

Supplementary Material

Barbituric and thiobarbituric acid derived chromophores as anticancer agents

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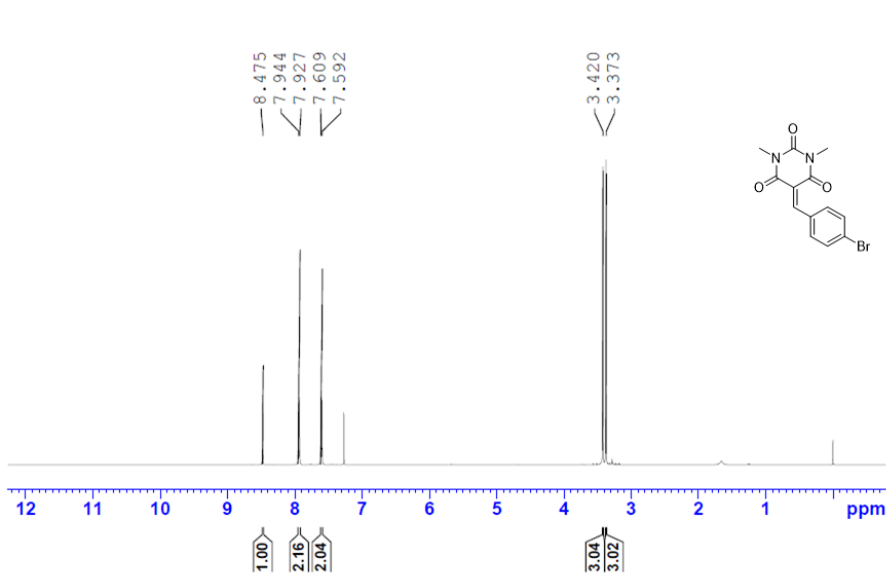
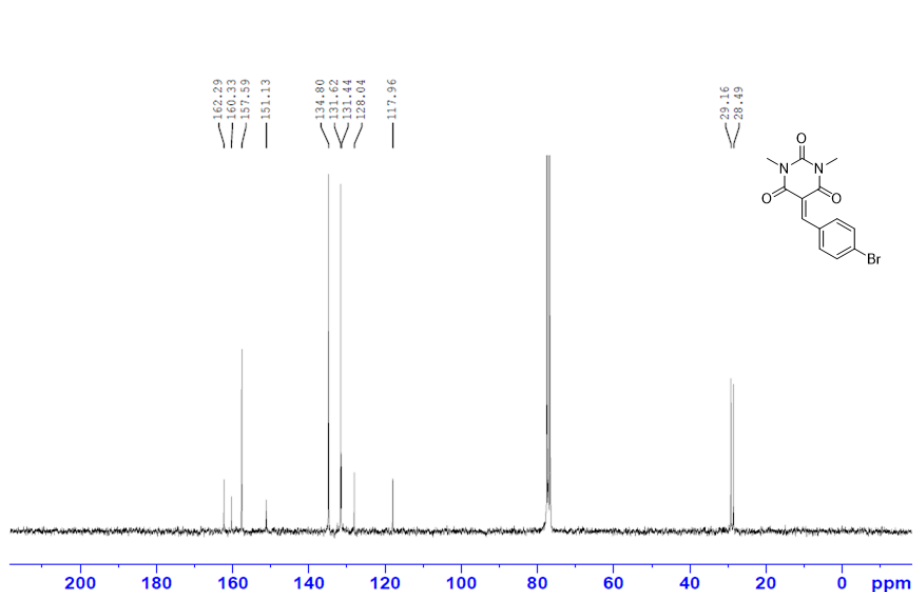
^ePeptide Sciences Laboratory, School of Physics and Chemistry, University of KwaZulu-Natal, Westville Campus, Durban 4000, South Africa

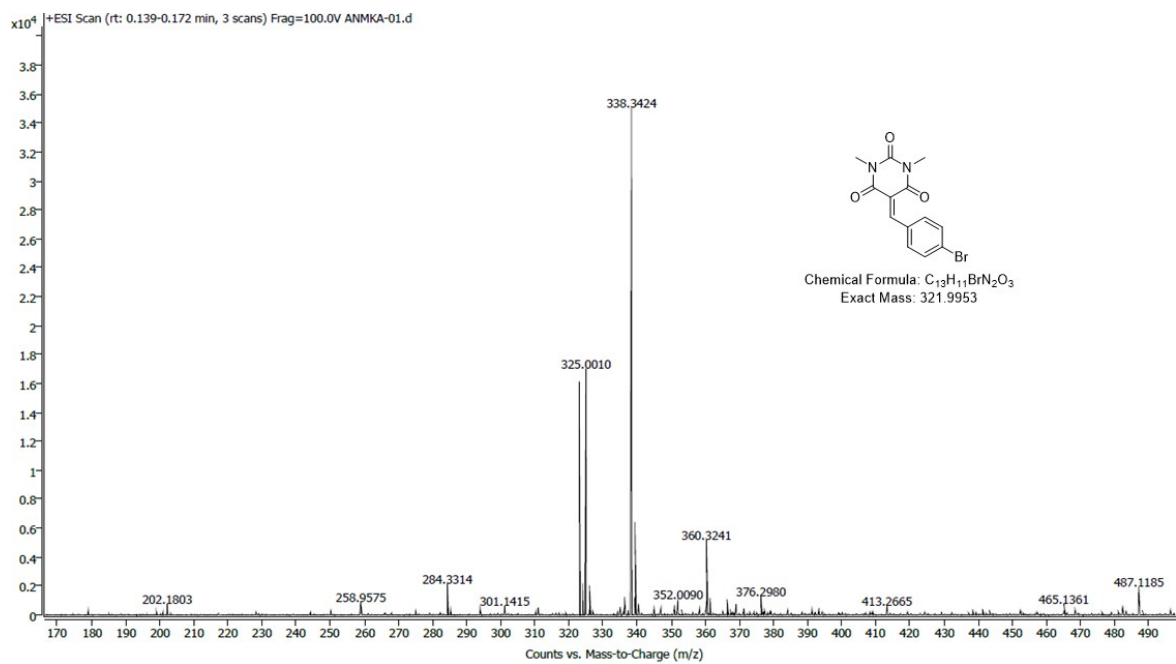
Email: lrsingh.iict@csir.res.in; anamika.aug14@gmail.com

#These authors contributed equally

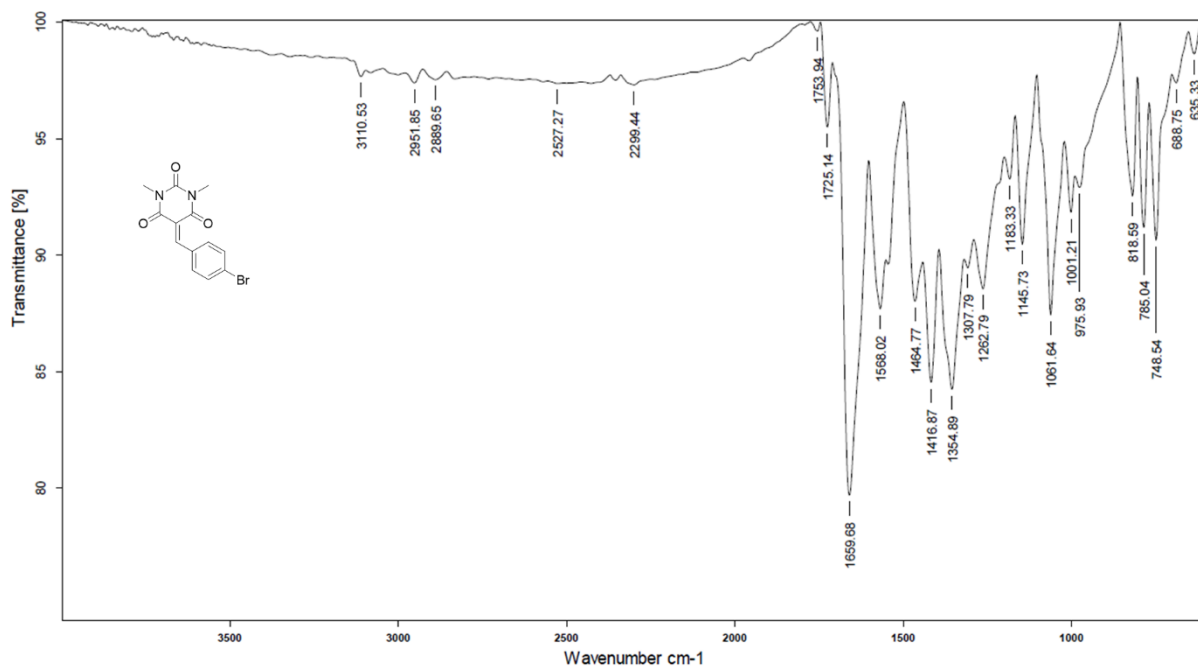
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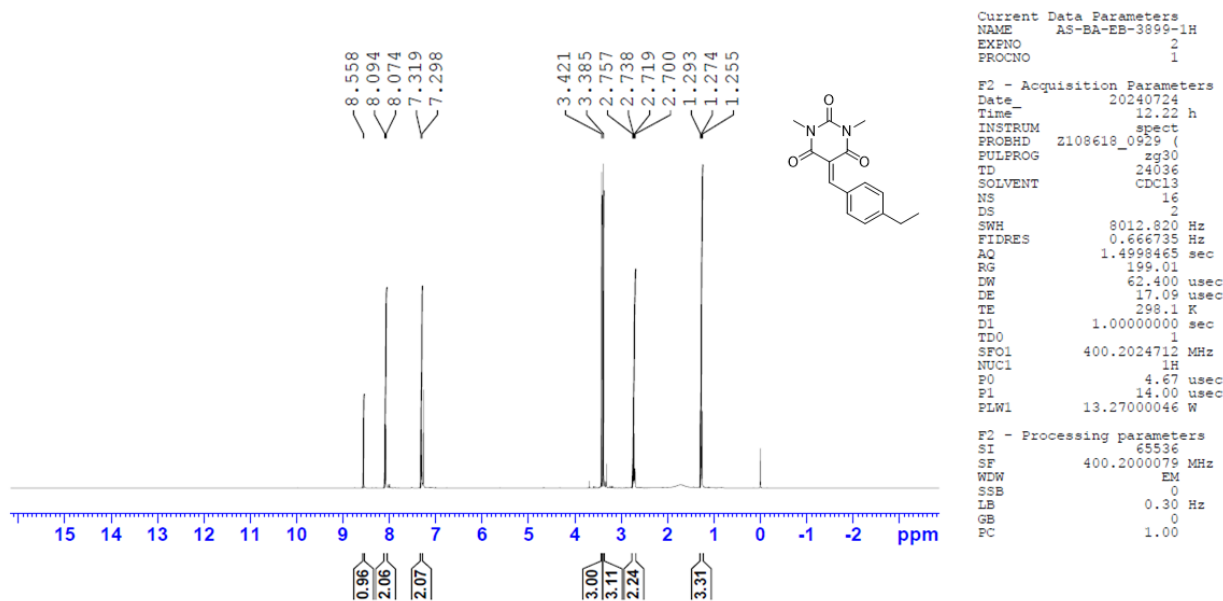
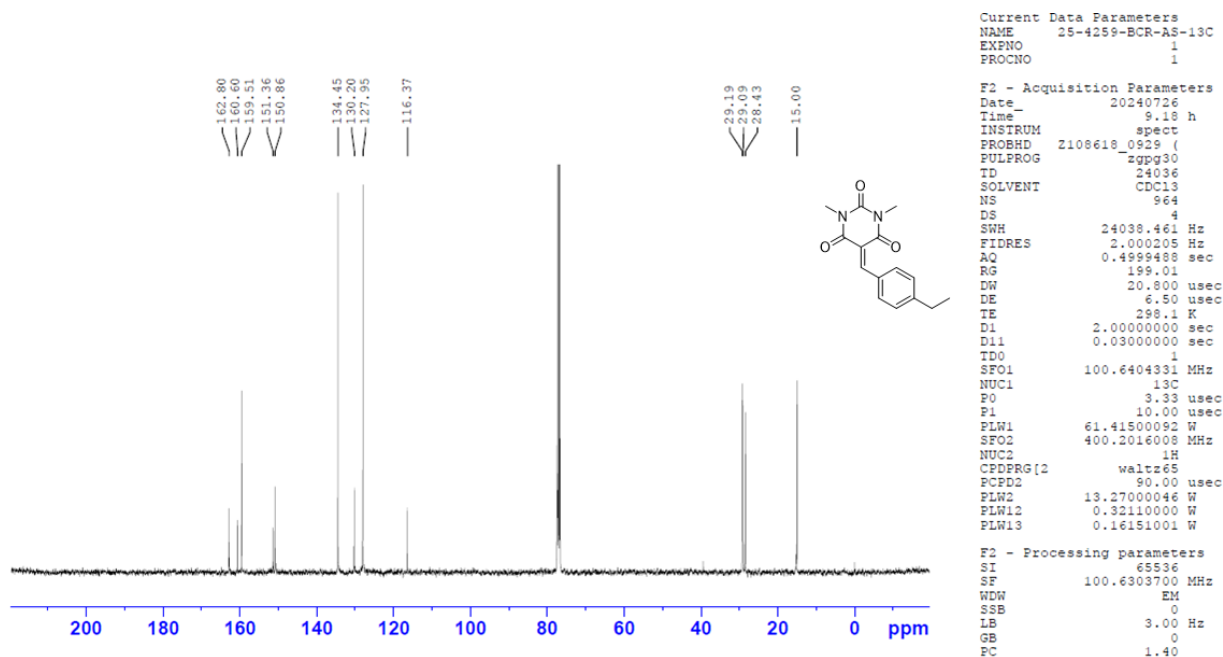
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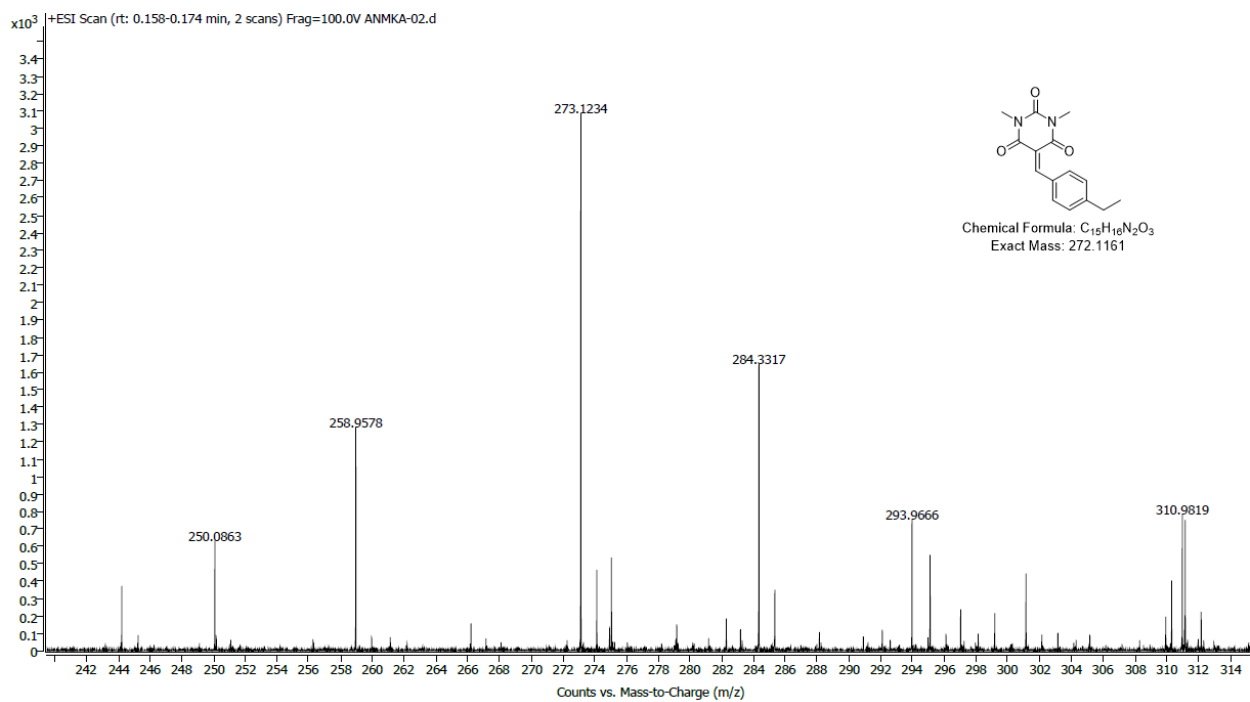


HRMS of 1

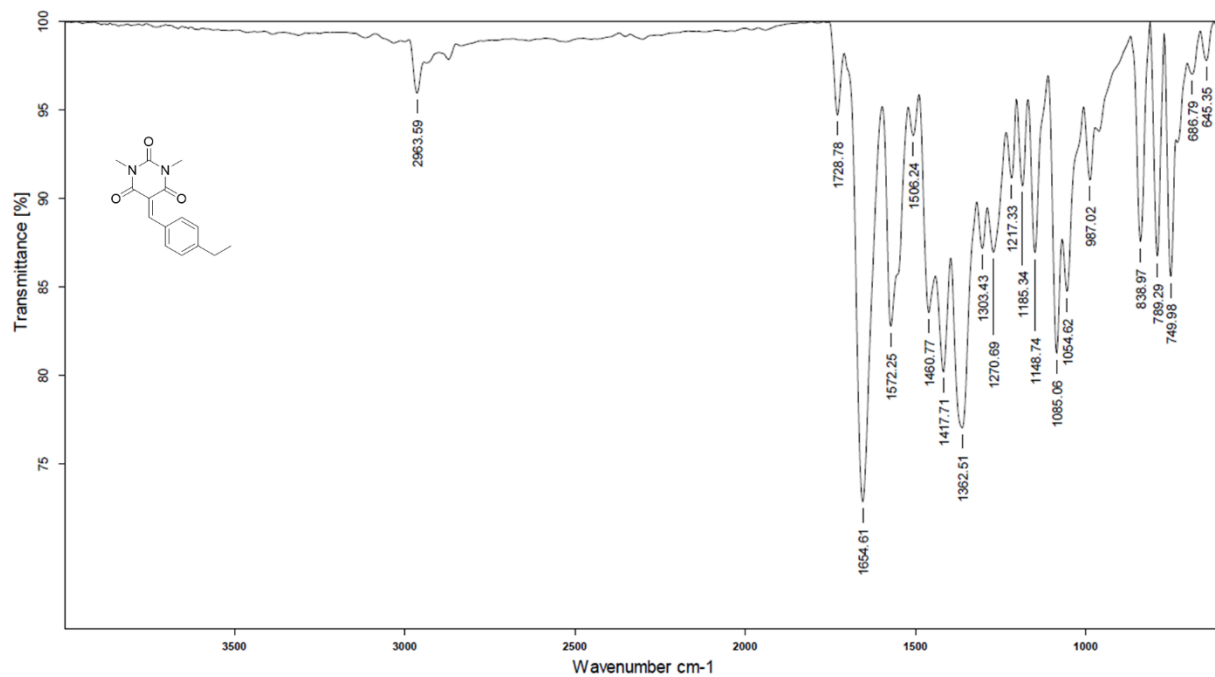


IR of 1

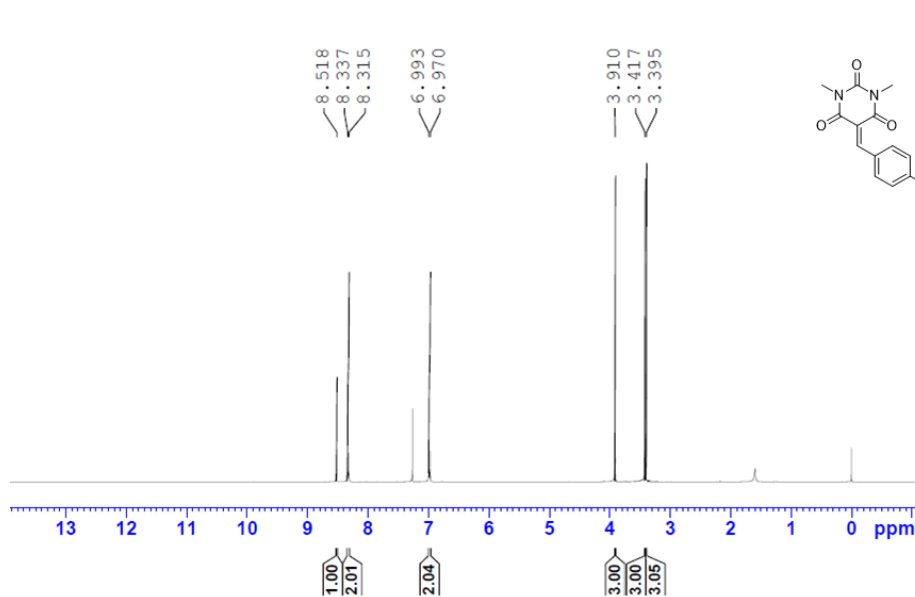
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HRMS of 2



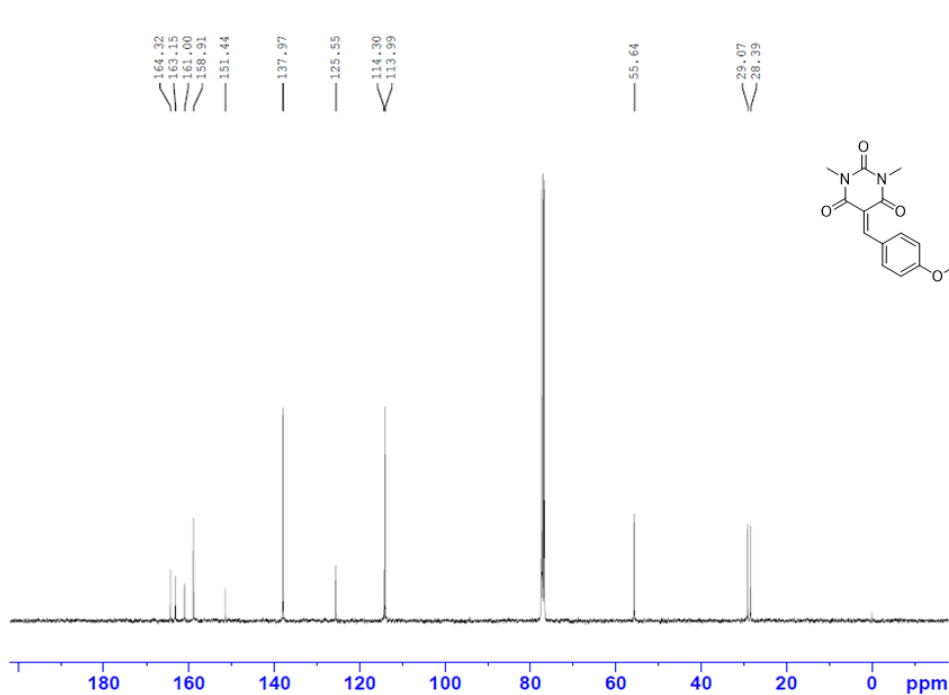
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 PULPROG zg30
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 SOLVENT CDCl3
 NS 16
 DS 2
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 FIDRES 0.666735 Hz
 AQ 1.4998465 sec
 RG 186.53
 DW 62.400 usec
 DE 17.77 usec
 TE 298.2 K
 D1 1.00000000 sec
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 NUC1 1H
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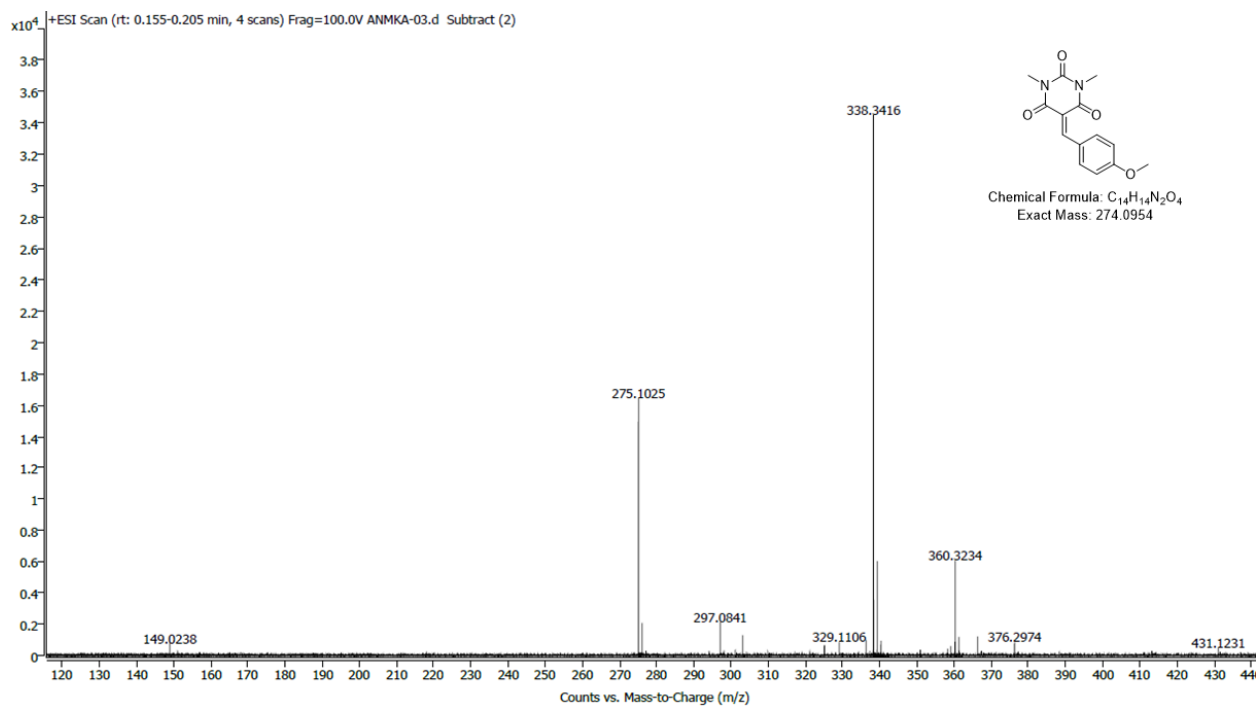
¹H NMR of 3

