

Supplementary Material

Alkyne Substituted Fimbroliide Analogues as Novel Bacterial Quorum Sensing Inhibitors

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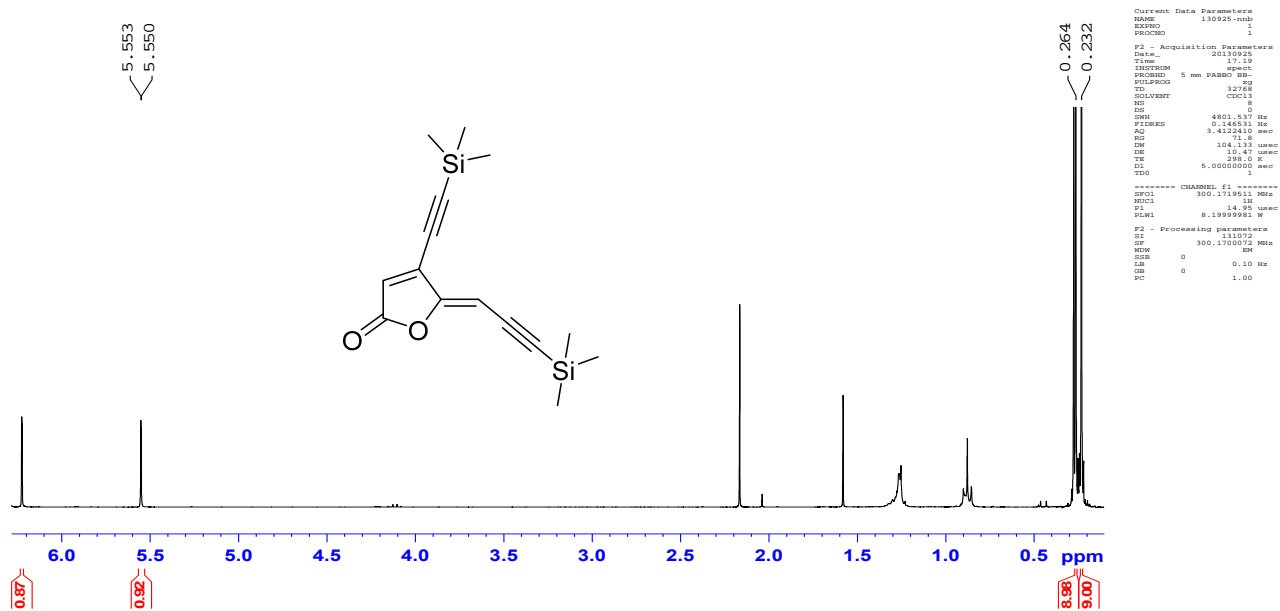
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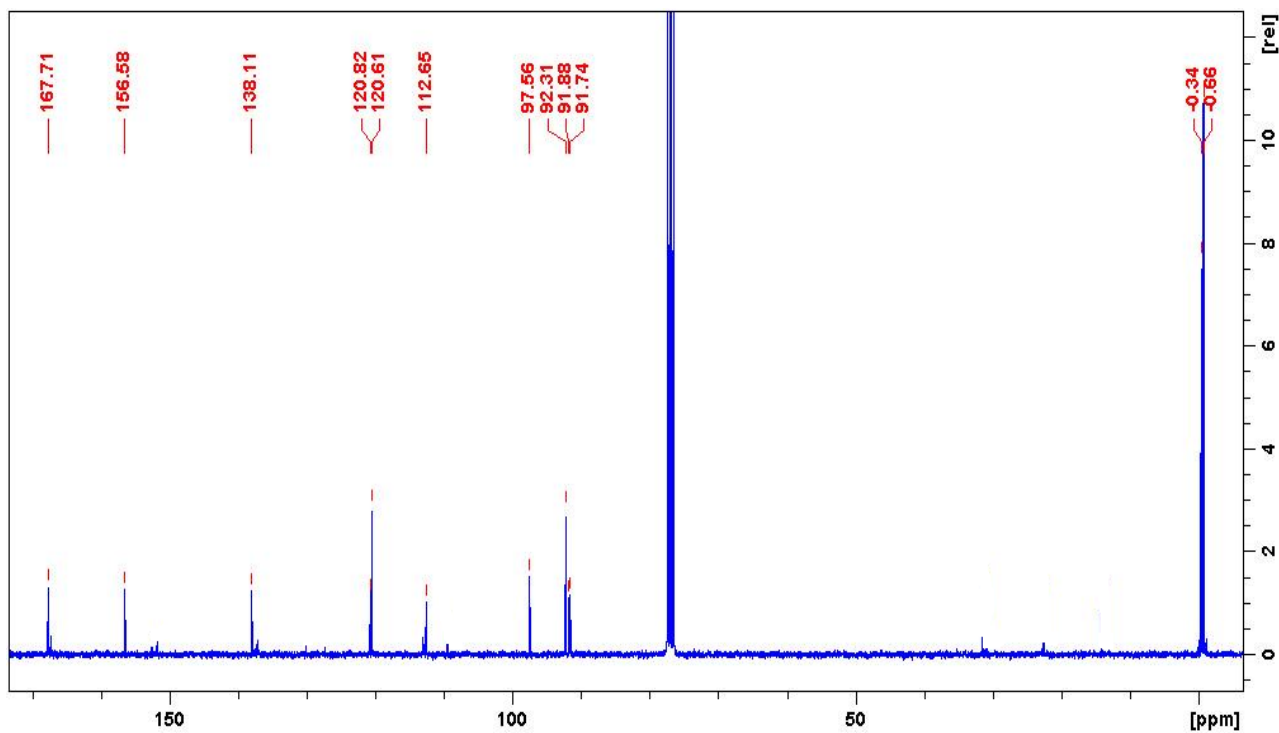
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¹H NMR spectrum of Compound # 11

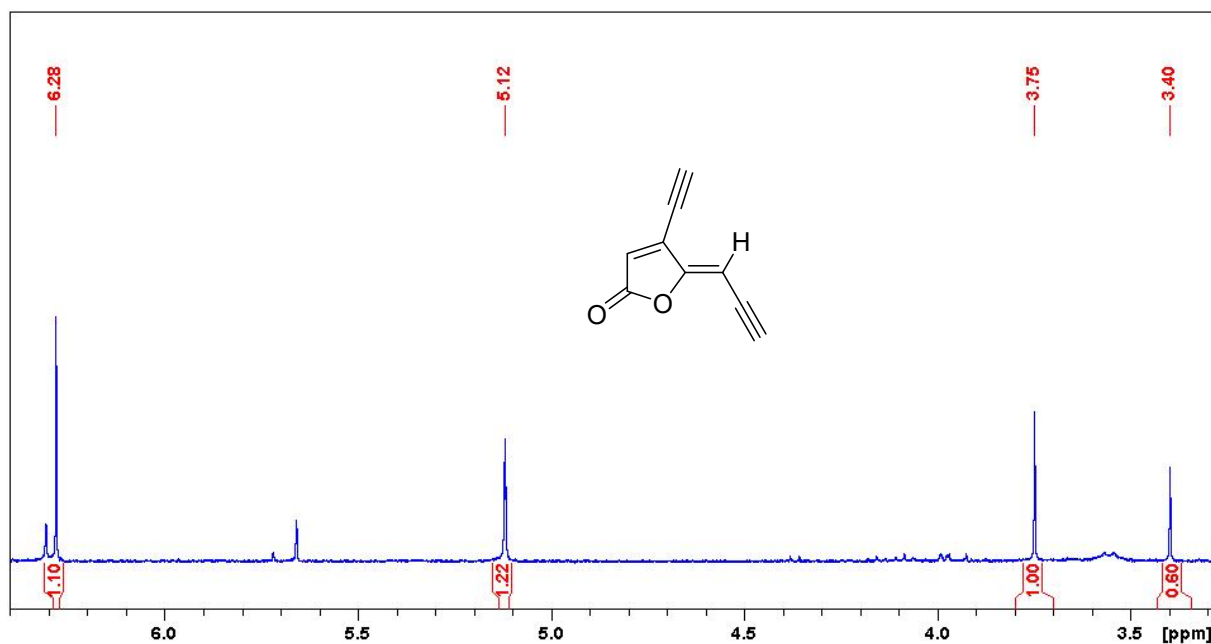
Supervisor Kumar
Fu 30- silyl protection - Fr1
1H CDCl3 F:\ nnb 23



