

Efficient Photodynamic Killing of Gram-Positive Bacteria by Synthetic Curcuminoids

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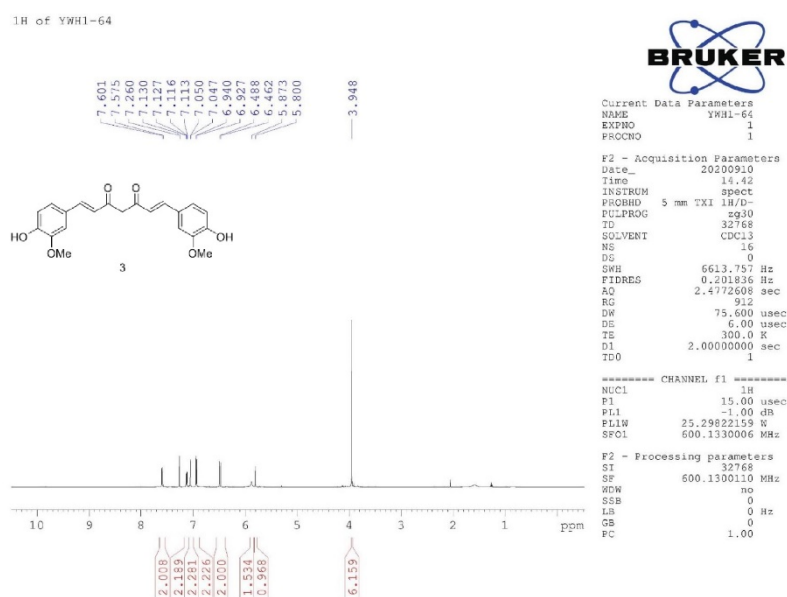


Figure S1. ¹H NMR (600 MHz, CDCl₃) of compound 3.

¹³C of YWH1-64

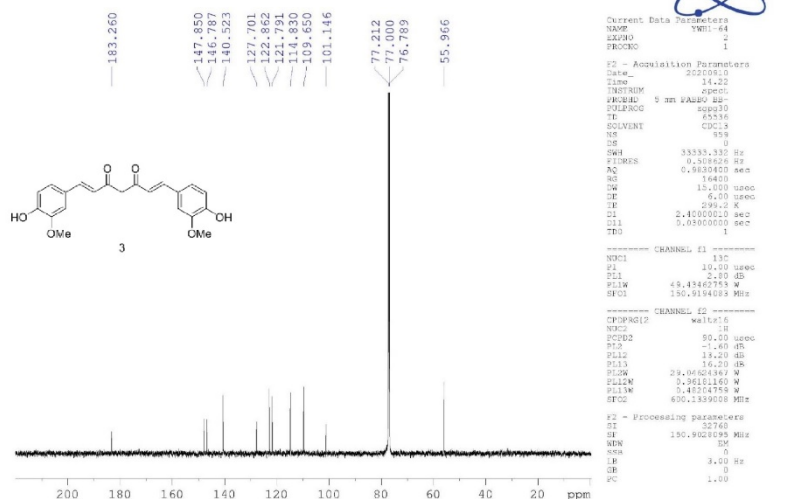


Figure S2. ¹³C NMR (150 MHz, CDCl₃) of compound 3.

¹H of YWH1-116

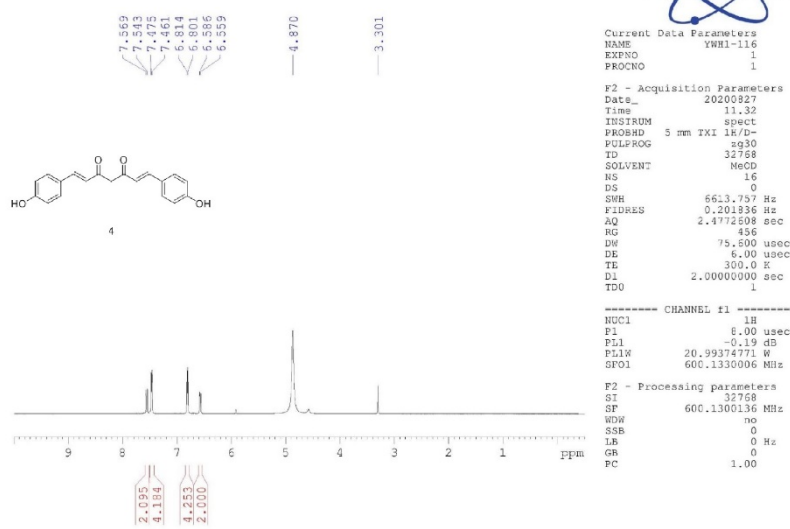


Figure S3. ¹H NMR (600 MHz, CD₃OD) of compound 4.

¹³C of YWH1-116

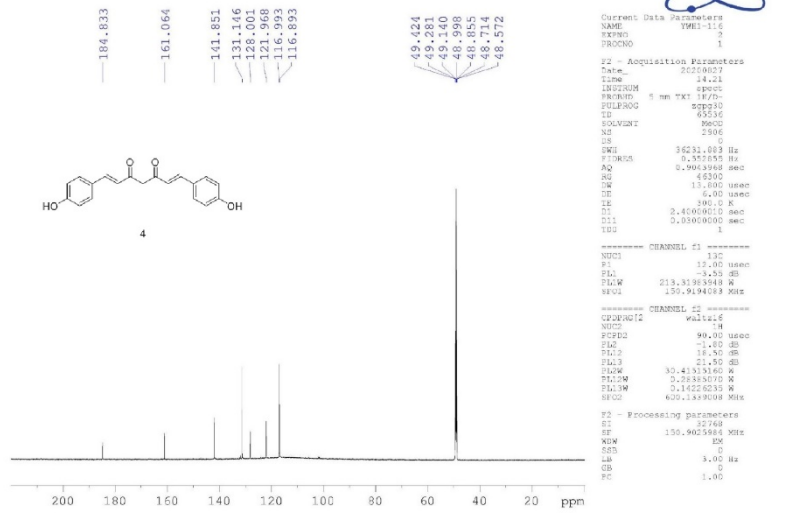


Figure S4. ¹³C NMR (150 MHz, CD₃OD) of compound 4.

