

# **Design, nanogel synthesis, anti-proliferative and *in silico* ADMET of pyrazoles and/or pyrimidines as Topo-II Inhibitors and DNA intercalators**

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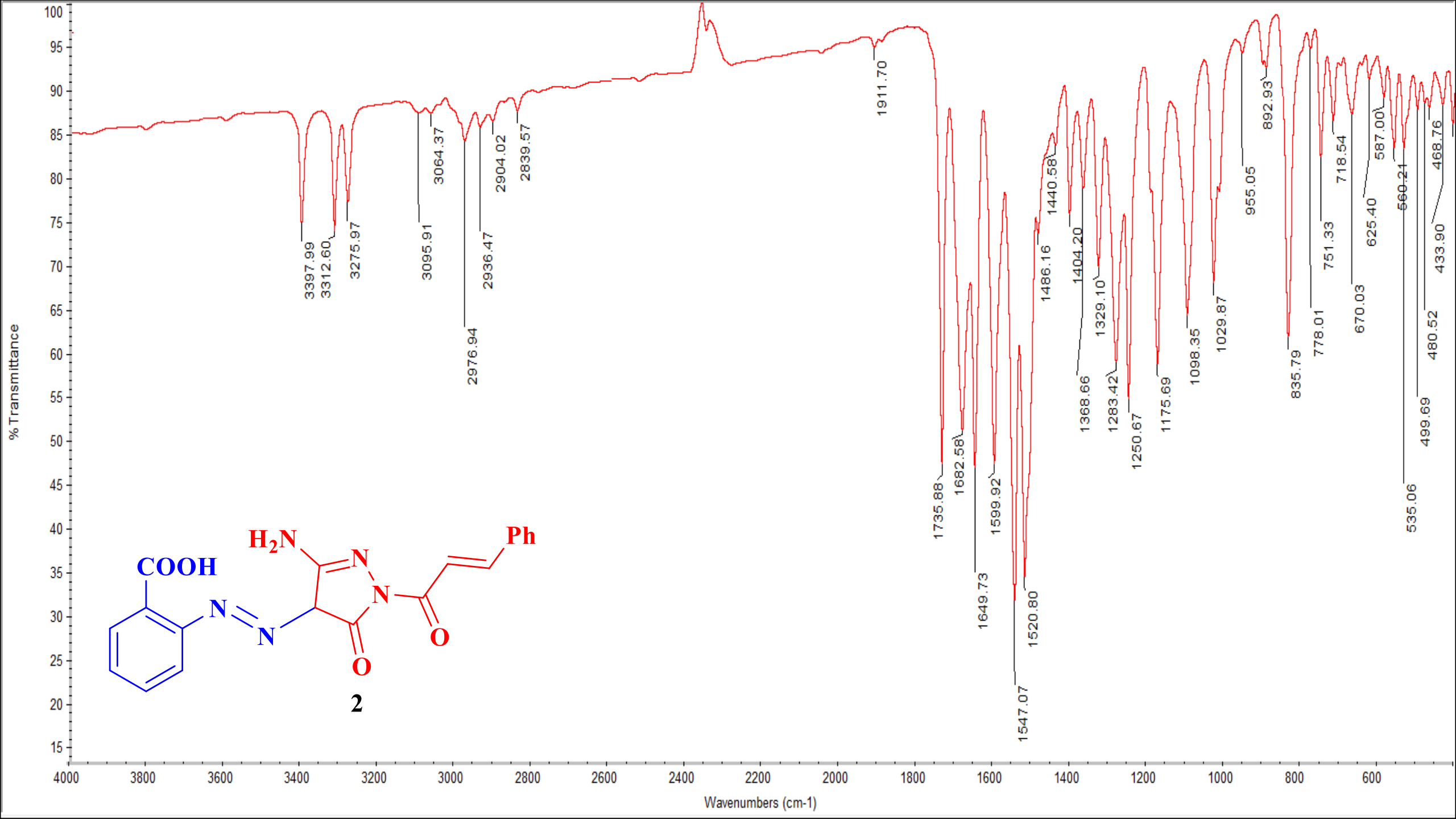
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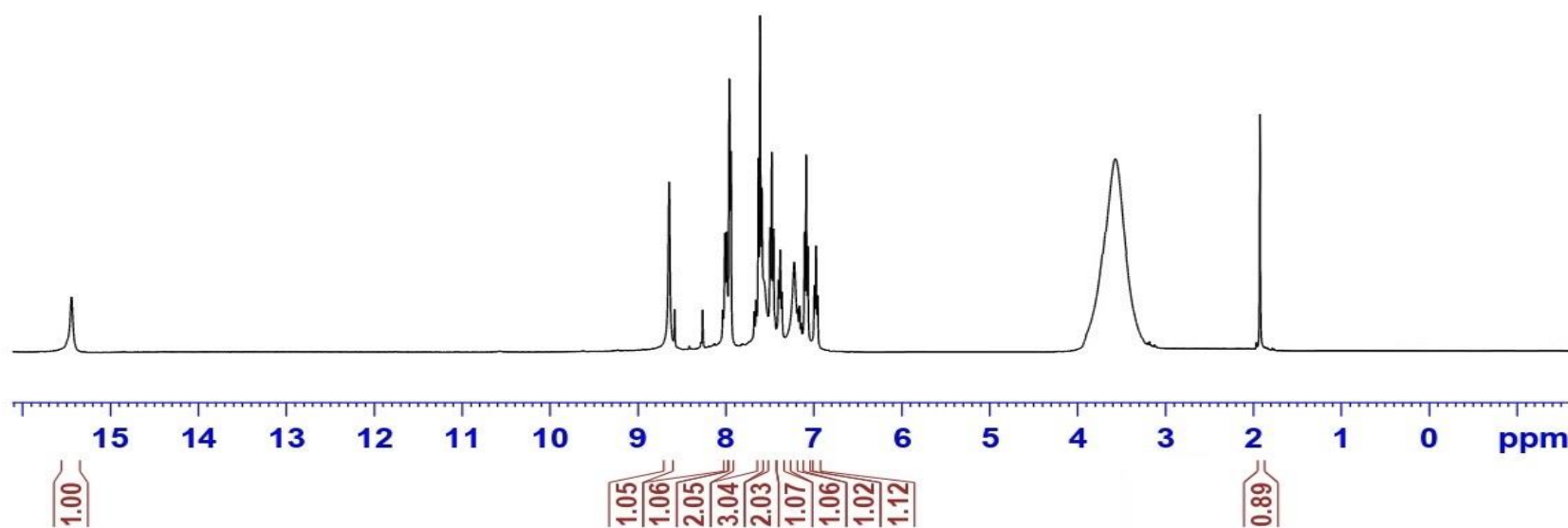
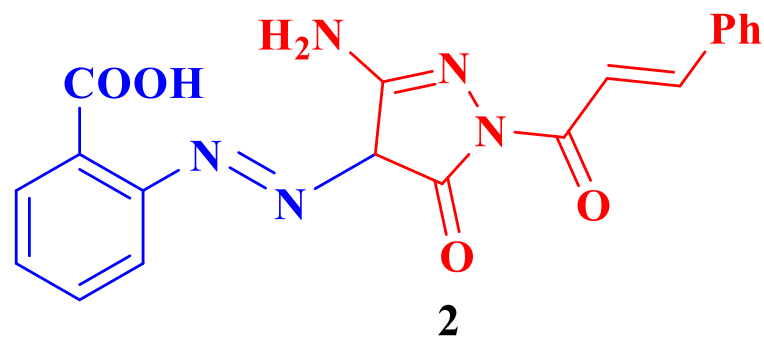
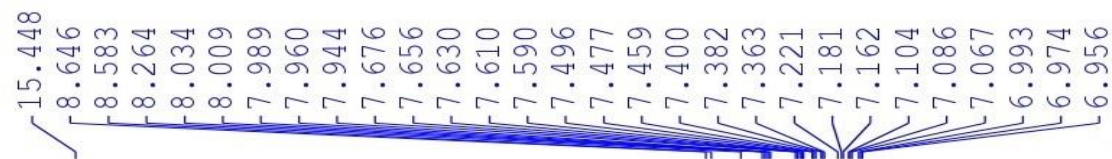
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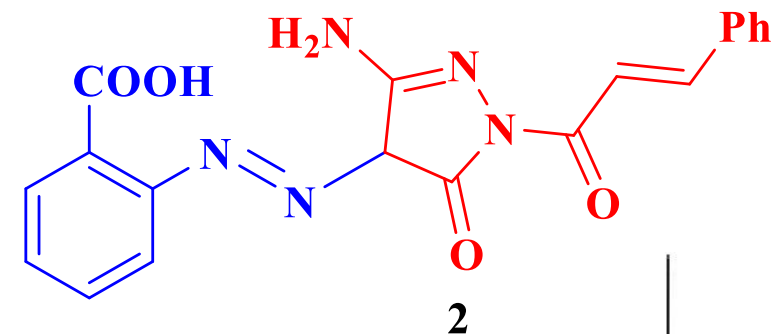
REC10-Hnmr-RR



