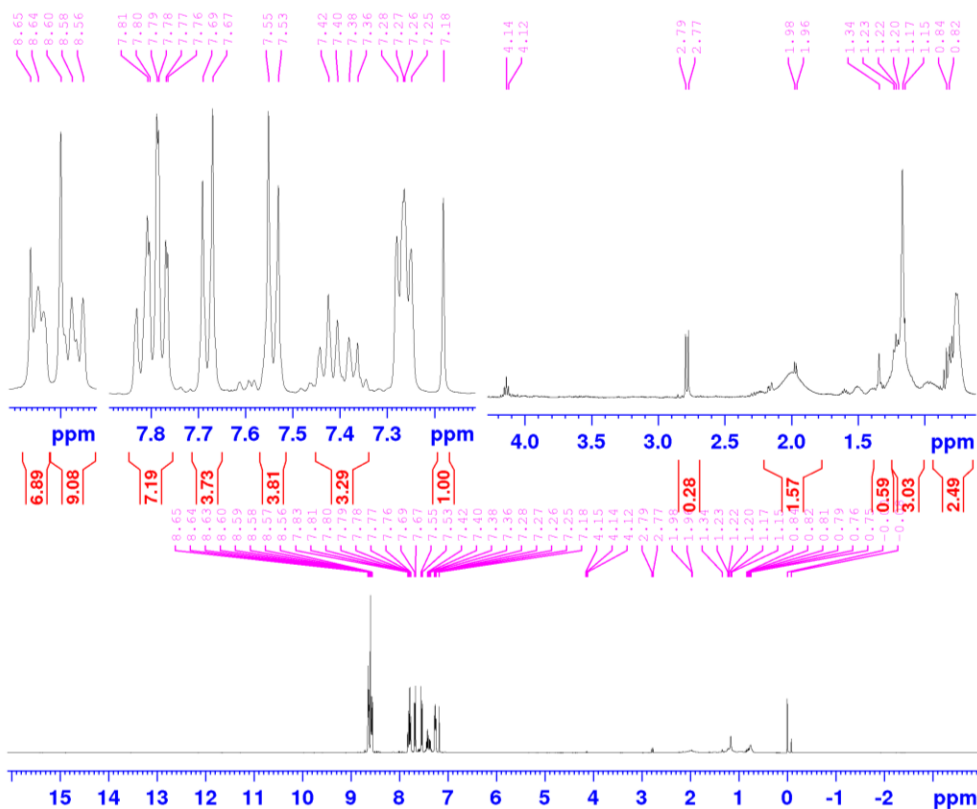


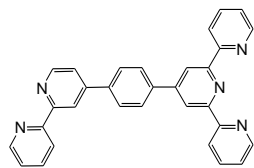
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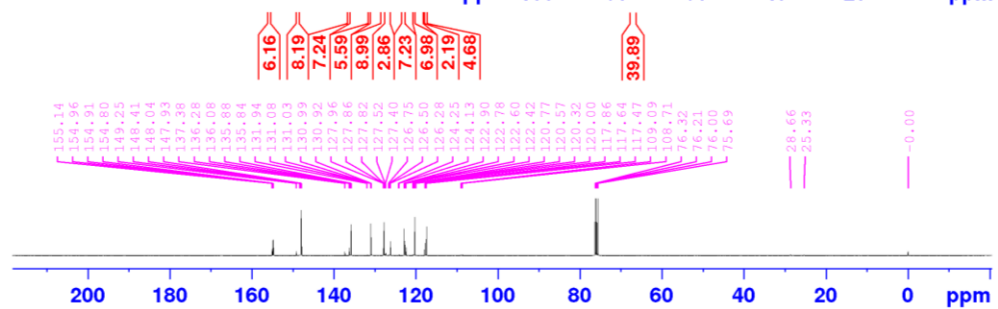
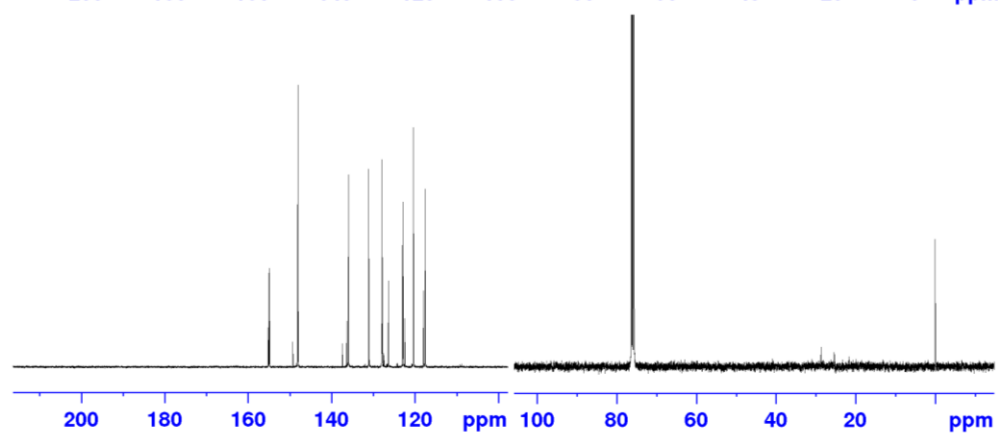
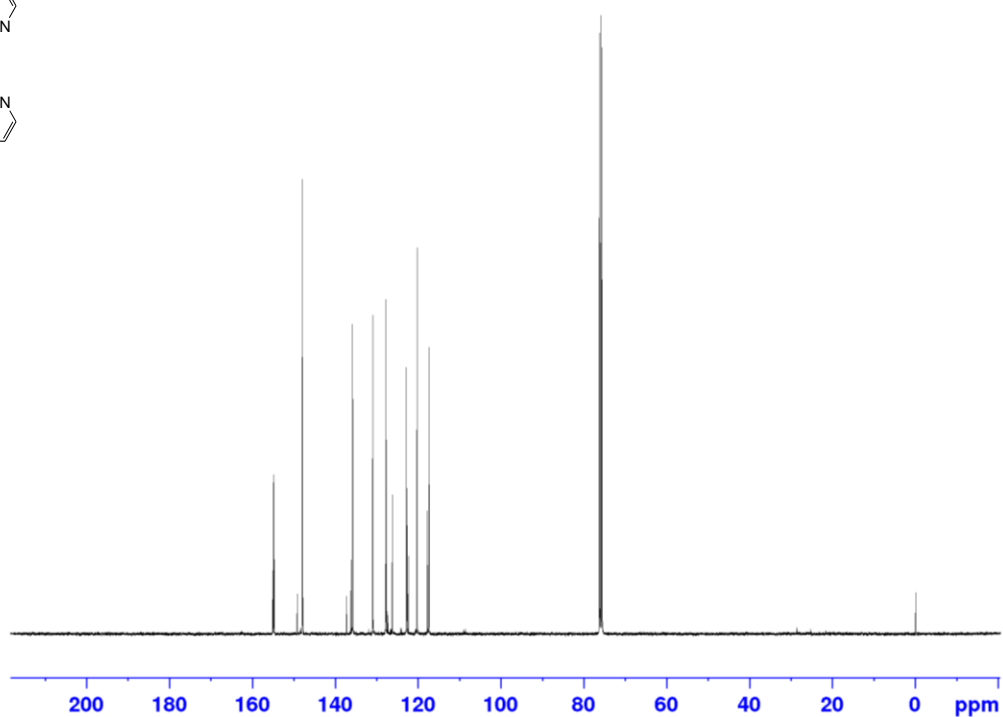
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SOLVENT  CDCl3
NS        32
DS        2
SWH       8012.820 Hz
FIDRES   0.244532 Hz
AQ        4.0894665 sec
RG        103.76
DM        62.400 usec
DE        6.50 usec
TE        292.4 K
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TDO       -
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NUC1      1H
P1        14.00 usec
PL1       13.0000000 W