¹H of KYL1-P3

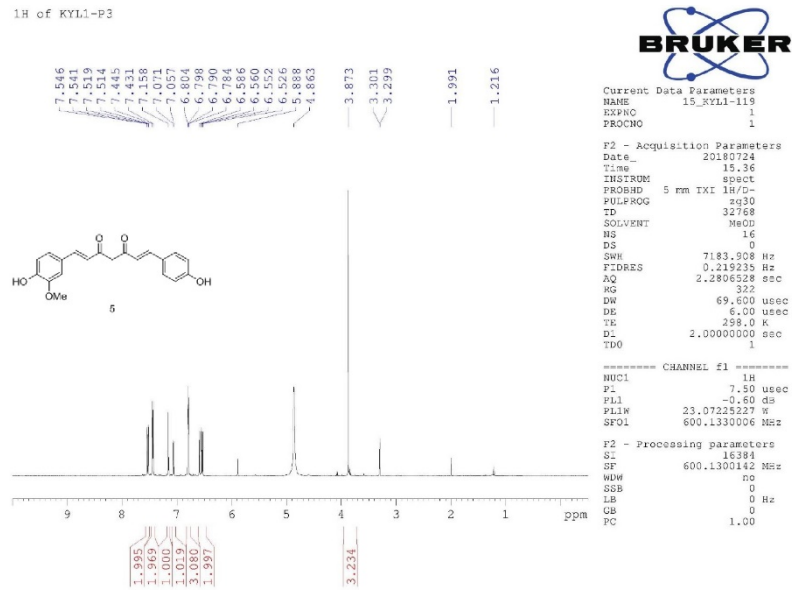
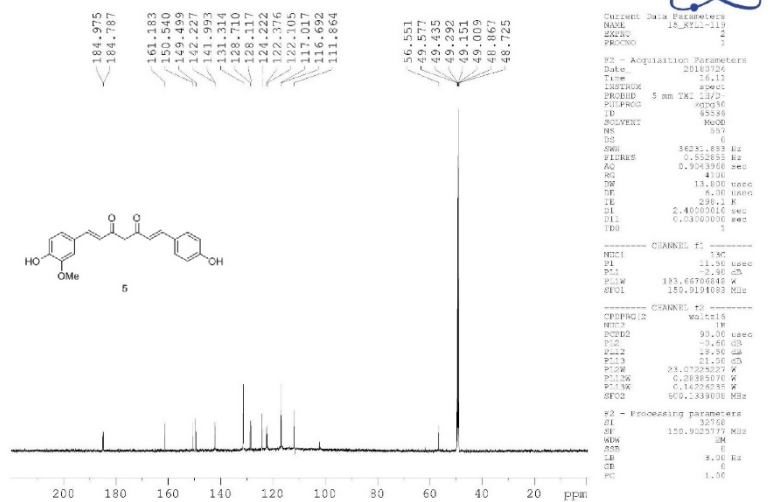
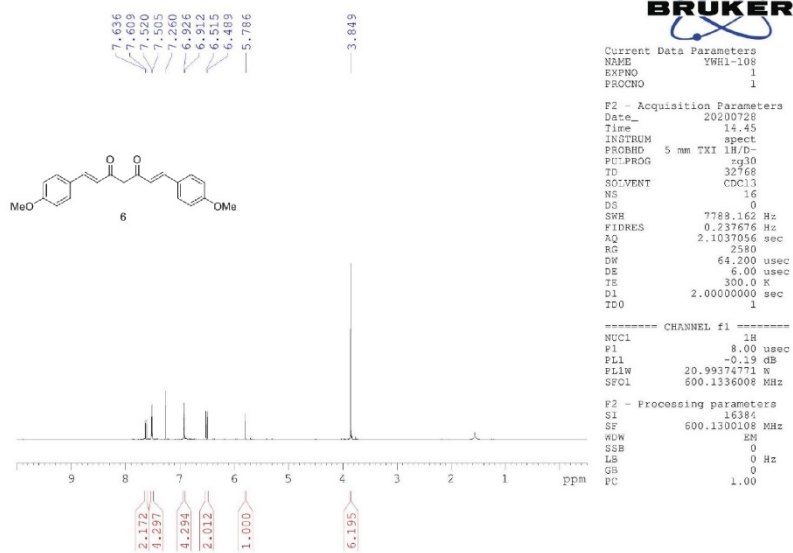


Figure S5. ¹H NMR (600 MHz, CD₃OD) of compound 5.

Figure S6. ¹³C NMR (150 MHz, CD₃OD) of compound 5.Figure S7. ¹H NMR (600 MHz, CDCl₃) of compound 6.

¹³C of YWH1-108

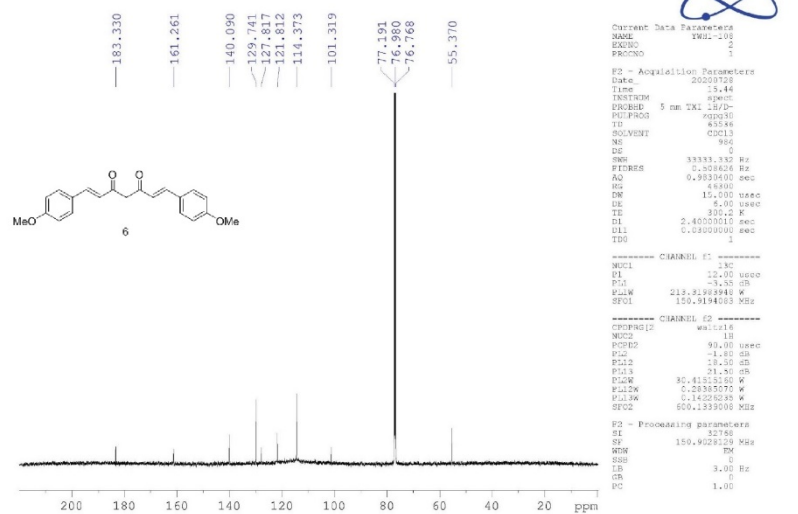


Figure S8. ¹³C NMR (150 MHz, CDCl₃) of compound 6.

¹H of YWH1-107

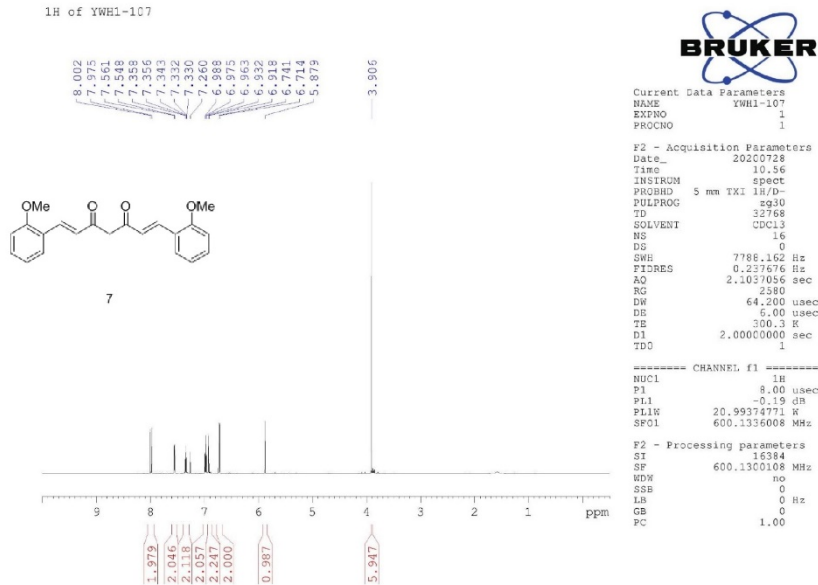
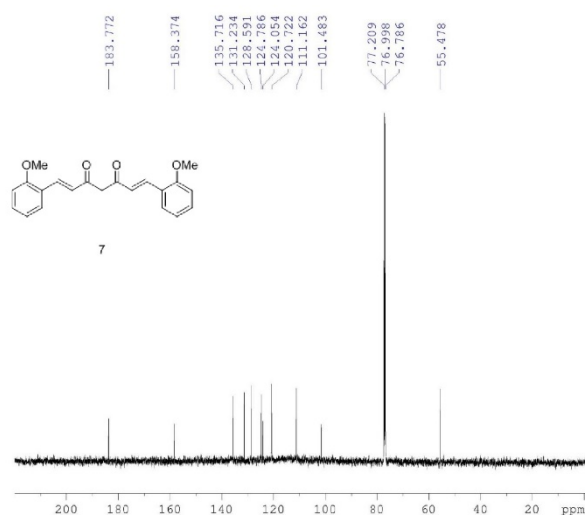


Figure S9. ¹H NMR (600 MHz, CDCl₃) of compound 7.

