

Synthesis of Alkyne-Substituted Dihydropyrrolones as Bacterial Quorum Sensing Inhibitors of *Pseudomonas aeruginosa*

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Crystal Structure Details

Table S1. Experimental details for compound 18

Crystal data	
Chemical formula	C ₂₅ H ₂₁ NO
<i>M_r</i>	351.43
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.8068 (7), 20.8376 (15), 10.6832 (6)
β (°)	104.884 (2)
<i>V</i> (Å ³)	1894.7 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.07
Crystal size (mm)	0.05 × 0 × 0
Data collection	
Diffractometer	Bruker D8 Quest
Absorption correction	Multi-scan <i>SADABS2016/2</i> (Bruker, 2016/2) was used for absorption correction. <i>wR2(int)</i> was 0.1421 before and 0.0847 after correction. The Ratio of minimum to maximum transmission is 0.7998. The λ/2 correction factor is Not present.
<i>T_{min}</i> , <i>T_{max}</i>	0.596, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	52956, 3532, 2377
<i>R_{int}</i>	0.119
(sin θ/λ) _{max} (Å ⁻¹)	0.606
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.049, 0.146, 1.12
No. of reflections	3532
No. of parameters	245
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.19, -0.19

Computer programs: *SAINT* V8.38A (Bruker, 2018), *SHELXT* 2014/5 (Sheldrick, 2014), *SHELXL* 2018/3 (Sheldrick, 2015), *Olex2* 1.5 (Dolomanov *et al.*, 2009).

Table S2. X-ray Experimental details for compound 26

Chemical formula	C ₁₉ H ₁₂ BrNO
<i>M_r</i>	350.21
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	105
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.944 (4), 9.578 (3), 13.798 (4)
β (°)	105.385 (6)
<i>V</i> (Å ³)	1521.9 (8)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	2.70
Crystal size (mm)	0.27 × 0.09 × 0.03
Data collection	
Diffractometer	Bruker D8Quest
Absorption correction	Multi-scan <i>SADABS2016/2</i> (Bruker, 2016/2) was used for absorption correction. <i>wR2(int)</i> was 0.1015 before and 0.0523 after correction. The Ratio of minimum to maximum transmission is 0.8415. The λ/2 correction factor is Not present.
<i>T</i> _{min} , <i>T</i> _{max}	0.627, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	47699, 3512, 2917
<i>R</i> _{int}	0.045
(sin θ/λ) _{max} (Å ⁻¹)	0.651
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.026, 0.068, 1.05
No. of reflections	3512
No. of parameters	199
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.34, -0.51

Computer programs: *SAINT* V8.38A, *SHELXT* 2014/5, *SHELXL*, *Olex2*

Table S3. Selected geometric parameters (Å, °)

Br01—C8	1.9009 (19)	C7—C8	1.381 (3)
C1—C2	1.345 (3)	C8—C9	1.381 (3)
C1—C4	1.470 (3)	C9—C10	1.384 (3)
C1—C5	1.476 (2)	C11—C12	1.420 (3)
N1—C3	1.370 (2)	C12—C13	1.199 (3)
N1—C4	1.390 (2)	C13—C14	1.436 (3)
O1—C3	1.234 (2)	C14—C15	1.396 (3)
C2—C3	1.470 (3)	C14—C19	1.397 (3)
C4—C11	1.346 (3)	C15—C16	1.384 (3)
C5—C6	1.397 (3)	C16—C17	1.383 (3)
C5—C10	1.394 (3)	C17—C18	1.379 (3)
C6—C7	1.389 (3)	C18—C19	1.390 (3)
C2—C1—C4	107.83 (16)	C7—C8—Br01	120.05 (14)
C2—C1—C5	127.53 (17)	C9—C8—Br01	118.16 (14)
C4—C1—C5	124.41 (16)	C9—C8—C7	121.76 (17)
C3—N1—C4	110.91 (15)	C8—C9—C10	118.86 (18)
C1—C2—C3	108.96 (17)	C9—C10—C5	120.77 (18)
N1—C3—C2	106.07 (16)	C4—C11—C12	122.31 (17)
O1—C3—N1	125.35 (17)	C13—C12—C11	176.4 (2)
O1—C3—C2	128.59 (18)	C12—C13—C14	179.2 (2)
N1—C4—C1	106.13 (16)	C15—C14—C13	119.68 (18)
C11—C4—C1	128.18 (17)	C15—C14—C19	119.65 (18)
C11—C4—N1	125.31 (16)	C19—C14—C13	120.66 (18)
C6—C5—C1	122.30 (17)	C16—C15—C14	119.87 (19)
C10—C5—C1	118.44 (17)	C17—C16—C15	120.29 (19)
C10—C5—C6	119.26 (17)	C18—C17—C16	120.20 (19)
C7—C6—C5	120.20 (17)	C17—C18—C19	120.3 (2)
C8—C7—C6	119.14 (18)	C18—C19—C14	119.64 (19)

Table S4. Selected hydrogen-bond parameters

$D-H\cdots A$	$D-H$ (Å)	$H\cdots A$ (Å)	$D\cdots A$ (Å)	$D-H\cdots A$ (°)
$N1-H1\cdots O1^i$	0.88	2.01	2.855 (2)	161.0
$C15-H15\cdots O1^i$	0.95	2.67	3.341 (3)	127.9

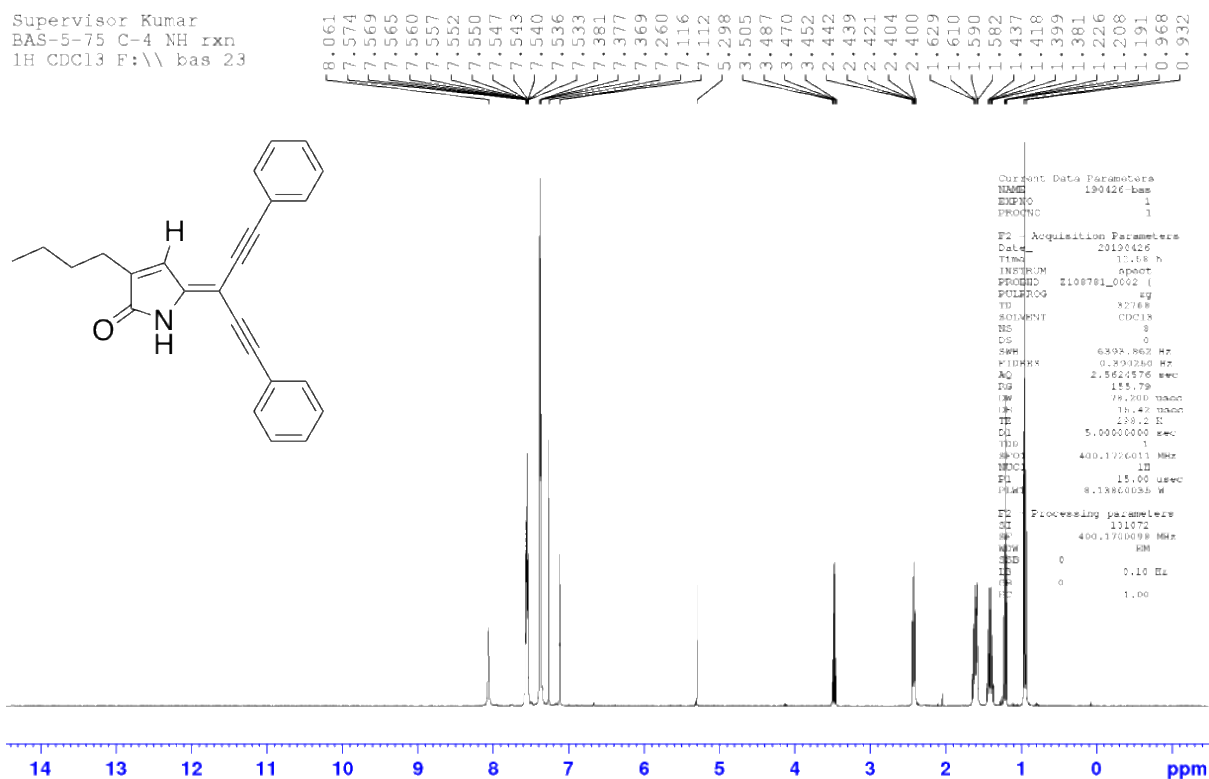
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Supplementary File S1

