

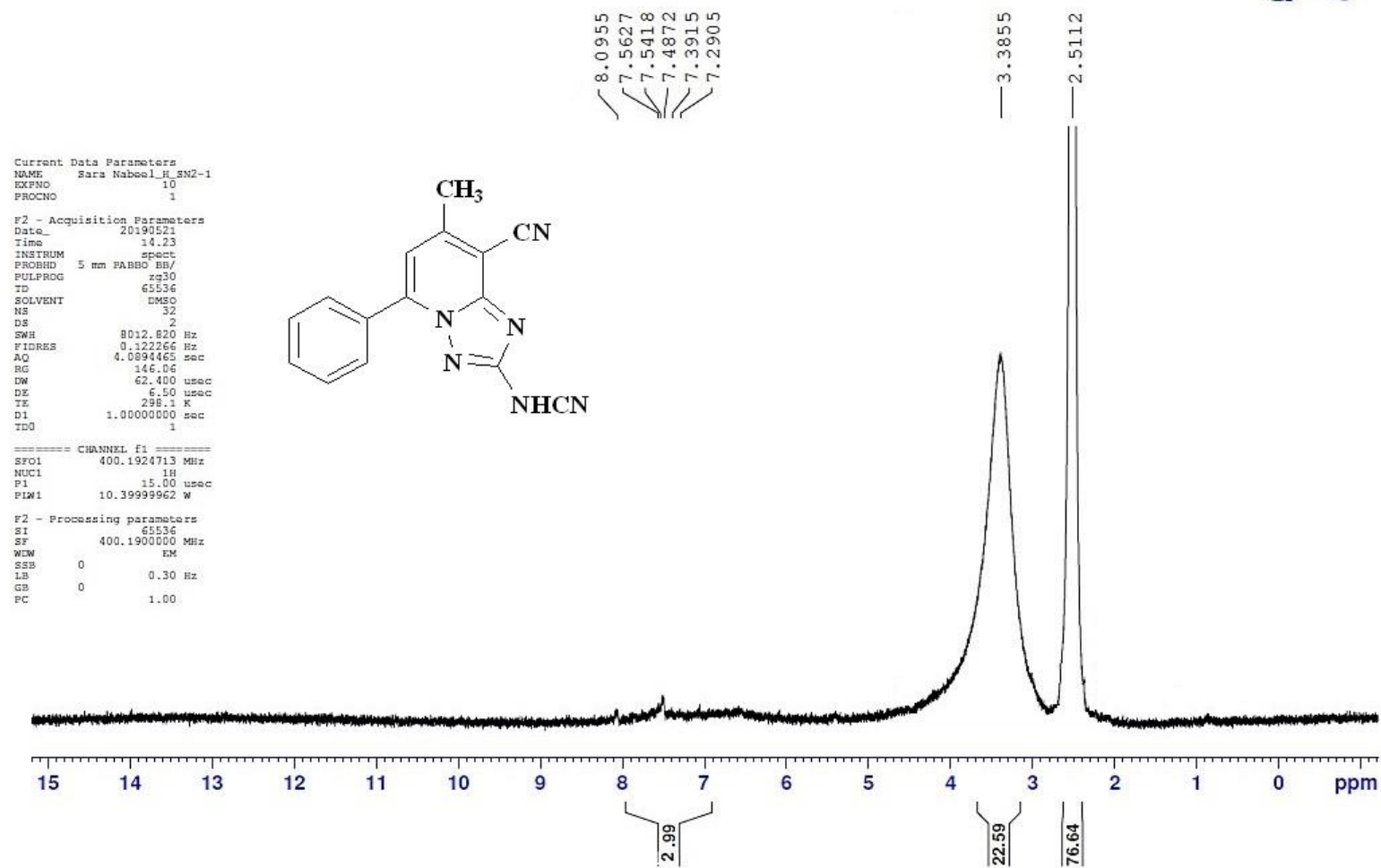
# **Synthesis Of Pyrido-Annulated [1,2,4,5]Tetrazines, [1,2,4]Triazepine, And [1,2,4,5]Tetrazepines For Anticancer, DFT, And Molecular Docking Studies.**

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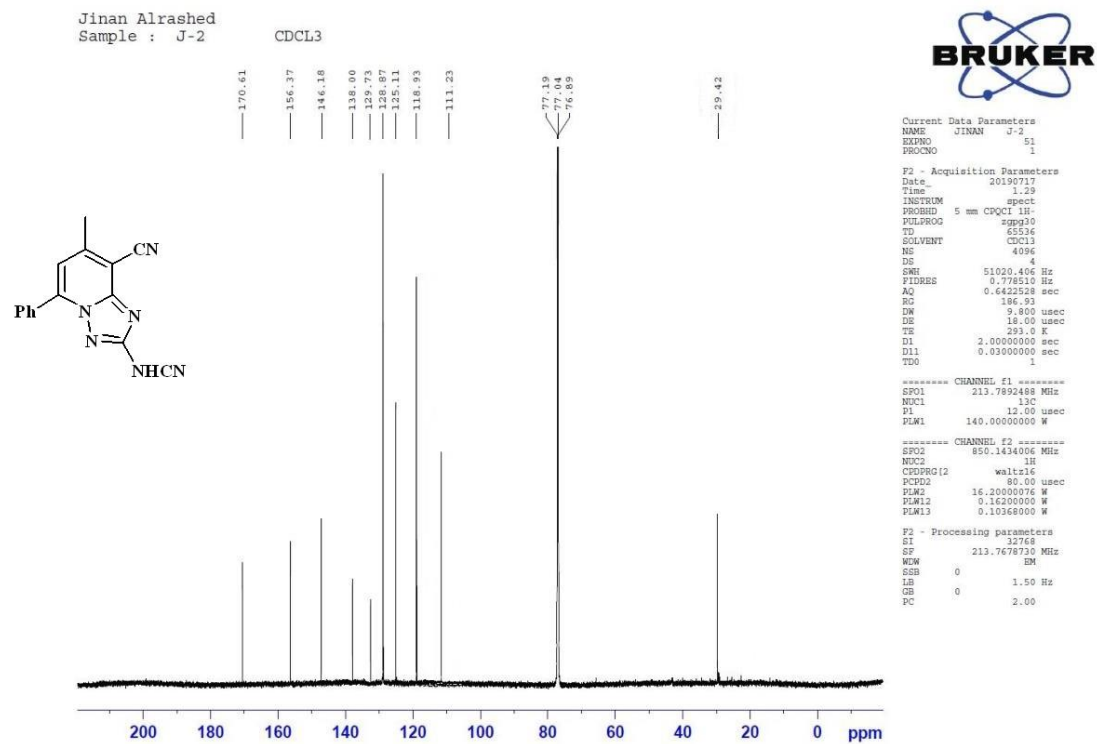
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[eman.sadek.1612@gmail.com](mailto:eman.sadek.1612@gmail.com).**

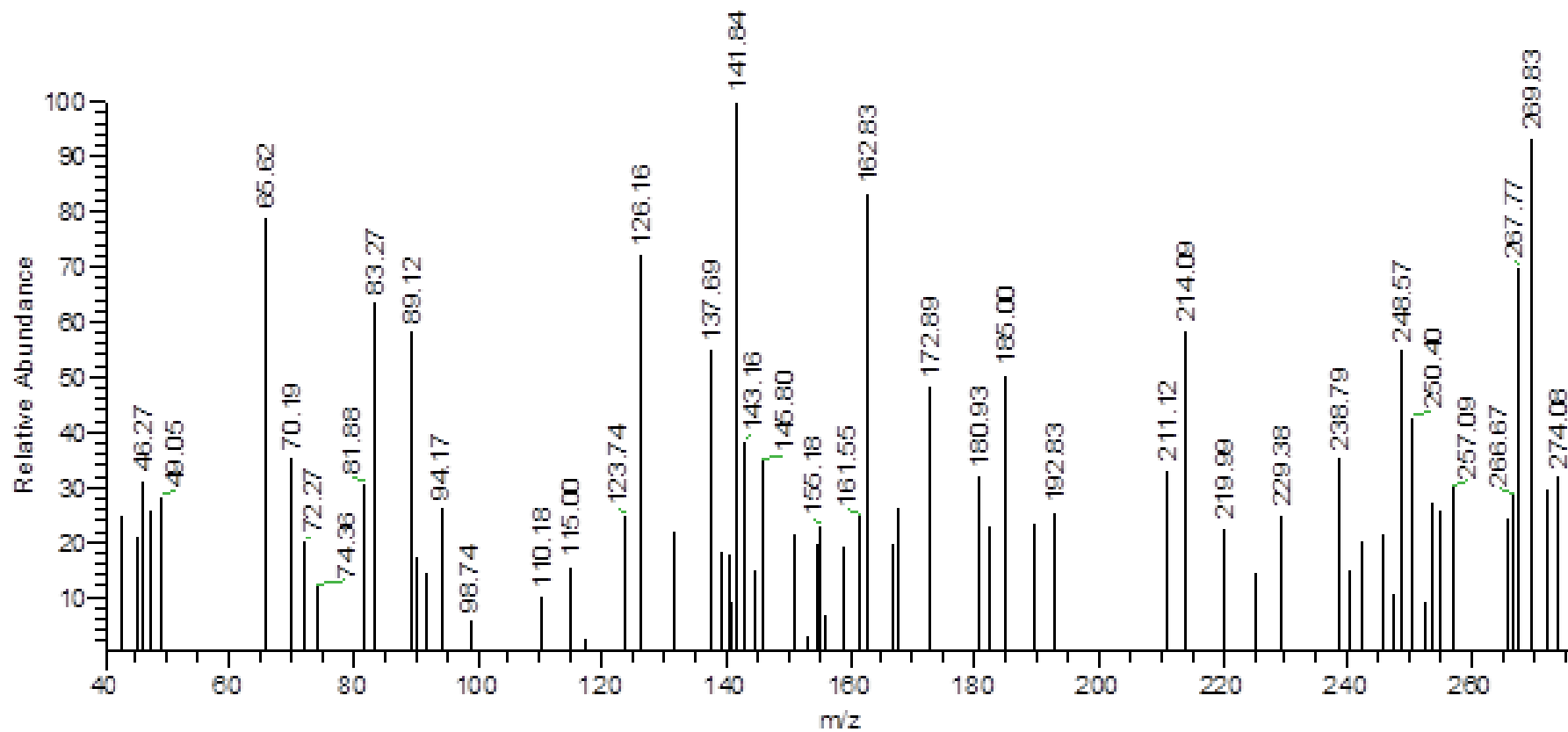


Supplementary fig. (1): <sup>1</sup>H NMR for compound 2.



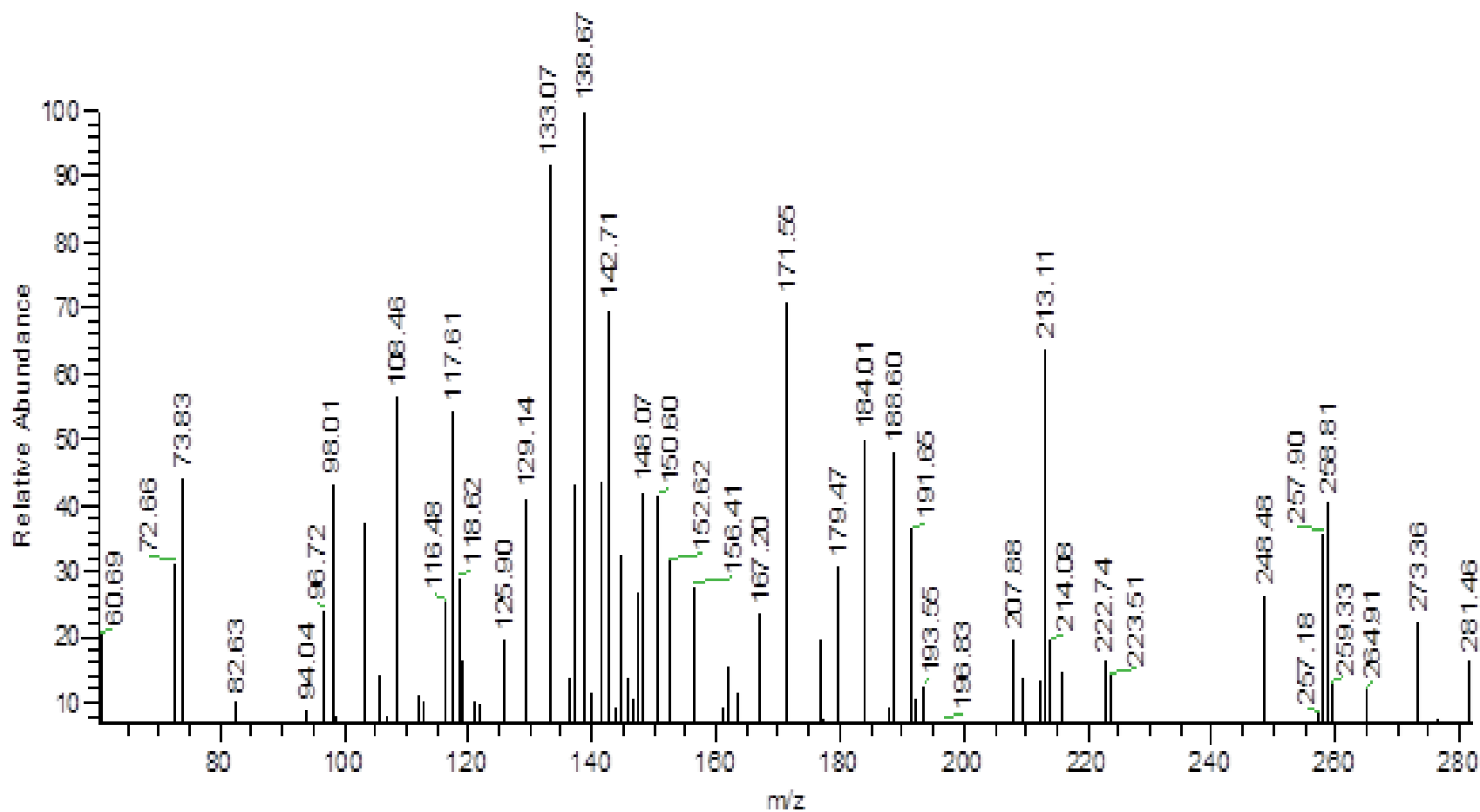
Supplementary fig. (2): <sup>13</sup>C NMR for compound 2.

eman-sadek-2 #139-140 RT: 2.34-2.36 AV: 2 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.61E2  
T: + c EI Full ms [40.00-1000.00]

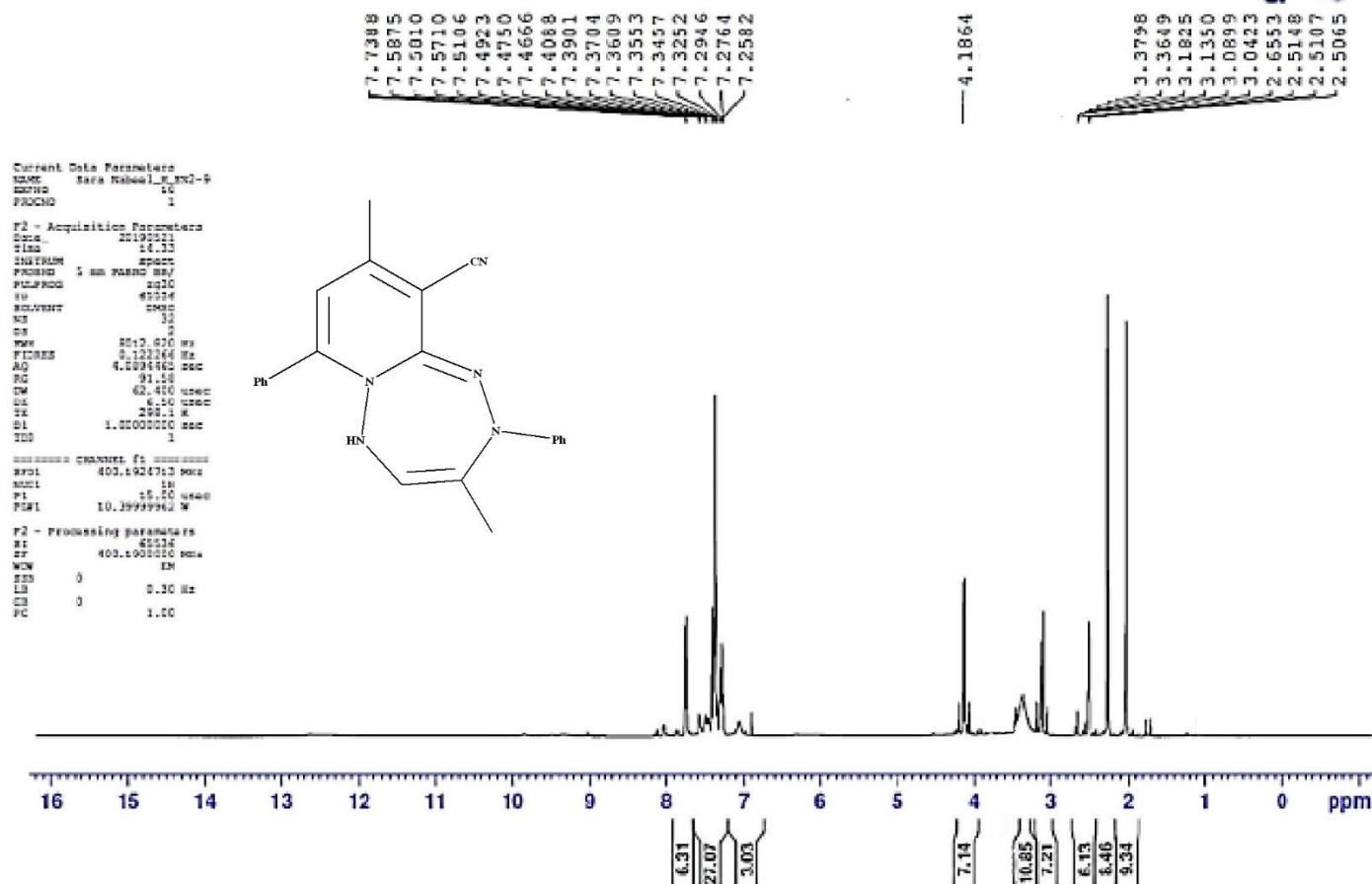


Supplementary fig. (3): mass spectrum for compound 2.

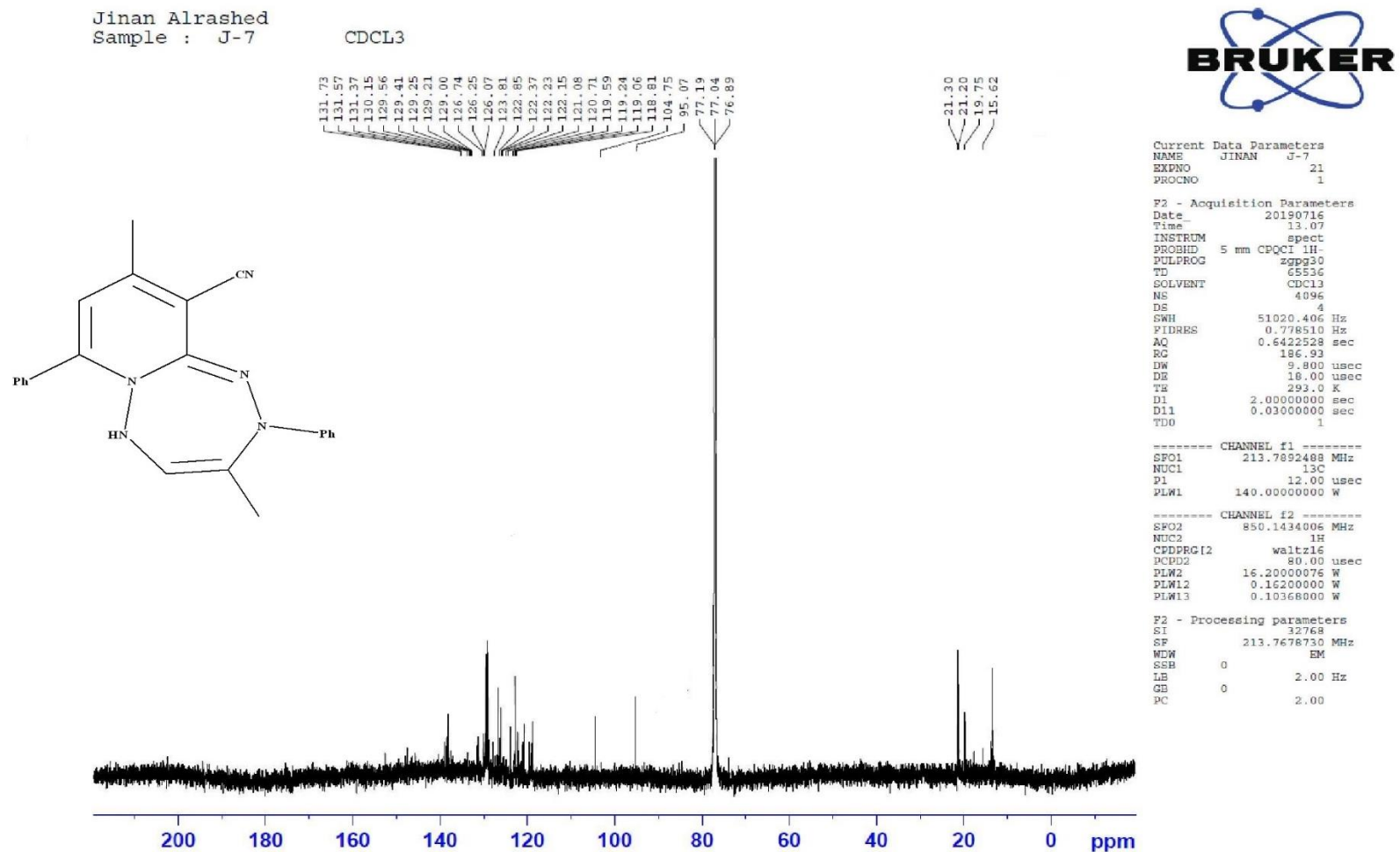
eman-sadek-4#162-165 RT: 2.73-2.78 AV: 4 SB: 28 1.21-1.34 ,0.87-1.14 NL: 1.68E2  
T: + c EI Full ms [40.00-1000.00]



Supplementary fig. (4): mass spectrum for compound 3.

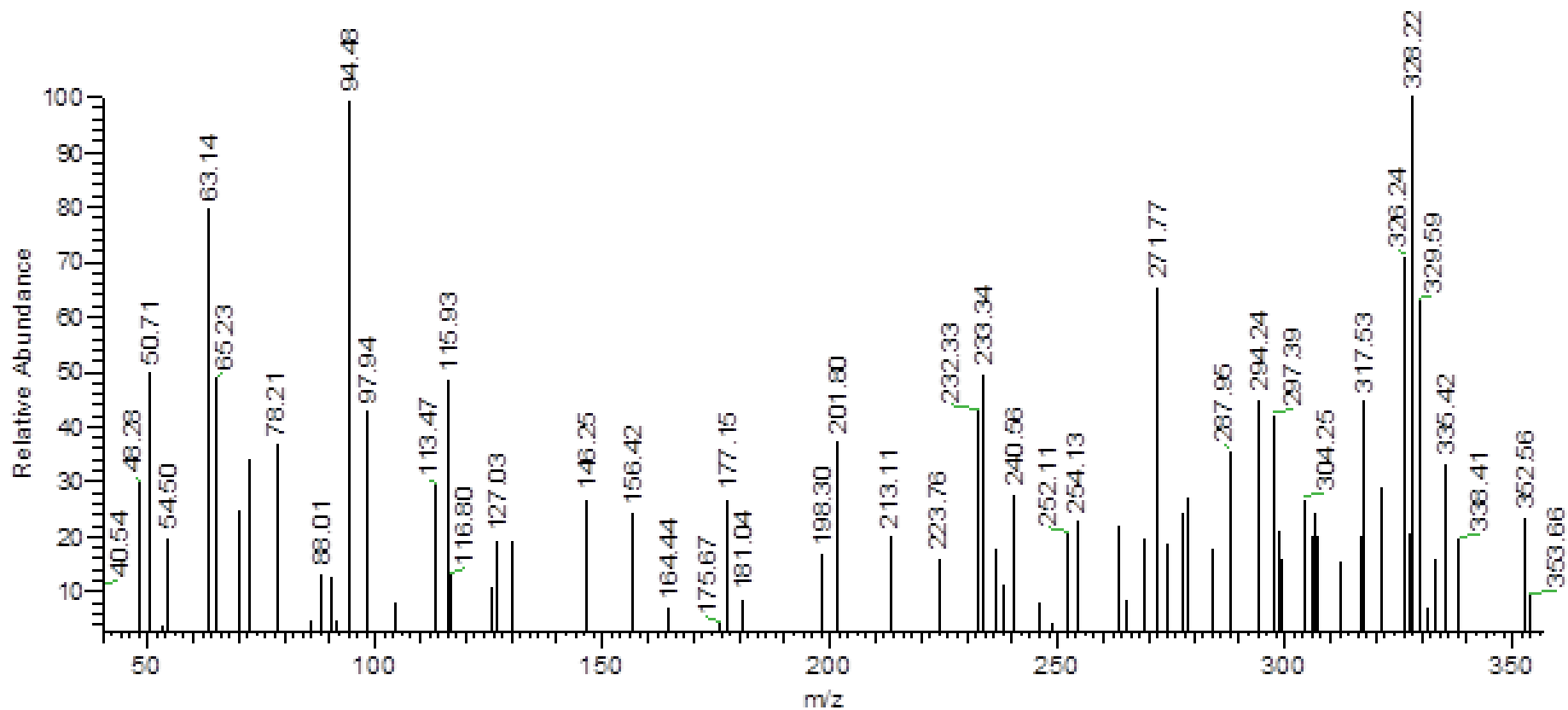


Supplementary fig. (5): <sup>1</sup>H NMR for compound 4.