13C of YWH1-107

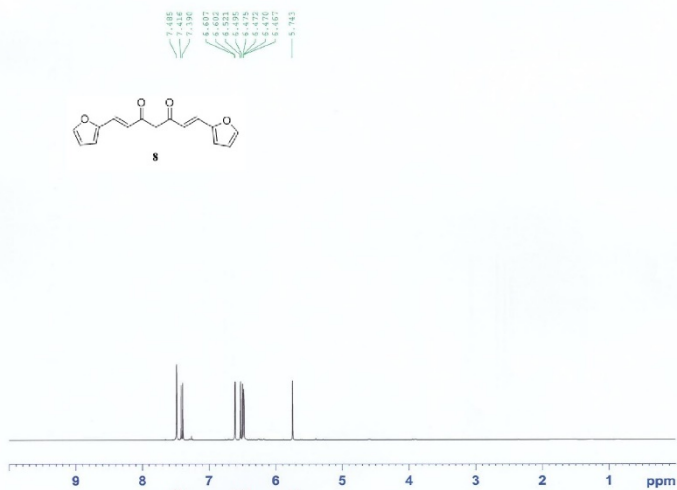


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PROCNO   1
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PULPROG  zgpg30
TE       300.2
SOLVENT  CDCl3
NS       0
DS       0
SWH      33333.332 Hz
FIDRES   0.308625 Hz
AQ       0.5830400 sec
RG       48800
DM       15.000 usec
DE       6.00 usec
TE       300.2 K
D1       2.4500000 sec
D11      0.0300000 sec
TWO      1
----- CHANNEL f1 -----
NUC1     13C
P1       12.00 usec
PL1      -1.50 dB
PL12     15.00 dB
PL13     21.50 dB
PL14     30.4133180 W
PL15     0.23382070 W
PL16     4.14226255 W
SFO1     600.1380000 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
P2       50.00 usec
PL2      -1.80 dB
PL22     15.00 dB
PL23     21.50 dB
PL24     30.4133180 W
PL25     0.23382070 W
PL26     4.14226255 W
SFO2     600.1380000 MHz
----- Processing parameters -----
SI       32768
SF       150.908129 MHz
WDW      EM
SSB      0
LB       3.00 Hz
GB       0
PC       1.00
  
```

Figure S10. ¹³C NMR (150 MHz, CDCl₃) of compound 7.

1H of CJK1-106



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NAME      CJK1-106
EXPNO    1
PROCNO   1
Date_    20200914
Time     15:58
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PROBHD   5 mm TXI 1H/D-
PULPROG  zg30
TE       32768
SOLVENT  CDCl3
NS       0
DS       0
SWH      6513.757 Hz