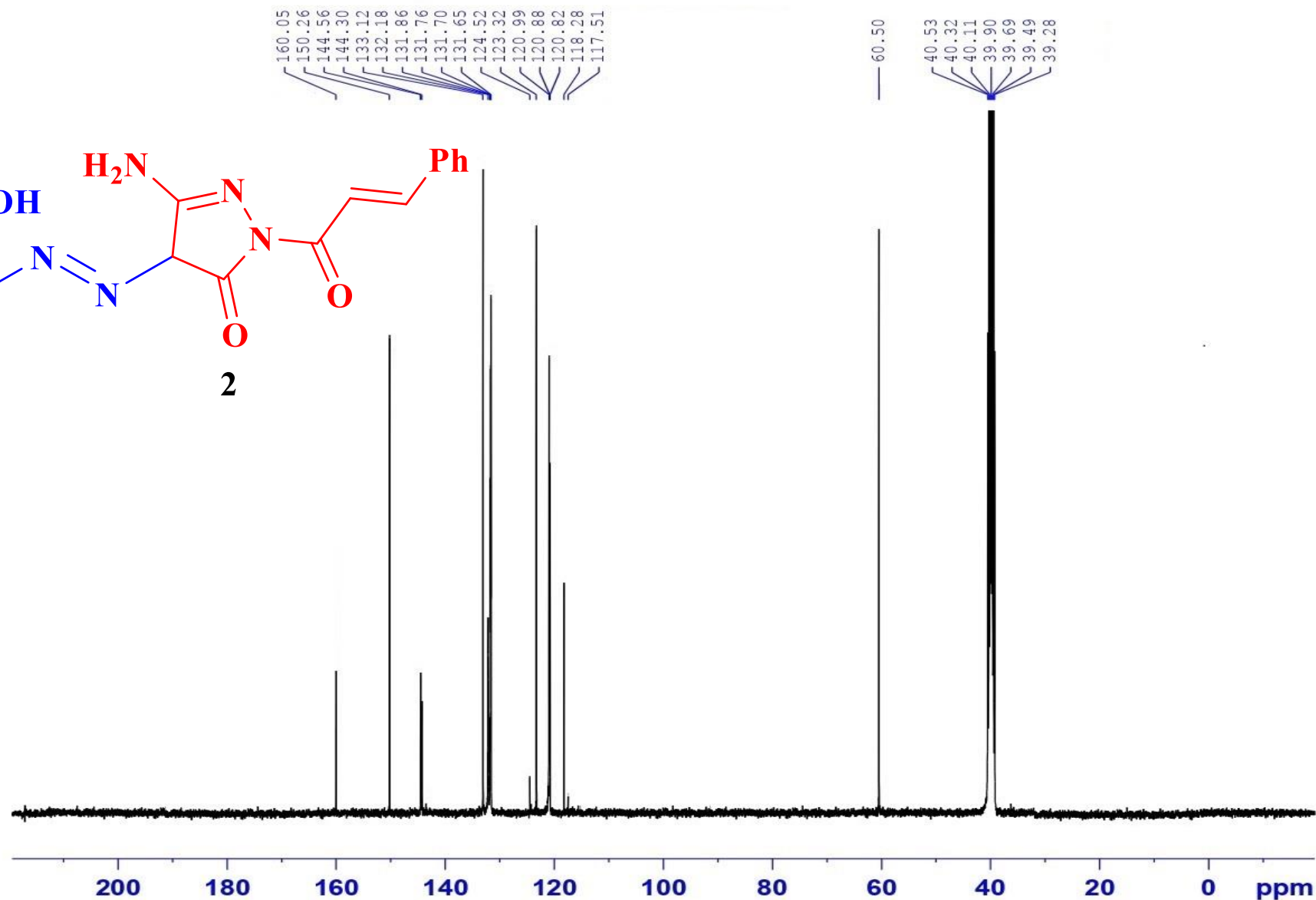
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 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 4.0894465 sec  
 RG 59.56  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2024712 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 13.00000000 W