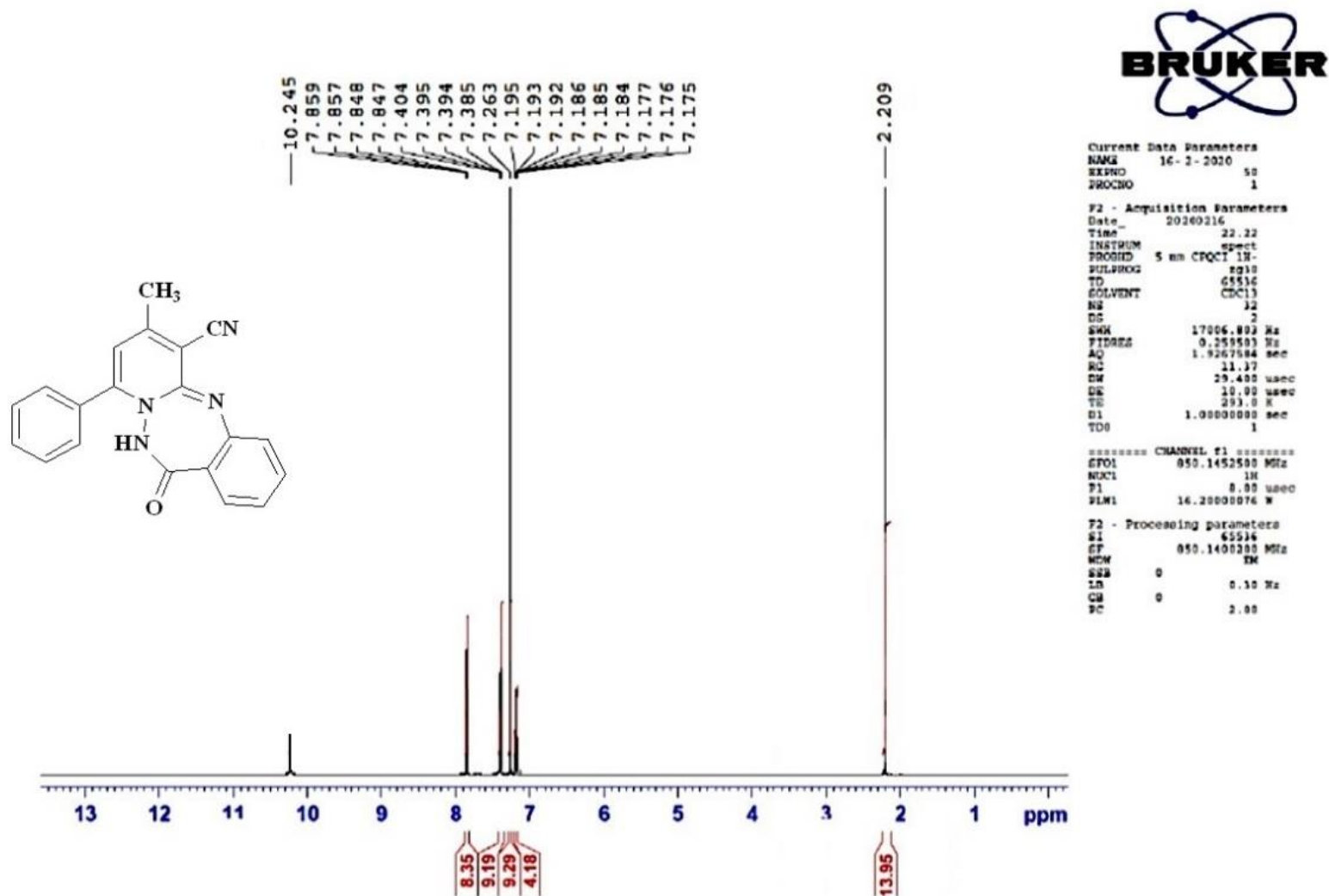
Supplementary fig. (6): <sup>13</sup>C NMR for compound 4.

eman-sadek-5 #167-169 RT: 2.81-2.85 AV: 3 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.58E2  
T: + c EI Full ms [40.00-1000.00]

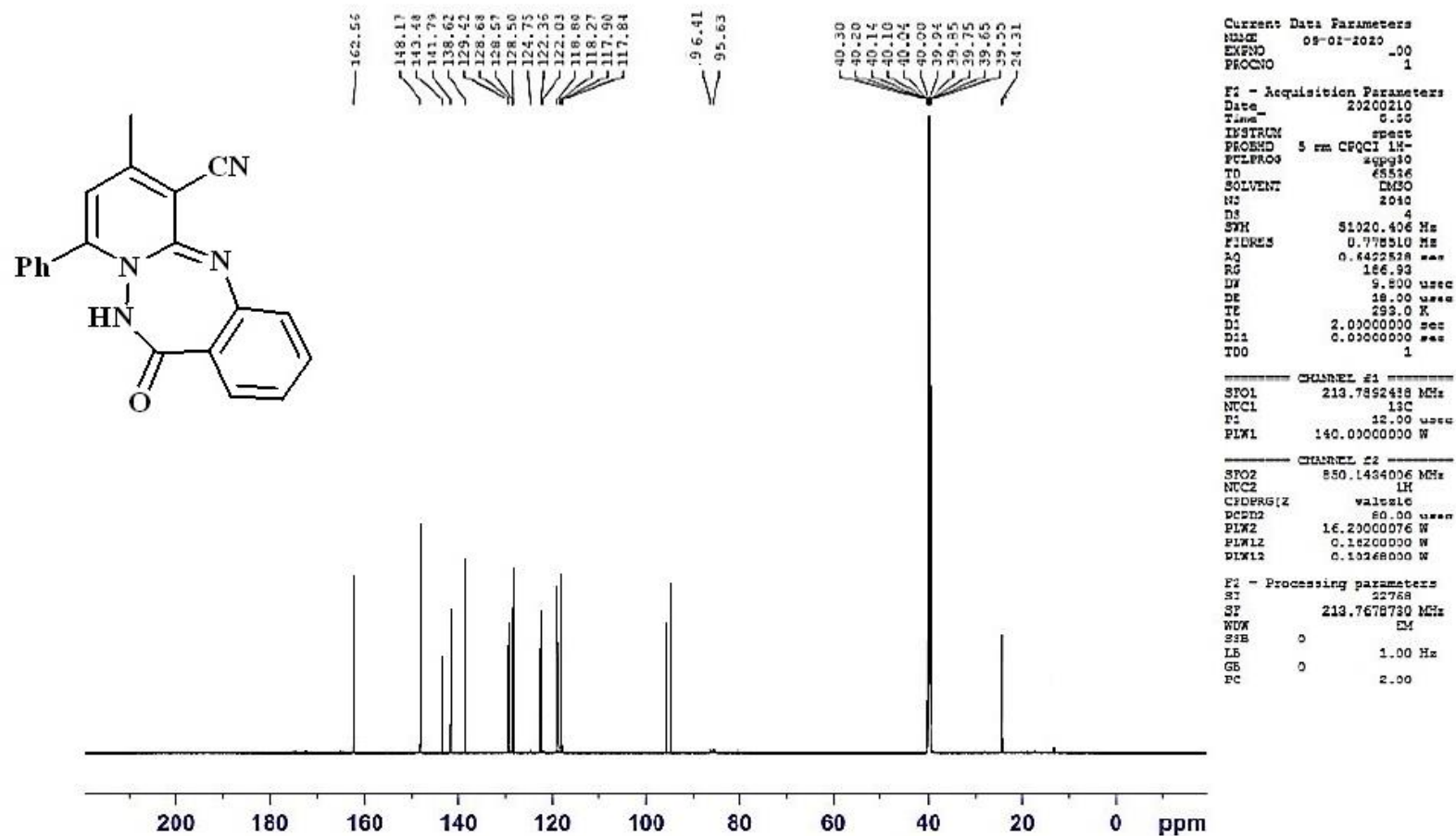


Supplementary fig. (7): mass spectrum for compound 4.



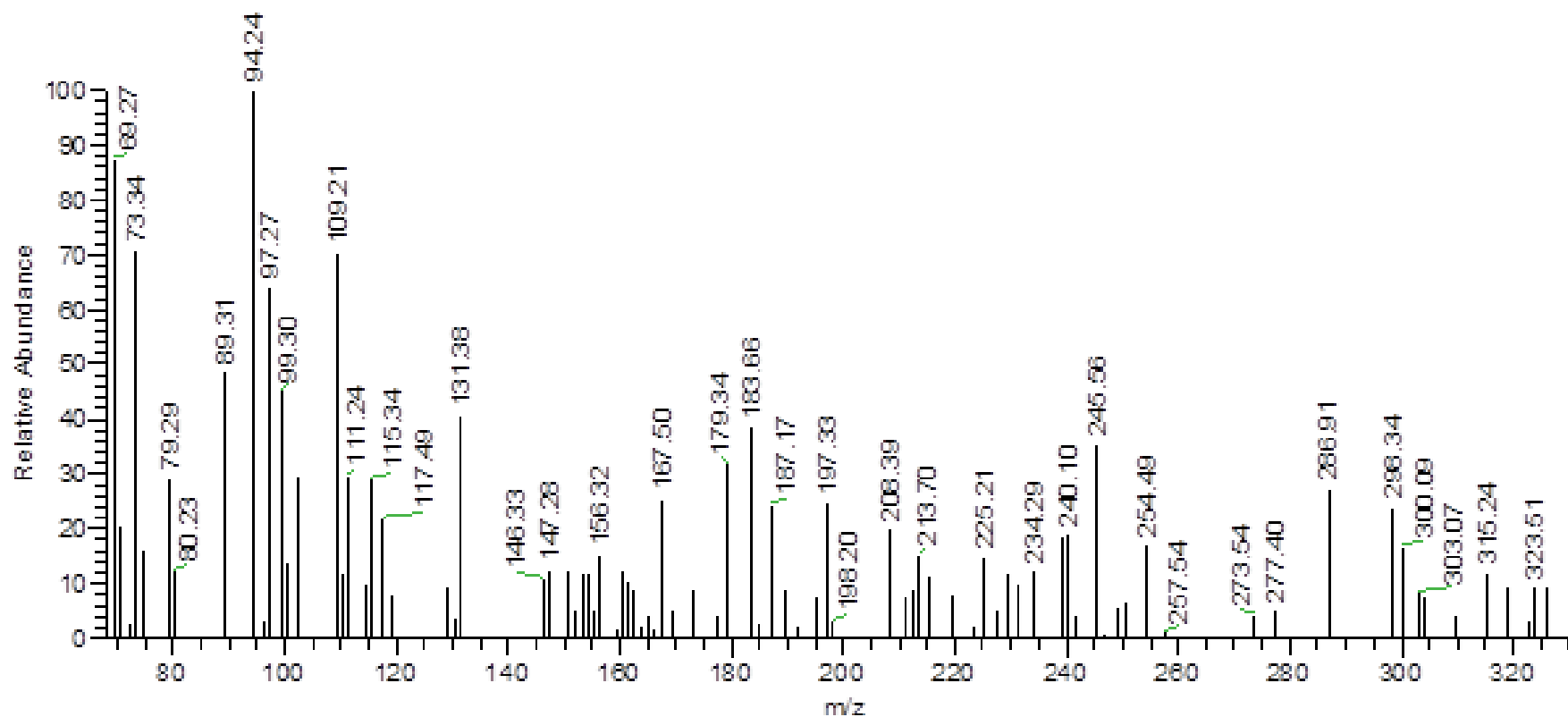


Supplementary fig. (8): <sup>1</sup>H NMR for compound 5.

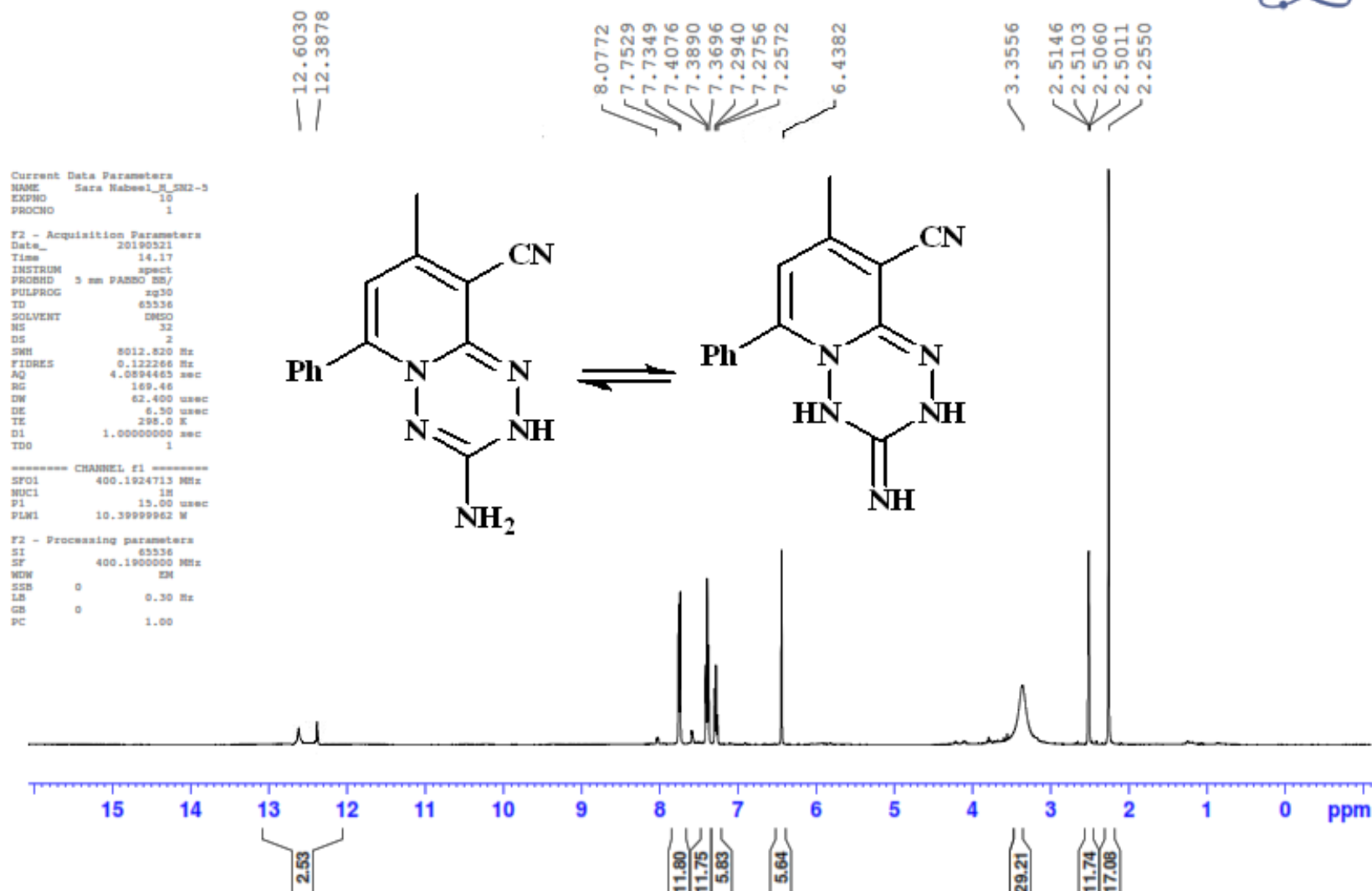


Supplementary fig. (9): <sup>13</sup>C NMR for compound 5.

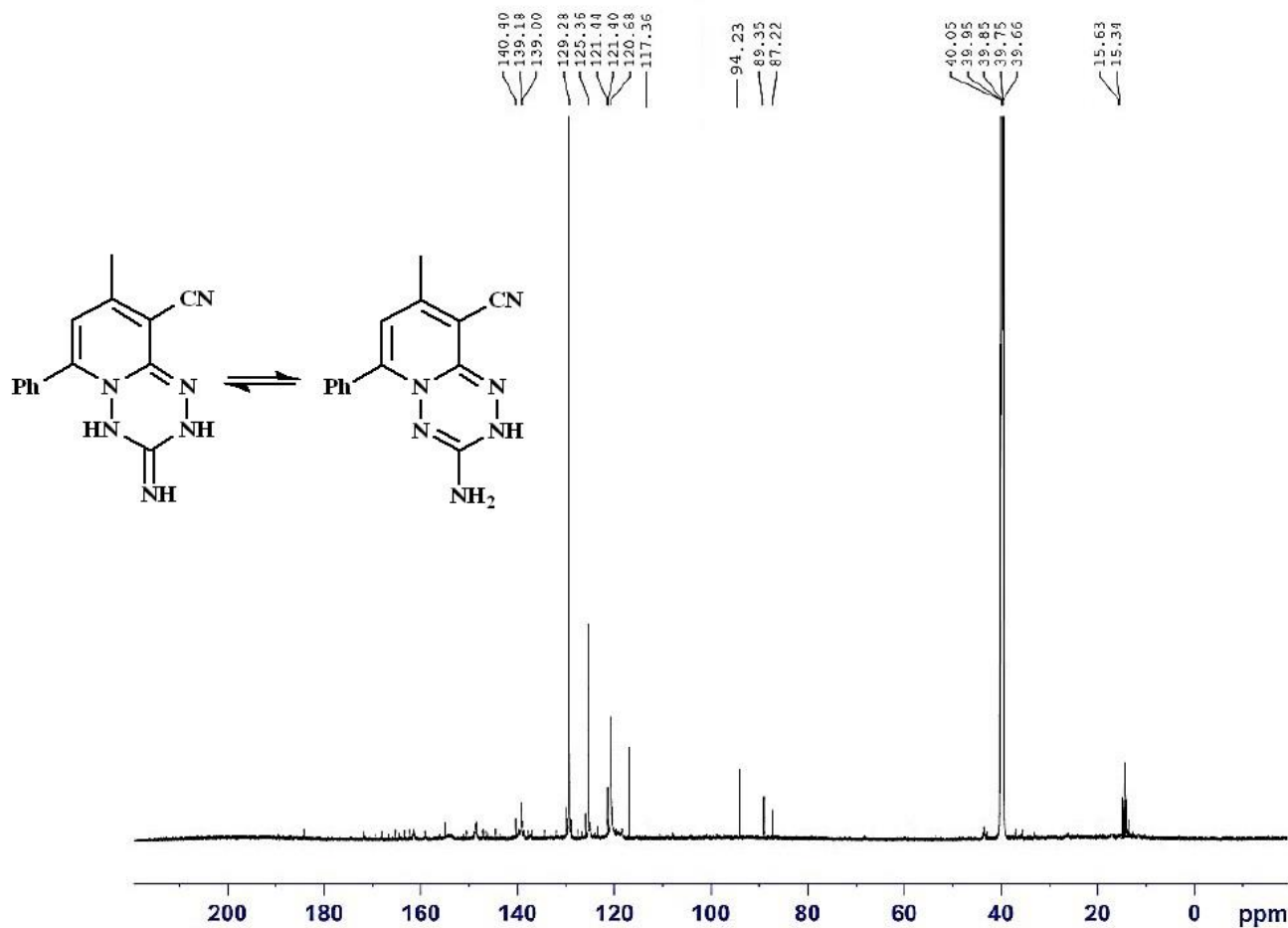
eman-sadek-8 #81-84 RT: 1.04-1.09 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 2.45E2  
T: + c EI Full ms [40.00-1000.00]



Supplementary fig. (10): mass spectrum for compound 5.



Supplementary fig. (11): <sup>1</sup>H NMR for compound 7.



Current Data Parameters  
 NAME 09-02-2020  
 EXPNO 60  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200209  
 Time 20.56  
 INSTRUM spect  
 PROBHD 5 mm CPQCI 1H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2048  
 DS 4  
 SWH 51020.406 Hz  
 FIDRES 0.778510 Hz  
 AQ 0.6422528 sec  
 RG 186.93  
 DW 9.000 usec  
 DE 18.00 usec  
 TE 293.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

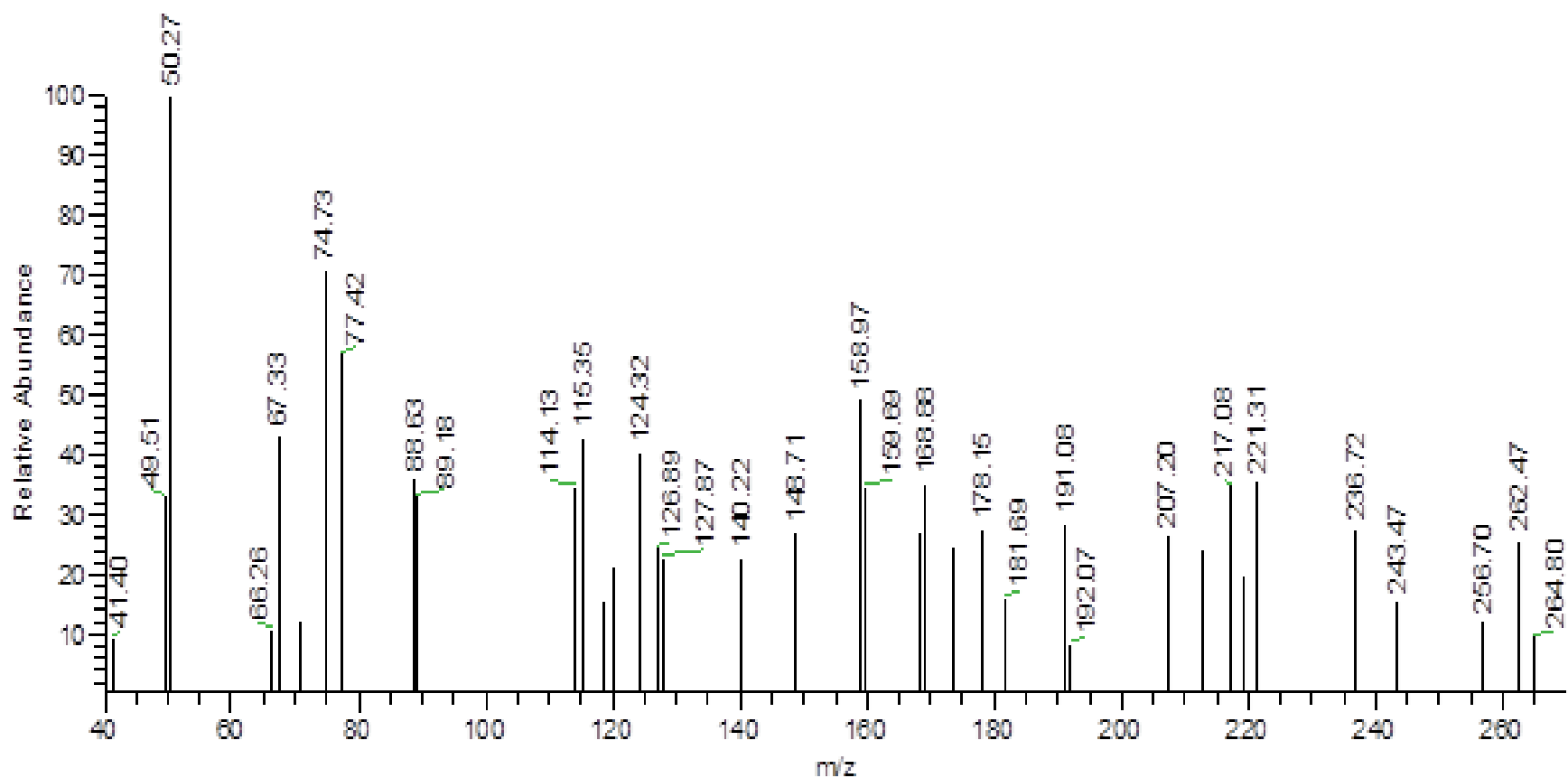
===== CHANNEL f1 =====  
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 NUC1 13C  
 P1 12.00 usec  
 PLW1 140.0000000 W

===== CHANNEL f2 =====  
 SFO2 500.1434006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 16.20000076 W  
 PLW12 0.16200000 W  
 PLW13 0.10360000 W

F2 - Processing parameters  
 SI 32768  
 SF 213.7678739 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 2.00

Supplementary fig. (12): <sup>13</sup>C NMR for compound 7.