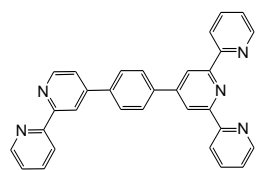
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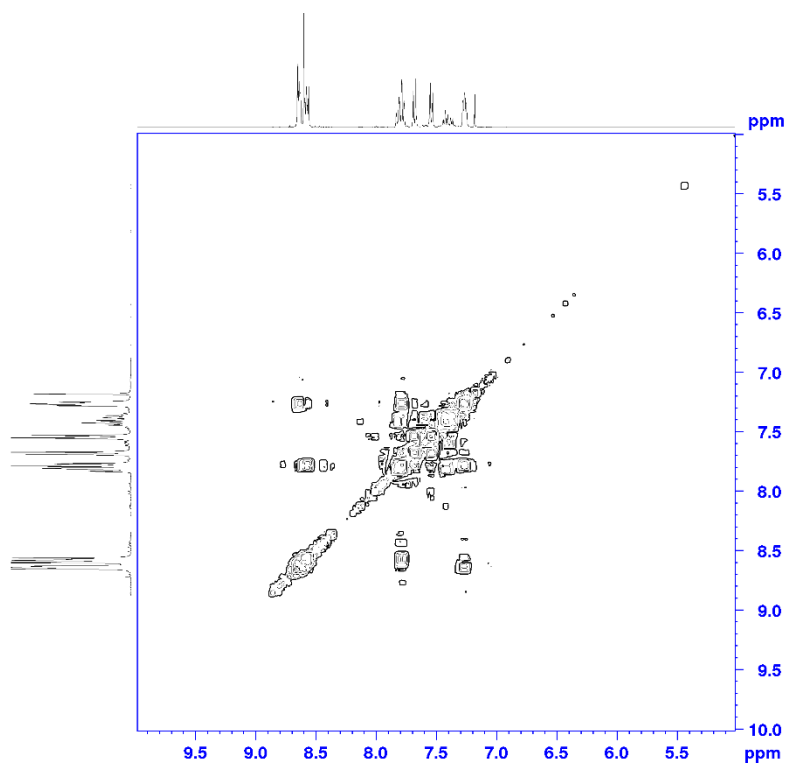
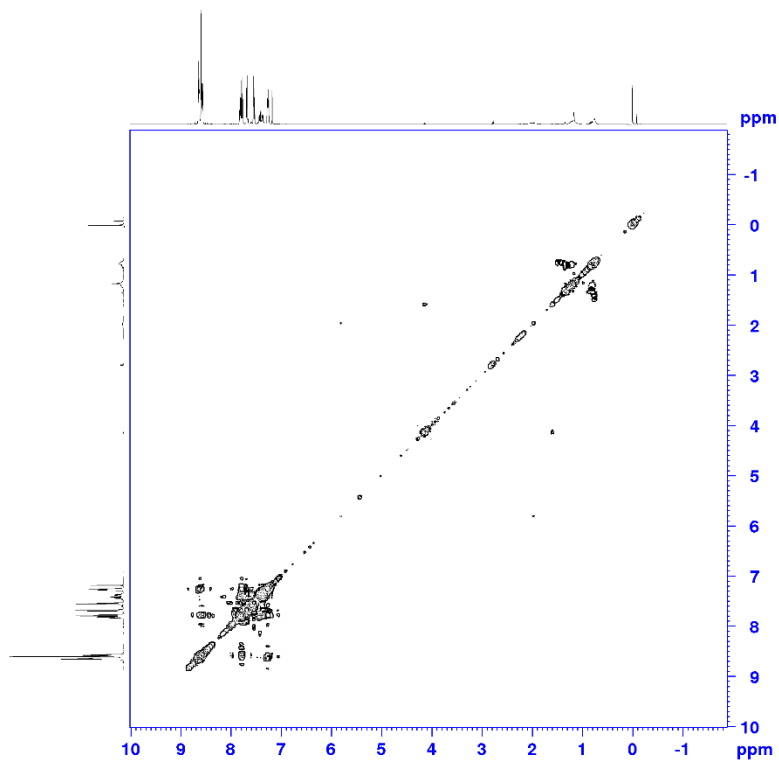