F2 - Processing parameters  
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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

# REC10-CNMR-DMSO-SH

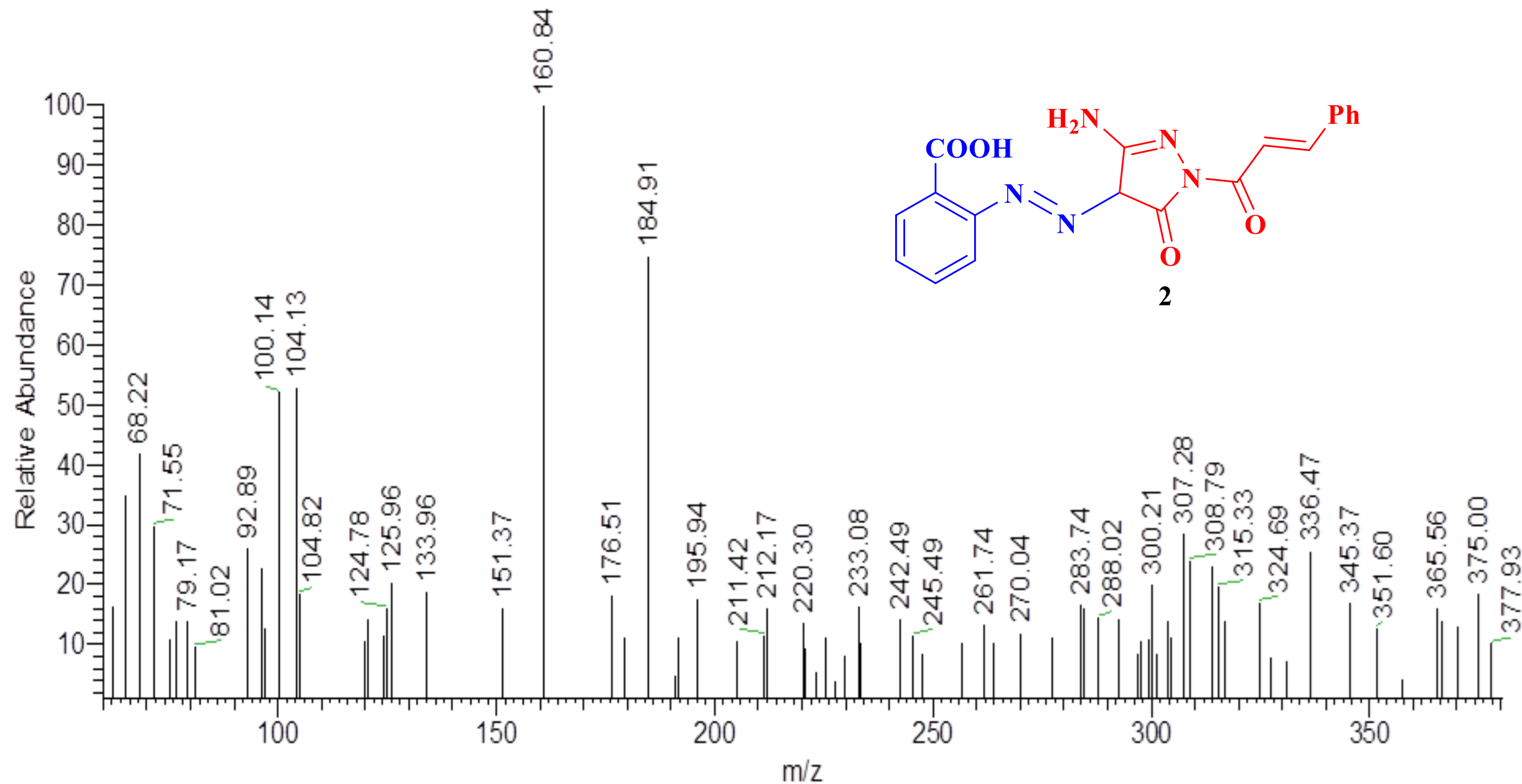


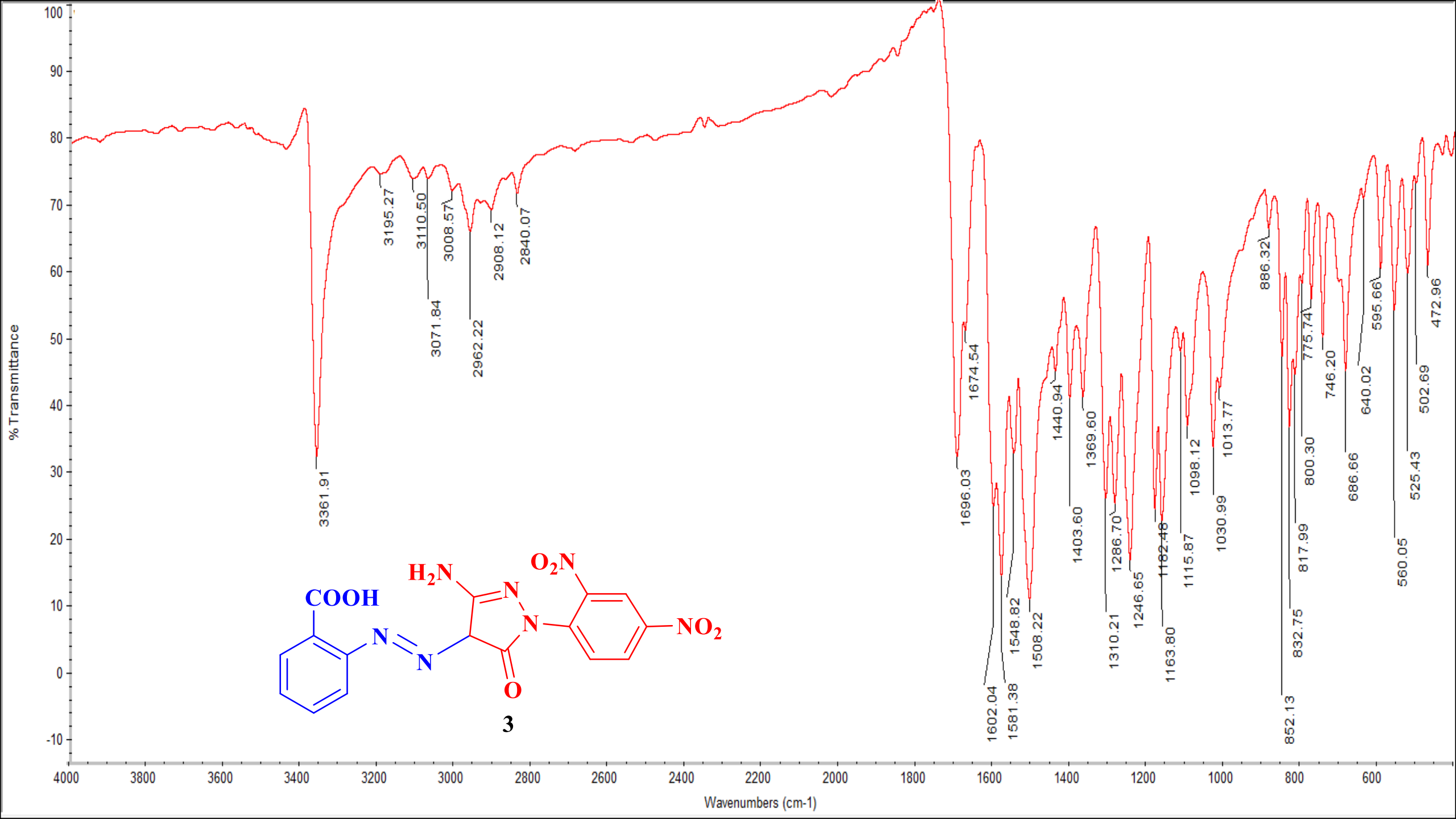
2



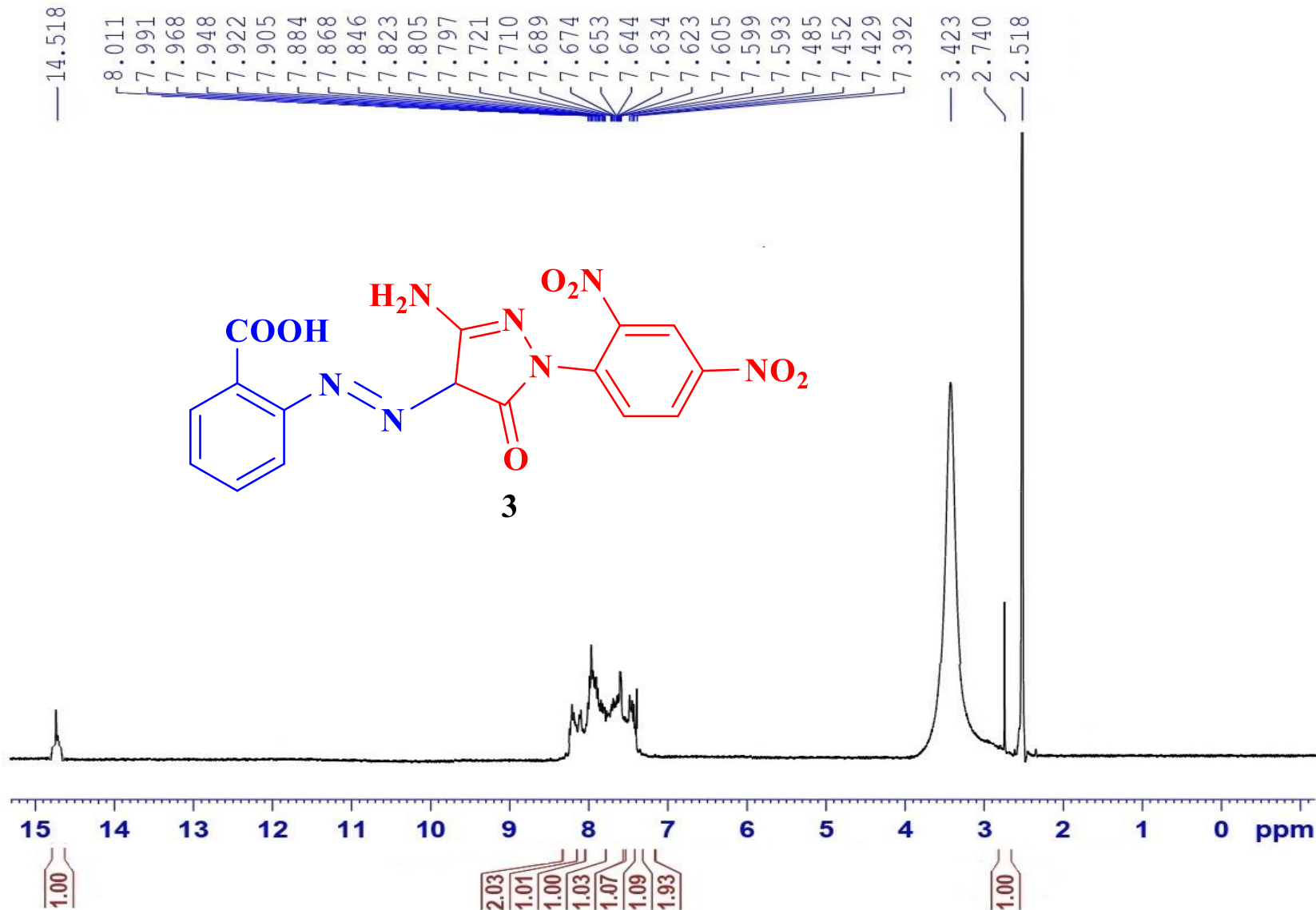
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 Time\_ 4.24 h  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.732896 Hz  
 AQ 1.2621488 sec  
 RG 88.24  
 DW 20.800 usec  
 DE 8.50 usec  
 TE 296.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1  
 SFO1 100.6204231 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 47.00000000 W  
 SFO2 400.2016008 MHz  
 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD2 90.00 usec  
 PLW2 13.00000000 W  
 PLW12 0.29249999 W  
 PLW13 0.14713000 W  
  