¹³C NMR spectrum of Compound # 11

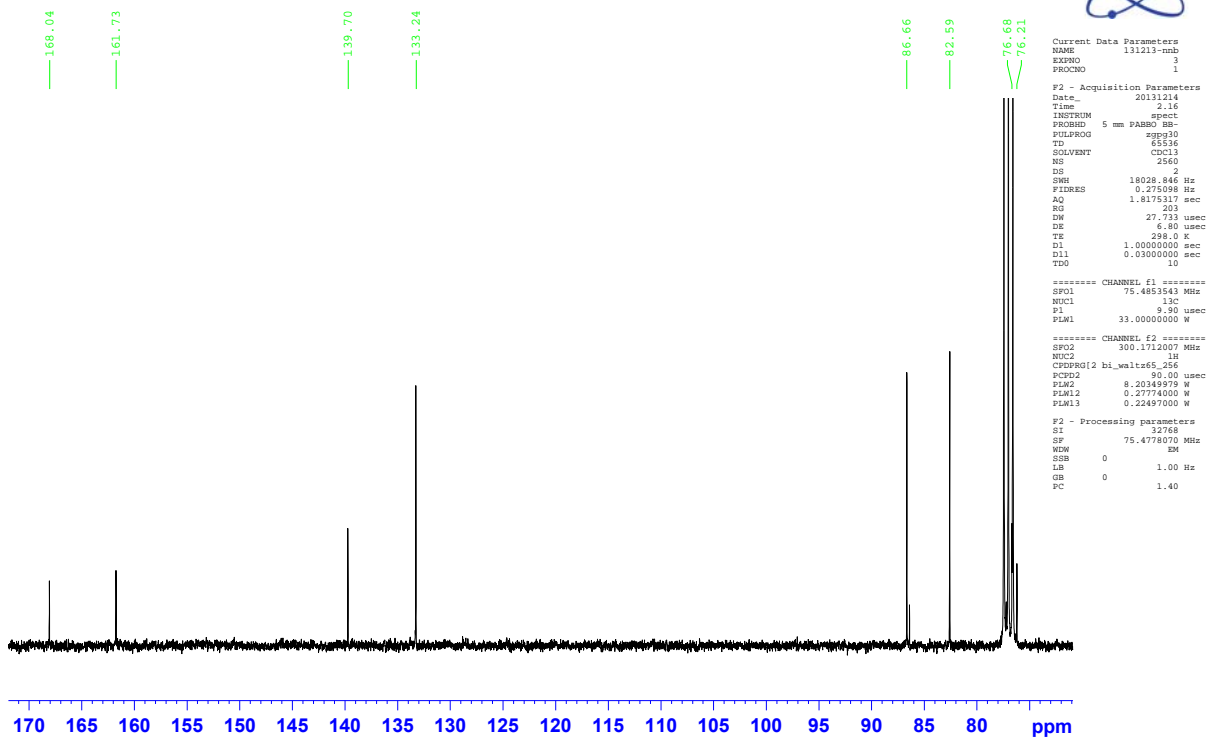


¹H NMR spectrum of Compound # 13



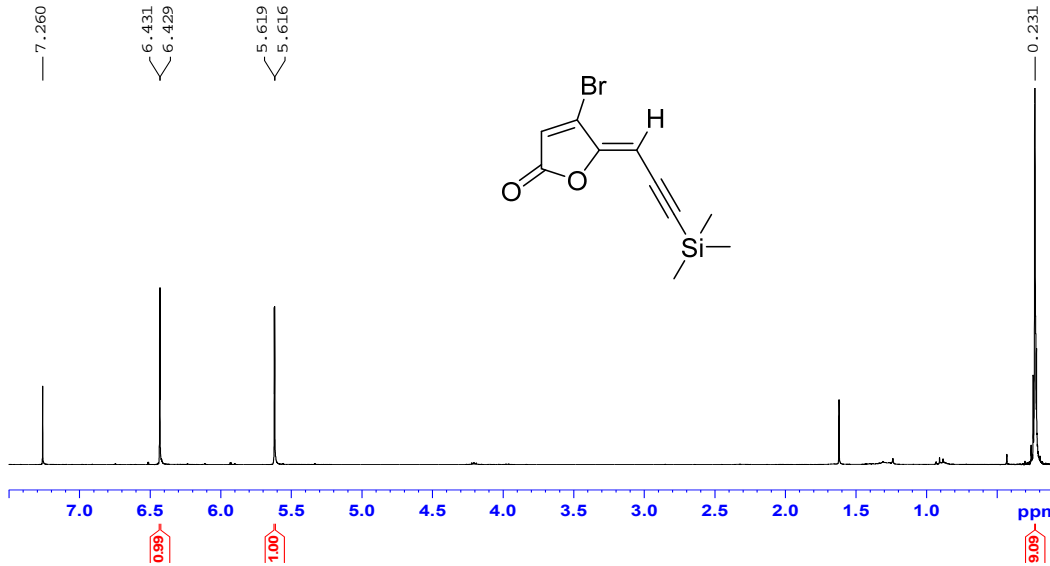
¹³C NMR spectrum of Compound # 13

Supervisor Kumar
Furanone 30+ TMS acetylene_deprotected-disubstituted
13C.night CDCl3 F:\ nmb 22



¹H NMR spectrum of Compound # 12

Supervisor Kumar
 Comp 30 dimer-Fr1
 1H CDC13 F:\ nnb 31



```

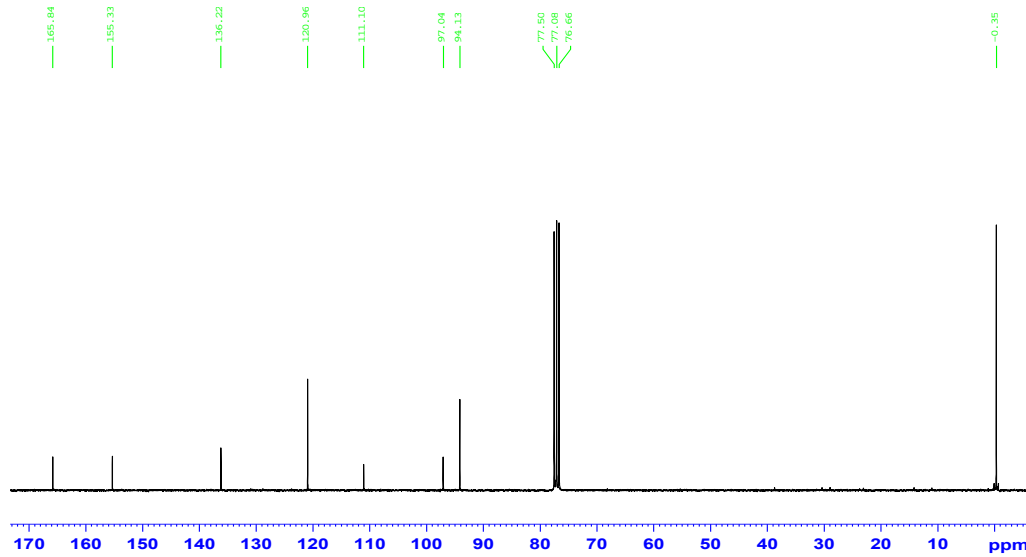
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¹³C NMR spectrum of Compound # 12

Supervisor Kumar
 Comp 30 dimer-Fr1
 13C.night CDC13 F:\ nnb 54



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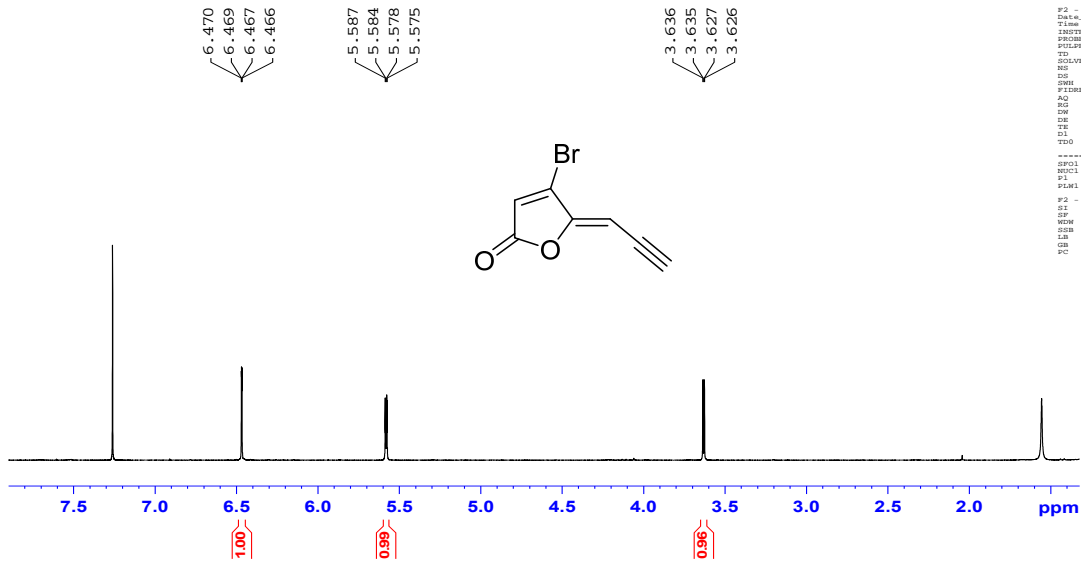
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PLM3     0.22819100 M
PLM3     0.18335000 M

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¹H NMR spectrum of Compound # 14

Supervisor Kumar
Fu 30- Silyl deprotected
1H CDCl3 F:\ nmb 8



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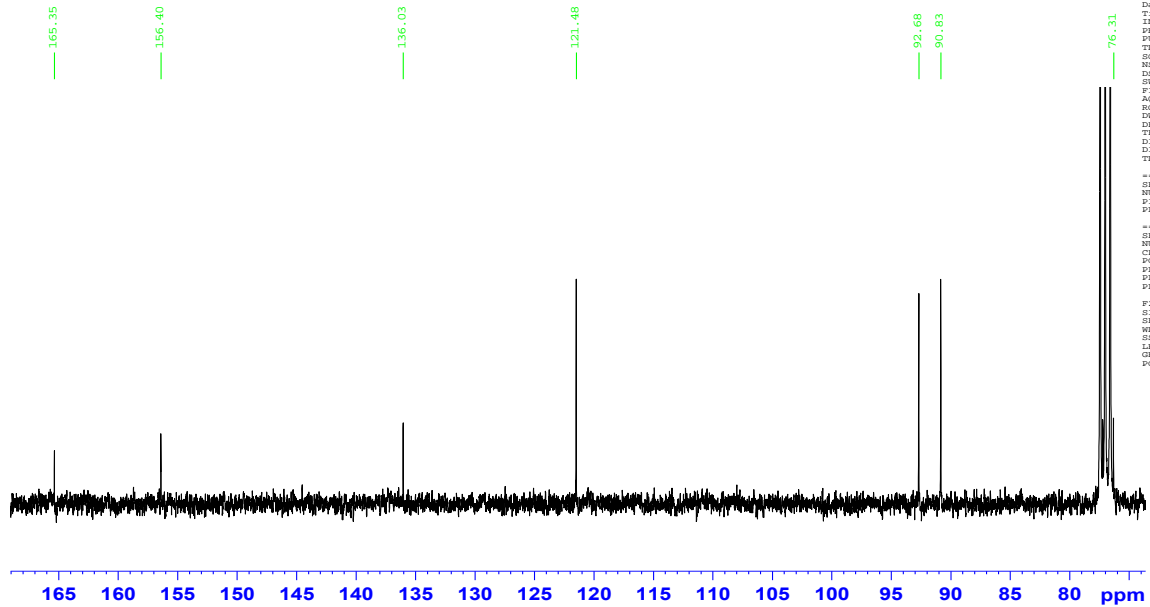
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TE        298.0 K
D1        5.0000000 sec
TDO       1

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SSB       0
LB        0.10 Hz
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PC        1.00
```