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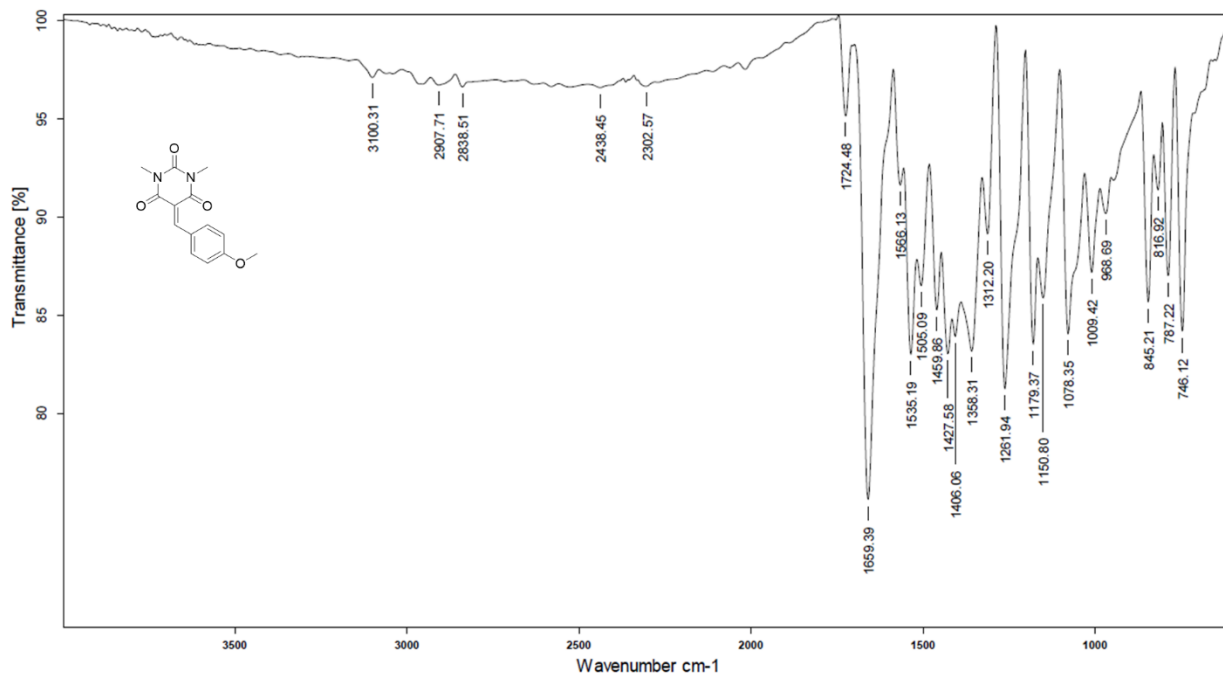
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 NS 1024
 DS 4
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 FIDRES 2.000240 Hz
 AQ 0.4999400 sec
 RG 209.58
 DW 14.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.33 usec
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 NUC2 1H
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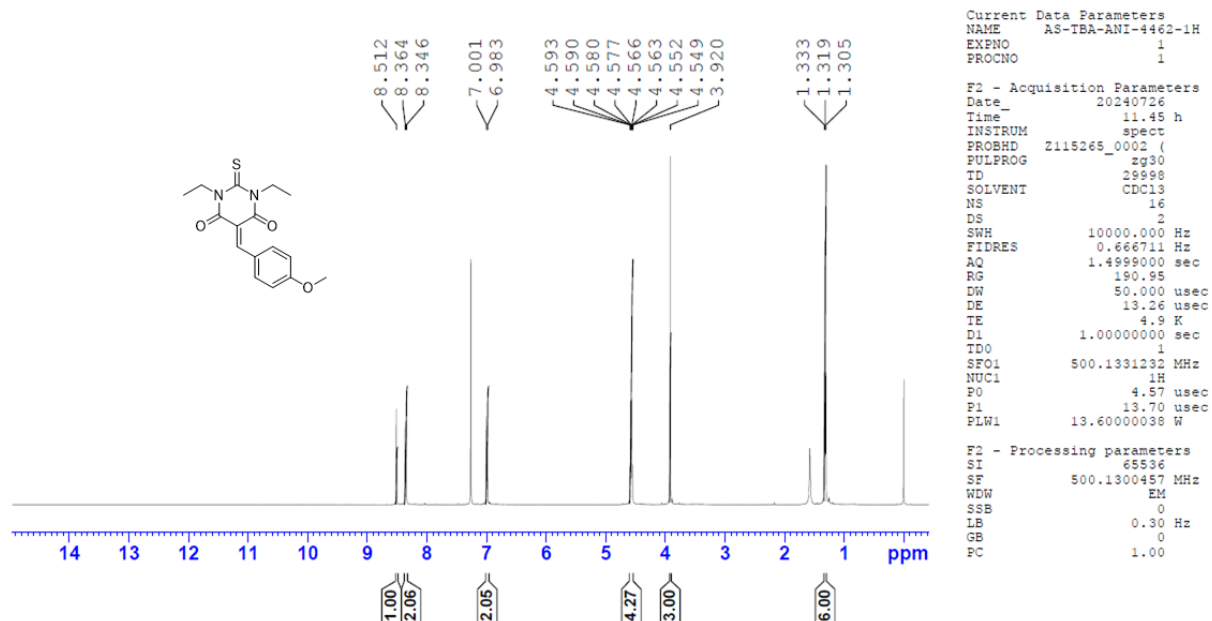
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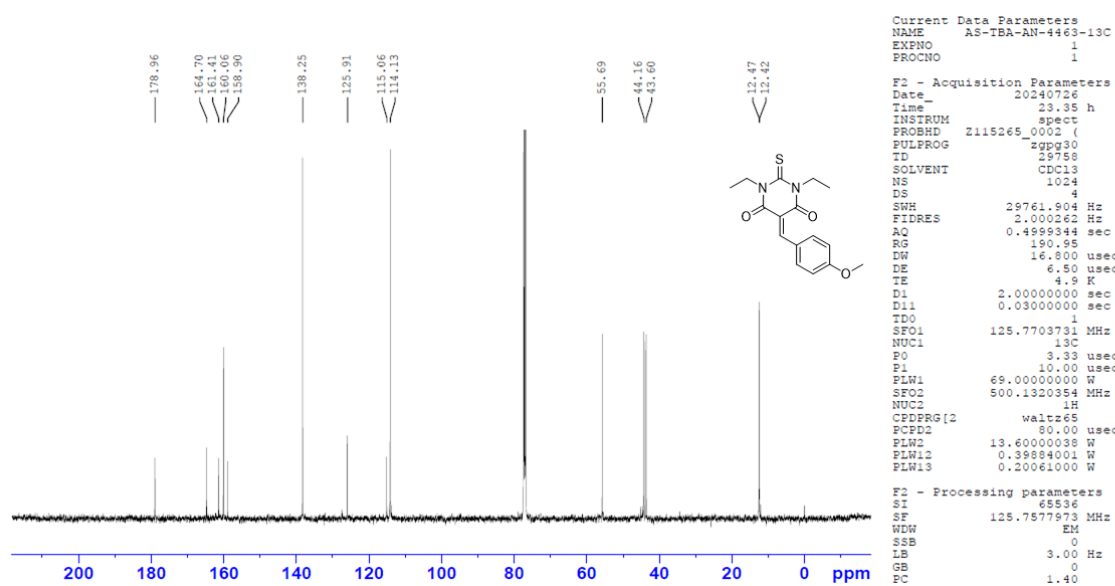
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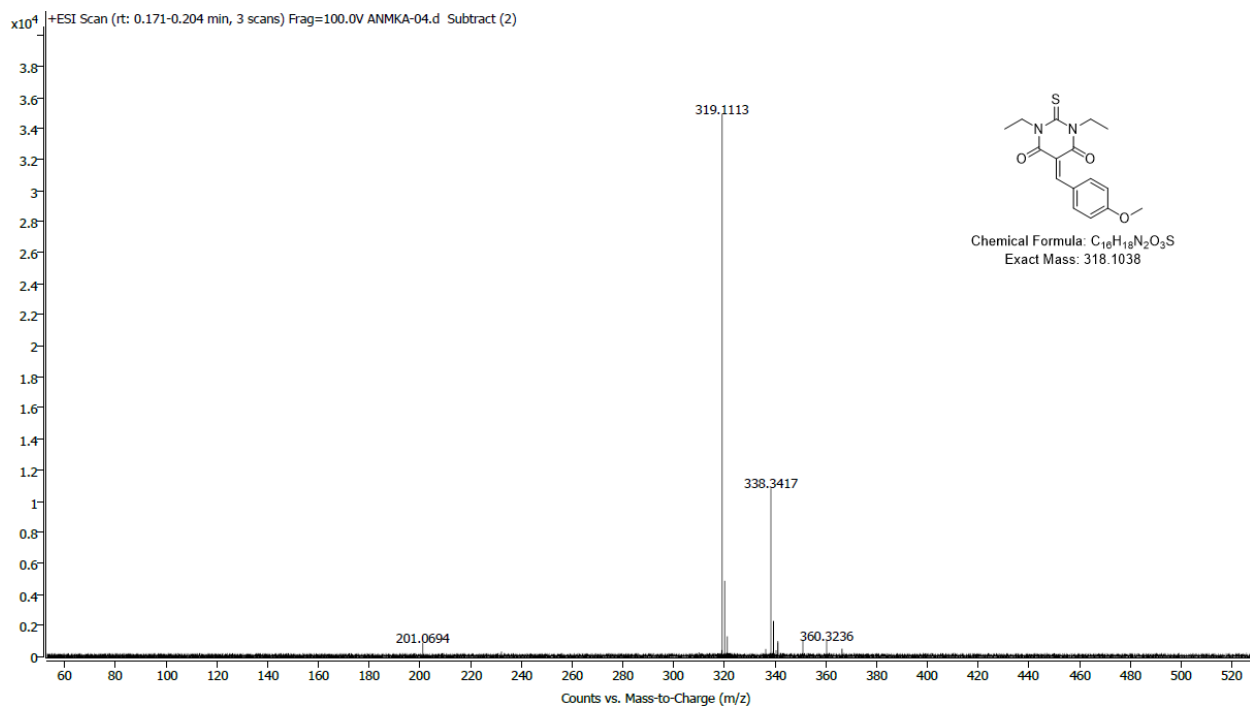
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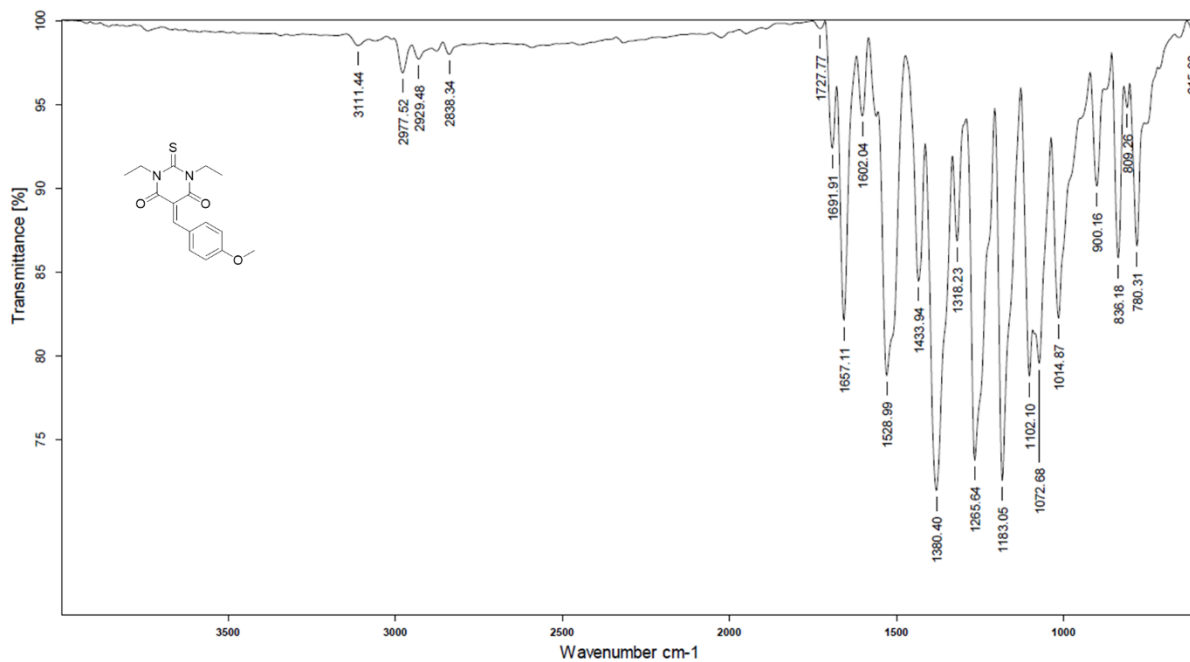
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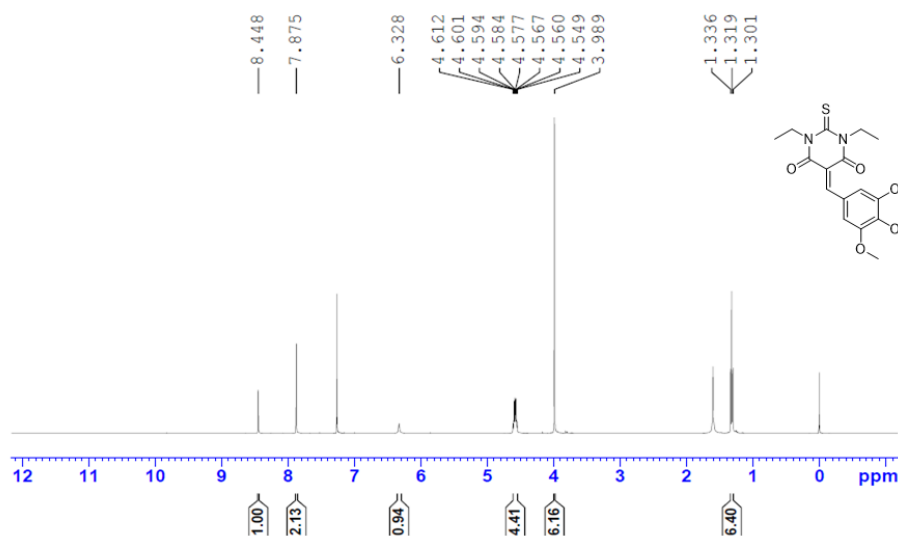
¹³C NMR of 4



HRMS of 4



IR of 4



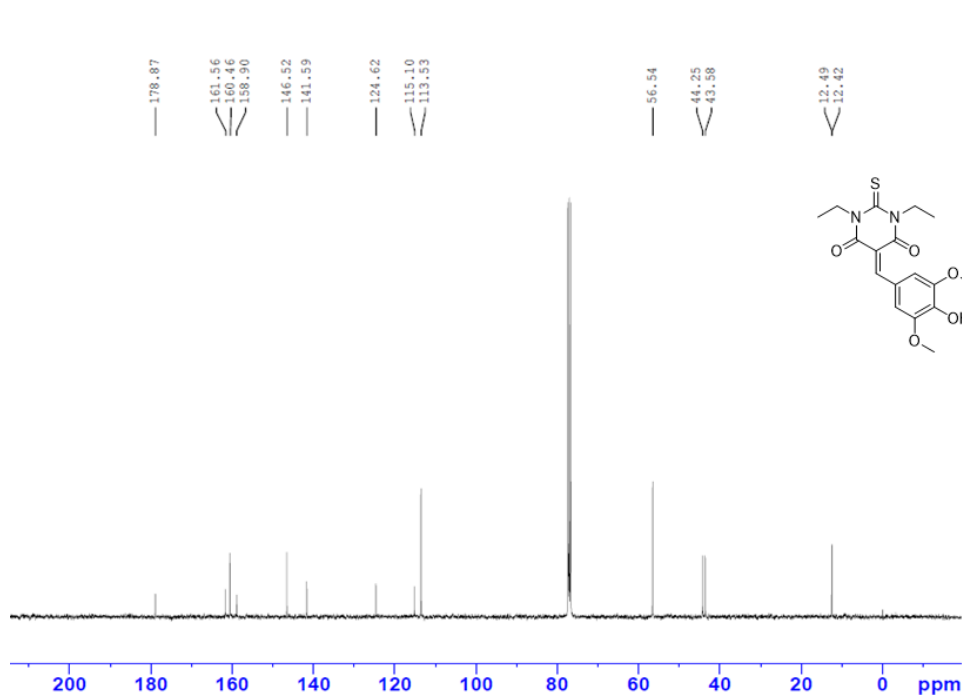
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TD         24036
SOLVENT   CDCl3
NS         16
DS         2
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FIDRES     0.666735 Hz
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RG         199.01
DW         62.400 usec
DE         17.09 usec
TE         298.1 K
D1         1.00000000 sec
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NUC1       1H
P0         4.67 usec
P1         14.00 usec
PLW1      13.27000046 W

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¹H NMR of 5



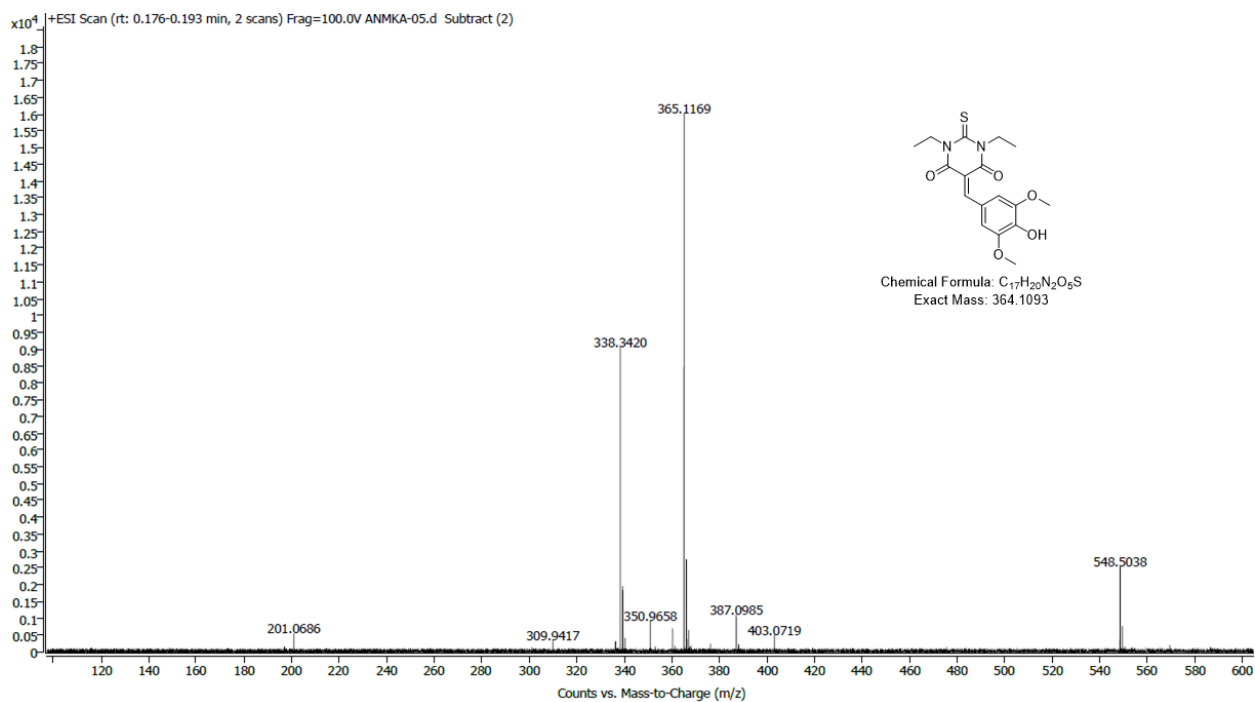
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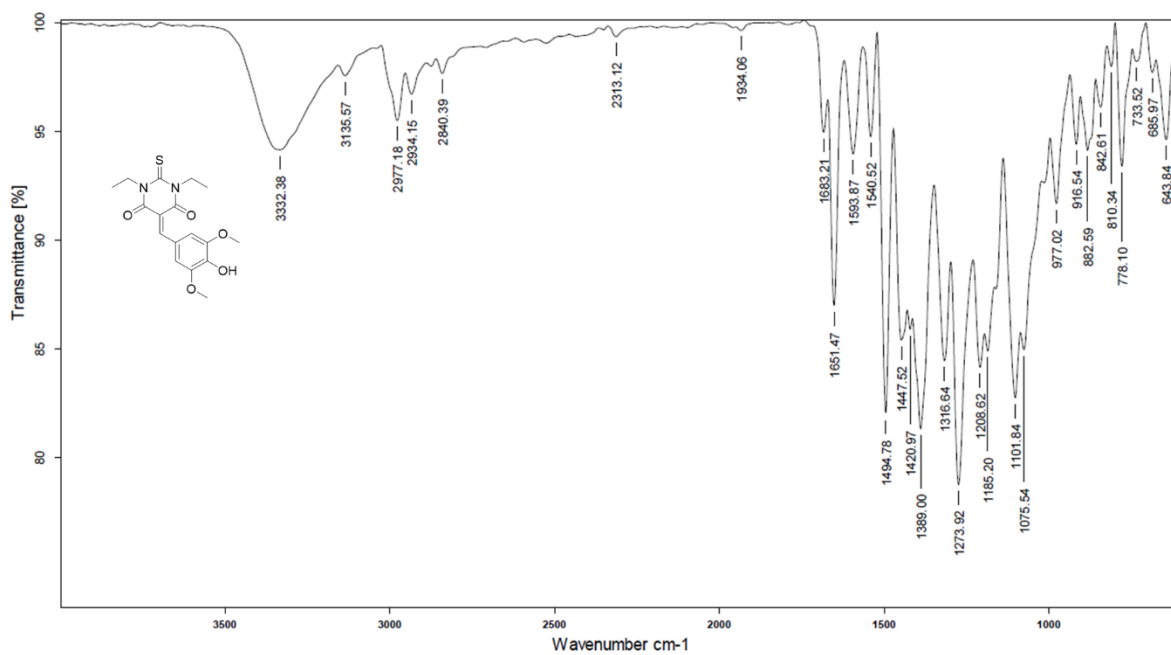
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SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     2.000205 Hz
AQ         0.4999488 sec
RG         209.58
DW         20.800 usec
DE         6.50 usec
TE         298.2 K
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D11        0.03000000 sec
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NUC1       13C
P0         3.33 usec
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PLW1      82.48899841 W
SFO2      400.1316005 MHz
NUC2       1H
CPDPRG2   waltz65
PCPD2     90.00 usec
PLW2      17.39800072 W
PLW12     0.21479000 W
PLW13     0.10804000 W