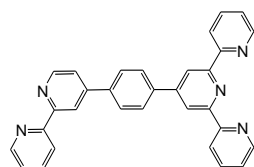
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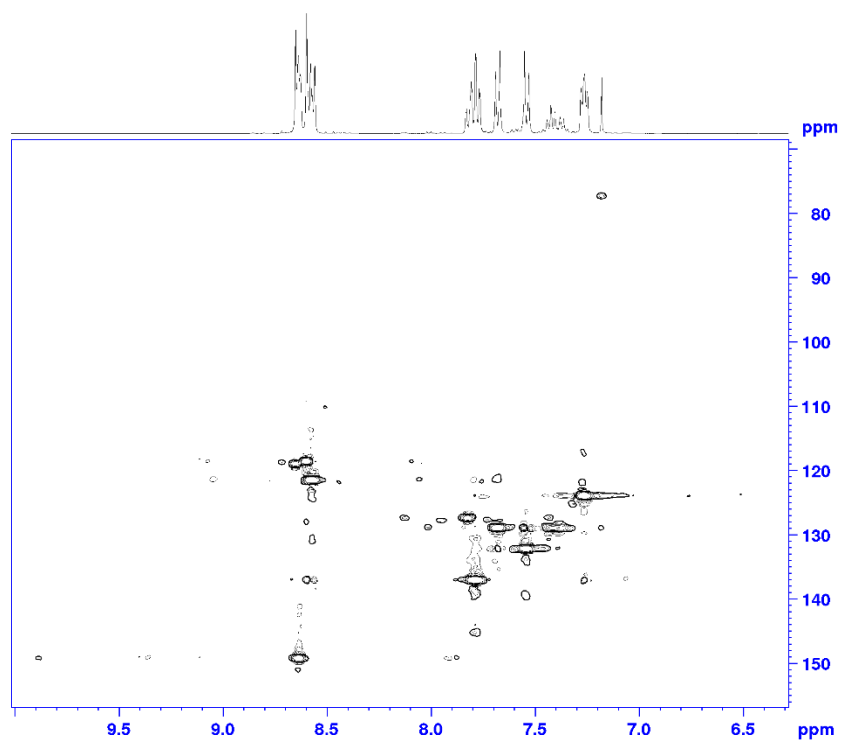
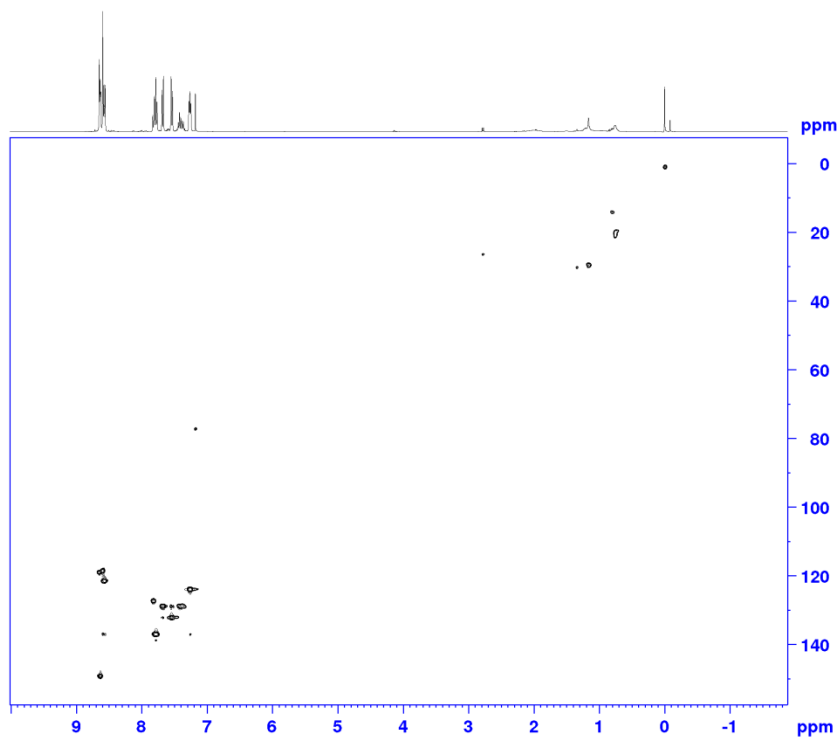


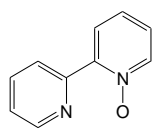
Compound (I)