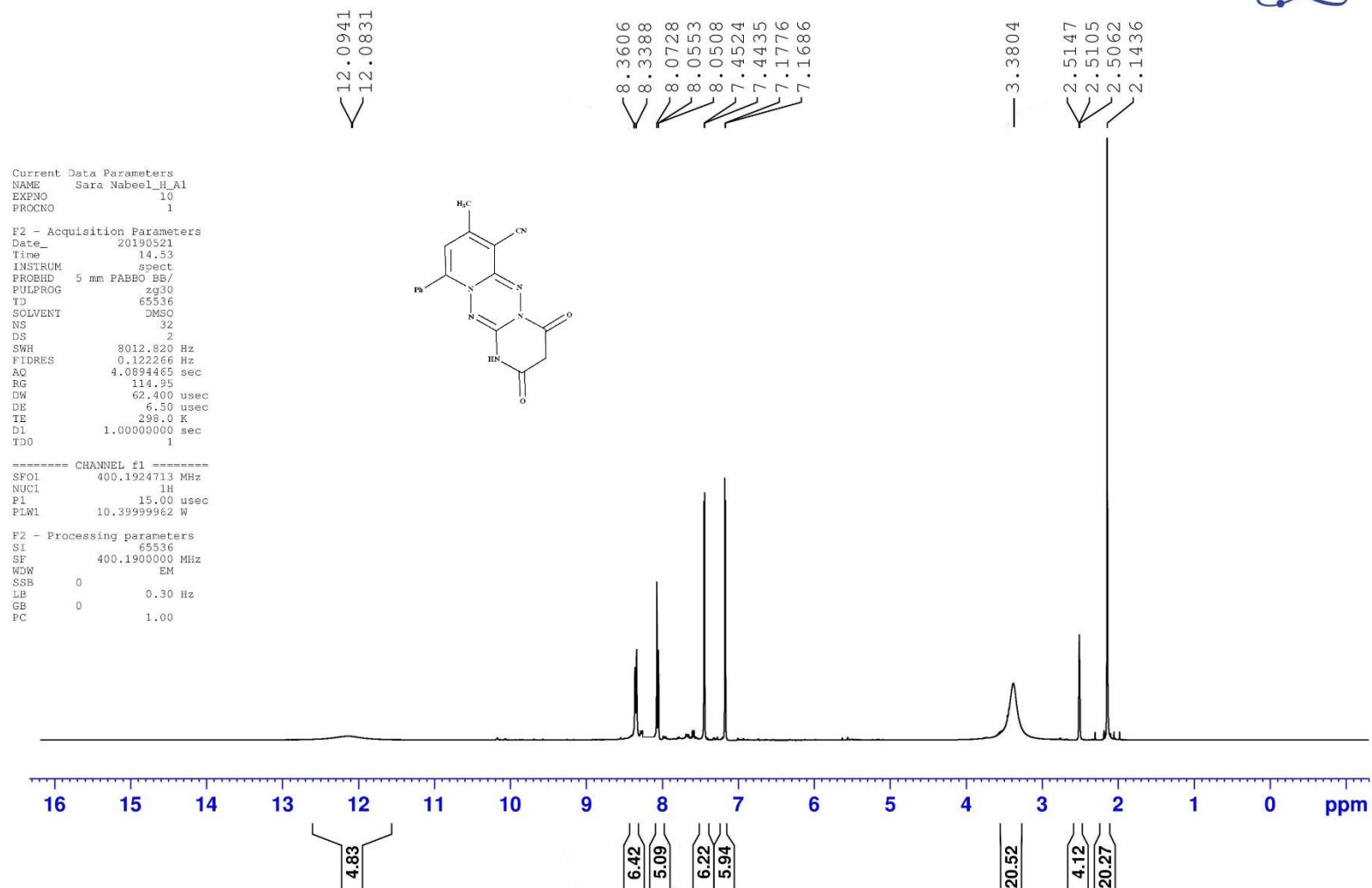
eman-sadek-8 #179-182 RT: 3.01-3.08 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.09E2  
T: + c EI Full ms [40.00-1000.00]



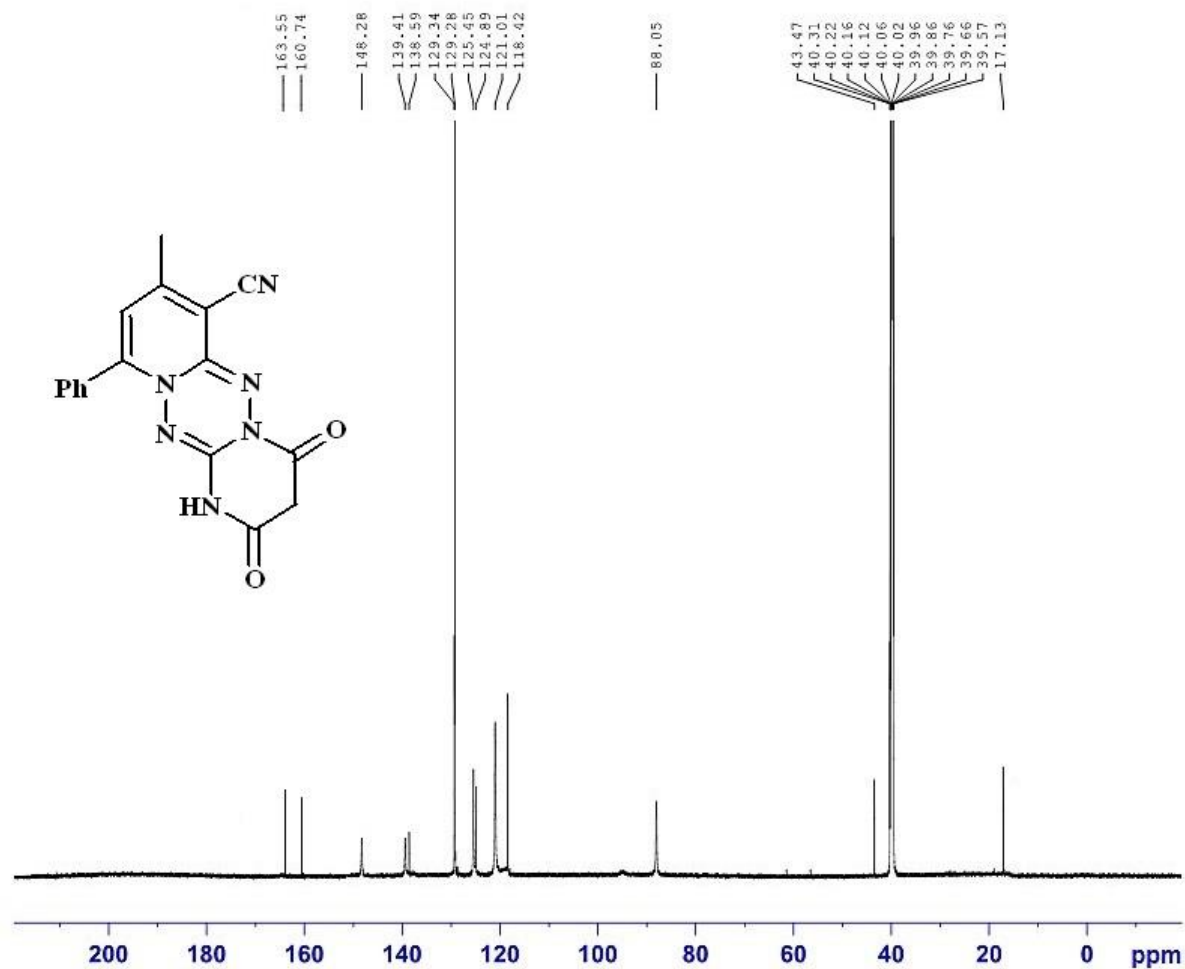
Supplementary fig. (13): mass spectrum for compound 7.

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Supplementary fig. (14): <sup>1</sup>H NMR for compound 8.



Current Data Parameters  
 NAME JINAN J-9 09-02-2020  
 EXPNO 70  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200209  
 Time\_ 23.59  
 INSTRUM spect  
 PROBHD 5 mm CPQCI 1H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2048  
 DS 4  
 SWH 51020.406 Hz  
 FIDRES 0.778510 Hz  
 AQ 0.6422528 sec  
 RG 186.93  
 DW 9.800 usec  
 DE 18.00 usec  
 TE 292.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 213.7892488 MHz  
 NUC1 13C  
 P1 12.00 usec  
 PLW1 140.00000000 W

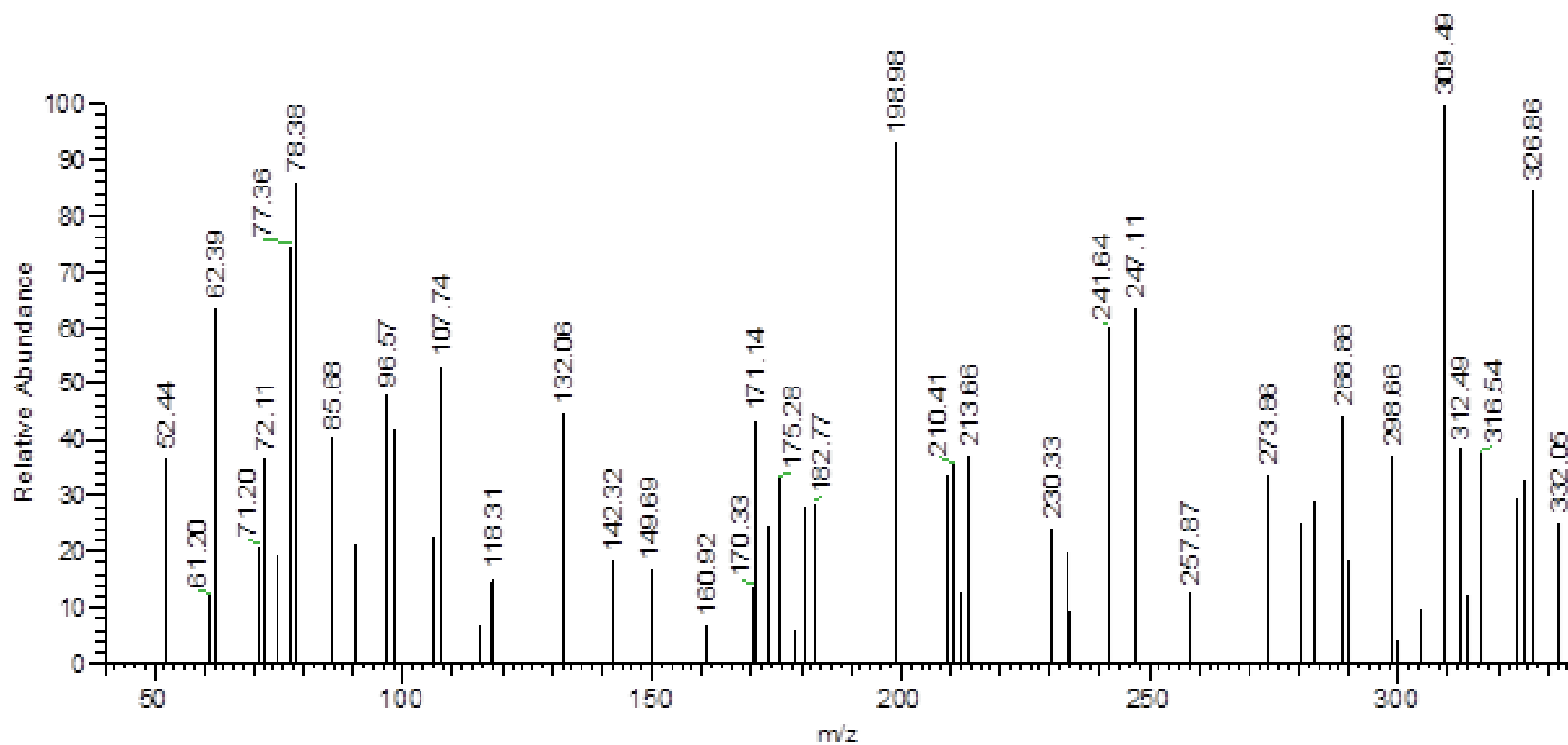
===== CHANNEL f2 =====  
 SFO2 850.1434006 MHz  
 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD2 80.00 usec  
 PLW2 16.20000076 W  
 PLW12 0.16200000 W  
 PLW13 0.10365000 W

F2 - Processing parameters  
 SI 32768  
 SF 213.7678730 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 2.00

Supplementary fig. (15): <sup>13</sup>C NMR for compound 8.



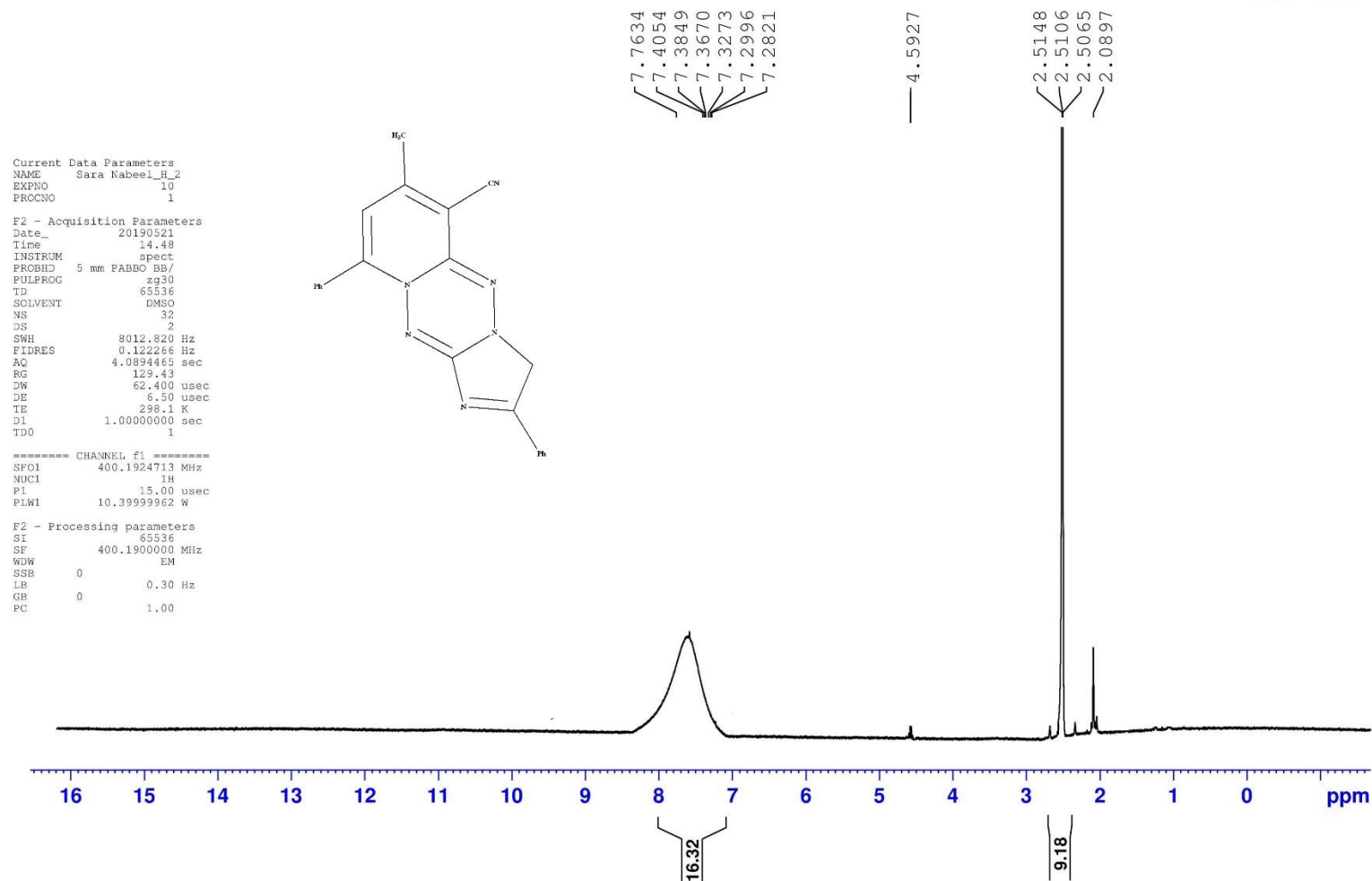
eman-sadek-9#115-117 RT: 1.94-1.97 AV: 3 SB: 26 1.21-1.34 ,0.87-1.14 NL: 9.18E1  
T: + c EI Full ms [40.00-1000.00]



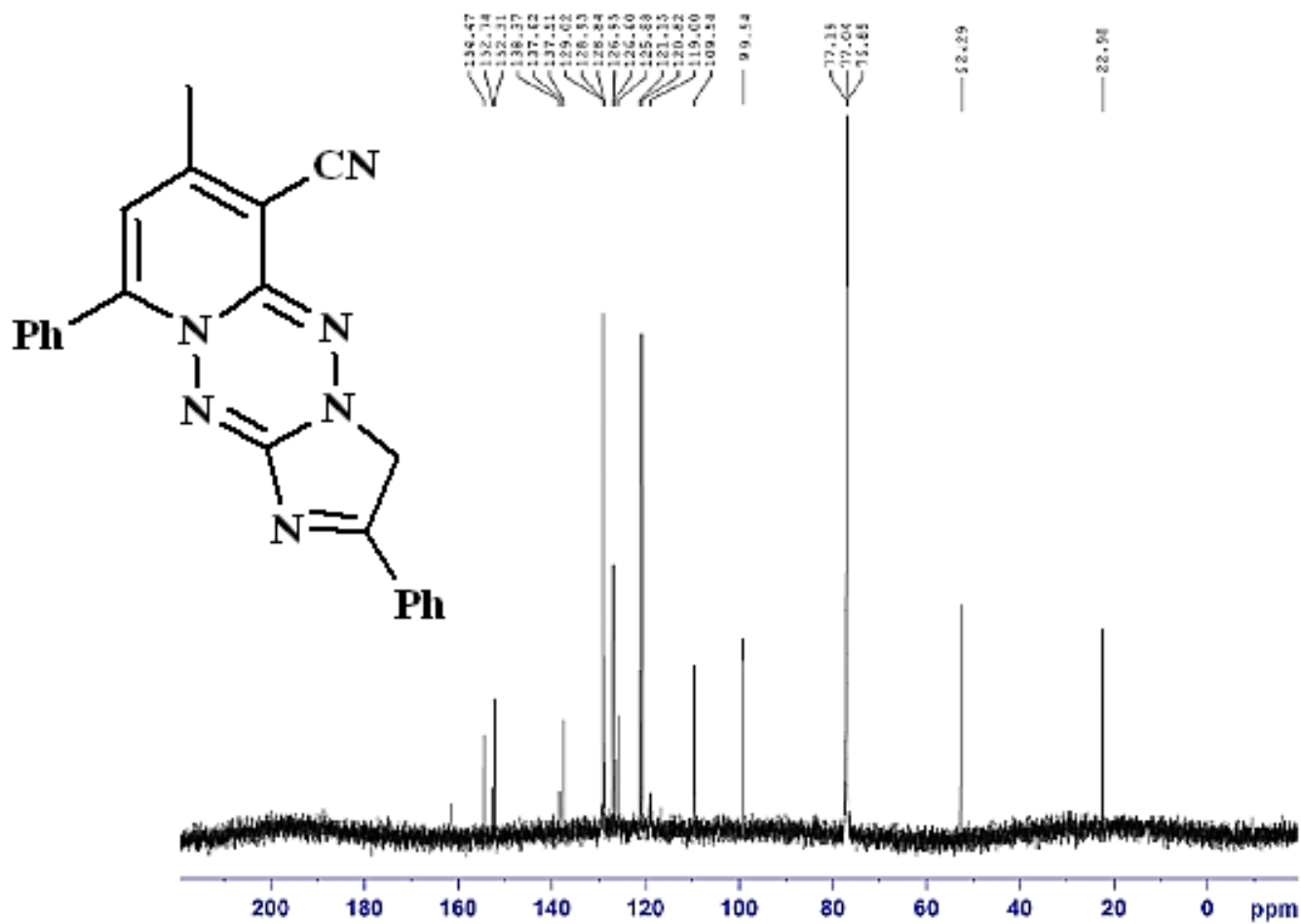
Supplementary fig. (16): mass spectrum for compound 8.

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Supplementary fig. (17): <sup>1</sup>H NMR for compound 9.



Current Data Parameters  
 NAME 03-02-2020  
 EXNO 18  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 23/02/24  
 Time 15:48  
 INSTRUM spect  
 PROBRD 5 mm CPDQ 1H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1000  
 DS 4  
 SWH 51320.404 Hz  
 FIDRES 0.775310 Hz  
 AQ 0.6122321 sec  
 RG 126.93  
 DM 9.800 umsec  
 DE 18.00 usec  
 TE 293.2 K  
 D1 2.01000100 sec  
 D11 0.01000000 sec  
 TDO 1

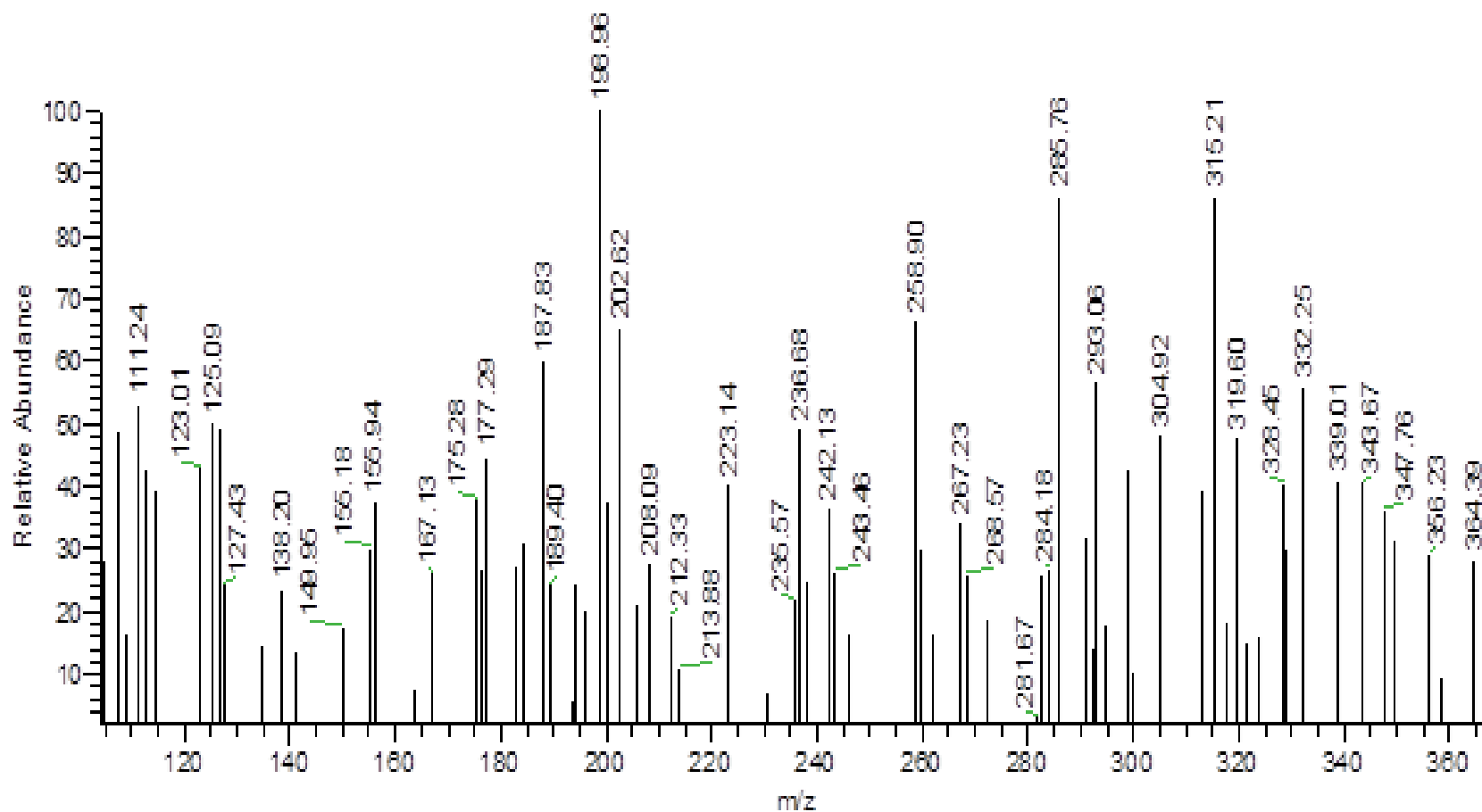
===== CHANNEL f1 =====  
 SFO1 213.3692468 MHz  
 NUCL1 13C  
 P1 12.00 usec  
 PCW1 140.01000000 W