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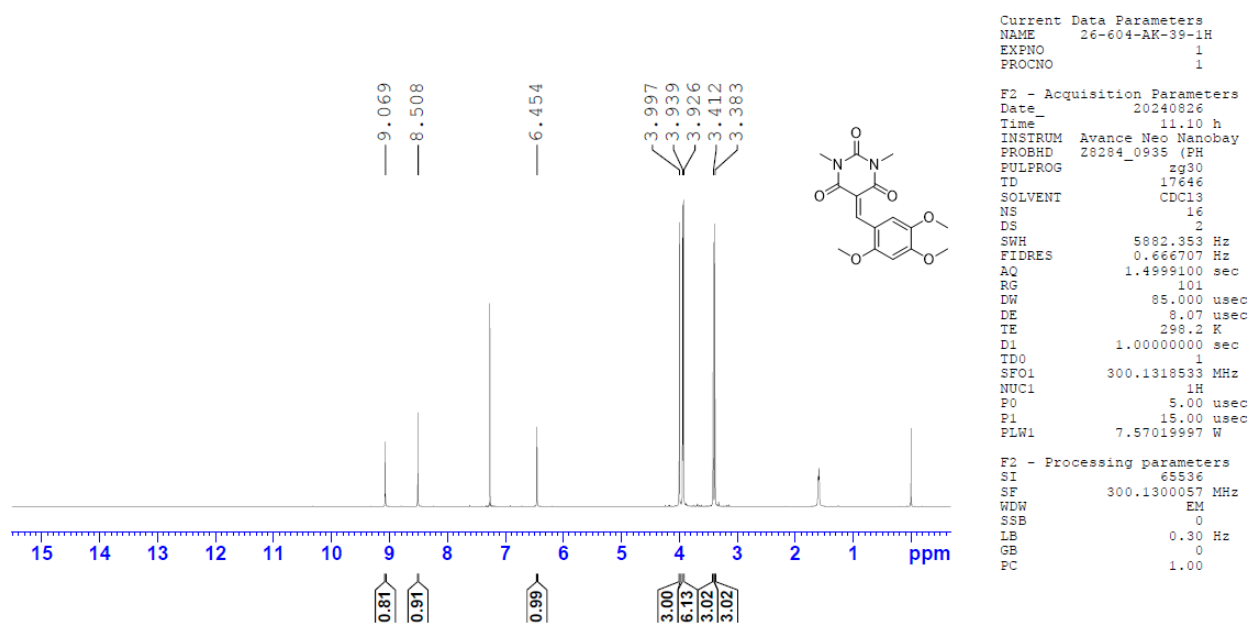
¹³C NMR of 5



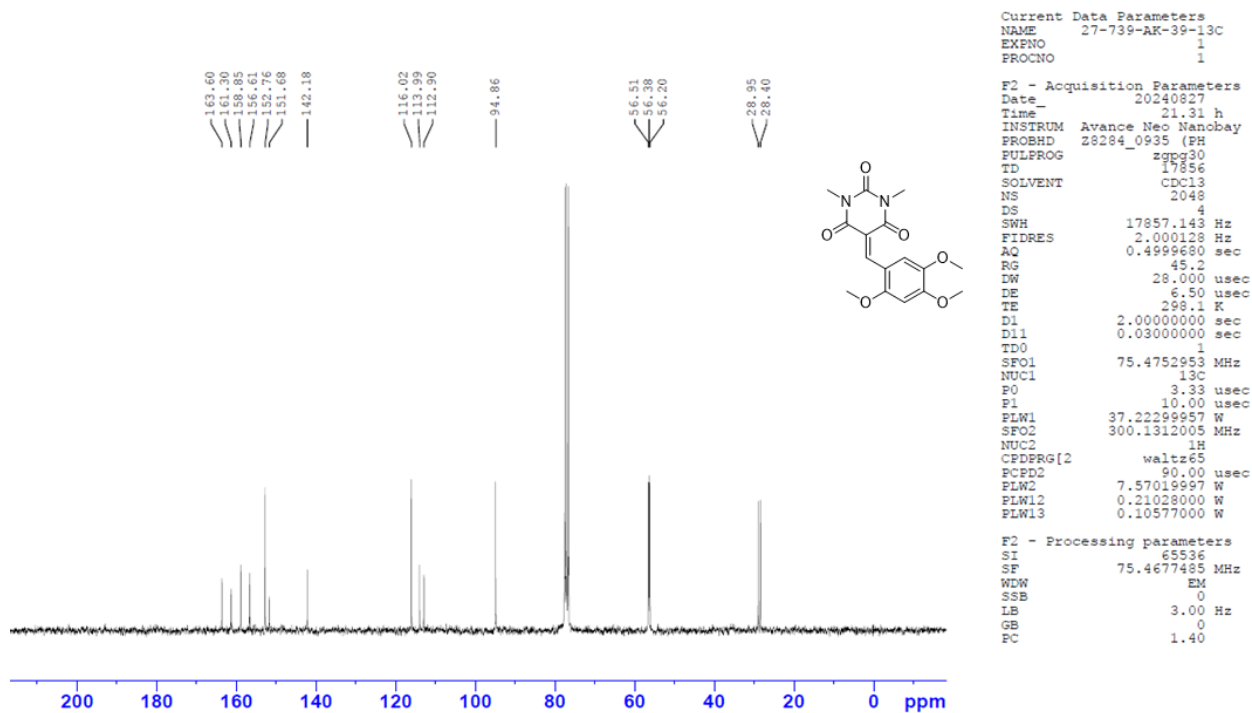
HRMS of 5



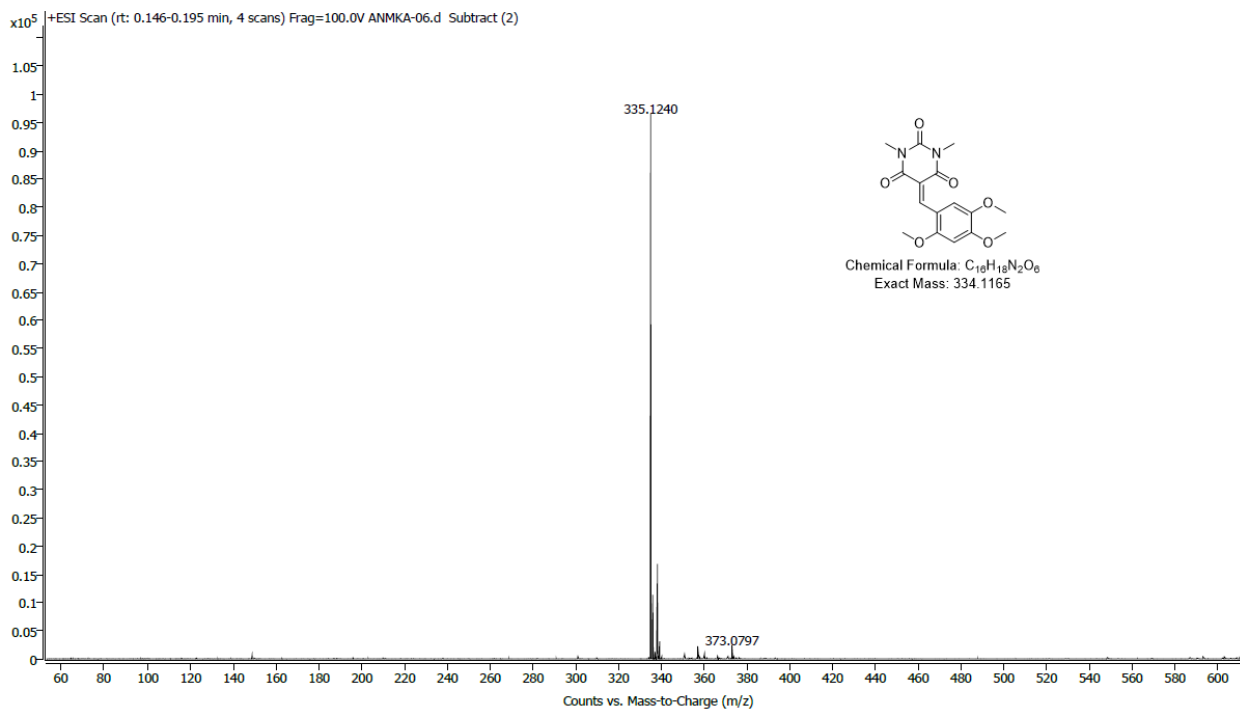
IR of 5



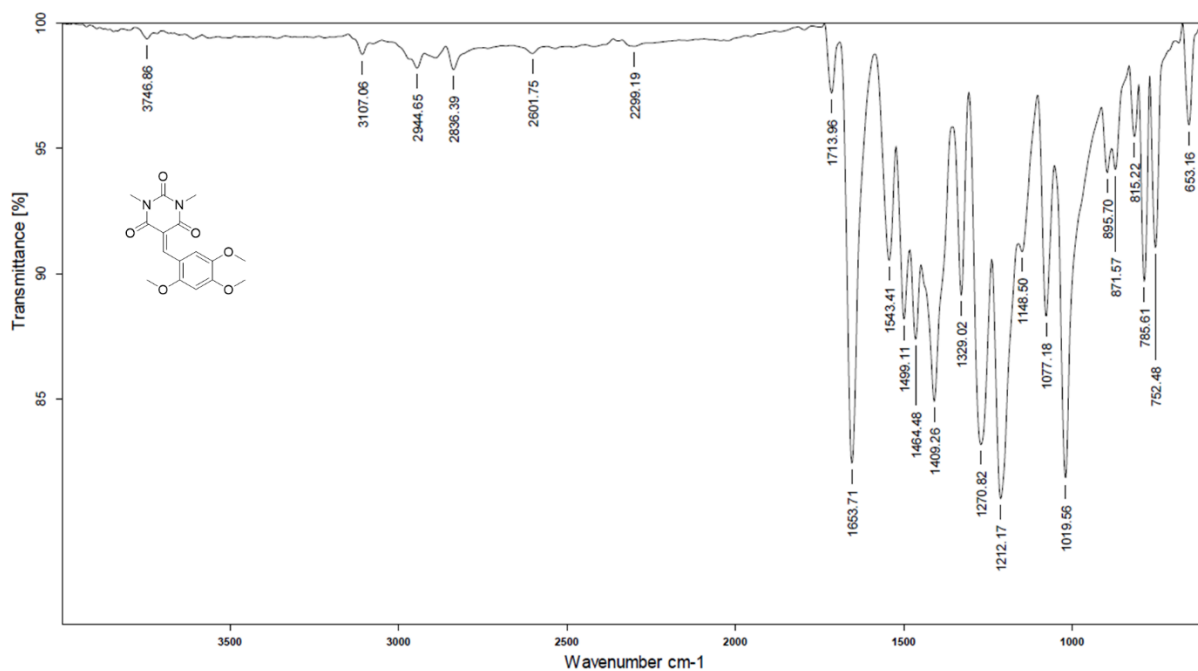
¹H NMR of 6



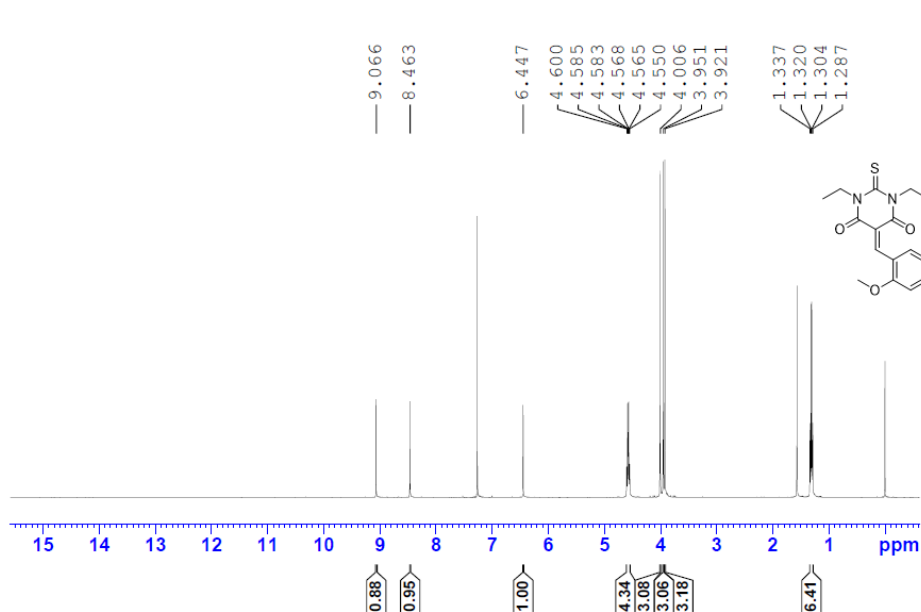
¹³C NMR of 6



HRMS of 6



IR of 6



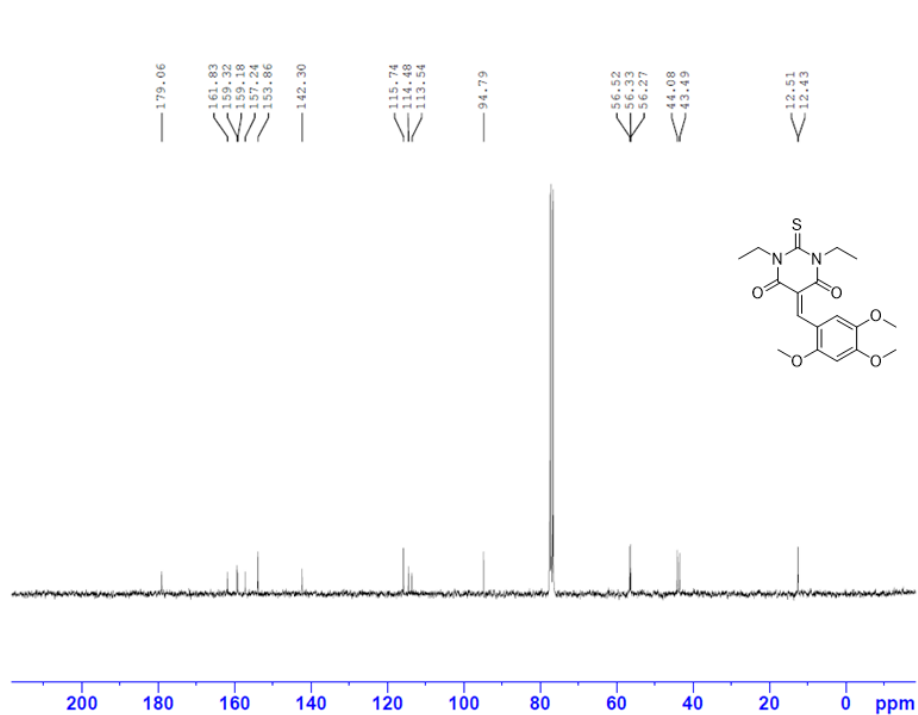
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PROCNO    1

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PULPROG   zg30
TD         24036
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.666735 Hz
AQ         1.4989465 sec
RG         199.01
DW         62.400 usec
DE         17.09 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1
SFO1       400.2024712 MHz
NUC1       1H
FO         4.67 usec
P1         14.00 usec
PLW1       13.27000046 W

F2 - Processing parameters
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¹H NMR of 7



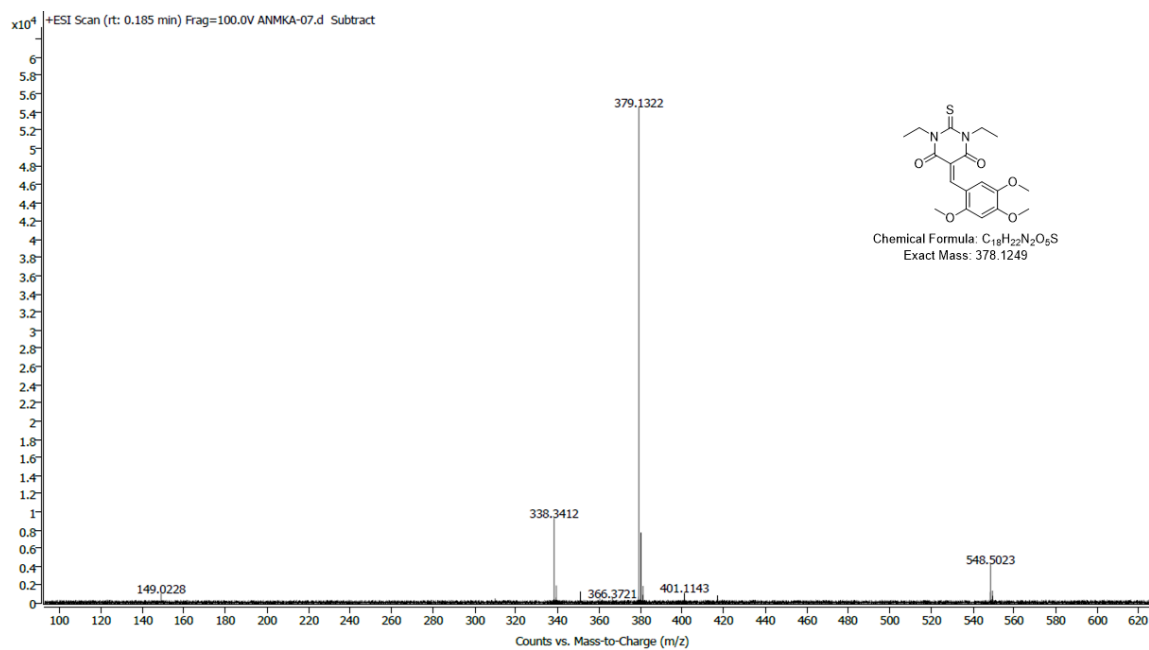
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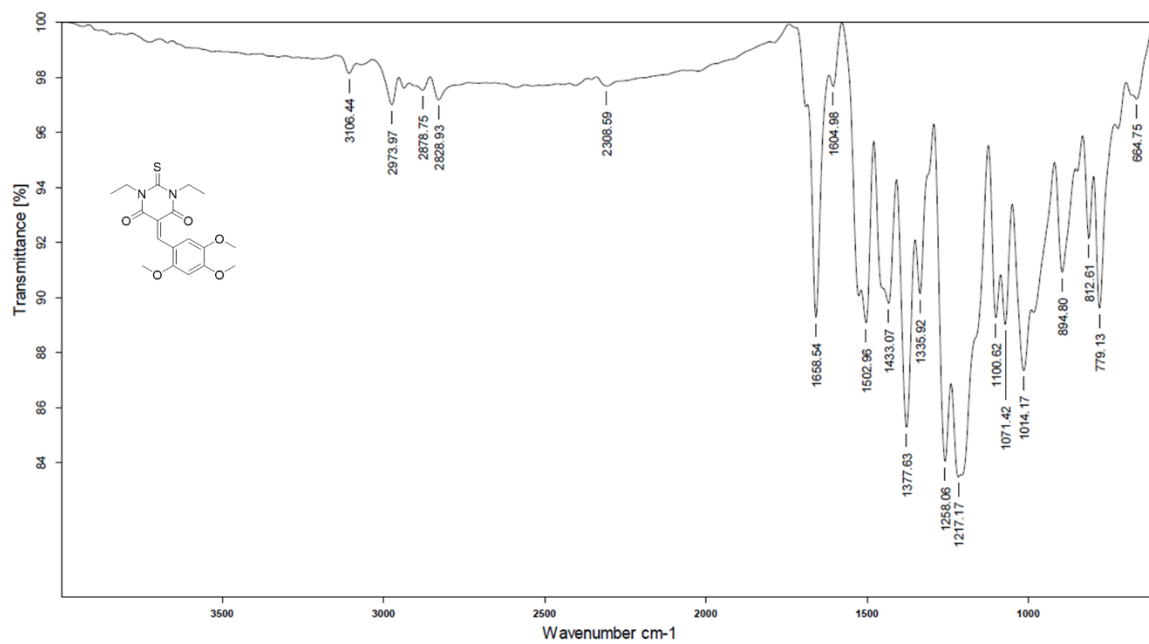
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D1         4.00000000 sec
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SFO1       75.4752953 MHz
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NUC2       1H
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PCPD2     90.00 usec
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PLW13      0.11406000 W

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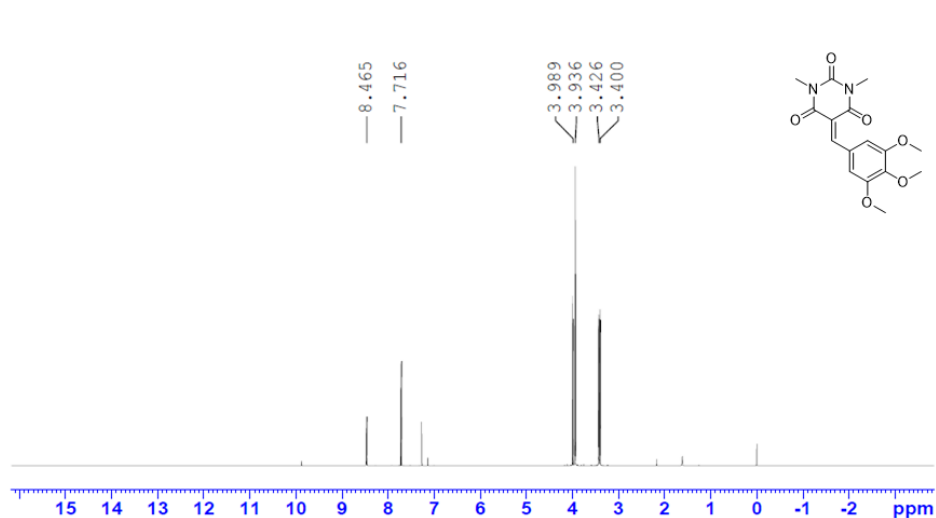
¹³C NMR of 7



HRMS of 7



IR of 7



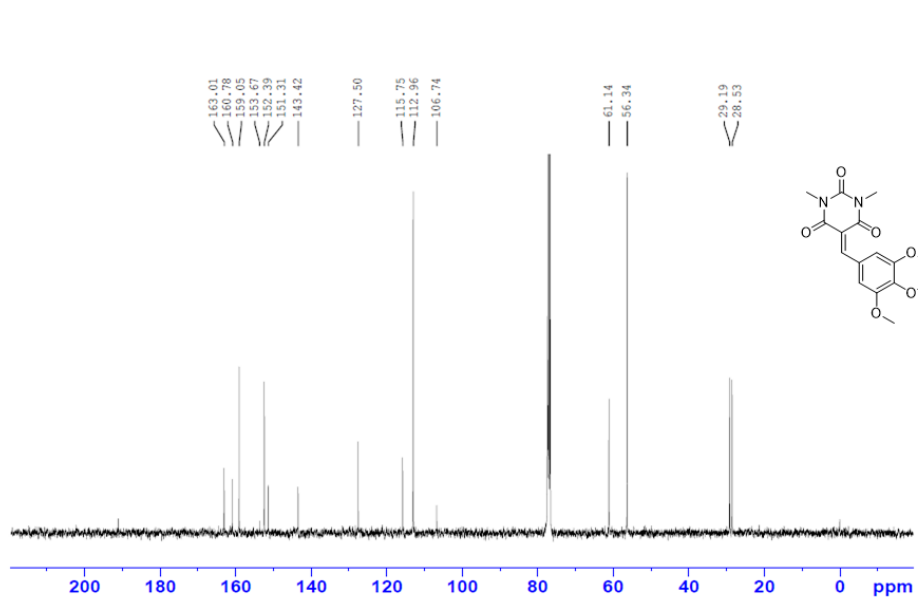
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PULPROG  zg30
TD       24036
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.666735 Hz
AQ       1.4998465 sec
RG       127.55
DW       62.400 usec
DE       17.09 usec
TE       298.2 K
D1       1.0000000 sec
TD0      1
SFO1     400.2024712 MHz
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PLW1     13.27000046 W

