Electronic Supplementary Information (ESI)

High-throughput DoE synthesis of chalcones and pyrazolines for fluorescent sensing

Alexander Ciupa*

General Experimental

Chemicals, solvents and reagents were purchased from commercial sources and used without further purification. PE refers to petroleum ether, bp 40-60 °C. Spectroscopy was performed with CHROMASOLV® gradient grade acetonitrile for HPLC, ≥99.9%, from Sigma-Aldrich.

The metal complexes used in this study were: LiCl, NaCl, KCl, $CaCl_2$, $MgCl_2$, $CuCl_2$, $NiCl_2$, $ZnCl_2$, $CdCl_2$, $RuCl_3$, $CoCl_2$, $MnCl_2$, $PbCl_2$, $ZnCl_2$ and HgI_2.

NMR spectra were obtained on a Bruker Avance III (400 MHz) spectrometer and processed via TopSpin® software. The chemical shifts are recorded in parts per million (ppm) with reference to tetramethylsilane. The coupling constants J are quoted to the nearest 0.5 Hz and are not corrected.

High resolution Mass spectroscopy was performed on Bruker Quadrupole Time-of-Flight (qToF) mass spectrometer.

UV/Vis spectroscopy was performed on an Thermo Scientific Varioskan LUX Multimode Microplate Reader with 360 nm excitation and measurement at 380-650 nm.

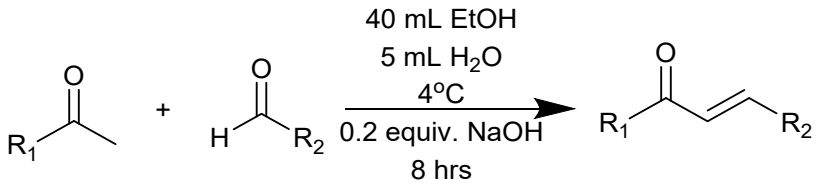
A 100 Watt 365 nm Analytikjena High intensity UV lamp was used to image the sensors in cuvettes with 5.0 equivalent indicated metal, sensor concentration was 20 µM, solvent was MeCN.

All figures were plotted using SigmaPlot® 14.5 software.

JMP Student edition 18 was used for all DoE studies.

Optimised synthetic conditions (S0)

Claisen–Schmidt condensation



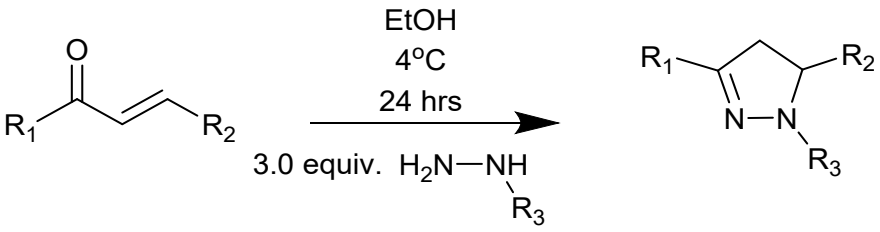
The following general procedure was used to synthesize chalcones **C1-C27**:

10 mmol of the required aromatic ketone was added to a stirred solution of 10 mmol of the required aromatic aldehyde in 40 mL EtOH, 5 mL H_2O, followed by 0.2 equiv. NaOH (2 mmol) and stirring continued at 4°C in a standard laboratory fridge. After 8 hrs the solution was removed from the fridge, the EtOH removed under vacuum and the resultant solid washes with copious amounts of cold H_2O, then dried in a freeze dryer. Recrystallisation from EtOH provided the required product without further purification.

See ESI S7 for ^{1}H and ^{13}C NMR spectra for **C1-C27**

See ESI S8 for characterisation details.

Pyrazoline formation



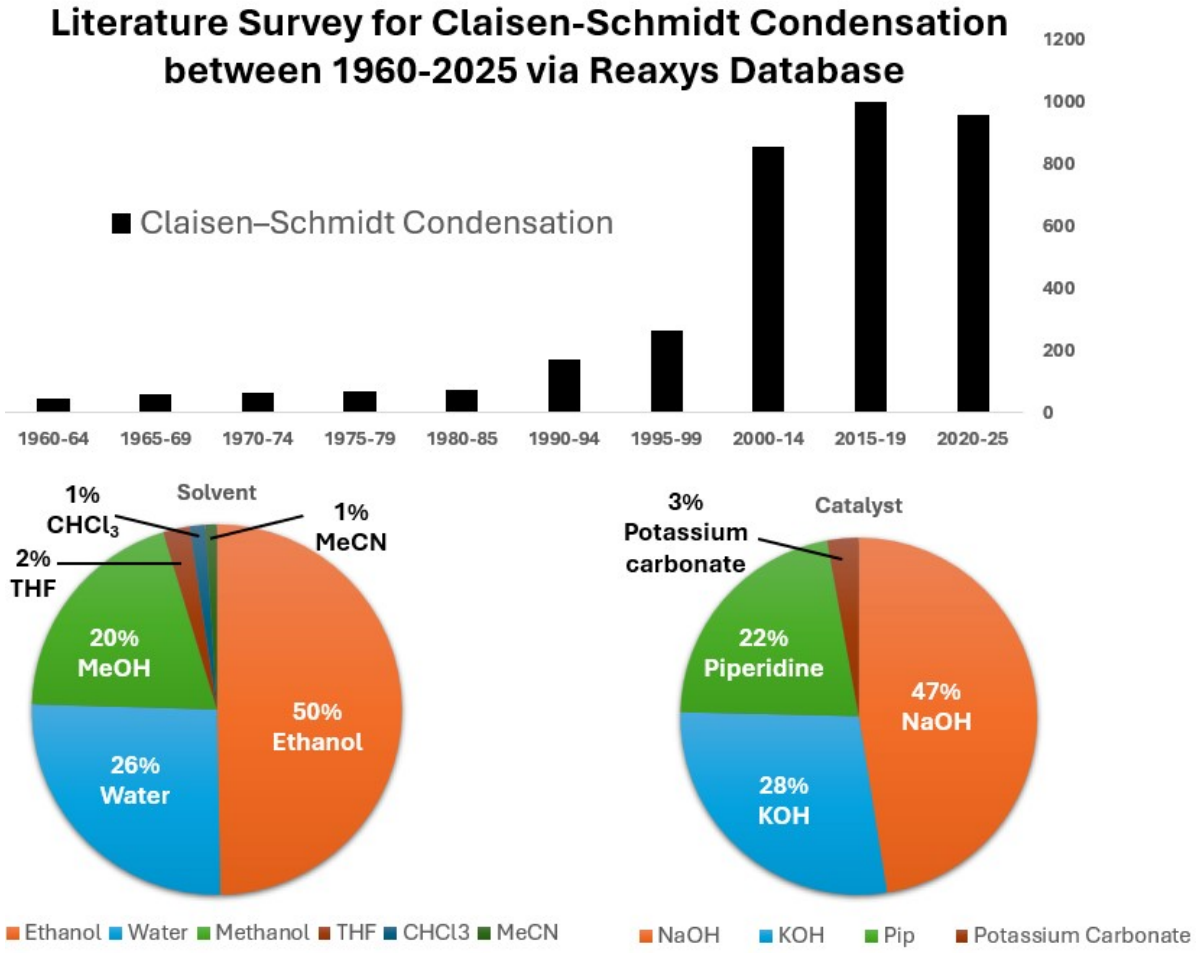
The following general procedure was used to synthesize pyrazolines **P1-P11:**

6 mmol of the required hydrazine was added to a stirred chalcone solution (2 mmol) in 20 mL EtOH with stirring continued at 4°C in a standard laboratory fridge. After 24 hrs the solution was removed from the fridge, the EtOH removed under vacuum and the resultant solid washed with copious amounts of cold H_2O, then dried in a freeze dryer. Recrystallization from EtOH provided the required pyrazoline without further purification.

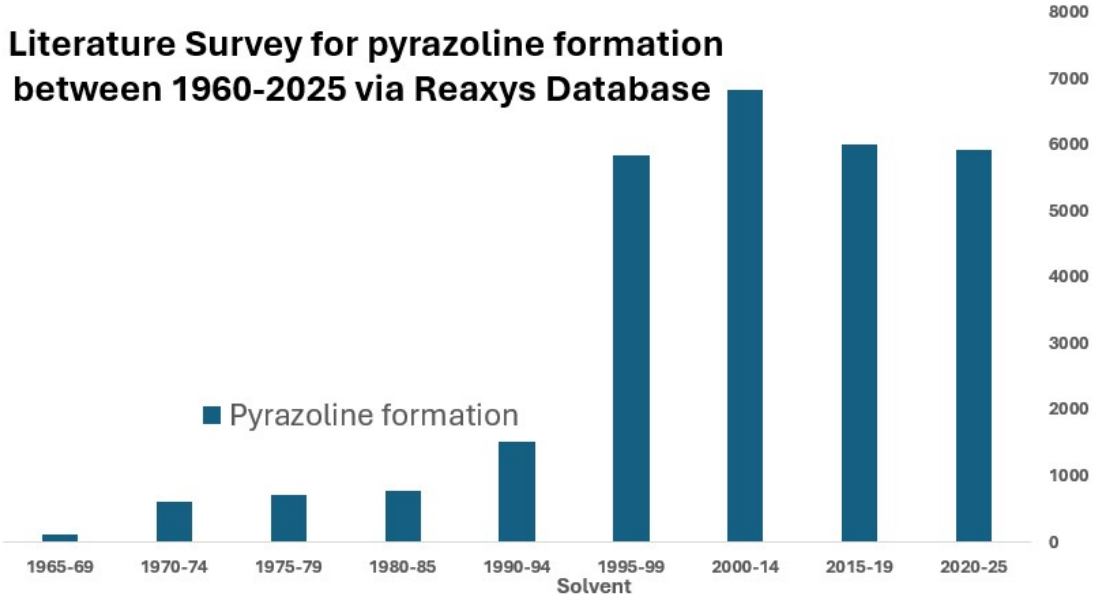
See S7 for ^{1}H and ^{13}C NMR spectra for **P1-P11**

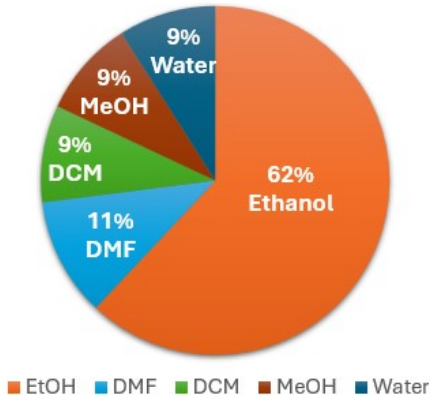
See S9 for characterisation details.

Claisen-Schmidt condensations reported between 1960 and 2025 *via* the Reaxys database (S1)

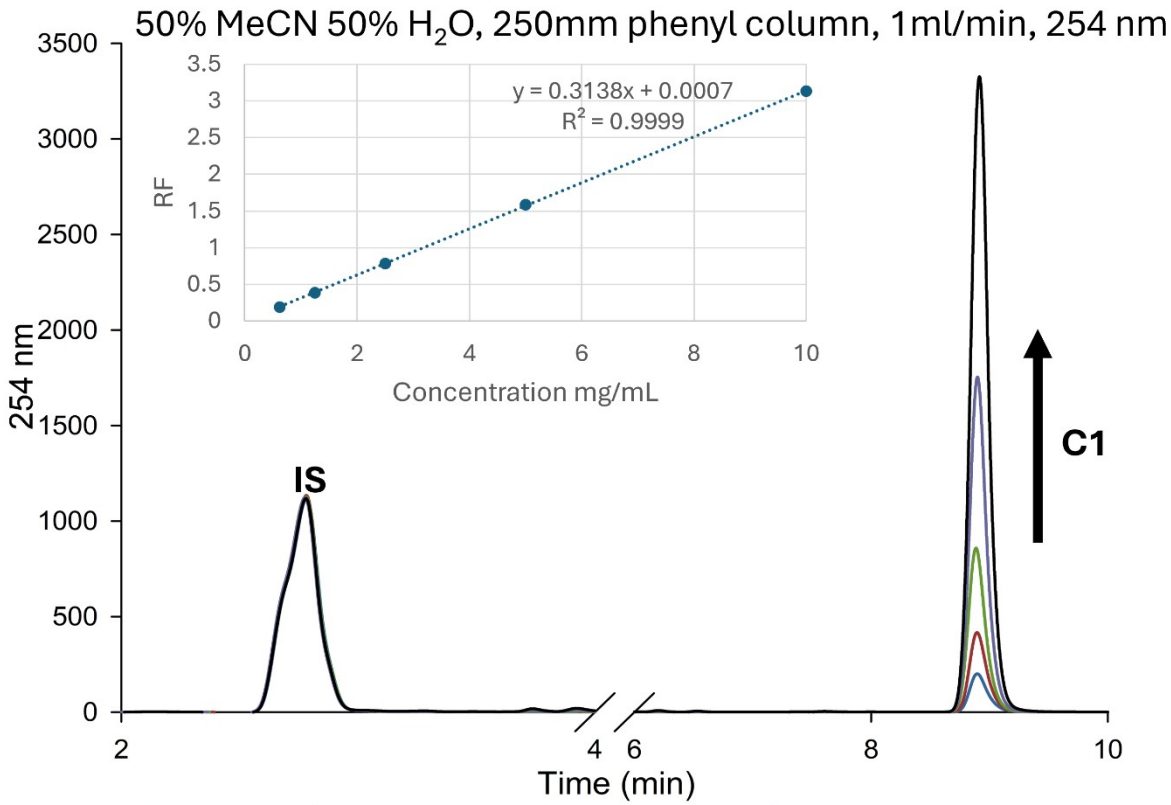


Pyrazoline synthesis reported between 1960 and 2025 *via* the Reaxys database (S2)



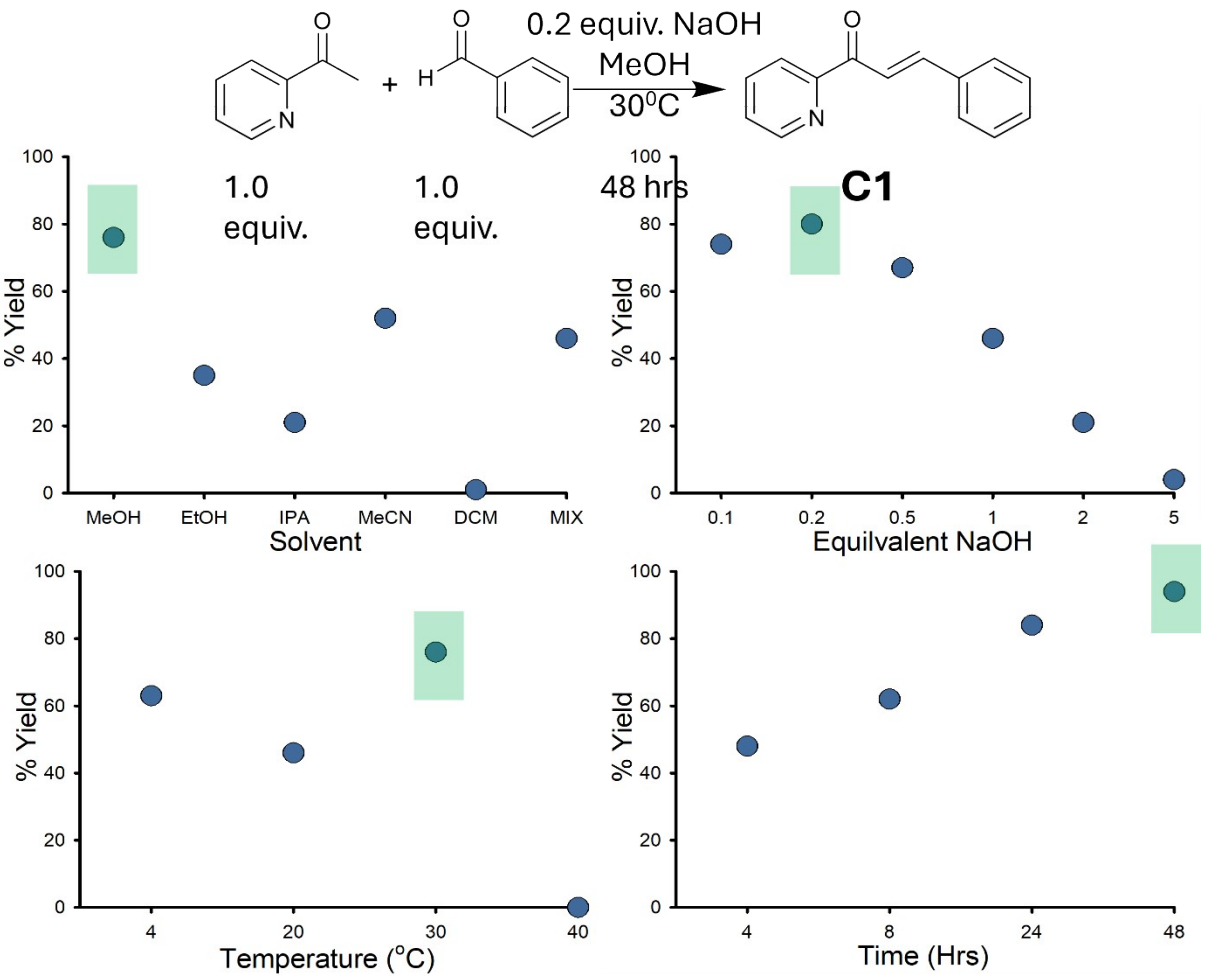


LC-MS calibration curve for C1 formation (S3)

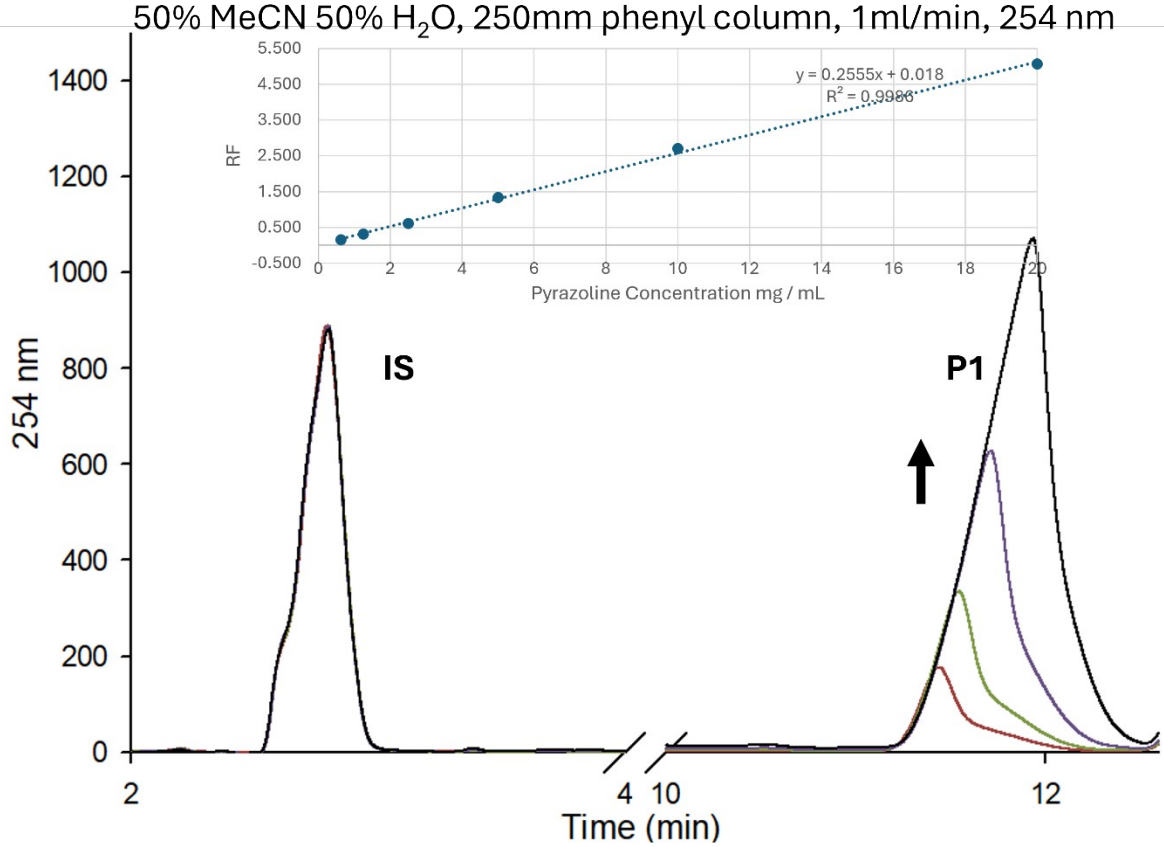


	1st Repeat			2nd Repeat			3rd Repeat			
Concentration mg/mL	AUC 1	IC 1	AVE 1	AUC 2	IC 2	AVE 2	AUC 3	IC 3	AVE 3	FINAL AVE
0.625	2229	11455	0.19459	2221	11483	0.19342	2231	11600	0.19233	0.193
1.25	4563	11701	0.38997	4448	11443	0.38871	4481	11526	0.38877	0.389
2.5	9026	11534	0.78256	9008	11520	0.78194	9009	11523	0.78183	0.782
5	18166	11418	1.591	18118	11415	1.58721	18161	11472	1.58307	1.587
10	35786	11403	3.1383	35624	11334	3.14311	35844	11515	3.11281	3.131

Initial parameter screening for DoE using OFAT approach (S4)



LC-MS calibration curve for P1 formation (S4)



	1st Repeat			2nd Repeat			3rd Repeat			
Concentration mg/mL	AUC 1	IC 1	AVE 1	AUC 2	IC 2	AVE 2	AUC 3	IC 3	AVE 3	FINAL AVE
0.625	1609	10532	0.15277	1613	10548	0.15292	1592	10571	0.1506	0.152
1.25	3356	10776	0.31143	3287	10622	0.30945	3290	10647	0.30901	0.310
2.5	6668	10807	0.61701	6666	10983	0.60694	6670	10889	0.61254	0.612
5	14227	10682	1.33187	14327	10803	1.32621	14361	10796	1.33021	1.329
10	29338	10887	2.69477	28896	10687	2.70385	29394	10876	2.70265	2.700
20	53734	10639	5.05066	53259	10528	5.0588	53636	10557	5.08061	5.063

C1 DoE Analysis report (S5)

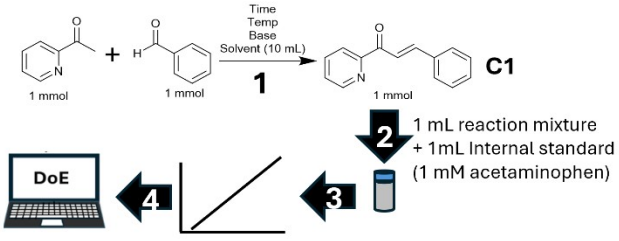
Fully replicated (in triplicate) 5 x 4 x 4 x4 custom DoE