FIDRES   0.201836 Hz
AQ       2.4773865 sec
RG       256
DM       75.600 usec
DE       6.00 usec
TE       300.2 K
D1       2.0000000 sec
TWO      1
----- CHANNEL f1 -----
NUC1     1H
P1       8.00 usec
PL1      -0.15 dB
PL12     20.99374771 W
SFO1     600.1380000 MHz
SI       16384
SF       600.1380000 MHz
WDW      EM
SSB      0
LB       0.00 Hz
GB       0
PC       1.00
  
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Figure S11. ¹H NMR (600 MHz, CDCl₃) of compound 8.

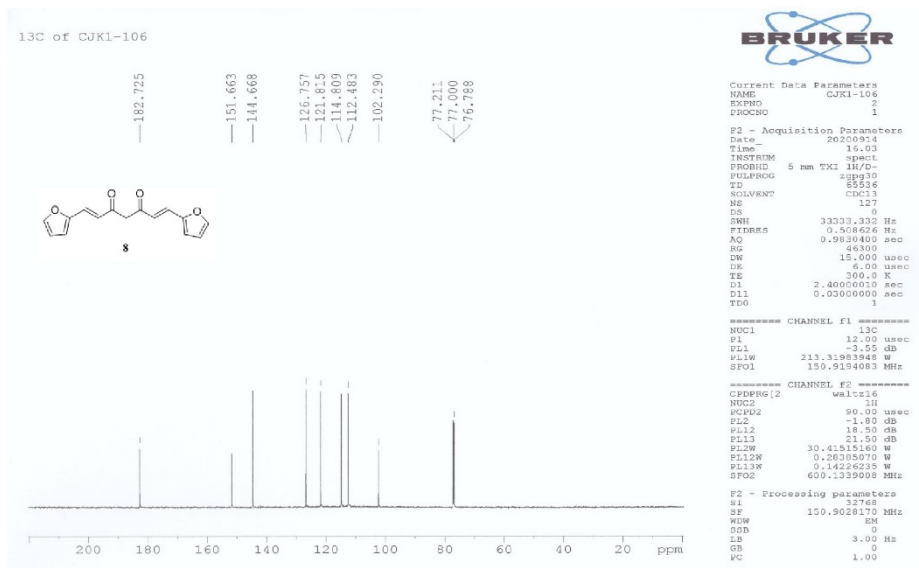


Figure S12. ¹³C NMR (150 MHz, CDCl₃) of compound 8.

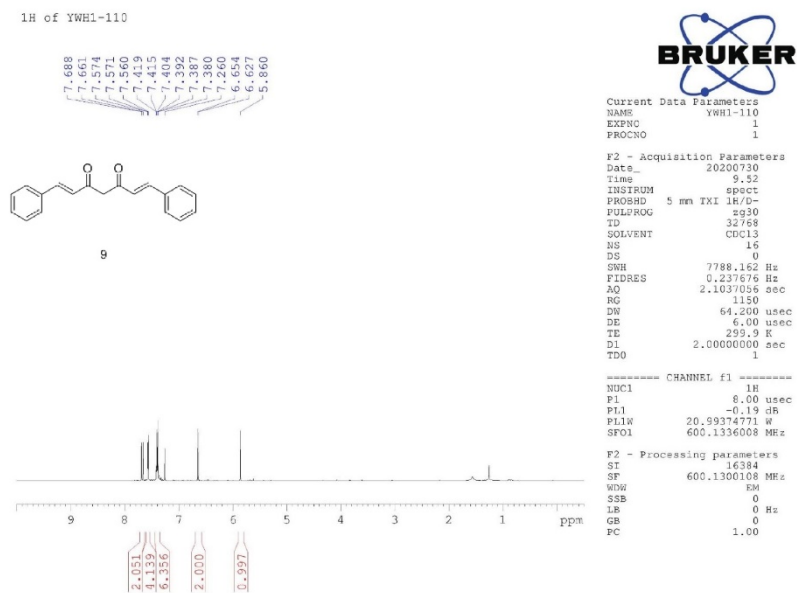


Figure S13. ¹H NMR (600 MHz, CDCl₃) of compound 9.

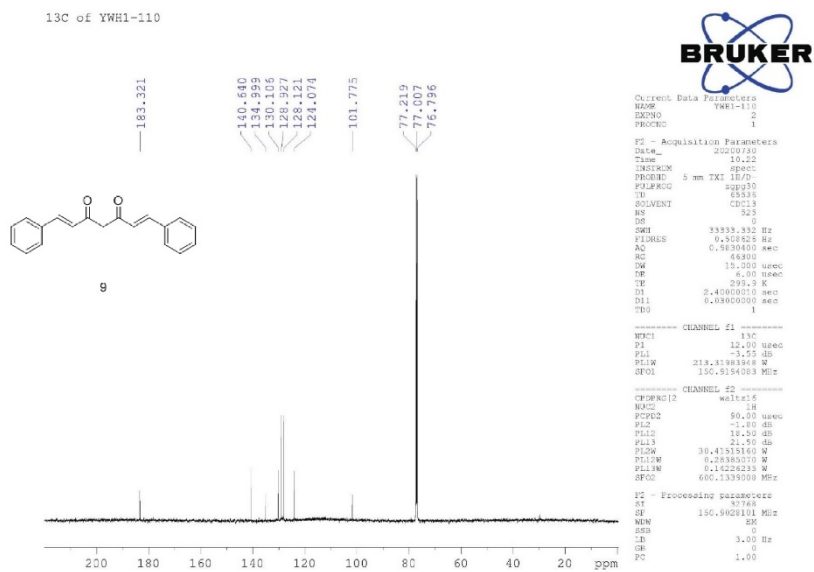


Figure S14. ¹³C NMR (150 MHz, CDCl₃) of compound 9.

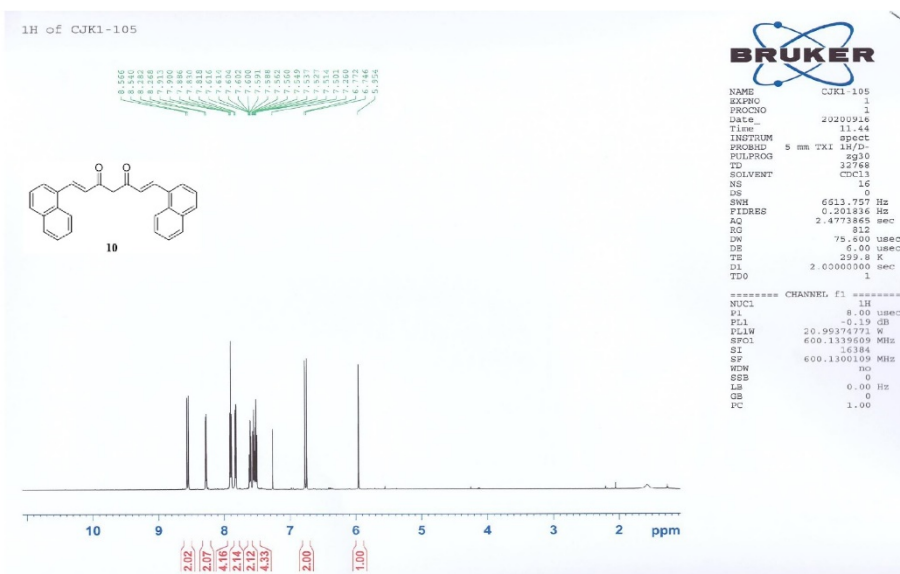


Figure S15. ¹H NMR (600 MHz, CDCl₃) of compound 10.

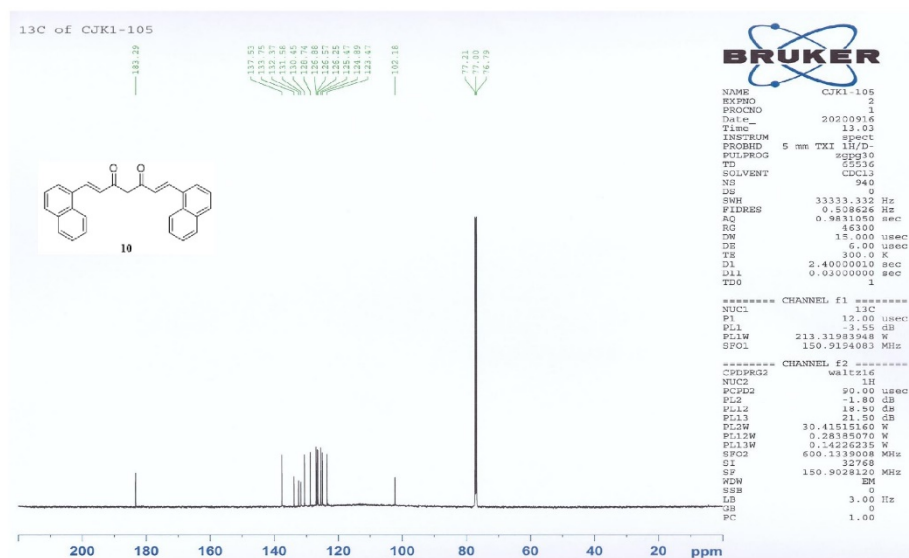


Figure S16. ¹³C NMR (150 MHz, CDCl₃) of compound 10.

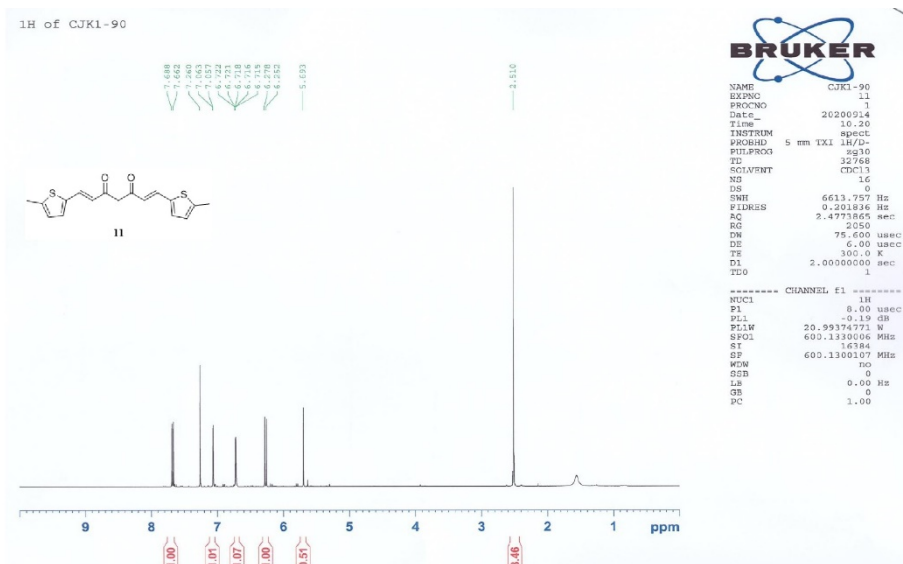


Figure S17. ¹H NMR (600 MHz, CDCl₃) of compound 11.

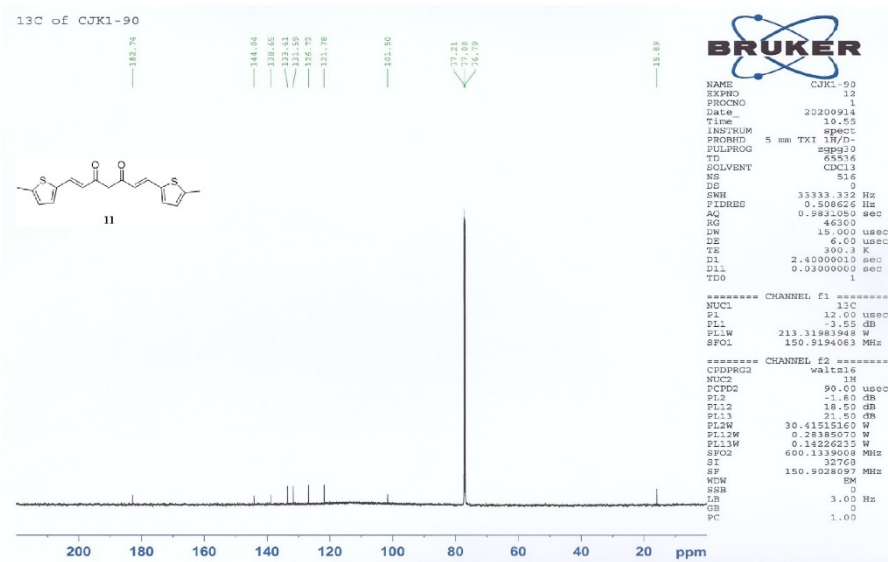


Figure S18. ¹³C NMR (150 MHz, CDCl₃) of compound 11.

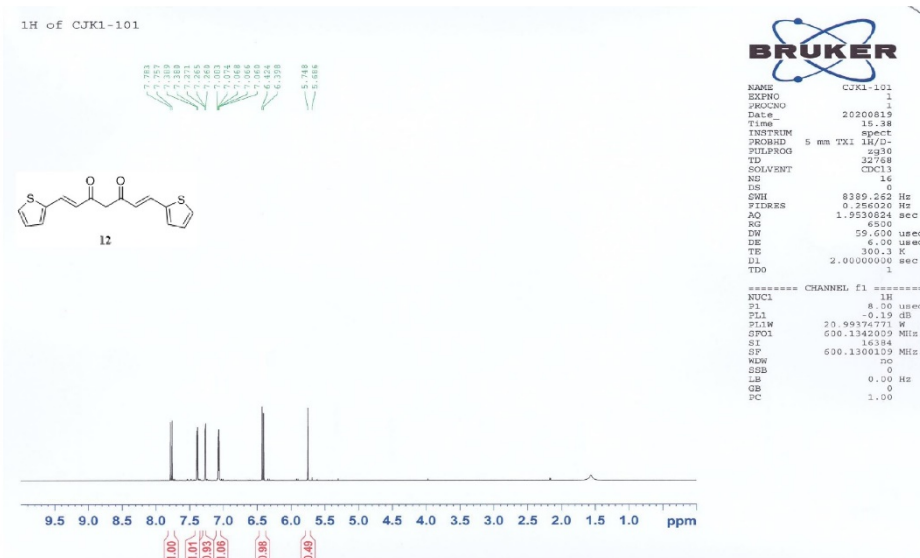


Figure S19. ¹H NMR (600 MHz, CDCl₃) of compound 12.

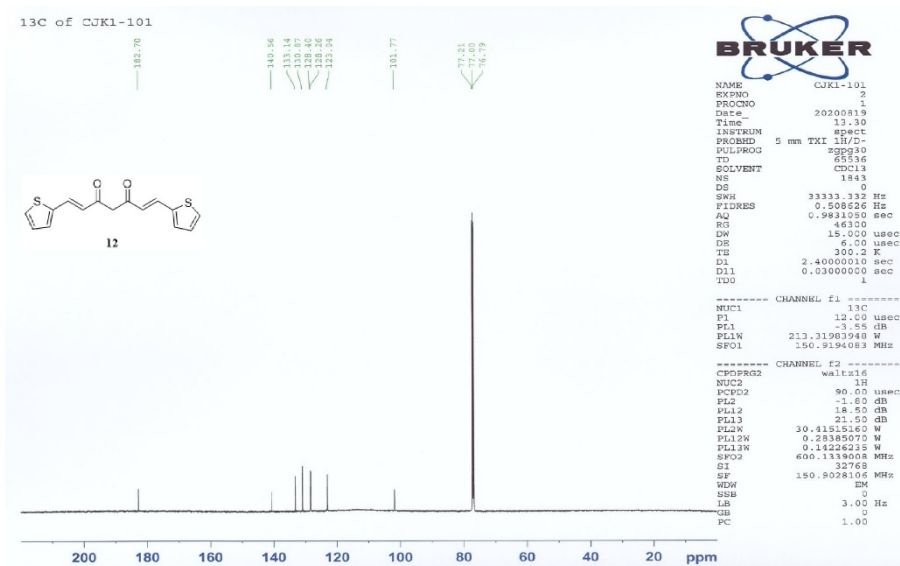


Figure S20. ¹³C NMR (150 MHz, CDCl₃) of compound 12.