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 SF 100.6203700 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

REC10 #85 RT: 1.44 P: + NL: 7.78E2  
T: {0,0} + c EI Full ms [40.00-1000.00]





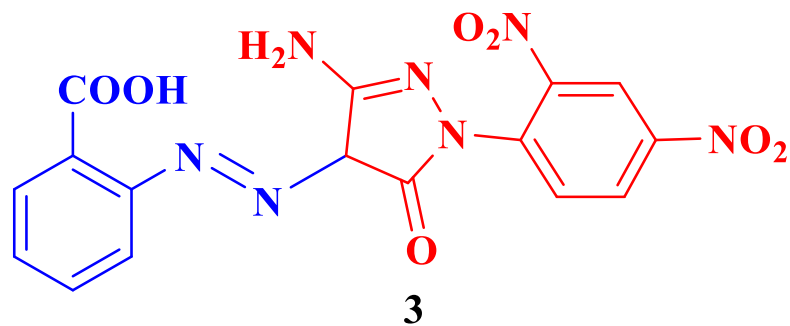
REC3-Hnmr-RR



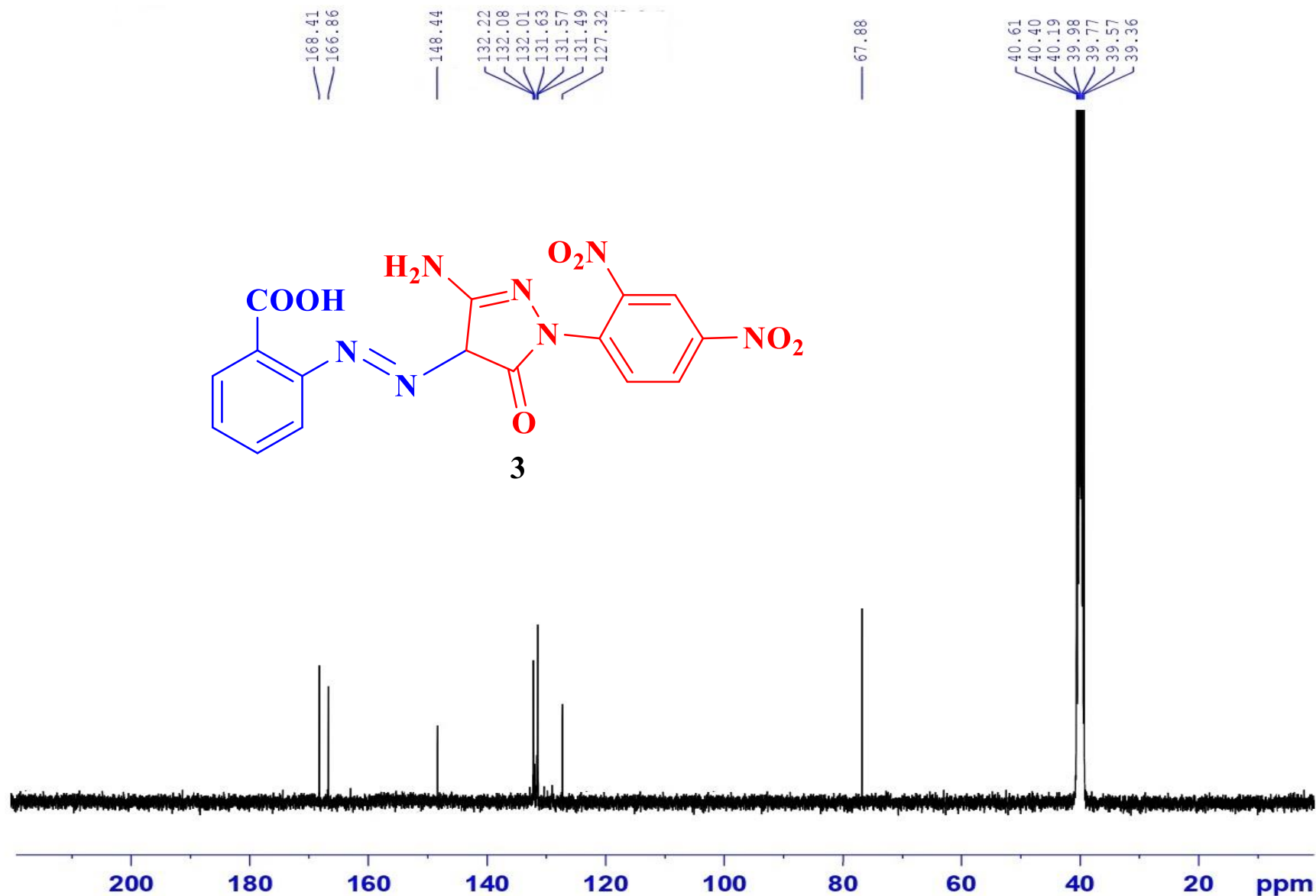
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 PROBHD z108618\_0945 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 4.0894465 sec  
 RG 197.77  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2024712 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 13.00000000 W

F2 - Processing parameters  
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 GB 0  
 PC 1.00