Experimental Factor	Factor Level	Controlled variables	Measured Response
Solvent	• MeOH • EtOH • IPA • MeCN • DCM — 5 levels	• Solvent Volume (10mL) • Reaction flask dimensions • Same batch of reagents • Same User • Same lab location	• **C1** formation as calculated by LC-MS
Base	• 0.2 equiv. • 1 equiv. • 2 equiv. • 5 equiv. — 4 levels		
Temperature	• 4°C • 20°C • 40°C • 50°C — 4 levels		
Time	• 4 hrs • 8 hrs • 24 hrs • 48 hrs — 4 levels		

This custom design DoE was configured to analyse four different factors between 4-5 factor levels; each treatment was measured in triplicate and in a random order. This custom design was configured to maximise factor number and level within a manageable timeframe. Further details below:

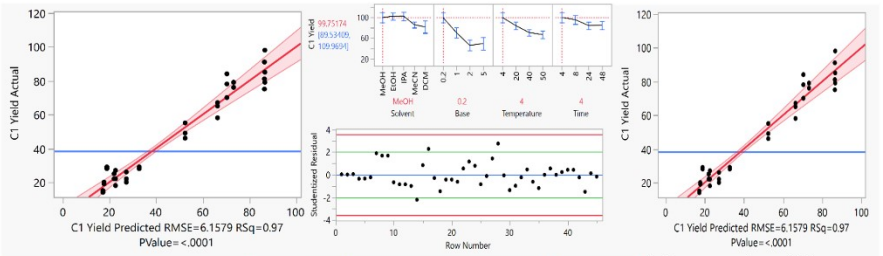
Σ	Solvent	Base	Temperature	Time	C1 Yield
1	DCM	5	20	48	0.1
2	DCM	5	20	48	0.01
3	DCM	5	20	48	0.2
4	EtOH	5	50	48	1.1
5	EtOH	5	50	48	1.2
6	EtOH	5	50	48	1.8
7	EtOH	2	40	4	29
8	EtOH	2	40	4	28
9	EtOH	2	40	4	28
10	EtOH	2	4	48	29
11	EtOH	2	4	48	28
12	EtOH	2	4	48	28
13	EtOH	0.2	20	4	81
14	EtOH	0.2	20	4	75
15	EtOH	0.2	20	4	91
16	EtOH	0.2	4	24	98
17	EtOH	0.2	4	24	85
18	EtOH	0.2	4	24	79
19	IPA	2	20	48	15
20	IPA	2	20	48	15
21	IPA	2	20	48	14
22	IPA	1	4	4	76
23	IPA	1	4	4	79
24	IPA	5	40	4	27
25	IPA	5	40	4	18
26	IPA	5	40	4	22
27	MeCN	0.2	4	48	78
28	MeCN	0.2	4	48	84
29	MeCN	0.2	4	48	70
30	MeCN	2	4	8	20

Σ	Solvent	Base	Temperature	Time	C1 Yield
31	MeCN	2	4	8	22
32	MeCN	2	4	8	26
33	MeCN	0.2	50	4	55
34	MeCN	0.2	50	4	49
35	MeCN	0.2	50	4	46
36	MeOH	1	50	48	22
37	MeOH	1	50	48	25
38	MeOH	1	50	48	22
39	MeOH	5	20	24	19
40	MeOH	5	20	24	20
41	MeOH	5	20	24	20
42	MeOH	0.2	40	8	65
43	MeOH	0.2	40	8	58
44	MeOH	0.2	40	8	67
45	DCM	1	40	24	7



Workflow:

1) Trial reaction (see table above for factor level)
2) Aliquot taken at require timepoint with internal standard added
1) HPLC analysis to determine **C1** yield
2) Input % yield into DoE



Source	Logworth	PValue
Base(0.2,5)	18.244	0.00000
Base*Base	16.124	0.00000
Temperature(4,50)	11.773	0.00000
Solvent	7.086	0.00000
Time(4,48)	5.844	0.00000
Time*Time	1.830	0.01479
Temperature*Temperature	0.839	0.14483

Most significant factor

Least significant factor

Nominal factors expanded to all levels

Term	Scaled Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-6.107036	4.201006	-1.45	0.1552
Solvent[MeOH]	5.4183894	2.353151	2.30	0.0275*
Solvent[EtOH]	7.8568501	1.67254	4.70	<.0001*
Solvent[IPA]	8.1134899	2.257764	3.59	0.0010*
Solvent[MeCN]	-8.703456	2.638225	-3.30	0.0023*
Solvent[DCM]	-12.68527	3.167603	-4.00	0.0003*
Base(0.2,5)	-25.32253	1.405045	-18.02	<.0001*
Base*Base	37.455219	2.440638	15.35	<.0001*
Temperature(4,50)	-16.59914	1.541182	-10.77	<.0001*
Temperature*Temperature	4.6833364	3.138254	1.49	0.1448
Time(4,48)	-7.654497	1.312997	-5.83	<.0001*
Time*Time	8.7256684	3.397786	2.57	0.0148*

Response C1 Yield

Effect Summary

Source	Logworth	PValue
Solvent*Temperature	18.701	0.00000
Solvent*Base	17.716	0.00000
Base*Time	9.606	0.00000
Solvent*Time	9.026	0.00000
Base*Temperature	4.505	0.00003
Temperature*Time	4.089	0.00008

Factor-Factor Interactions

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	15	37926.694	2528.45	126.9759
Error	29	577.471	19.91	Prob > F
C. Total	44	38504.166		<.0001*

DoE summary: Base, temperature, solvent and time are significant factors for the formation of **C1**. These factors are interacting with each other and therefore DoE is ideal for optimising these reaction conditions. **Ideal conditions**: MeOH, 0.2 equiv. NaOH, 4°C and 8 hrs reaction time.

P1 DoE Analysis report (S6)

Fully replicated (in triplicate) 3 x 4 x 3 x3 custom DoE For P1

Experimental Factor	Factor Level	Controlled Variables	Measured Response
Solvent	• MeOH • EtOH • IPA — 3 levels	• Solvent Volume (10mL) • Reaction flask dimensions • Same batch of reagents • Same User • Same lab location	• **P1** formation as calculated by LC-MS
Temperature	• 4°C • 20°C • 50°C • 80°C — 4 levels		
Hydrazine	• 2 equiv. • 3 equiv. • 4 equiv. — 3 levels		
Time	• 4 hrs • 8 hrs • 24 hrs — 3 levels		

This custom design DoE was configured to analyse four different factors between 3-4 factor levels; each treatment was measured in triplicate and in a random order. This design was configured to maximise factor number and level within a manageable timeframe. Further details below:

Σ	Solvent	Temperature	Equilvalent	Time	P1 Yield
1	EtOH	4	1.5	8	38
2	EtOH	4	1.5	8	43
3	EtOH	4	1.5	8	43
4	EtOH	4	1.5	24	52
5	EtOH	4	1.5	24	50
6	EtOH	4	1.5	24	40
7	EtOH	20	1	4	8
8	EtOH	20	1	4	9
9	EtOH	20	1	4	9
10	EtOH	20	1	8	10
11	EtOH	20	1	8	9
12	EtOH	20	1	8	8
13	IPA	4	1.5	8	30
14	IPA	4	1.5	8	28
15	IPA	4	1.5	8	24
16	IPA	4	1.5	24	32
17	IPA	4	1.5	24	30
18	IPA	4	1.5	24	32
19	IPA	4	2	8	9
20	IPA	4	2	8	8
21	IPA	4	2	8	10
22	IPA	20	2	4	1
23	IPA	20	2	4	1
24	IPA	20	2	4	0
25	IPA	50	1	8	3
26	IPA	50	1	8	4
27	IPA	50	1	8	4
28	IPA	80	1	4	10
29	IPA	80	1	4	11
30	IPA	80	1	4	•
31	IPA	80	1	8	3
32	IPA	80	1	8	4
33	IPA	80	1	8	4
34	IPA	80	2	4	1
35	IPA	80	2	4	1

Σ	Solvent	Temperature	Equilvalent	Time	P1 Yield
35	IPA	80	2	4	4
36	IPA	80	2	8	8
37	IPA	80	2	8	10
38	IPA	80	2	8	7
39	MeOH	4	1	4	3
40	MeOH	4	1	4	2
41	MeOH	4	1	4	2
42	MeOH	20	1	4	3
43	MeOH	20	1	4	6
44	MeOH	20	1	8	5
45	MeOH	20	1	8	4
46	MeOH	20	1	8	5
47	MeOH	20	1	4	3
48	MeOH	20	1	4	6
49	MeOH	20	2	8	5
50	MeOH	20	2	8	4
51	MeOH	20	2	8	5
52	MeOH	50	1.5	4	14
53	MeOH	50	1.5	4	14
54	MeOH	50	1.5	4	18
55	MeOH	80	1	4	14
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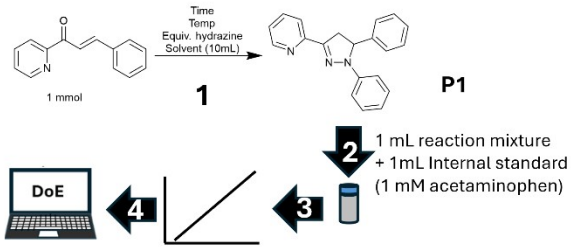
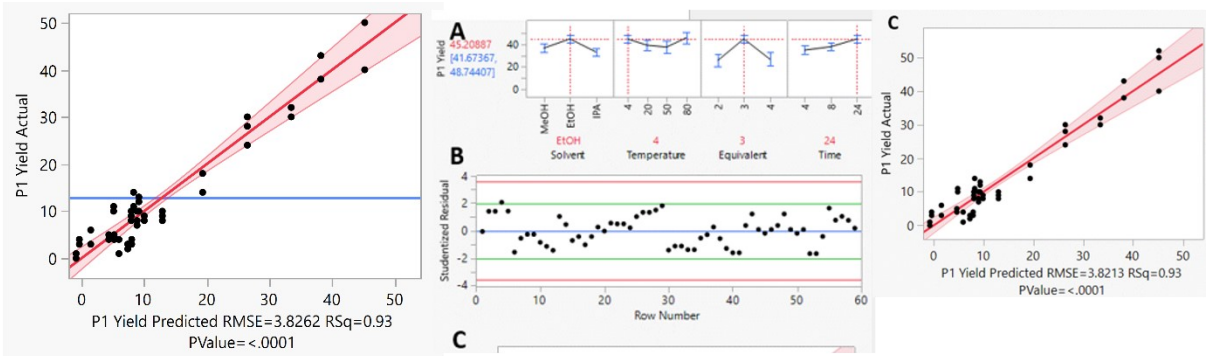
58	MeOH	80	2	4	12
59	MeOH	80	2	4	10

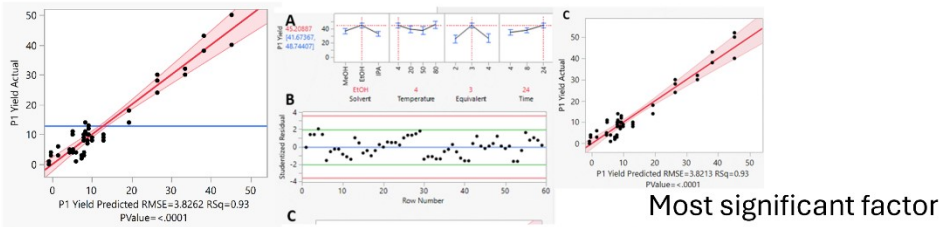


Workflow:

1) Trial reaction (see table above for factor level)
2) Aliquot taken at require timepoint with internal standard added
1) HPLC analysis to determine **P1** yield
2) Input % yield into DoE



Source	Logworth	PValue	
Equilvalent*Equilvalent	12.543	0.00000	
Solvent	7.709	0.00000	
Temperature	5.341	0.00000	
Time(4,24)	3.949	0.00011	
Time*Time	0.399	0.39895	
Equilvalent(1,2)	0.290	0.51299	^



Most significant factor

Source	Logworth	PValue	
Equilvalent*Equilvalent	12.543	0.00000	
Solvent	7.709	0.00000	
Temperature	5.341	0.00000	
Time(4,24)	3.949	0.00011	
Time*Time	0.399	0.39895	
Equilvalent(1,2)	0.290	0.51299	^

Least significant factor

Source	Logworth	PValue
Solvent*Temperature	15.087	0.00000
Temperature*Equilvalent	11.868	0.00000
Equilvalent*Time	5.121	0.00001
Solvent*Equilvalent	2.158	0.00695
Temperature*Time	1.368	0.04281
Solvent*Time	0.150	0.70825
Time(4,24)	.	.
Equilvalent(1,2)	.	.
Temperature	.	.
Solvent	.	.

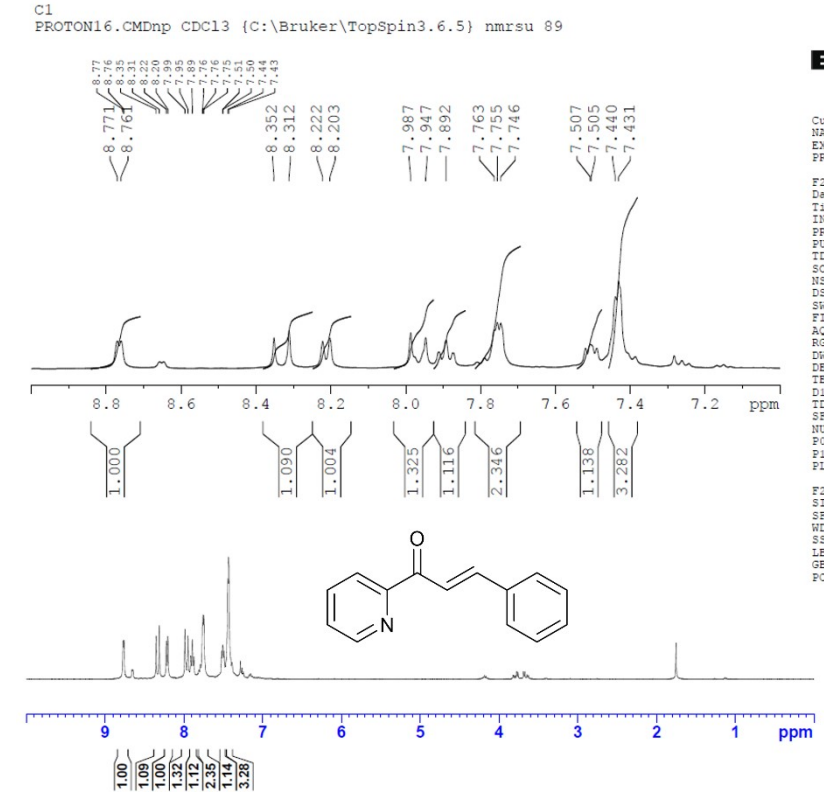
Factor-Factor Interactions

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	15	10167.669	677.845	138.3778
Error	43	210.636	4.899	Prob > F
C. Total	58	10378.305		<.0001*

DoE summary: Hydrazine equiv., solvent, temperature and time are significant factors for the formation of **P1**. These factors are interacting with each other and therefore DoE is ideal for optimising these reaction conditions. **Ideal conditions**: EtOH, 3 equiv. hydrazine, 4°C and 24 hrs reaction time.

NMR Spectra (S7)



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DE                 6.50 usec
TE                298.0 K
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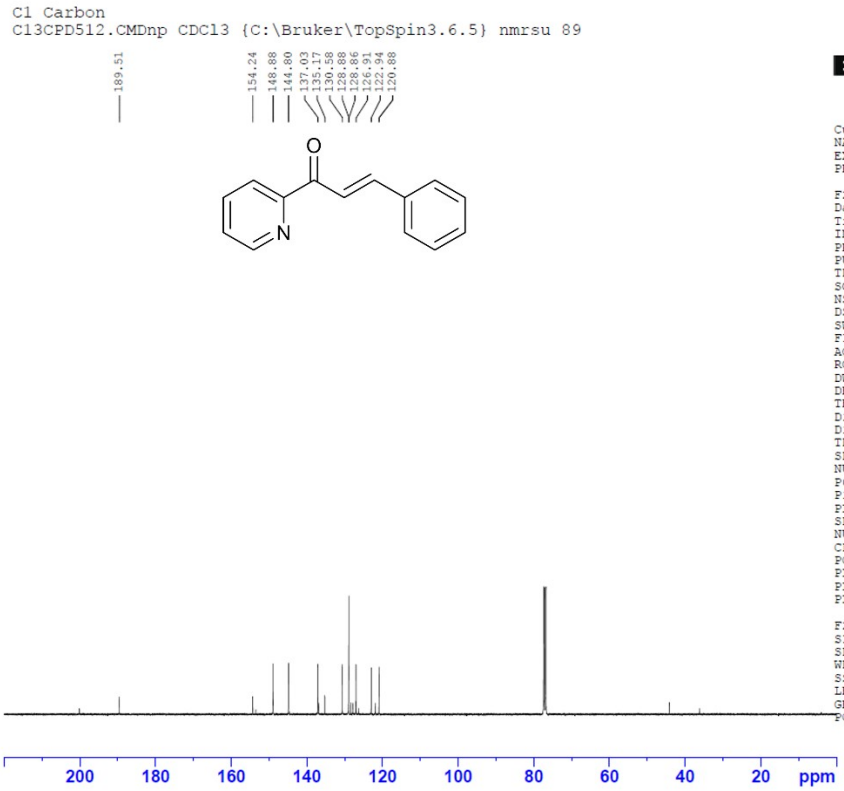

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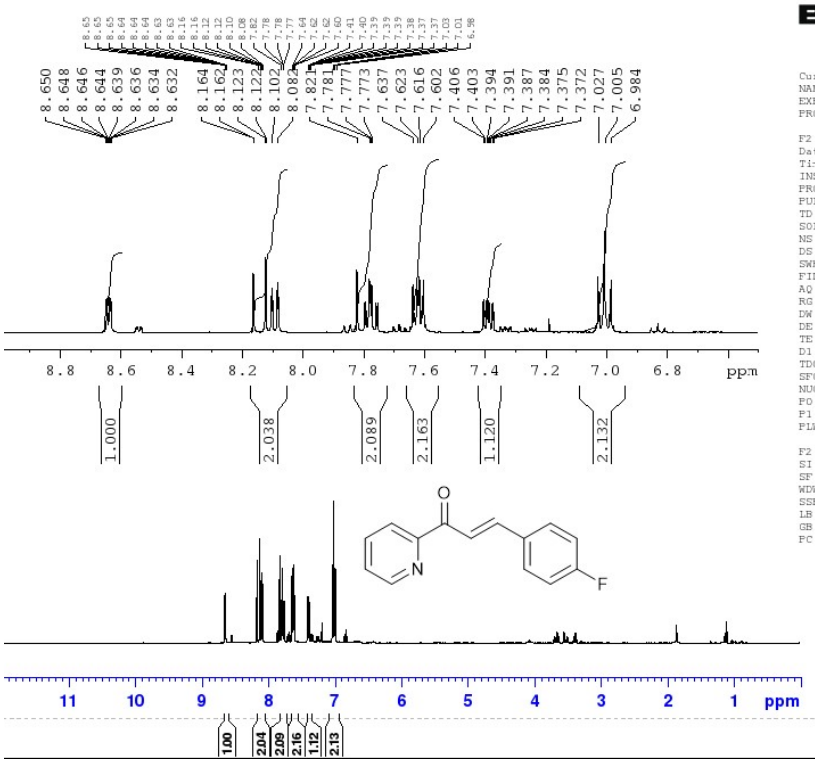

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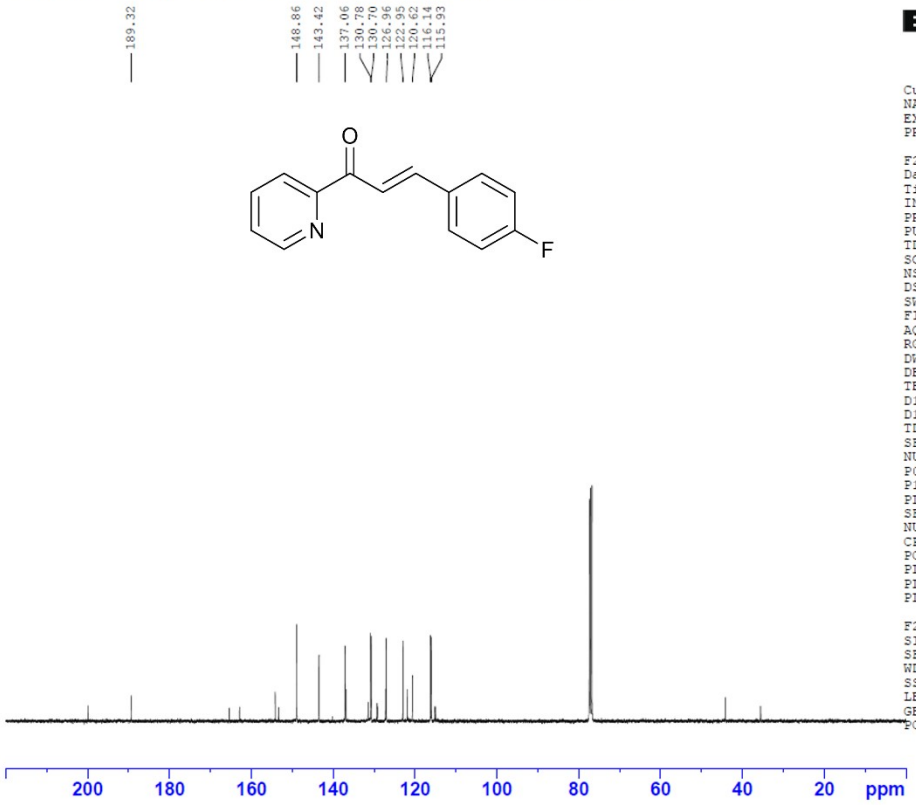