¹³C NMR spectrum of Compound # 14

Supervisor Kumar
Fu-30 Fr2 Silyl deprotected
13C.night CDCl3 F:\ nmb 33



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PROCNO   1

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FIDRES   0.278098 Hz
AQ        1.8175377 sec
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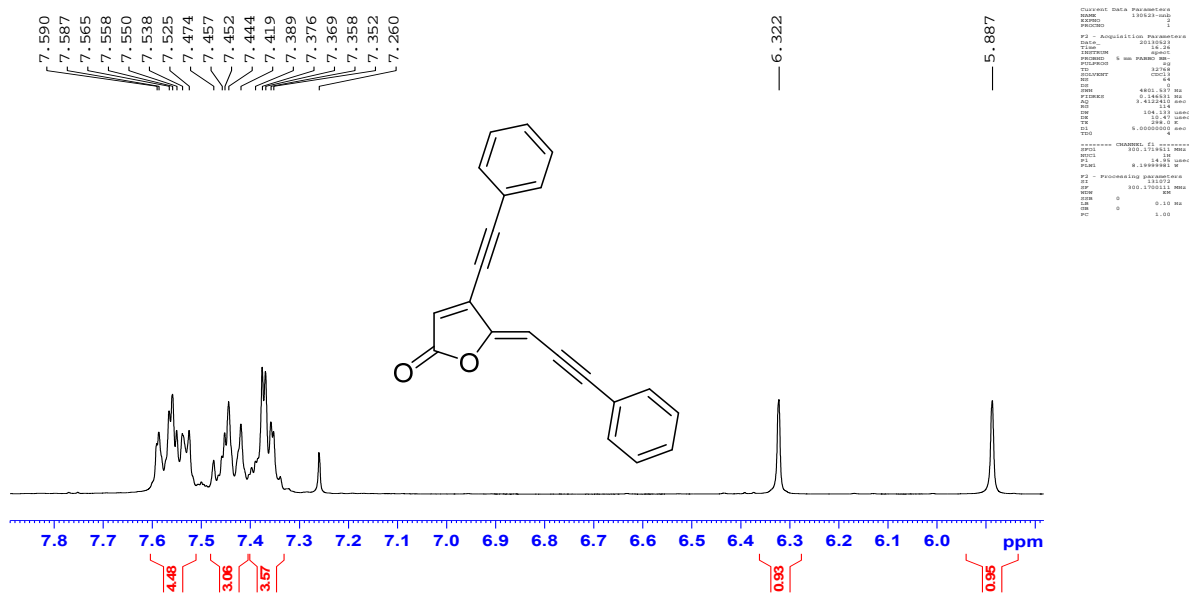
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NUC2     1H
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PLM2     0.22635889 W
PLM3     0.18335000 W

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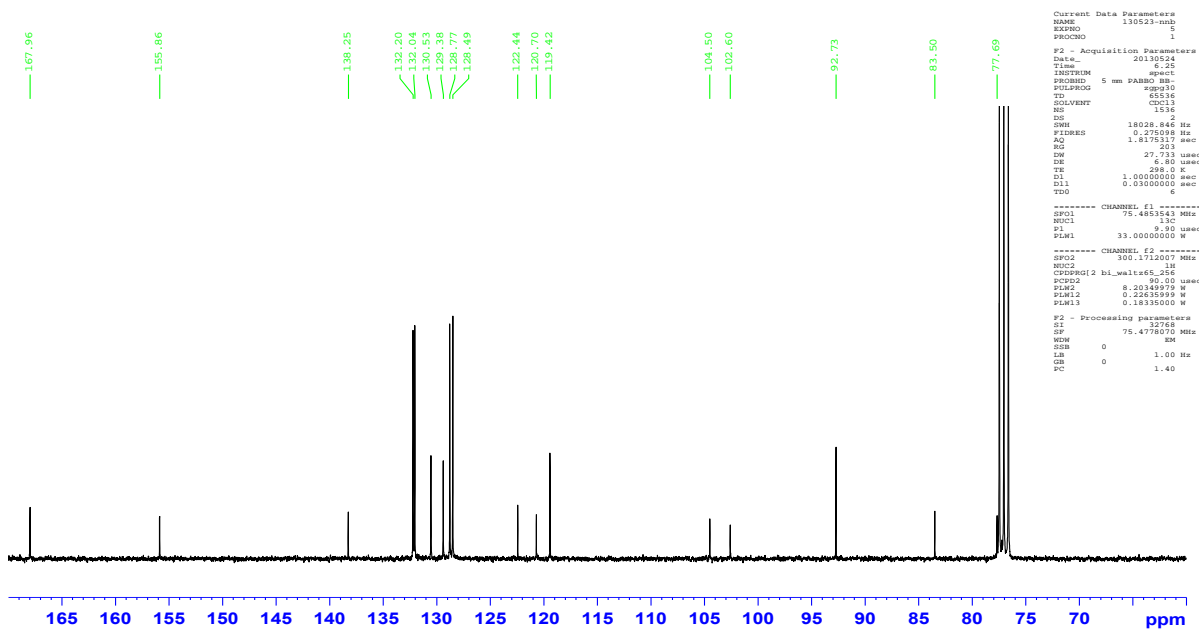
¹H NMR spectrum of Compound # 17a