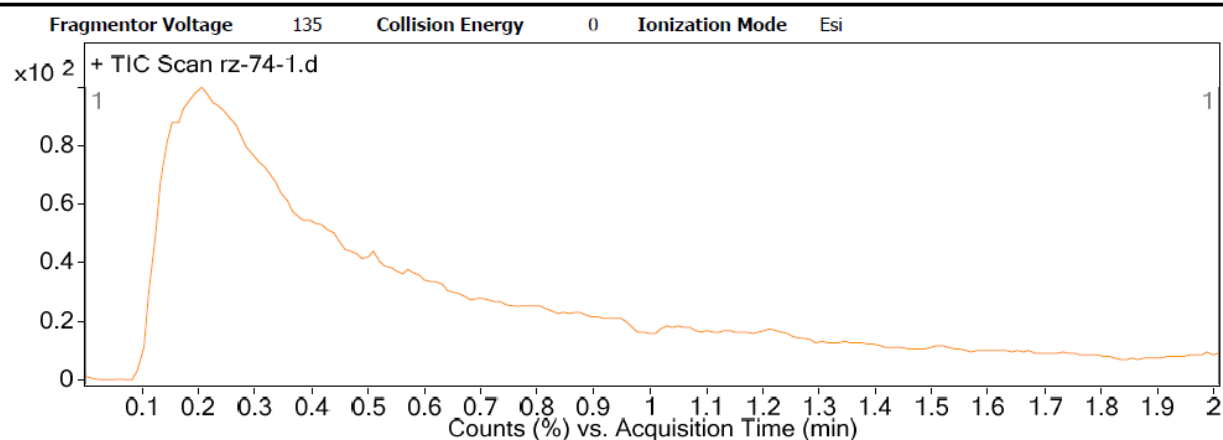
Compound (I)



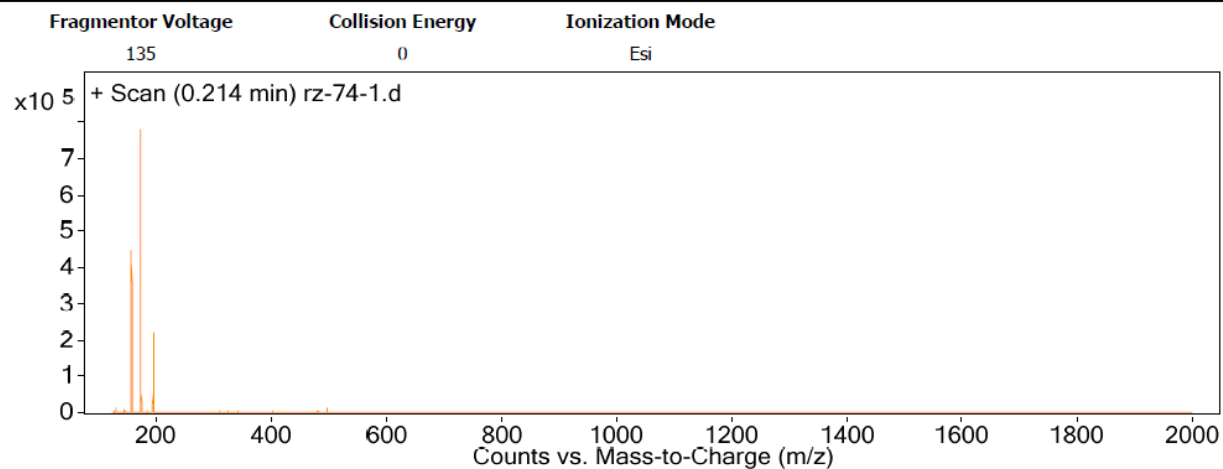


$C_{10}H_8N_2O$
 Exact Mass: 172.06
 Mol. Wt.: 172.18
 C, 69.76; H, 4.68; N, 16.27; O, 9.29

Compound (1)

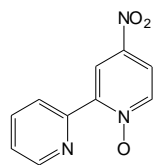


User Spectra



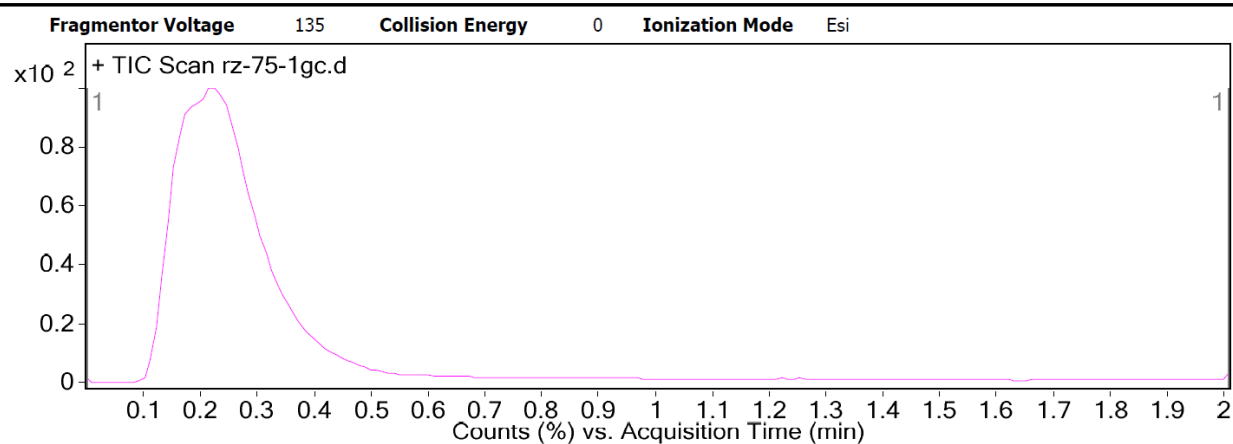
Peak List

m/z	z	Abund.
154.9		45805
155.9		89524
156.9	1	445062
157.9	1	49977
172.9	1	778221
173.9	1	98347
194.8		220209