BRUKER

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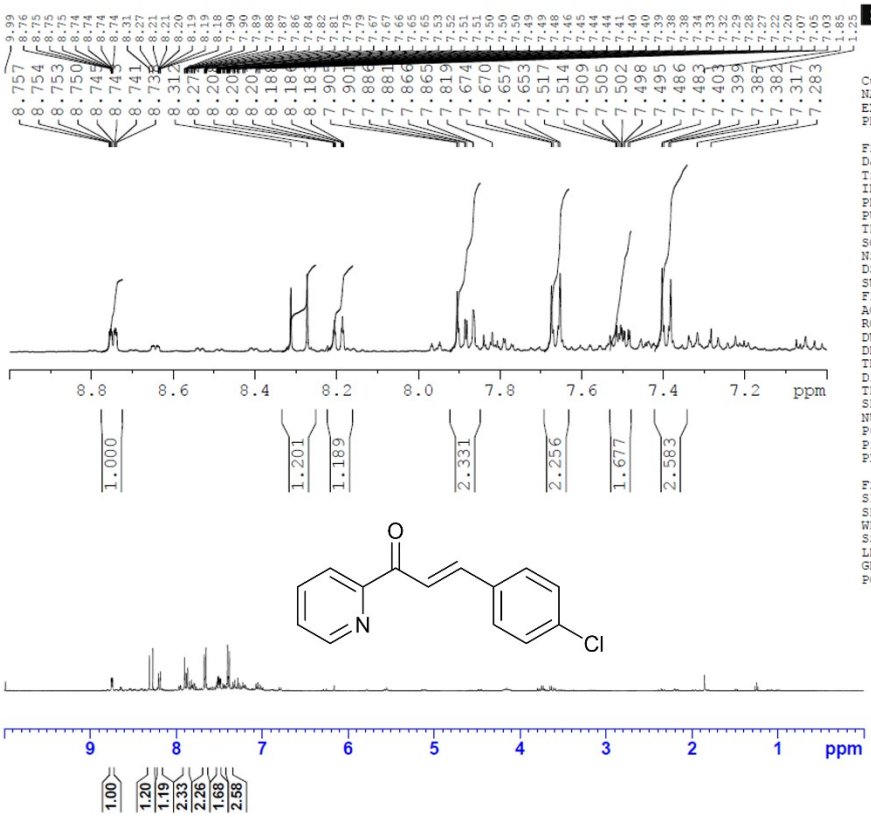
Current Data Parameters
NAME      Sep10-2025-Alex
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_           20250910
Time              10.59 h
INSTRUM             av400
PROBHD    Z163739_1011 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ             1.4155777 sec
RG                209.43
DW                21.600 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6384215 MHz
NUC1                  13C
P0                 2.67 usec
P1                 8.00 usec
PLW1          98.76699829 W
SFO2          400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C3
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 91



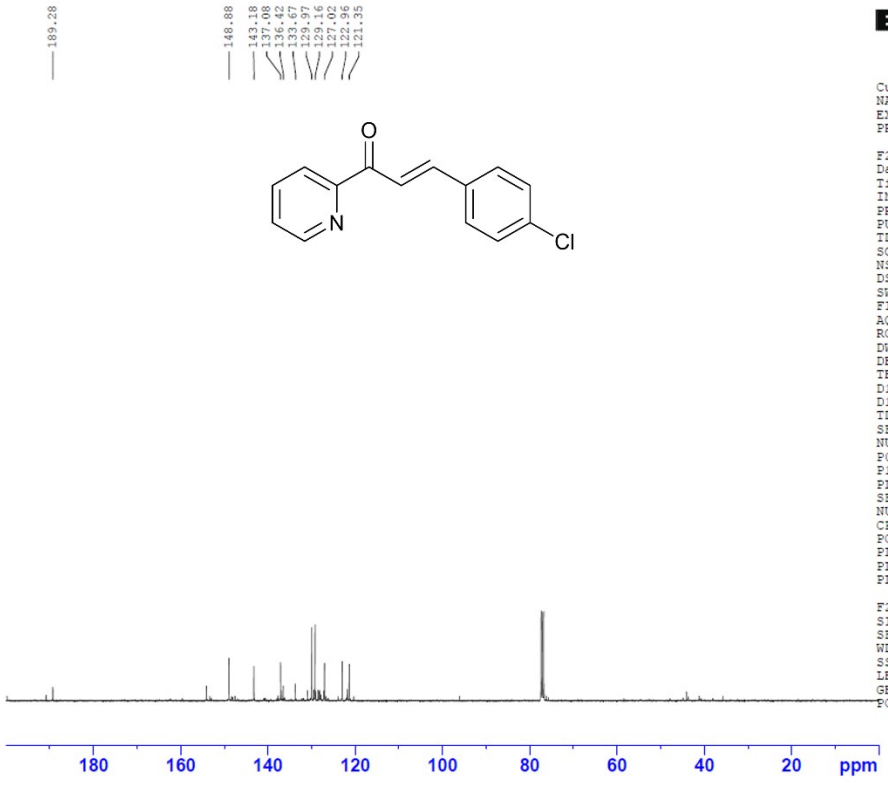
BRUKER

Current Data Parameters
NAME Sep10-2025-Alex
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250910
Time 9.15 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 55.93
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C3 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 91



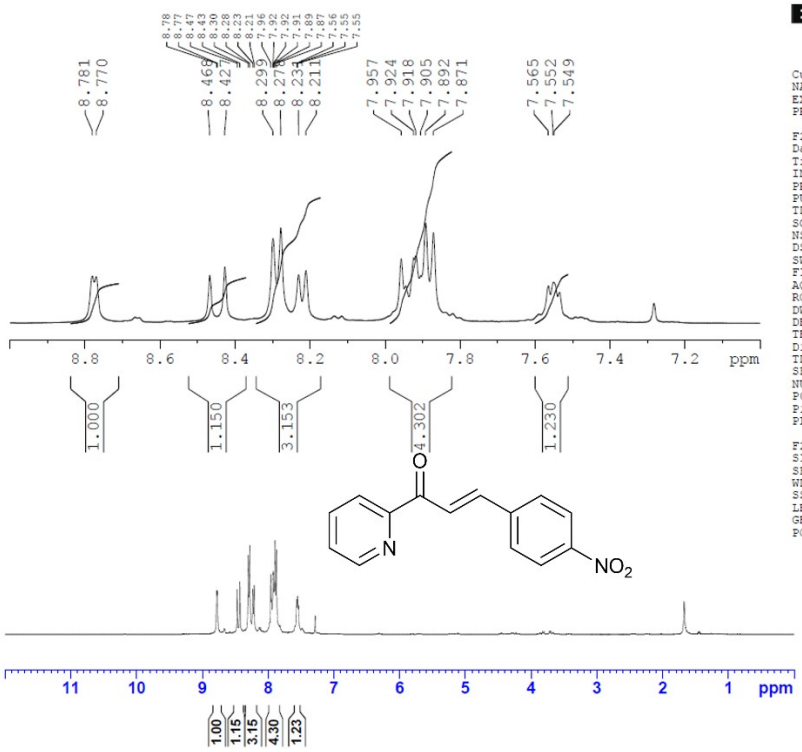
BRUKER

Current Data Parameters
NAME Sep10-2025-Alex
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250910
Time 11.34 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C15
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 25



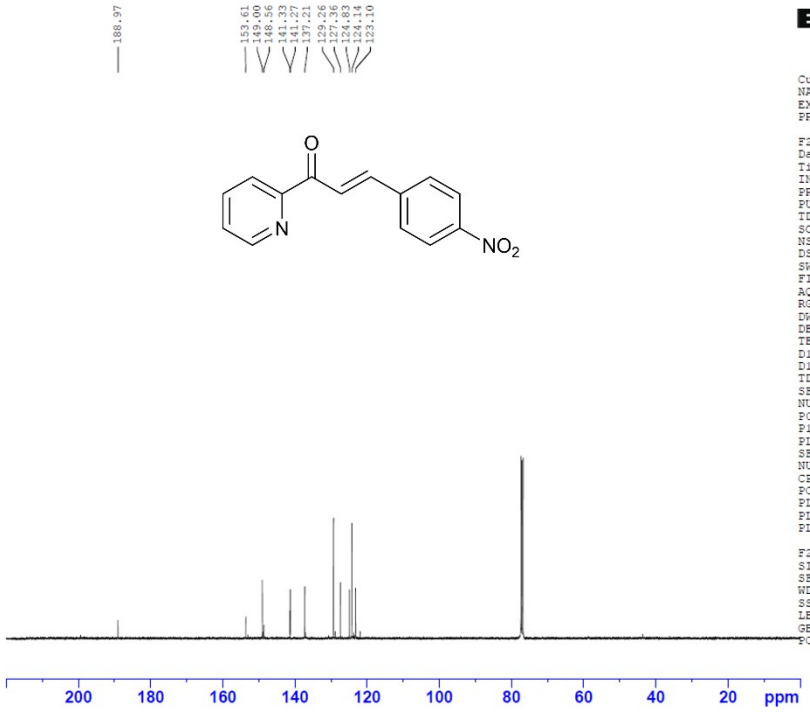
BRUKER

Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250911
Time 8.58 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C15 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 25



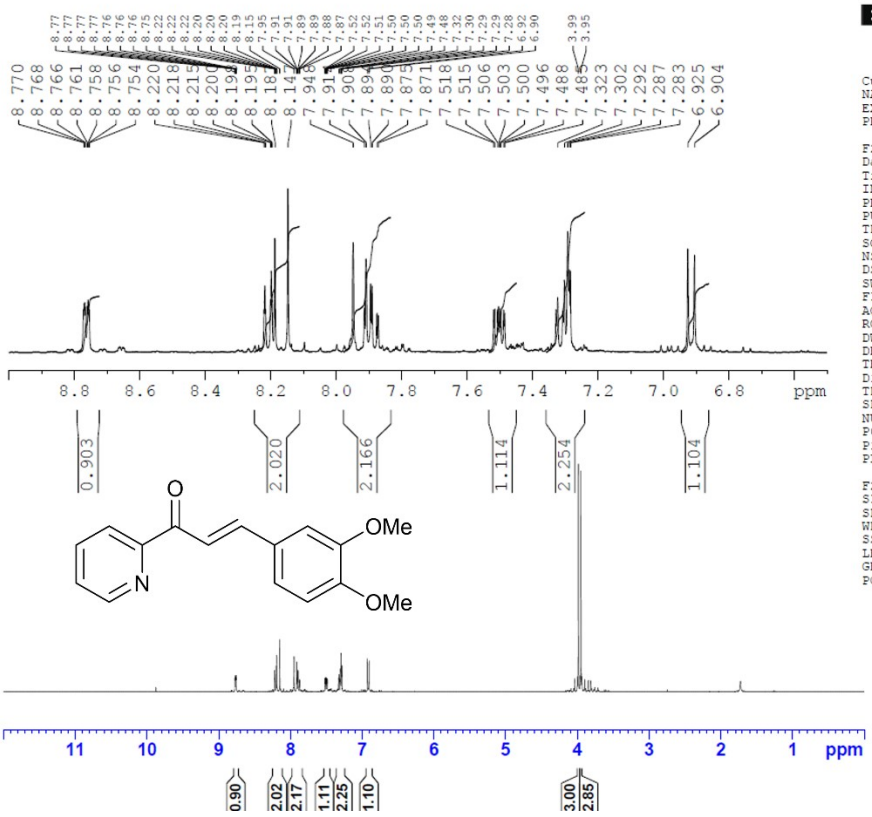
BRUKER

Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250911
Time 9.58 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C16
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 26



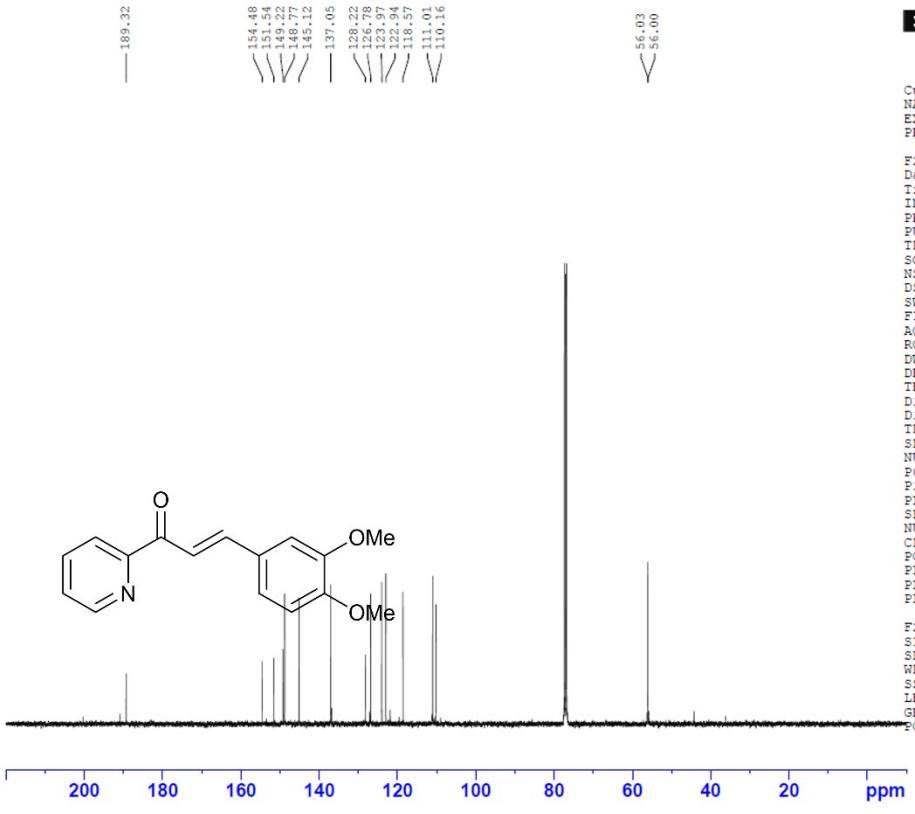
BRUKER

Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250911
Time 9.03 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C16 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 26



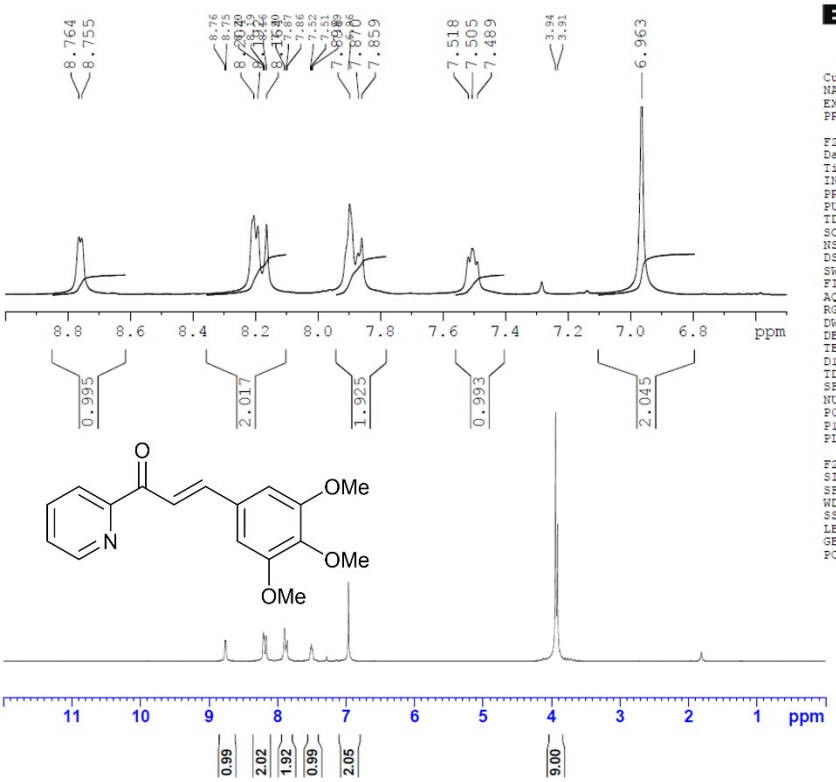
BRUKER

Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250911
Time 10.32 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C17
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 27

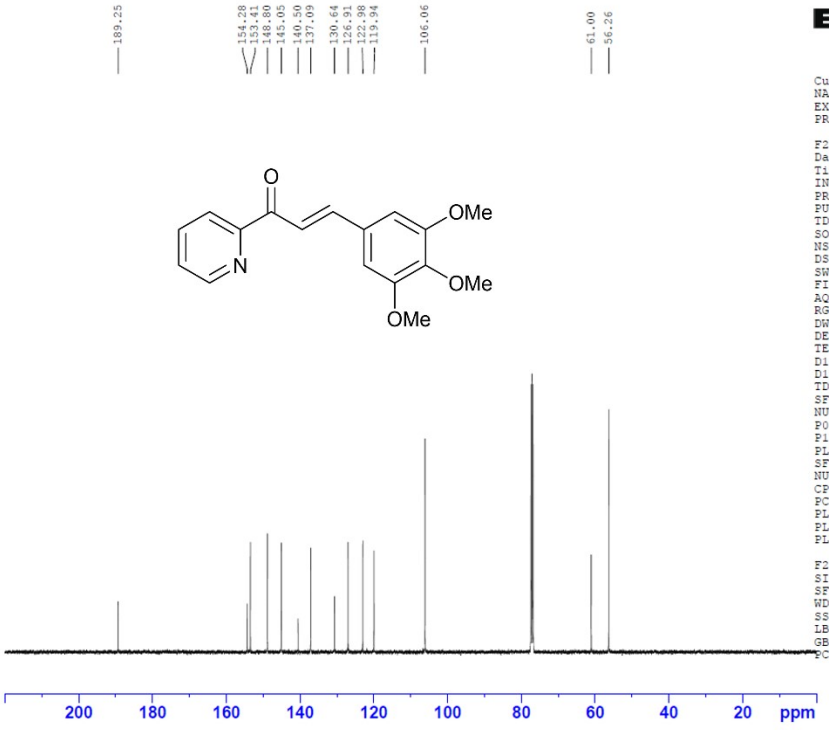


Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250911
Time 9.11 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 63.64
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

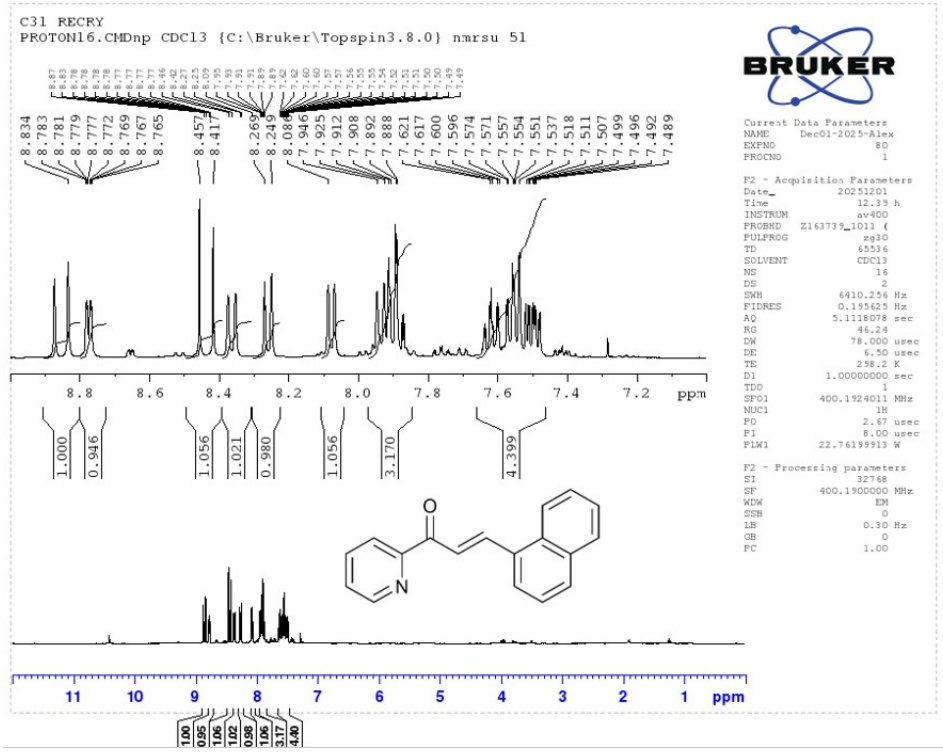
C17 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 27

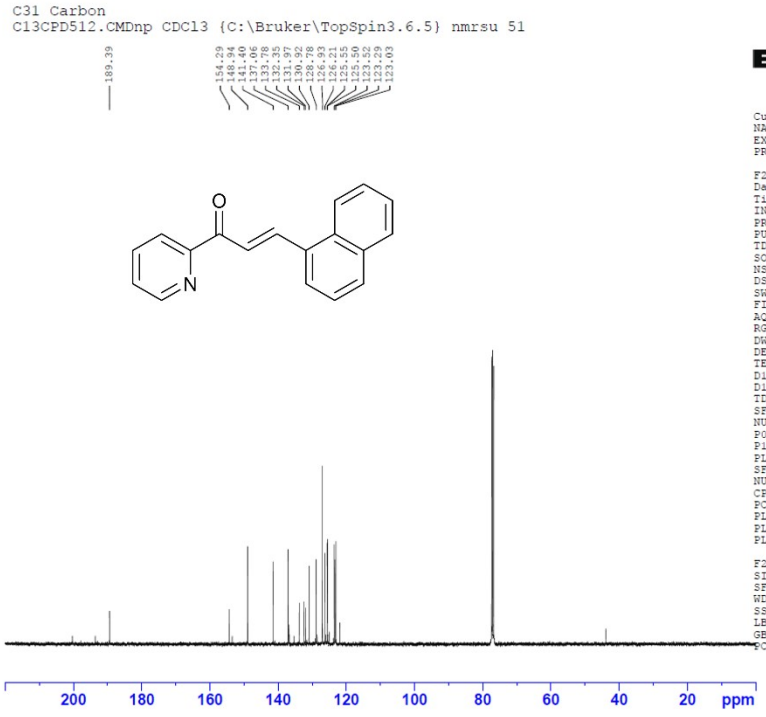


Current Data Parameters
NAME Sep11-2025-Alex
EXPNO 80
PROCNO 1

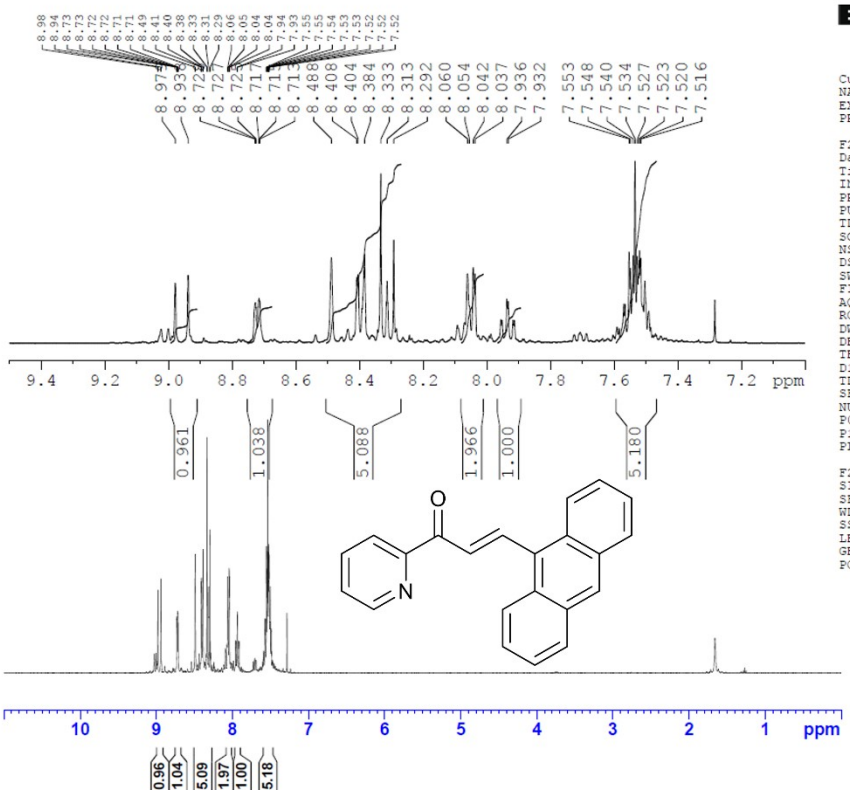
F2 - Acquisition Parameters
Date_ 20250911
Time 12.13 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