Supervisor Kumar
 Comp 30+ Ph acetylene- Fr2
 1H CDC13 F:\nmb 35



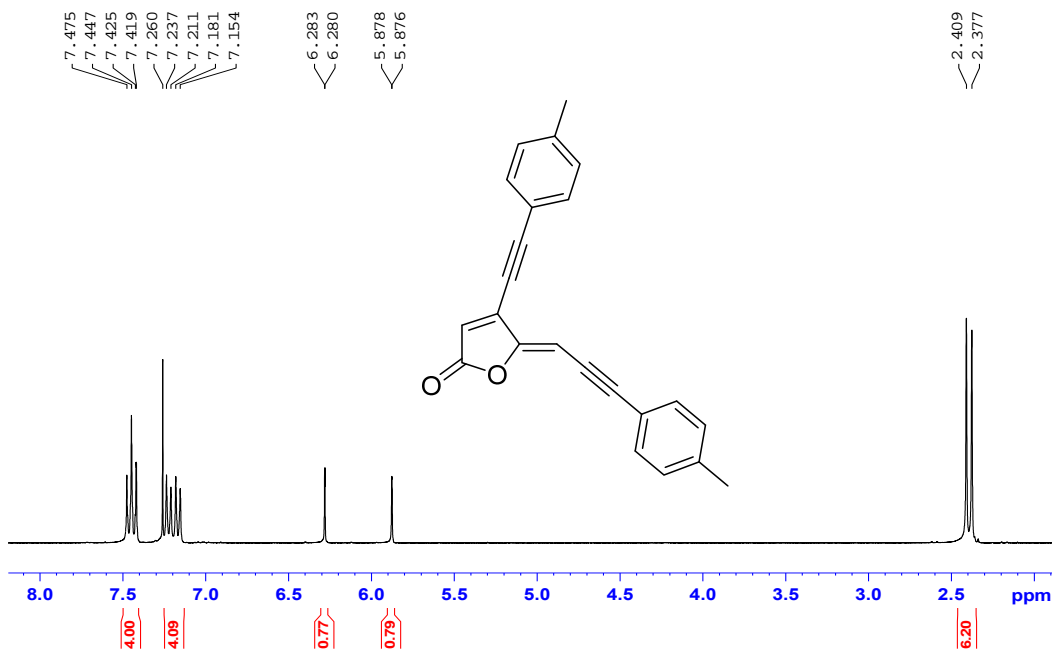
¹³C NMR spectrum of Compound # 17a

Supervisor Kumar
 Comp 30+ Ph acetylene-Fr2
 13C.night CDC13 F:\nmb 10



¹H NMR spectrum of Compound # 17b

Supervisor Kumar
 Furanone 30 + 4- methyl ph acetylene- Dried
 1H CDC13 F:\ nnb 31



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EXPNO    2
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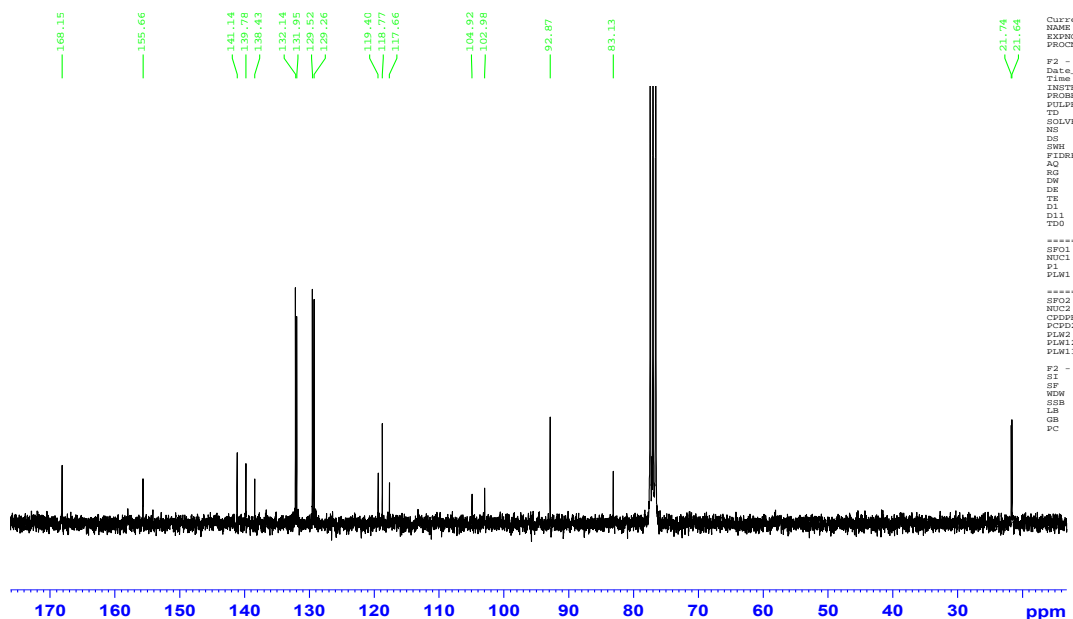
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D1       5.0000000 sec
TDO      1

----- CHANNEL f1 -----
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¹³C NMR spectrum of Compound # 17b

Supervisor Kumar
 Furanone 30 + 4-methyl phenylacetylene- Dried
 13C.night CDC13 F:\ nnb 44



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PROCNO   1

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D11      0.0300000 sec
TDO      8

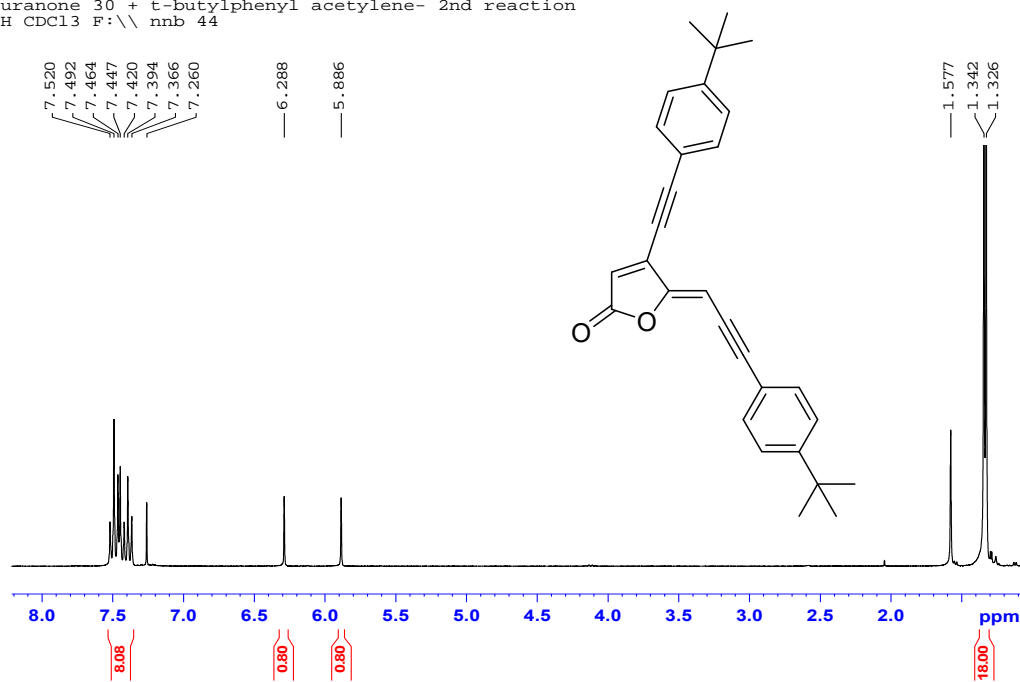
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NUC2     1H
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PCPD2    90.00 usec
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PLW12    0.27774000 W
PLW13    0.22497000 W

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LB       1.00 Hz
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PC       1.40
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¹H NMR spectrum of Compound # 17c

Supervisor Kumar
 Furanone 30 + t-butylphenyl acetylene- 2nd reaction
 1H CDCl3 F:\ nnb 44



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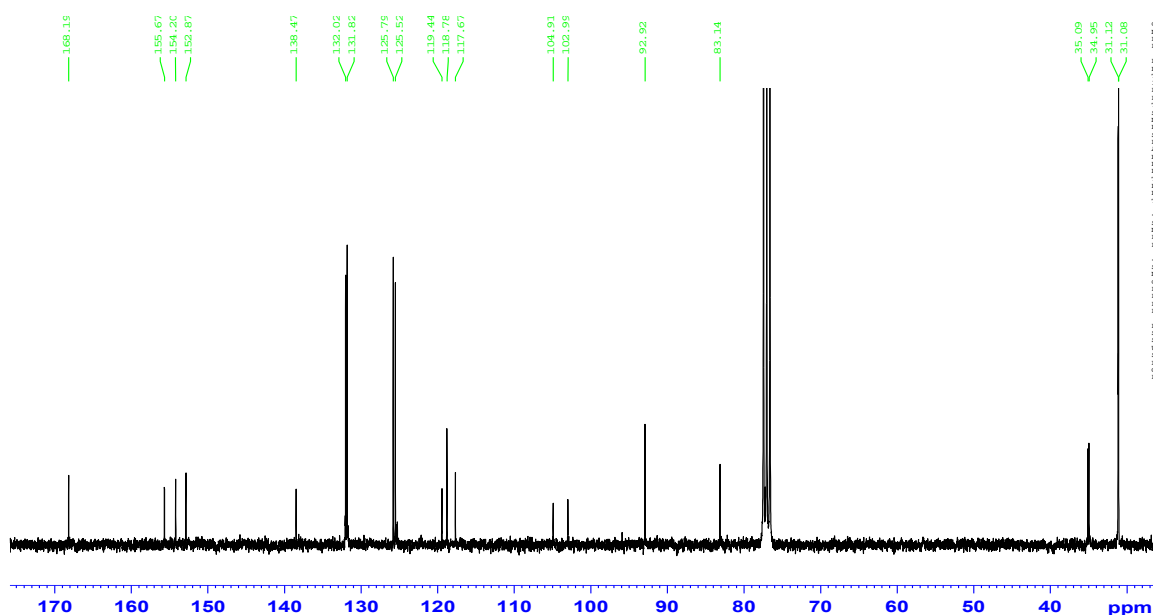
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TE        298.20 K
D1        5.00000000 sec
TD0       1