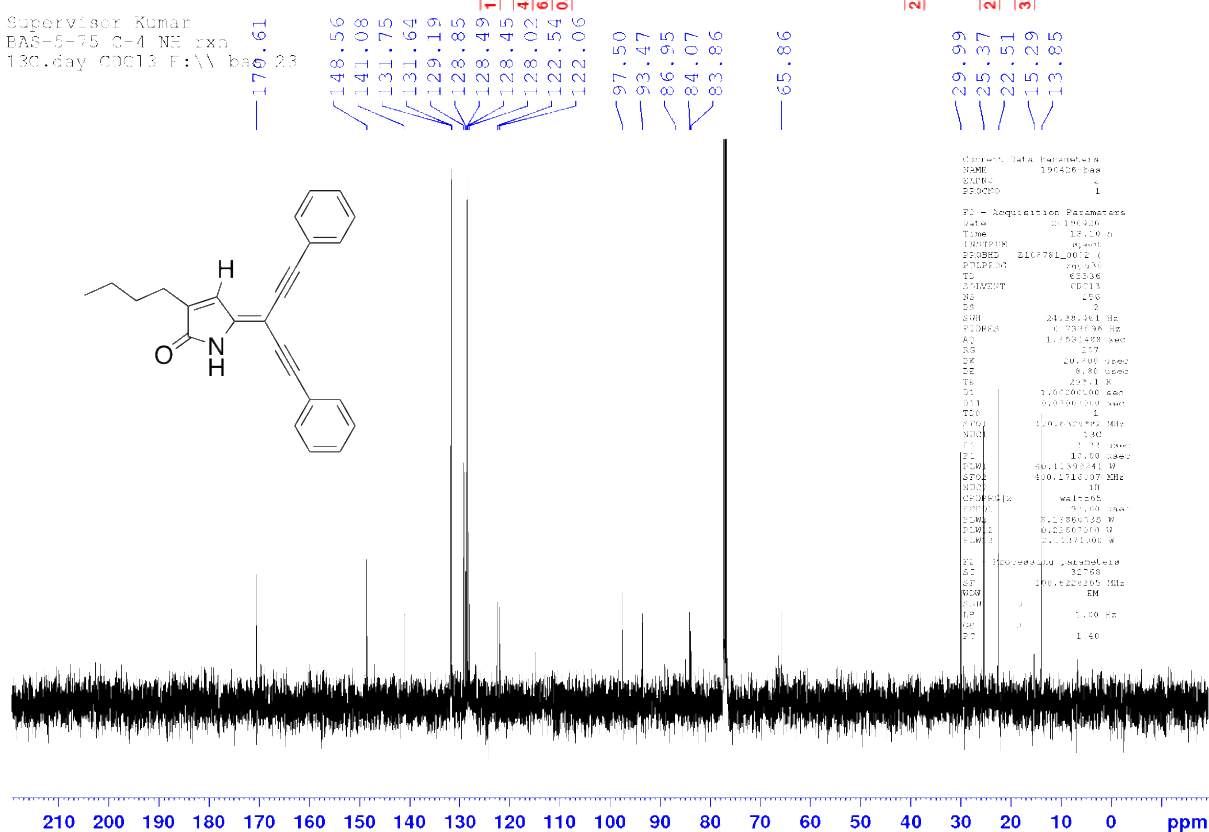
NMR Spectral Data

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Supervisor Kumar
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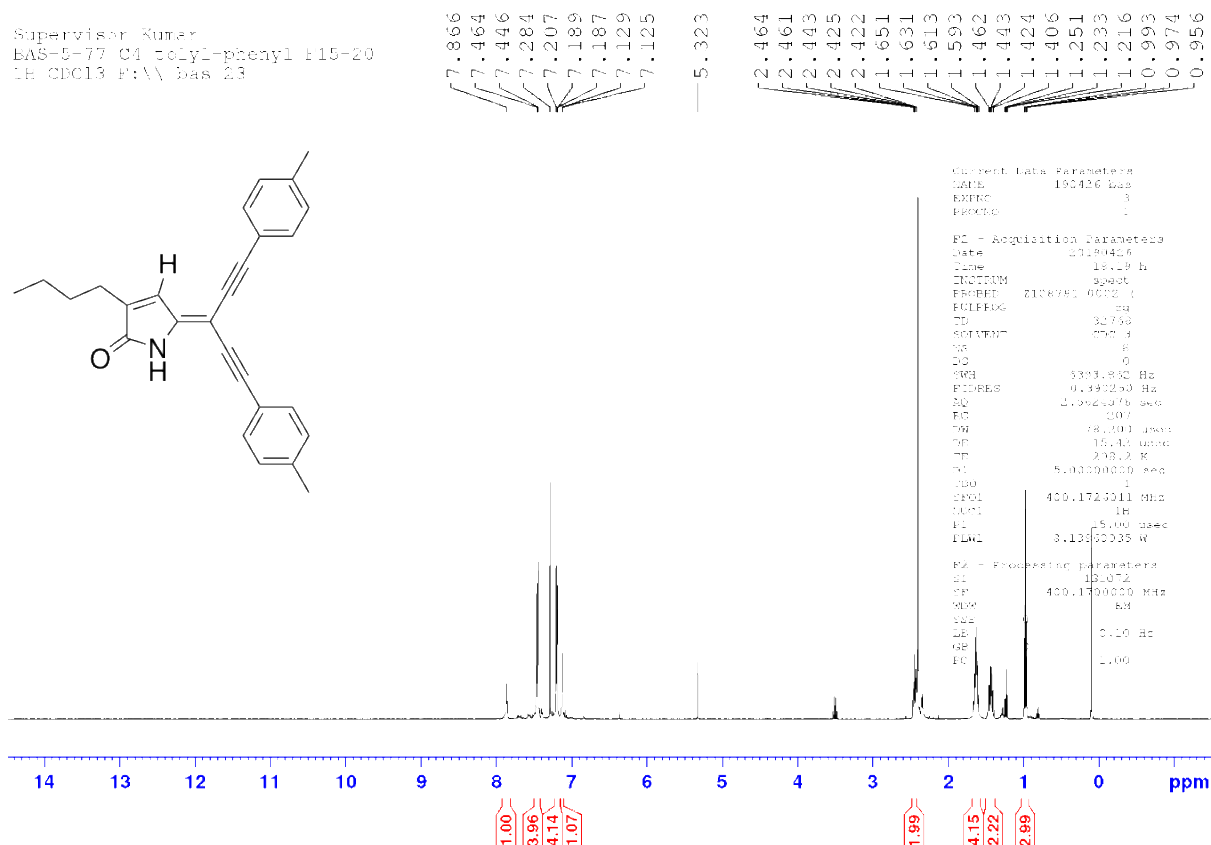


Supervisor Kumar
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13C day CDCl3 F:\bas 23

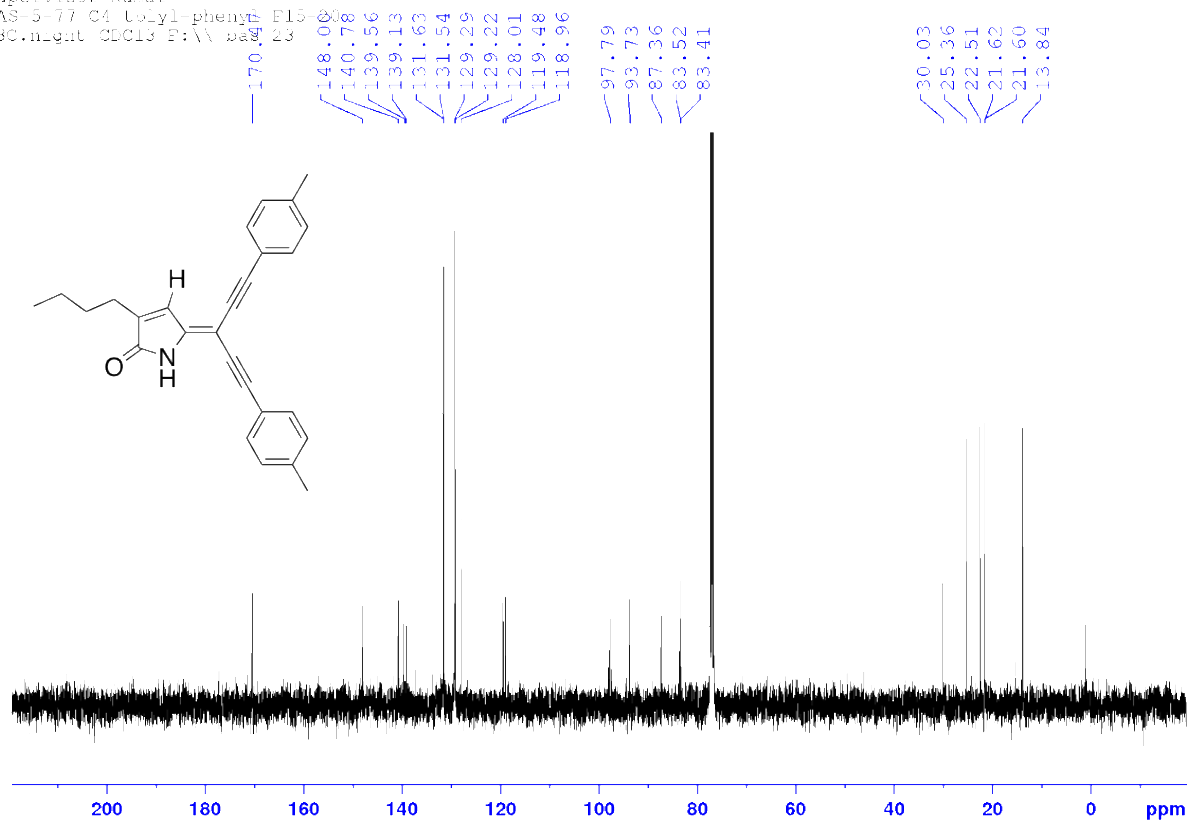


3-butyl-5-(1,5-di-p-tolylpenta-1,4-diy-3-ylidene)-1,5-dihydro-2H-pyrrol-2-one (19)

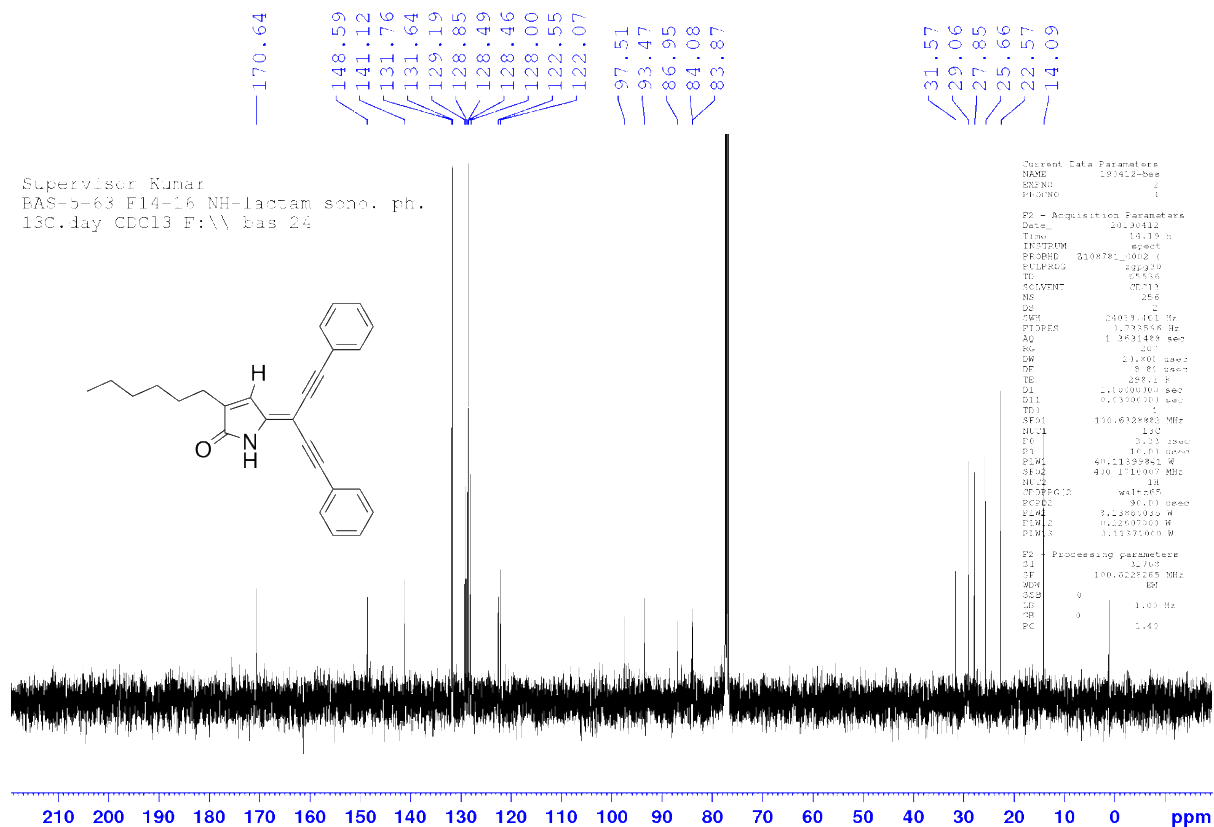
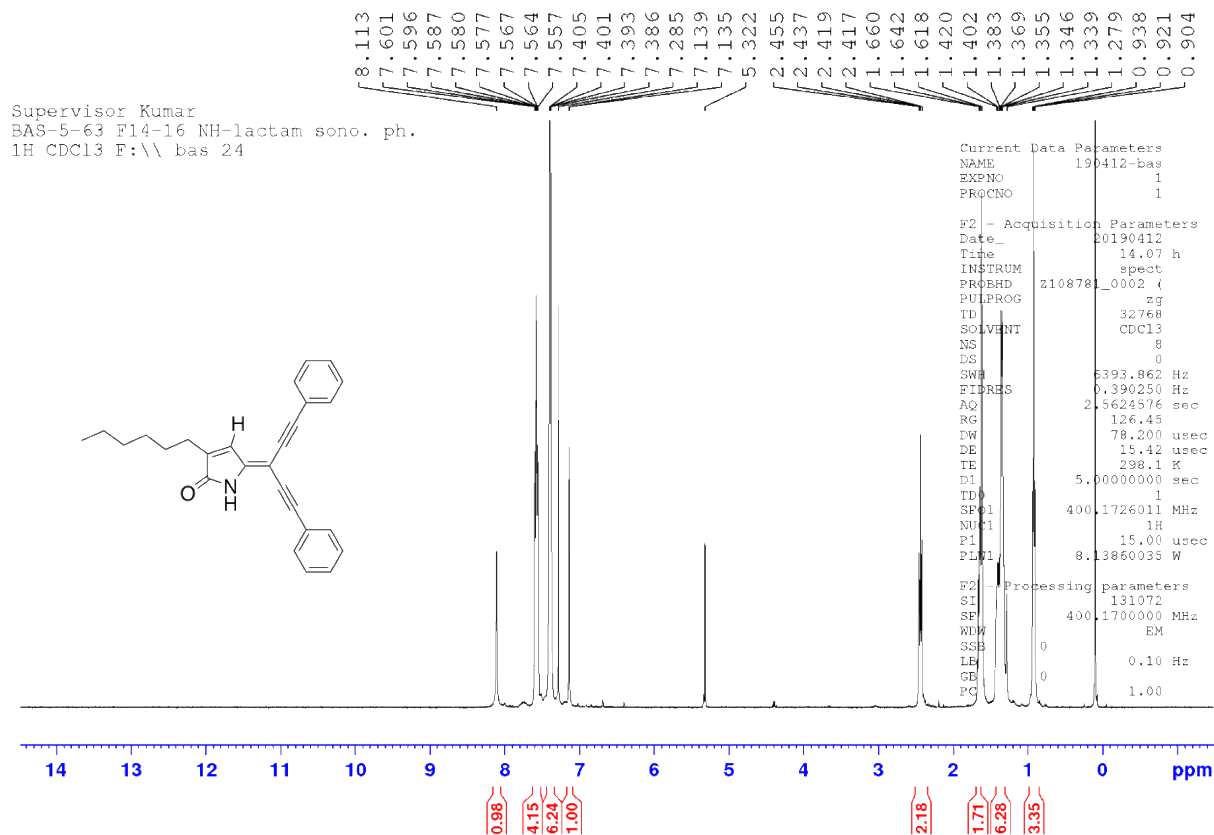
Supervisor: Kumar
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1H CDCl3 F:\N bas 23