C31 RECRY
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 51
8.834
8.783
8.781
8.779
8.777
8.772
8.769
8.767
8.765
8.457
8.417
8.269
8.249
8.086
7.946
7.925
7.912
7.908
7.892
7.888
7.621
7.617
7.600
7.596
7.574
7.571
7.557
7.554
7.551
7.537
7.518
7.511
7.507
7.499
7.496
7.492
7.489
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
1.000
0.946
1.056
1.021
0.980
1.056
3.170
4.399
O
N
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.95
1.06
1.02
0.98
1.06
3.17
4.40
BRUKER
Current Data Parameters
NAME Dec01-2025-Alex
EXPNO 80
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251201
Time 12.39 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 46.24
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


C31 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 51
189.39
154.29
148.94
141.46
137.06
133.78
132.35
131.92
130.97
128.78
126.93
126.21
125.55
125.50
123.52
123.29
123.03
O
N
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME Sep23-2025-Alex
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20250923
Time 14.50 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76698829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W
F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C32
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 52



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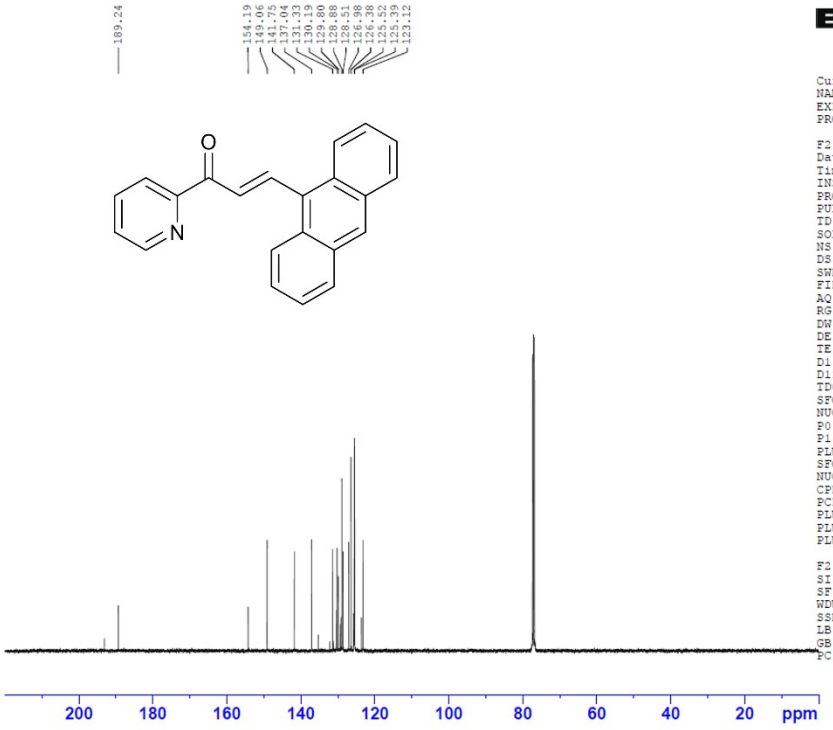
```
Current Data Parameters
NAME       Sep23-2025-Alex
EXPNO                  20
PROCNO                  1

F2 - Acquisition Parameters
Date_            20250923
Time                13.56 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               5.1118078 sec
RG                 104.12
DW                 78.000 usec
DE                  6.50 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                    1
SFO1           400.1924011 MHz
NUC1                  1H
P0                  2.67 usec
P1                  8.00 usec
PLW1           22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C32 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 52



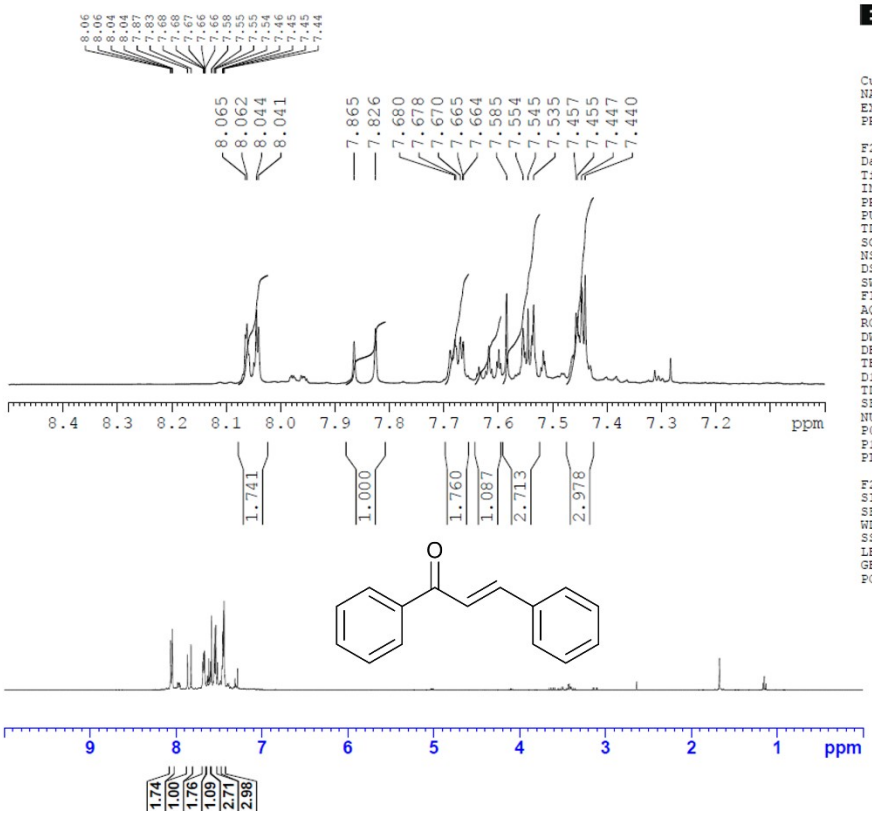
BRUKER

```
Current Data Parameters
NAME       Sep23-2025-Alex
EXPNO                  50
PROCNO                  1

F2 - Acquisition Parameters
Date_            20250923
Time                15.25 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH             23148.148 Hz
FIDRES           0.706425 Hz
AQ               1.4155777 sec
RG                 209.43
DW                 21.600 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           100.6384215 MHz
NUC1                  13C
P0                  2.67 usec
P1                  8.00 usec
PLW1           98.76699829 W
SFO2           400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2           22.76199913 W
PLW12           0.17985000 W
PLW13           0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C5
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 55

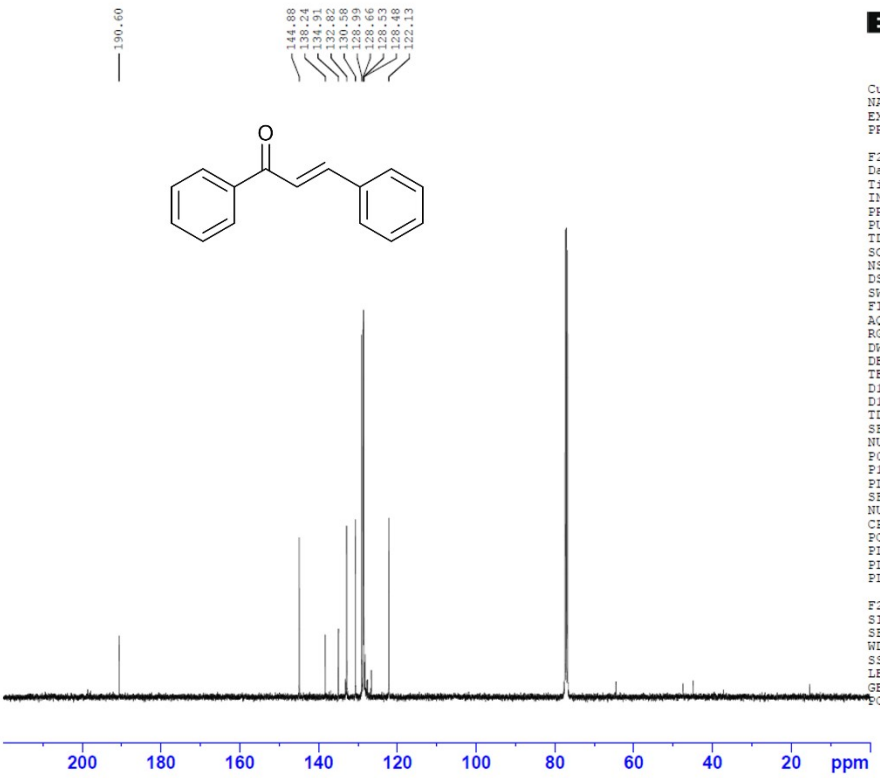


Current Data Parameters
NAME Sep09-2025-Alex
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250909
Time 11.02 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C5 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 55

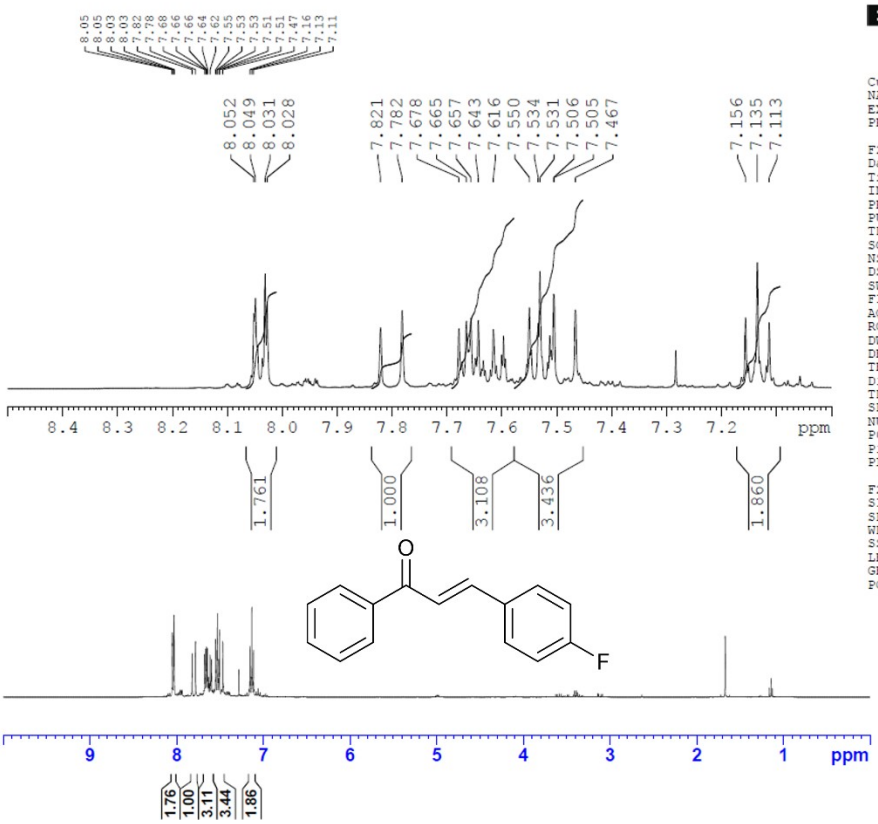


Current Data Parameters
NAME Sep09-2025-Alex
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250909
Time 13.42 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 use
DE 6.50 use
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 use
P1 8.00 use
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 use
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C6
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 56

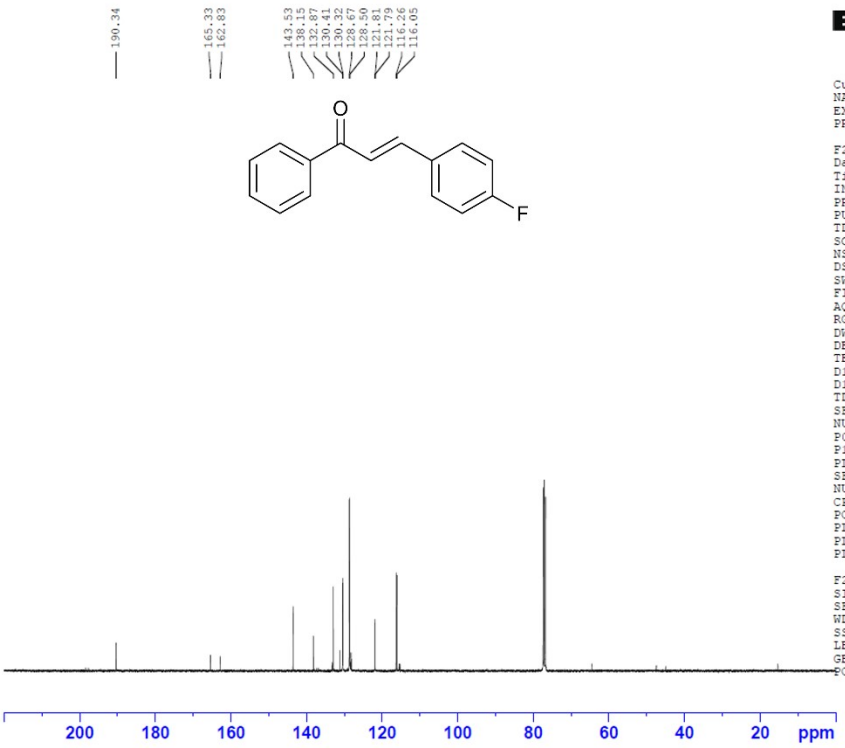


```
Current Data Parameters
NAME      Sep09-2025-Alex
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20250909
Time              11.08 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118078 sec
RG                104.12
DW                78.000 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C6 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 56

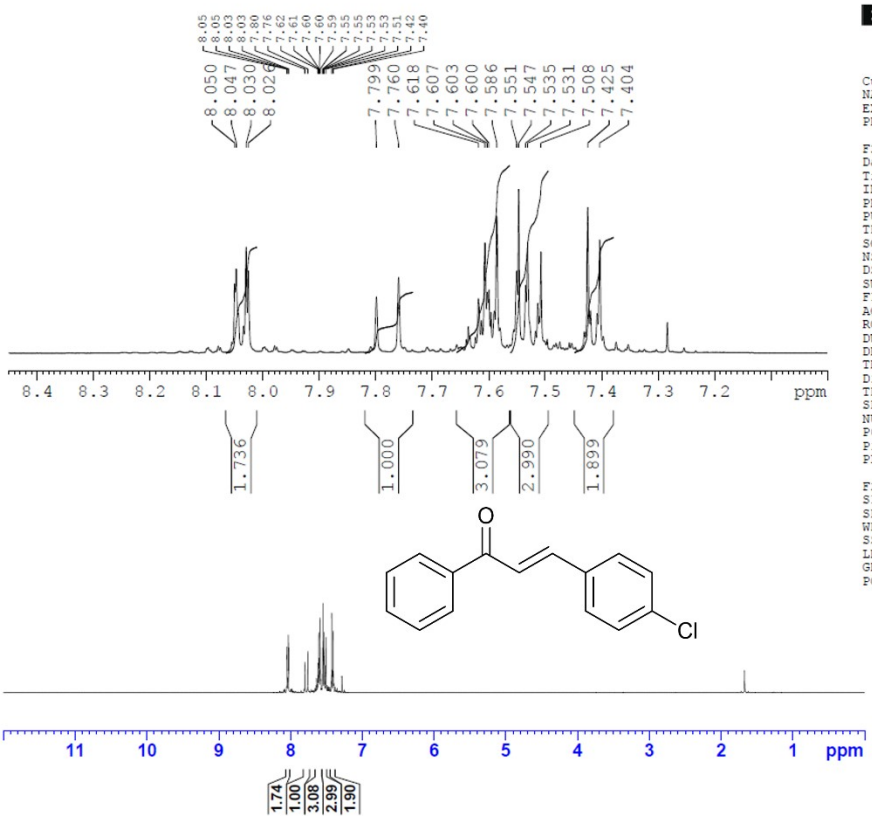


```
Current Data Parameters
NAME      Sep09-2025-Alex
EXPNO                100
PROCNO                 1

F2 - Acquisition Parameters
Date_           20250909
Time              14.28 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155777 sec
RG                209.43
DW                21.600 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6384215 MHz
NUC1                  13C
P0                 2.67 usec
P1                 8.00 usec
PLW1          98.76699829 W
SFO2          400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C7
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 90



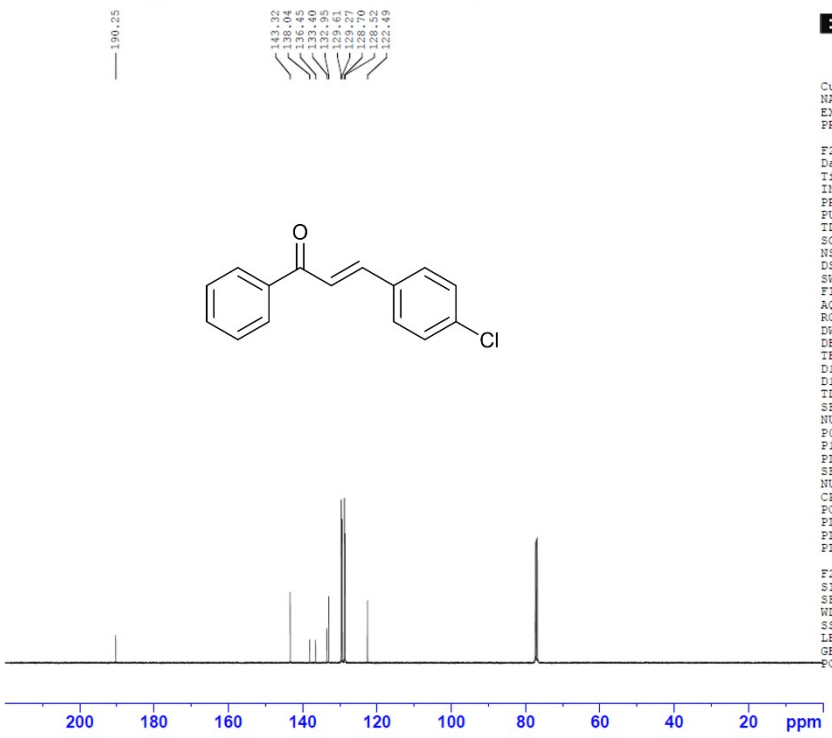
BRUKER

```
Current Data Parameters
NAME      Sep19-2025-Alex
EXPNO                 20
PROCNO                 1

F2 - Acquisition Paramet
Date_           20250919
Time              10.01
INSTRUM            av400
PROBHD   Z163739_1011 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6410.256
FIDRES         0.195625
AQ             5.1118078
RG                104.12
DW                78.000
DE                  6.50
TE                298.0
D1            1.00000000
TD0                   1
SFO1         400.1924011
NUC1                1H
P0                 2.67
P1                 8.00
PLW1         22.76199913

F2 - Processing paramete
SI                32768
SF           400.1900000
WDW                  EM
SSB                   0
LB                 0.30
GB                    0
PC                 1.00
```

C7 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 90



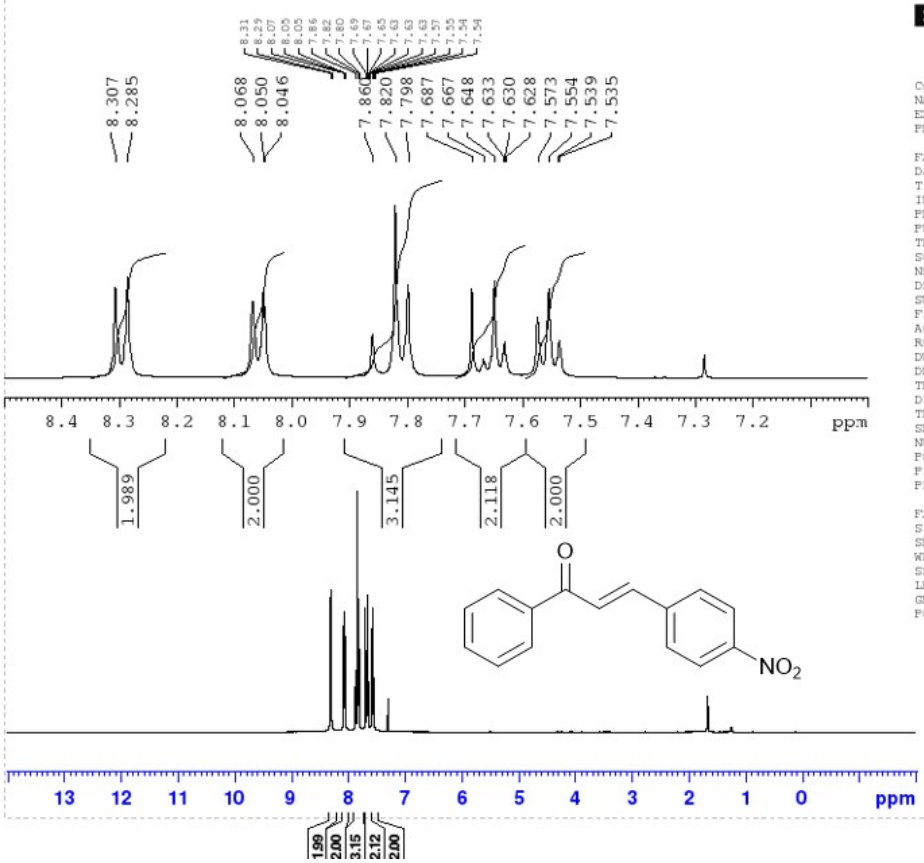
BRUKER

```
Current Data Parameters
NAME      Sep19-2025-Alex
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameter
Date_           20250919
Time              12.09 h
INSTRUM            av400
PROBHD   Z163739_1011 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23148.148 Hz
FIDRES         0.706425 Hz
AQ             1.4155777 se
RG                209.43
DW                21.600 us
DE                 6.50 us
TE                298.0 K
D1            2.00000000 se
D11           0.03000000 se
TD0                   1
SFO1         100.6384215 MH
NUC1                13C
P0                 2.67 us
P1                 8.00 us
PLW1         98.76699829 W
SFO2         400.1916008 MH
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 us
PLW2         22.76199913 W
PLW12         0.17985000 W
PLW13         0.09046300 W

F2 - Processing parameters
SI                32768
SF           100.6278555 MH
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

C19 RECRY
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 28



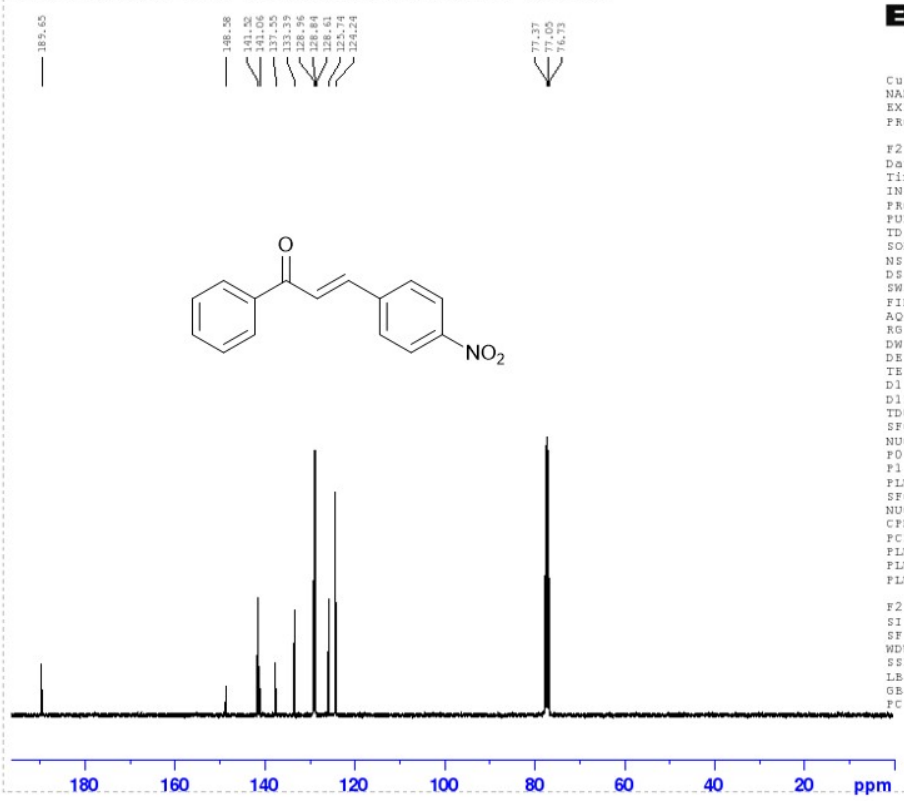
BRUKER