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PLW1     8.1939995 W

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WDW       EM
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¹³C NMR spectrum of Compound # 17c

Supervisor Kumar
 Furanone 30+ t-butylphenylacetylene- Double substituted
 13C.night CDCl3 F:\ nnb 1



```

Current Data Parameters
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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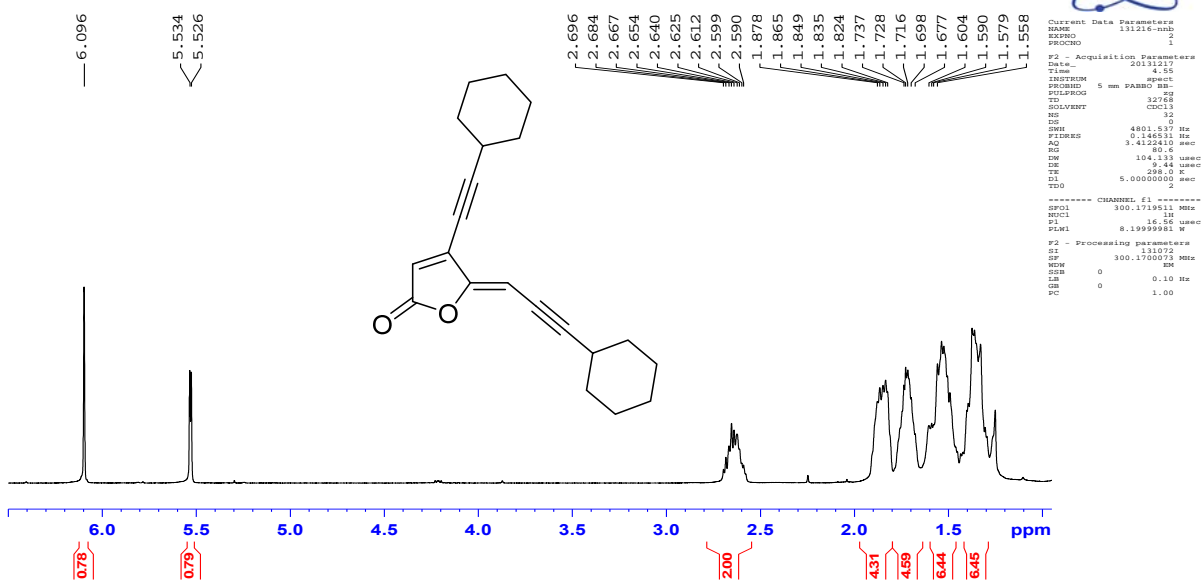
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NUC2      1H
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PCPD2    40.10 usec
PLW2     8.20349979 W
PLW3     0.27774800 W
PLW13    0.22497000 W

F2 - Processing parameters
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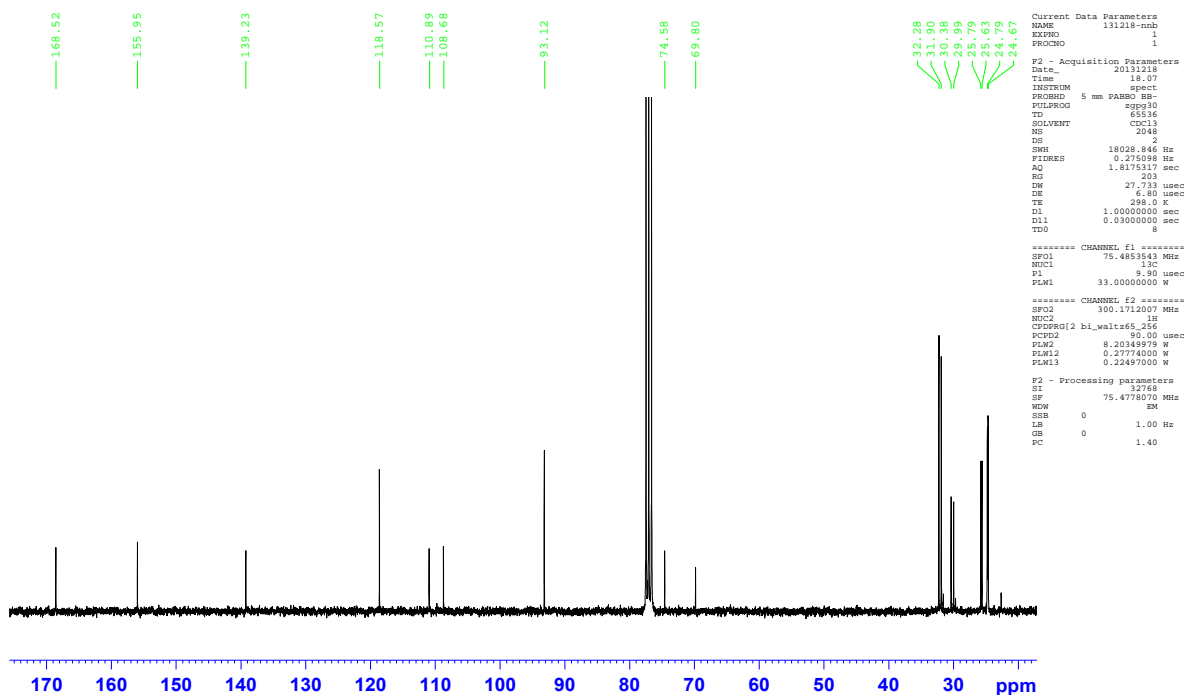
¹H NMR spectrum of Compound # 17d

Supervisor Kumar
 Furanone 30 + Cyclohexylacetylene- column 3 -Fr1
 1H CDCl3 F:\ nmb 5



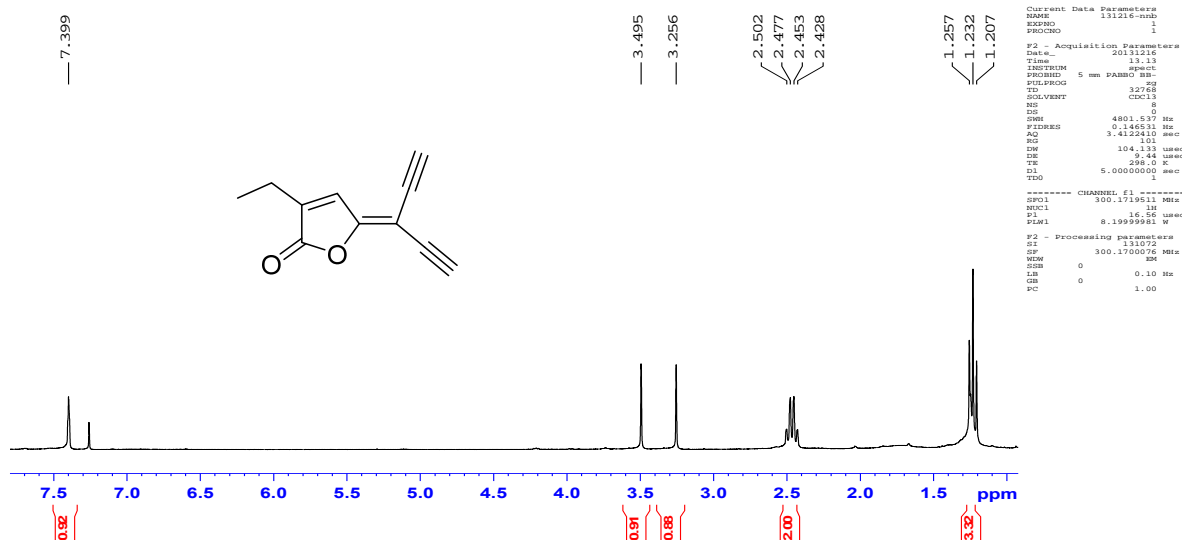
¹³C NMR spectrum of Compound # 17d

Supervisor Kumar
 Furanone 30 + Cyclohexylacetylene- Good fraction
 13C.night CDCl3 F:\ nmb 41