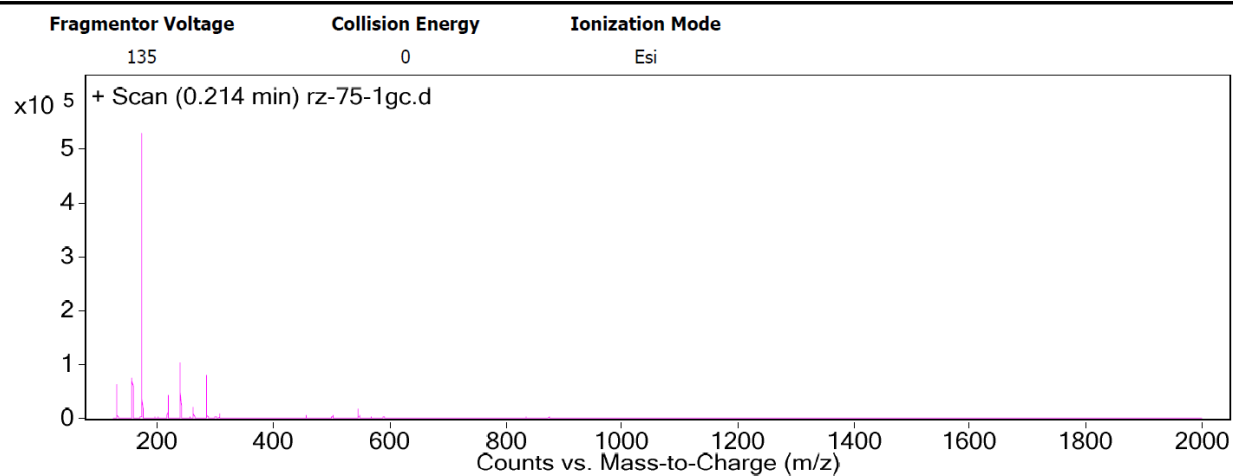


$C_{10}H_7N_3O_3$
 Exact Mass: 217.05
 Mol. Wt.: 217.18
 C, 55.30; H, 3.25; N, 19.35; O, 22.10

Compound (2)

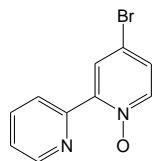


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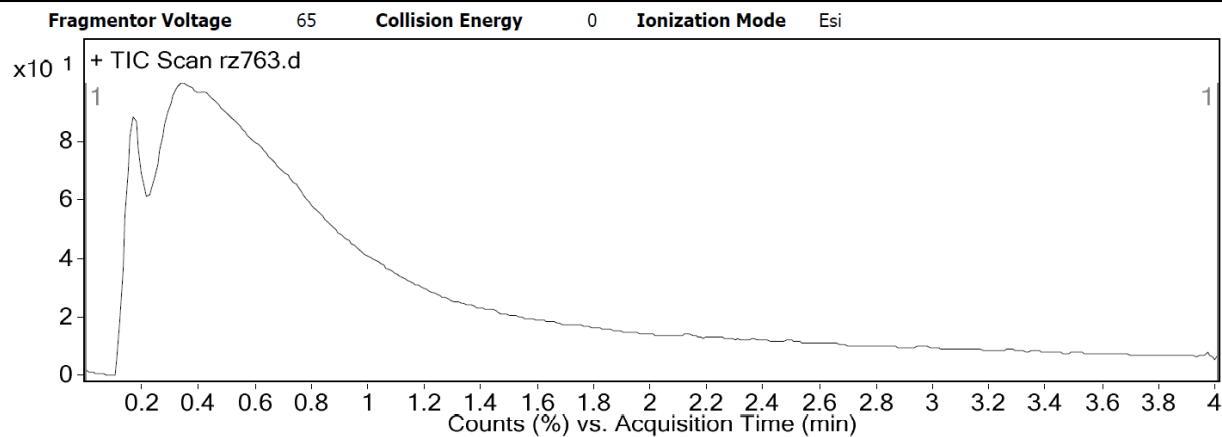
Peak List

<i>m/z</i>	<i>z</i>	Abund.
130		63176
156.9		73568
172.9	1	527497
173.9	1	64954
217.9		41811
239.9		104099
284.8		80357