```
Current Data Parameters
NAME      Nov26-2025-Alex
EXPNO                  80
PROCNO                  1

F2 - Acquisition Parameters
Date_           20251126
Time              12.52 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118078 sec
RG                104.12
DW                78.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SF01          400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C19 RECRY
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 28



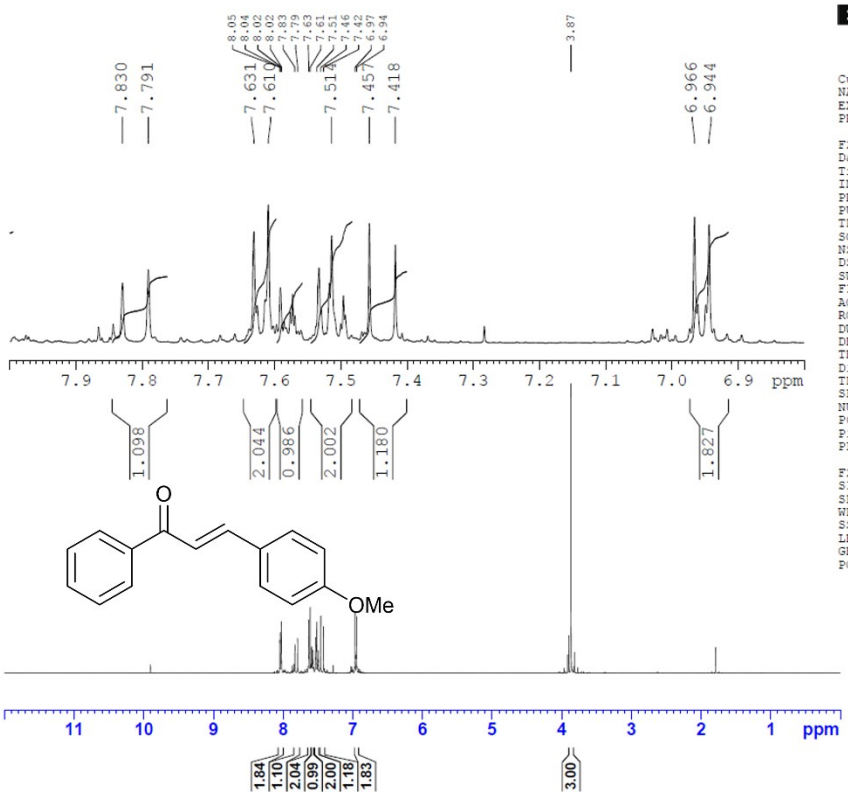
BRUKER

```
Current Data Parameters
NAME      Nov26-2025-Alex
EXPNO                 120
PROCNO                  1

F2 - Acquisition Parameters
Date_           20251126
Time              14.45 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155577 sec
RG                209.43
DW                21.600 use
DE                 6.50 use
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6384215 MHz
NUC1                  13C
P0                 2.67 use
P1                 8.00 use
PLW1          98.76699829 W
SFO2          400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 use
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C18W
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 45

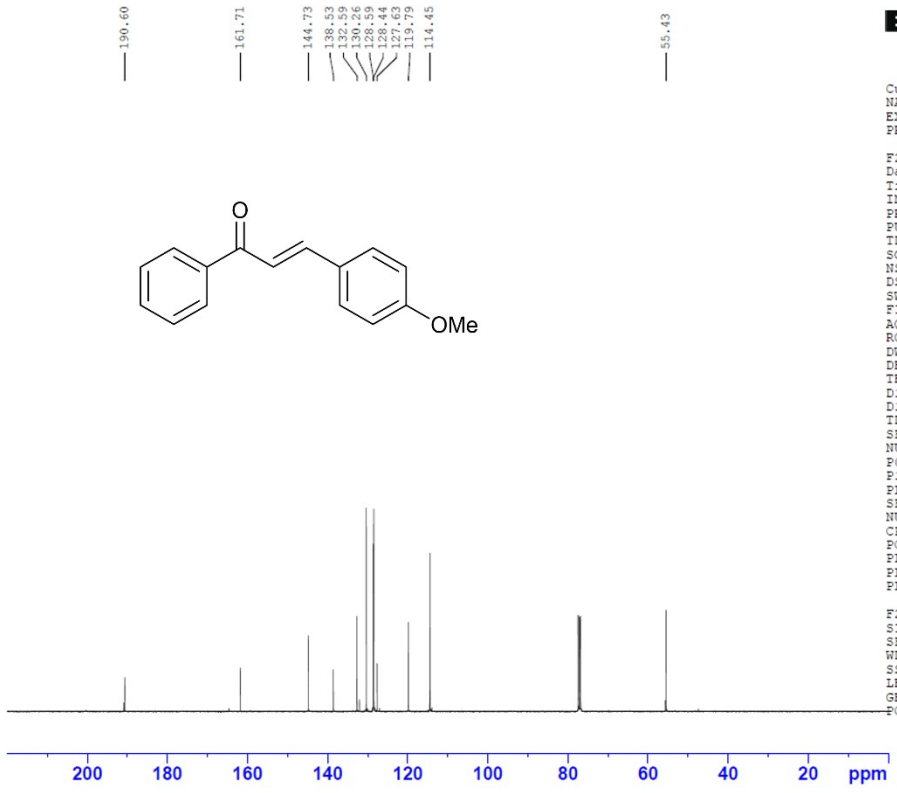


```
Current Data Parameters
NAME      Sep17-2025-Alex
EXPNO                 90
PROCNO                 1

F2 - Acquisition Parameters
Date_           20250917
Time              12.20 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               5.1118078 sec
RG                  50.17
DW                 78.000 usec
DE                  6.50 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                     1
SFO1           400.1924011 MHz
NUC1                   1H
P0                  2.67 usec
P1                  8.00 usec
PLW1           22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C18W Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 45

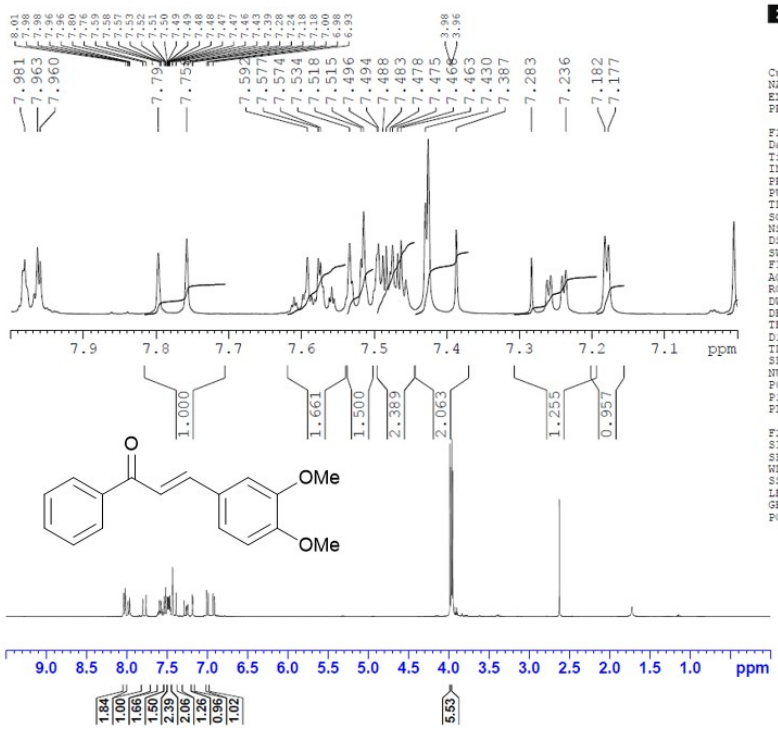


```
Current Data Parameters
NAME      Sep17-2025-Alex
EXPNO                110
PROCNO                 1

F2 - Acquisition Parameters
Date_           20250917
Time              14.06 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH             23148.148 Hz
FIDRES           0.706425 Hz
AQ               1.4155777 sec
RG                  209.43
DW                 21.600 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1           100.6384215 MHz
NUC1                   13C
P0                  2.67 usec
P1                  8.00 usec
PLW1           98.76699829 W
SFO2           400.1916008 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2           22.76199913 W
PLW12           0.17985000 W
PLW13           0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C15
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 47



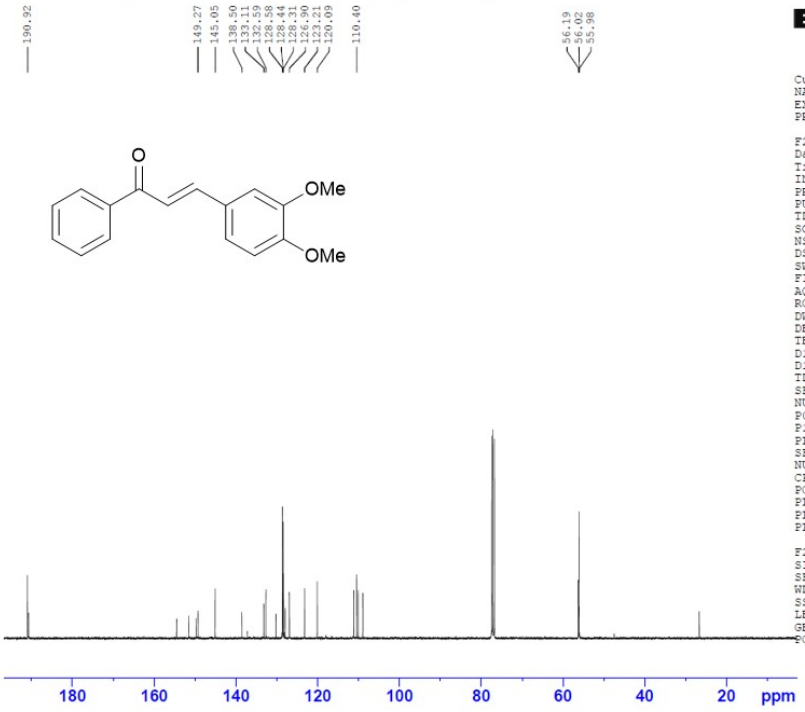
BRUKER

```
Current Data Parameters
NAME      Oct20-2025-Alex
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251020
Time              10.56 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ               5.1118078 sec
RG                 63.64
DW                78.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          22.76199913 W

F2 - Processing parameters
SI                 32768
SF          400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C15
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 47