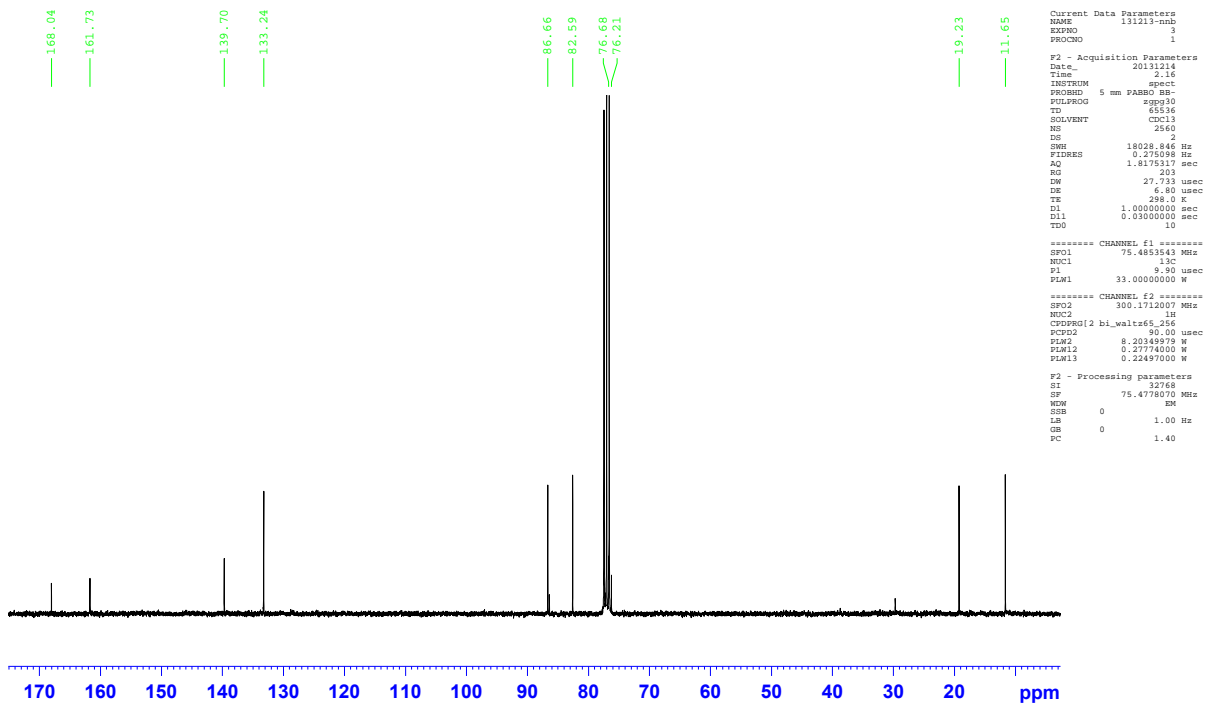
¹H NMR spectrum of Compound # 18a

Supervisor Kumar
 Furanone 17 + TMS Acetylene- Deprotected- Dried- 2nd reaction- Good
¹H CDCl₃ F:\ nnb 42



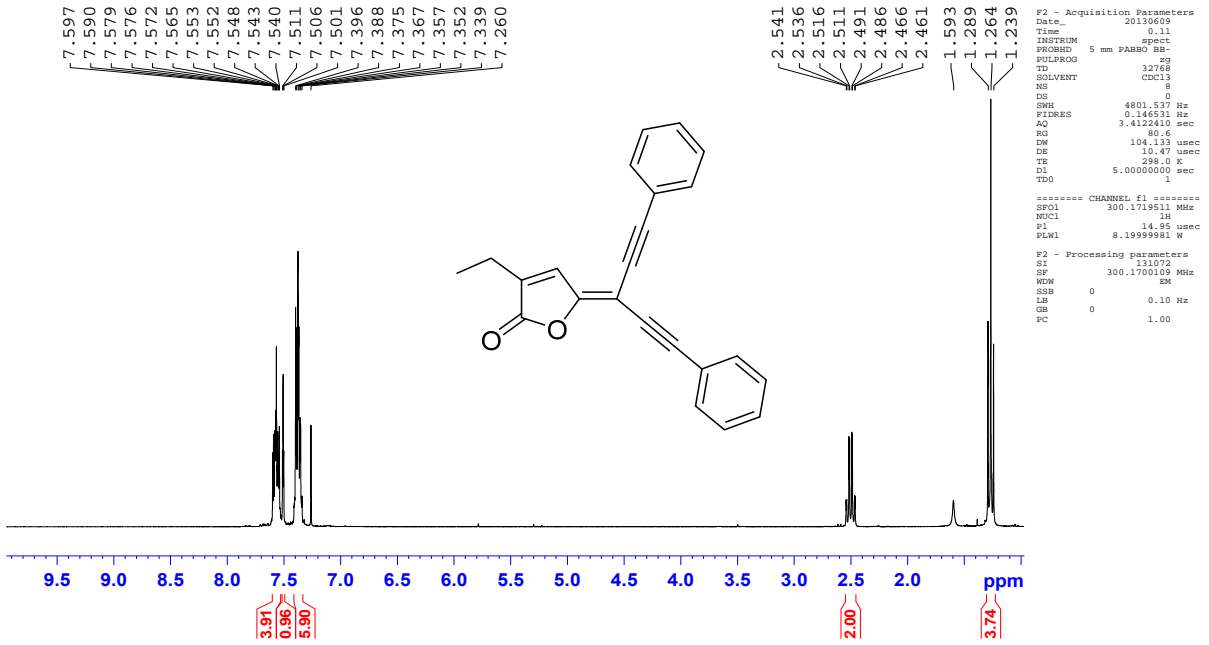
¹³C NMR spectrum of Compound # 18a

Supervisor Kumar
 Furanone 17+ TMS acetylene- TBAF dprotection-2nd reaction -dried
¹³C.night CDCl₃ F:\ nnb 22



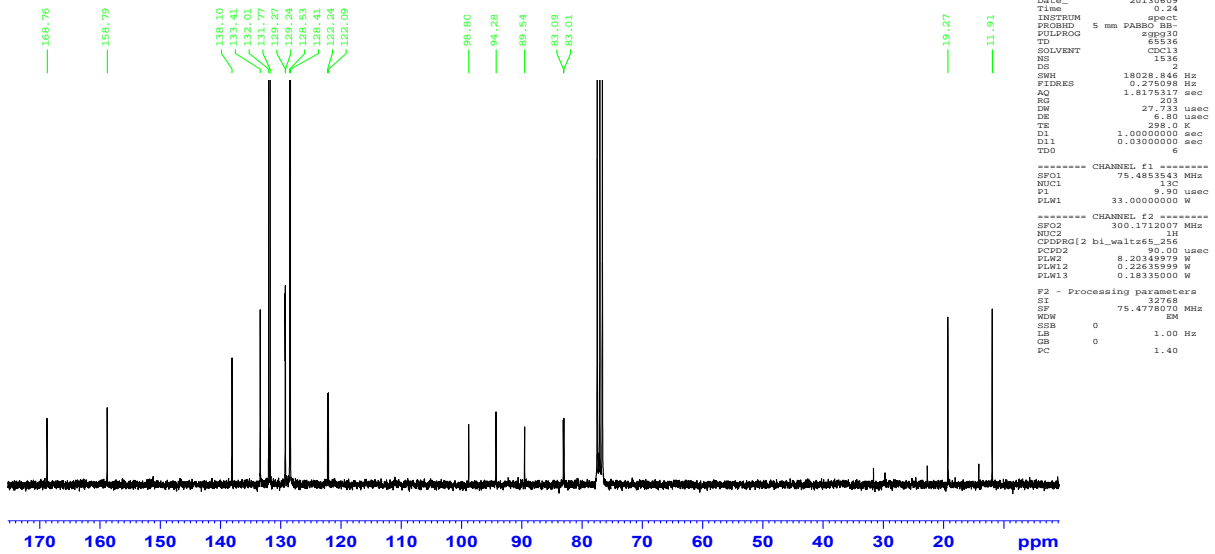
¹H NMR spectrum of Compound # 18b

Supervisor Kumar
Comp 17+ Phenylacetylene- Trial 3 (Degassing the solvent with Ar)
1H CDC13 F:\nmb 13



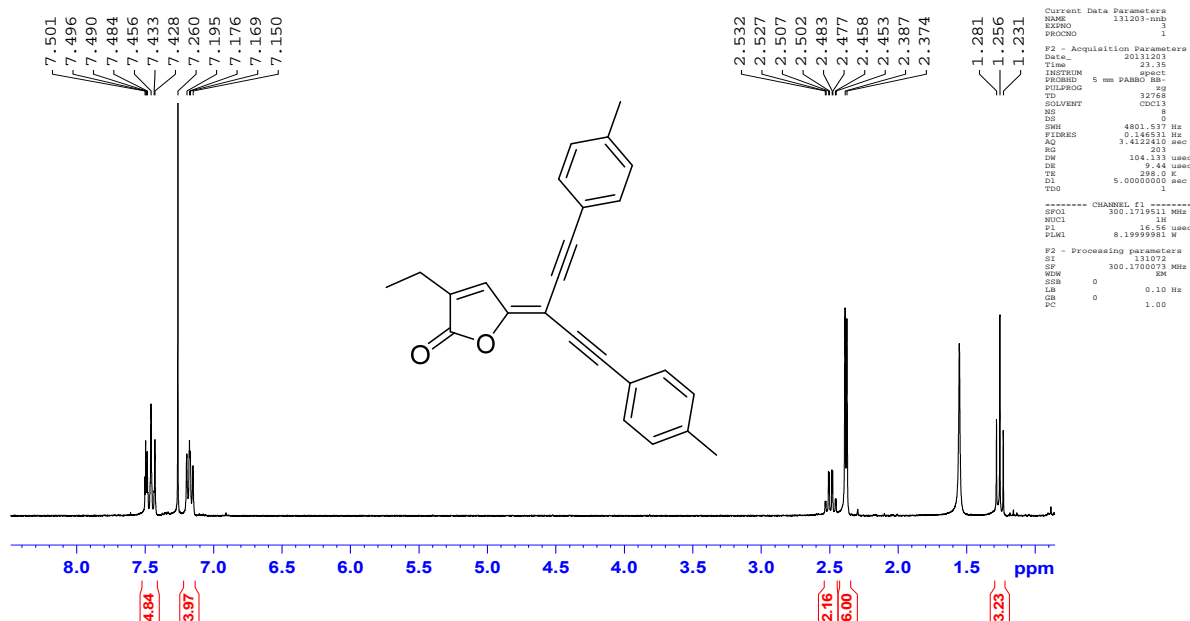
¹³C NMR spectrum of Compound # 18b

Supervisor Kumar
Comp 17+ Phenylacetylene- Trial 3 (Degassing the solvent with Ar)
13C.night CDC13 F:\nmb 13



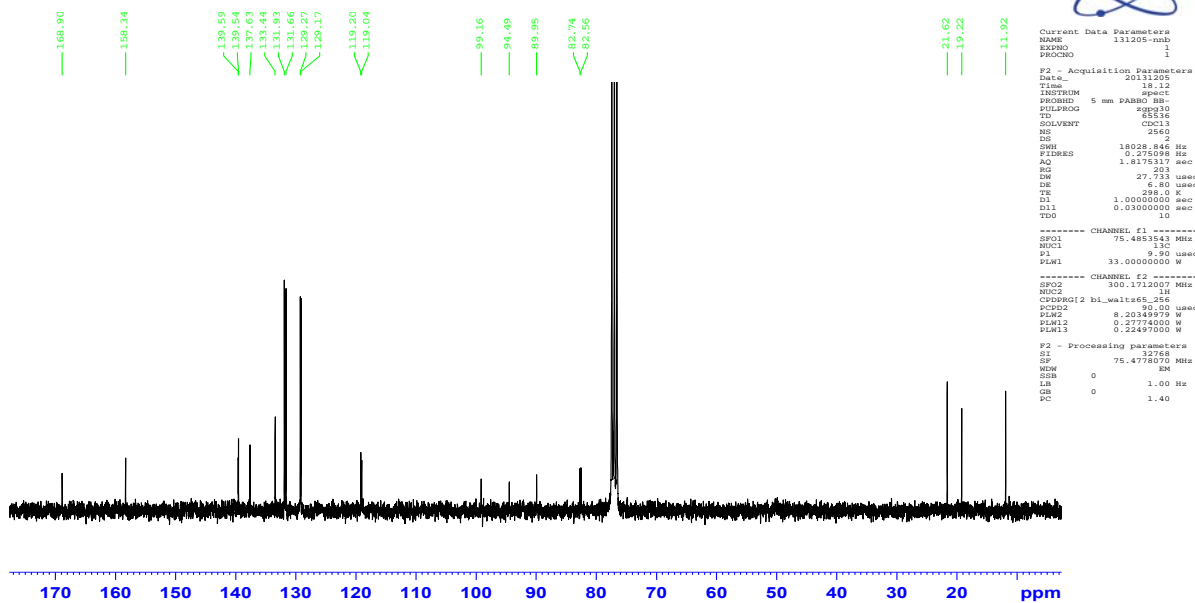
¹H NMR spectrum of Compound # 18c

Supervisor Kumar
Furanone 17 + 4- methyl ph acetylene- Dried
1H CDCl3 F:\ nnb 32



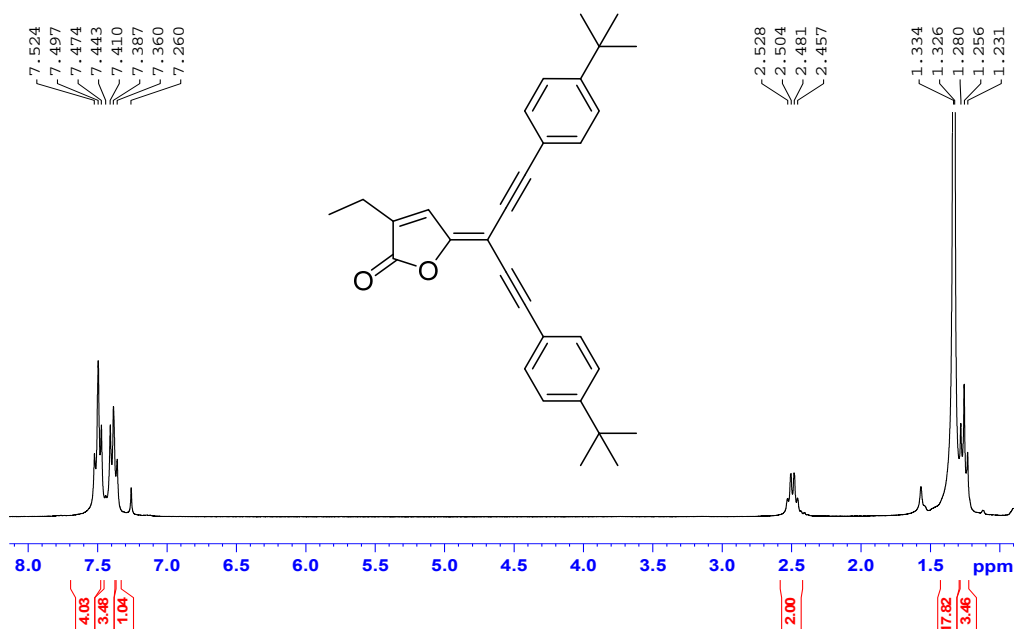
¹³C NMR spectrum of Compound # 18c

Supervisor Kumar
Furanone 17 + 4-methyl phenylacetylene- Dried
13C.night CDCl3 F:\ nnb 42



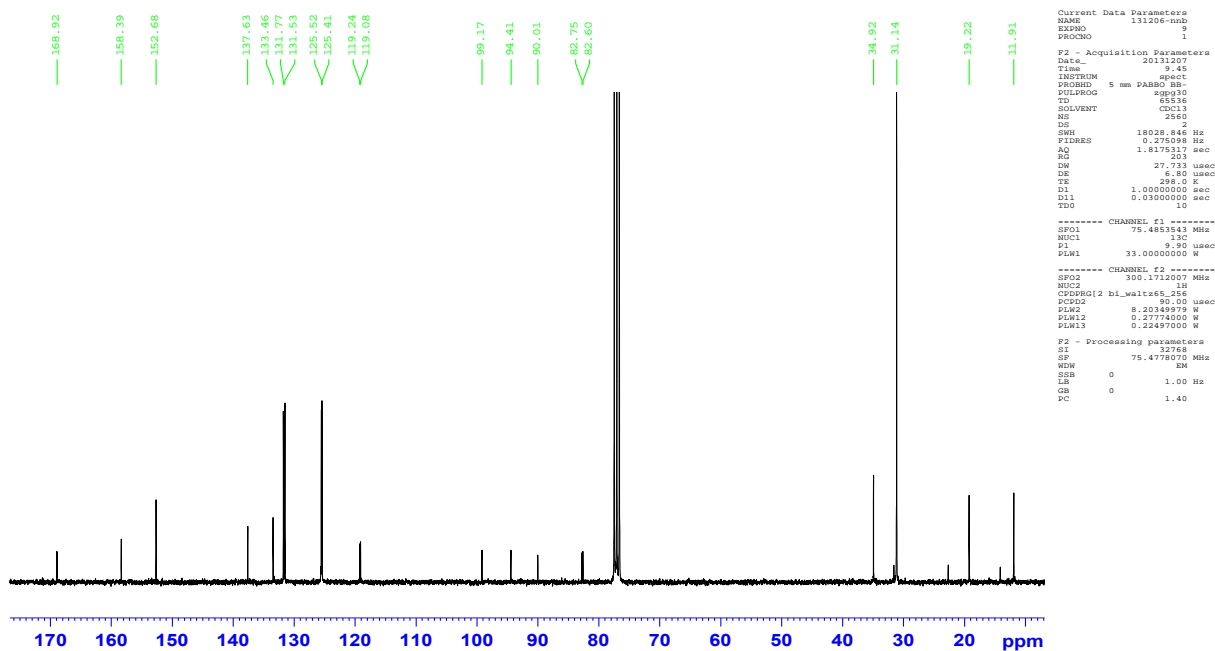