# REC3-Cnmr-HG



3

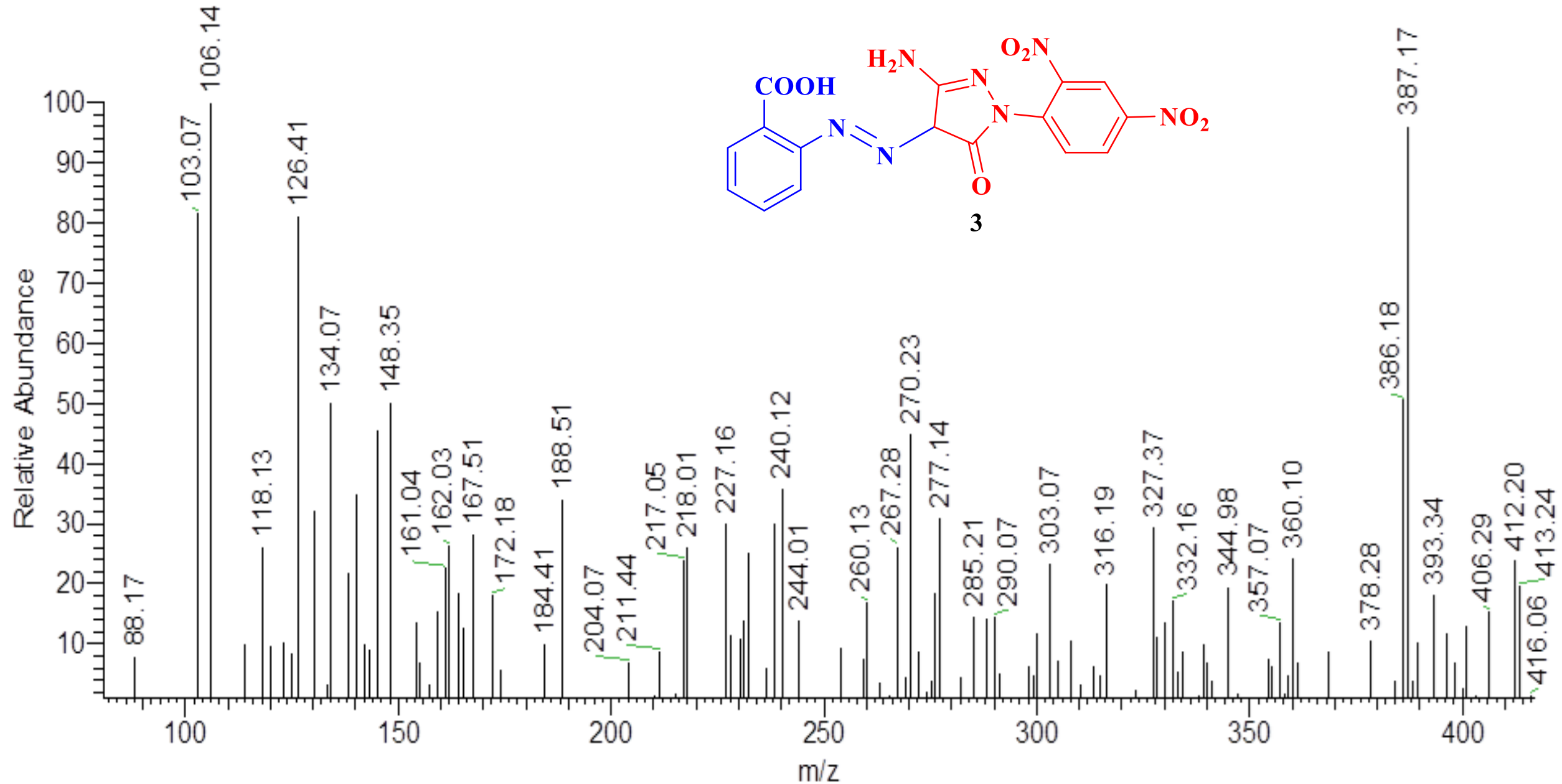


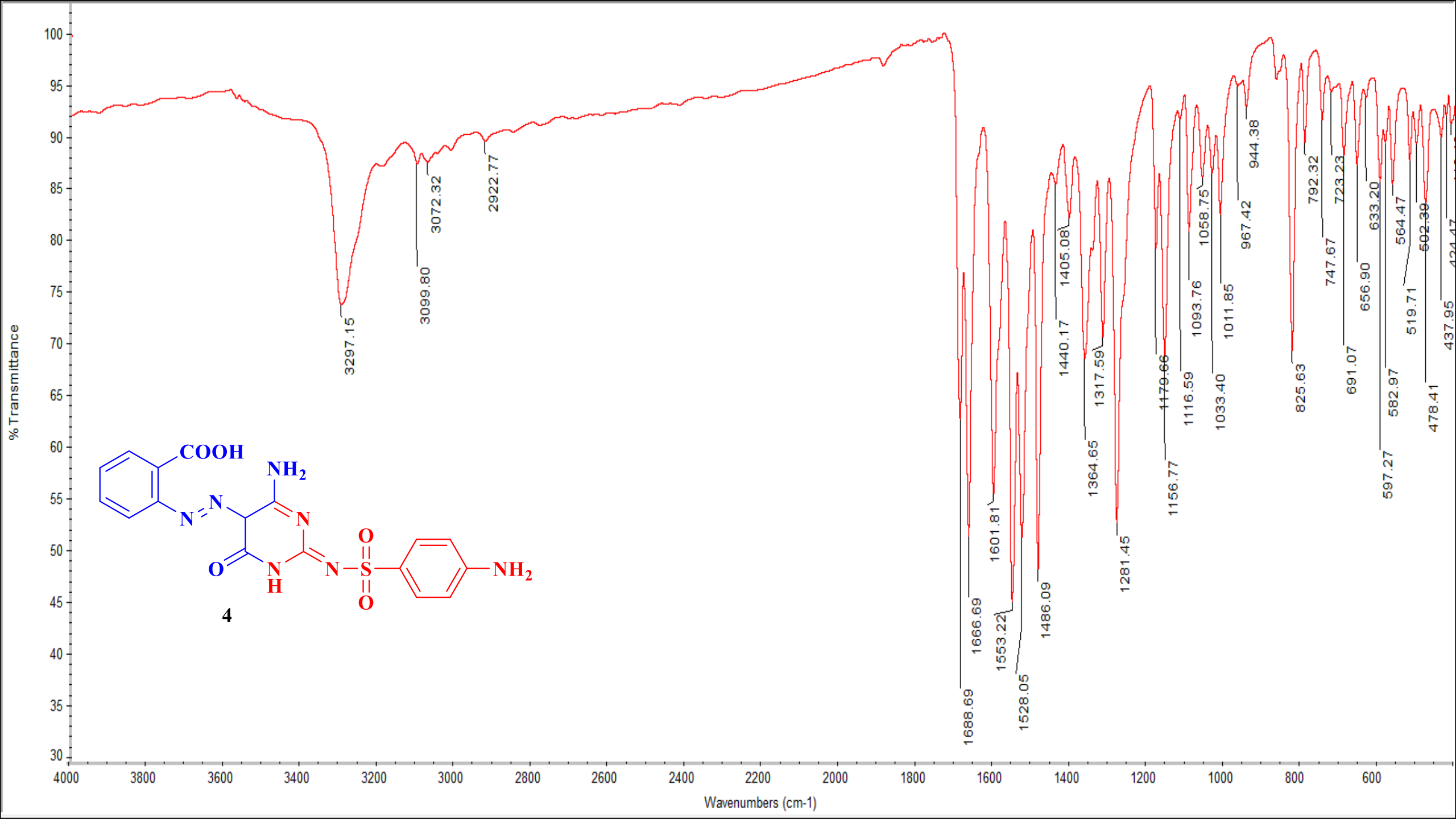
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Time 19.49 h  
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PULPROG 65536  
TD 2100  
SOLVENT DMSO  
NS 2100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 197.77  
DW 20.800 usec  
DE 6.50 usec  
TE 296.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6404331 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 47.00000000 W  
SFO2 400.2016008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.00000000 W  
PLW12 0.29249999 W  
PLW13 0.14713000 W