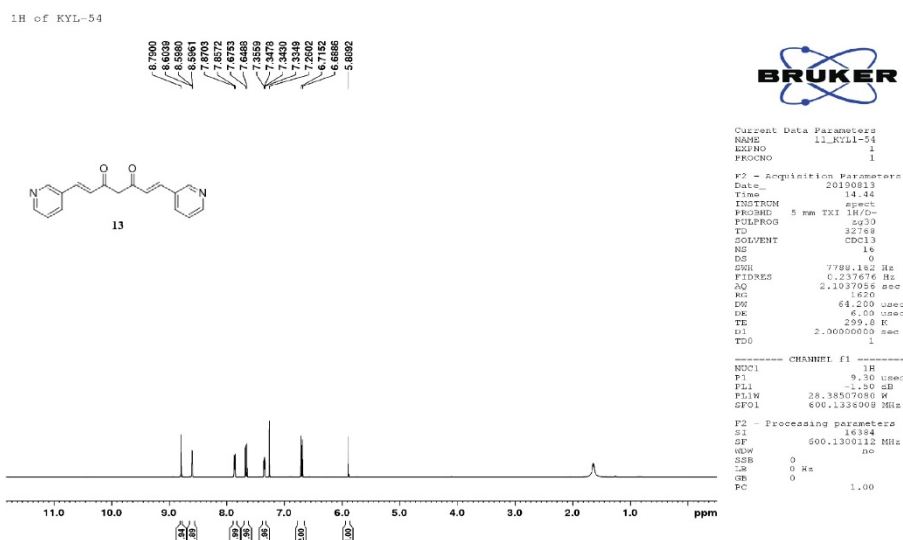


Figure S21. ¹H NMR (600 MHz, CDCl₃) of compound 13.

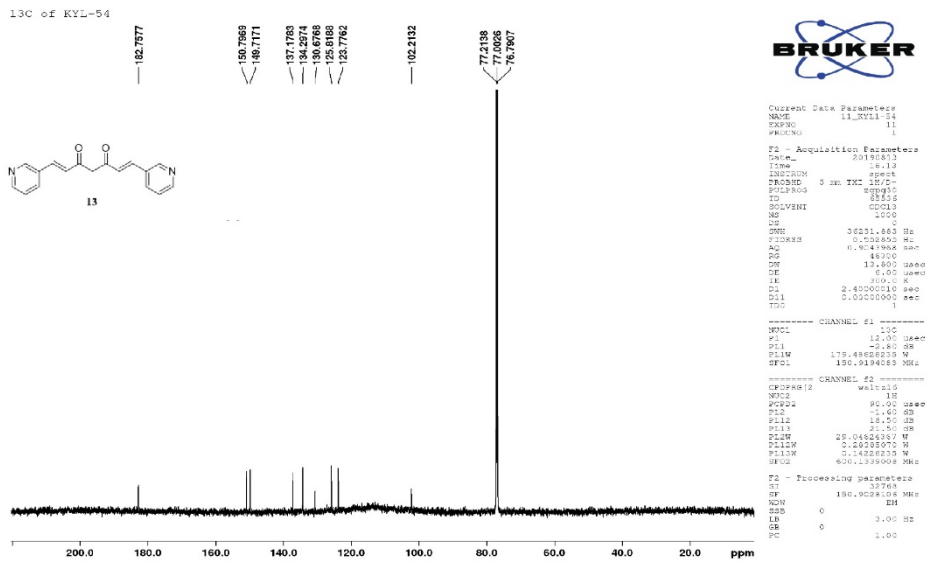


Figure S22. ¹³C NMR (150 MHz, CDCl₃) of compound 13.

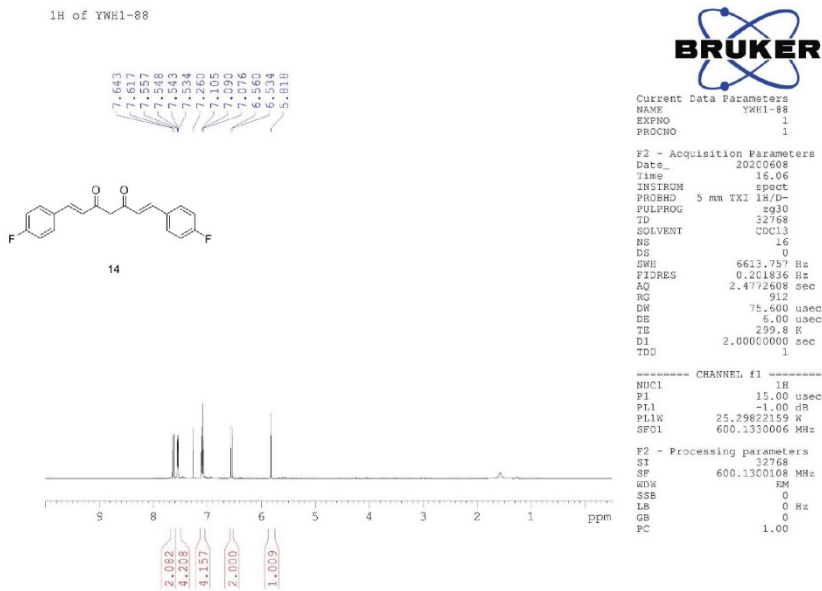
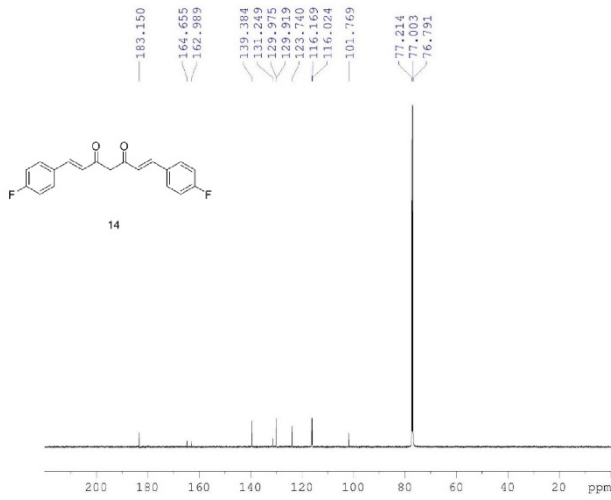


Figure S23. ¹H NMR (150 MHz, CDCl₃) of compound 14.

13C of YWH1-88



Current Data Parameters
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EXPNO 1
PROCNO 1

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Time 14.50
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PROBHD 5 mm 1A5BQ us-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1813
DS 4
SWH 33333.333 Hz
FIDRES 0.328625 Hz
AQ 0.8828123 sec
RG 44300
WM 15.000 usec
DE 4.00 usec
TE 296.2 K
D1 2.4000000 sec
D11 0.0300000 sec
TDD

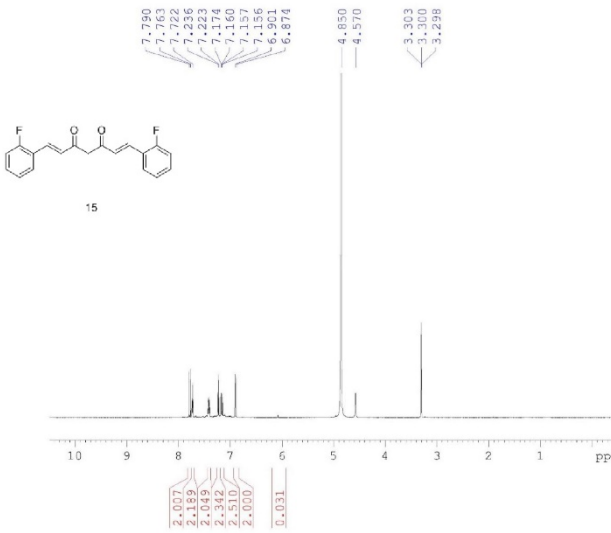
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NUC1 13C
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PL1 2.00 dB
PL1W 45.4846375 W
SFO1 100.628125 MHz

CHANNEL #2
CPDPRG2 waltz16
NUC1 1H
PCPD 90.00 usec
PL2 -1.00 dB
PL12 13.20 dB
PL13 14.20 dB
PL14 14.20 dB
PL15 14.20 dB
PL16 14.20 dB
PL17 14.20 dB
PL18 14.20 dB
PL19 14.20 dB
PL20 14.20 dB
PL21 14.20 dB
PL22 14.20 dB
PL23 14.20 dB
PL24 14.20 dB
PL25 14.20 dB
PL26 14.20 dB
PL27 14.20 dB
PL28 14.20 dB
PL29 14.20 dB
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PL32 14.20 dB