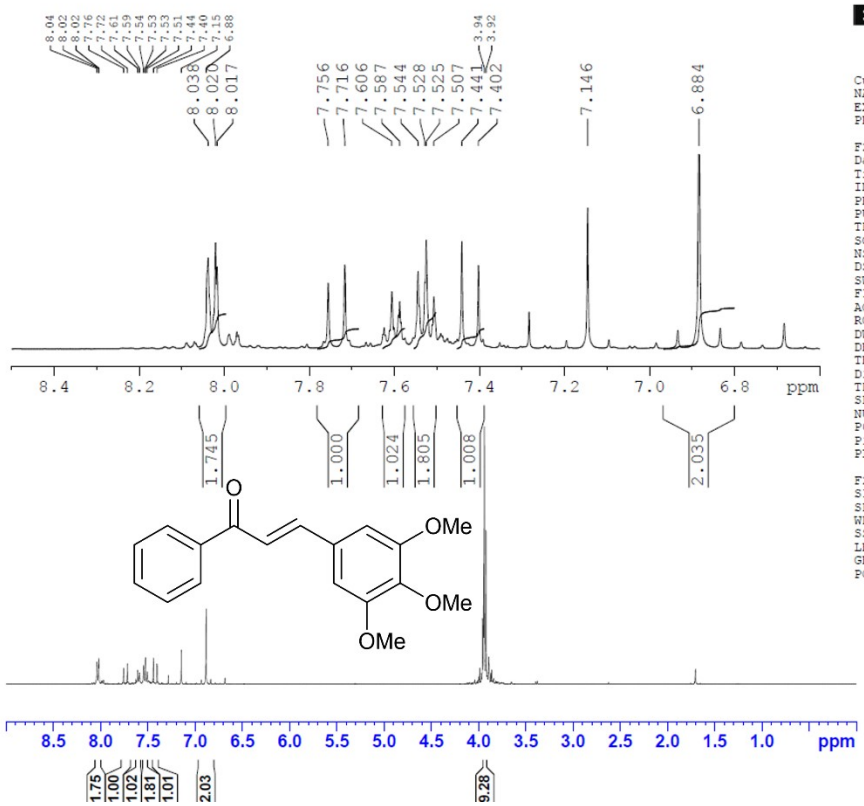
BRUKER

```
Current Data Parameters
NAME      Oct20-2025-Alex
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251020
Time              11.28 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ               1.4155777 sec
RG                 209.43
DW                21.600 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6384215 MHz
NUC1                  13C
P0                 2.67 usec
P1                 8.00 usec
PLW1          98.76699829 W
SFO2         400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF          100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C21
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 28

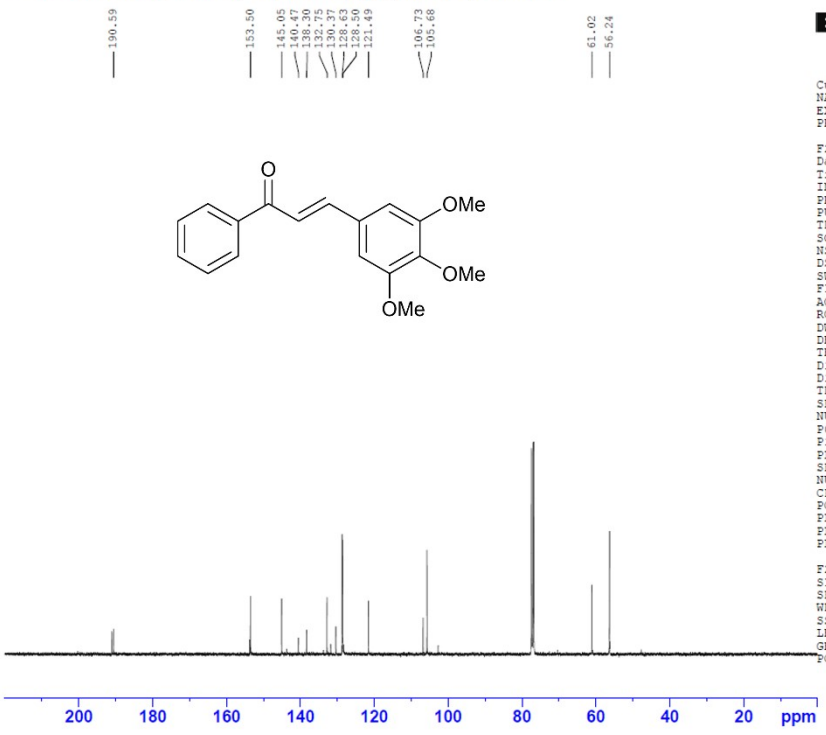


Current Data Parameters
NAME Sep12-2025-Alex
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250912
Time 10.50 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 71.26
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C21
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 28

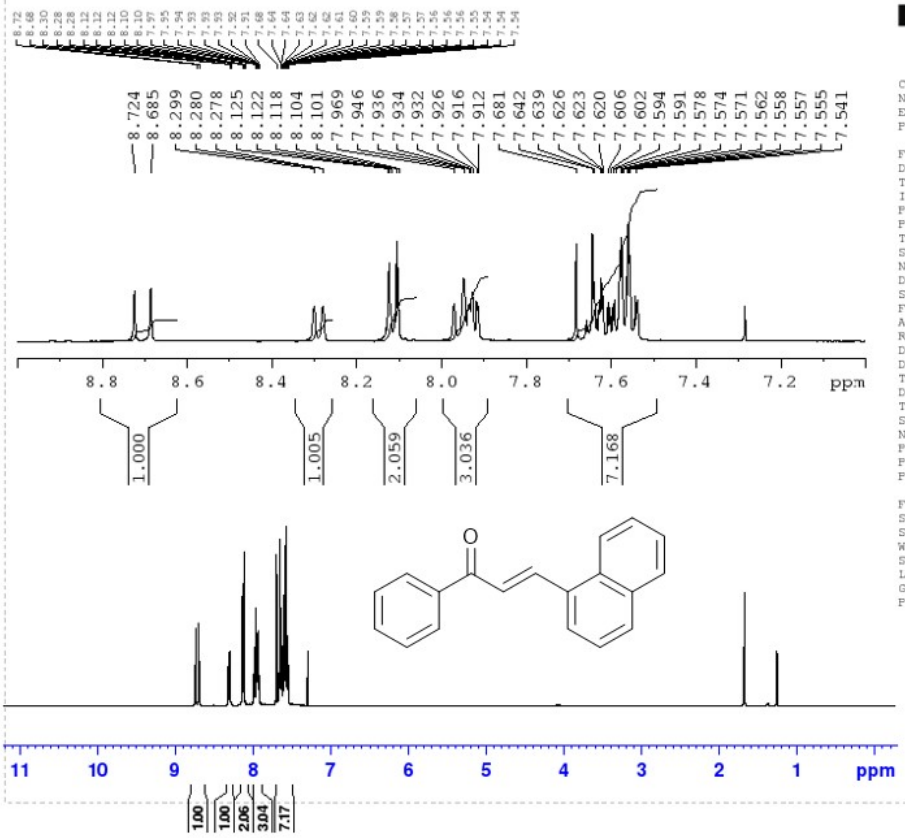


Current Data Parameters
NAME Sep12-2025-Alex
EXPNO 80
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250912
Time 12.24 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C22
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 1

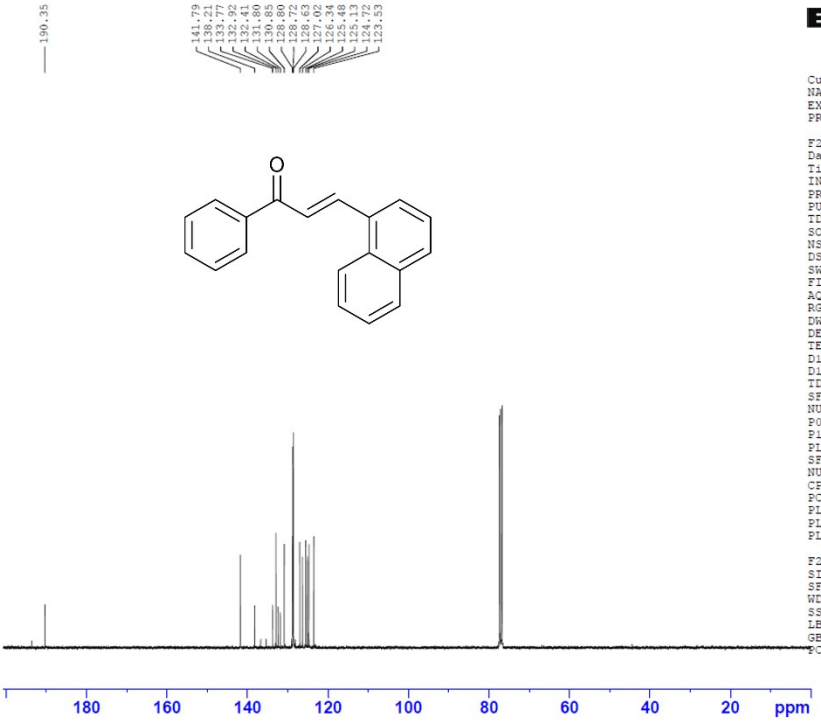


Current Data Parameters
NAME Nov28-2025-Alex
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251128
Time 12.49 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C22W Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 40

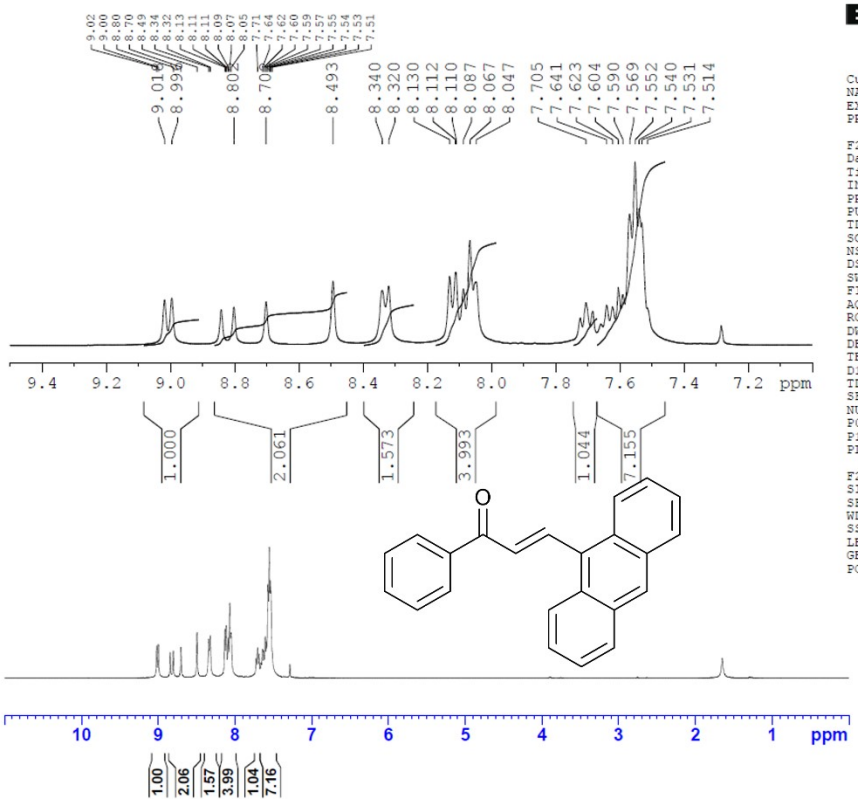


Current Data Parameters
NAME Sep17-2025-Alex
EXPNO 170
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250917
Time 16.34 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C23
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 80

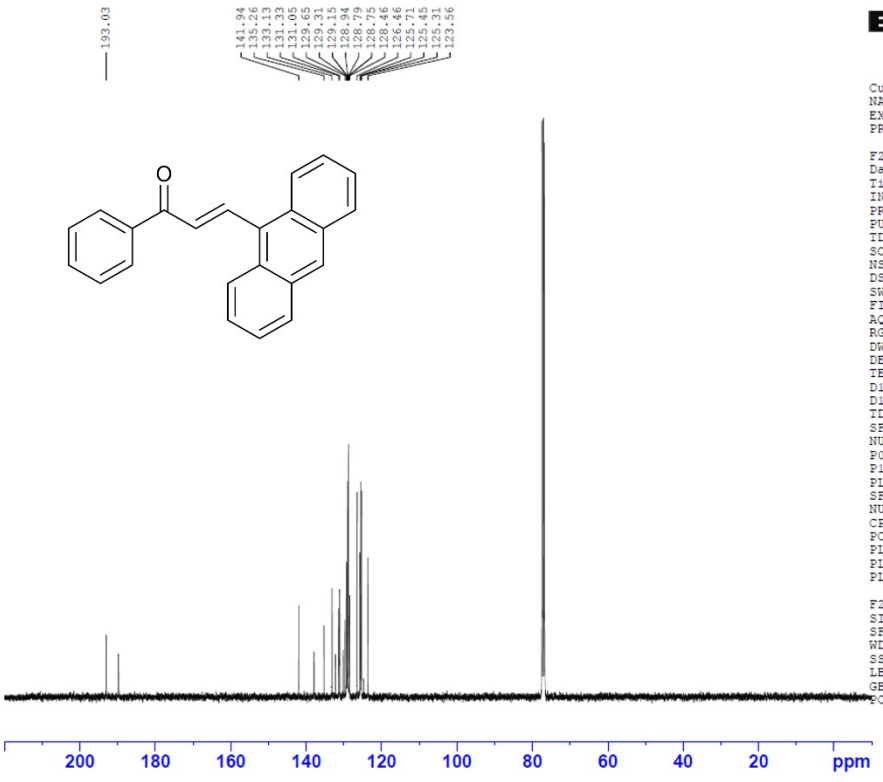


Current Data Parameters
NAME Sep17-2025-Alex
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250917
Time 9.08 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C23 CARBON
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 80

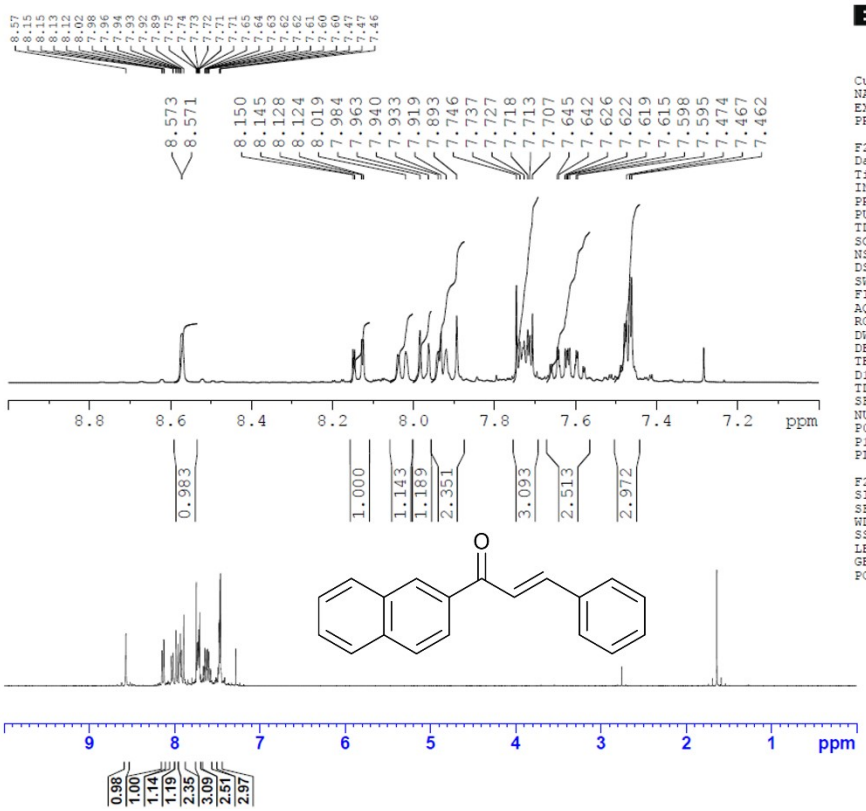


Current Data Parameters
NAME Sep17-2025-Alex
EXPNO 80
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250917
Time 11.14 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C9
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 59

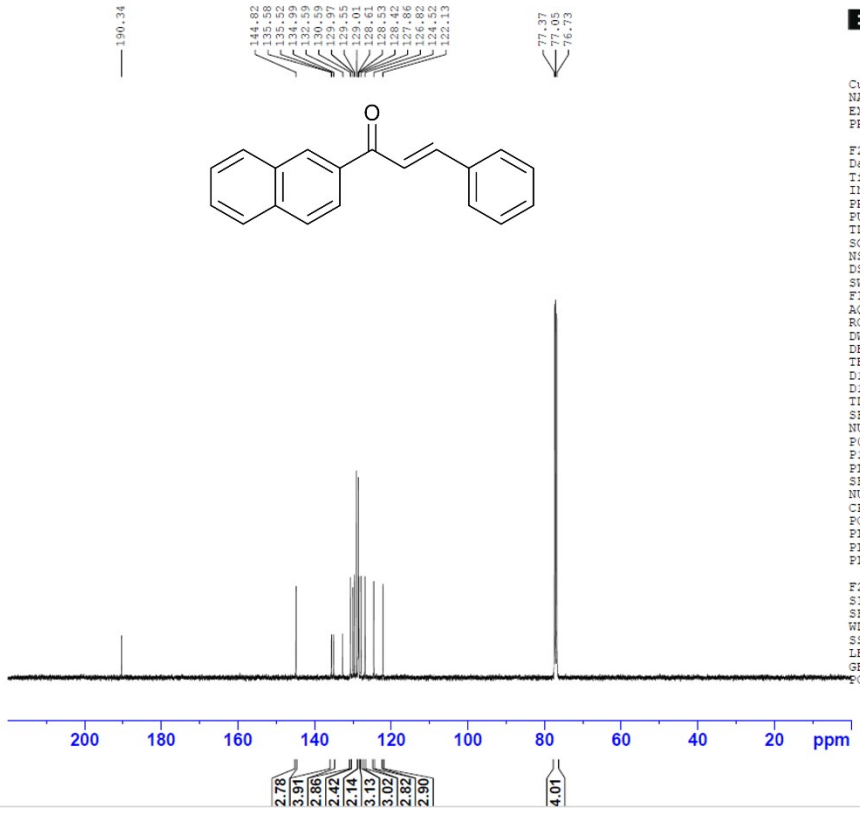


Current Data Parameters
NAME Sep09-2025-Alex
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250909
Time 11.30 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

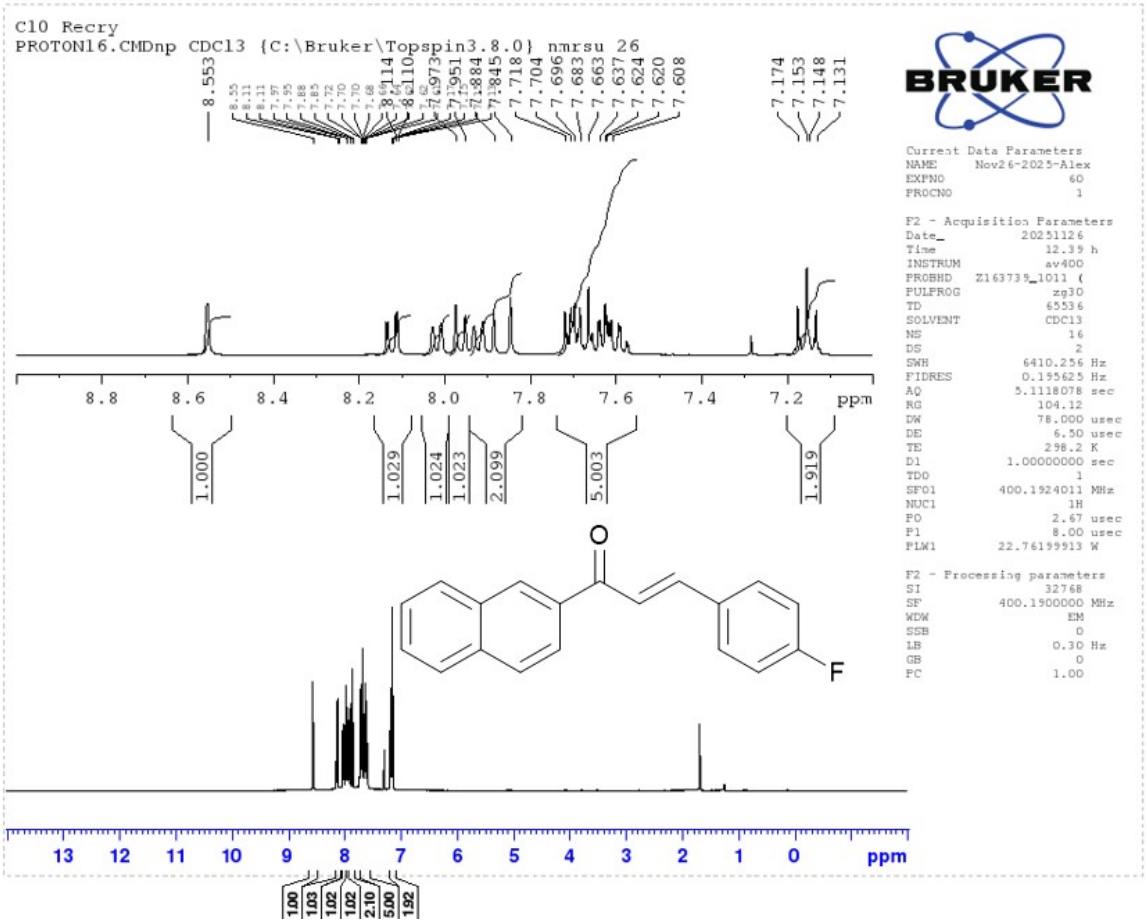
C9 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 59

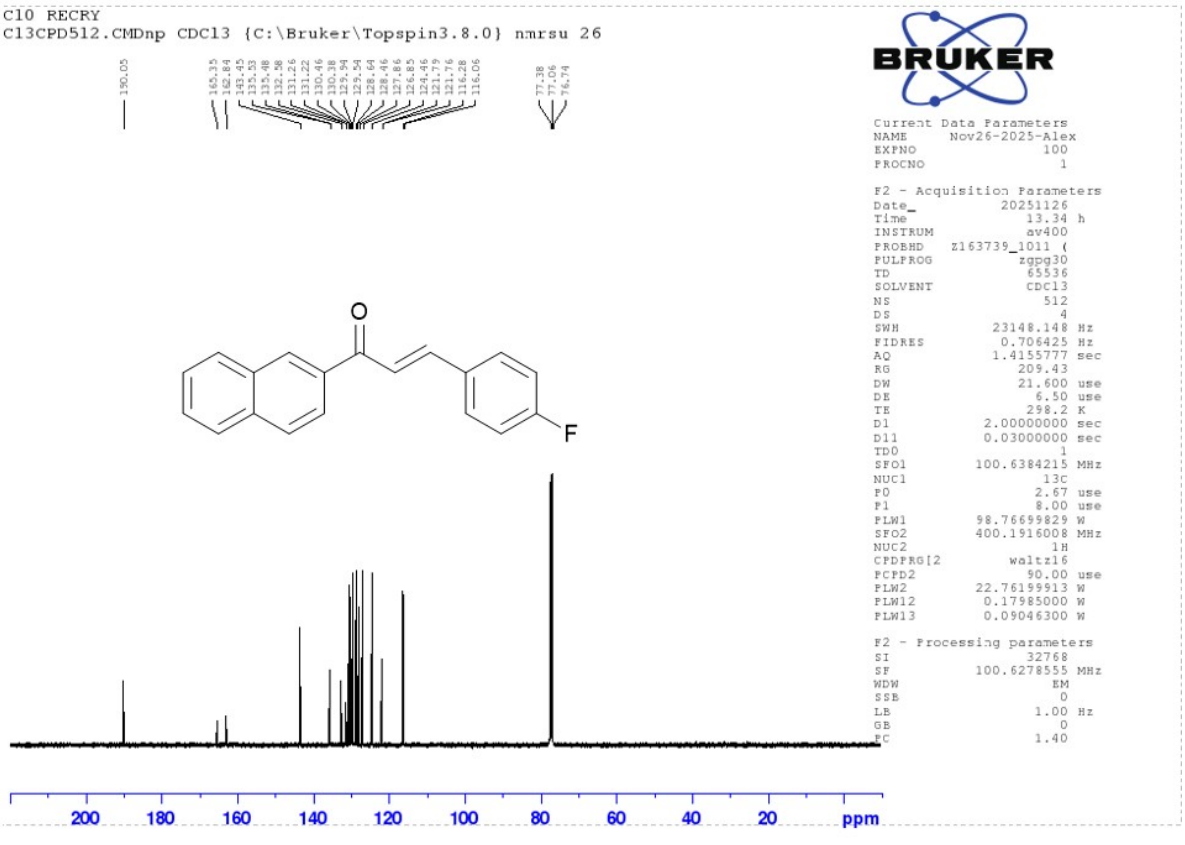


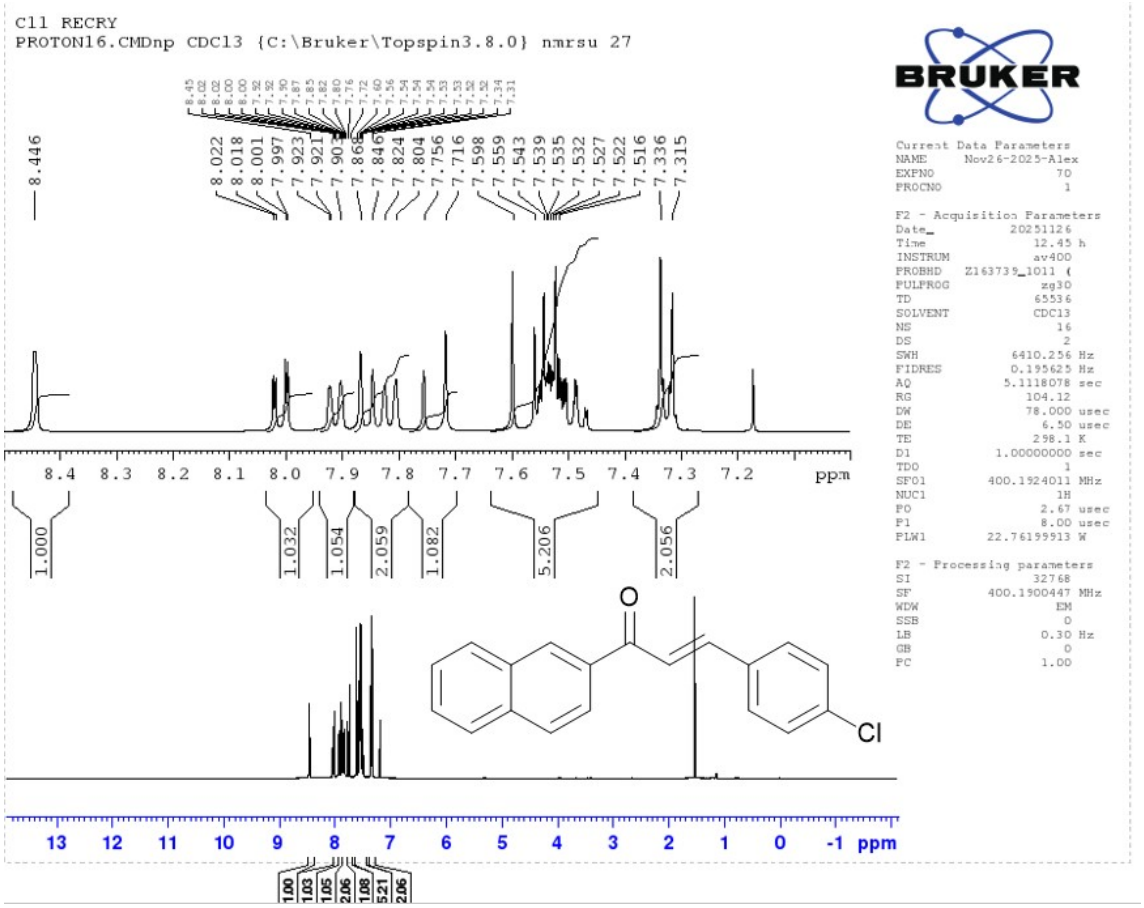
Current Data Parameters
NAME Sep09-2025-Alex
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250909
Time 17.09 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


C10 Recry
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 26
8.553
8.114
8.110
7.973
7.951
7.884
7.845
7.718
7.704
7.696
7.683
7.663
7.637
7.624
7.620
7.608
7.174
7.153
7.148
7.131
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
1.000
1.029
1.024
1.023
2.099
5.003
1.919
O
F
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.02
1.02
2.10
5.00
1.92
Current Data Parameters
NAME Nov26-2025-Alex
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251126
Time 12.39 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W
F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


C10 RECRY
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 26
190.05
165.35
162.84
143.45
135.53
135.48
132.58
131.26
131.22
130.46
130.38
129.94
129.54
128.64
128.46
127.86
126.85
124.46
121.79
121.76
116.28
116.06
77.38
77.06
76.74
O
F
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Nov26-2025-Alex
EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251126
Time 13.34 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.41555777 sec
RG 209.43
DW 21.600 use
DE 6.50 use
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 use
P1 8.00 use
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 use
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W
F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

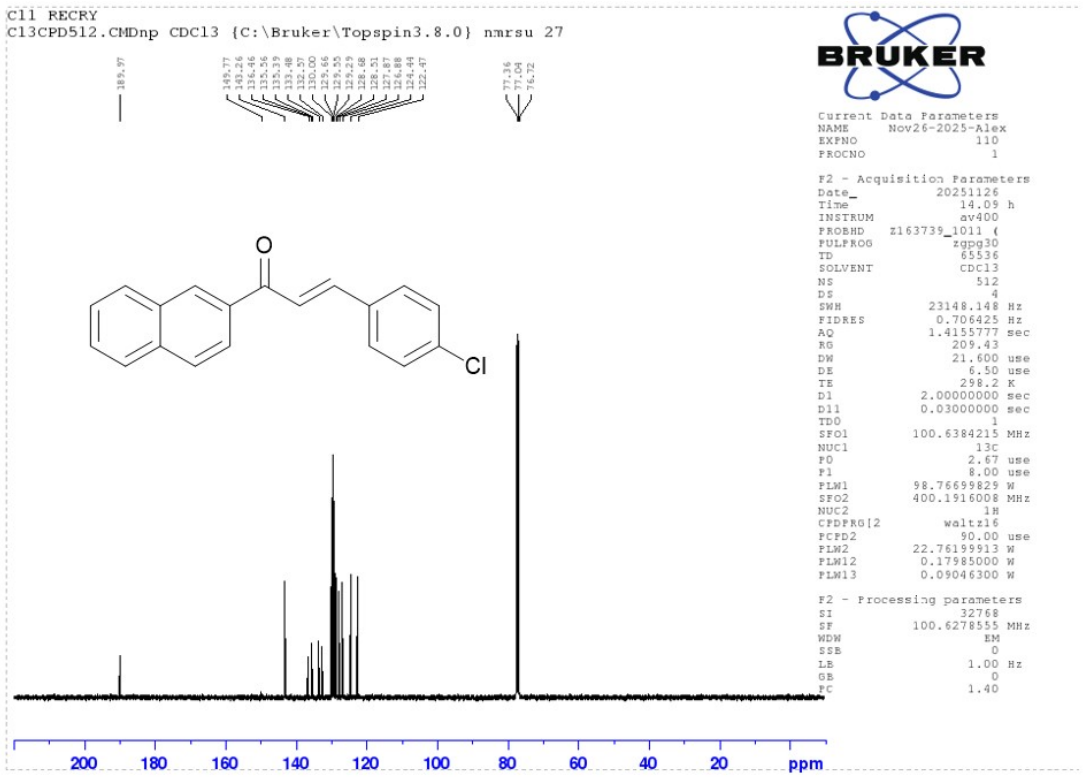


BRUKER

```
Current Data Parameters
NAME        Nov26-2025-Alex
EXPNO                   70
PROCNO                   1

F2 - Acquisition Parameters
Date_             20251126
Time                12.45 h
INSTRUM             av400
PROBHD    Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES             0.195625 Hz
AQ              5.1118078 sec
RG                  104.12
DW                78.000 usec
DE                 6.50 usec
TE                 298.1 K
D1              1.00000000 sec
TD0                    1
SF01           400.1924011 MHz
NUC1                   1H
P0                 2.67 usec
P1                 8.00 usec
PLW1           22.76199913 W

F2 - Processing parameters
SI                 32768
SF             400.1900447 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