¹H NMR spectrum of Compound # 18d

Supervisor Kumar
Furanone 17 + t-Bu phe acetyleneRC
1H CDCl3 F:\n nb 41



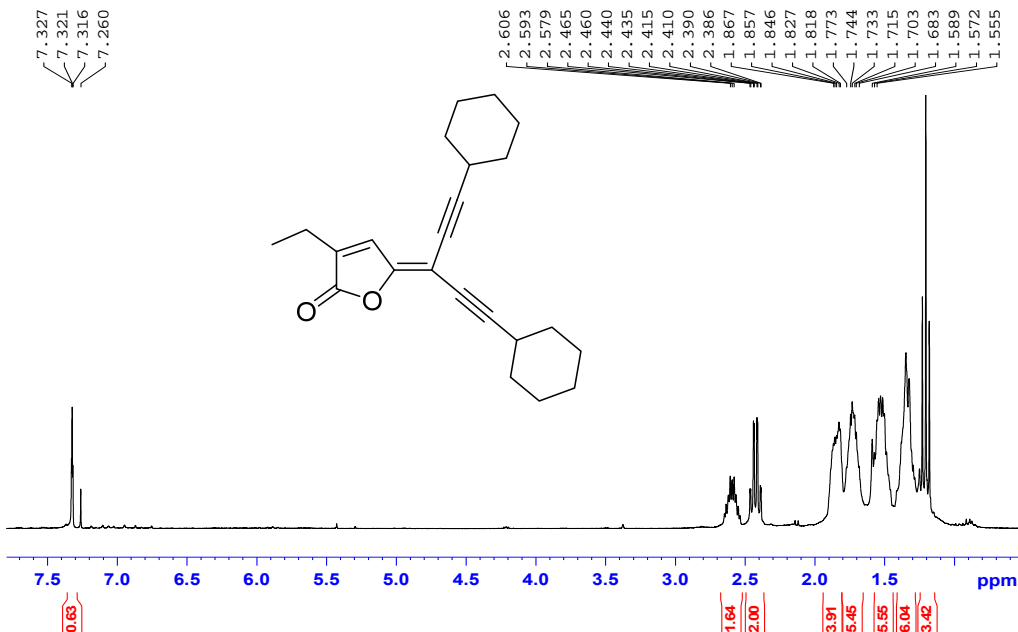
¹³C NMR spectrum of Compound # 18d

Supervisor Kumar
Furanone 17+ t-butylphenylacetylene-
13C.night CDCl3 F:\n nb 31



¹H NMR spectrum of Compound # 18e

Supervisor Kumar
 Furanone 17 + Cyclohexylacetylene
¹H CDCl₃ F:\ nmb 33



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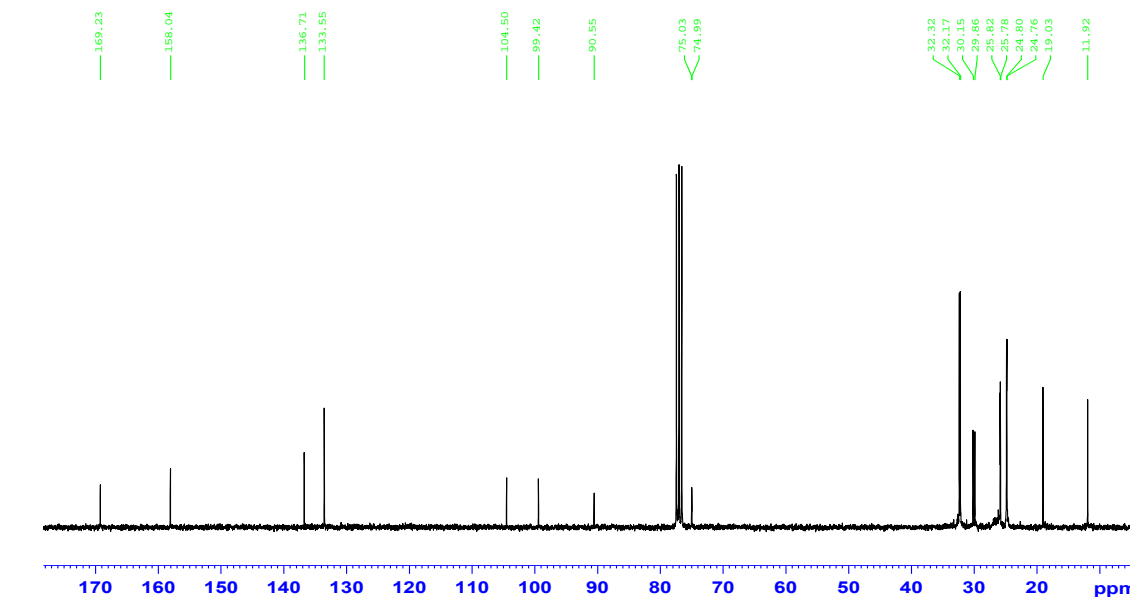
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FIDRES   0.146531 Hz
AQ       3.4122610 sec
RG       40.3
RW       104.133 usec
DE       9.44 usec
TE       298.0 K
D1       5.0000000 sec
TDO      1

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NUC1    13C
P1      18.58 usec
PLM1    8.19999981 W

F2 - Processing parameters
SI      300.1700073 MHz
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LB      0.10 Hz
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PC      1.00
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¹³C NMR spectrum of Compound # 18e

Supervisor Kumar
 Furanone 17 + Cyclohexylacetylene
¹³C.night CDCl₃ F:\ nmb 29