===== CHANNEL f2 =====  
 SFO2 601.1434004 MHz  
 NUCL2 1H  
 CPDPRG2 waltz16  
 PCPD2 30.00 usec  
 PCW2 16.11000016 W  
 PCW12 0.13200000 W  
 PCW13 0.13260000 W

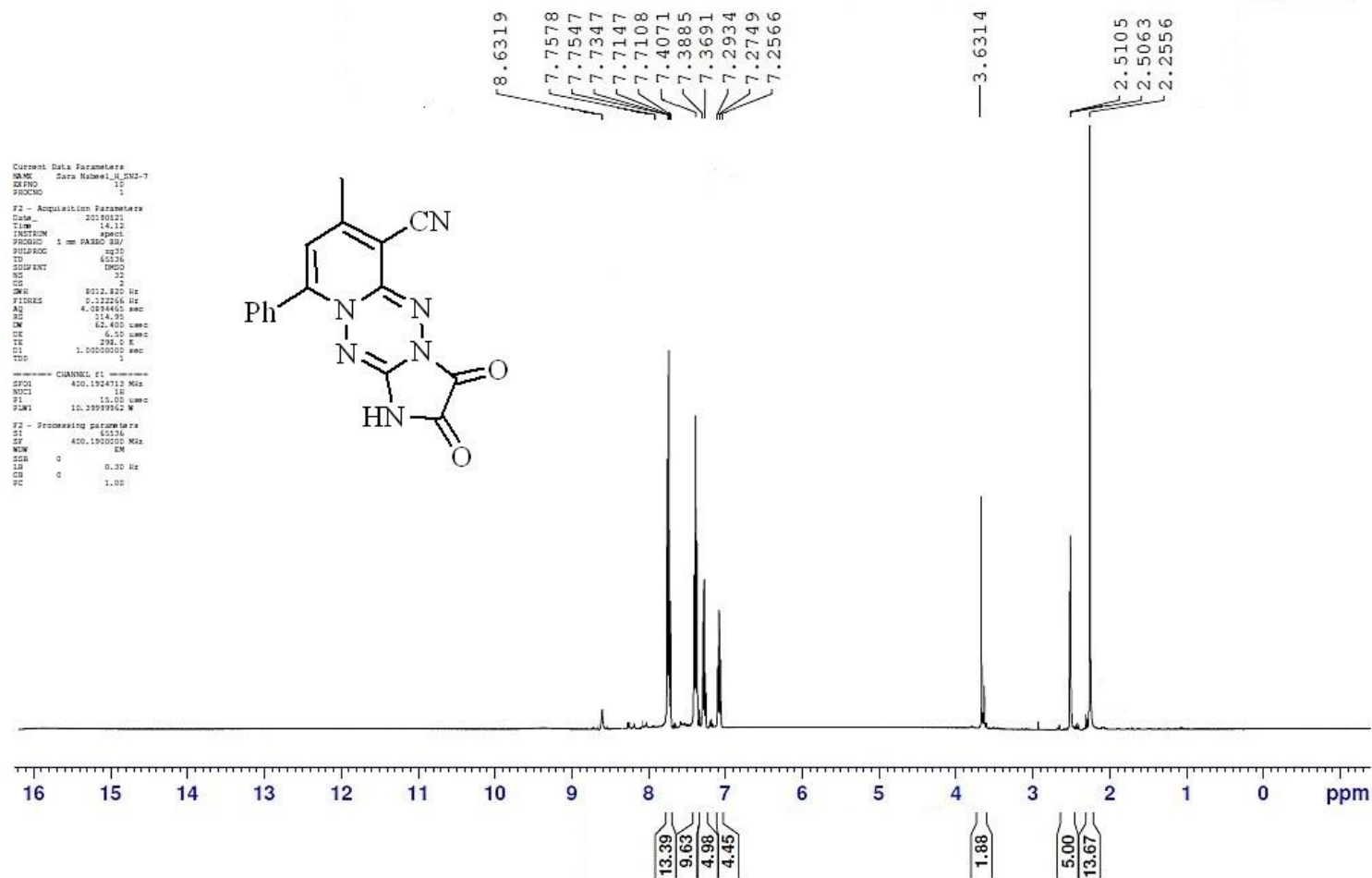
F2 - Processing parameters  
 SI 32768  
 SF 213.3695738 MHz  
 GDM MH  
 SWH 0  
 LB 2.00 MHz  
 GB 0  
 PC 2.00

Supplementary fig. (18): <sup>13</sup>C NMR for compound 9.

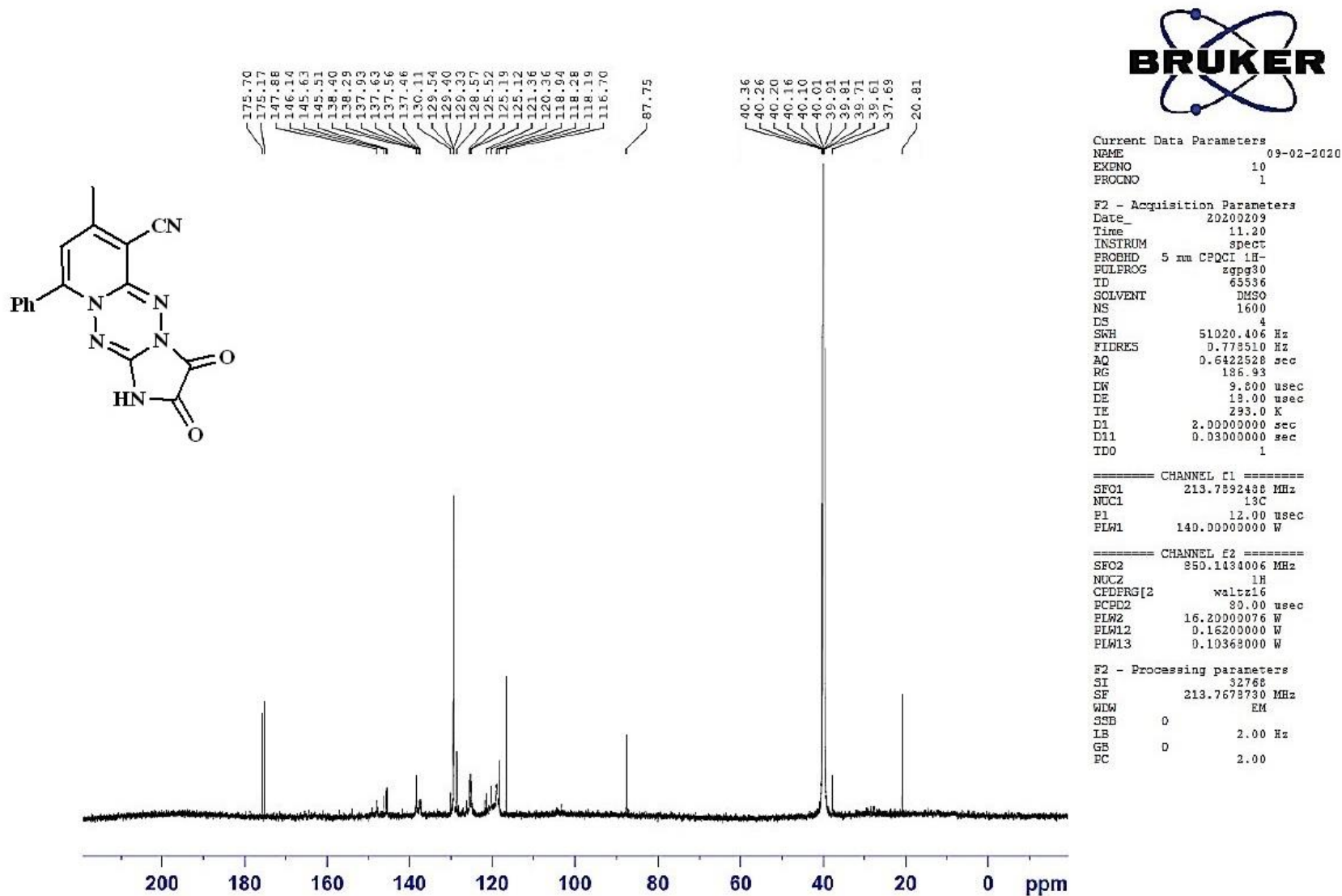
eman-sadek-10 #189-191 RT: 3.18-3.21 AV: 3 SB: 26 1.21-1.34, 0.87-1.14 NL: 8.87E1  
T: + c EI Full ms [40.00-1000.00]



Supplementary fig. (19): mass spectrum for compound 9.

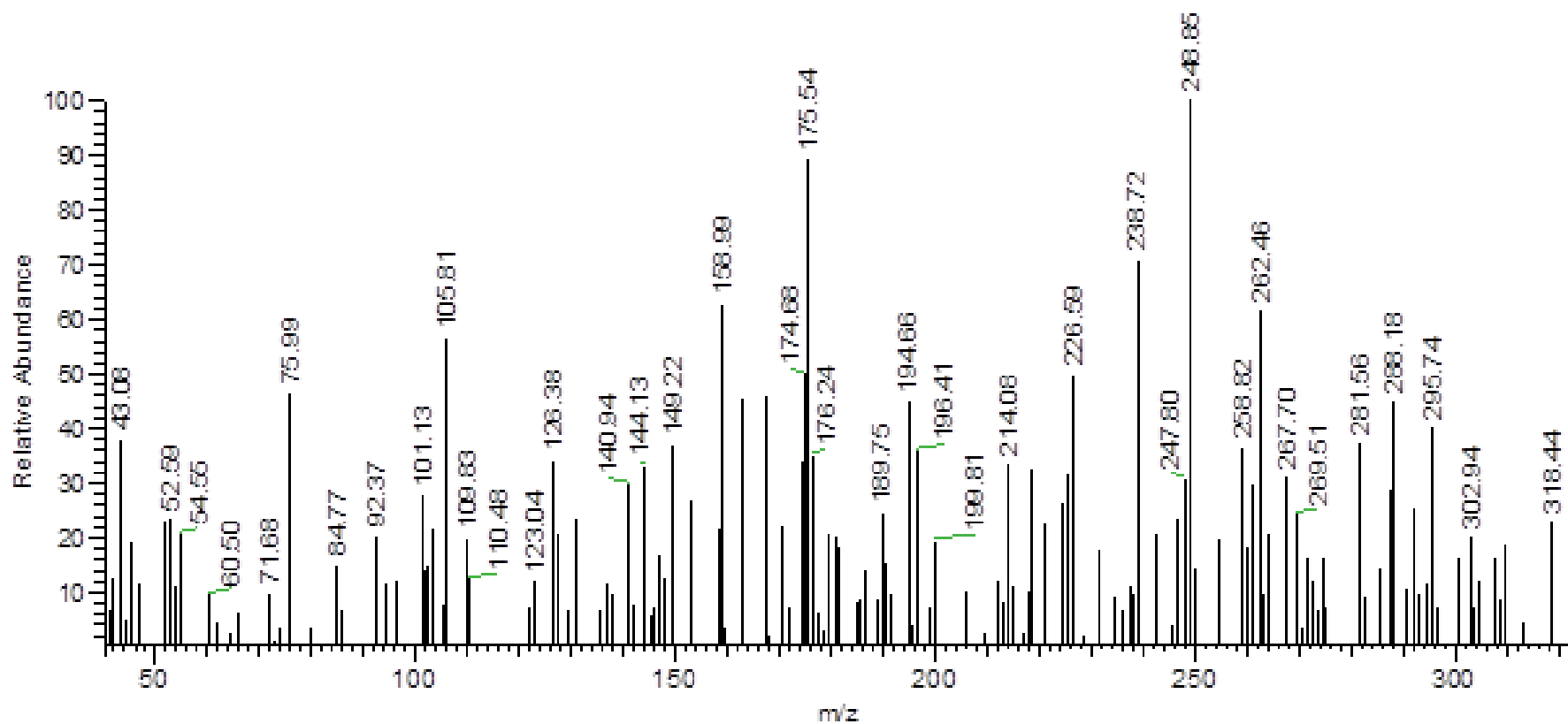


Supplementary fig. (20): <sup>1</sup>H NMR for compound 10.

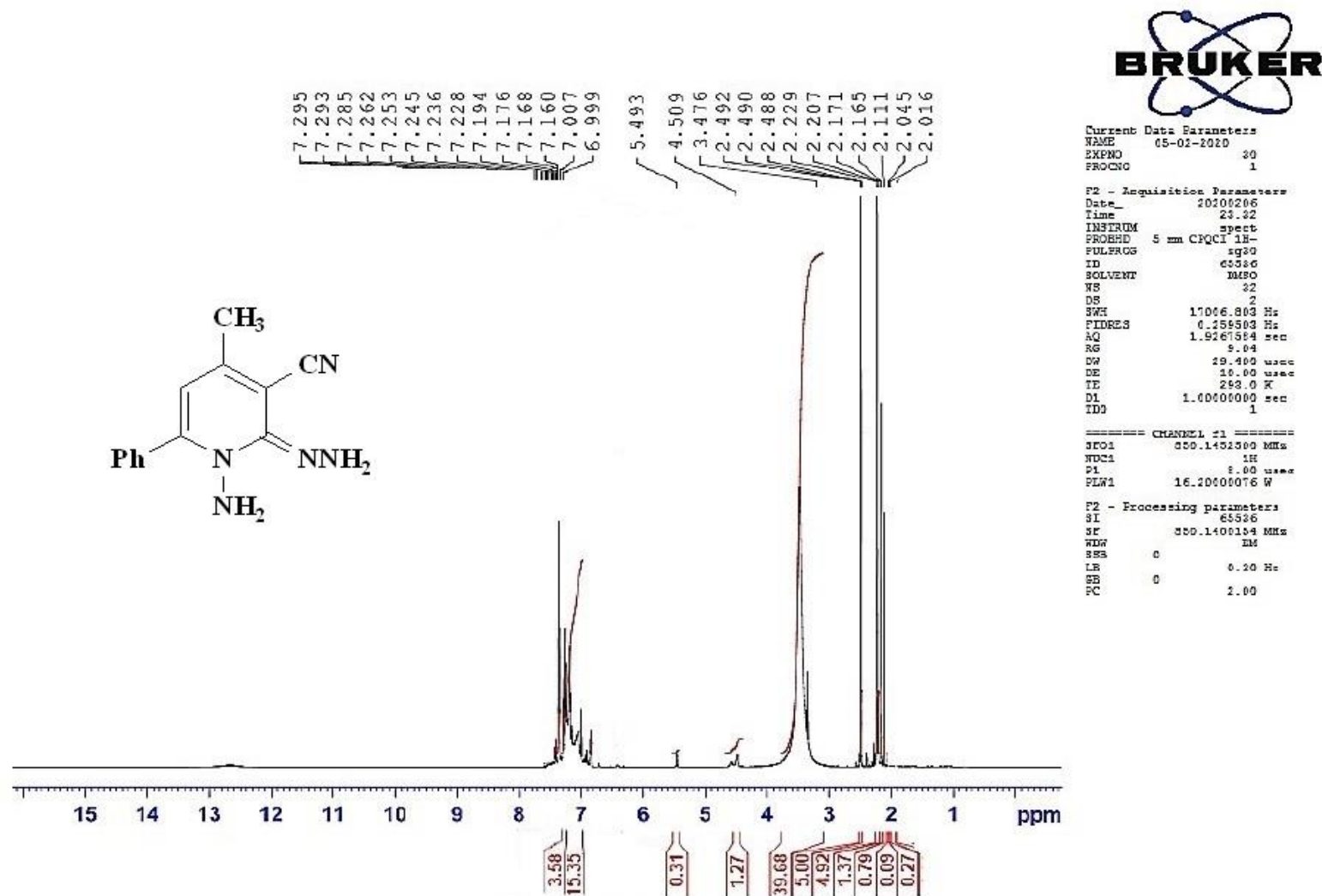


Supplementary fig. (21): <sup>13</sup>C NMR for compound 10.

eman-sadek-11 #145-147 RT: 2.44-2.48 AV: 3 SB: 26 1.21-1.34, 0.87-1.14 NL: 2.01E2  
T: + c EI Full ms [40.00-1000.00]

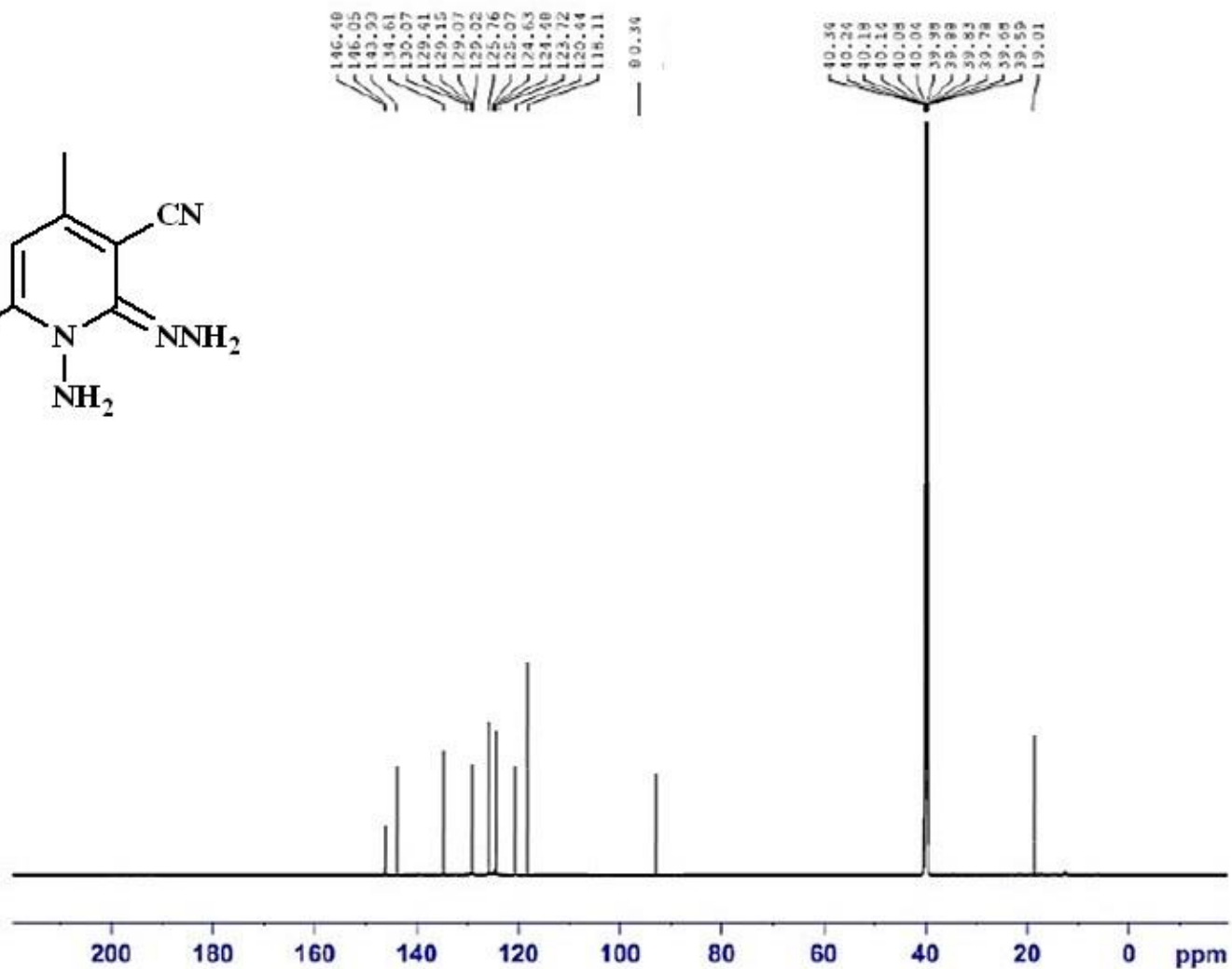
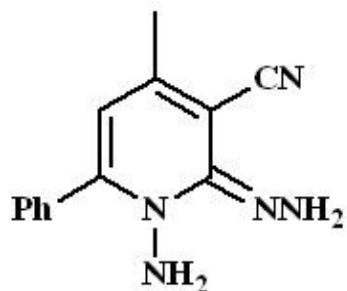


Supplementary fig. (22): mass spectrum for compound 10.



Supplementary fig. (23): <sup>1</sup>H NMR for compound 11.





Current Data Parameters  
 NAME 16-02-2020  
 EXPTNO 130  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200210  
 Time\_ 5.31  
 INSTRUM spect  
 P1 5 mm CPQCI 13-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1200  
 DS 4  
 SWH 51020.496 Hz  
 FIDRES 0.776810 Hz  
 AQ 0.6412528 sec  
 RS 186.30  
 DW 9.800 usec  
 DE 10.00 usec  
 TE 302.0 K  
 D1 2.00000000 sec  
 D11 0.02000000 sec  
 ID0 1

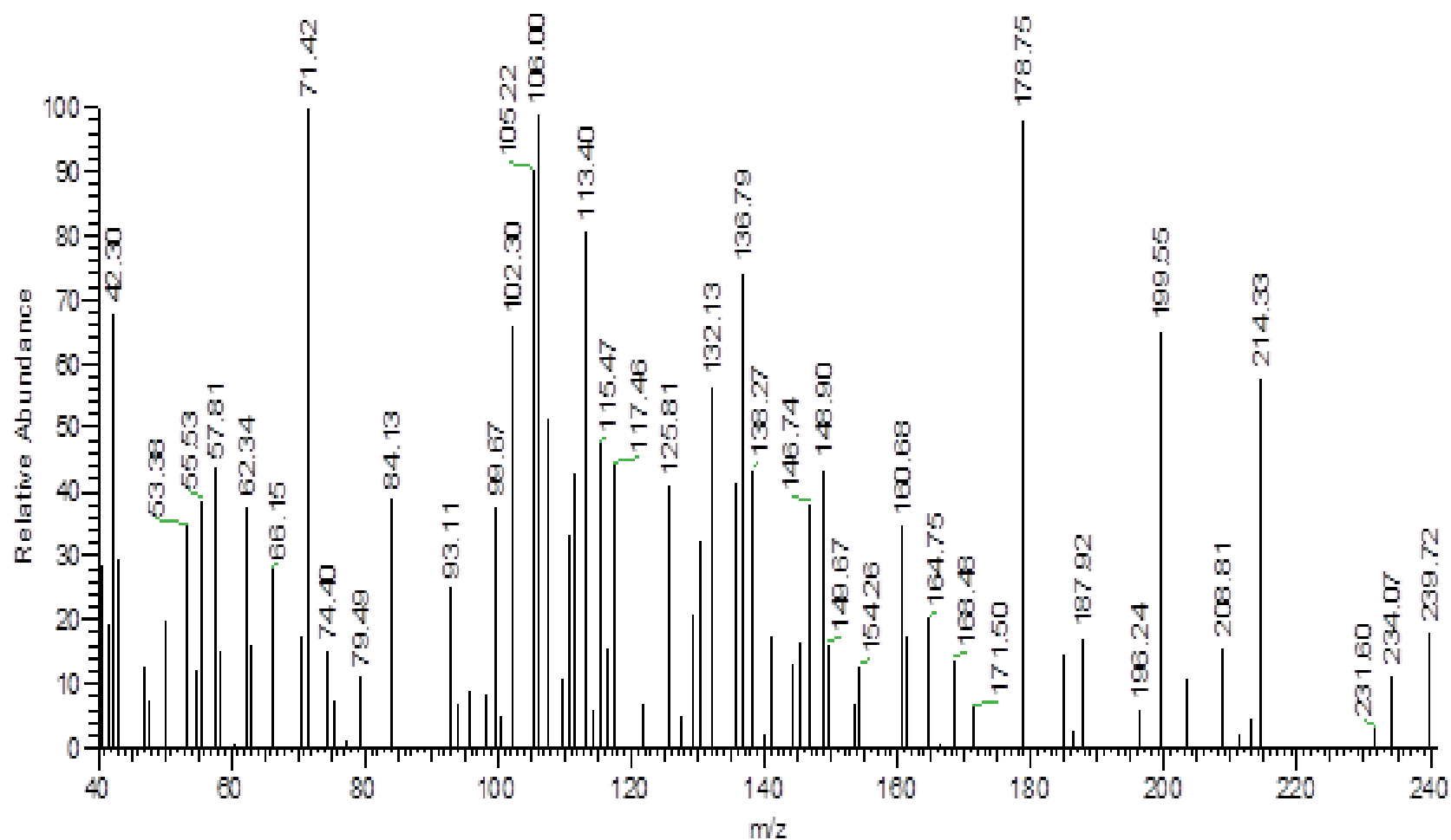
===== CHANNEL f1 =====  
 SFO1 213.7672438 MHz  
 NUQ1 13C  
 P1 12.00 usec  
 PLW1 140.0000000 W