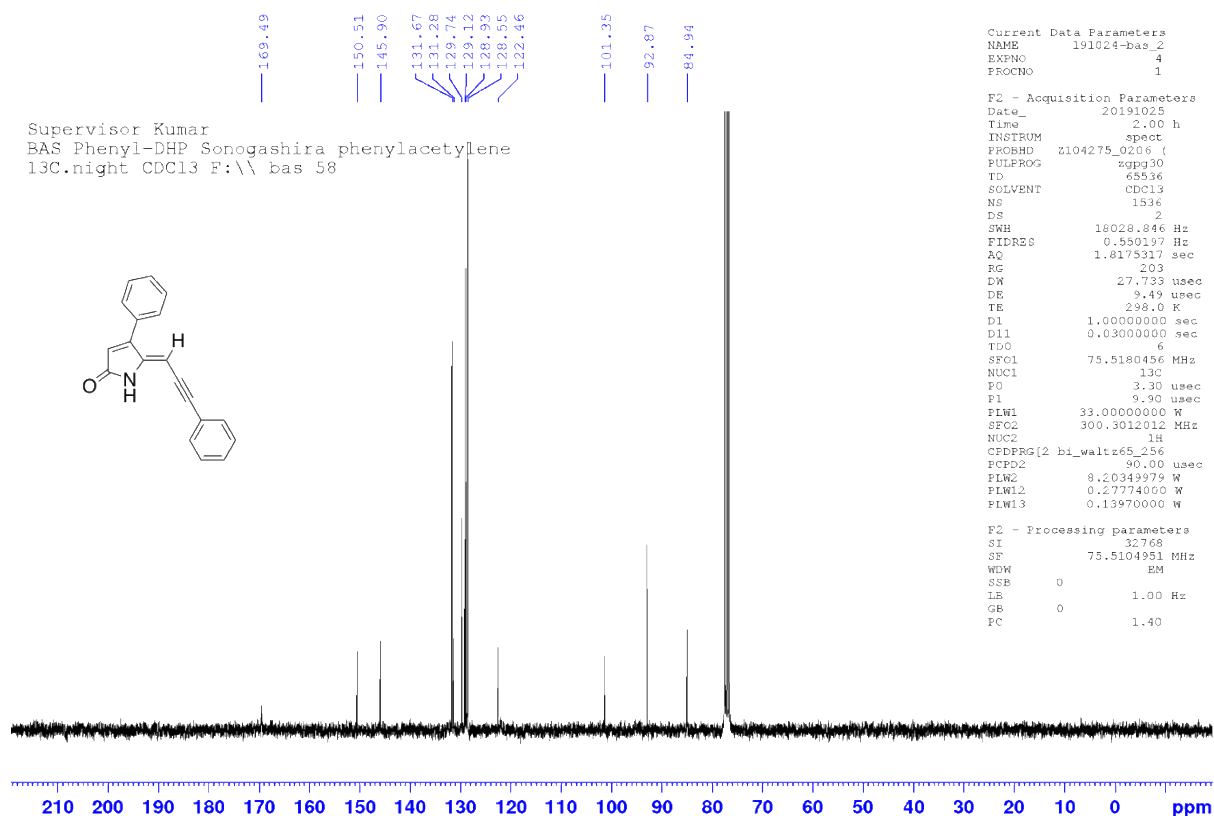
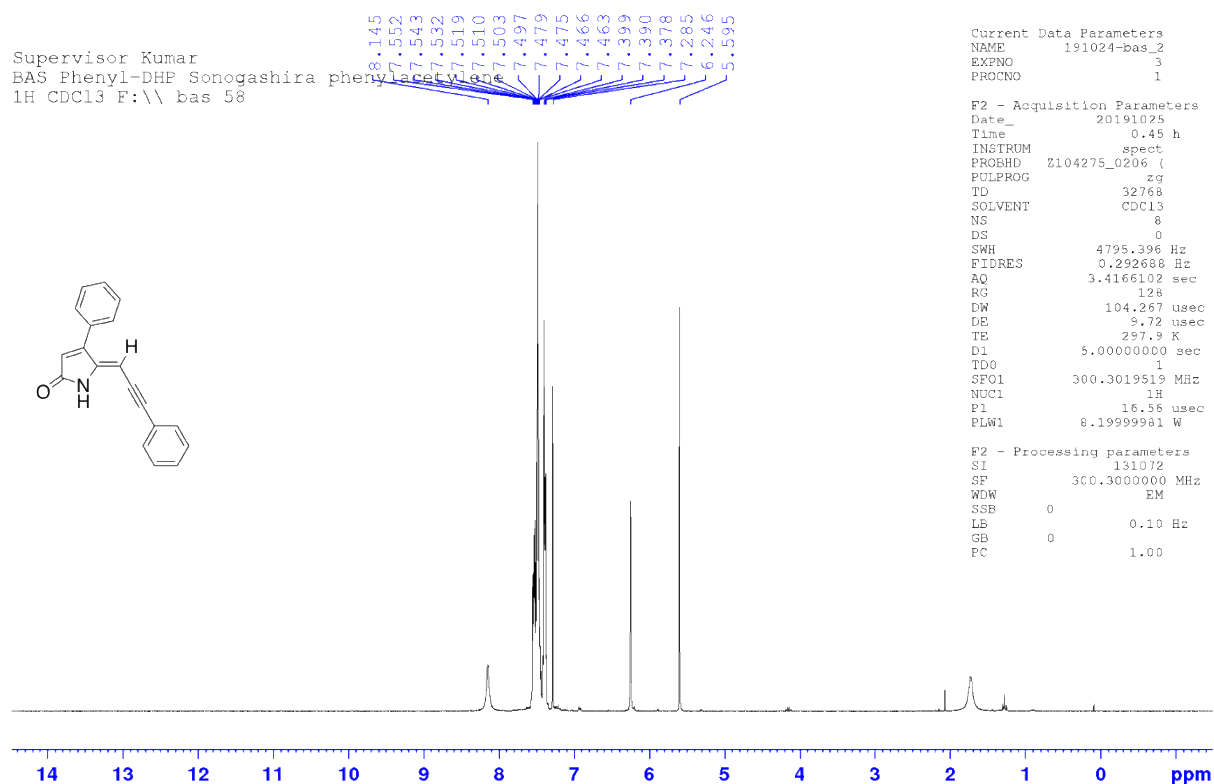
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BAS-5-77 C4 tolyl-phenyl F15-20
13C NMR CDCl3 F:\N bas 23



5-(1,5-Diphenylpenta-1,4-diyn-3-ylidene)-3-hexyl-1,5-dihydro-2H-pyrrol-2-one (20)

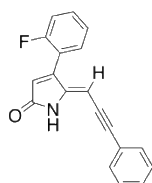


(Z)-4-Phenyl-5-(3-phenylprop-2-yn-1-ylidene)-1,5-dihydro-2H-pyrrol-2-one (24)



(Z)-4-(2-Fluorophenyl)-5-(3-phenylprop-2-yn-1-ylidene)-1,5-dihydro-2H-pyrrol-2-one
(25)

Supervisor Kumar
BAS 2F-DHP Sonogashira
1H CDC13 F:\ bas 57



8.017
7.512
7.500
7.390
7.383
7.377
7.293
7.285
7.268
7.264
7.243
7.239
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7.225
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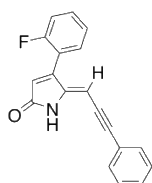
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143.79
141.63
131.49
131.38
130.85
130.82
129.16
128.57
124.38
124.32
122.40
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116.31
101.51
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84.81