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PL35 14.20 dB
PL36 14.20 dB
PL37 14.20 dB
PL38 14.20 dB
PL39 14.20 dB
PL40 14.20 dB
PL41 14.20 dB
PL42 14.20 dB
PL43 14.20 dB
PL44 14.20 dB
PL45 14.20 dB
PL46 14.20 dB
PL47 14.20 dB
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PL79 14.20 dB
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PL91 14.20 dB
PL92 14.20 dB
PL93 14.20 dB
PL94 14.20 dB
PL95 14.20 dB
PL96 14.20 dB
PL97 14.20 dB
PL98 14.20 dB
PL99 14.20 dB
PL100 14.20 dB

F2 - Processing parameters
SI 32768
SF 600.1330000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S24. ¹³C NMR (150 MHz, CDCl₃) of compound 14.

1H of YWH1-121



Current Data Parameters
NAME YWH1-121
EXPNO 1
PROCNO 1

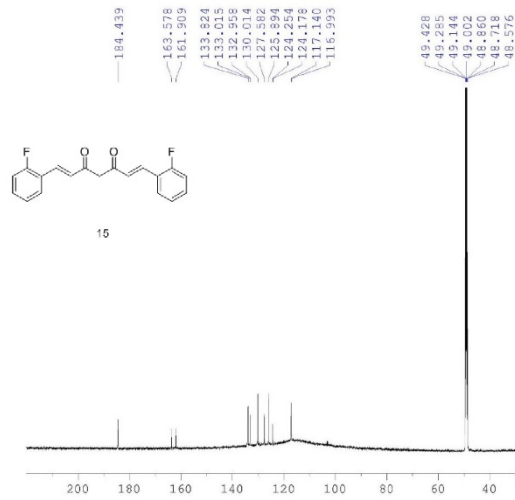
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Time 10.51
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PULPROG zg30
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4772608 sec
RG 724
WM 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1

CHANNEL #1
NUC1 1H
P1 8.00 usec
PL1 -0.19 dB
PL1W 20.9937472 W
SFO1 600.1330006 MHz

F2 - Processing parameters
SI 32768
SF 600.1330136 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S25. ¹H NMR (600 MHz, CD₃OD) of compound 15.

¹³C of YWH1-121

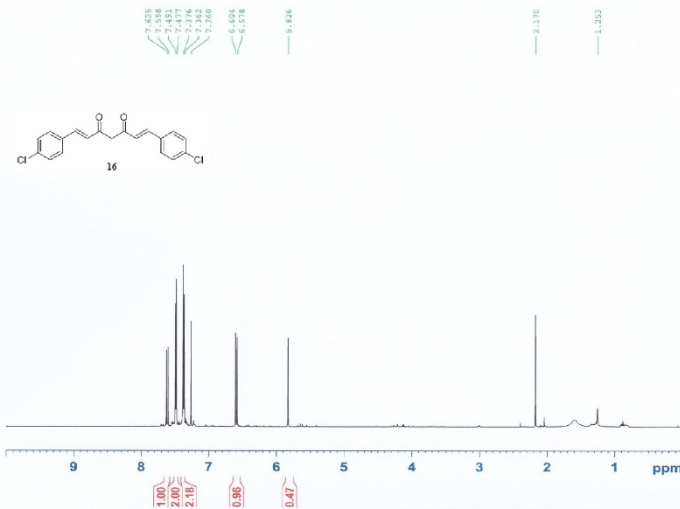


Current Data Parameters