===== CHANNEL f2 =====  
 SFO2 500.1364004 MHz  
 NUQ2 1H  
 CPDPRG2 waltz16  
 P1 80.00 usec  
 PLW2 15.20000074 W  
 PLW12 0.16200000 W  
 PLW13 0.10360000 W

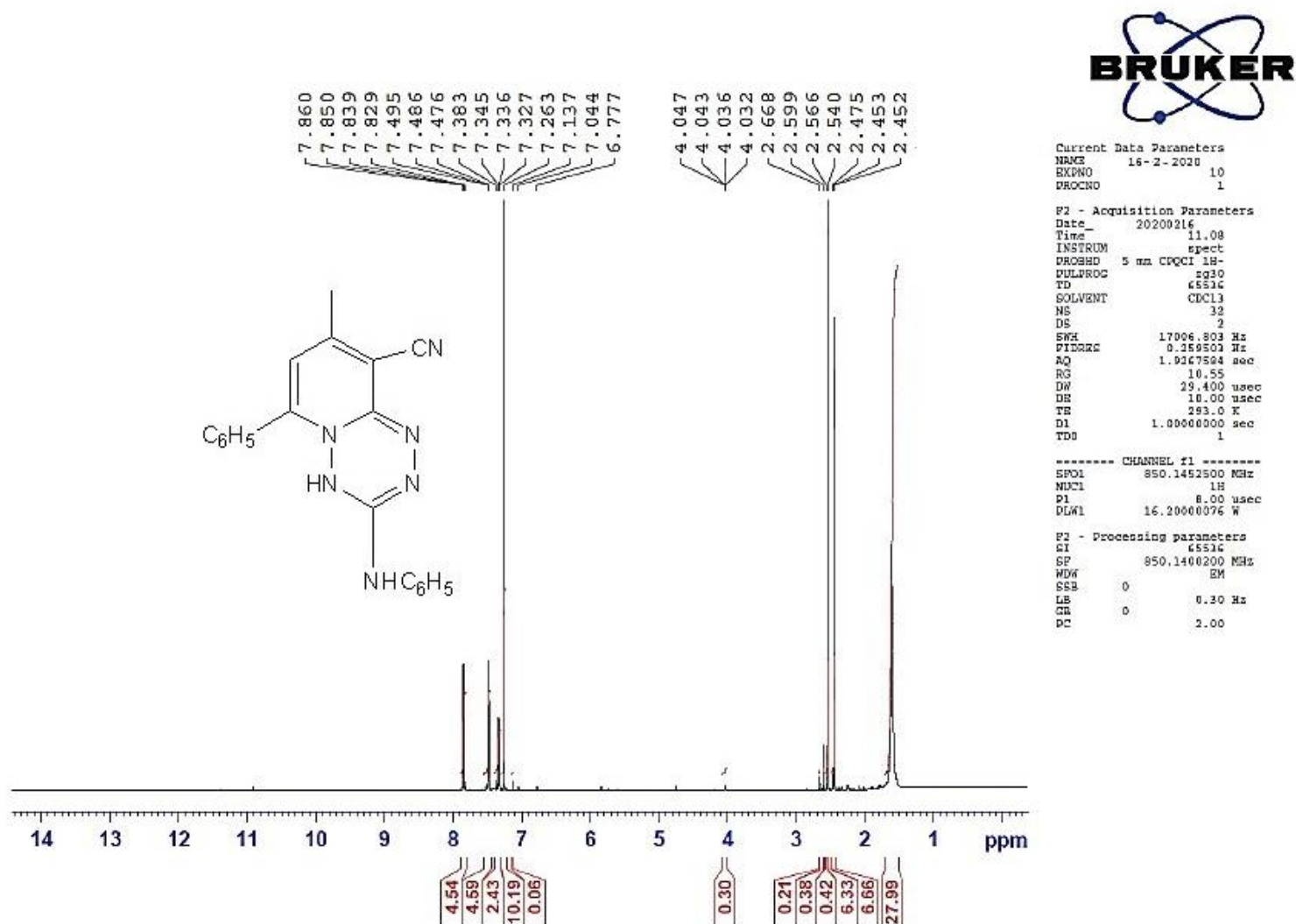
F2 - Processing parameters  
 SI 32768  
 SF 213.7678720 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

Supplementary fig. (24): <sup>13</sup>C NMR for compound 11.

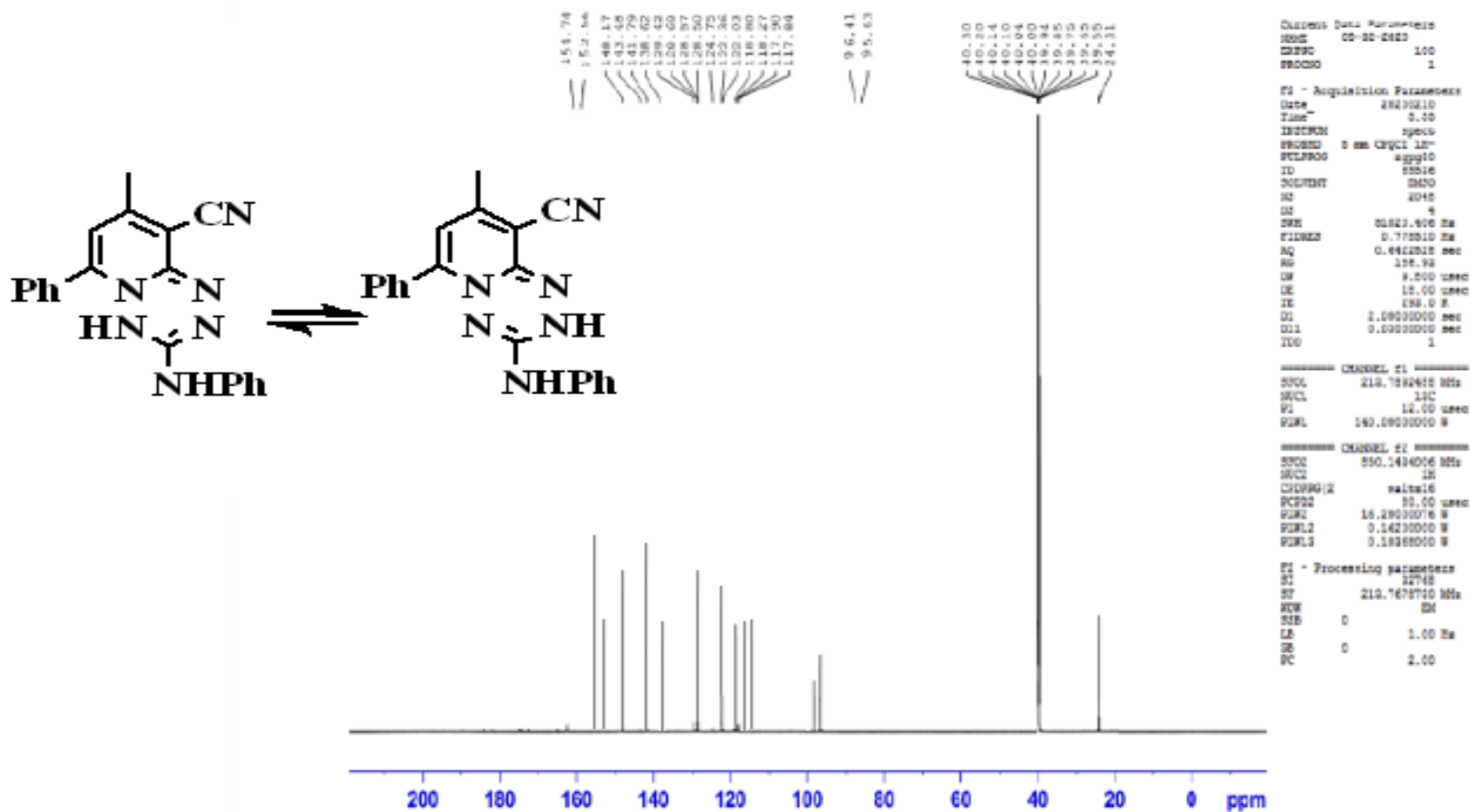
eman-sadek-12 #89-92 RT: 1.51-1.56 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.28E2  
T: + e EI Full ms [40.00-1000.00]



Supplementary fig. (25): mass spectrum for compound 11

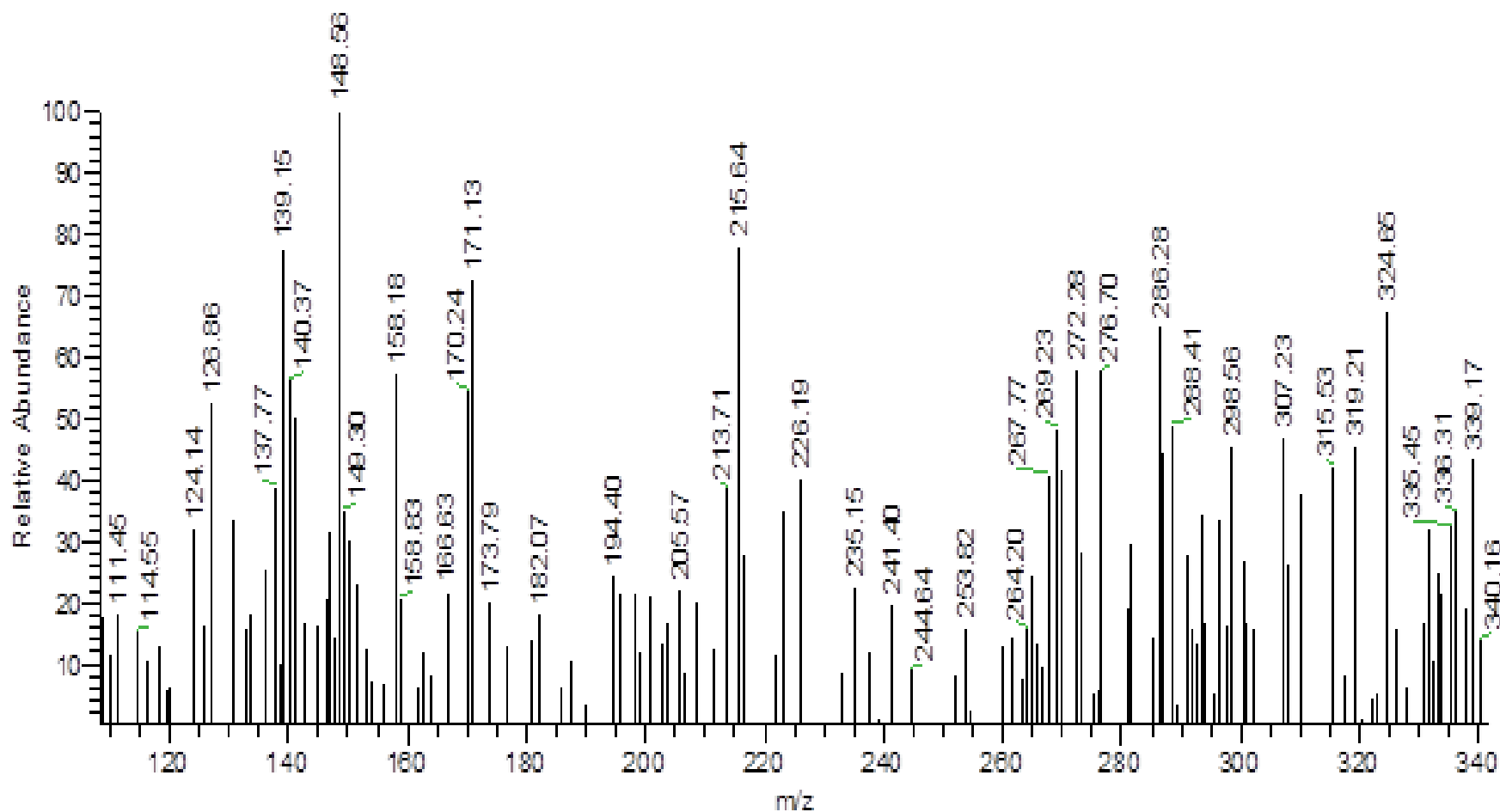


Supplementary fig. (26): <sup>1</sup>H NMR for compound 12.

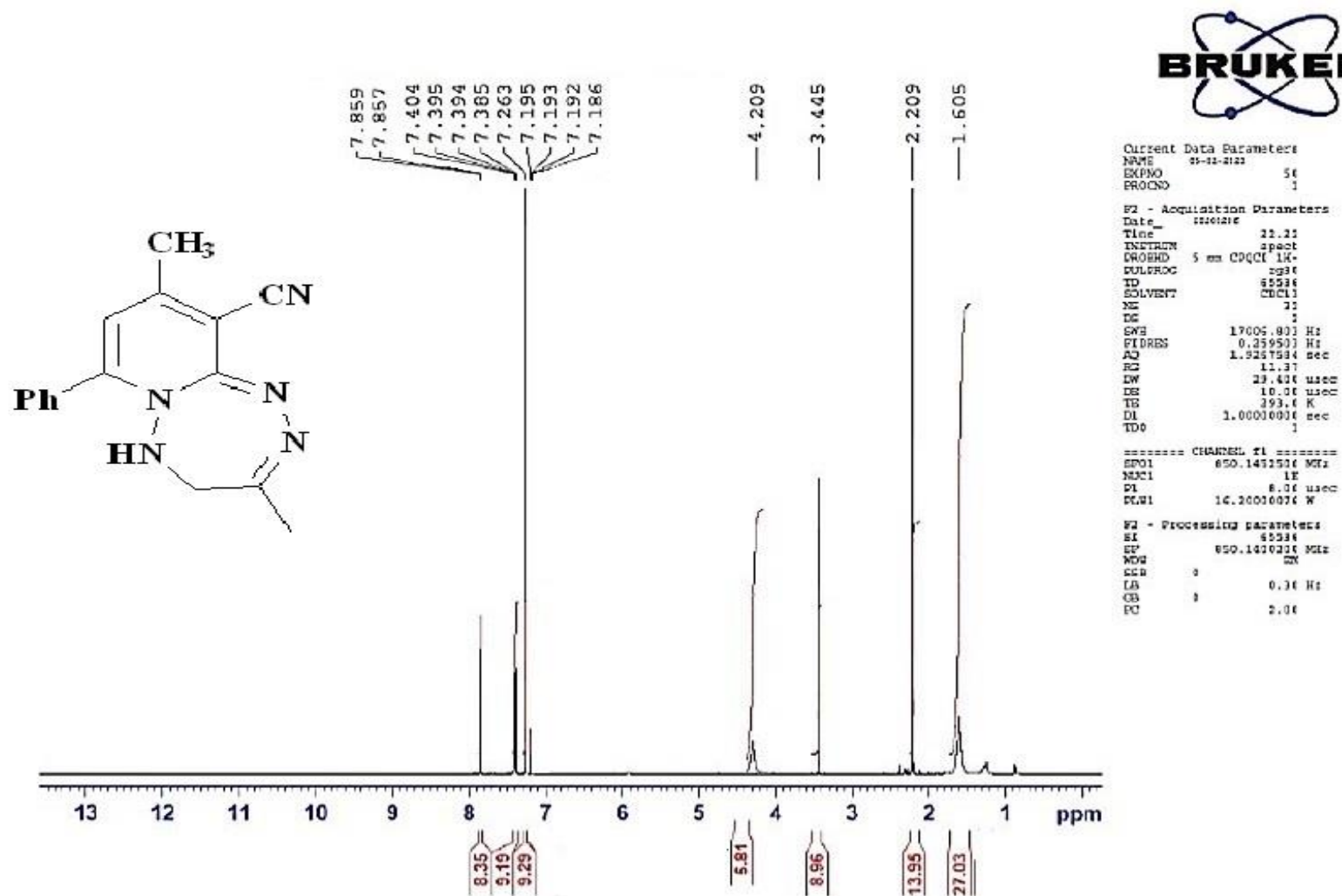


**Supplementary fig. (27):**  $^{13}\text{C}$  NMR for compound **12**.

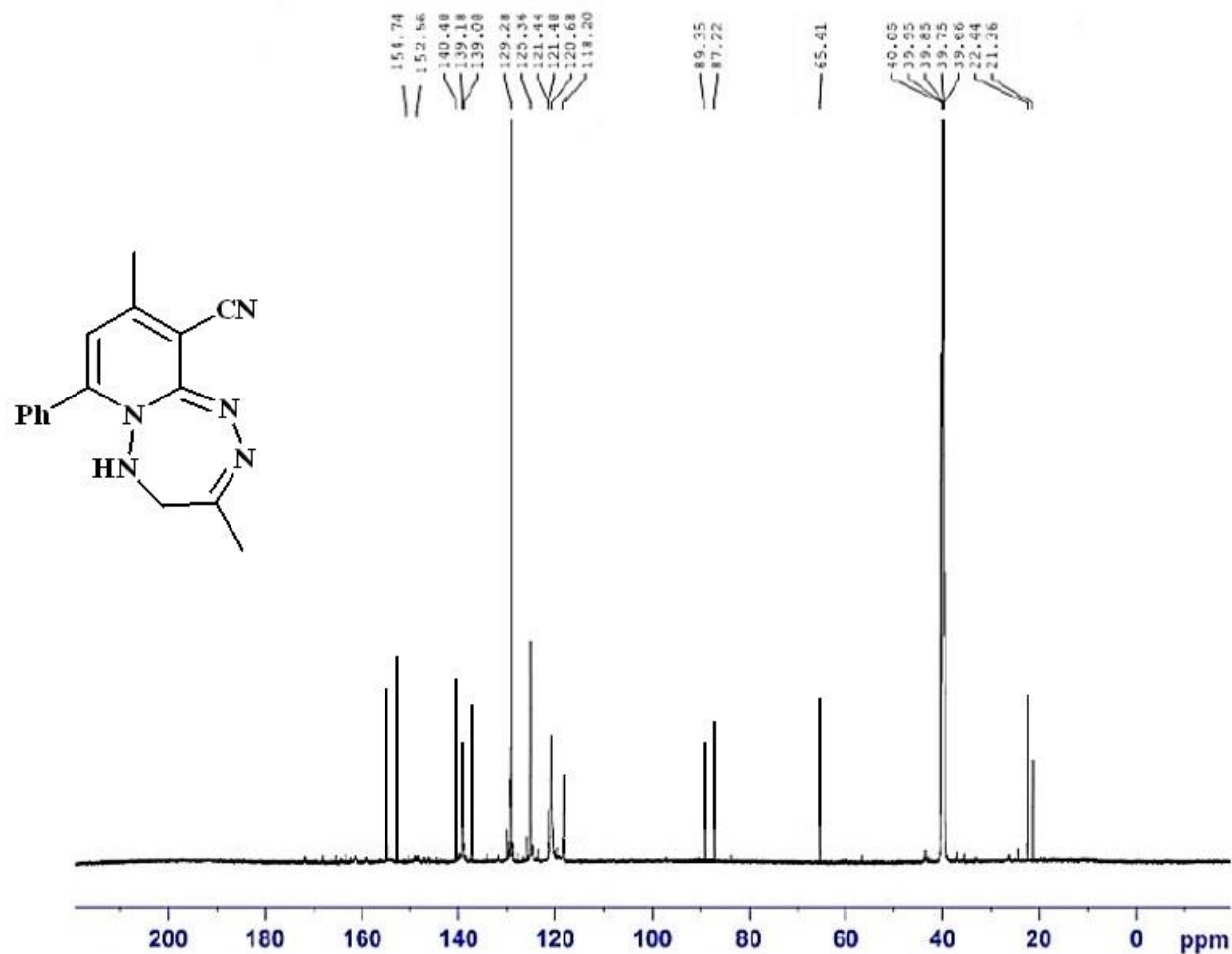
eman-sadek-13 #154-158 RT: 2.59-2.63 AV: 3 SB: 26 1.21-1.34, 0.87-1.14 NL: 1.98E2  
T: + cEI Full ms [40.00-1000.00]



Supplementary fig. (28): mass spectrum for compound 12.



Supplementary fig. (29): <sup>1</sup>H NMR for compound 13.



Current Data Parameters  
NAME 09-01-2020  
EXNO 60  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200209  
Time 20.56  
INSTRUM spect  
PROBHD 5 mm CPQCI 1H-  
PULPROG zgpg20  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 51020.405 KHz  
FIDRES 0.778510 KHz  
AQ 0.6422521 sec  
RG 128.94  
CW 9.500 usec  
EC 10.00 usec  
TE 293.0 K  
CA 2.30000000 sec  
C11 0.30000000 sec  
TD0 1

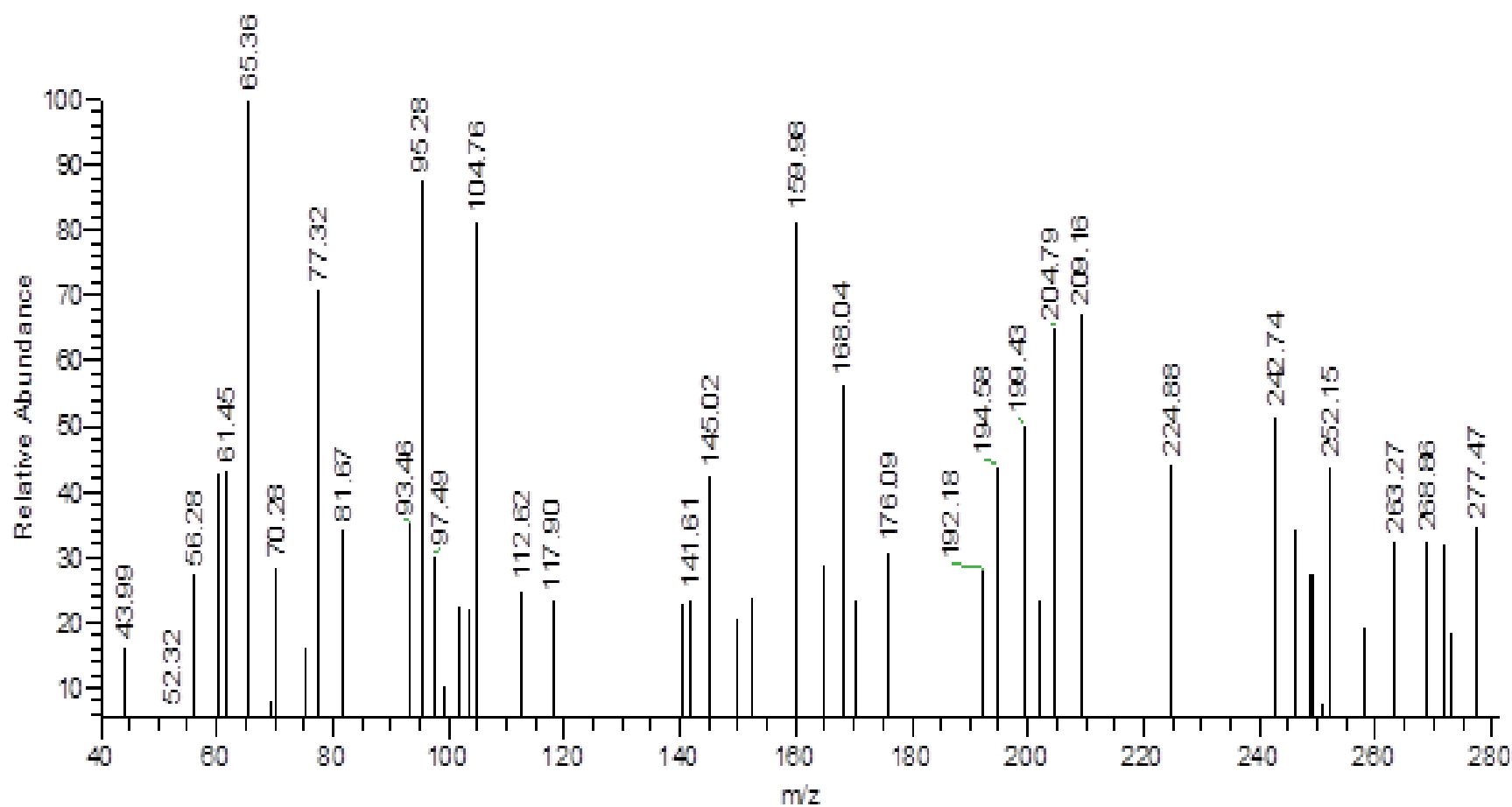
===== CHANNEL f1 =====  
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NUC1 13C  
P1 12.00 usec  
PLW1 140.90000000 W

===== CHANNEL f2 =====  
SFO2 800.1424006 MHz  
NUC2 1H  
CFDPRG[2] waltz16  
PCPD1 50.00 usec  
PLW2 16.20000076 W  
PLW12 0.16200000 W  
PLW13 0.10368000 W