Supervisor Kumar
BAS 2F-DHP Sonogashira
13C.night CDC13 F:\ bas 57



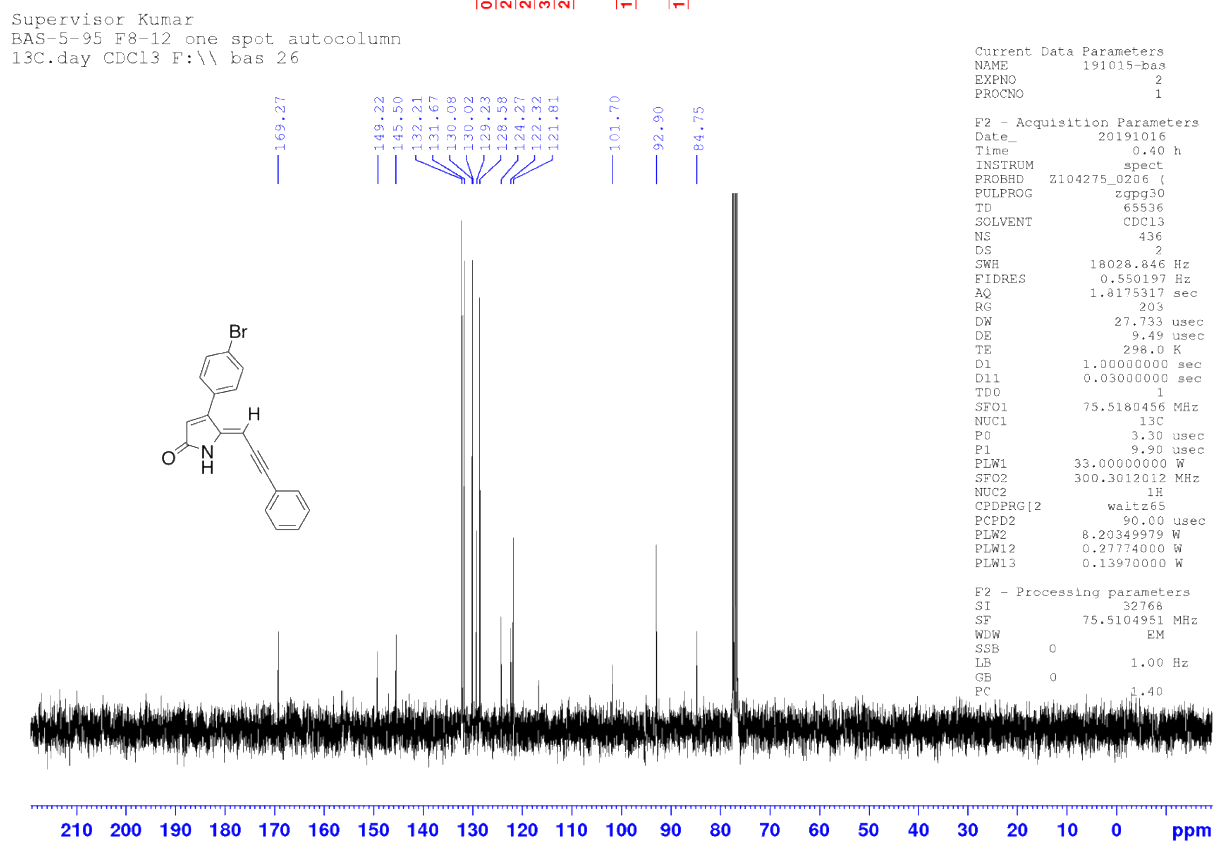
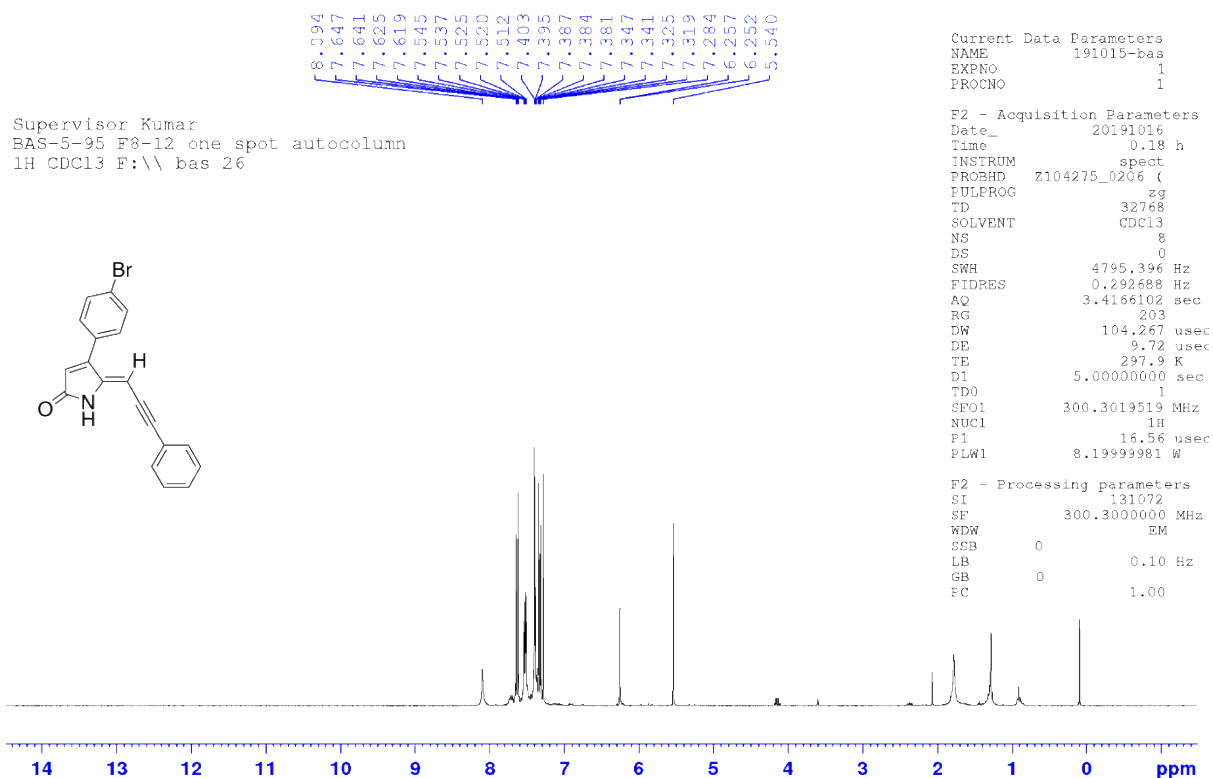
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P1 9.90 usec
PLW1 33.00000000 W
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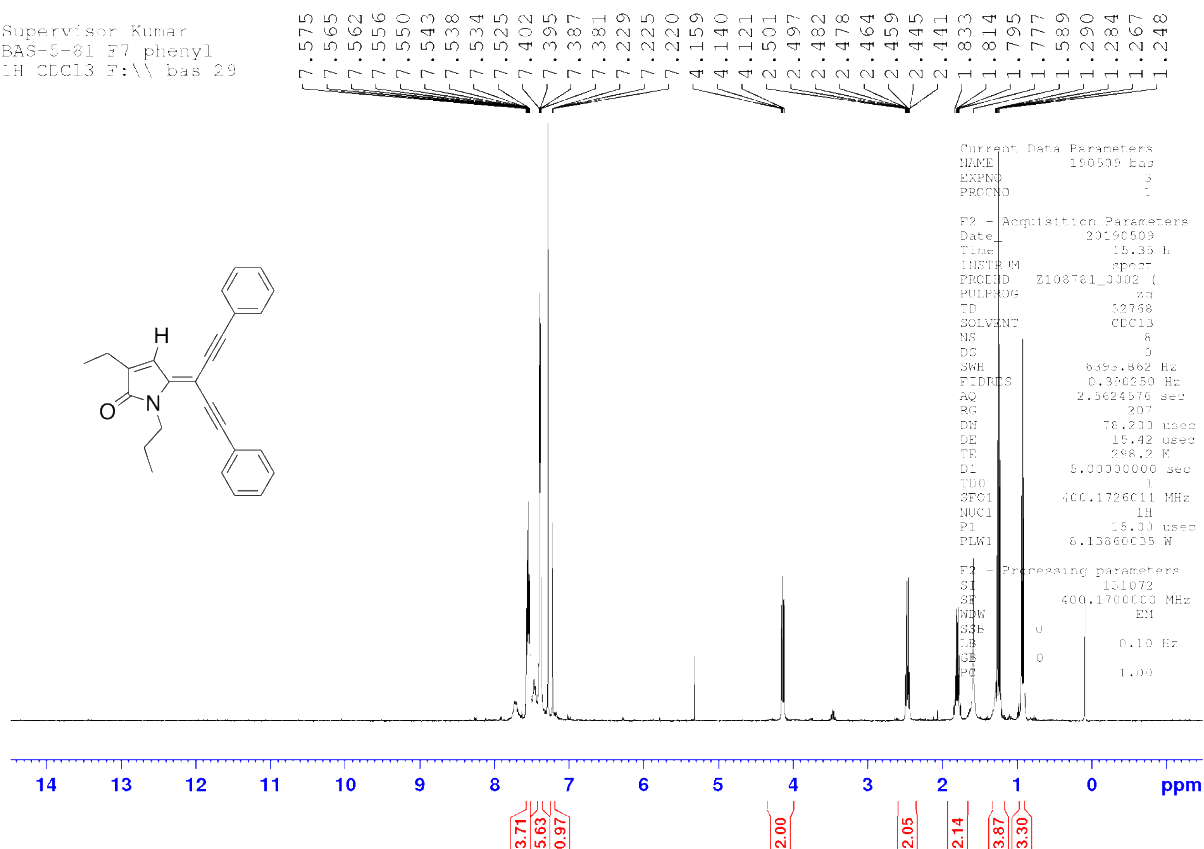
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(26)

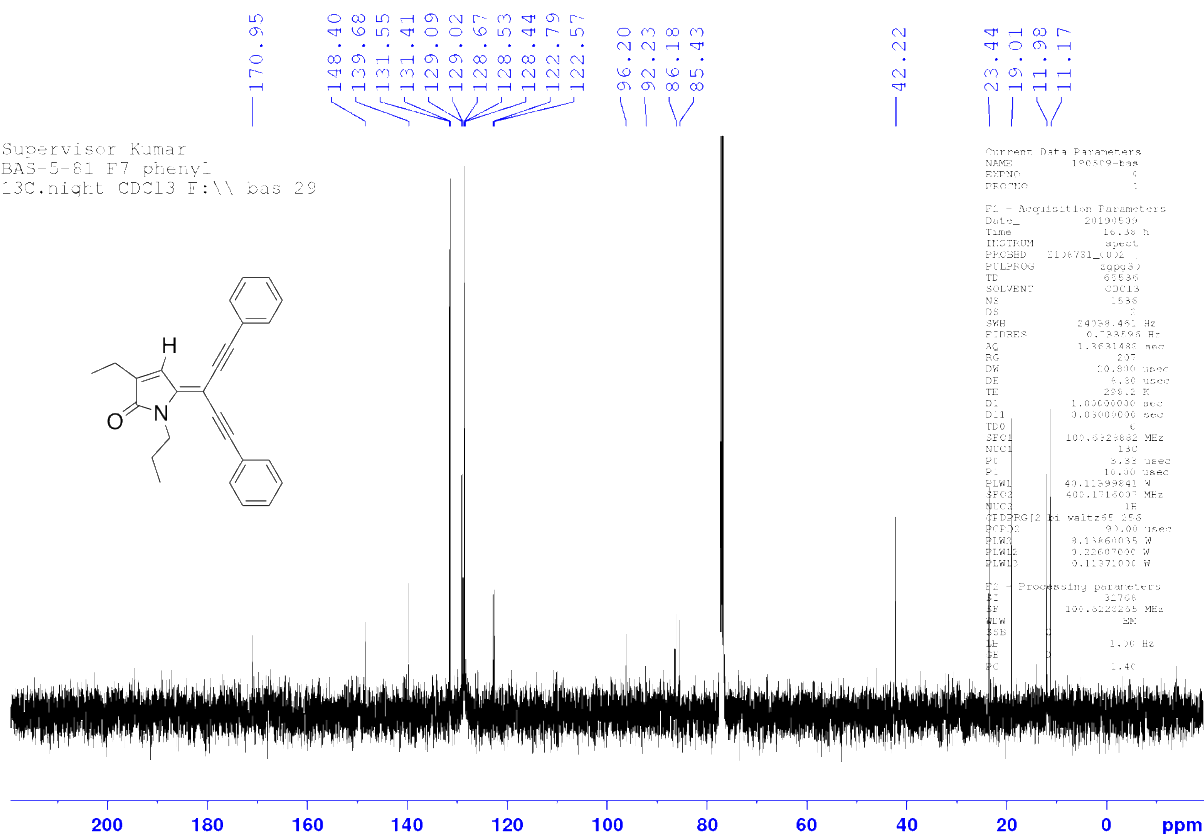


5-(1,5-Diphenylpenta-1,4-diyn-3-ylidene)-3-ethyl-1-propyl-1,5-dihydro-2H-pyrrol-2-one (36)