F2 - Processing parameters  
SI 32768  
SF 100.6303700 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

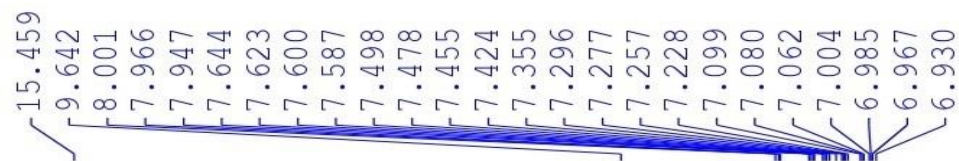


REC3 #237 RT: 3.98 P: + SB: 10 2.43 , 2.76-2.90 NL: 5.29E3  
T: {0,0} + c EI Full ms [40.00-1000.00]

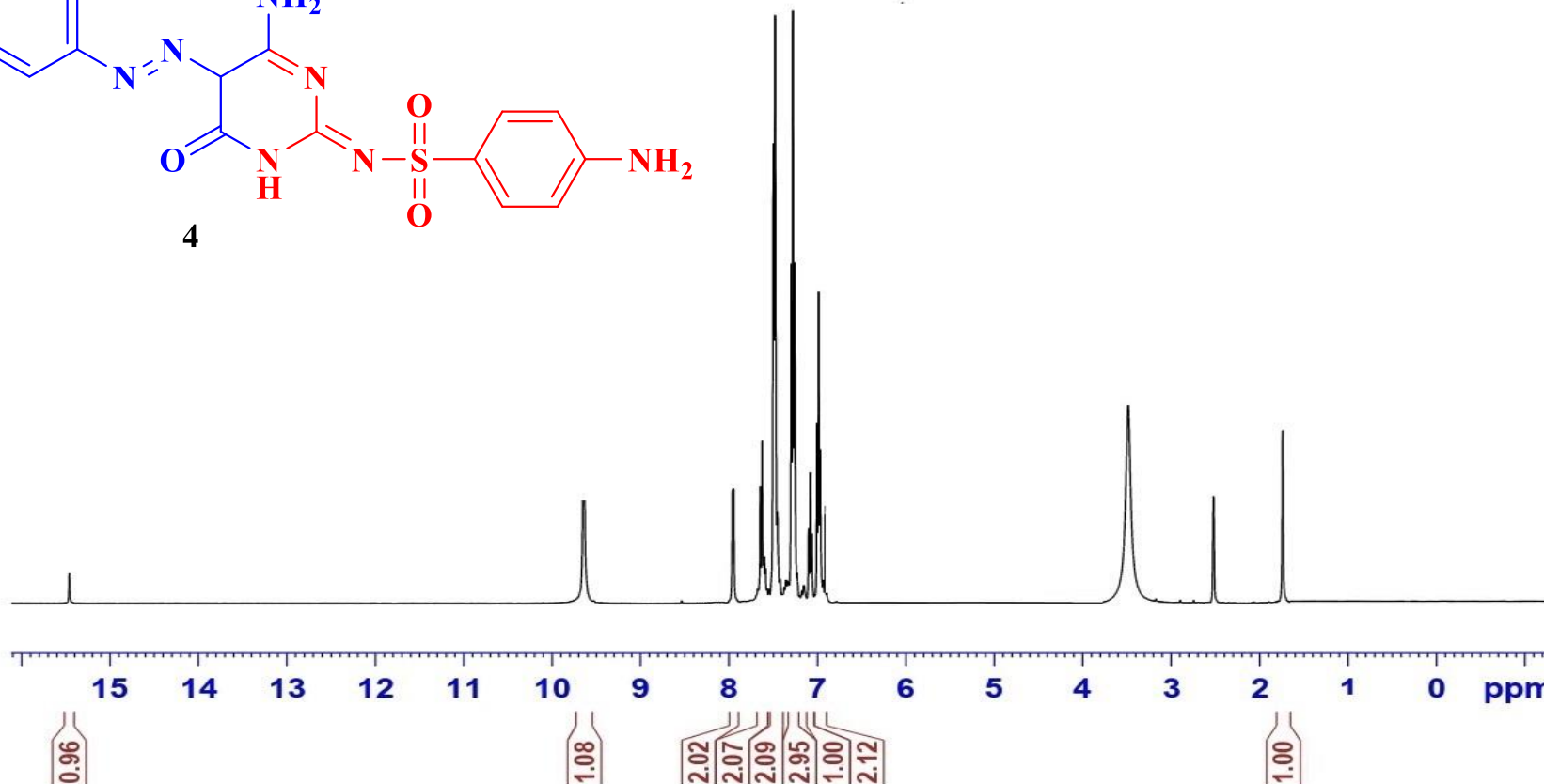
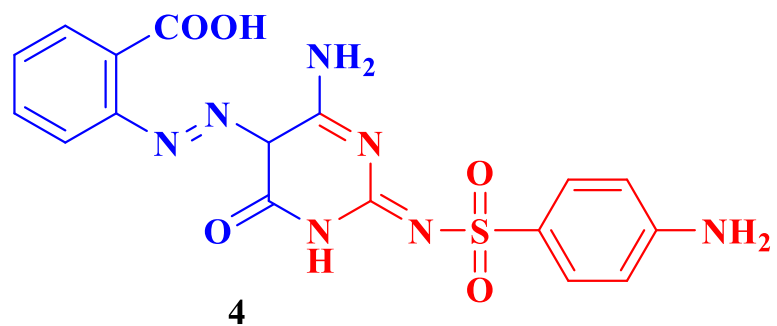