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¹H NMR of **8**



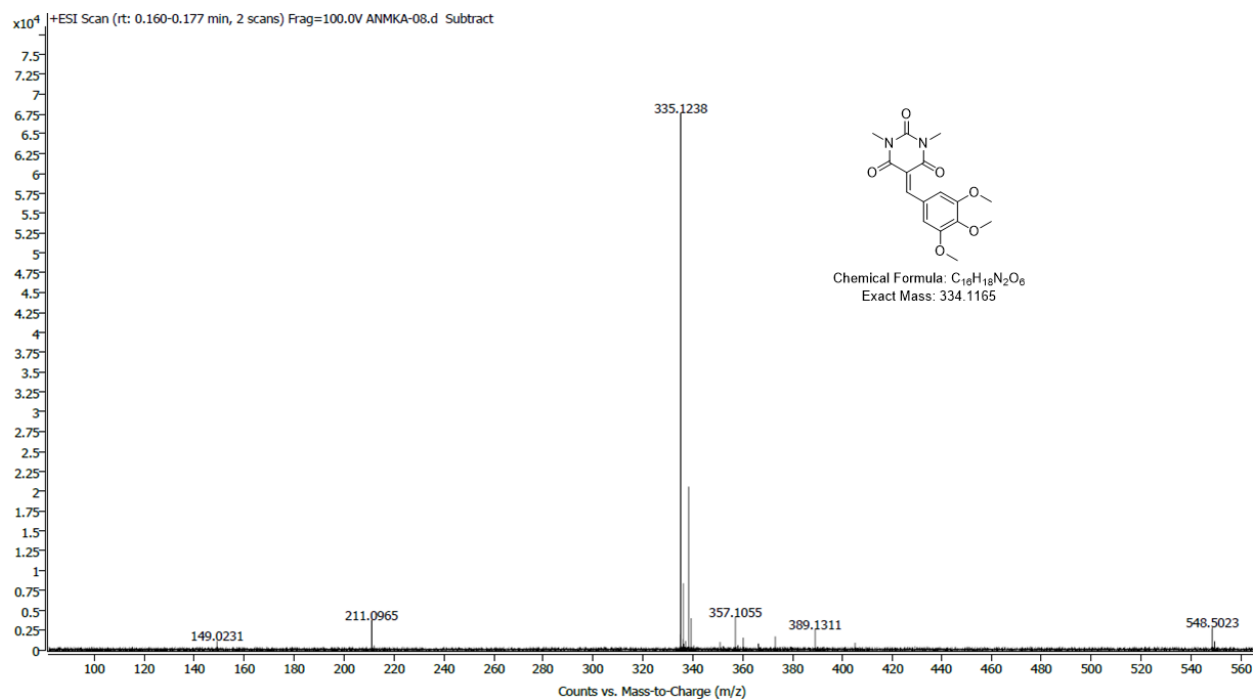
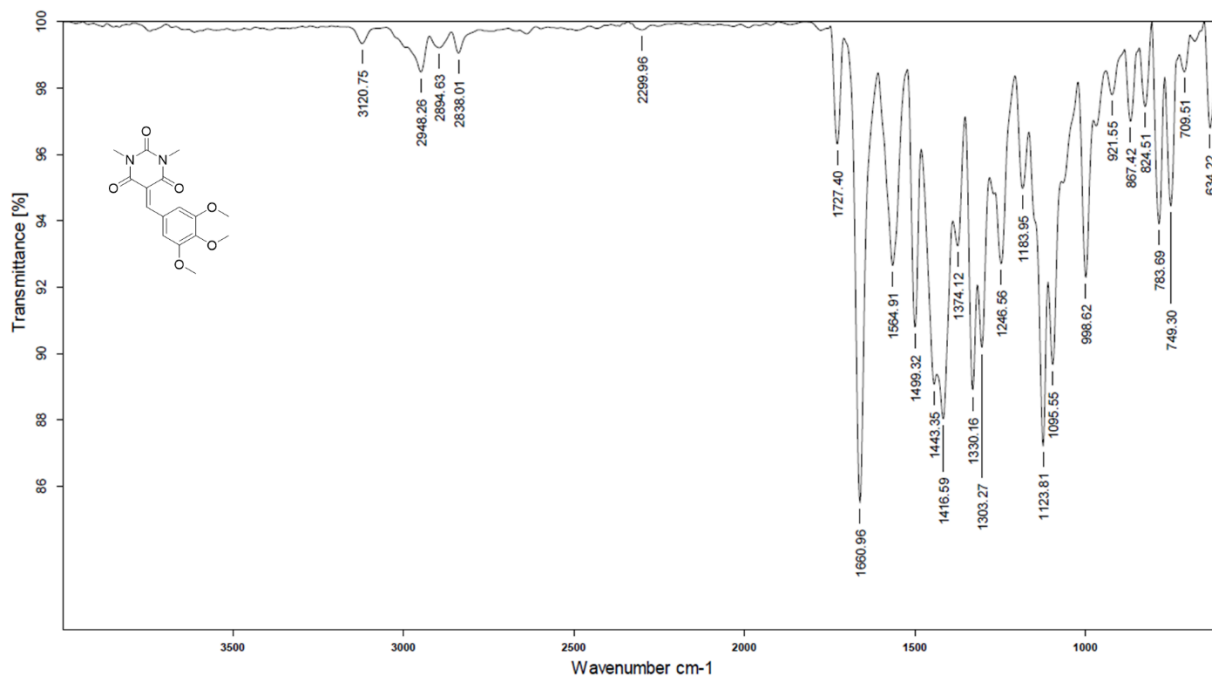
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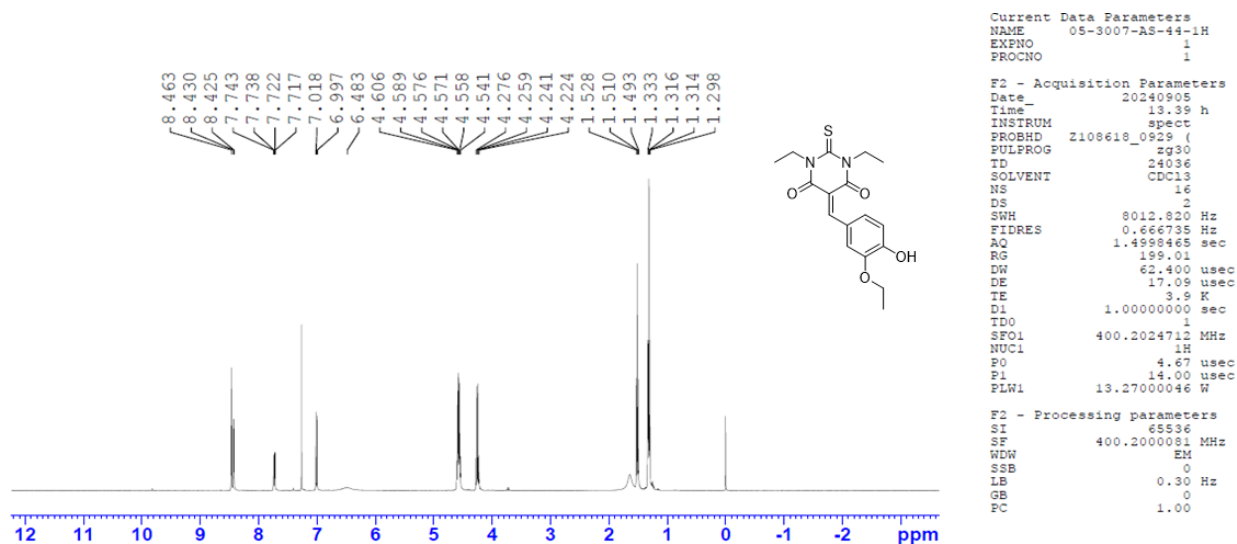
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SOLVENT  CDCl3
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FIDRES   2.000205 Hz
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RG       209.58
DW       20.800 usec
DE       6.50 usec
TE       298.2 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
FO       3.33 usec
PI       10.00 usec
PLW1     82.48899841 W
SFO2     400.1316005 MHz
NUC2     1H
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PCPD2    90.00 usec
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PLW12    0.21479000 W
PLW13    0.10804000 W

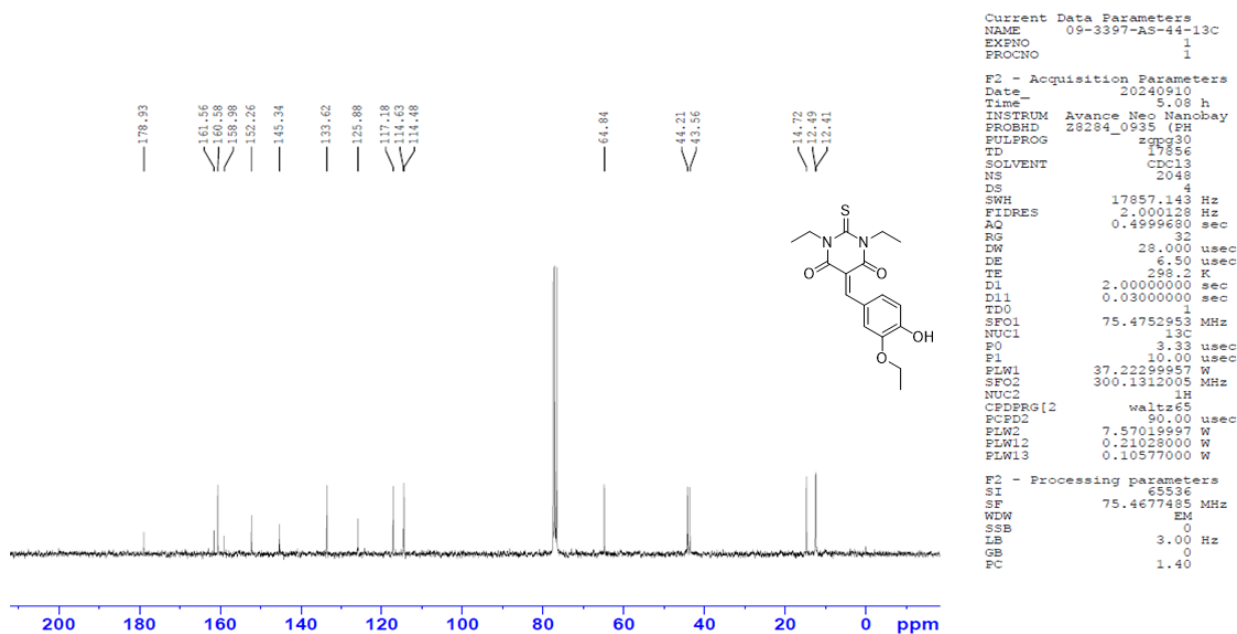
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¹³C NMR of **8**

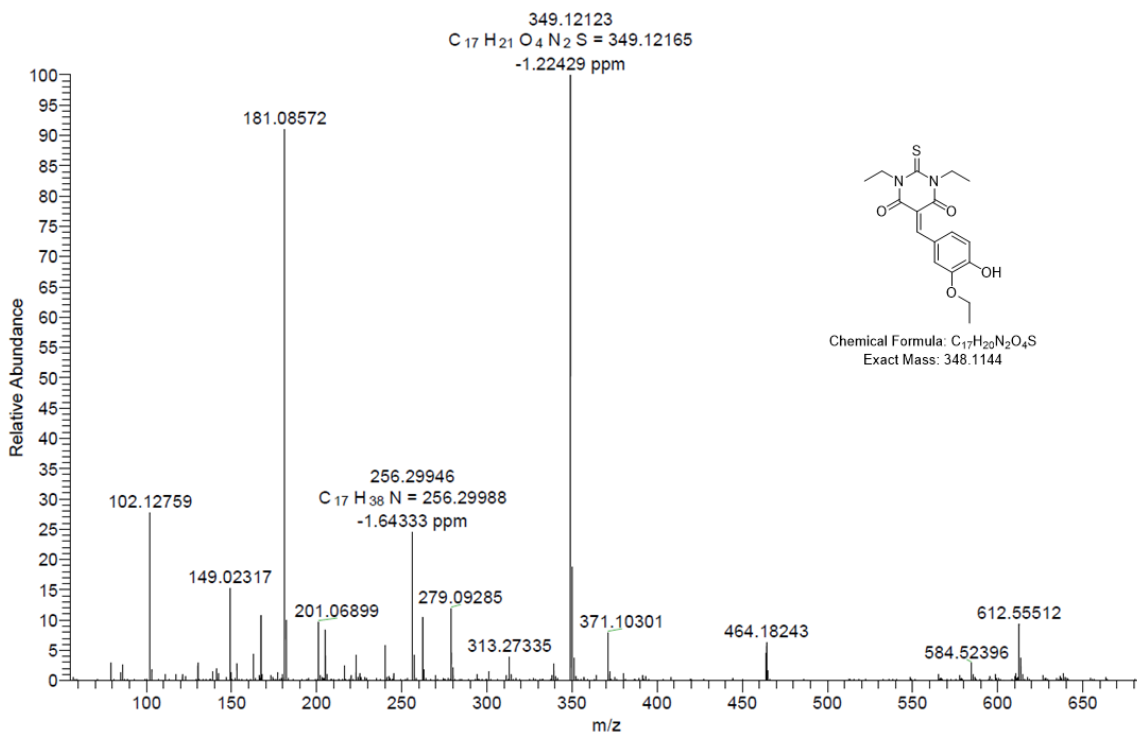
HRMS of **8**IR of **8**



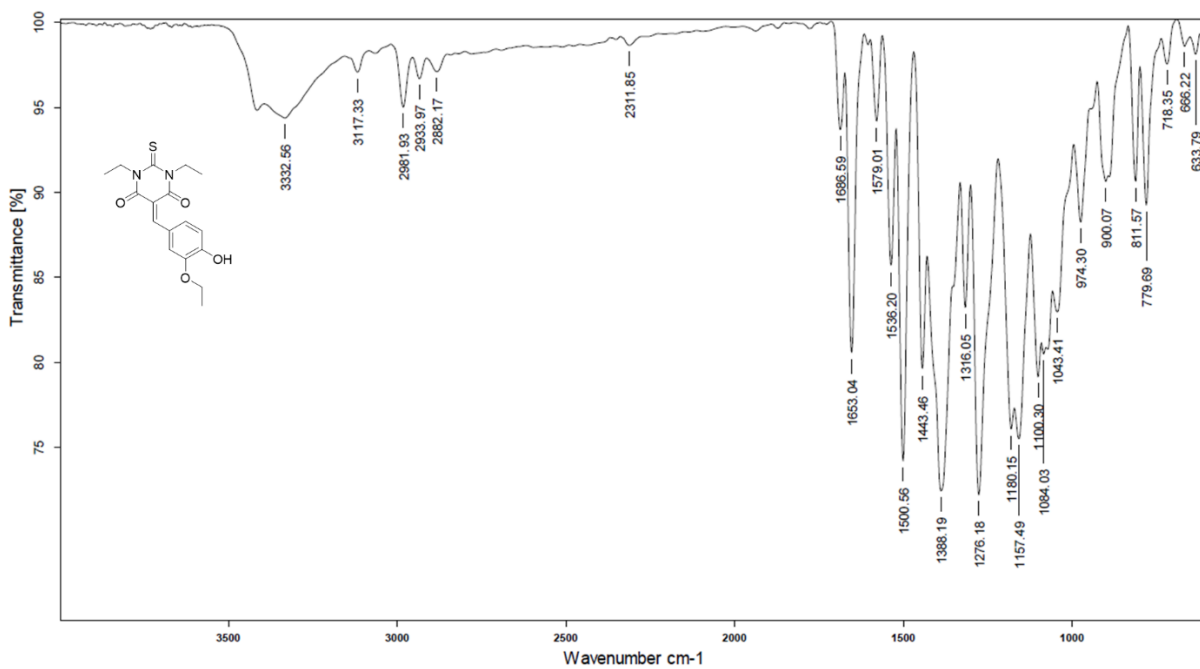
¹H NMR of 9



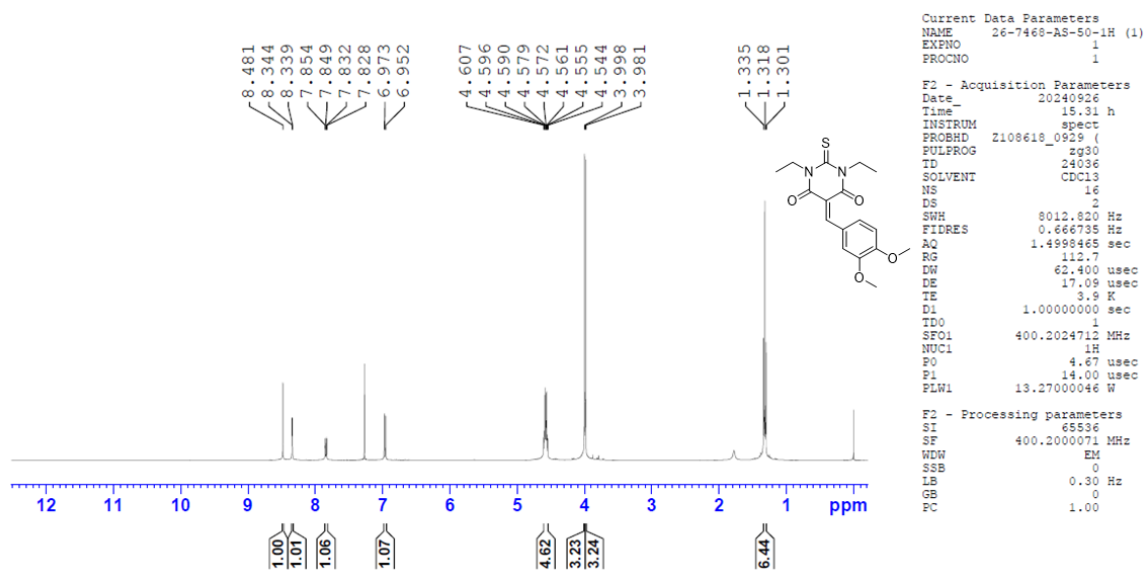
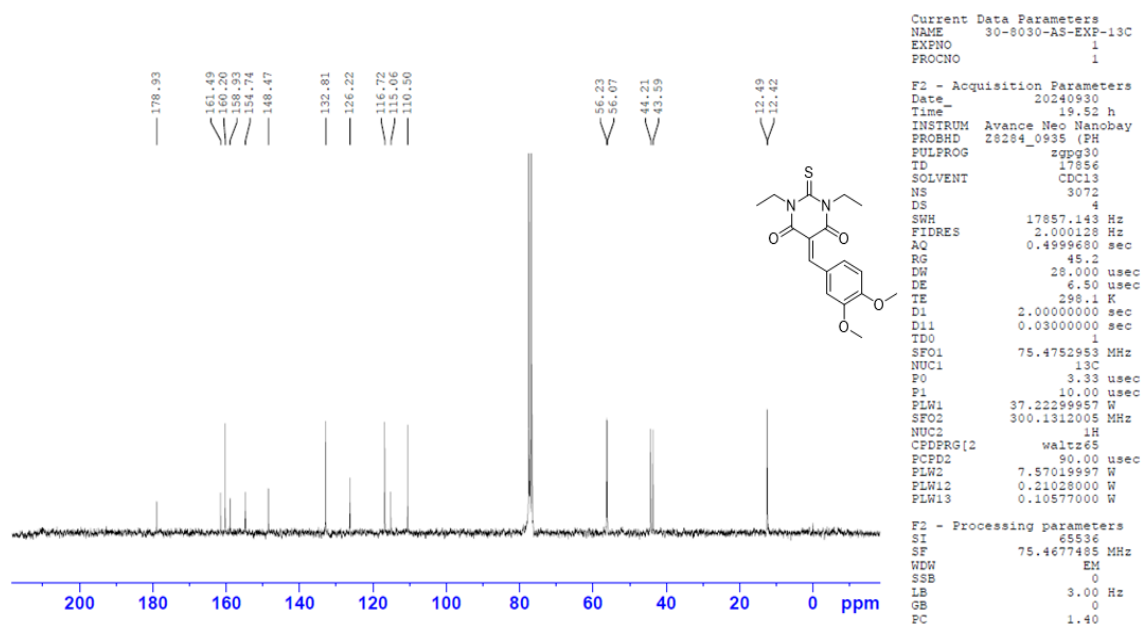
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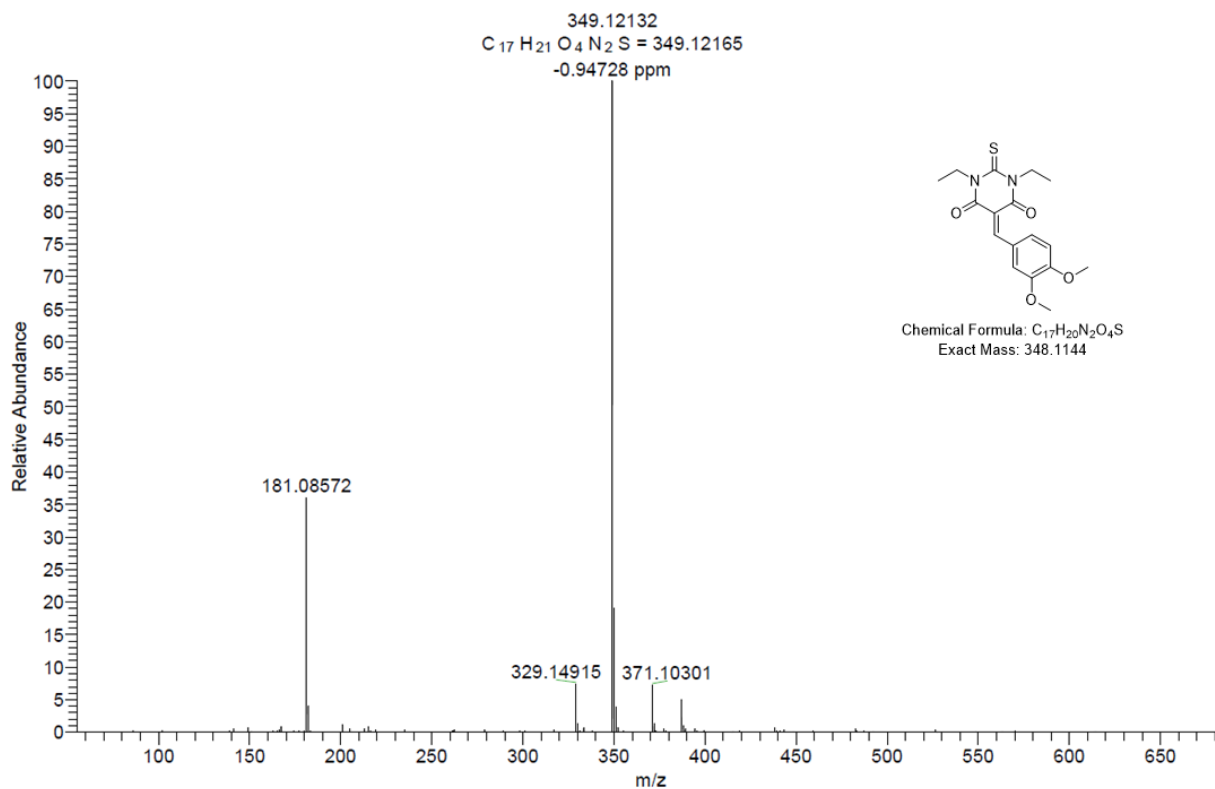