Supervisor Kumar
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1H CDCl3 F:\bas 29

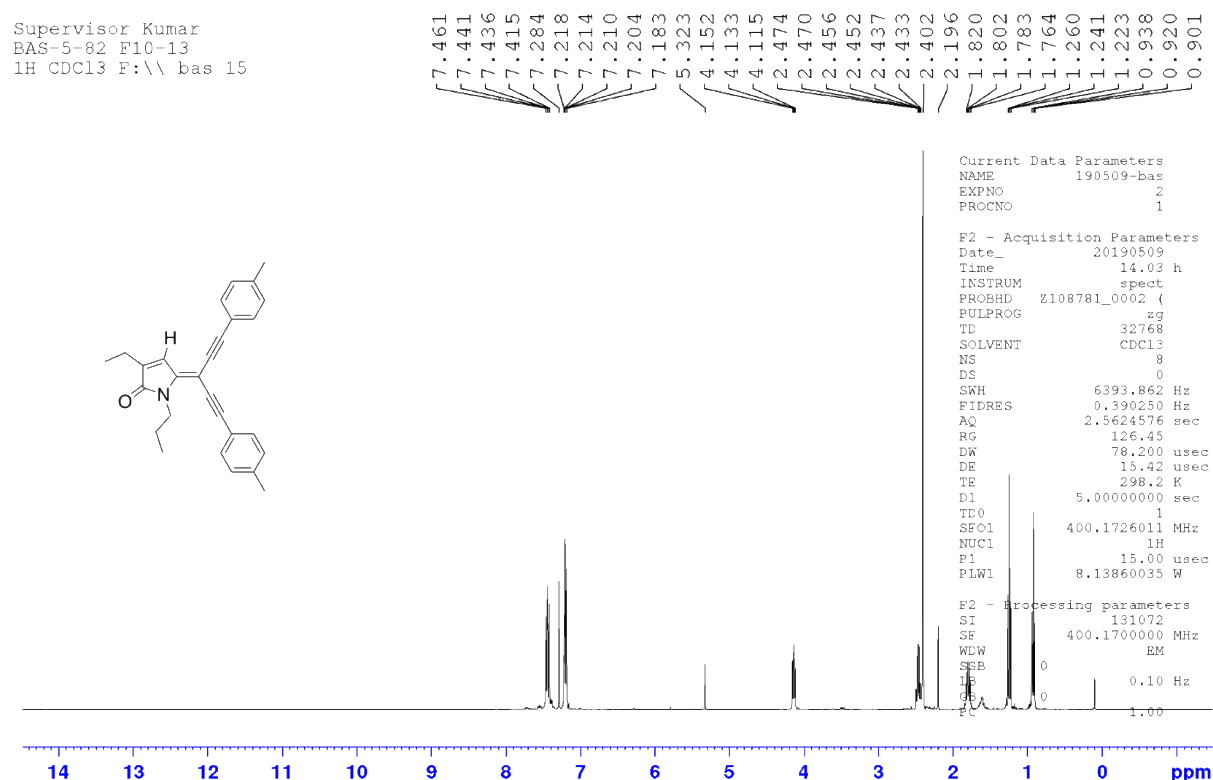


Supervisor Kumar
BAS-5-81 F7 phenyl
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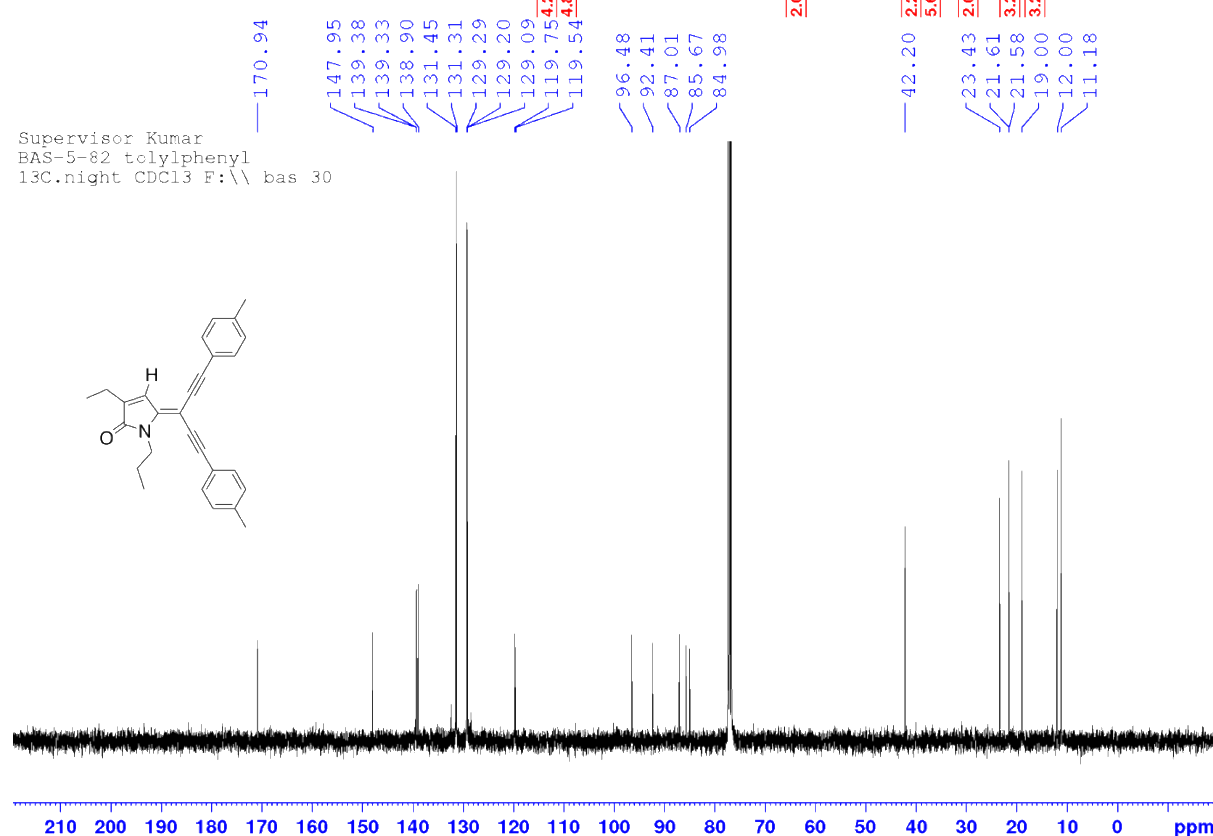


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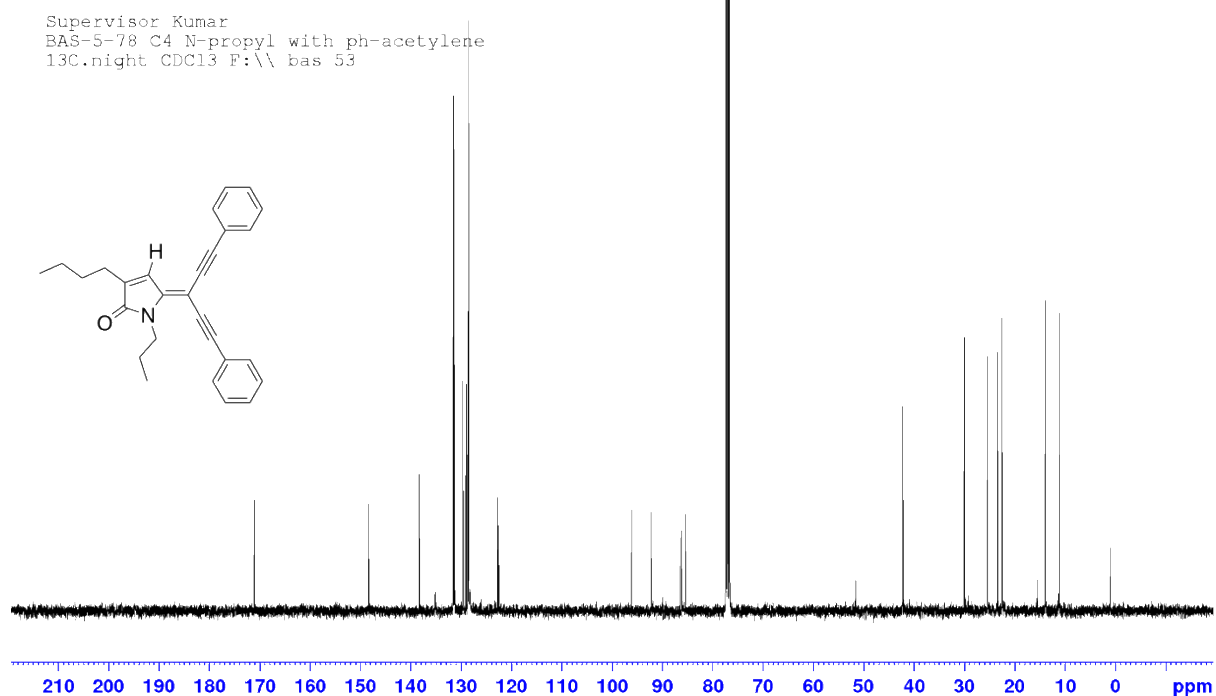
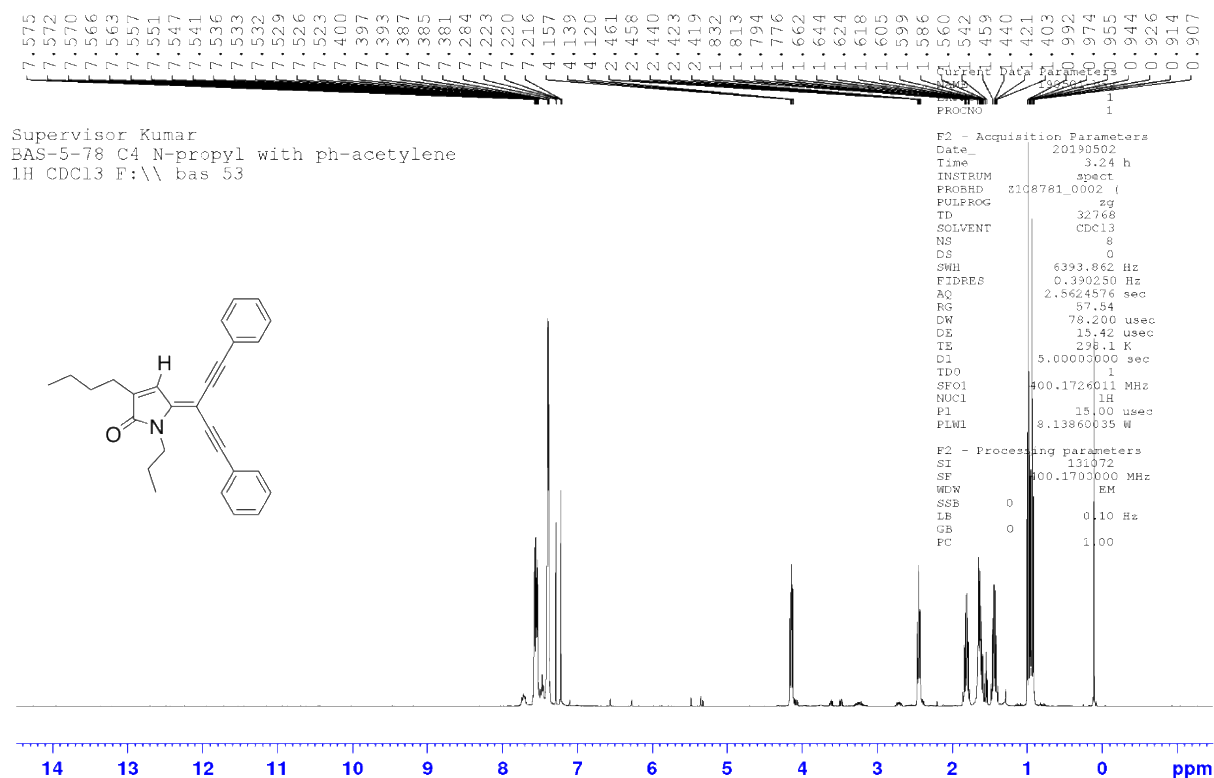
Supervisor Kumar
BAS-5-82 F10-13
1H CDC13 F:\ bas 15