F2 - Processing parameters  
SI 32768  
SF 213.7578730 MHz  
WDW EM  
SSB 0  
LB 2.00 KHz  
GB 0  
PC 2.00

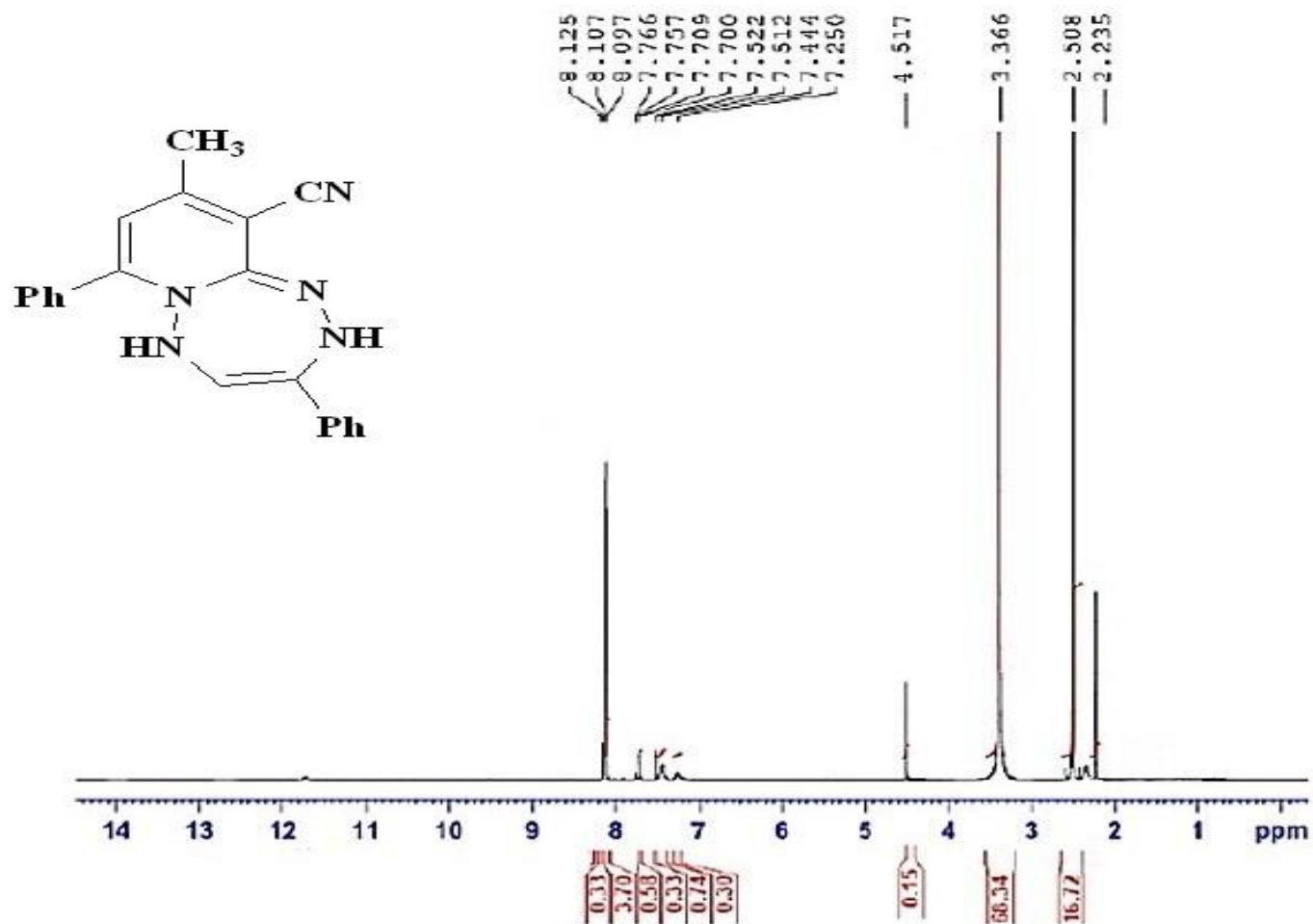
Supplementary fig. (30): <sup>13</sup>C NMR for compound 13.

eman-sadek-14 #155-157 RT: 2.81-2.84 AV: 3 SB: 26 1.21-1.34, 0.87-1.14 NL: 1.13E2  
T: + c EI Full ms [40.00-1000.00]



Supplementary fig. (31): mass spectrum for compound 13.





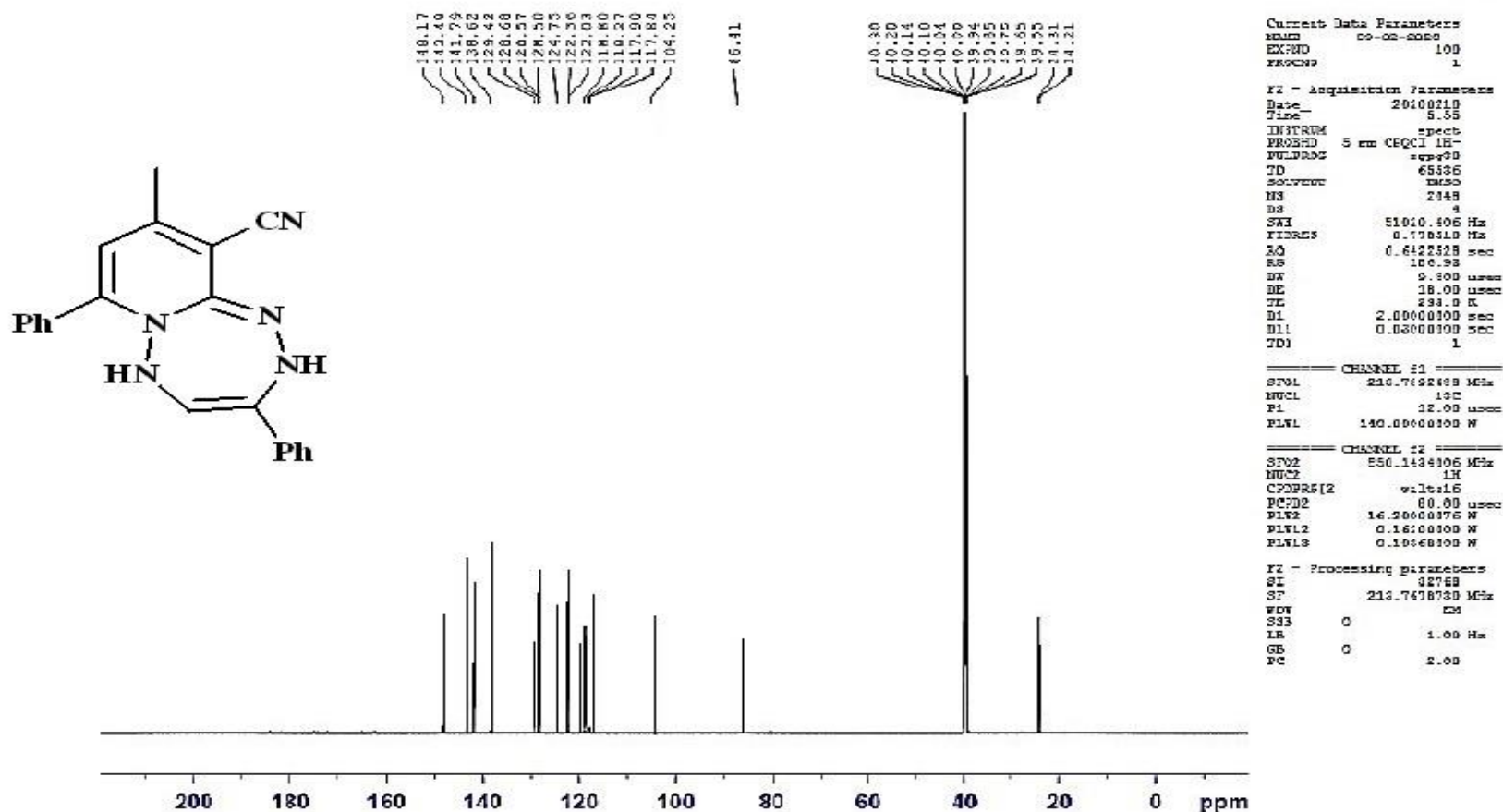
Current Data Parameters  
 NAME 35-12-2023  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230206  
 Time\_ 20.22  
 INSTRUM spect  
 PROBRG 5 - CPQCE 1D-  
 PULPROG zgpg  
 TO 65546  
 SOLVENT DMSO  
 NS 12  
 DS 2  
 SWH 17006.803 Hz  
 FIDRES 0.228003 Hz  
 AQ 1.6267554 sec  
 RG 11.87  
 DW 25.400 usec  
 DE 10.00 usec  
 TE 303.2 K  
 D1 1.00000000 sec  
 TD 1

===== CHANNEL f1 =====  
 FREQ1 500.1421000 MHz  
 P1 8.00 usec  
 PL1 16.40000070 dB

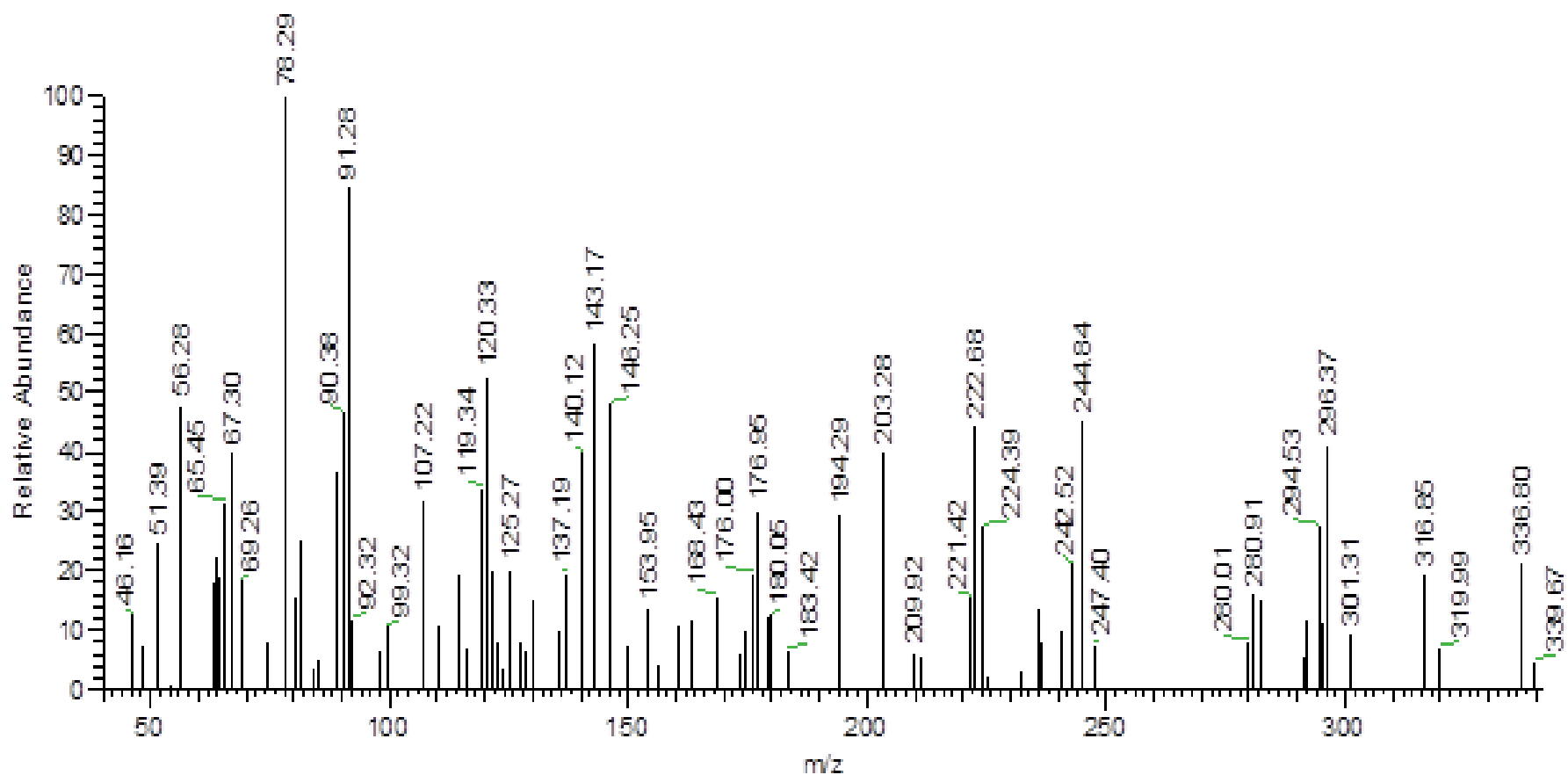
F2 - Processing parameters  
 SI 32768  
 SF 500.1420000 MHz  
 DS 4  
 SFO 0.80 Hz  
 XBU 0 2.00

Supplementary fig. (32): <sup>1</sup>H NMR for compound 14.

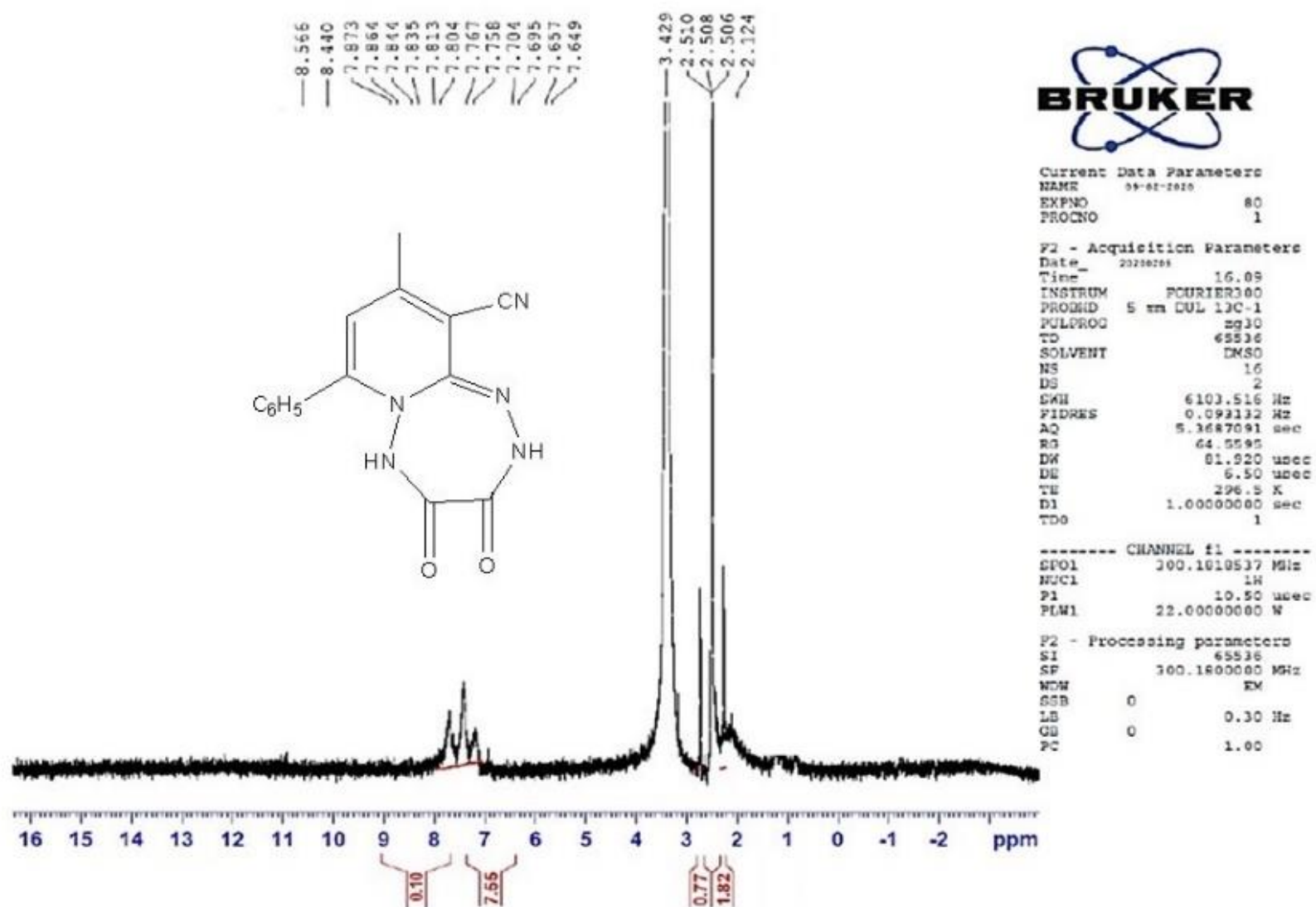


Supplementary fig. (33): <sup>13</sup>C NMR for compound 14.

eman-sadek-15 #205-208 RT: 3.45-3.46 AV: 2 SB: 26 1.21-1.34, 0.87-1.14 NL: 4.67E2  
T: + c EI Full ms [40.00-1000.00]

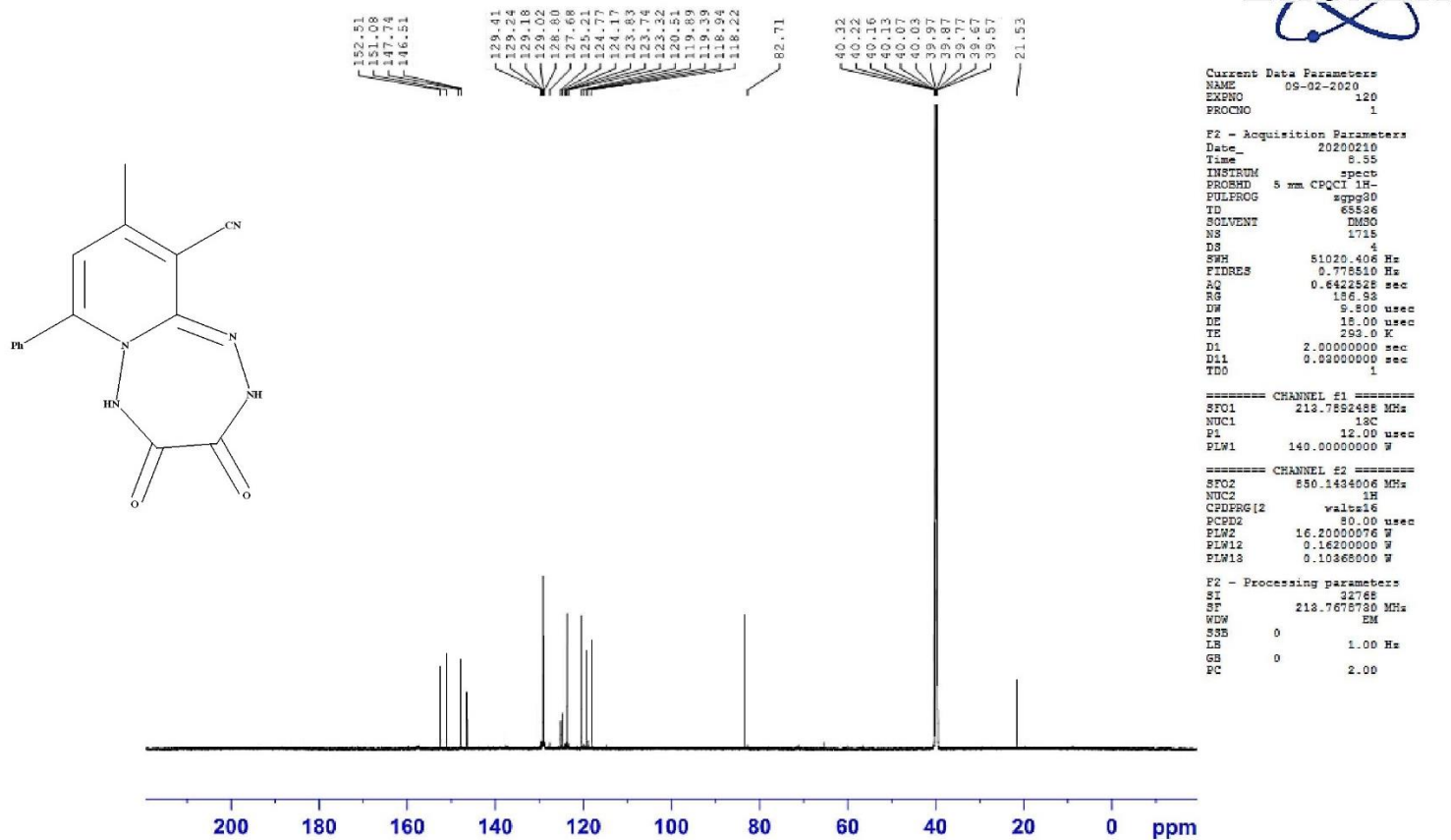


Supplementary fig. (34): mass spectrum for compound 14.

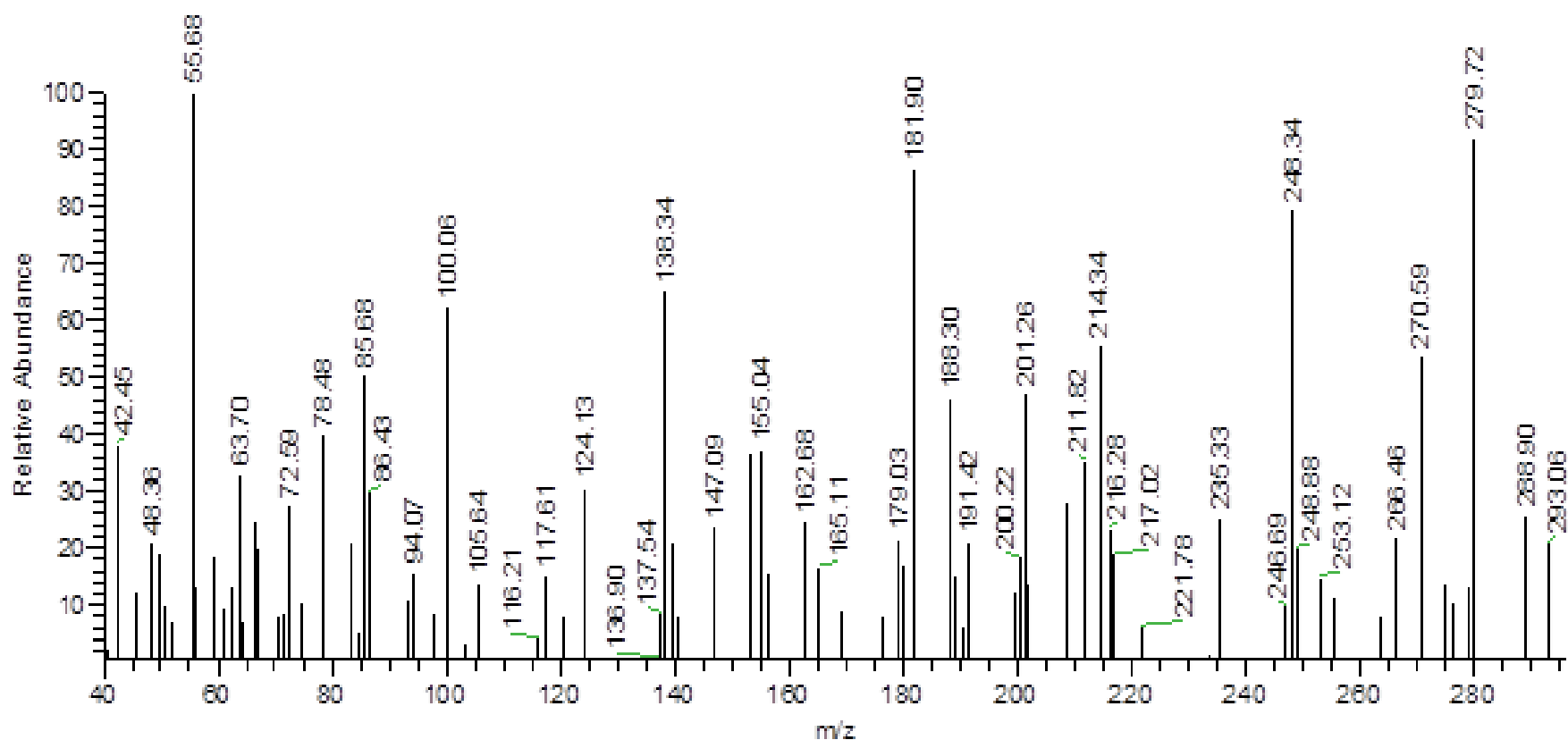


Supplementary fig. (35):  $^1\text{H}$  NMR for compound 15.