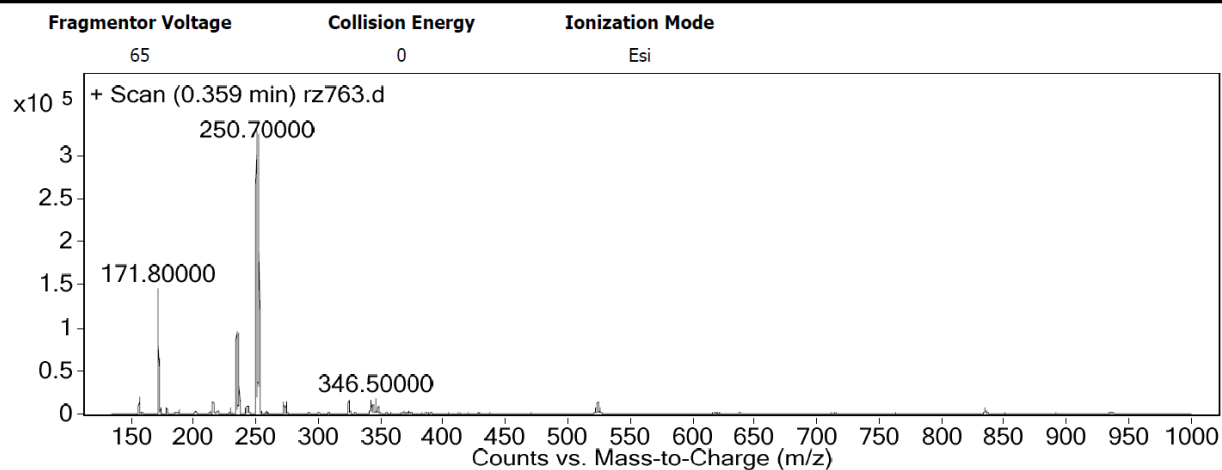


$C_{10}H_7BrN_2O$
 Exact Mass: 249.97
 Mol. Wt.: 251.08
 C, 47.84; H, 2.81; Br, 31.82; N, 11.16; O, 6.37

Compound (3)

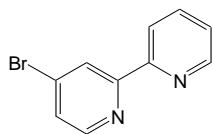


User Spectra



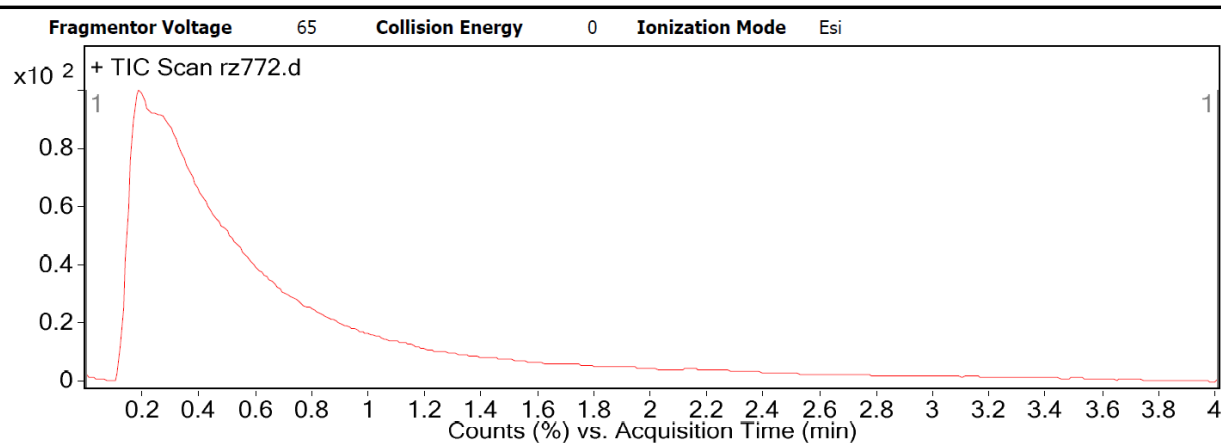
Peak List

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156.8		20045
171.8		145542
172.8		63254
234.7		95950
236.7		93766
250.7	1	327644
251.7	1	38004
252.7	1	324023
253.7	1	37049
346.5		18107

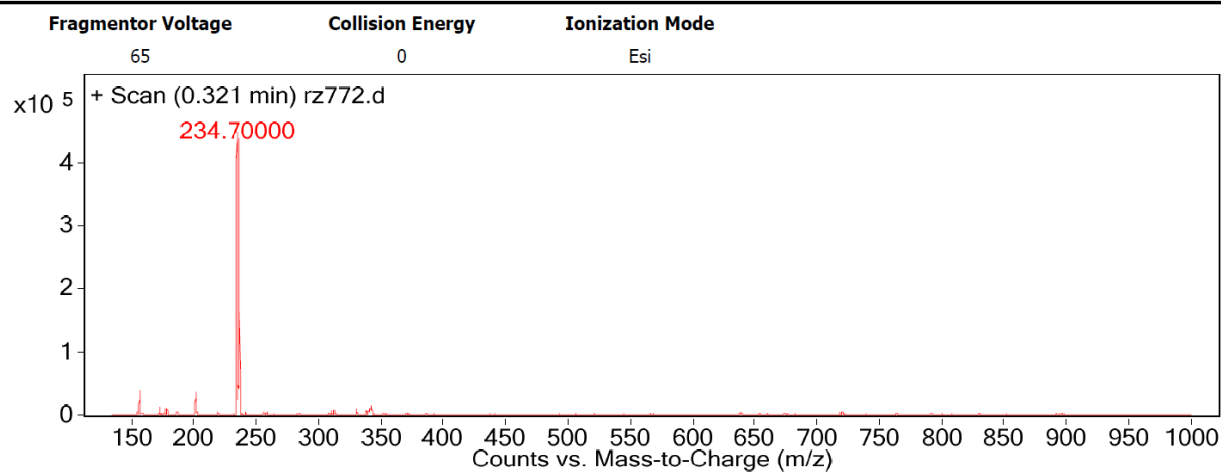


$C_{10}H_7BrN_2$
Exact Mass: 233.98
Mol. Wt.: 235.08
C, 51.09; H, 3.00; Br, 33.99; N, 11.92

Compound (4)