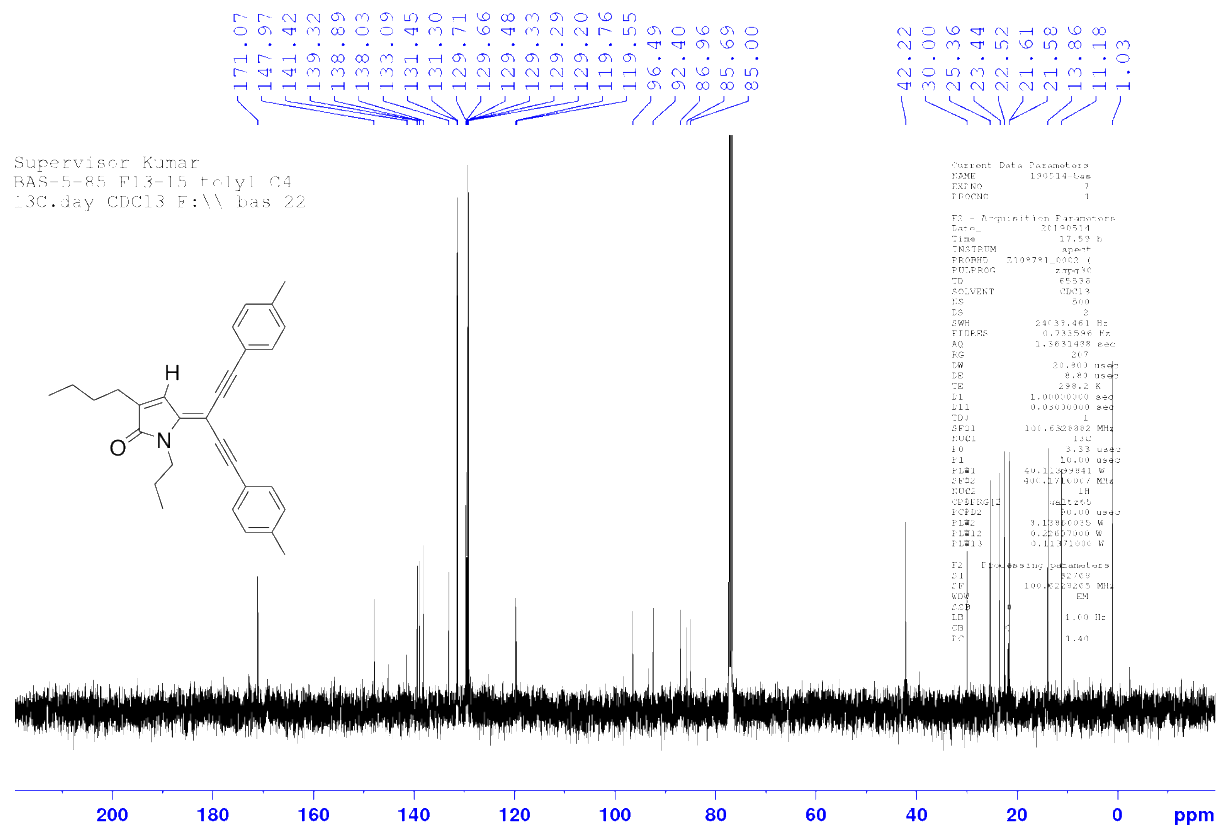
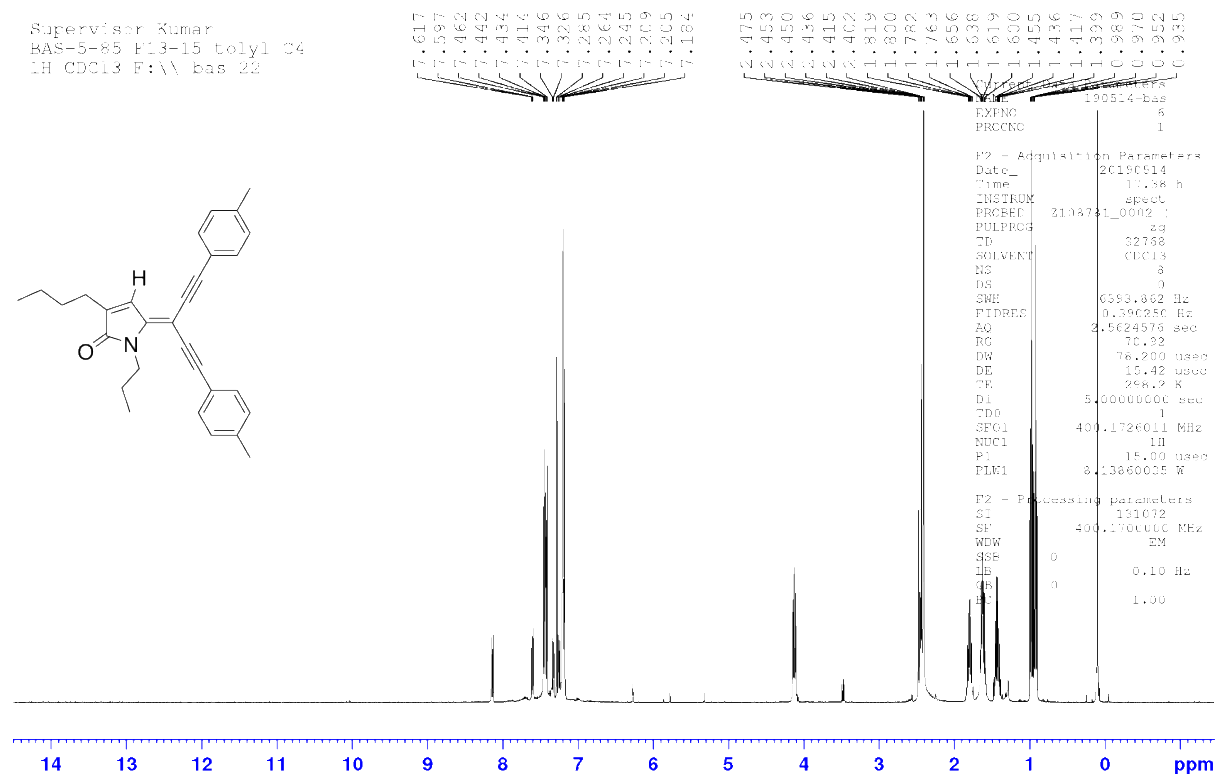
Supervisor Kumar
BAS-5-82 tolylphenyl
13C.night CDC13 F:\ bas 30



3-Butyl-5-(1,5-diphenylpenta-1,4-diyn-3-ylidene)-1-propyl-1,5-dihydro-2H-pyrrol- 2-one (38)