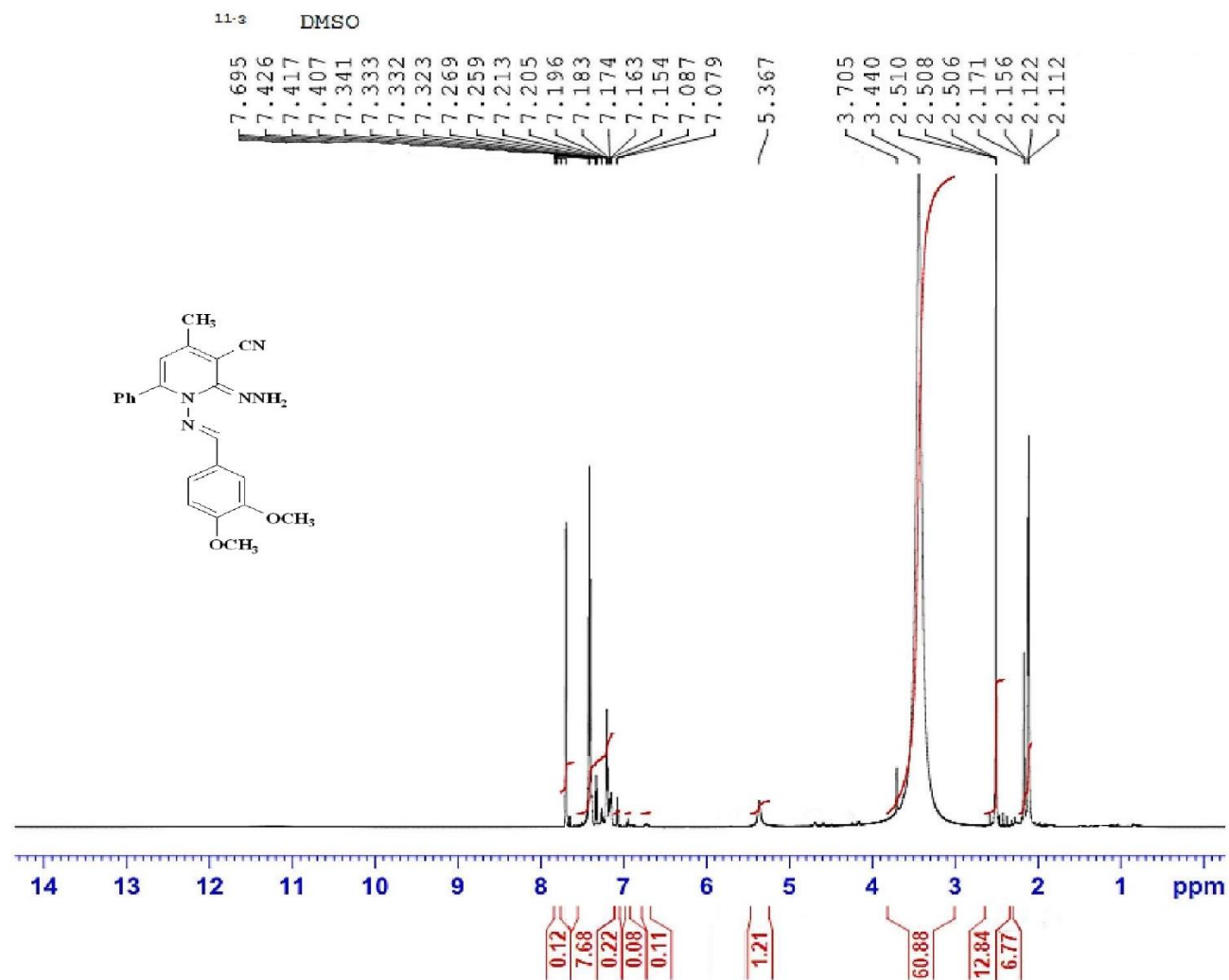
11.5

Supplementary fig. (36): <sup>13</sup>C NMR for compound 15.

eman-sadek-16 #83-85 RT: 1.41-1.44 AV: 3 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.45E2  
T: + c EI Full ms [40.00-1000.00]



Supplementary fig. (37): mass spectrum for compound 15.



Current Data Parameters  
 NAME 08-02-2020  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200206  
 Time\_ 22.04  
 INSTRUM spect  
 PROBHD 5 mm CPQCI 1H-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 17006.803 KHz  
 FIDRES 0.259503 KHz  
 AQ 1.9267584 sec  
 RG 10.55  
 DW 29.400 usec  
 DE 10.00 usec  
 TE 293.0 K  
 D1 1.00000000 sec  
 TD0 1

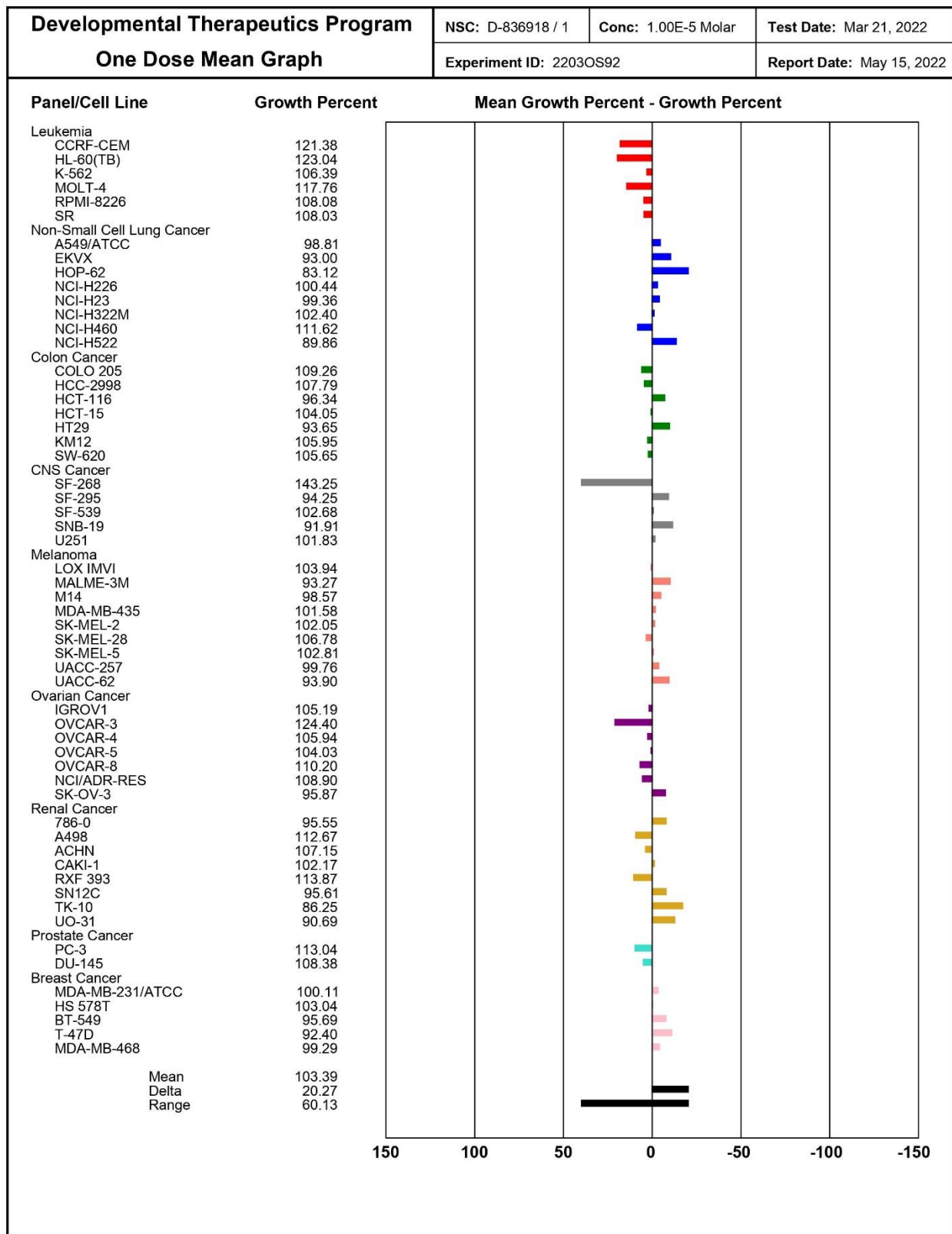
===== CHANNEL f1 =====  
 SFO1 850.1452500 MHz  
 NUC1 1H  
 P1 8.00 usec  
 PLW1 16.20000076 W

F2 - Processing parameters  
 SI 65536  
 SF 850.1400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 KHz  
 GB 0  
 FC 2.00

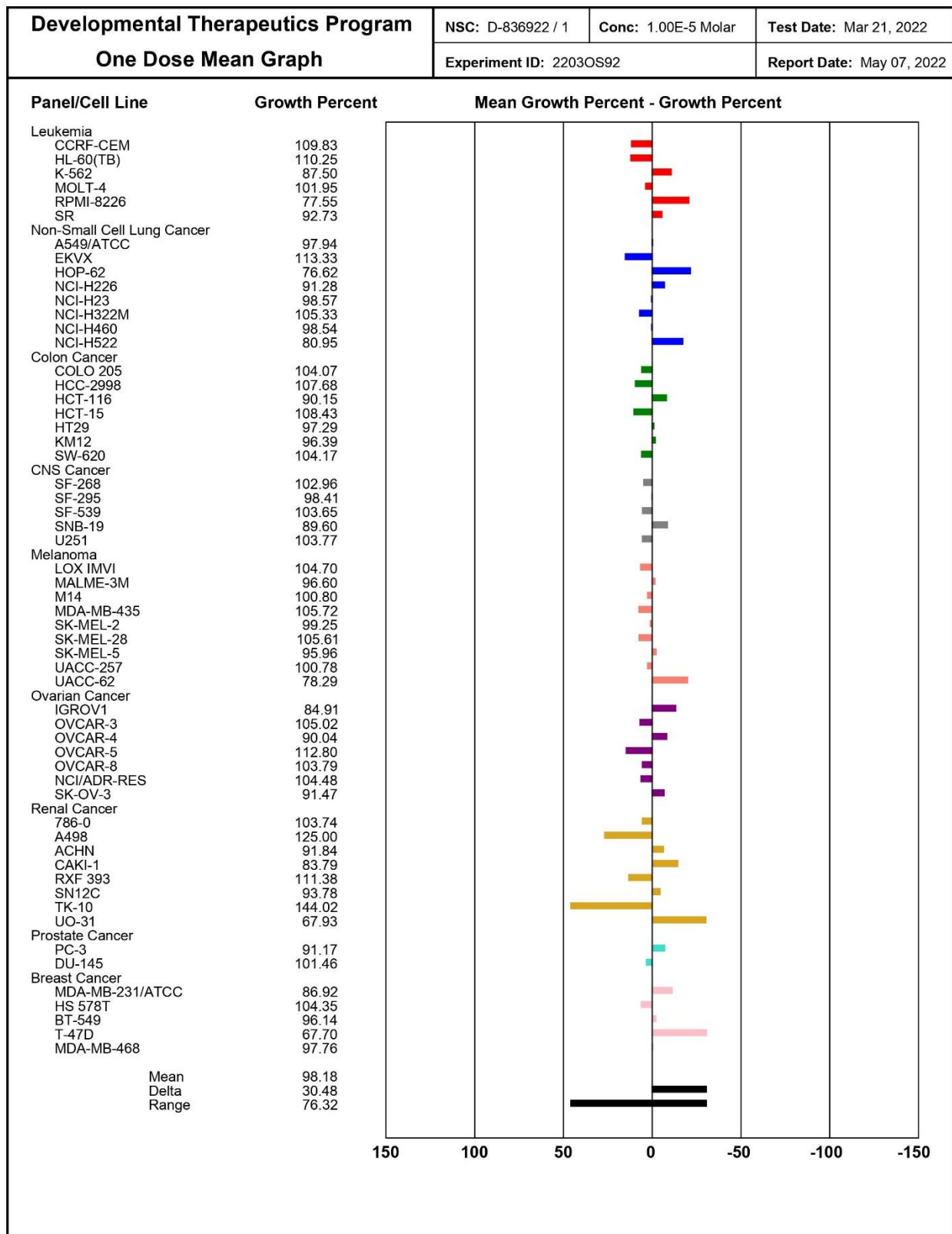
Supplementary fig. (38): <sup>1</sup>H NMR for compound 16.N