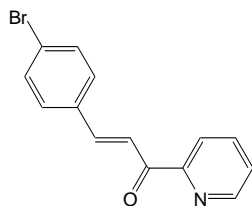


User Spectra



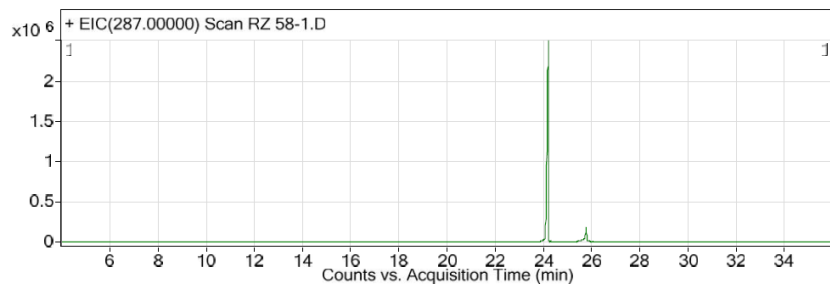
Peak List

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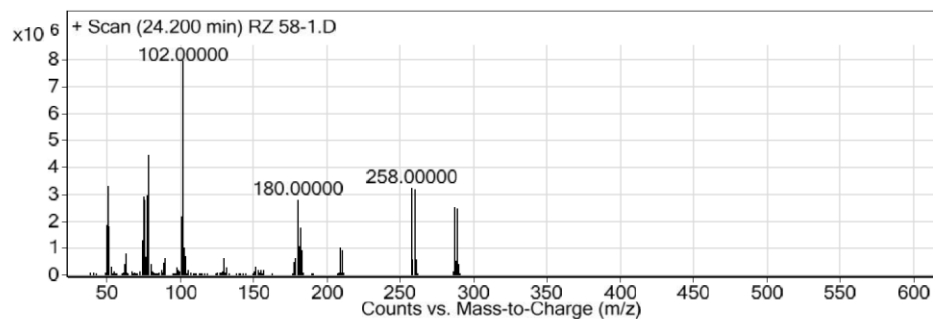
$C_{14}H_{10}BrNO$
Exact Mass: 286.99
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 C, 58.36; H, 3.50; Br, 27.73; N, 4.86; O, 5.55

Compound (7)



User Spectra

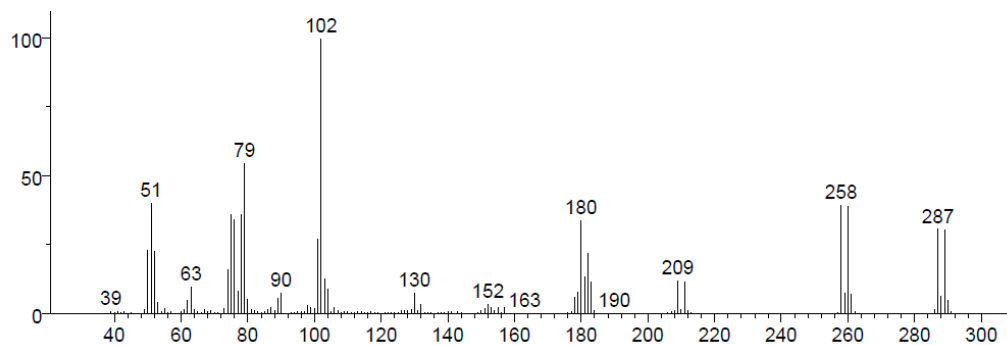
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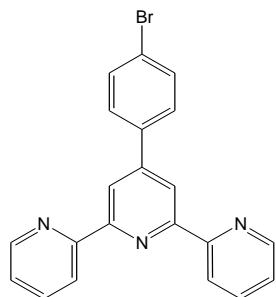


Peak List

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76	1	2762973
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79	1	4453592
102	1	8126465
180		2770680
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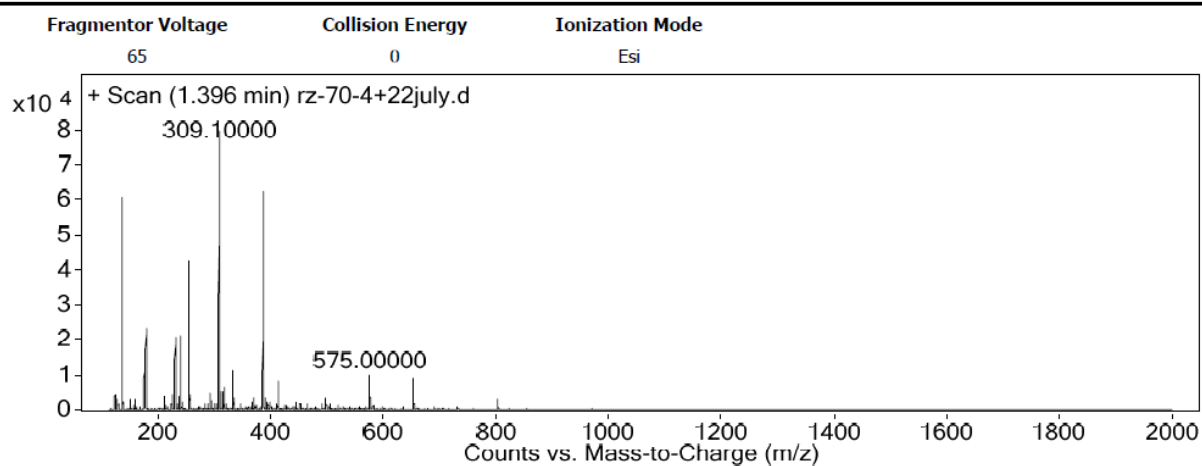




$C_{21}H_{14}BrN_3$
Exact Mass: 387.04
Mol. Wt.: 388.26
C, 64.96; H, 3.63; Br, 20.58; N, 10.82