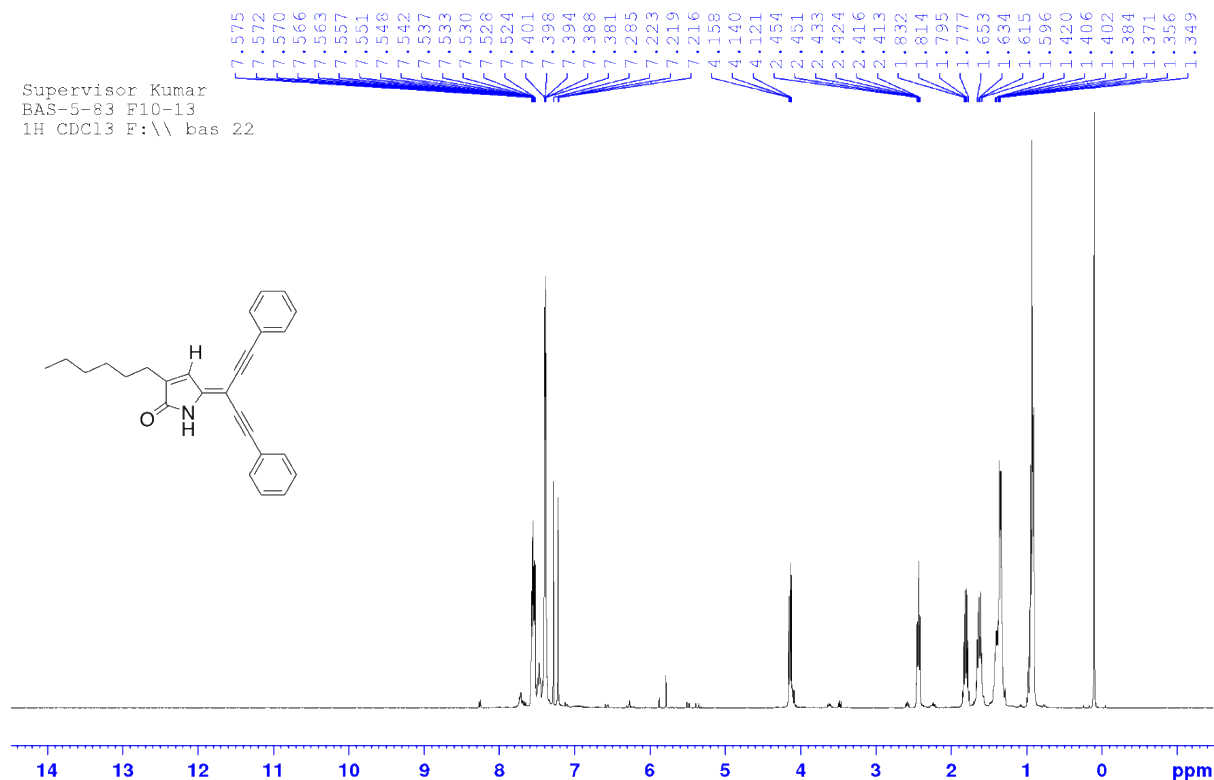


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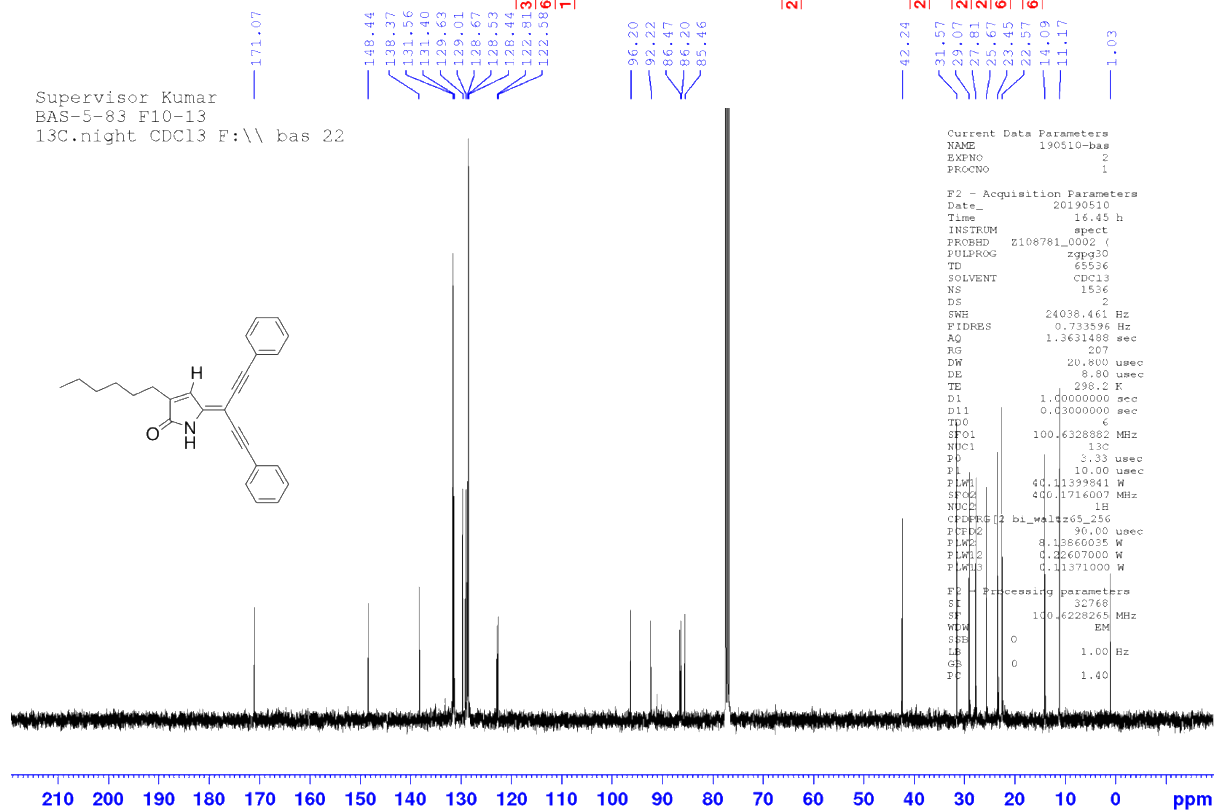


5-(1,5-Diphenylpenta-1,4-diyn-3-ylidene)-3-hexyl-1-propyl-1,5-dihydro-2H-pyrrol-2-one (40)

Supervisor Kumar
BAS-5-83 F10-13
1H CDC13 F:\ bas 22



Supervisor Kumar
BAS-5-83 F10-13
13C.night CDC13 F:\ bas 22



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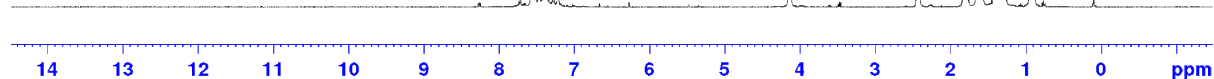
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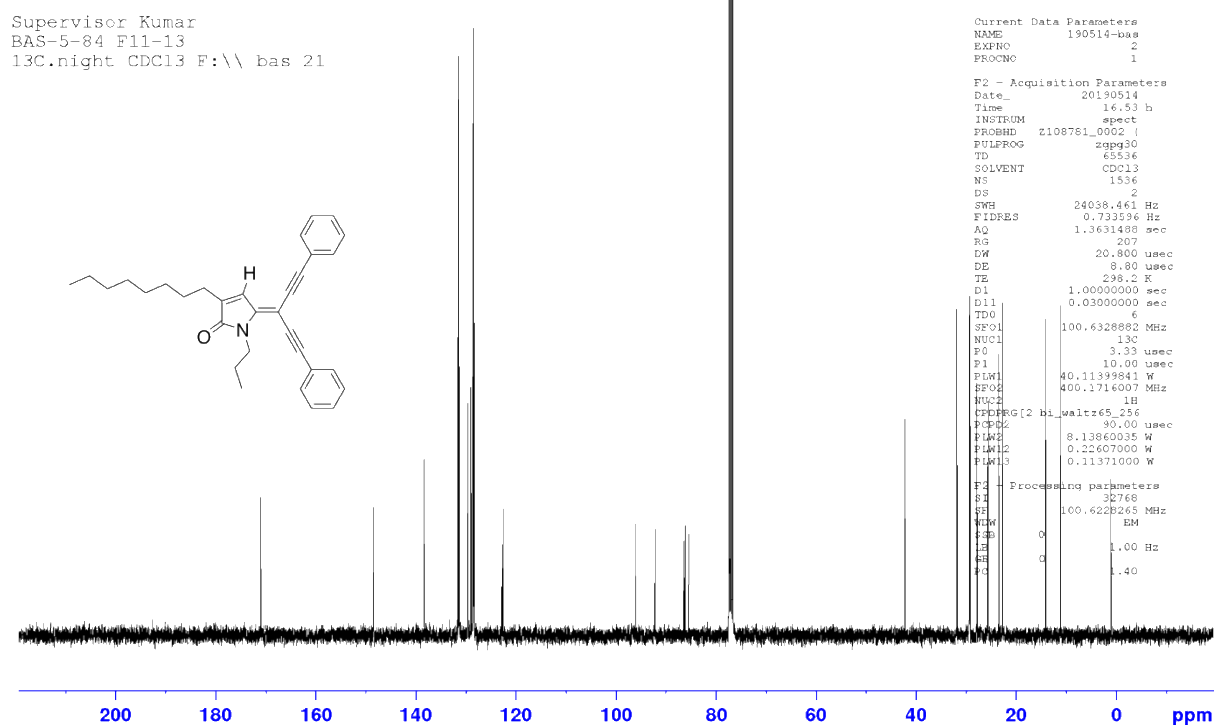
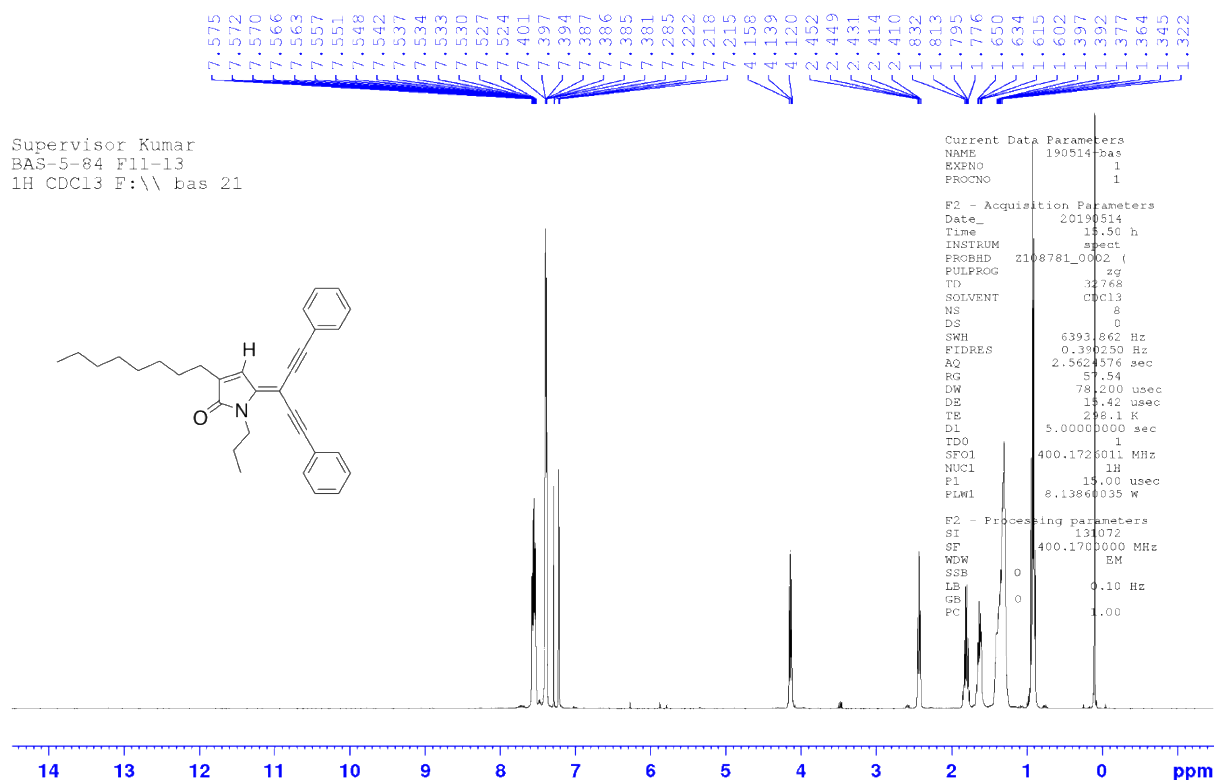
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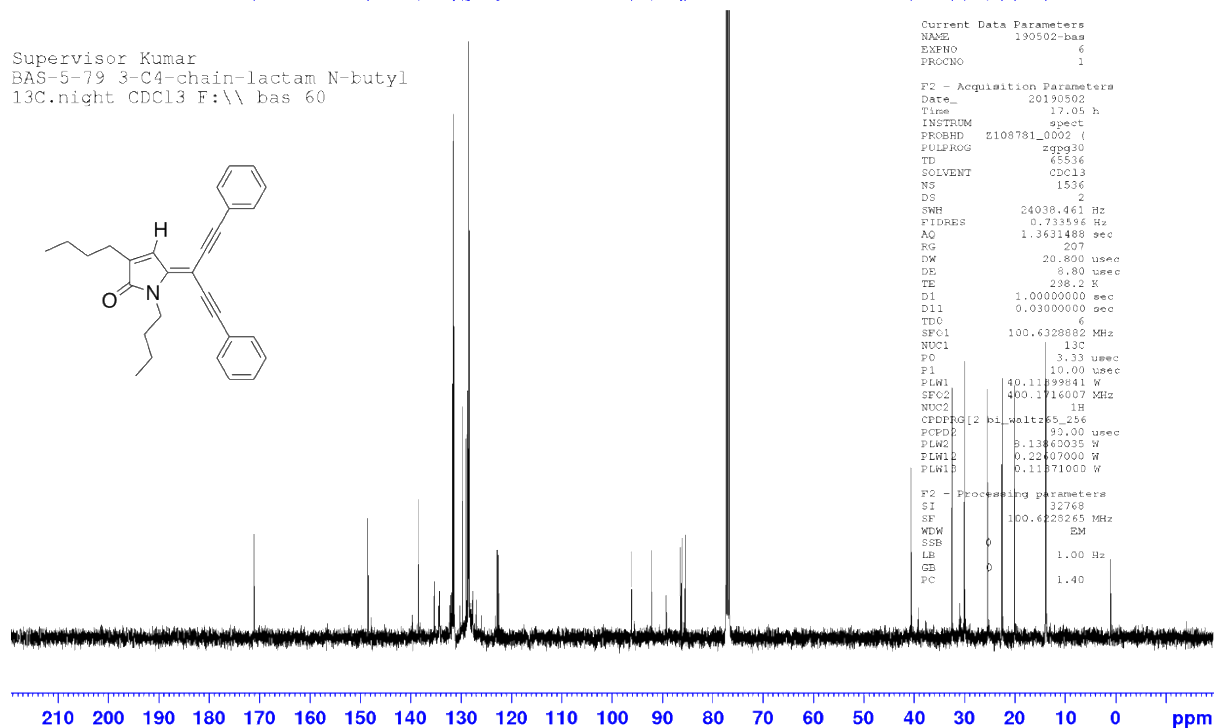
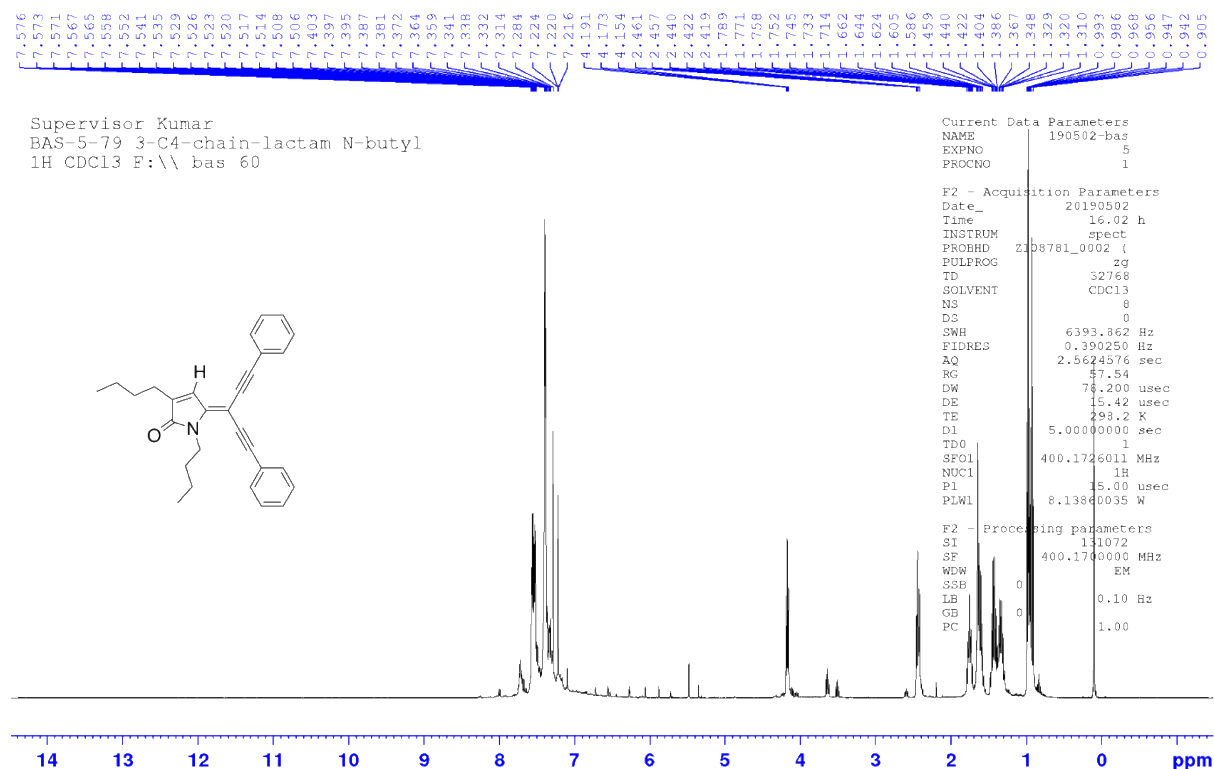
F2	Processing parameters	
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F8		100.6229265 MHz
WDW		EM
SSB	0	
RB		1.00 Hz
GB	0	
GC		1.40