REC14-Hnmr-RR



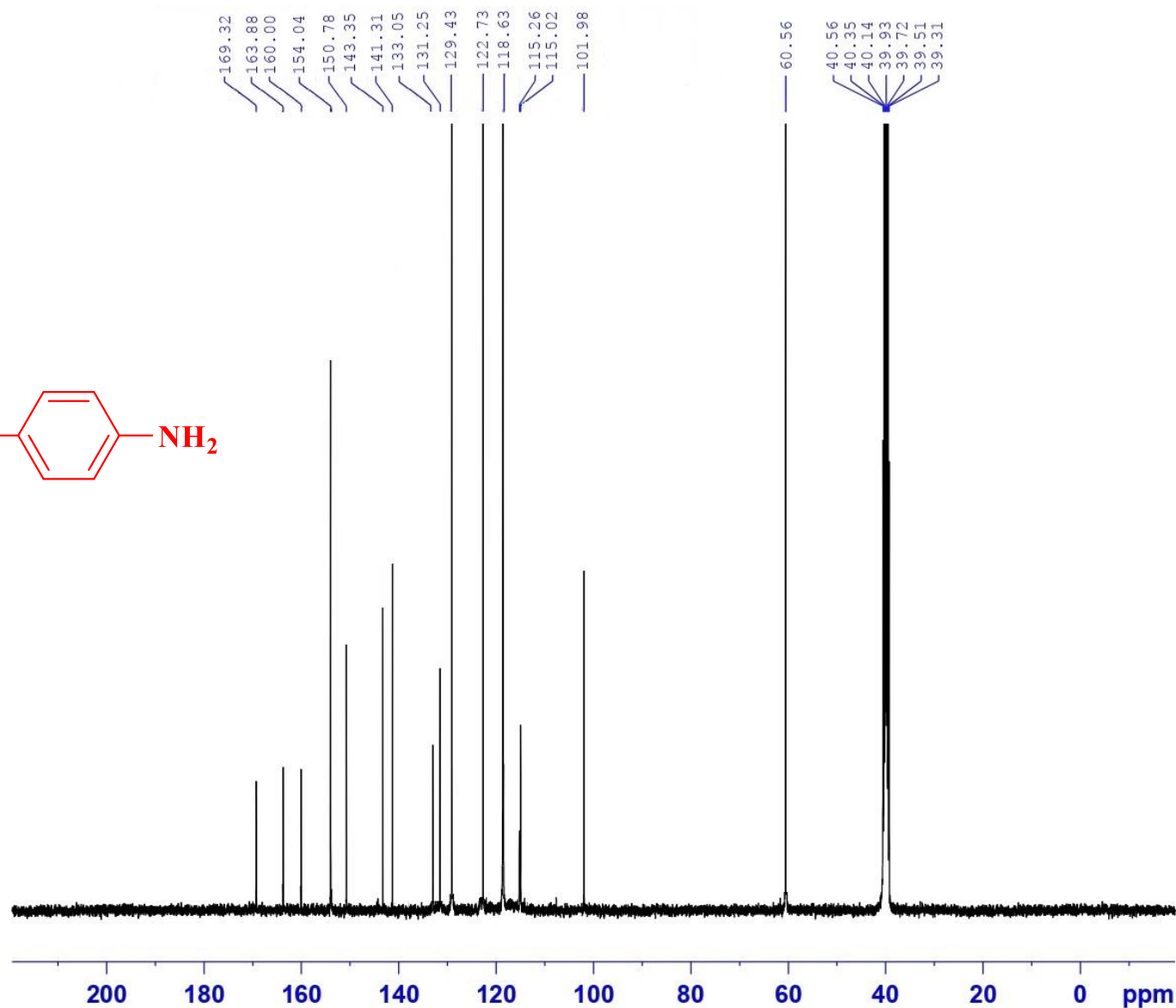
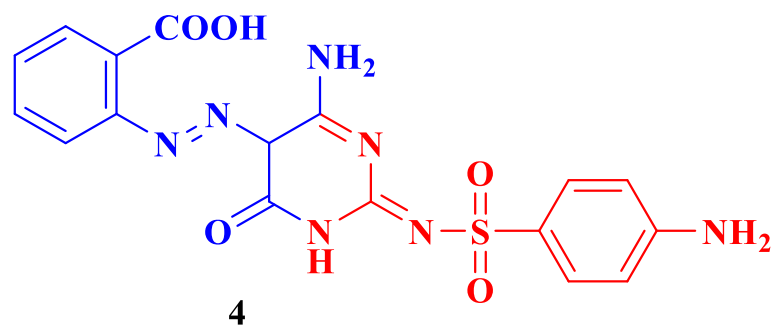
— 3.484  
— 2.520  
— 1.738



F2 - Acquisition Parameters  
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 Time\_ 15.88 h  
 INSTRUM spect  
 PROBHD zg30  
 PULPROG 65536  
 TD 16  
 SOLVENT DMSO  
 NS 2  
 DS 8012.820 Hz  
 SWH 0.244532 Hz  
 FIDRES 4.0894465 sec  
 AQ 58.17  
 RG 62.400 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2024712 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 13.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2000000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

# REC14-CNMR-DMSO-SH



F2 - Acquisition Parameters  
 Date\_ 20240629  
 Time 10.34 h  
 INSTRUM spect  
 PROCNO 2108618  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2200  
 DS 4  
 SSW 24028.461 Hz  
 FIDRES 0.722596 Hz  
 AQ 1.2621488 sec  
 RG 197.77  
 DW 20.800 usec  
 DE 8.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0200000 sec  
 TDO 1  
 SFO1 100.6204221 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLM1 47.0000000 W  
 SFO2 400.2016008 MHz  
 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD 90.00 usec  
 PLM2 12.0000000 W  
 PLM12 0.29249999 W  
 PLM13 0.14718000 W  
 F2 - Processing parameters  
 SI 227.68  
 SF 100.6203700 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

REC14 #93 RT: 1.57 P: + SB: 13 1.22-1.41, 1.31 NL: 6.88E2

T: {0,0} + c EI Full ms [40.00-1000.00]