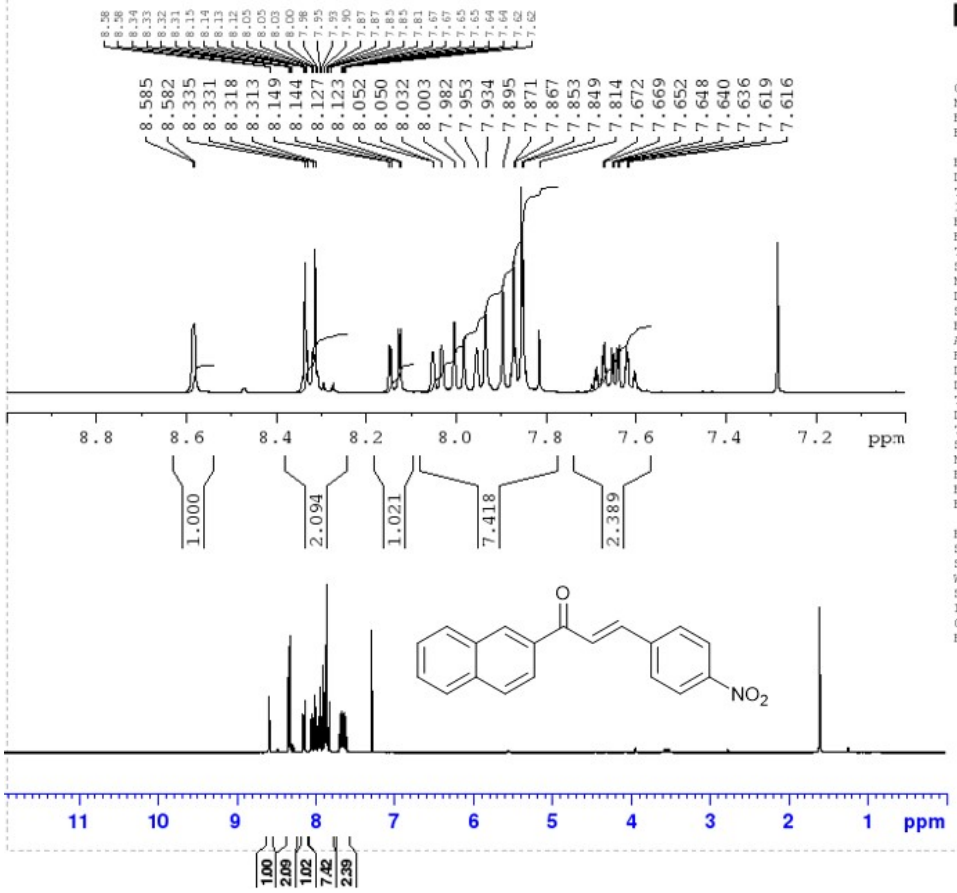
BRUKER

```
Current Data Parameters
NAME        Nov26-2025-Alex
EXPNO                  110
PROCNO                   1

F2 - Acquisition Parameters
Date_             20251126
Time                14.09 h
INSTRUM             av400
PROBHD    Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES             0.706425 Hz
AQ              1.4155777 sec
RG                  209.43
DW                21.600 use
DE                 6.50 use
TE                 298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SF01           100.6384215 MHz
NUC1                   13c
P0                 2.67 use
P1                 8.00 use
PLW1           98.76699829 W
SFO2           400.1916008 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 use
PLW2           22.76199913 W
PLW12           0.17985000 W
PLW13           0.09046300 W

F2 - Processing parameters
SI                 32768
SF             100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C25 RECRY
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 29

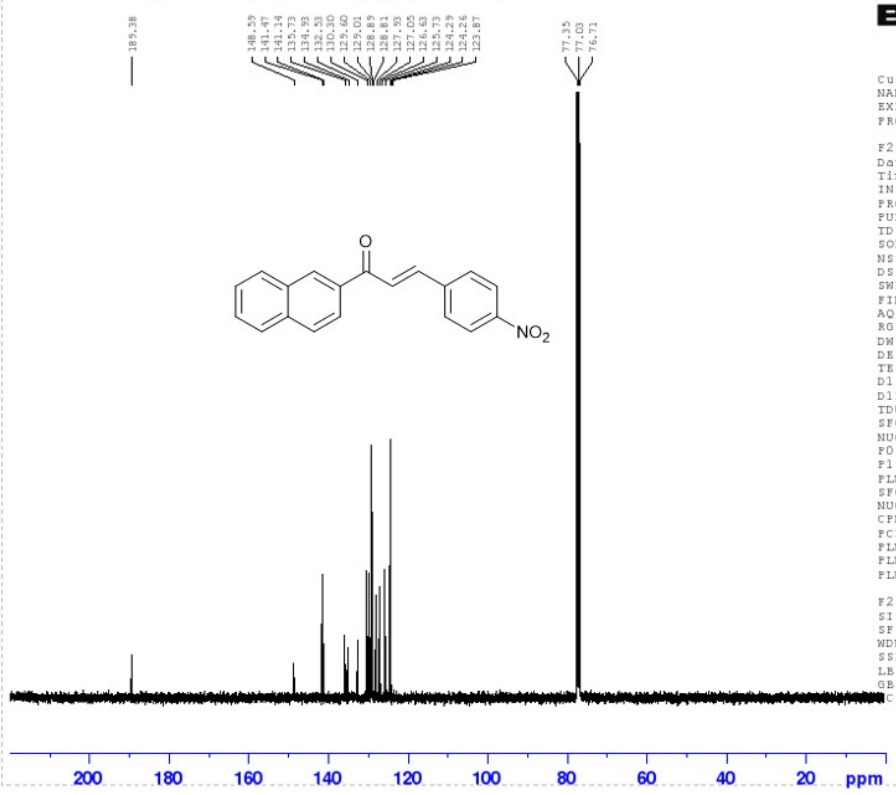


Current Data Parameters
NAME Nov26-2025-Alex
EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251126
Time 14.51 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 185.2
DW 78.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

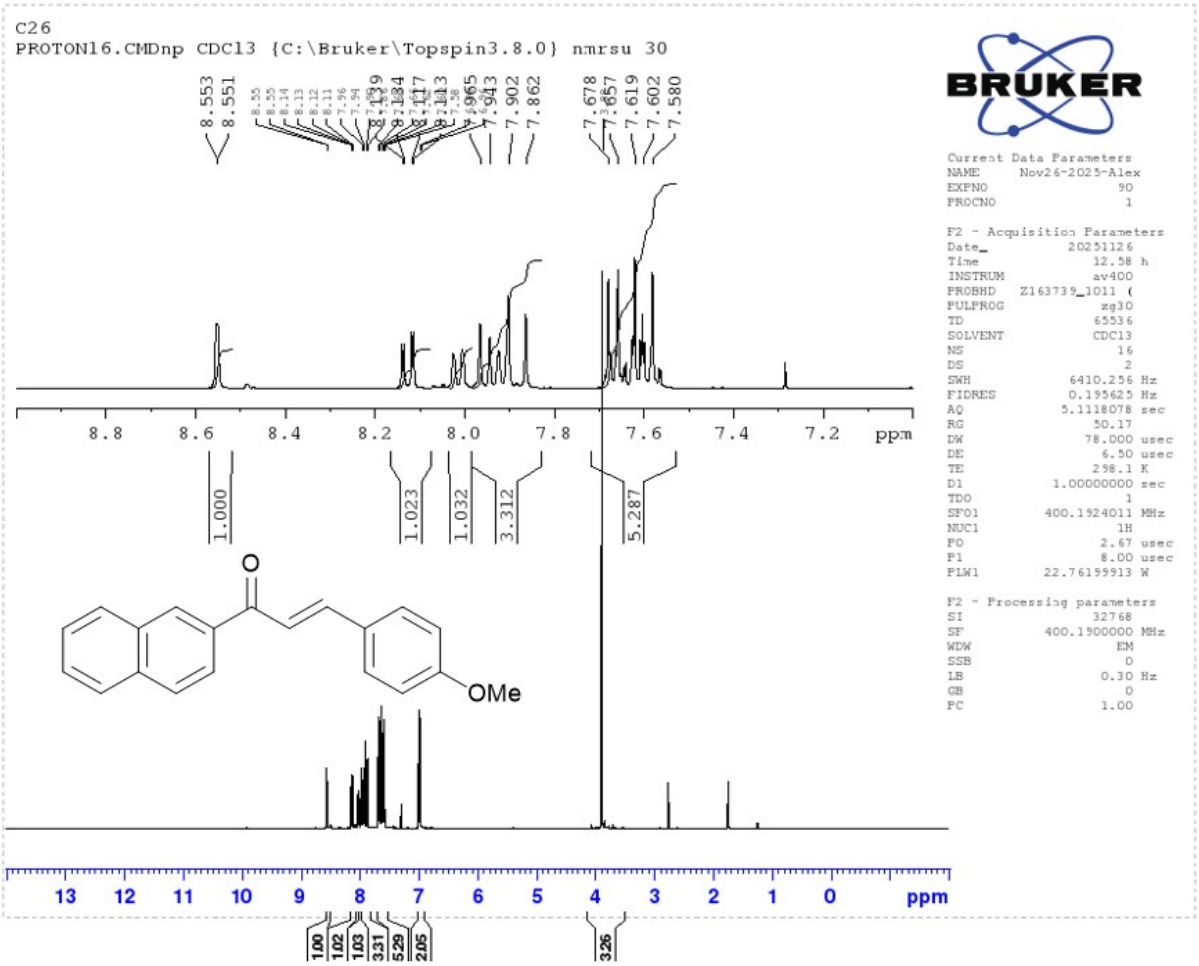
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 29



Current Data Parameters
NAME Nov26-2025-Alex
EXPNO 131
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251126
Time 15.22 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 use
DE 6.50 use
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 use
P1 8.00 use
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 use
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
C 1.40



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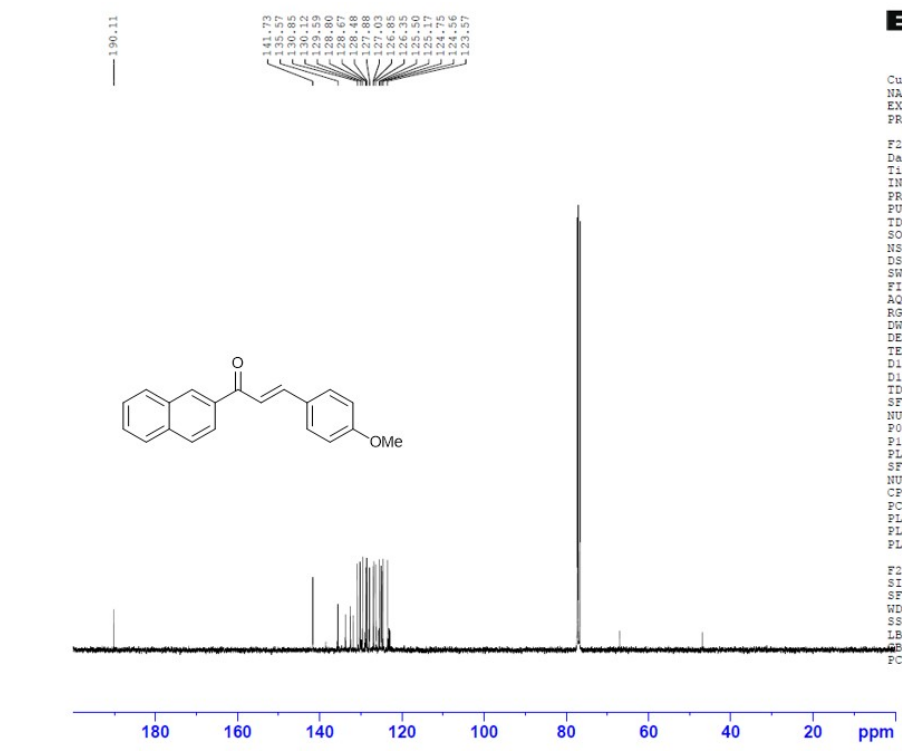
```
Current Data Parameters
NAME      Nov26-2025-Alex
EXPNO                  90
PROCNO                  1

F2 - Acquisition Parameters
Date_            20251126
Time                12.58 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118078 sec
RG                 50.17
DW                78.000 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
SFO1           400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1           22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



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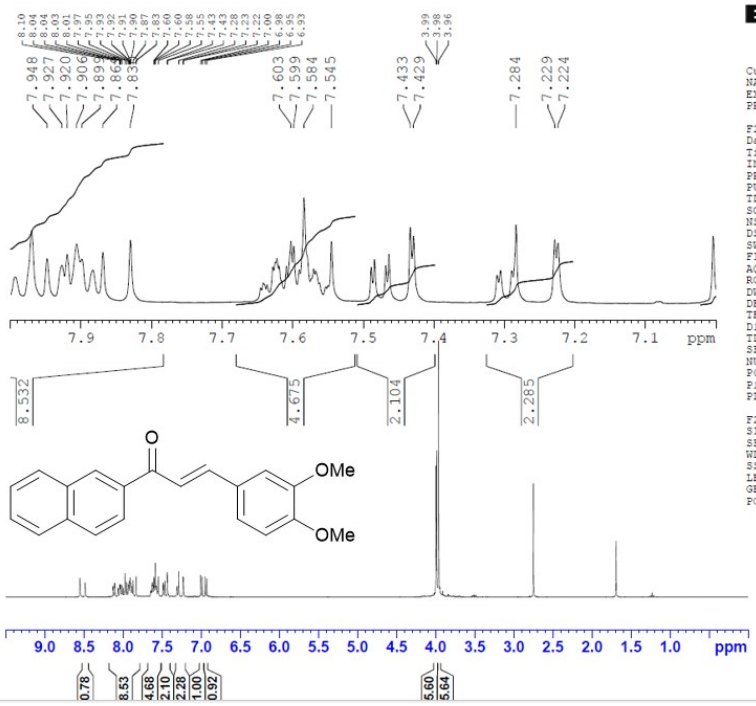
```
Current Data Parameters
NAME      Oct20-2025-Alex
EXPNO                  31
PROCNO                  1

F2 - Acquisition Parameters
Date_            20251020
Time                12.43 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155777 sec
RG                 209.43
DW                21.600 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           100.6384215 MHz
NUC1                  13C
P0                 2.67 usec
P1                 8.00 usec
PLW1           98.76699829 W
SFO2           400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2           22.76199913 W
PLW12           0.17985000 W
PLW13           0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C24
PROTON16.CMDnp CDC13 {C:\Bruker\TopSpin3.6.5} nmrsu 48



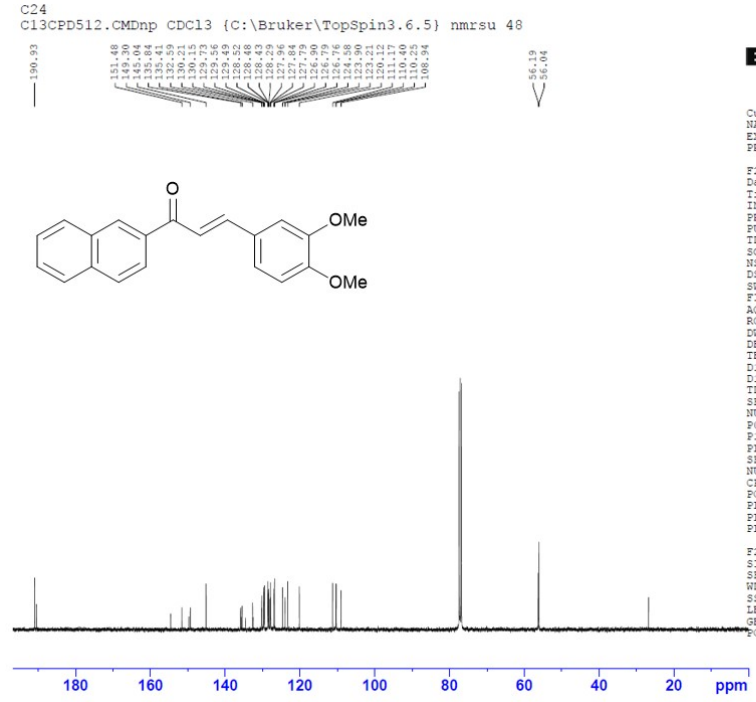
BRUKER

```
Current Data Parameters
NAME      Oct20-2025-Alex
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251020
Time              11.35 h
INSTRUM             av400
PROBHD    Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118078 sec
RG                 104.12
DW                 78.000 usec
DE                  6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C24
C13CPD512.CMDnp CDC13 {C:\Bruker\TopSpin3.6.5} nmrsu 48