5-(1,5-Diphenylpenta-1,4-diyn-3-ylidene)-3-octyl-1-propyl-1,5-dihydro-2H-pyrrol- 2-one (42)



1,3-Dibutyl-5-(1,5-diphenylpenta-1,4-diyn-3-ylidene)-1,5-dihydro-2H-pyrrol-2-one (43)



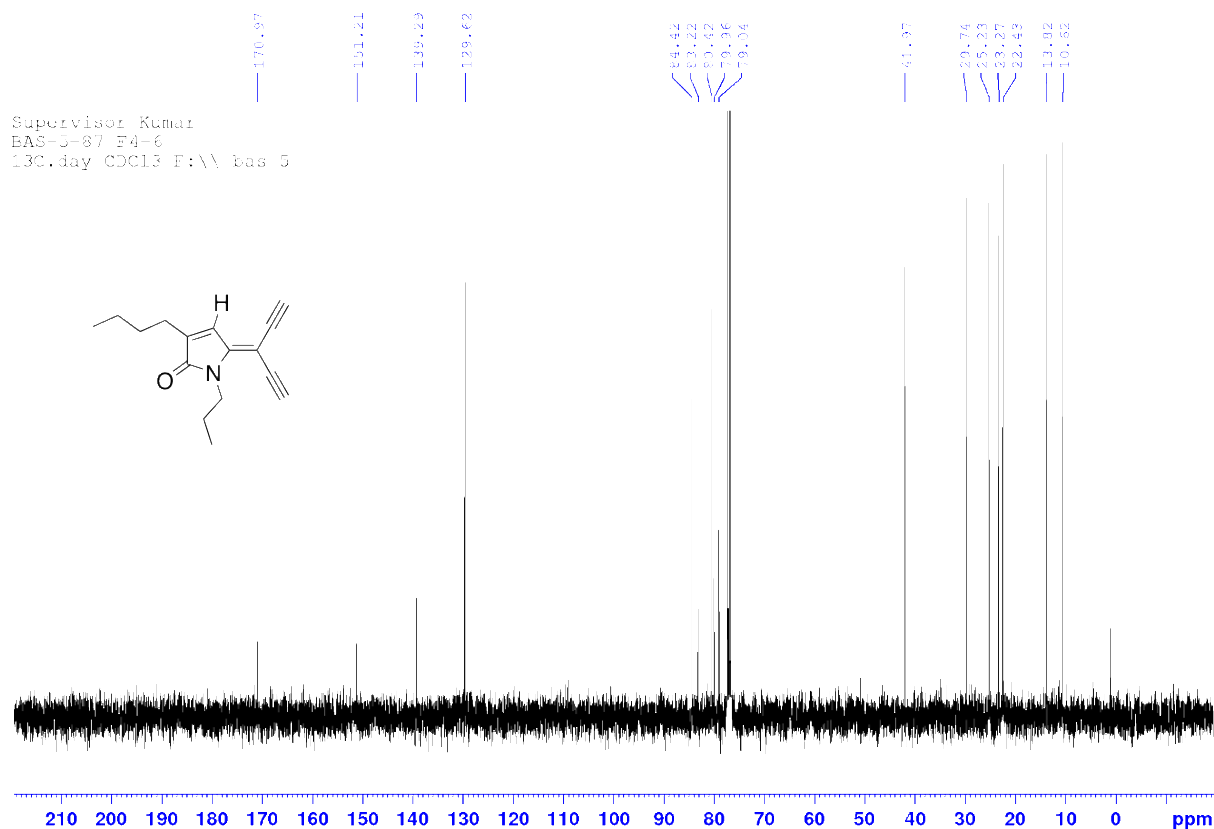
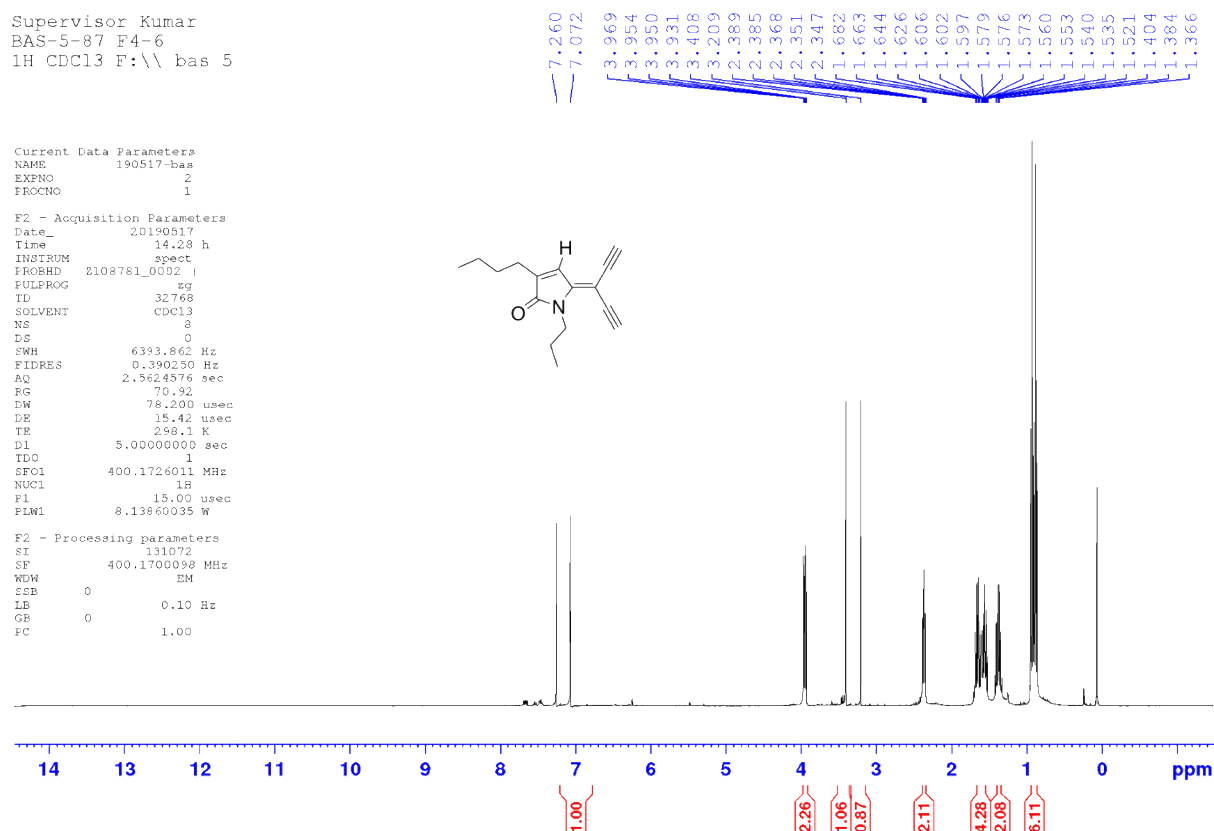
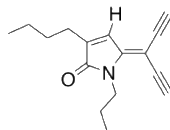
3-Butyl-5-(penta-1,4-diyn-3-ylidene)-1-propyl-1,5-dihydro-2H-pyrrol-2-one (44)

Supervisor Kumar
BAS-5-87 F4-6
1H CDC13 F:\ bas 5

Current Data Parameters
NAME 190517-bas
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190517
Time 14.28 h
INSTRUM spect
PROBHD E108781_0002
FULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.390250 Hz
AQ 2.5624576 sec
RG 70.92
DW 78.200 usec
DE 15.42 usec
TE 298.1 K
D1 5.00000000 sec
TD0 1
SFO1 400.1726011 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.13860035 W

F2 - Processing parameters
SI 131072
SF 400.1700098 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
FC 1.00



Supervisor Kumar
BAS-5-87 F4-6
13C.day CDCl3 F:\ bas 5