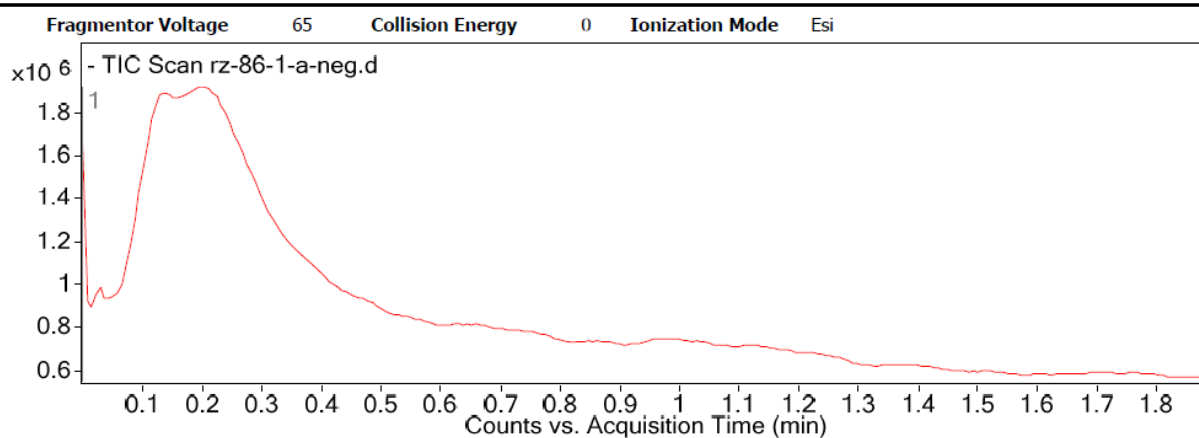
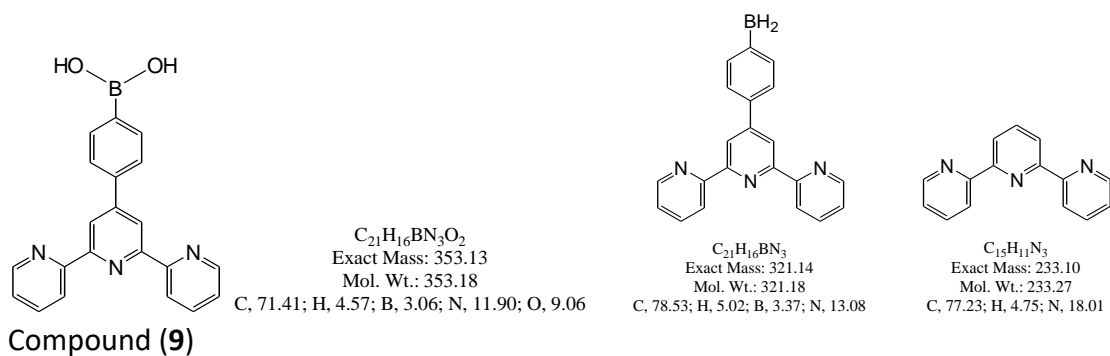
Compound (8)

User Spectra

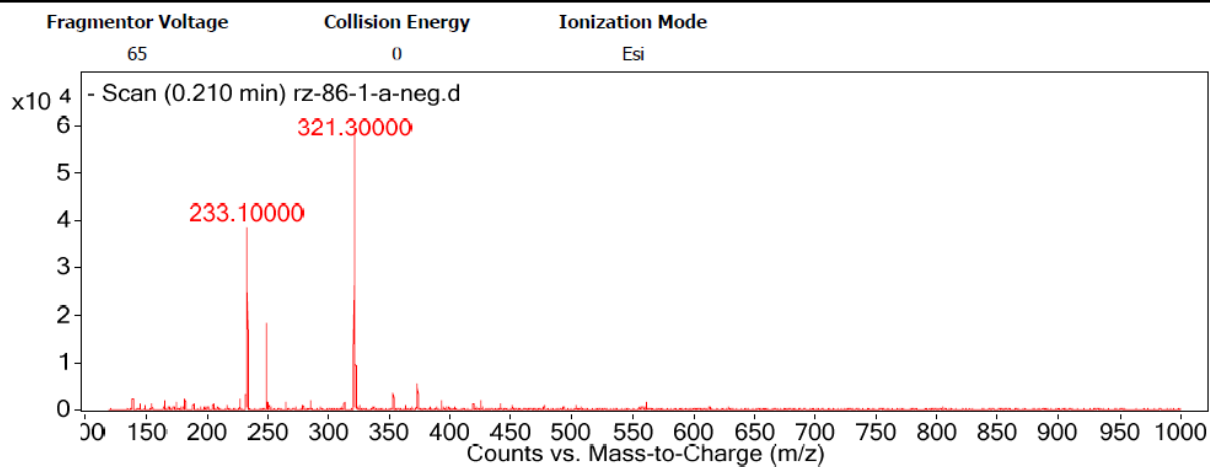


Peak List

m/z	z	Abund.
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179.1		23092
231		20807
241.1		21025
255.1	1	42546
309.1	1	79345
311		23628
333.1		11289
387.1	1	62110
389.1	1	10940

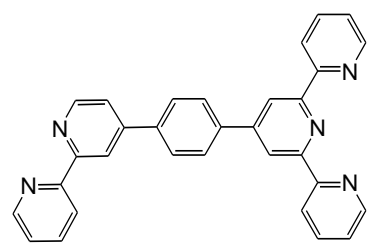


User Spectra



Peak List

<i>m/z</i>	Abund.
232.1	3083
233.1	38489
249	18316
321.3	59135
322.2	9630
353.1	3616
373.3	5449



Compound (I)

$C_{31}H_{21}N_5$
Exact Mass: 463.18
Mol. Wt.: 463.53
C, 80.32; H, 4.57; N, 15.11