HRMS of 9

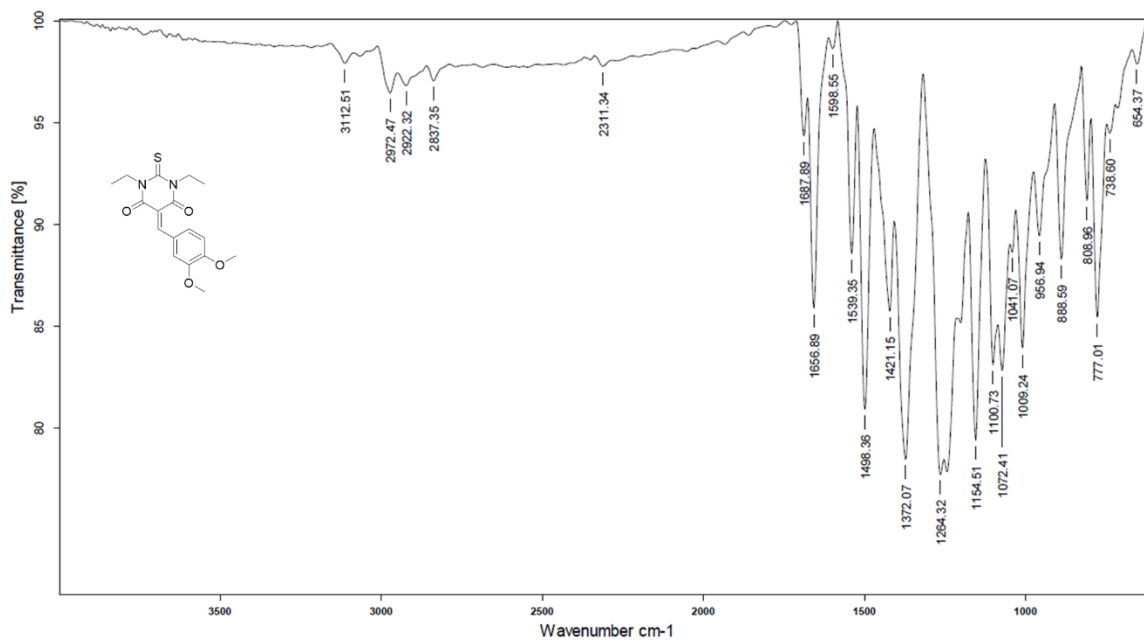


IR of 9

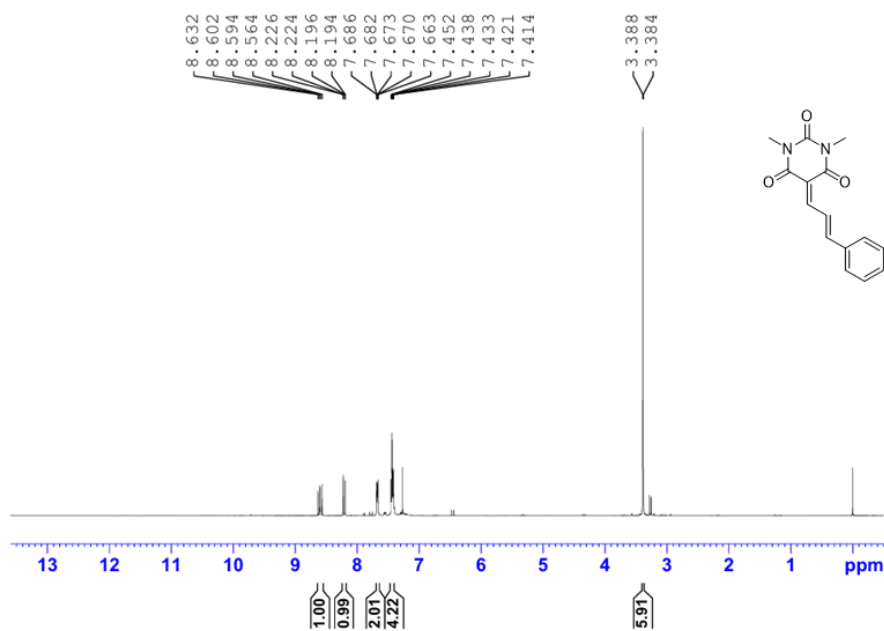
¹H NMR of **10**¹³C NMR of **10**



HRMS of 10



IR of 10

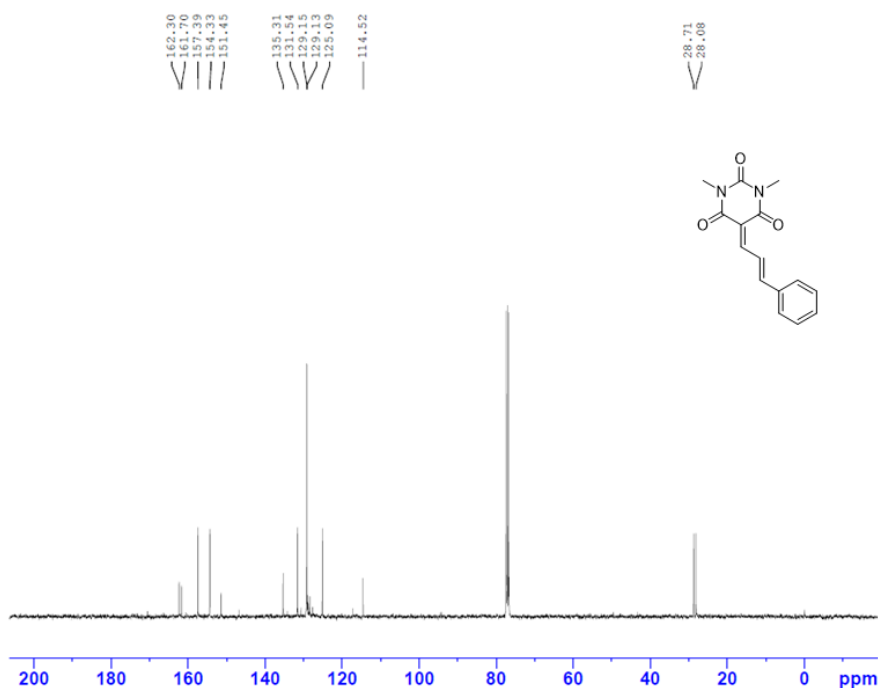


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 SOLVENT CDCl3
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 FIDRES 0.666735 Hz
 AQ 1.4999465 sec
 RG 176.03
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¹H NMR of 11

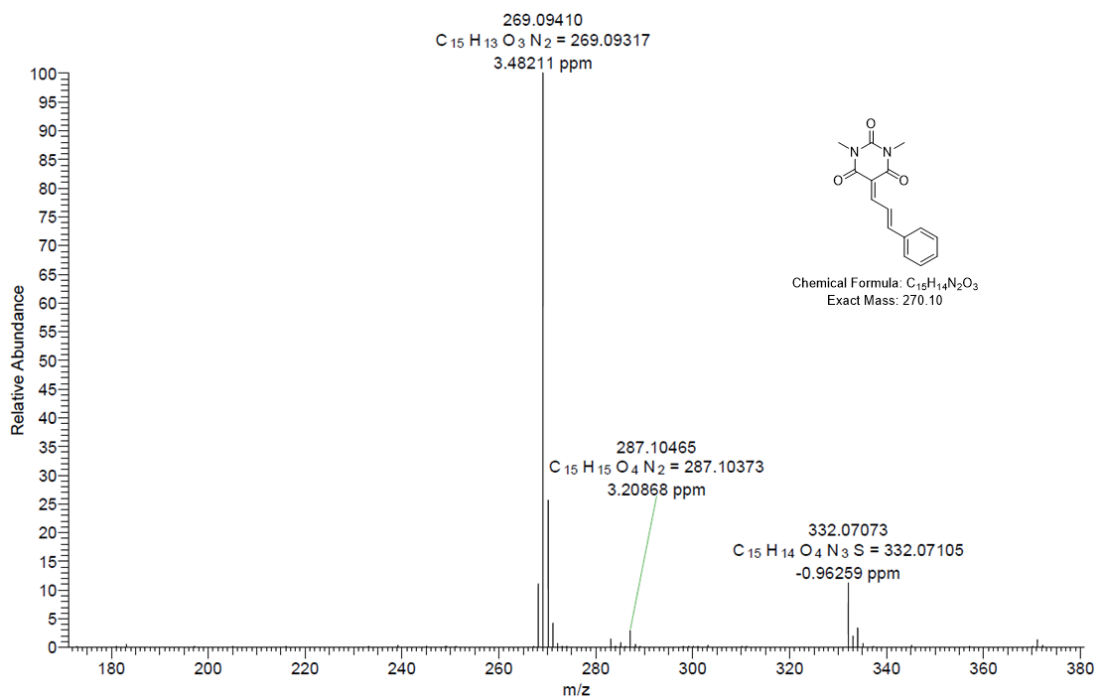


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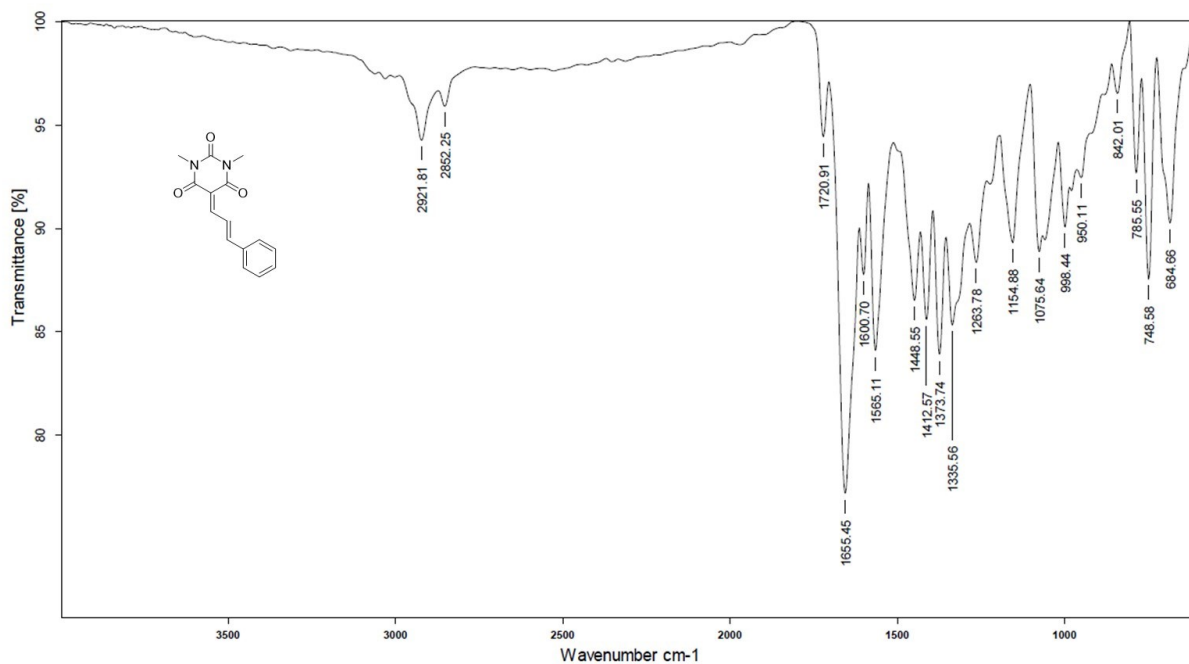
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 SOLVENT CDCl3
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 FIDRES 2.000205 Hz
 AQ 0.4999498 sec
 RG 198.97
 DW 20.800 usec
 DE 6.50 usec
 TE -4.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6354036 MHz
 NUC1 13C
 PO 3.33 usec
 P1 10.00 usec
 PLW1 39.94400024 W
 SFO2 400.1816007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 9.59899998 W
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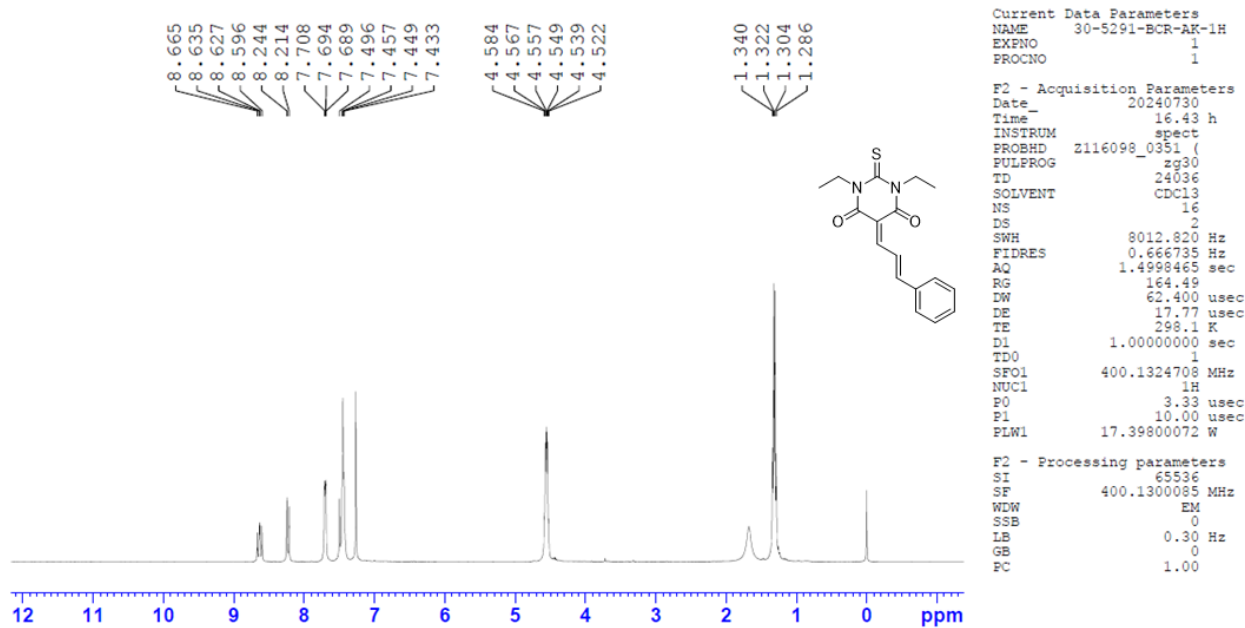
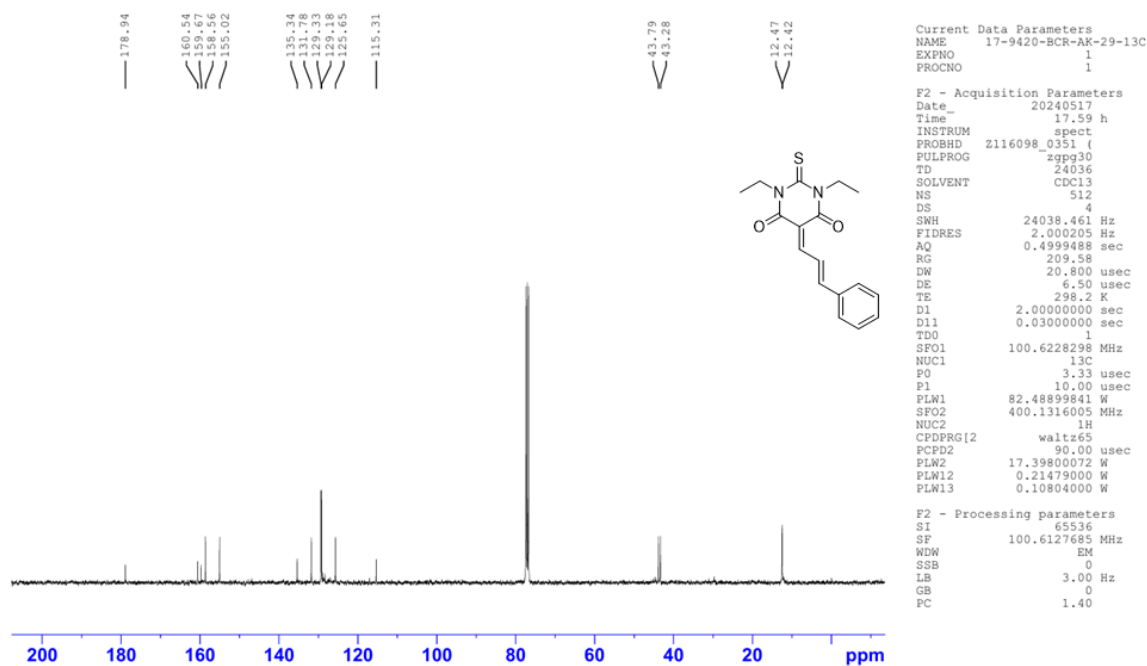
¹³C NMR of 11

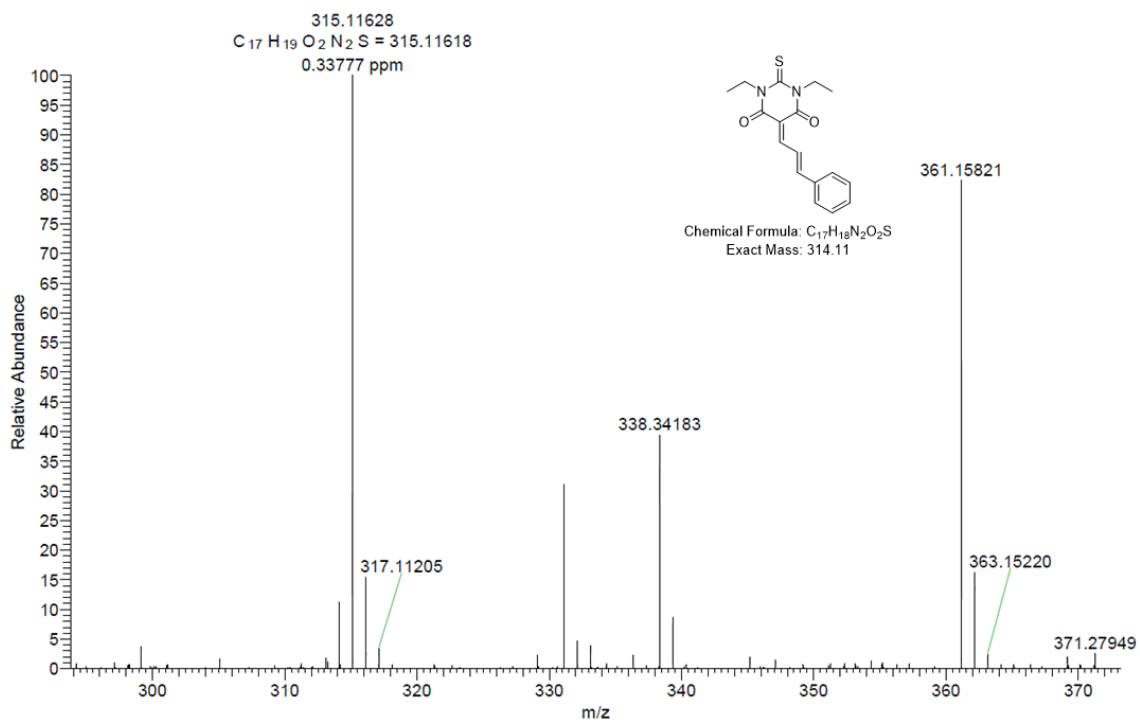


HRMS of 11

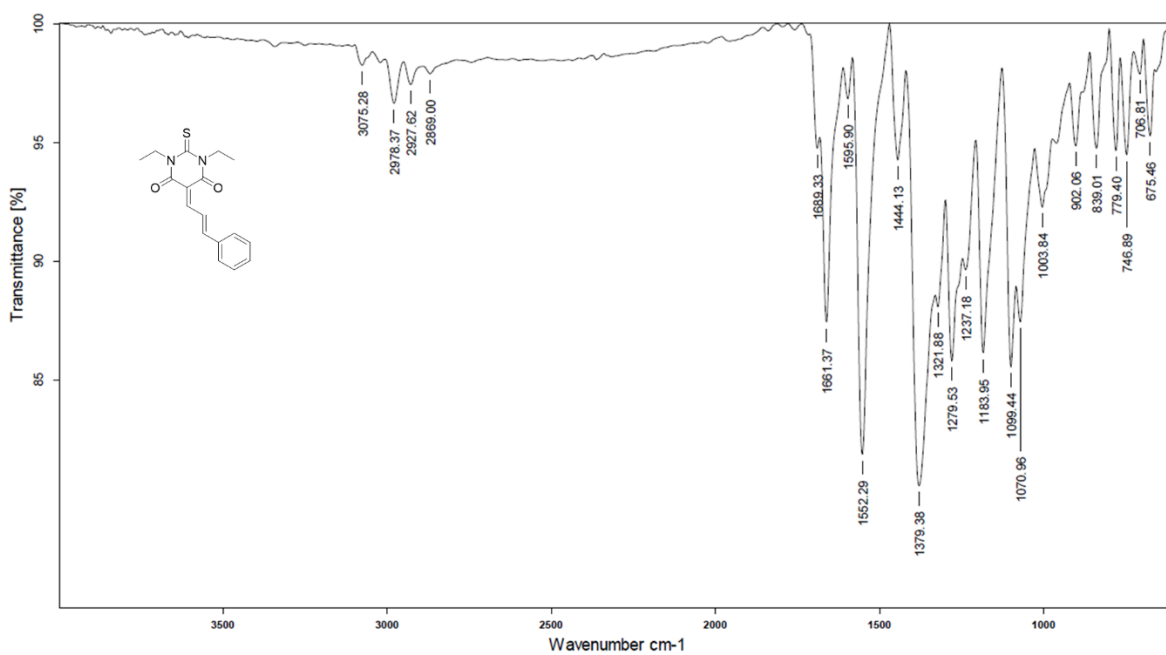


IR of 11

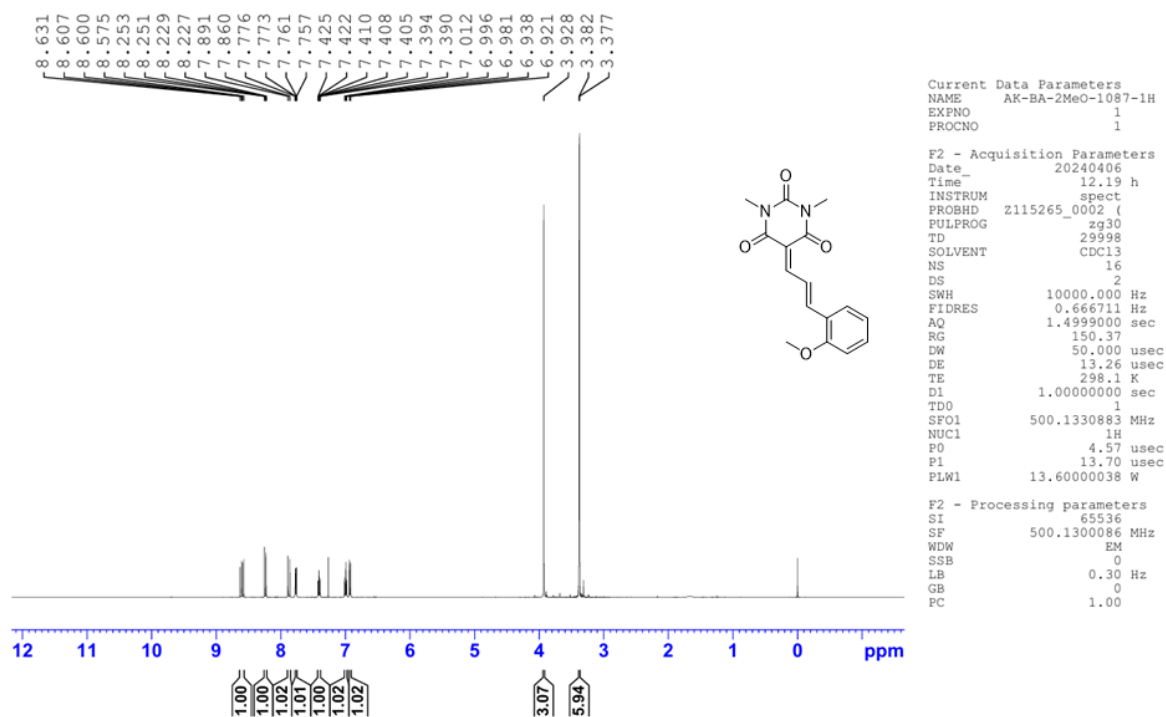
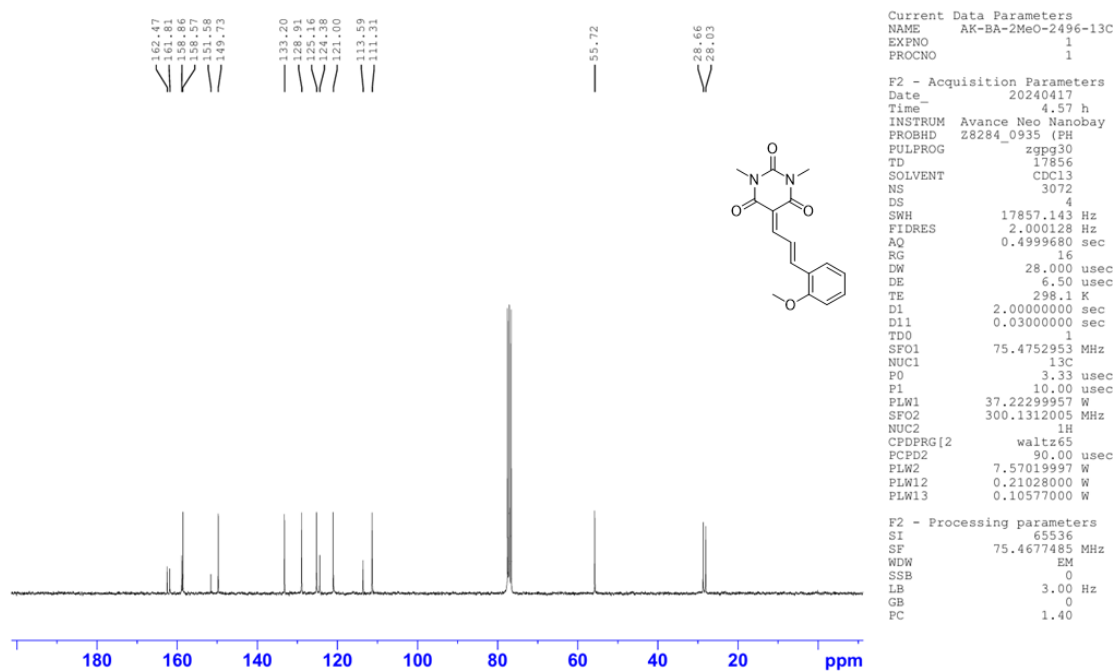
¹H NMR of 12¹³C NMR of 12