```
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EXPNO    5
PROCNO   1

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NS       2048
DS       2
SWH      18038.446 Hz
FIDRES   0.275098 Hz
AQ       1.8175117 sec
RG       203
RW       27.733 usec
DE       6.80 usec
TE       298.0 K
D1       1.0000000 sec
D11     0.0300000 sec
TDO      8

----- CHANNEL f1 -----
SFO1    75.4833643 MHz
NUC1    13C
P1      9.90 usec
PLM1    33.0000000 W

----- CHANNEL f2 -----
SFO2    300.1712007 MHz
NUC2    1H
CPDPRG2  bi_waltz16_256
P2PRG2   90.00 usec
PLM2     8.20349979 W
PLM3     0.27744000 W
PLM13    0.22497000 W

F2 - Processing parameters
SI      300.1700073 MHz
WDW     EM
SSB     0
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PC      1.40
```

Table S1: Percentage inhibition of QS activity in the *P. aeruginosa* MH602 *lasB* reporter strain by the acetylene-based fimbrolide analogues.

Compounds	QSI activity against PA MH602 at the indicated concentration / %			
	250 μ M	125 μ M	62.5 μ M	31.3 μ M
13	82.2 \pm 1.4 ^c	63.1 \pm 2.3 ^c	45.6 \pm 2.2 ^b	28.9 \pm 0.6 ^a
14	97.6 \pm 0.2 ^d	82.0 \pm 1.2 ^c	55.6 \pm 0.4 ^b	33.4 \pm 0.5 ^a
17a	13.3 \pm 0.1 ^a	NA	NA	NA
17b	11.2 \pm 1.2 ^a	NA	NA	NA
17c	13.2 \pm 1.4 ^a	7.0 \pm 1.9	NA	NA
17d	18.2 \pm 2.0 ^a	6.2 \pm 0.9	3.6 \pm 1.3	1.8 \pm 1.6
18a	31.8 \pm 1.2 ^a	12.4 \pm 1.4	9.4 \pm 0.7	5.6 \pm 1.0
18b	8.1 \pm 2.2 ^a	4.3 \pm 1.9	NA	NA
18c	3.14 \pm 1.3 ^a	NA	NA	NA
18d	15.5 \pm 1.0 ^a	7.7 \pm 0.7	5.6 \pm 1.0	3.0 \pm 1.4
18e	50.6 \pm 1.5 ^b	25.8 \pm 5.7	19.3 \pm 1.0	13.2 \pm 1.3
Furanone 30 (positive control), 4	89.7 \pm 4.6 ^c	64.2 \pm 3.5 ^b	41.4 \pm 2.7	26.0 \pm 5.2

^aNo growth inhibition; ^bGrowth inhibition \leq 15%; ^cGrowth inhibition \geq 20%; ^dGrowth inhibition \geq 50%; NA = no activity.

Table S2: Growth inhibition (%OD) of *P. aeruginosa* strain PAMH602 in presence of synthesized compounds at different concentrations.

Compounds	Percentage growth inhibition at the given concentration			
	250 μ M	125 μ M	62.5 μ M	31.3 μ M
13	26.3 \pm 0.7	16.9 \pm 0.9	11.9 \pm 1.0	6.6 \pm 0.6
14	57.1 \pm 0.9	30.1 \pm 0.5	3.8 \pm 0.4	0
17a	0	0	0	0
17b	0	0	0	0
17c	0	0	0	0
17d	0	0	0	0
18a	0	0	0	0
18b	0	0	0	0
18c	0	0	0	0
18d	0	0	0	0
18e	13.3 \pm 2.0	0	0	0
Furanone 30 (positive control), 4	24.4 \pm 3.4	11.5 \pm 4.4	0	0

Growth inhibition \pm standard deviation of mean from at least two independent experiments. Compounds tested twice in duplicate. 0 = No growth inhibition.