## **NCI anticancer data result**

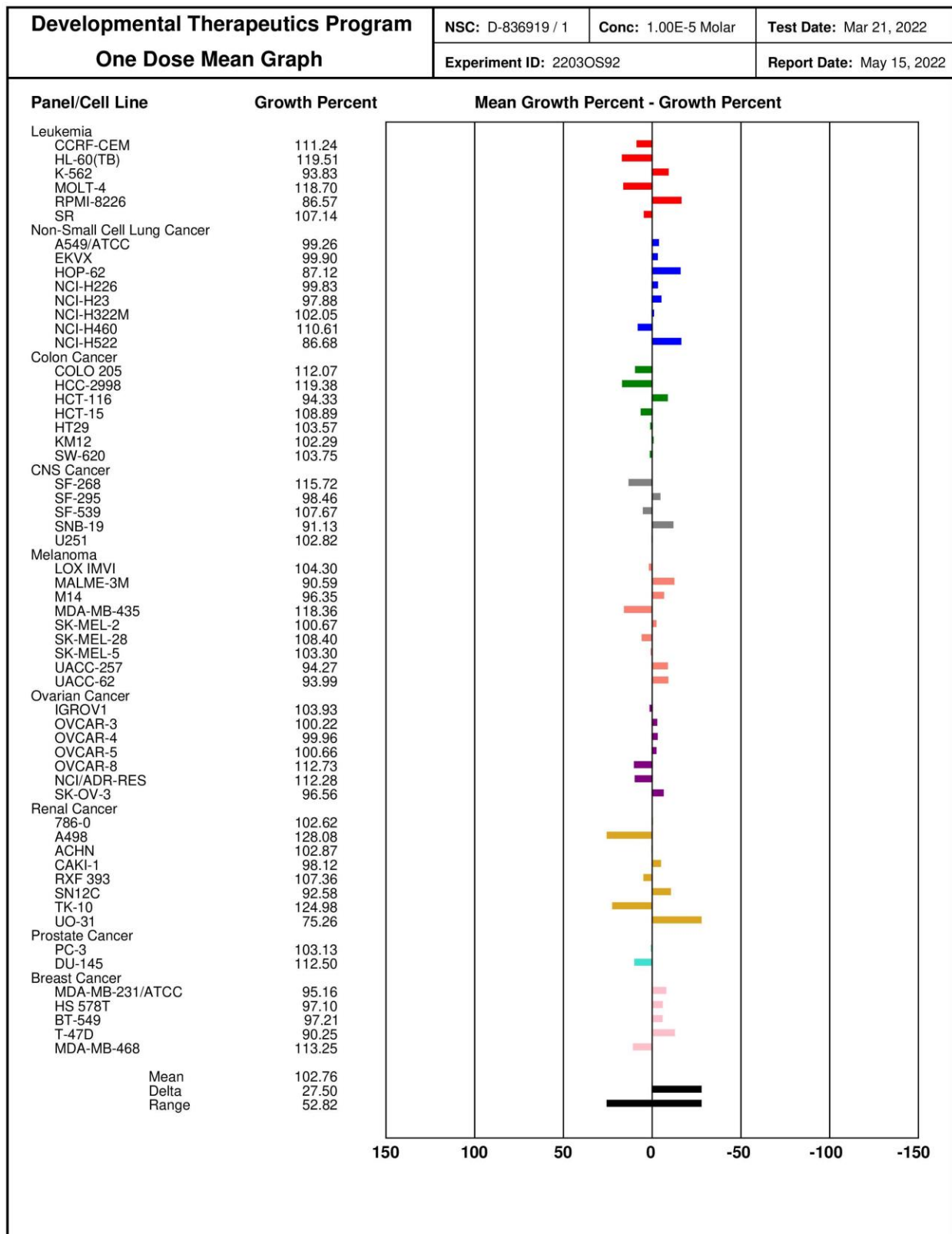




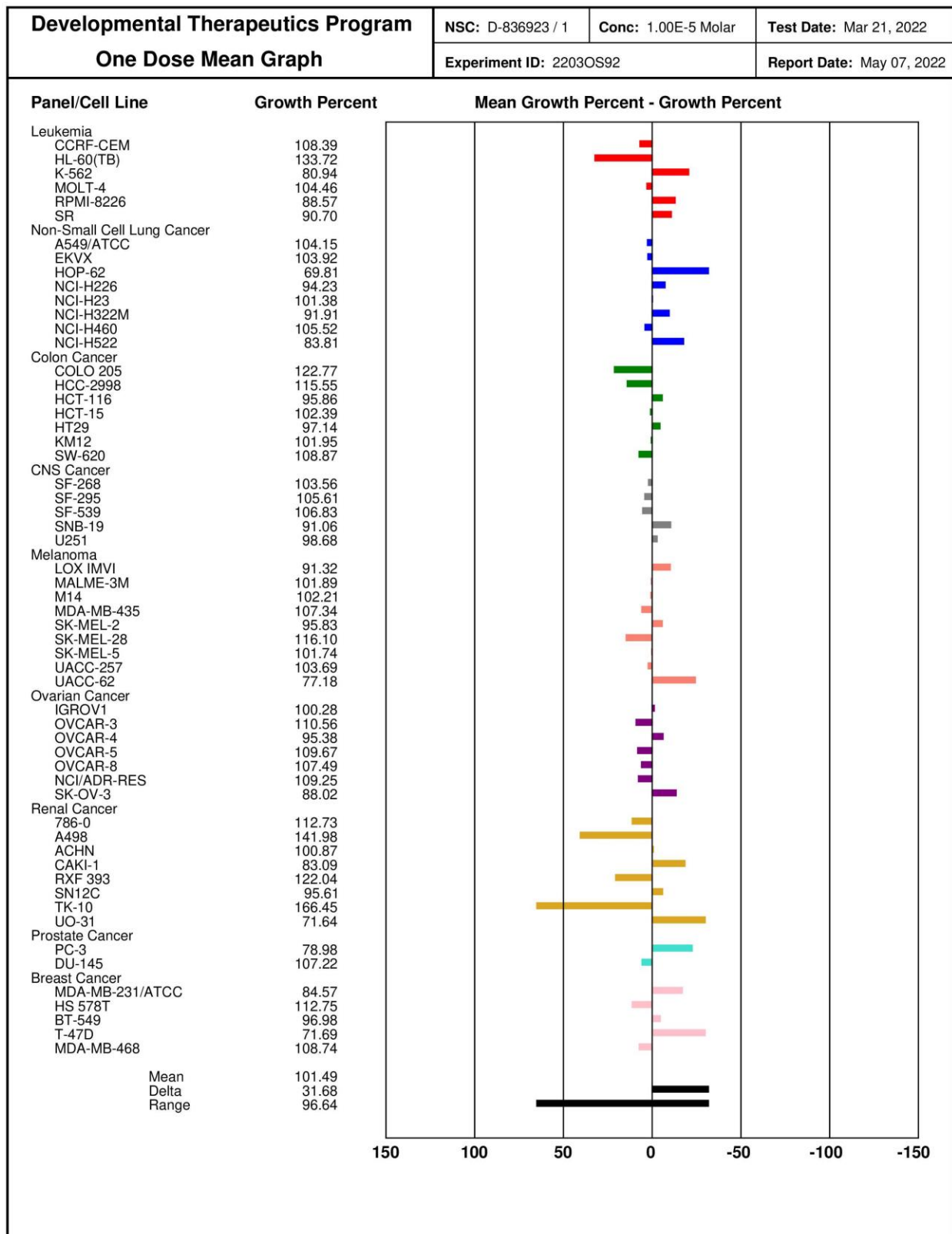
**Compound 2**



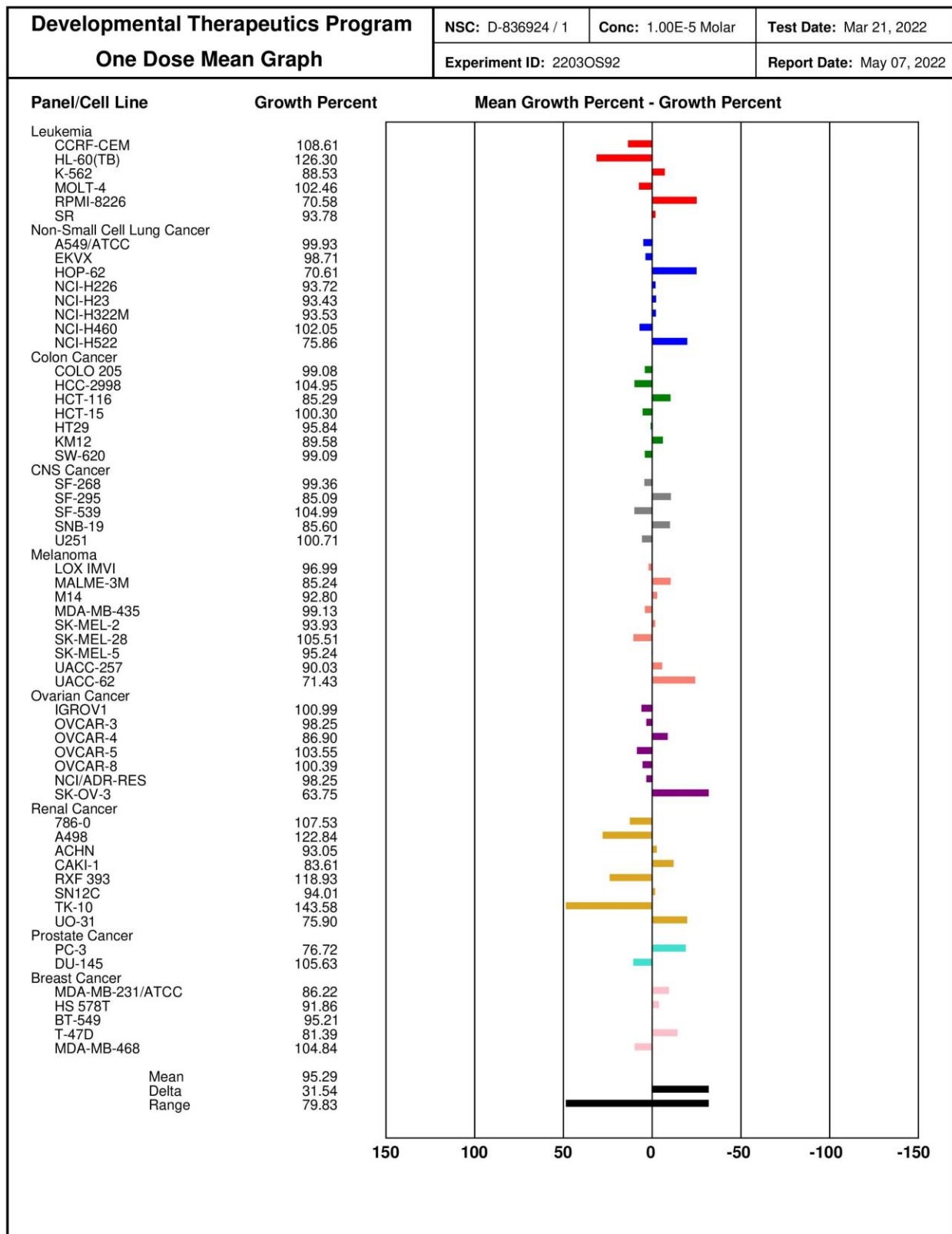
**Compound 4**



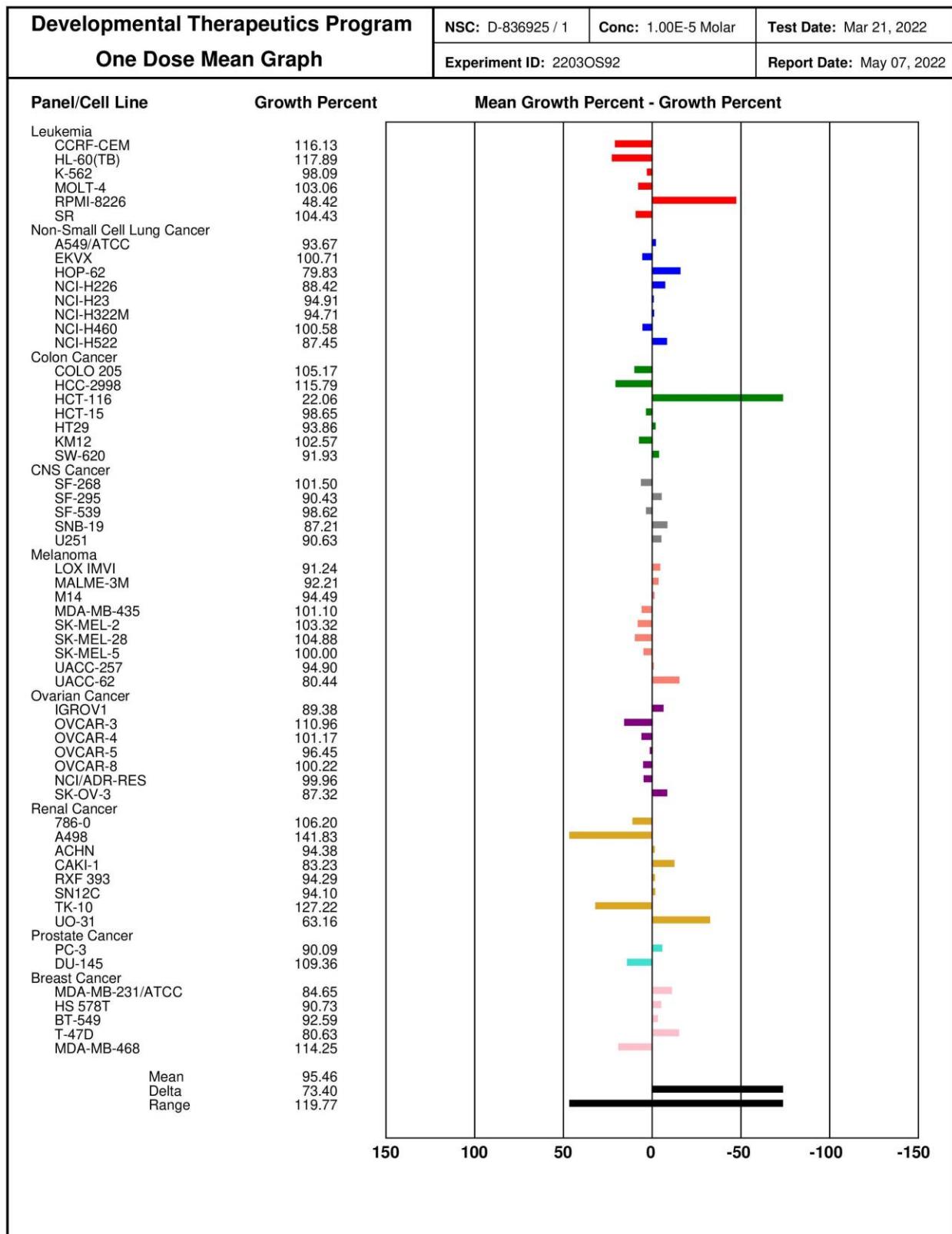
**Compound 5**



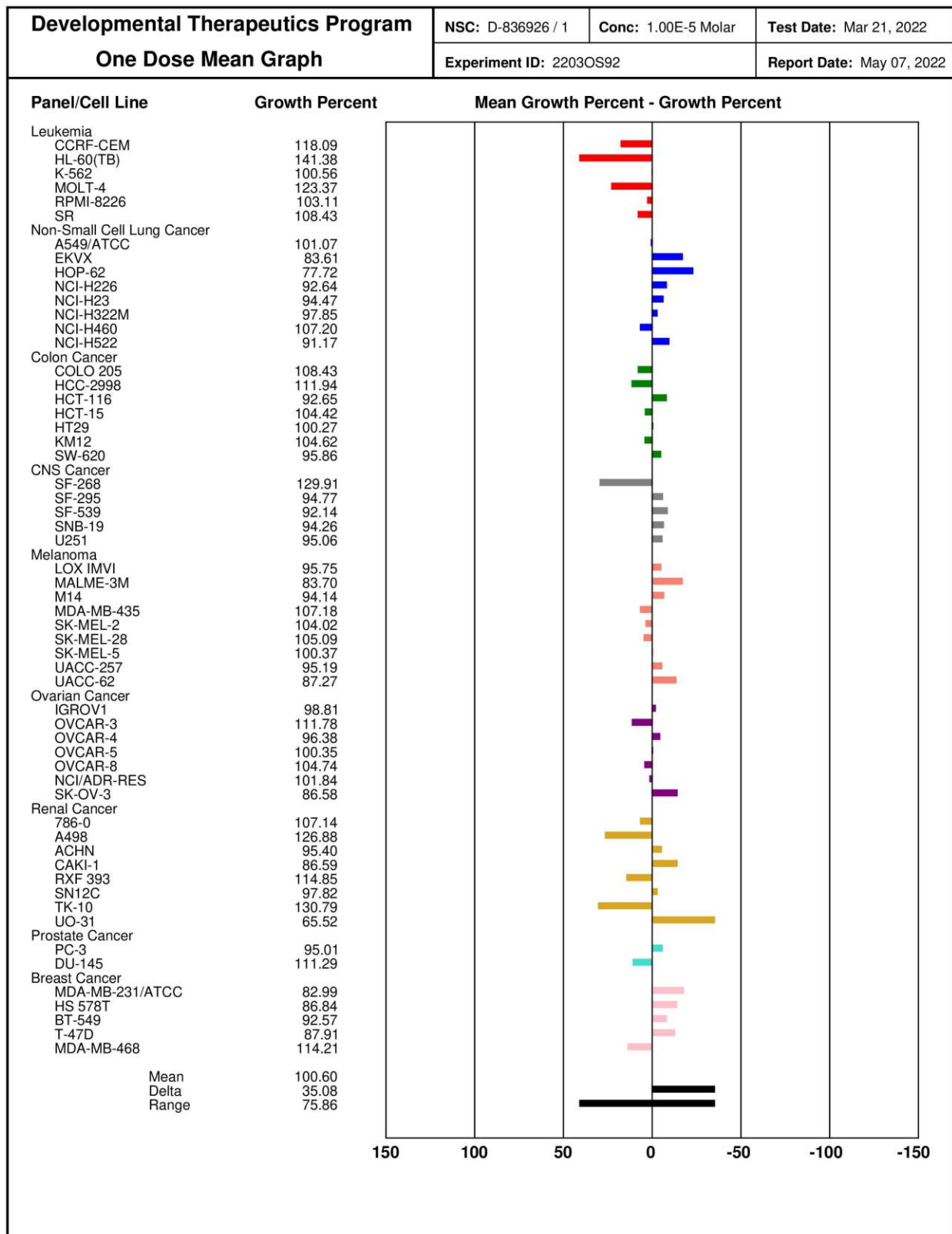
**Compound 7**



**Compound 8**

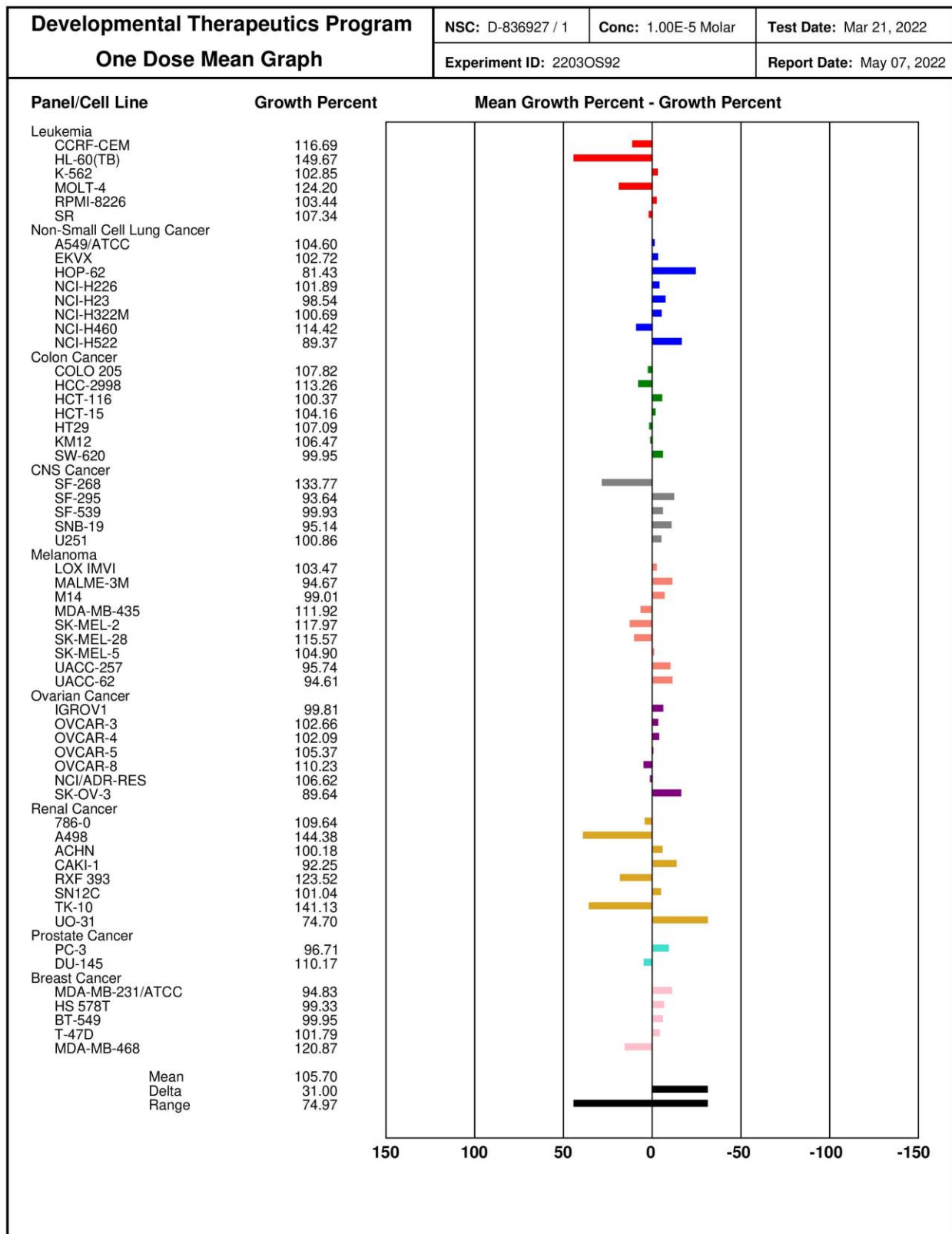


**Compound 9**



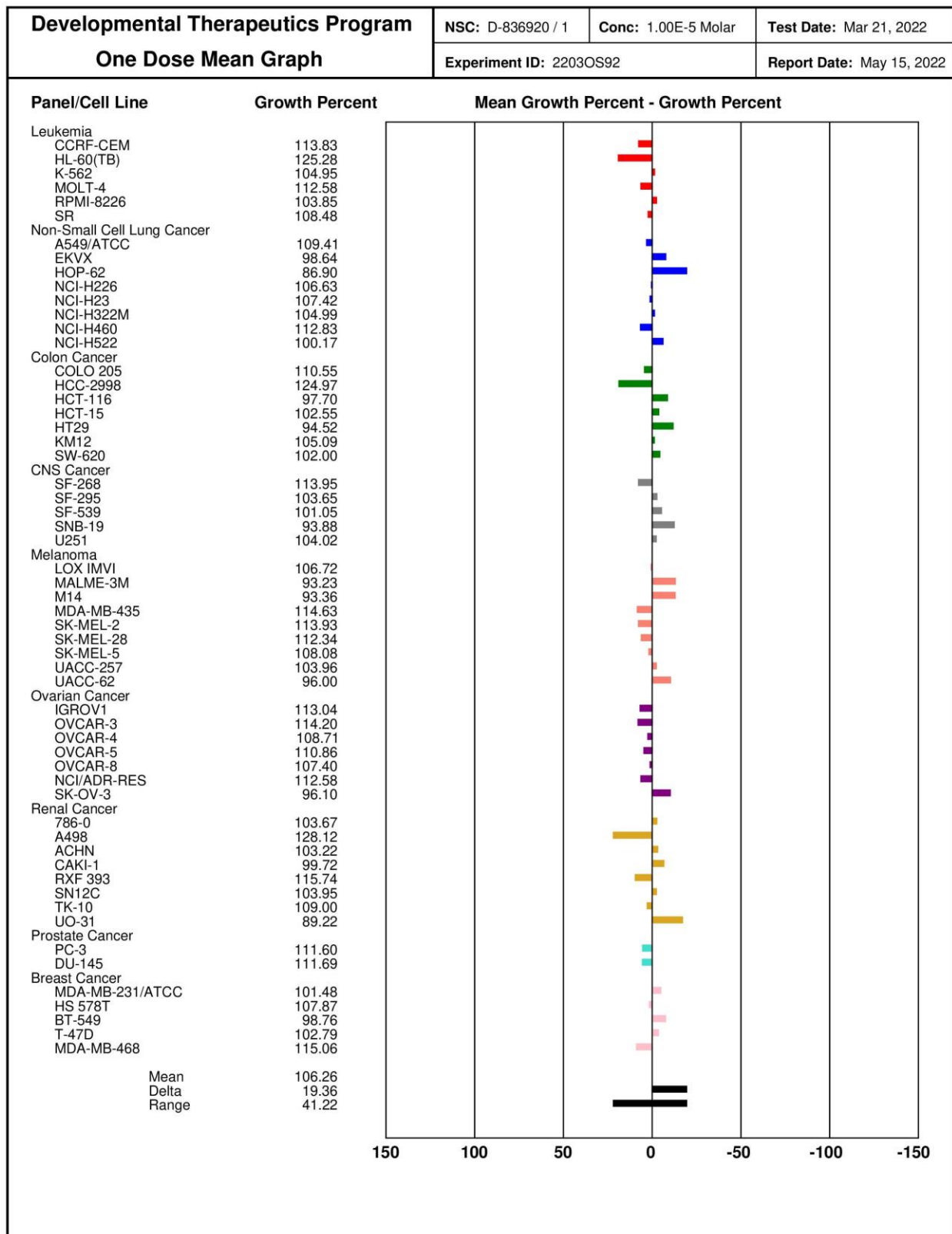
**Compound 10**



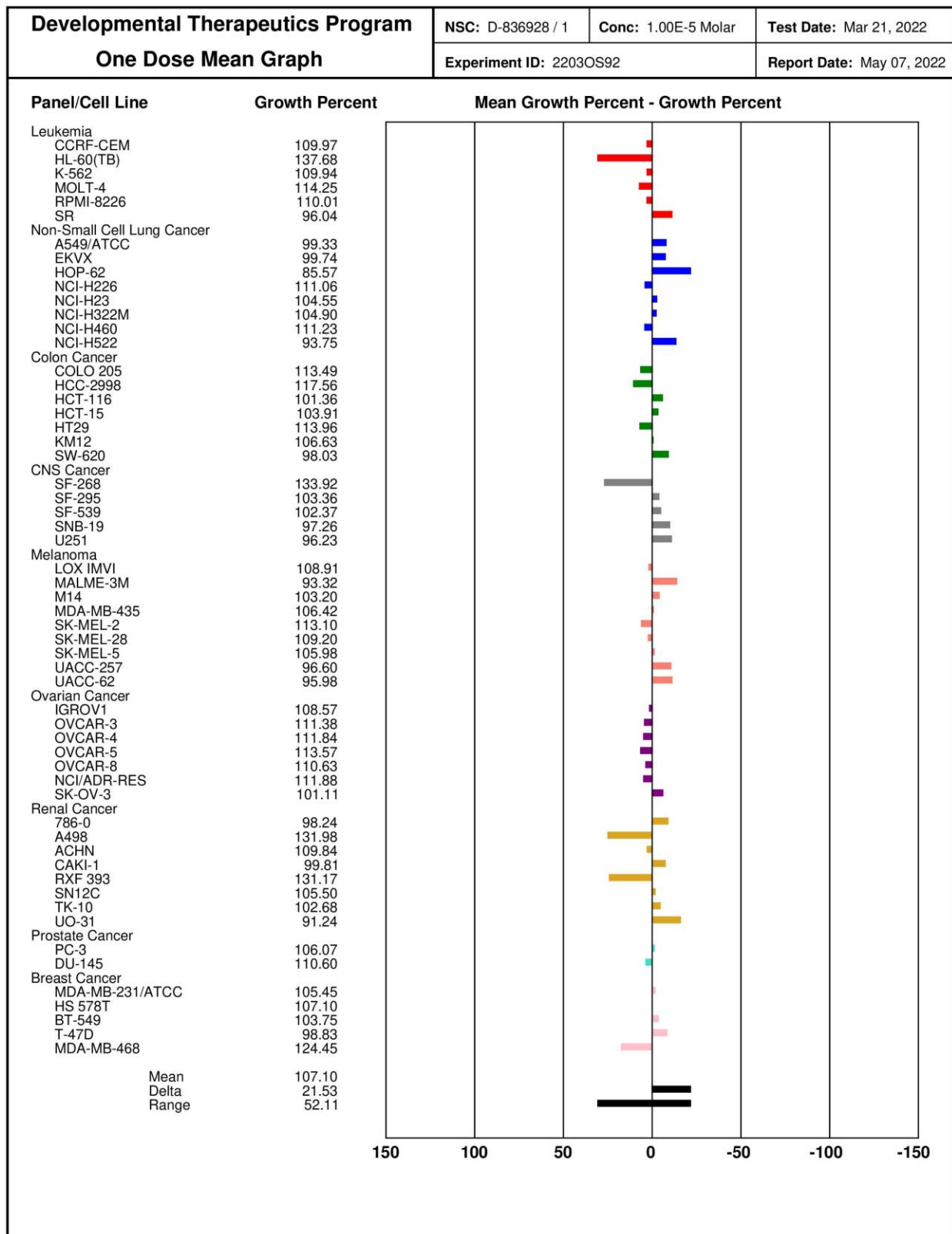


**Compound 12**

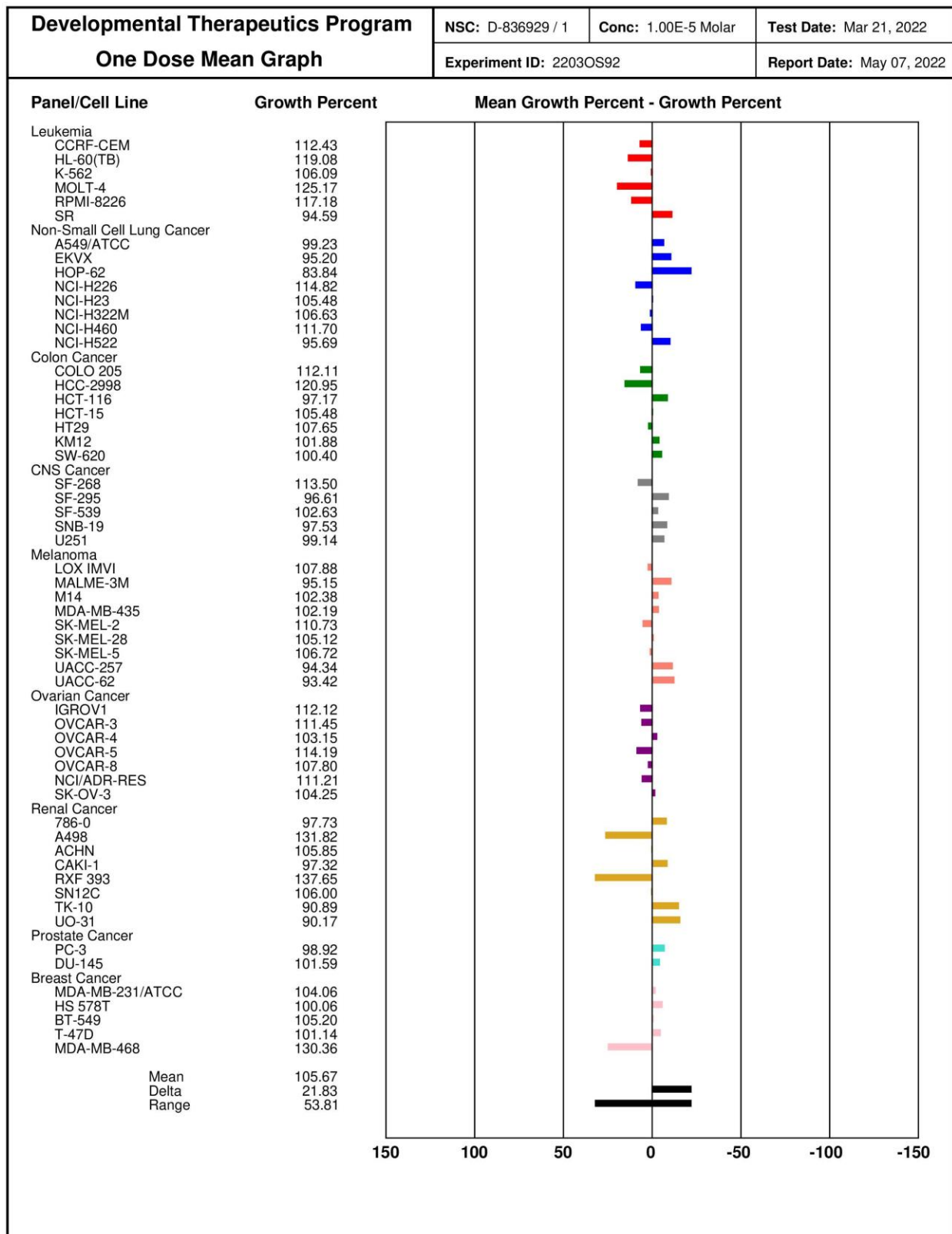




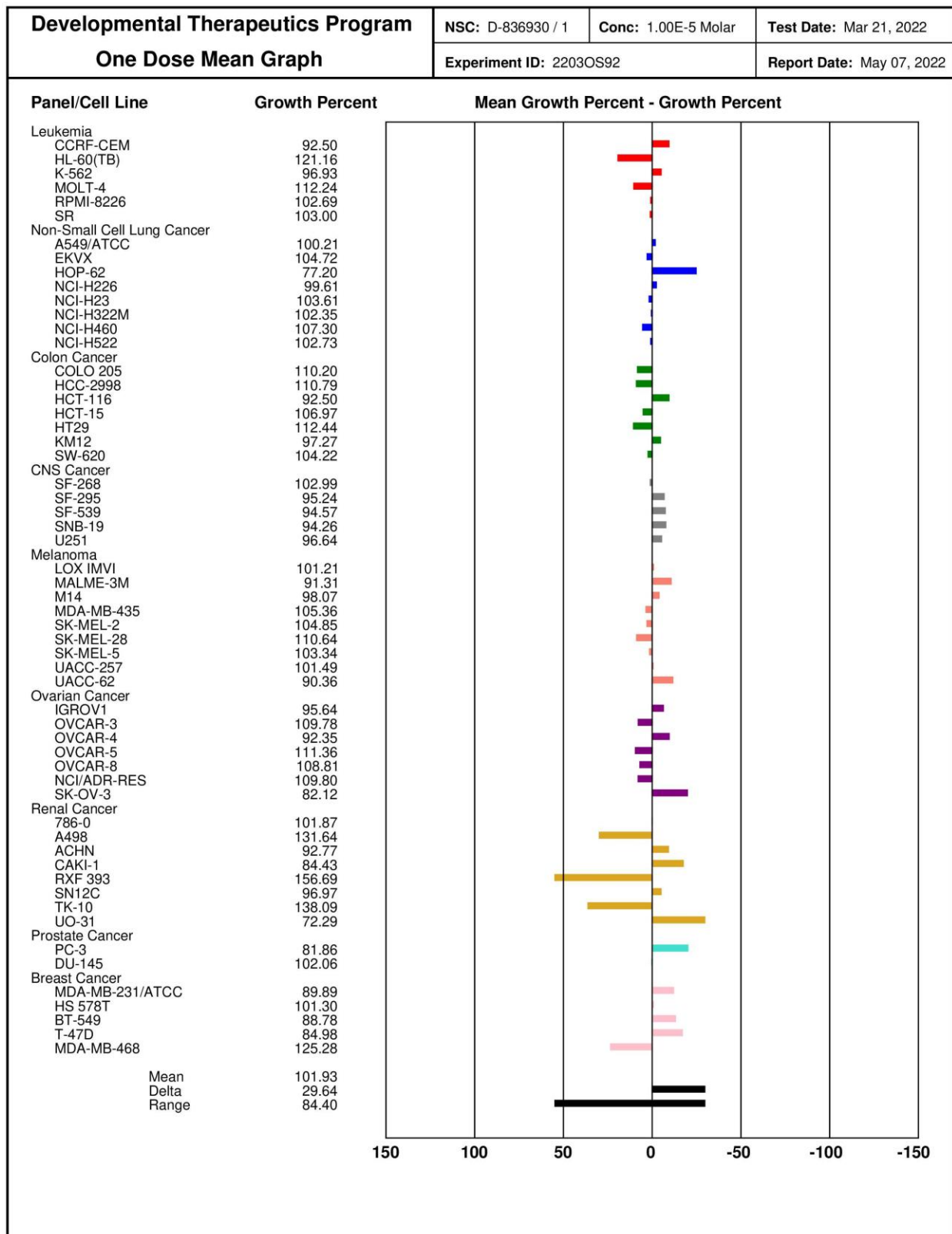
**Compound 13**



## Compound 14



**Compound 15**



**Compound 16**