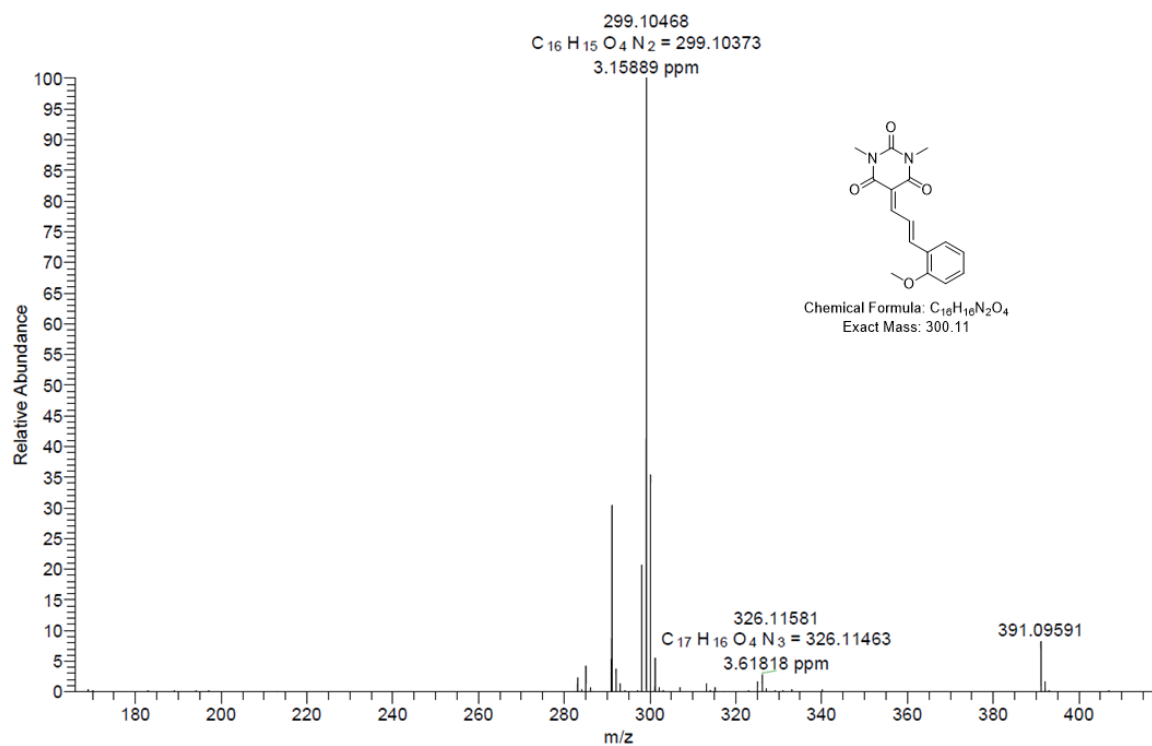


HRMS of 12

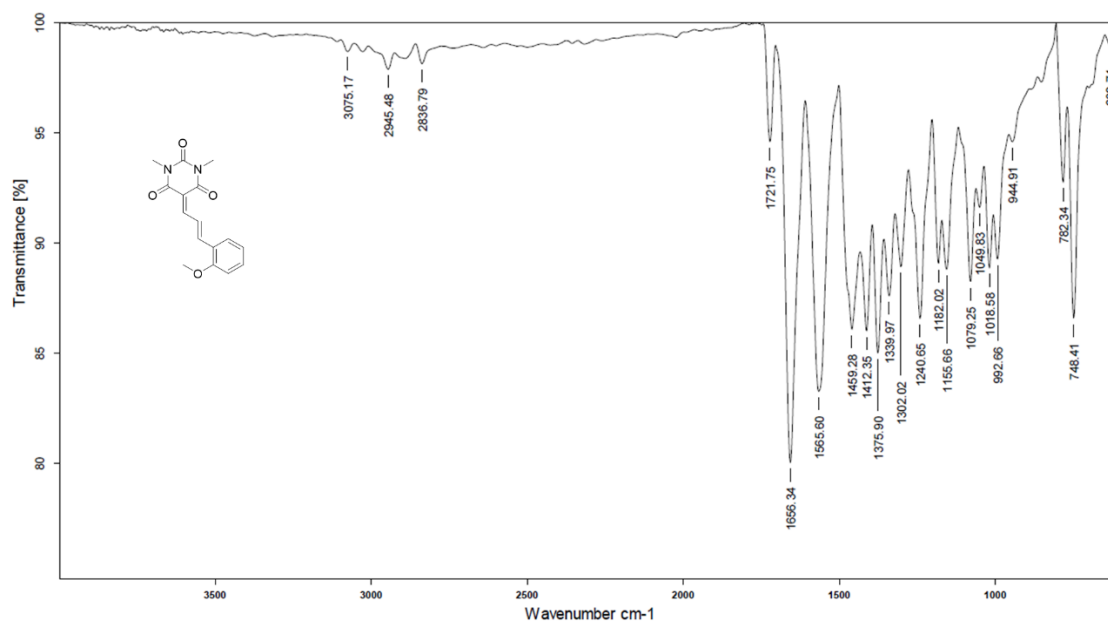


IR of 12

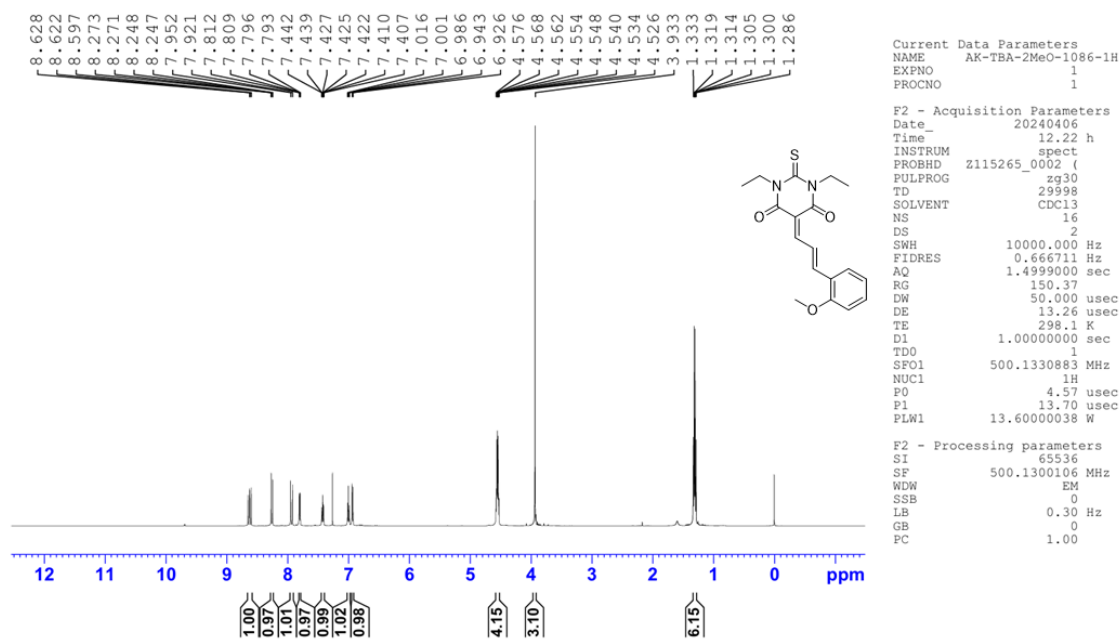
¹H NMR of **13**¹³C NMR of **13**



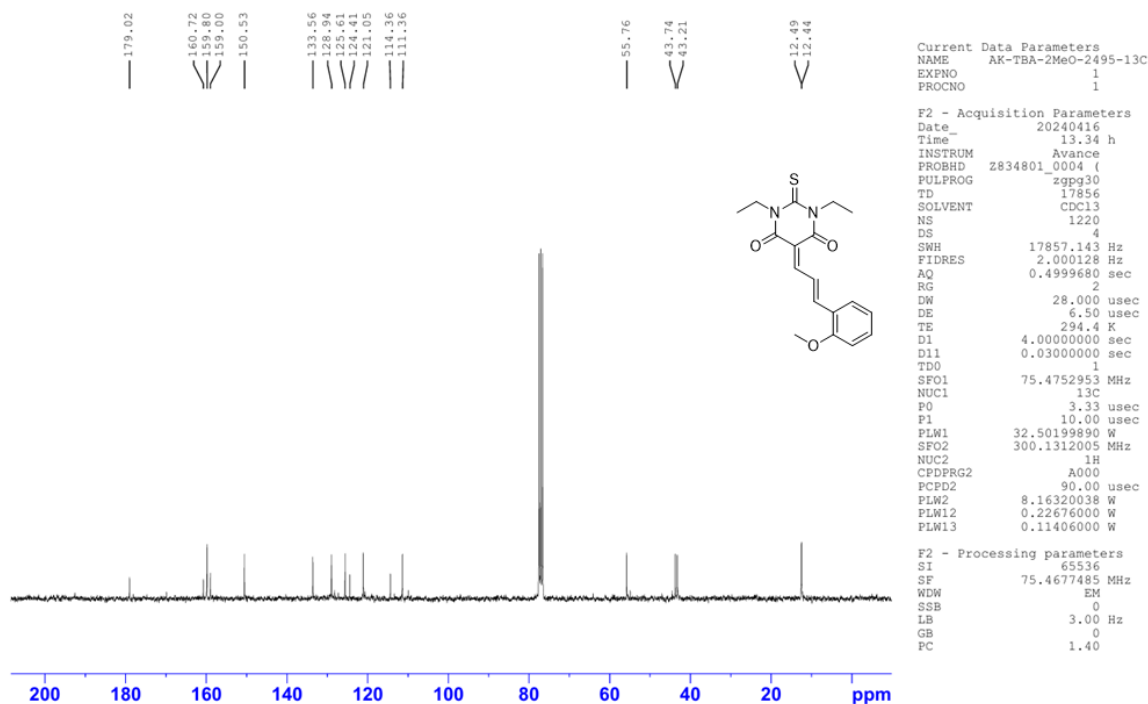
HRMS of 13



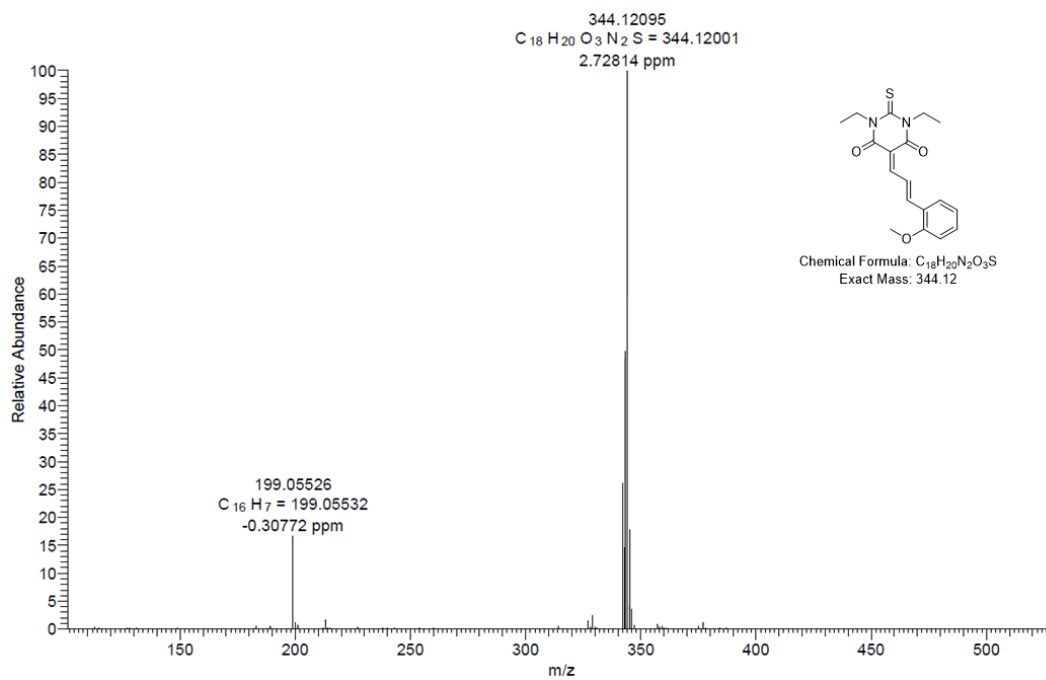
IR of 113



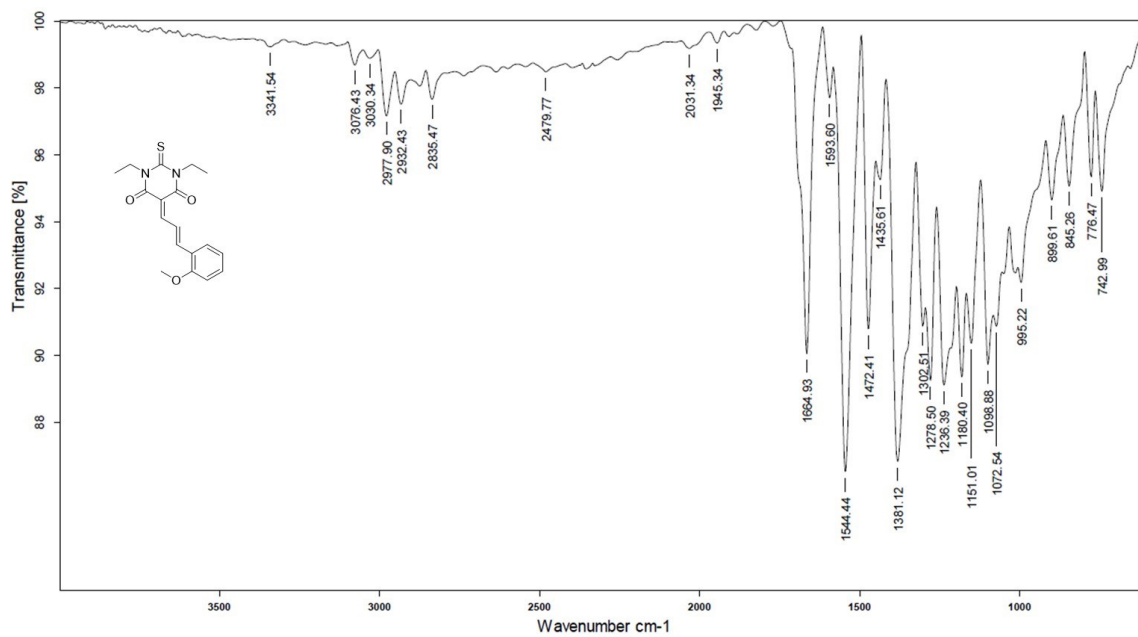
¹H NMR of 14



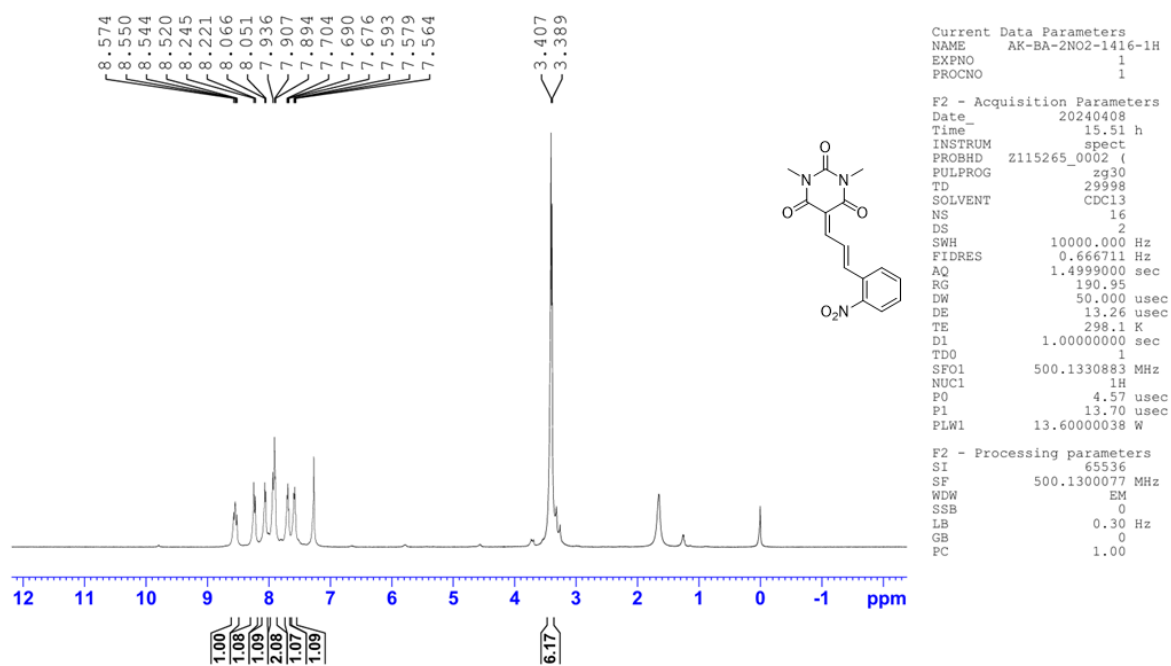
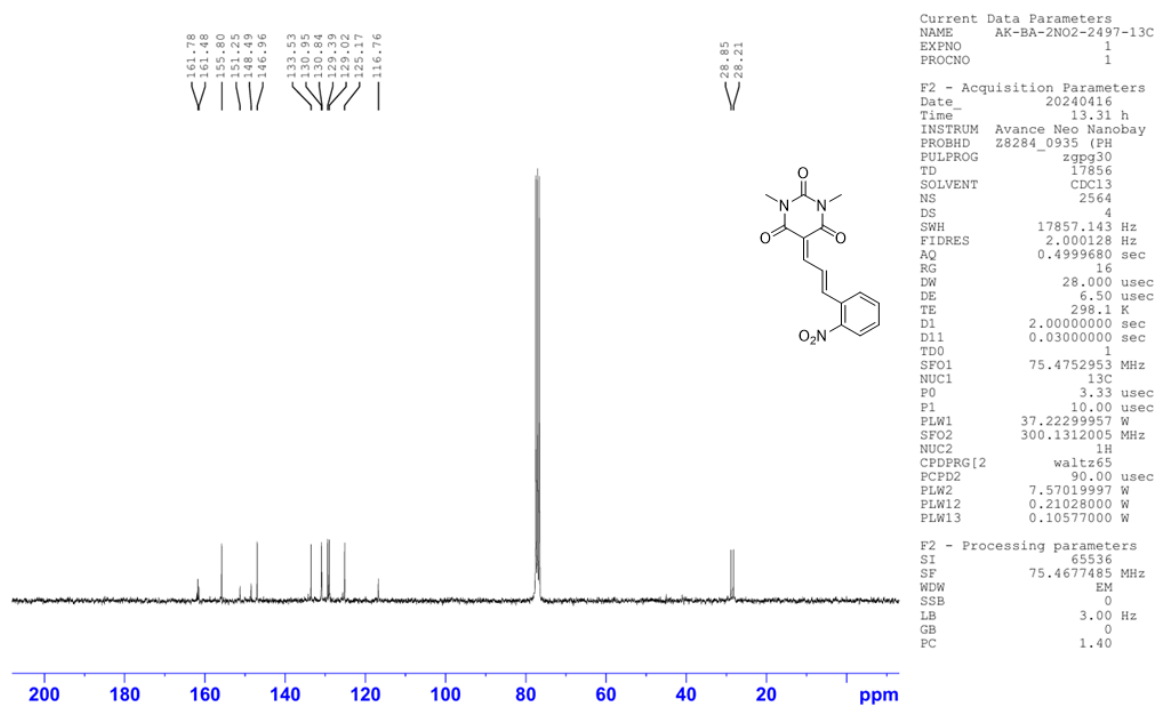
¹³C NMR of 14

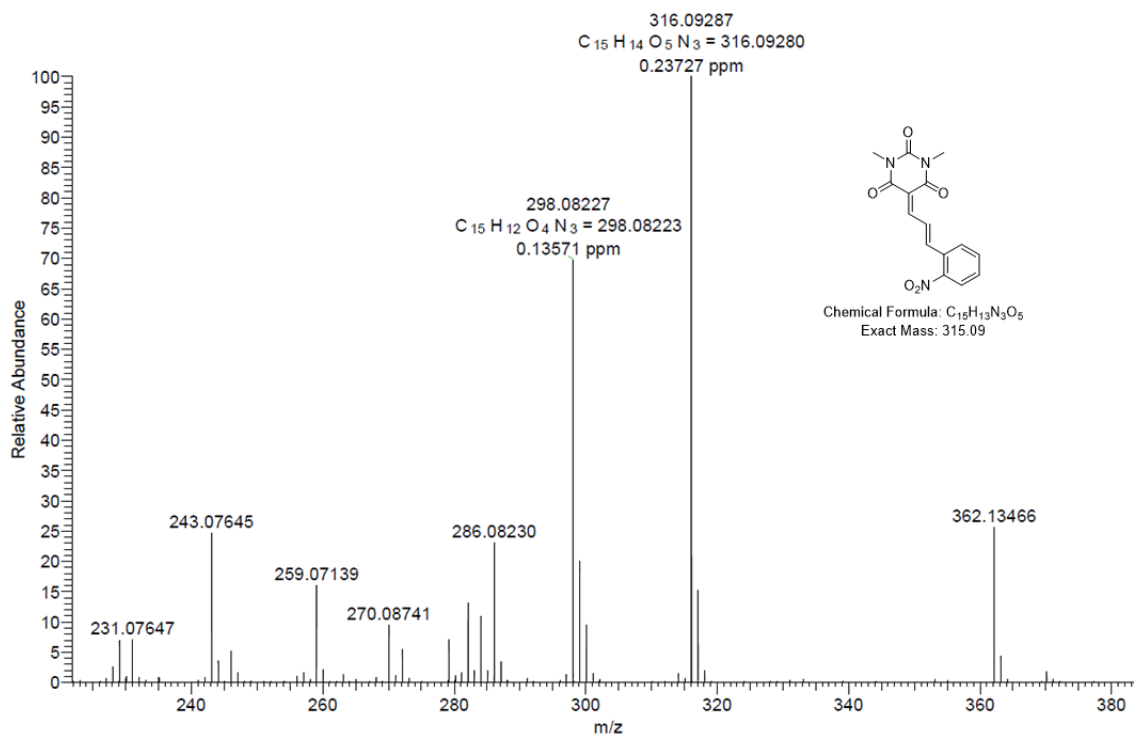
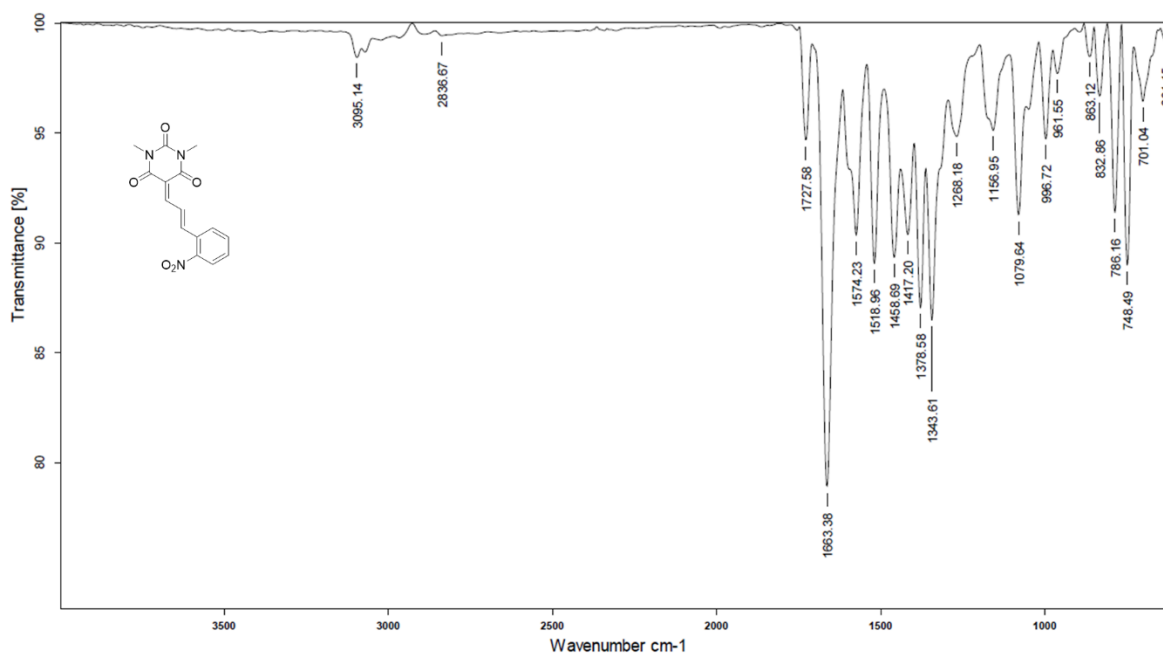