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Date 20200927
Time 14.17
INSTRUM spect
PROBHD 5 mm TXI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 36231.803 Hz
FIDRES 0.251858 Hz
AQ 0.9043968 sec
RG 3200
DW 13.800 usec
DE 6.00 usec
TE 300.2 K
D1 2.4000010 sec
D11 0.0500000 sec
TDO 1

===== CHANNEL f1 =====
NUCL 13C
P1 12.00 usec
PL1 -4.55 dB
PL12 18.40 dB
PL13 21.50 dB
PLW 30.4215160 W
PL13W 0.34226235 W
SFO1 100.6281500 MHz
SFO2 600.1339000 MHz
SI 32768
SF 150.9028114 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S26. ¹³C NMR (150 MHz, CD₃OD) of compound 15.

¹H of CJK1-102

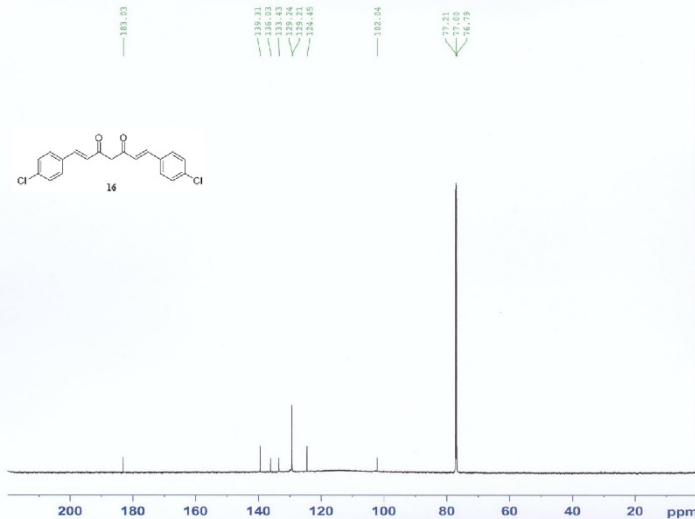


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PROCNO 1
Date 20200902
Time 14.16
INSTRUM spect
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PULPROG zgpg30
TD 33744
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.362 Hz
FIDRES 0.256020 Hz
AQ 1.9530824 sec
RG 4100
DW 59.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUCL 1H
P1 8.00 usec
PL1 0.19 dB
SFO1 200.9937771 MHz
SFO2 600.1342009 MHz
SI 16384
SF 600.1301005 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Figure S27. ¹H NMR (600 MHz, CDCl₃) of compound 16.

¹³C of CJK1-102



NAME CJK1-102
EXPNO 12
PROCNO 1
Date 20200902
Time 16.13
INSTRUM spect
PROBHD 5 mm TXI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1362
DS 0
SWH 33331.332 Hz
FIDRES 0.504626 Hz