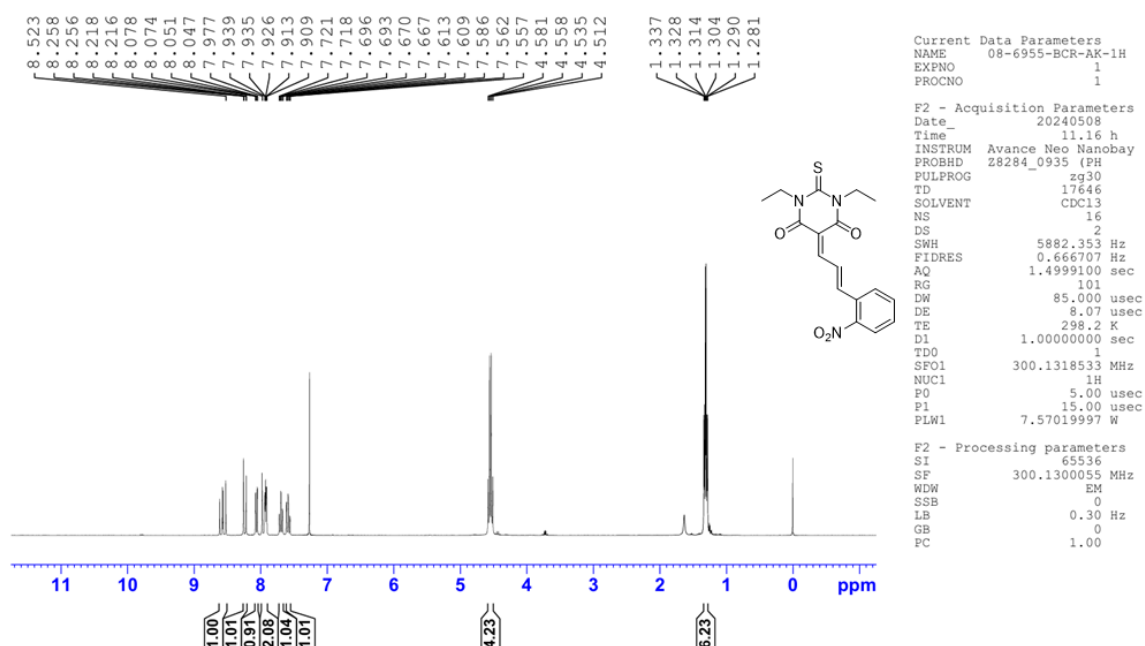
HRMS of 14



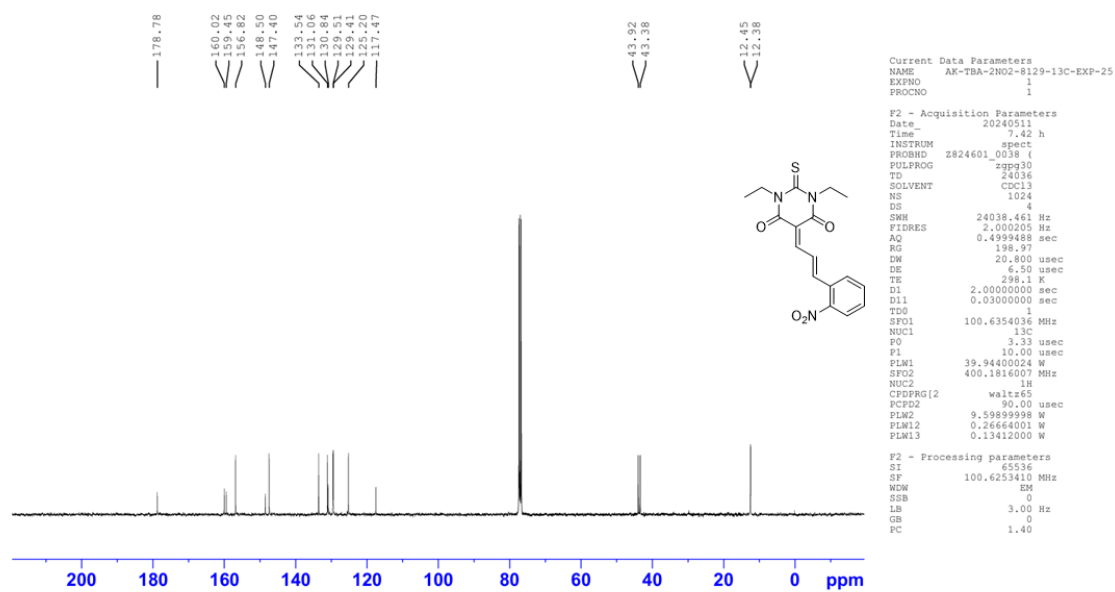
IR of 14

¹H NMR of **15**¹³C NMR of **15**

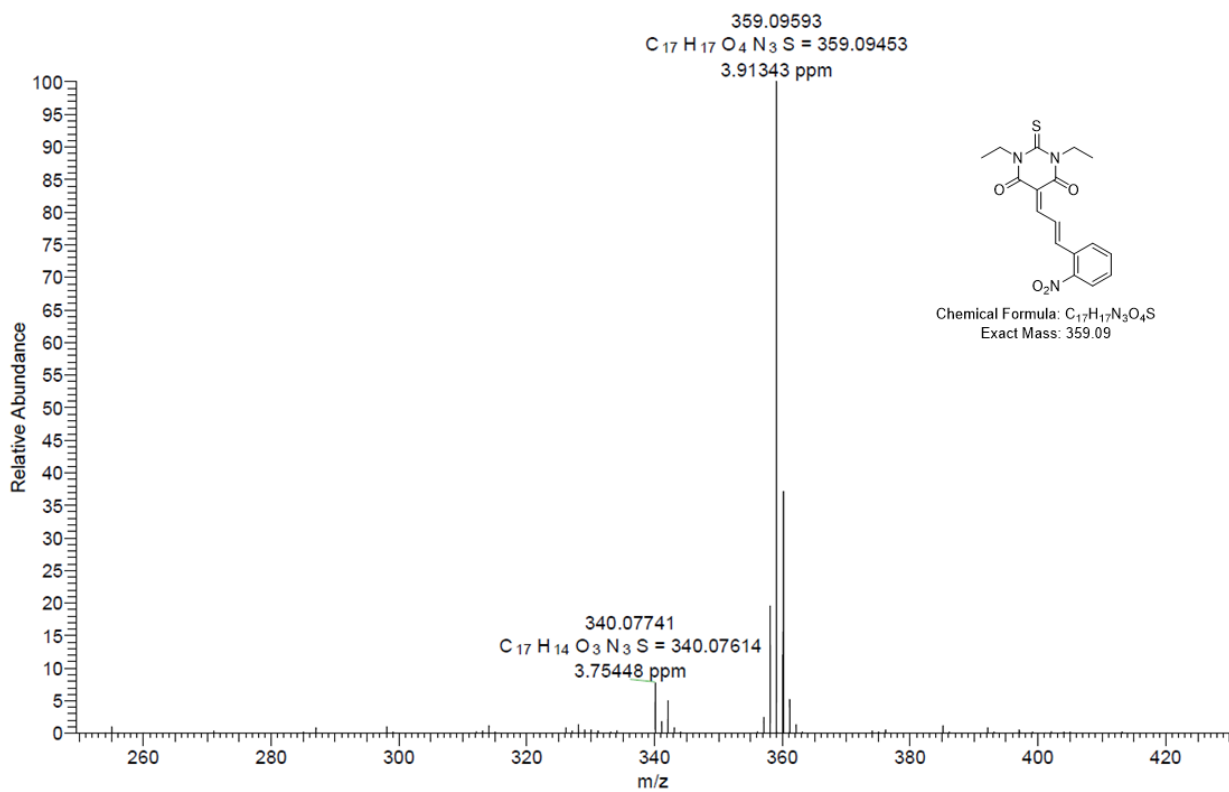
HRMS of **15**IR of **15**



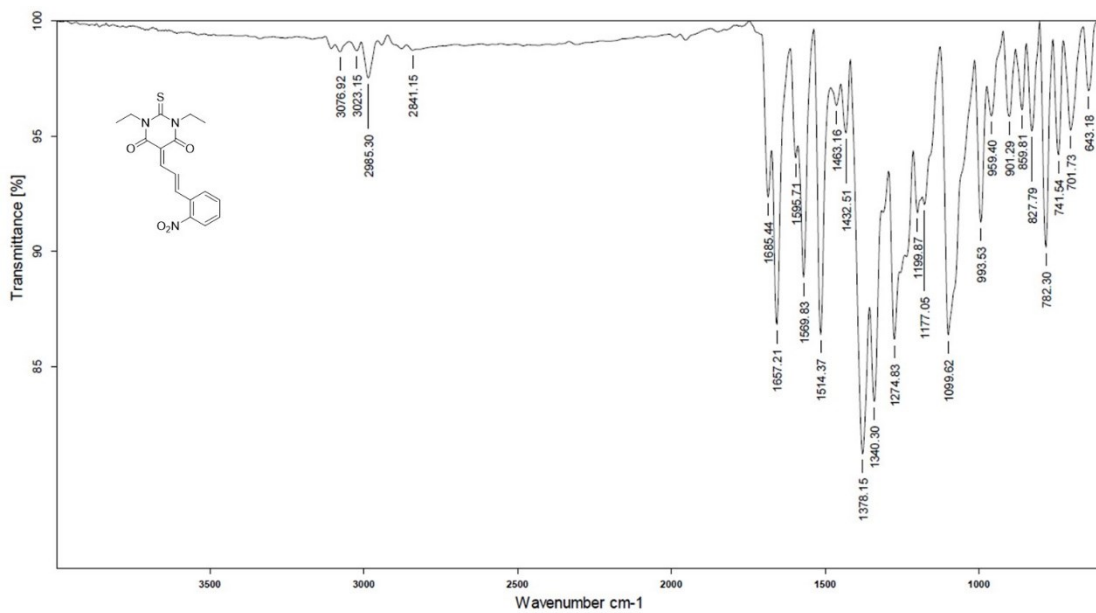
¹H NMR of 16



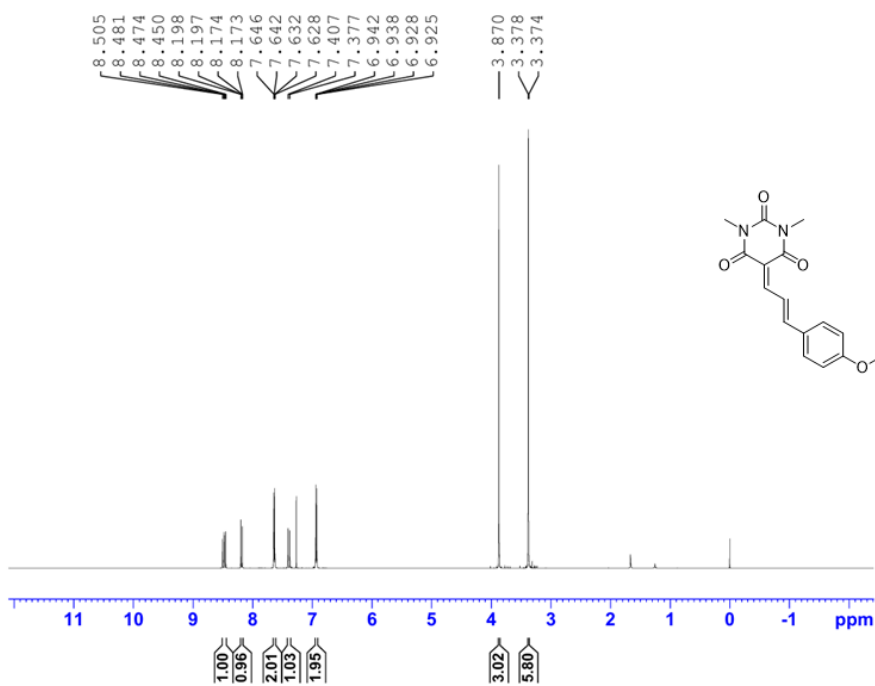
¹³C NMR of 16



HRMS of 16



IR of 16

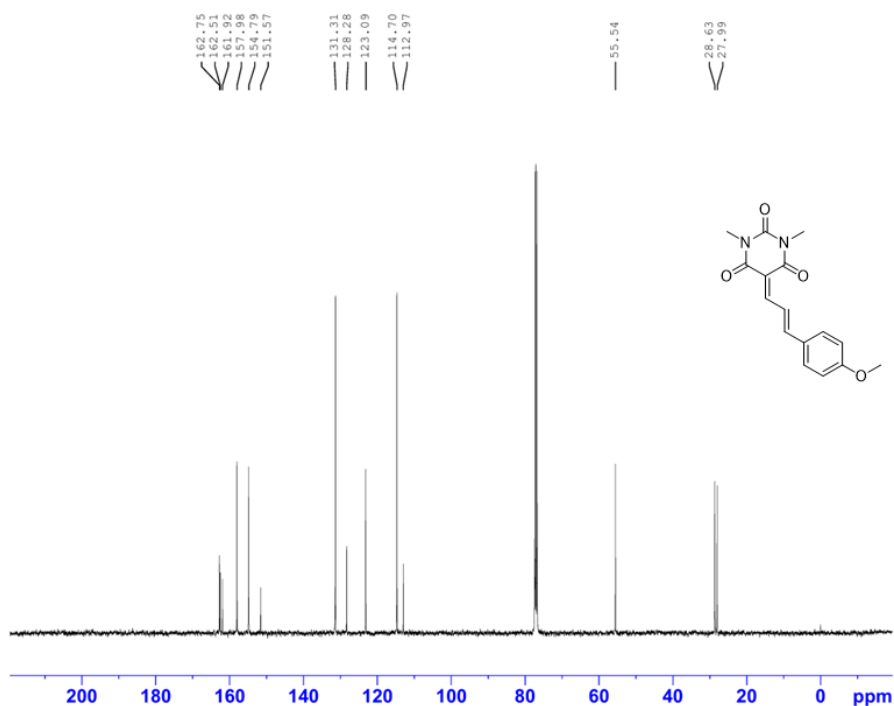


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 PROCNO 1

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 TD 29998
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.666711 Hz
 AQ 1.4999000 sec
 RG 137.48
 DW 50.000 usec
 DE 13.26 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.1330883 MHz
 NUC1 1H
 PO 4.57 usec
 P1 13.70 usec
 PLW1 13.60000038 W

F2 - Processing parameters
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¹H NMR of 17

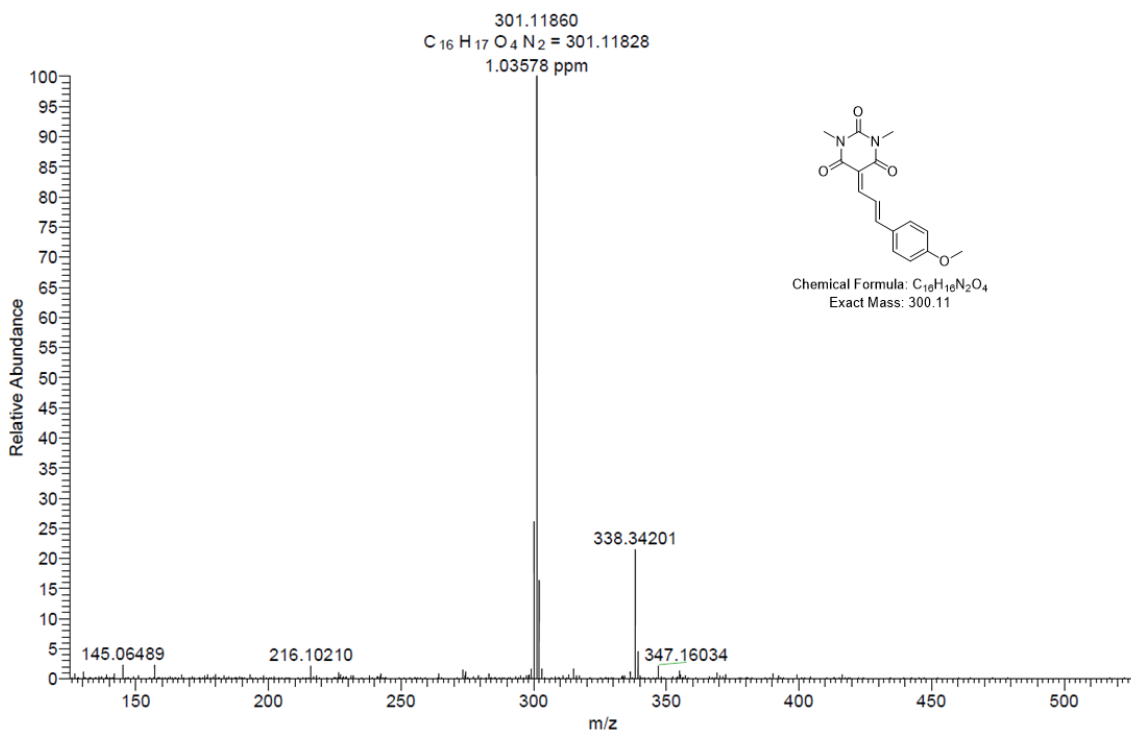


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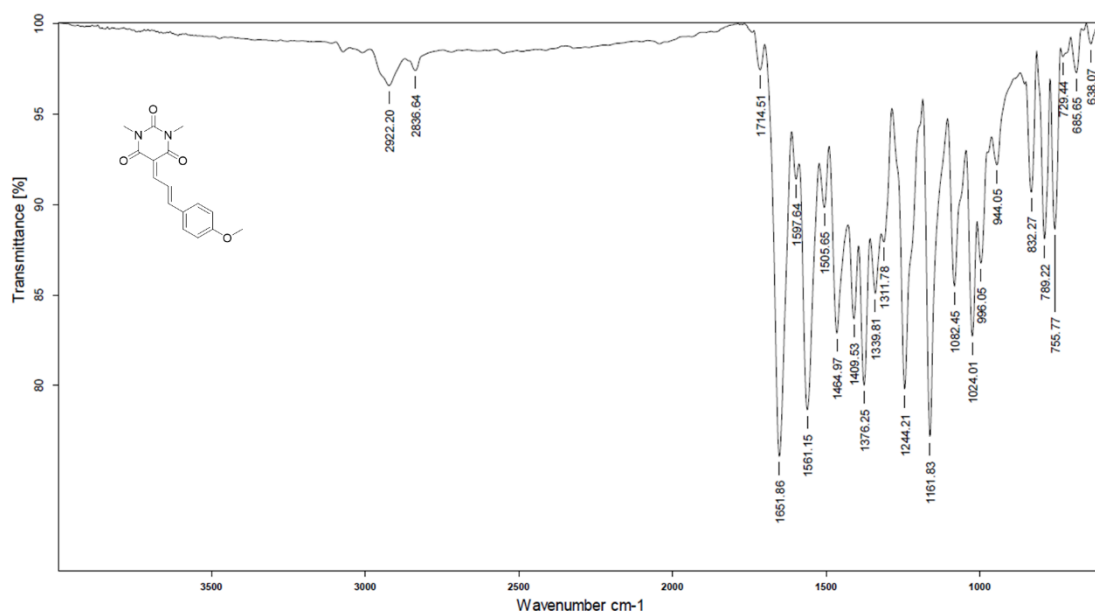
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 NS 1024
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 SWH 24038.461 Hz
 FIDRES 2.000205 Hz
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 RG 199.01
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.6404331 MHz
 NUC1 13C
 PO 3.33 usec
 P1 10.00 usec
 PLW1 61.41500092 W
 SFO2 400.2016008 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 13.27000046 W
 PLW12 0.32110000 W
 PLW13 0.16151001 W

F2 - Processing parameters
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 SSB 0
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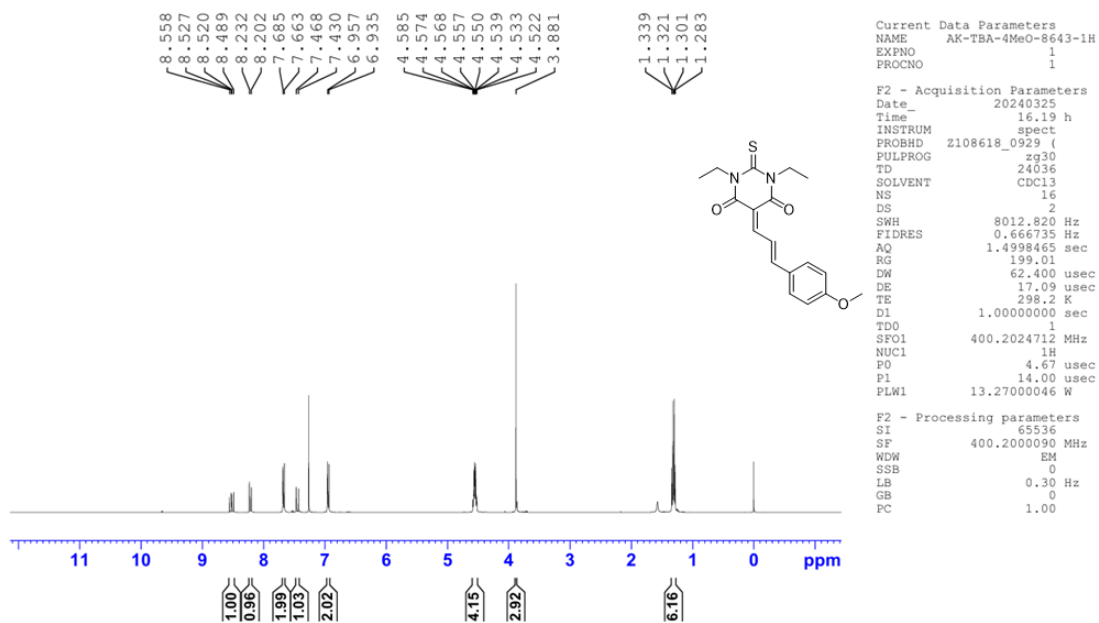
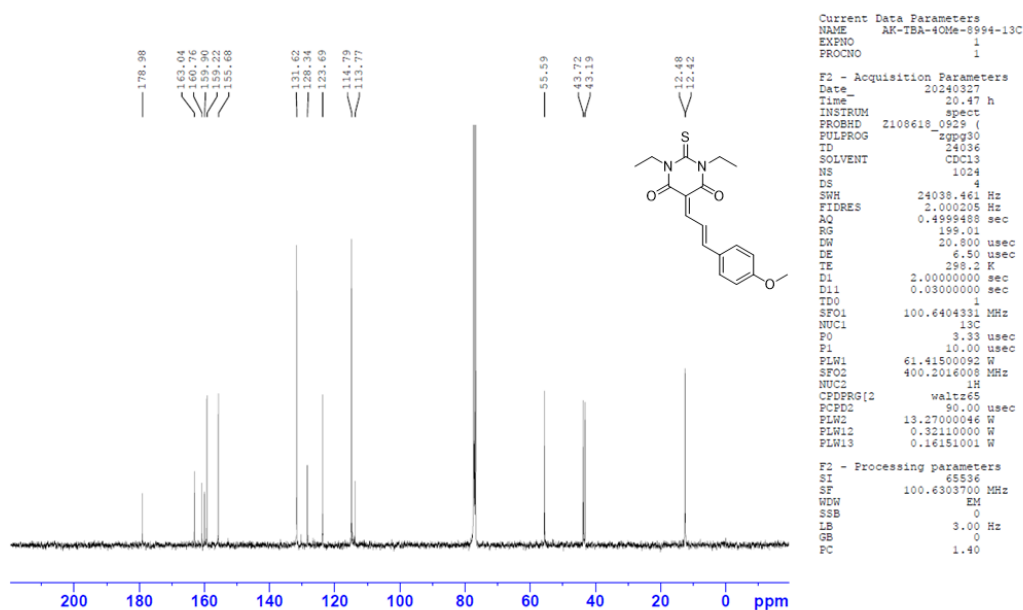
¹³C NMR of 17

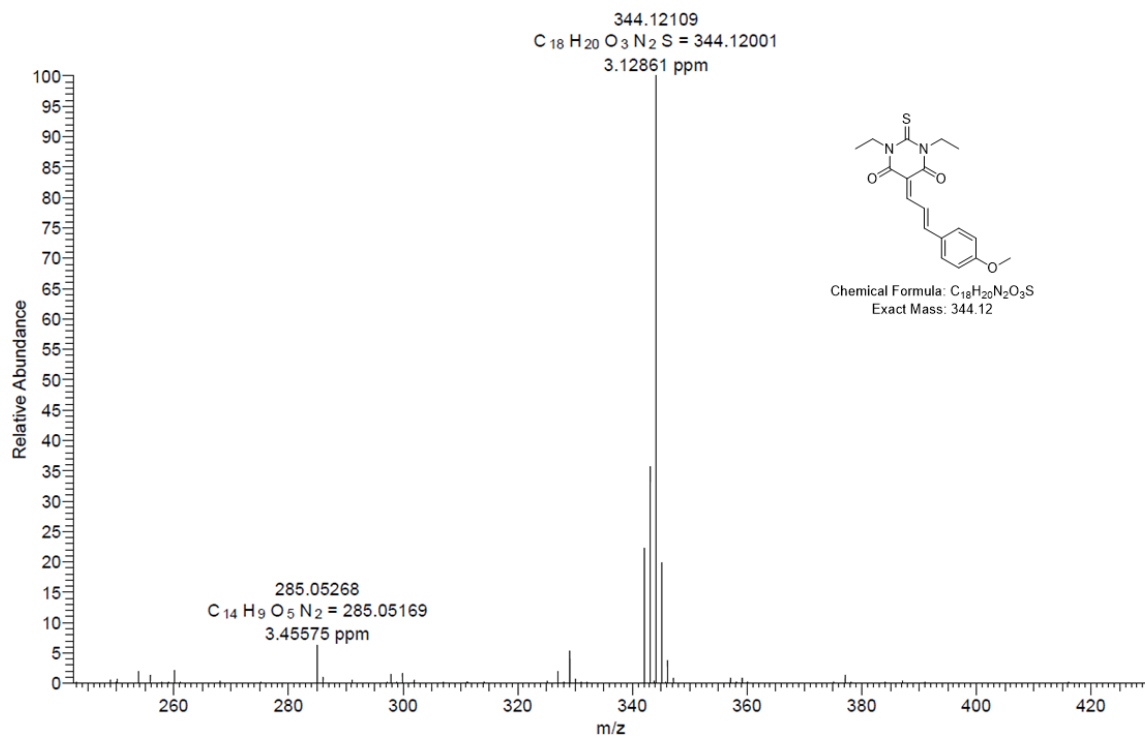


HRMS of 17

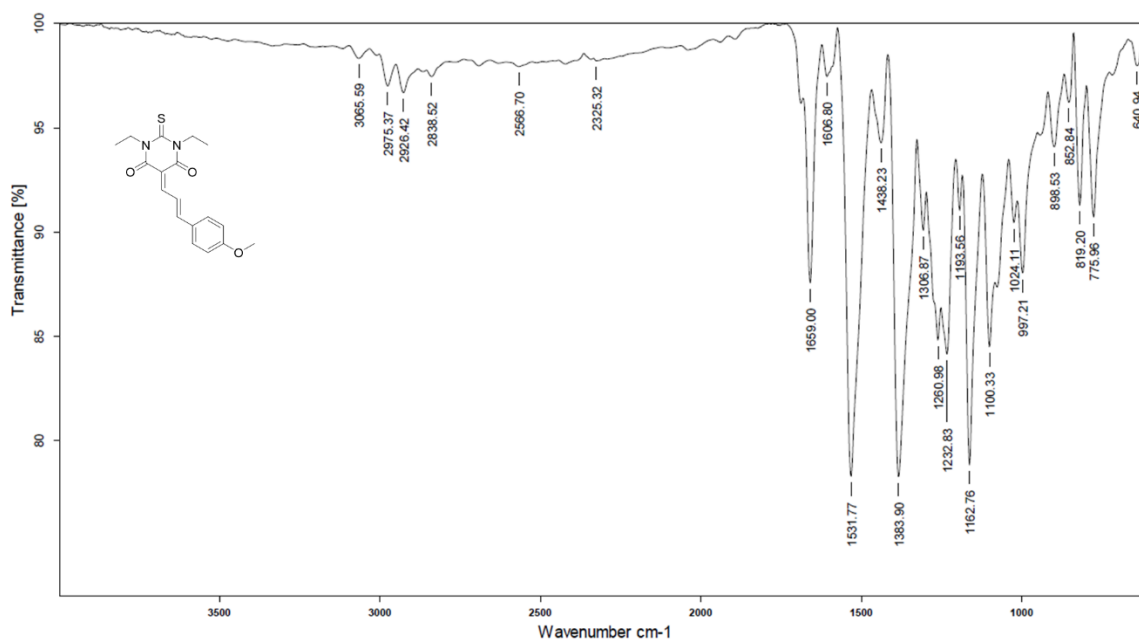


IR of 17

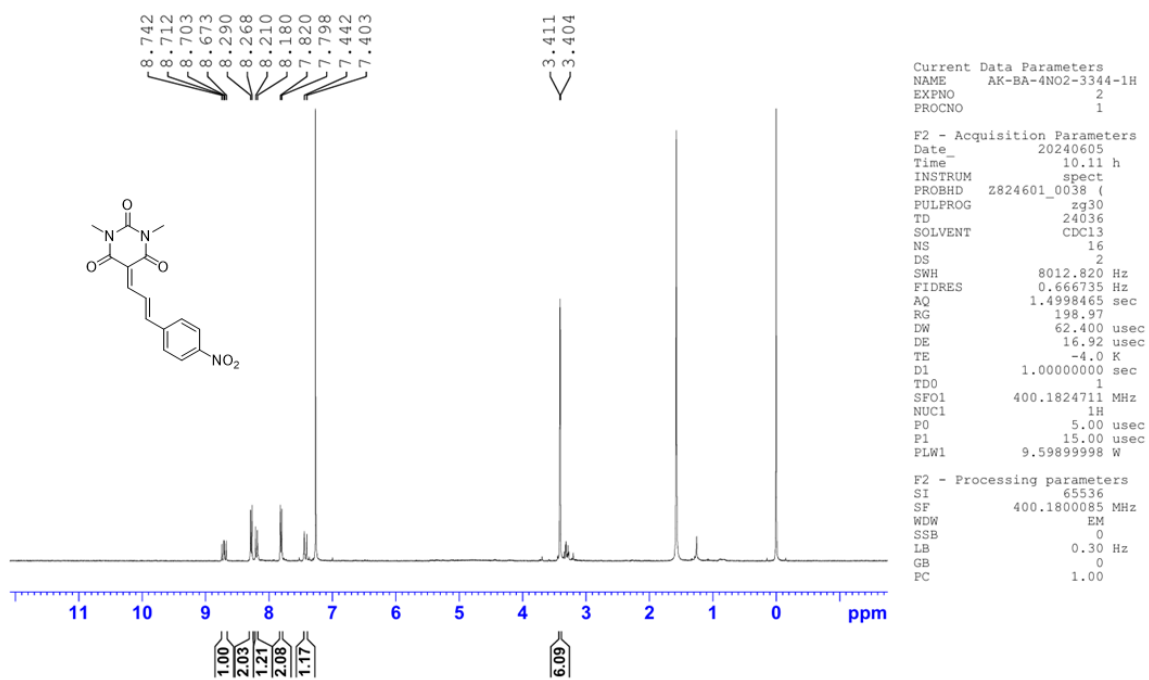
 ^1H NMR of **18** ^{13}C NMR of **18**



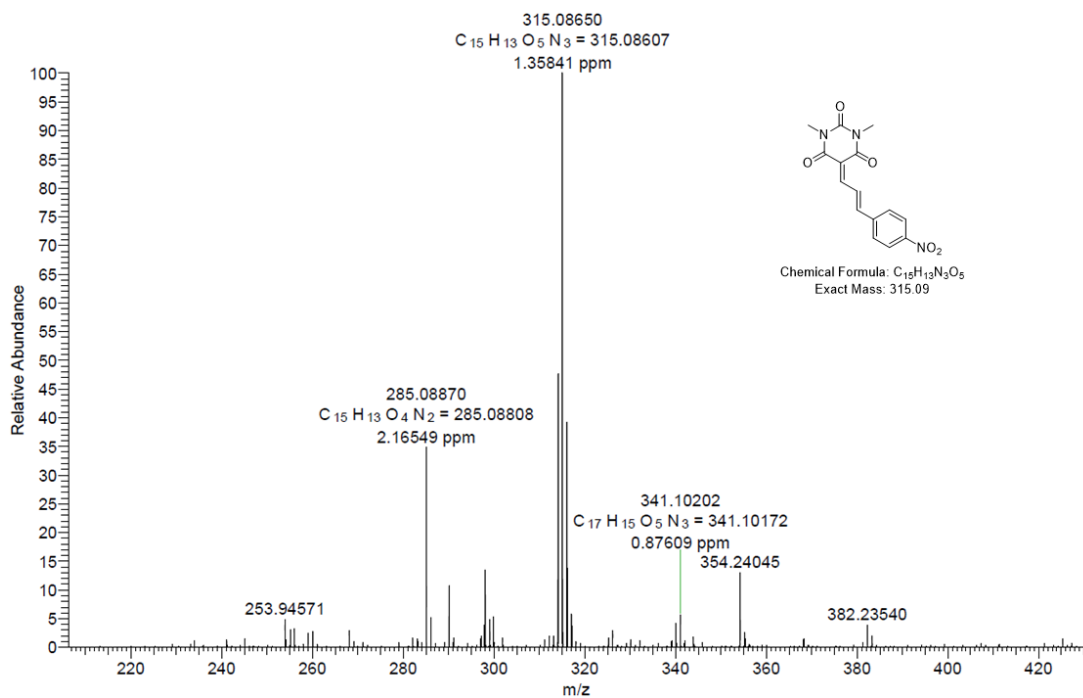
HRMS of 18



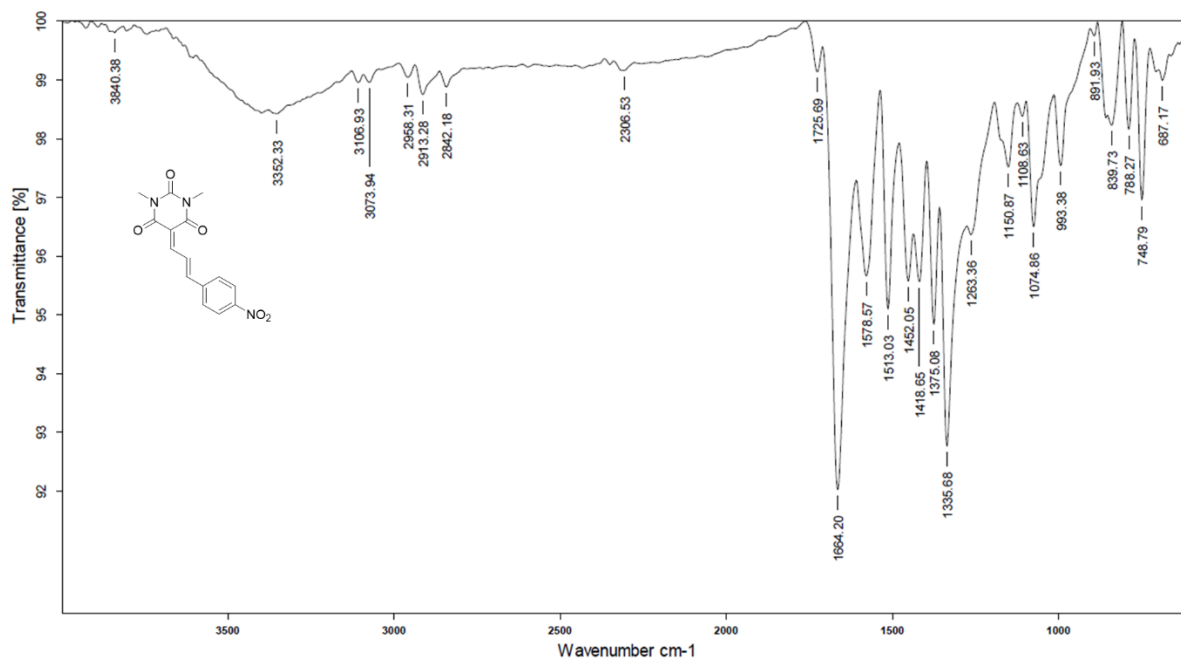
IR of 18



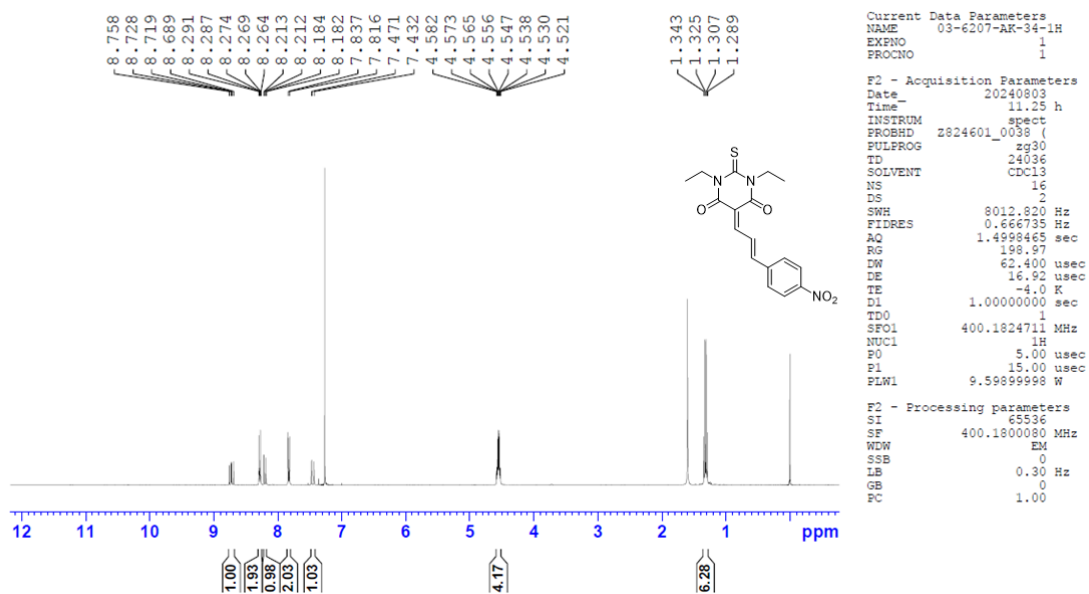
¹H NMR of 19

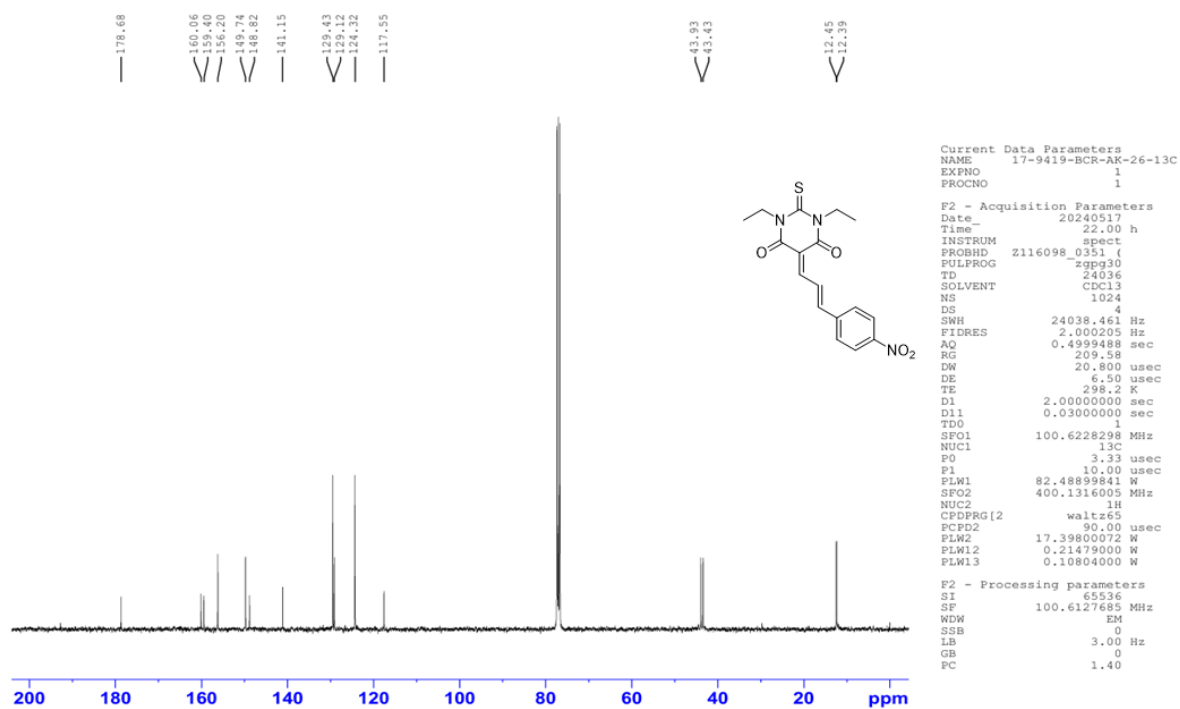
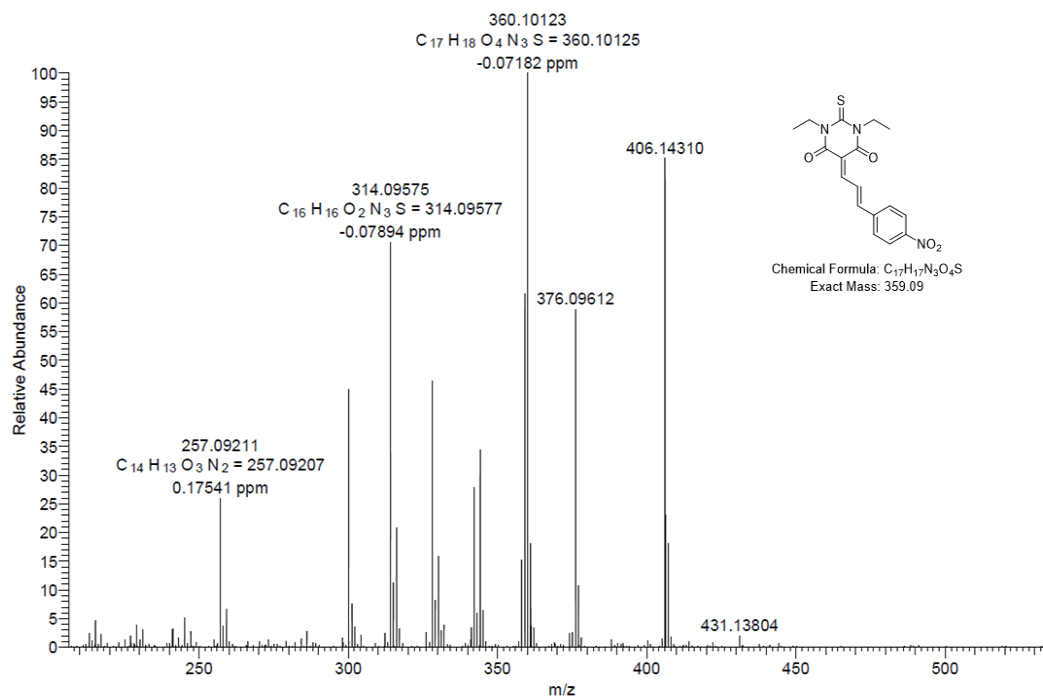


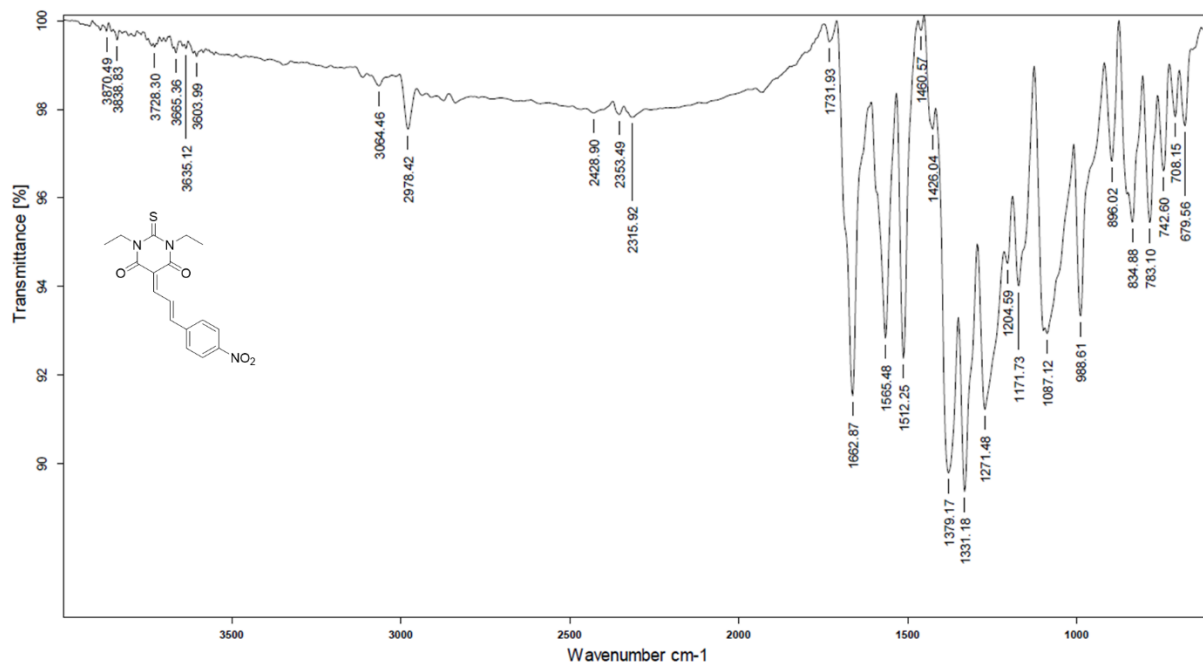
HRMS of 19



IR of 19

¹H NMR of 20

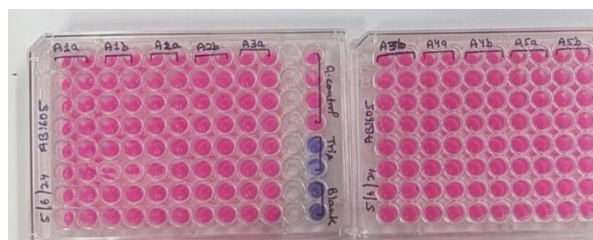
¹³C NMR of **20**HRMS of **20**



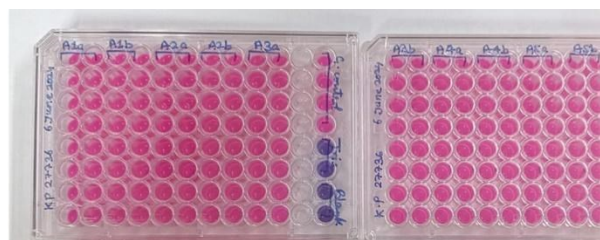
IR of 20

Table X. Minimum inhibitory concentrations (MIC) for the synthesized compounds **1-20**

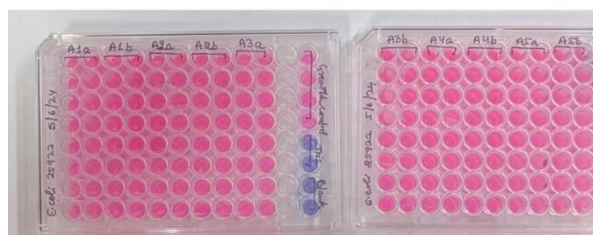
Compound Number	<i>Acinetobacter baumannii</i> ATCC (1605)	<i>Klebsiella pneumoniae</i> ATCC (27736)	<i>Escherichia coli</i> ATCC (25922)	<i>Pseudomonas aeruginosa</i> ATCC (27853)	<i>Staphylococcus aureus</i> ATCC (25923)
1	>50	>50	>50	>50	>50
2	>50	>50	>50	>50	>50
3	>50	>50	>50	>50	>50
4	>50	>50	>50	>50	>50
5	>50	>50	>50	>50	>50
6	>50	>50	>50	>50	>50
7	>50	>50	>50	>50	>50
8	>50	>50	>50	>50	>50
9	>50	>50	>50	>50	>50
10	>50	>50	>50	>50	>50
Meropenem	12.5	0.39	0.39	0.39	0.39
ciprofloxacin	25	0.39	0.39	0.39	0.39
Vancomycin	50	>50	>50	>50	0.78
Tigecycline	12.5	6.25	1.56	6.25	6.25



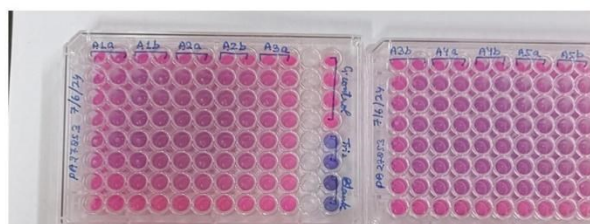
Acinetobacter baumannii ATCC 1605



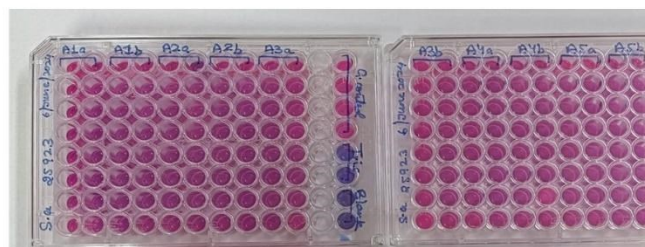
Klebsiella pneumoniae ATCC 27736



Escherichia coli ATCC 25922



Pseudomonas aeruginosa ATCC 27853



Staphylococcus aureus ATCC (25923)

Figure S21. 96-Well plate for MIC determination of the compounds **1-10**.