AQ 0.9831050 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.4000010 sec
D11 0.0500000 sec
TDO 1

===== CHANNEL f1 =====
NUCL 13C
P1 12.00 usec
PL1 -4.55 dB
PL12 18.40 dB
PL13 21.50 dB
PLW 30.4215160 W
PL13W 0.26185070 W
SFO1 100.6281500 MHz
SFO2 600.1339000 MHz
SI 32768
SF 150.9028114 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S28. ¹³C NMR (150 MHz, CDCl₃) of compound 16.

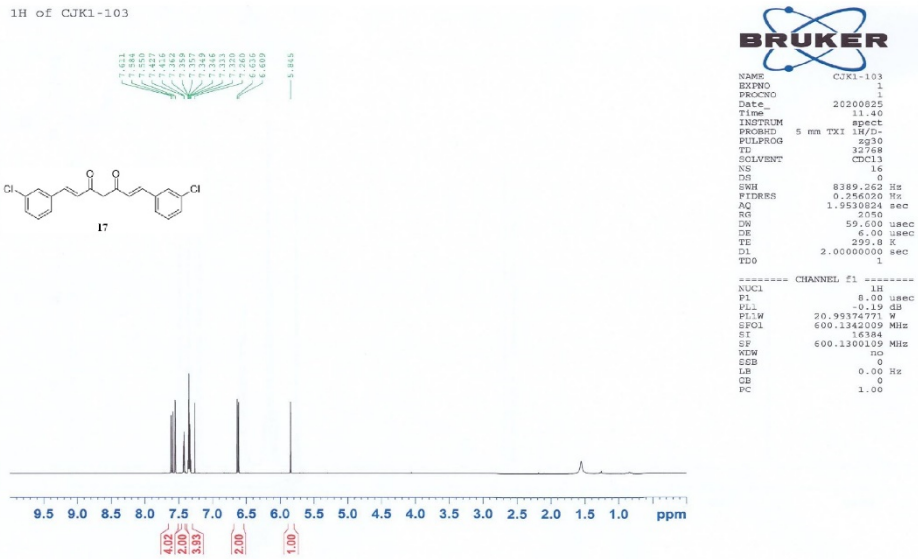


Figure S29. ¹H NMR (600 MHz, CDCl₃) of compound 17.

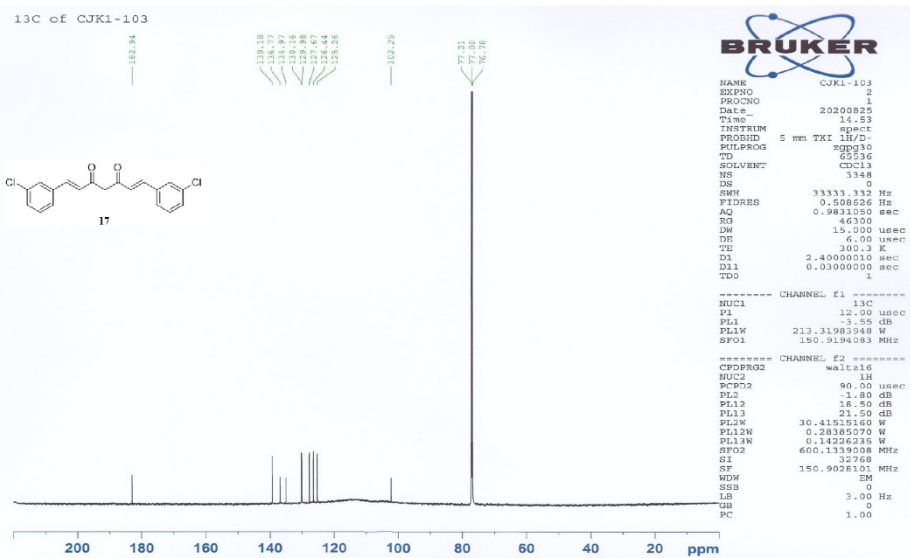


Figure S30. ¹³C NMR (150 MHz, CDCl₃) of compound 17.

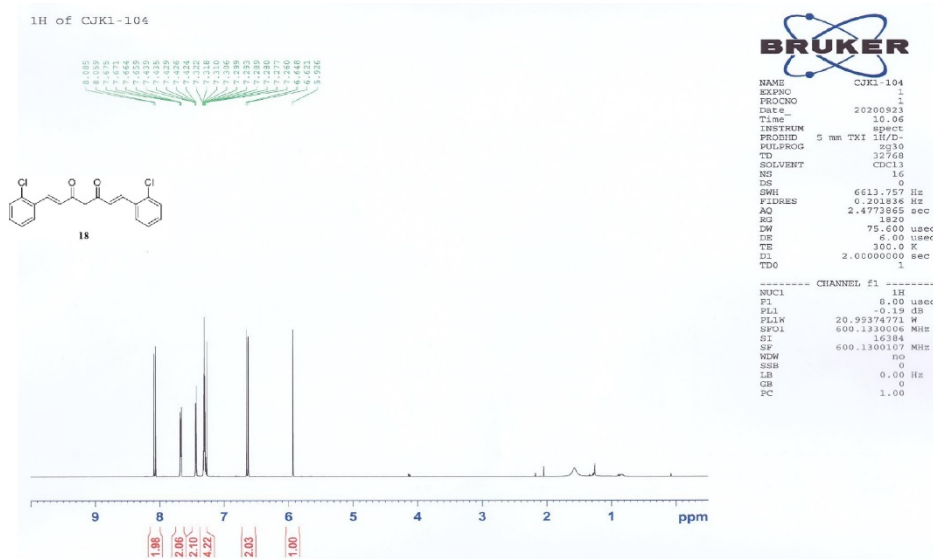


Figure S31. ¹H NMR (600 MHz, CDCl₃) of compound 18.

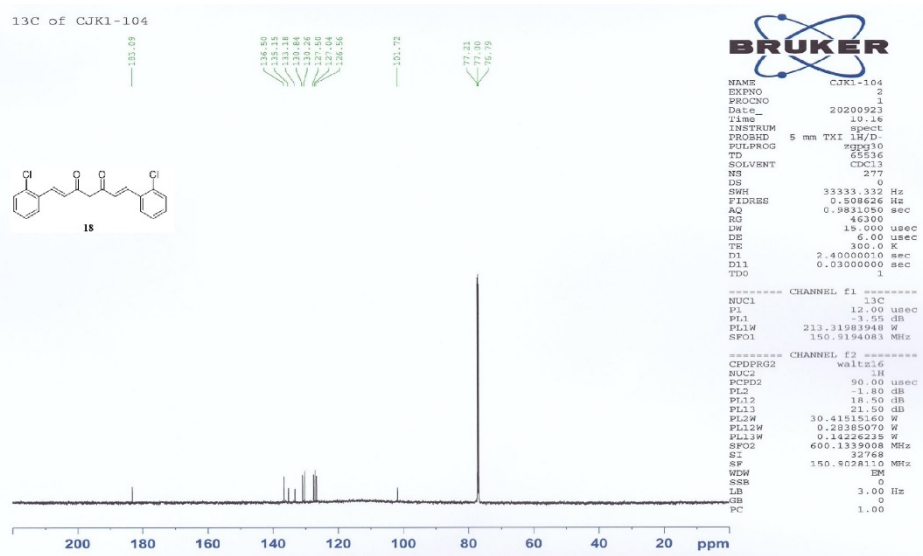


Figure S32. ¹³C NMR (150 MHz, CDCl₃) of compound 18.

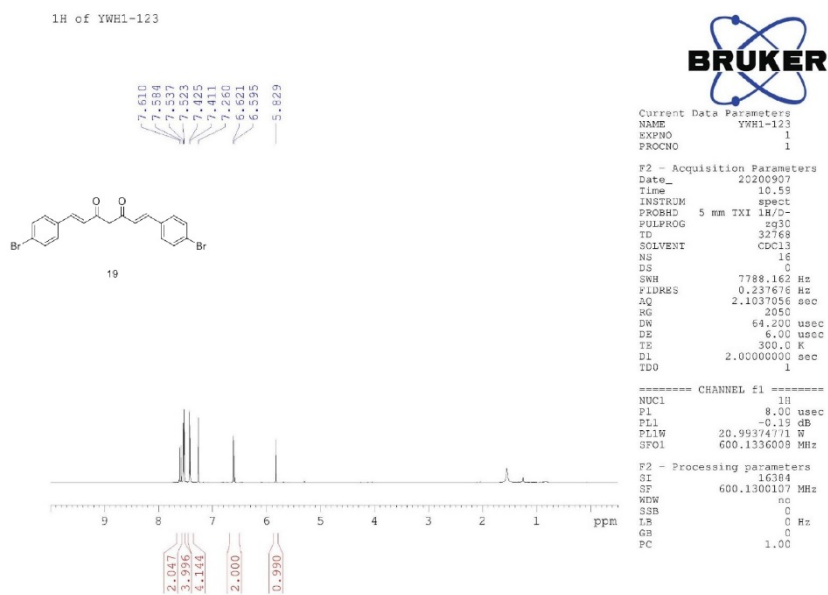


Figure S33. ¹H NMR (600 MHz, CDCl₃) of compound 19.

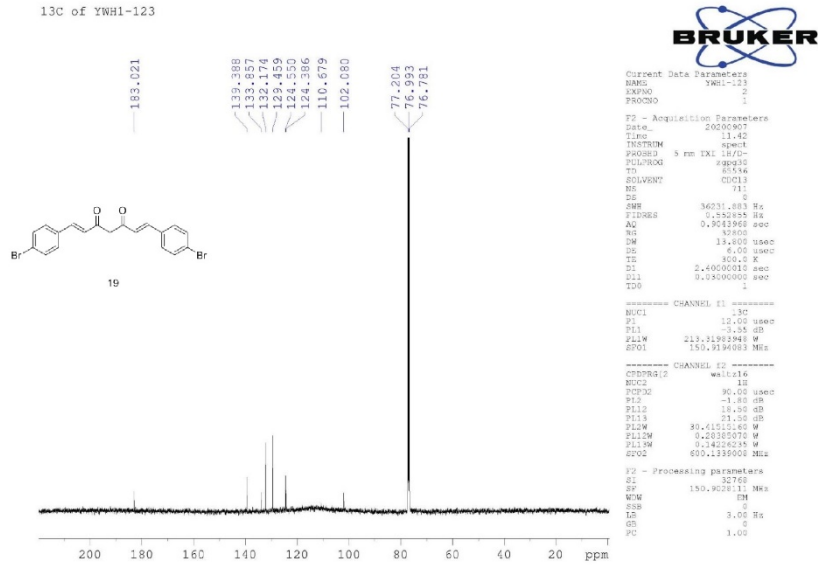


Figure S34. ¹³C NMR (150 MHz, CDCl₃) of compound 19.

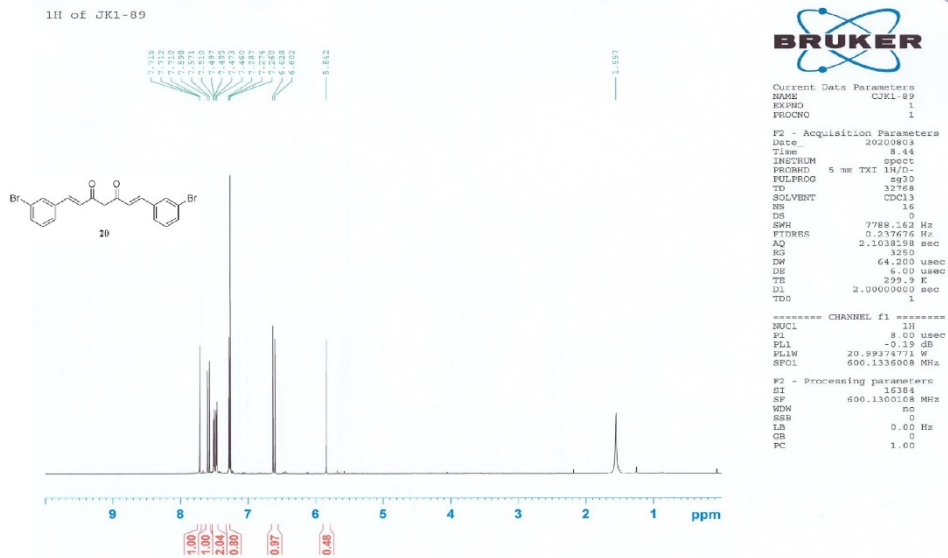


Figure S35. ¹H NMR (600 MHz, CDCl₃) of compound 20.

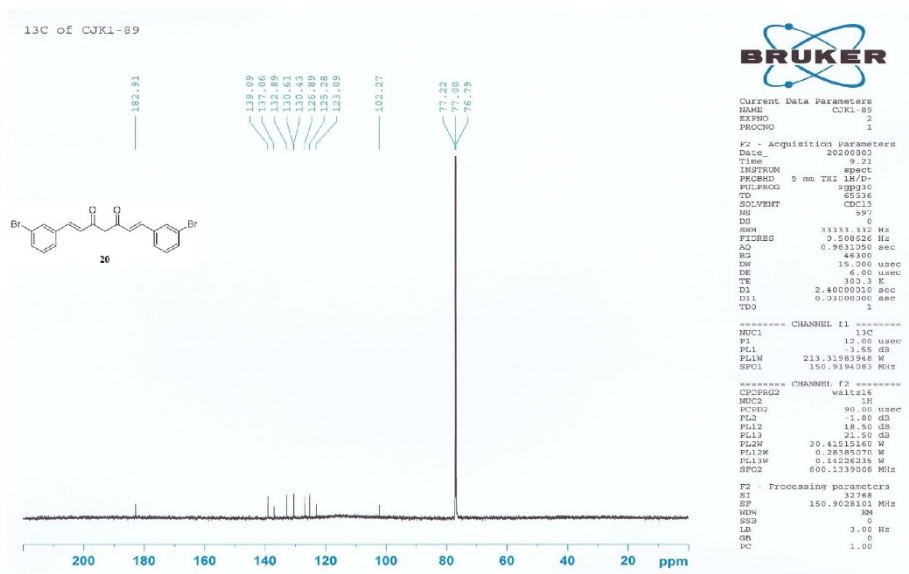


Figure S36. ¹³C NMR (150 MHz, CDCl₃) of compound 20.

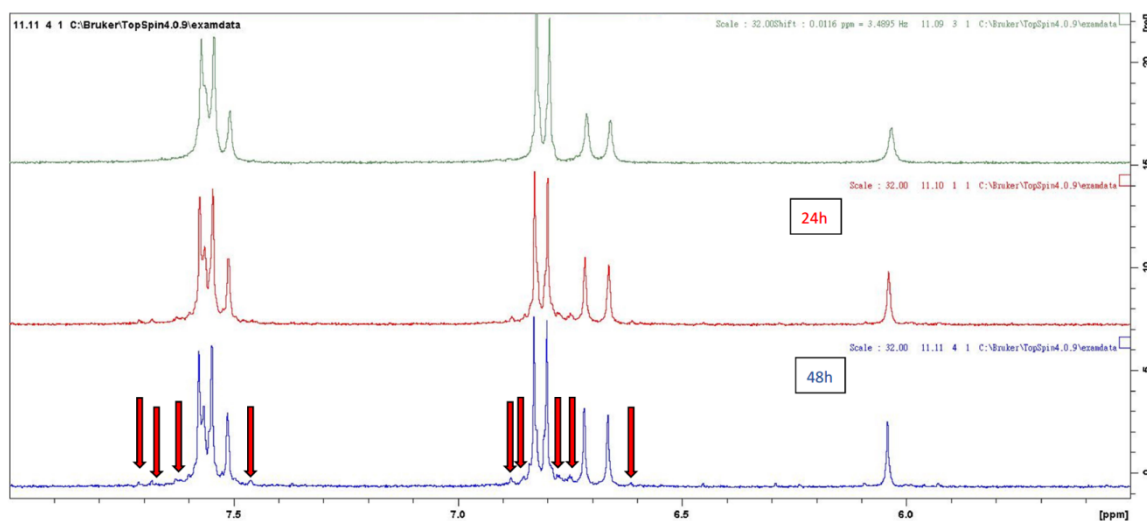


Figure S37. The NMR spectra of degraded compound 4 after storage at room temperature in the dark for 48 h. Arrows indicate the newly formed peaks.