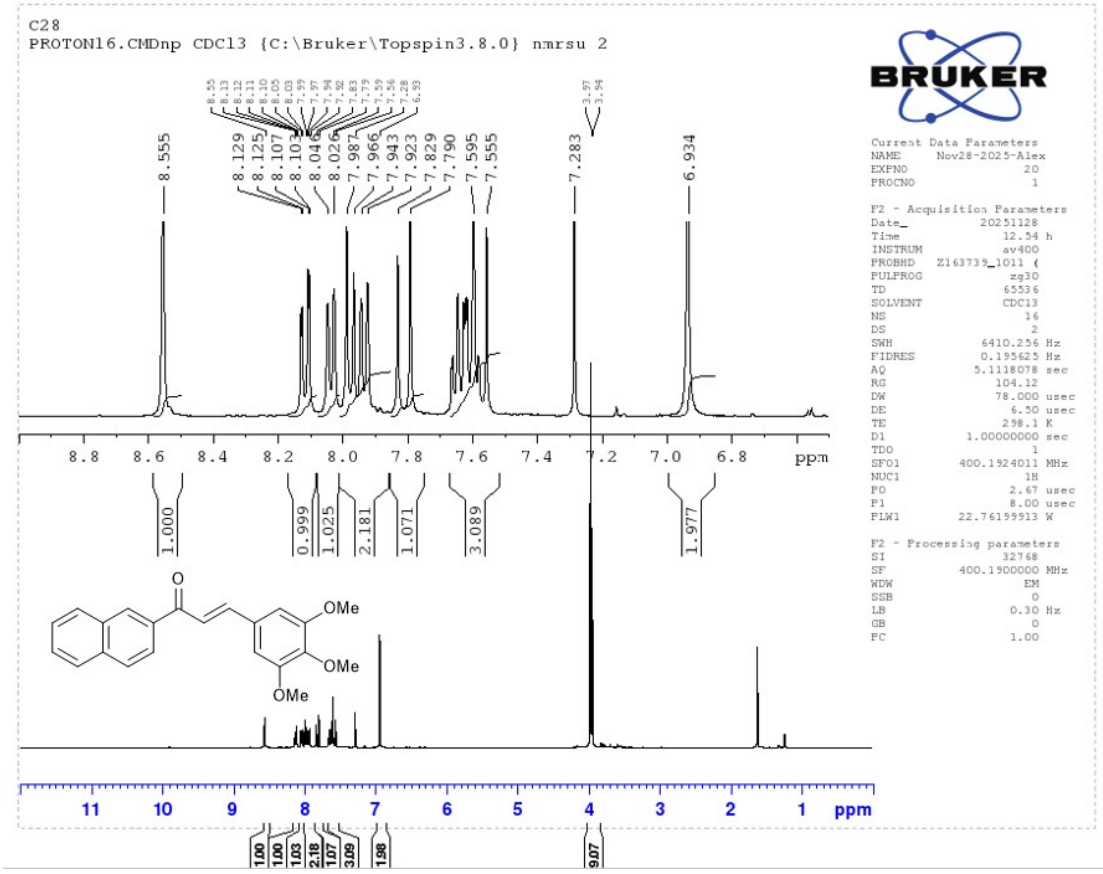


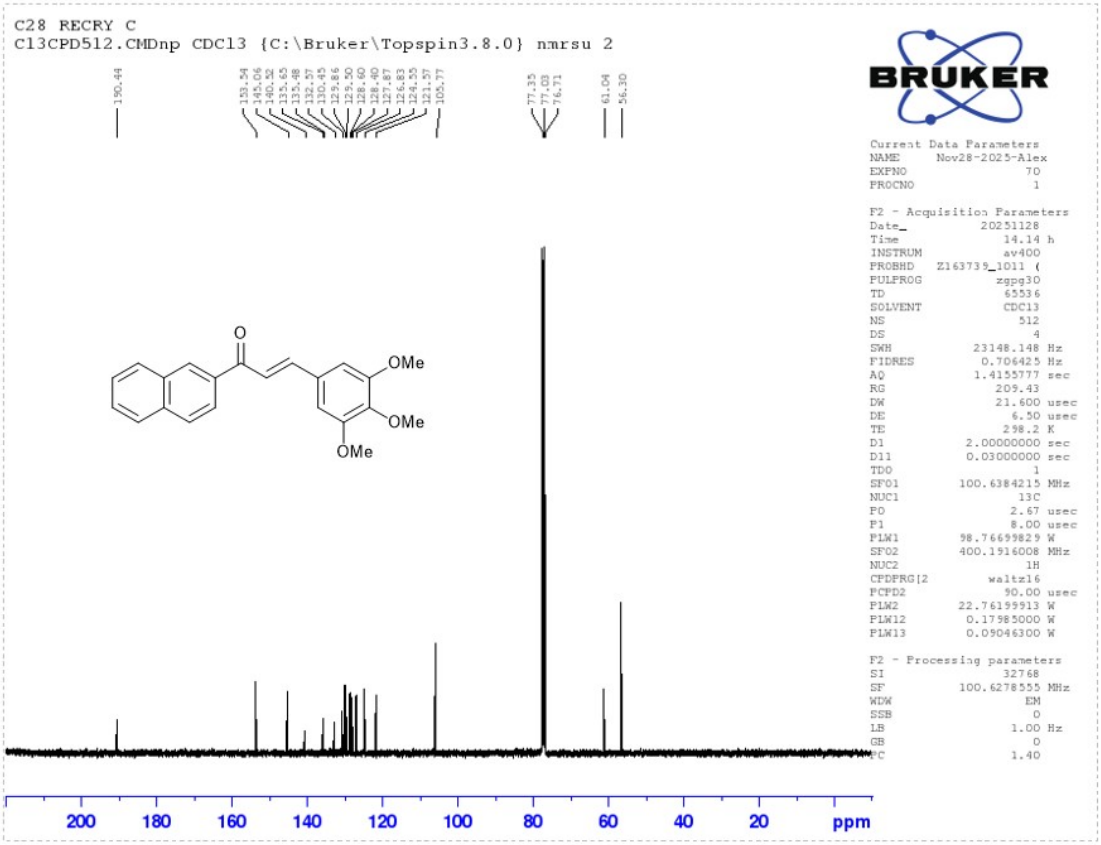
BRUKER

```
Current Data Parameters
NAME      Oct20-2025-Alex
EXPNO                 21
PROCNO                 1

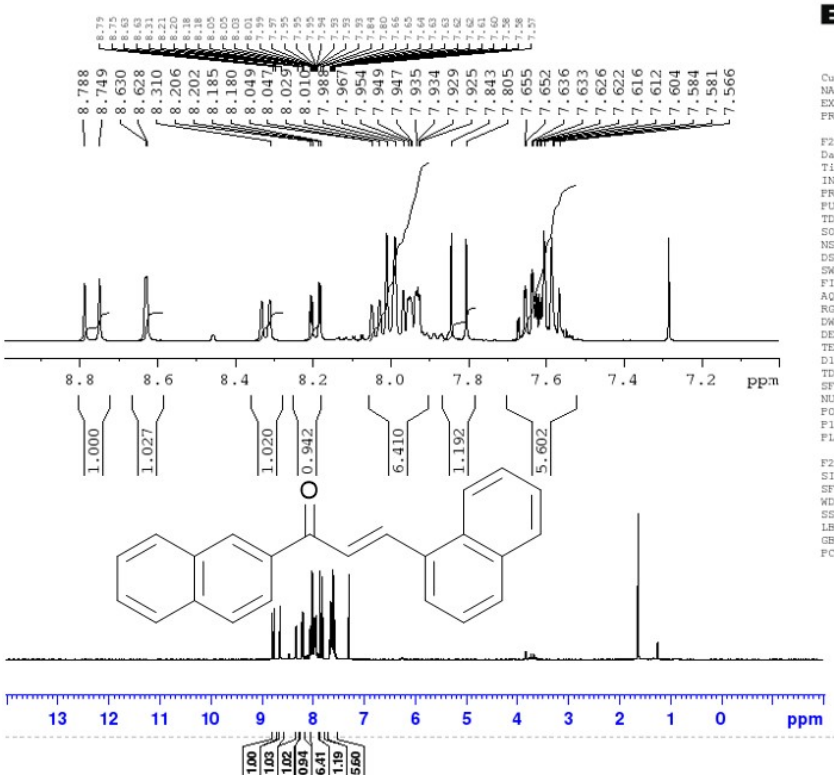
F2 - Acquisition Parameters
Date_           20251020
Time              12.06 h
INSTRUM             av400
PROBHD    Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155777 sec
RG                 209.43
DW                 21.600 usec
DE                  6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6384215 MHz
NUC1                  13C
P0                 2.67 usec
P1                 8.00 usec
PLW1          98.76699829 W
SFO2          400.1916008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


C28
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 2
8.555
8.129
8.125
8.107
8.103
8.046
8.026
7.987
7.966
7.943
7.923
7.829
7.790
7.595
7.555
7.283
6.934
ppm
1.000
0.999
1.025
2.181
1.071
3.089
1.977
OMe
OMe
OMe
Current Data Parameters
NAME Nov28-2025-Alex
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251128
Time 12.54 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W
F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


C28 RECRY C
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 2
190.44
153.54
145.06
140.52
135.65
132.98
131.37
130.45
125.86
125.50
128.40
128.40
127.87
126.83
124.55
121.57
105.77
77.35
77.03
76.71
61.04
56.30
ppm
OMe
OMe
OMe
Current Data Parameters
NAME Nov28-2025-Alex
EXPNO 70
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251128
Time 14.14 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76659829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W
F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C29
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 3



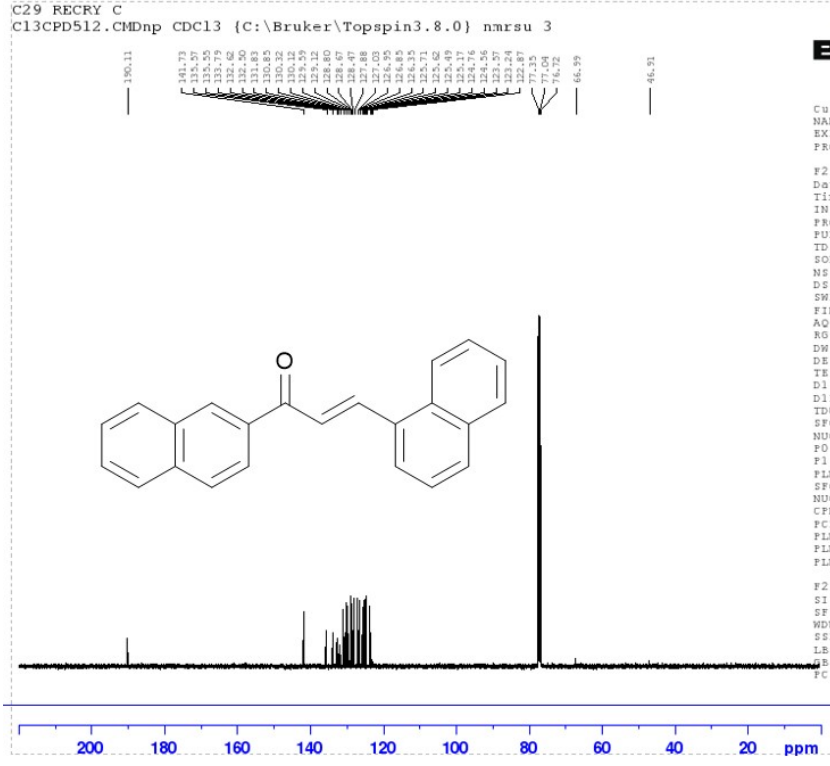
BRUKER

```
Current Data Parameters
NAME      Nov28-2025-Alex
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251128
Time              13.00 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118078 sec
RG                 104.12
DW                78.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SF01         400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1         22.76199913 W

F2 - Processing parameters
SI                 32768
SF          400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C29 RECRY C
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 3



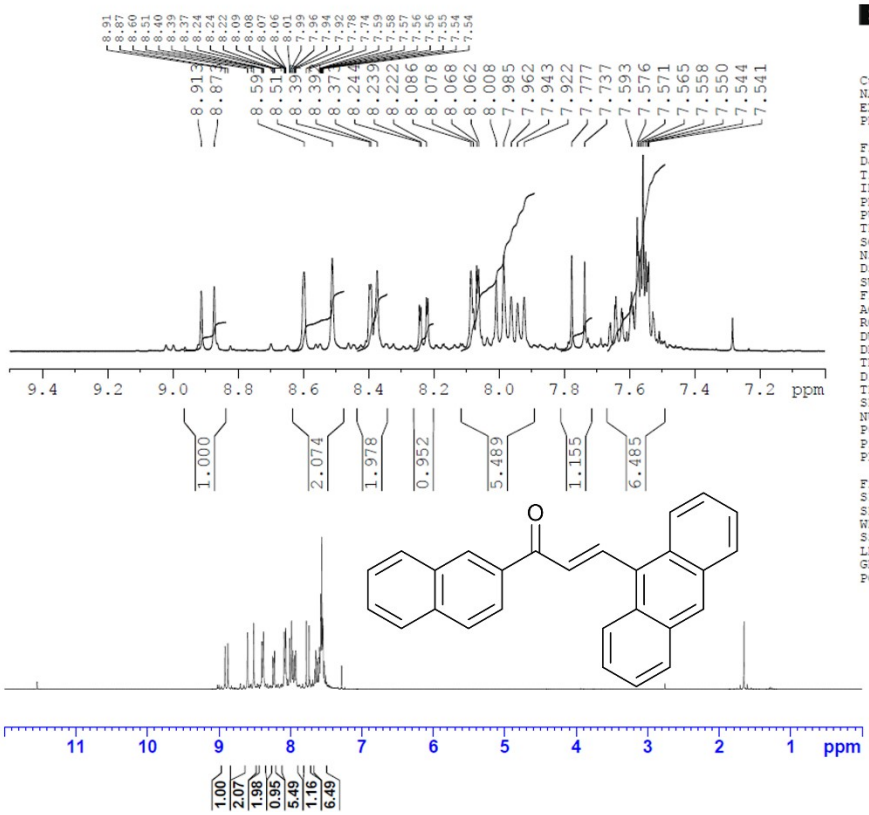
BRUKER

```
Current Data Parameters
NAME      Nov28-2025-Alex
EXPNO                 80
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251128
Time              14.48 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155577 sec
RG                 209.43
DW                21.600 use
DE                 6.50 use
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SF01         100.6384215 MHz
NUC1                  13C
P0                 2.67 use
P1                 8.00 use
PLW1         98.76699829 W
SF02         400.1916008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 use
PLW2         22.76199913 W
PLW12         0.17985000 W
PLW13         0.09046300 W

F2 - Processing parameters
SI                 32768
SF          100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

C30 Washed
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 65

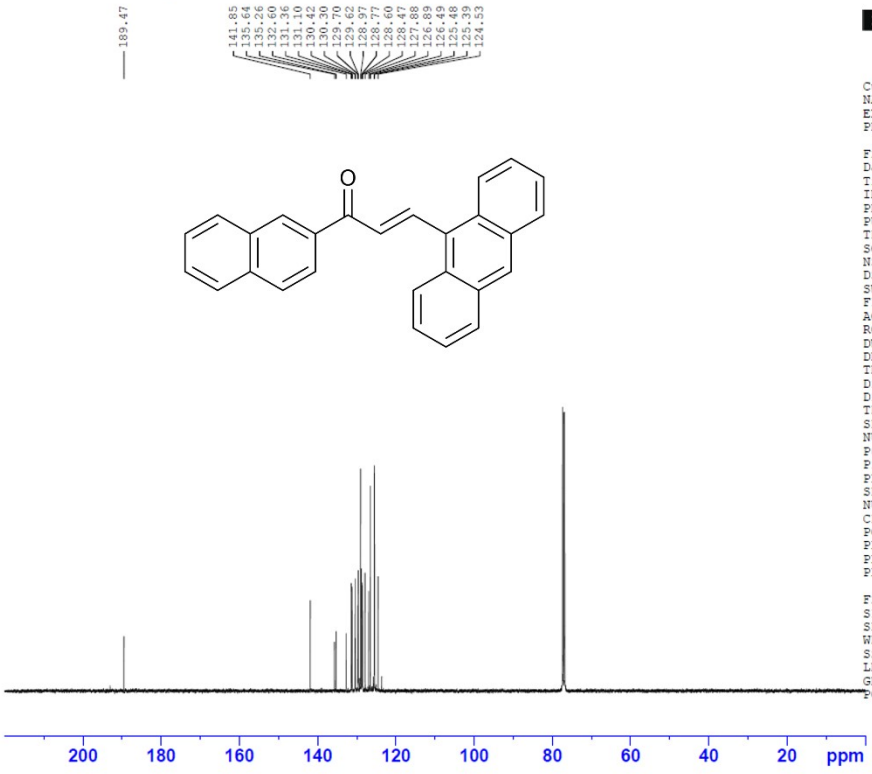


Current Data Parameters
NAME Sep24-2025-Alex
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250924
Time_ 15.45 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C30 Carbon
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 65

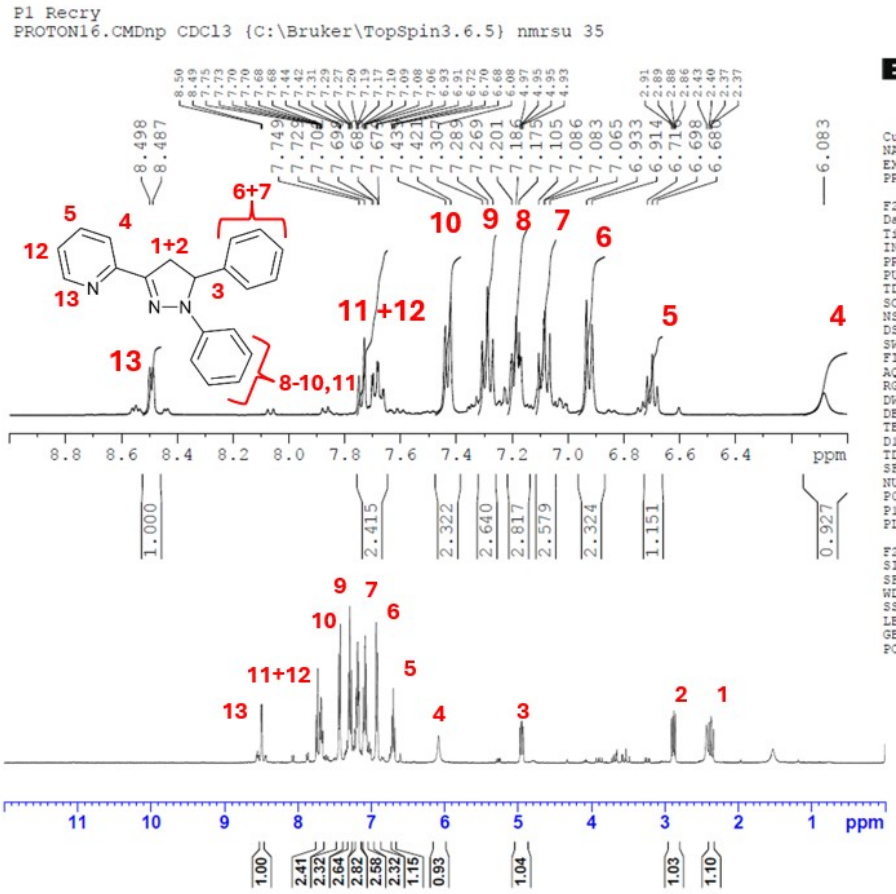


Current Data Parameters
NAME Sep24-2025-Alex
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250924
Time_ 18.51 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P1 Recry
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 35

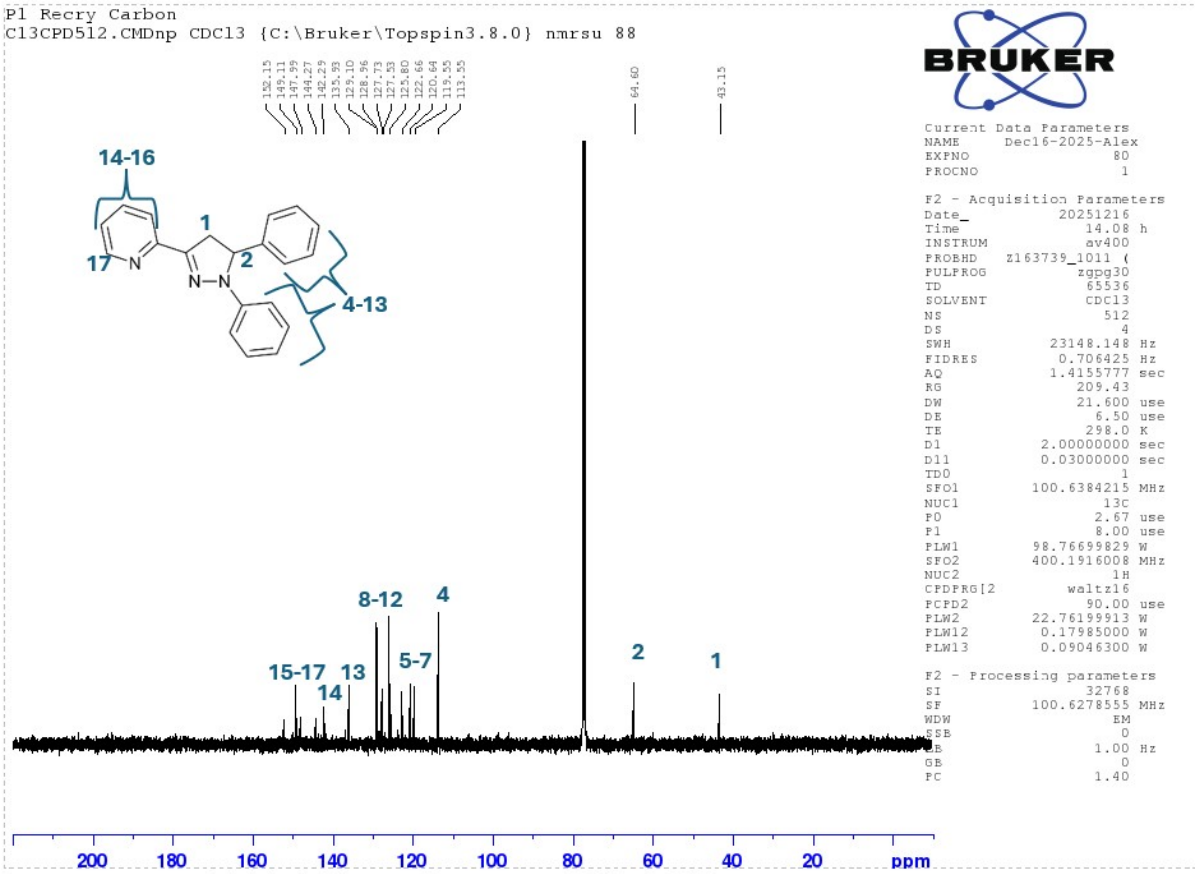


BRUKER

Current Data Parameters
NAME Oct10-2025-Alex
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251010
Time 10.07 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900435 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

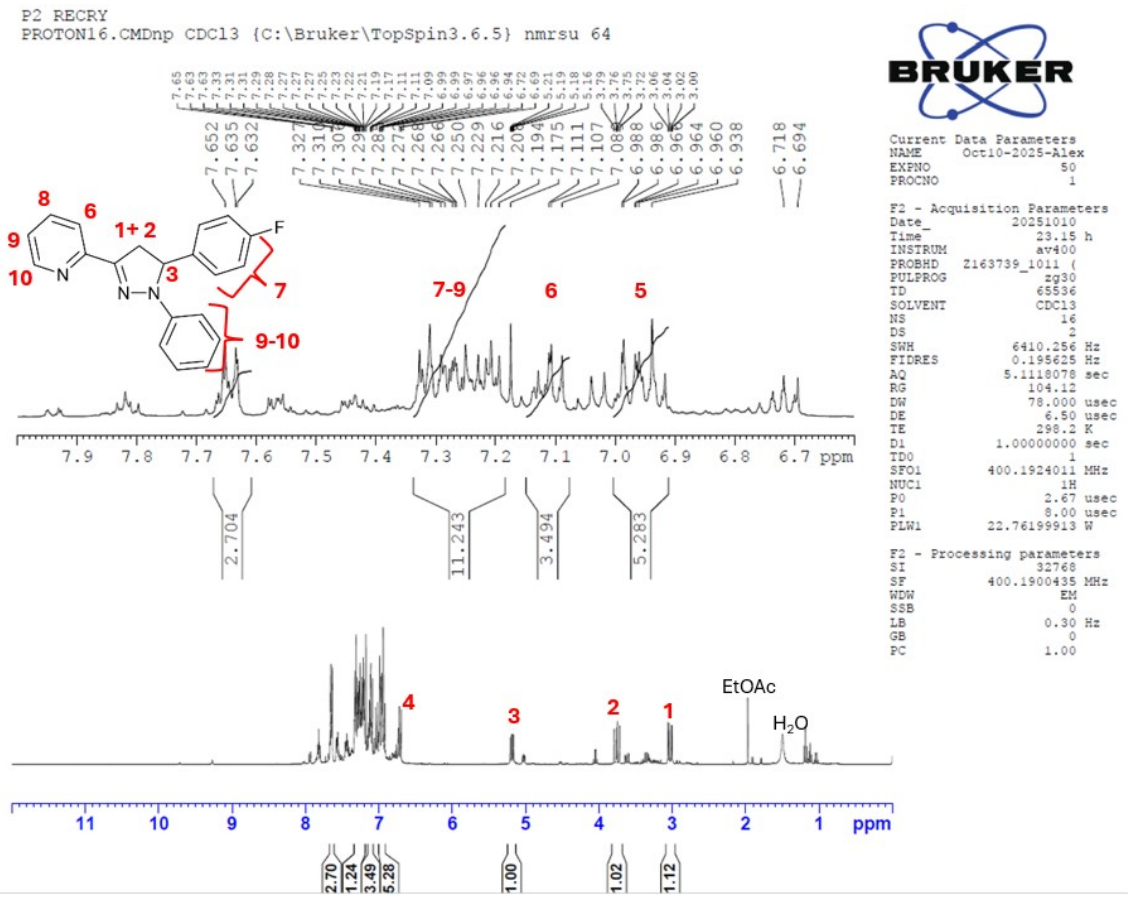


Current Data Parameters
NAME Dec16-2025-Alex
EXPNO 80
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251216
Time 14.08 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 use
DE 6.50 use
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 use
P1 8.00 use
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 use
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

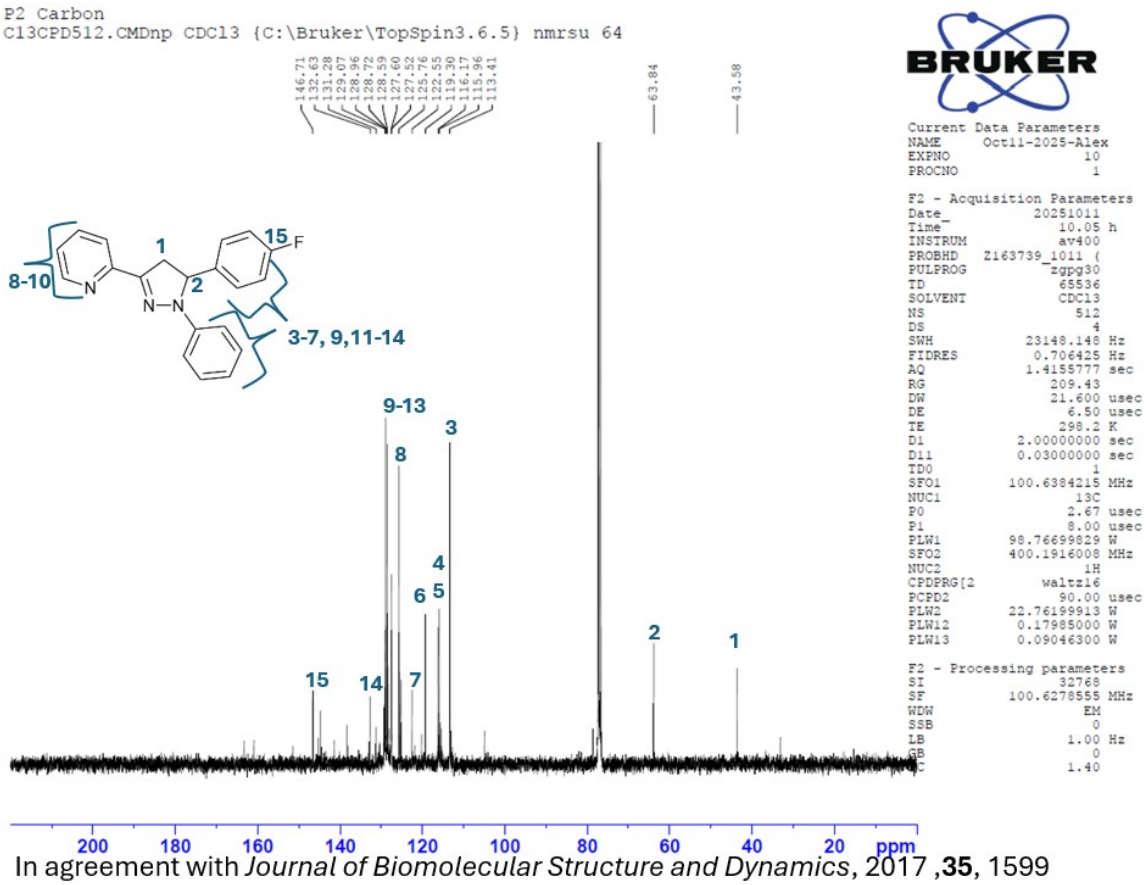
In agreement with *Med. Chem. Commun.*, 2013,**4**, 956



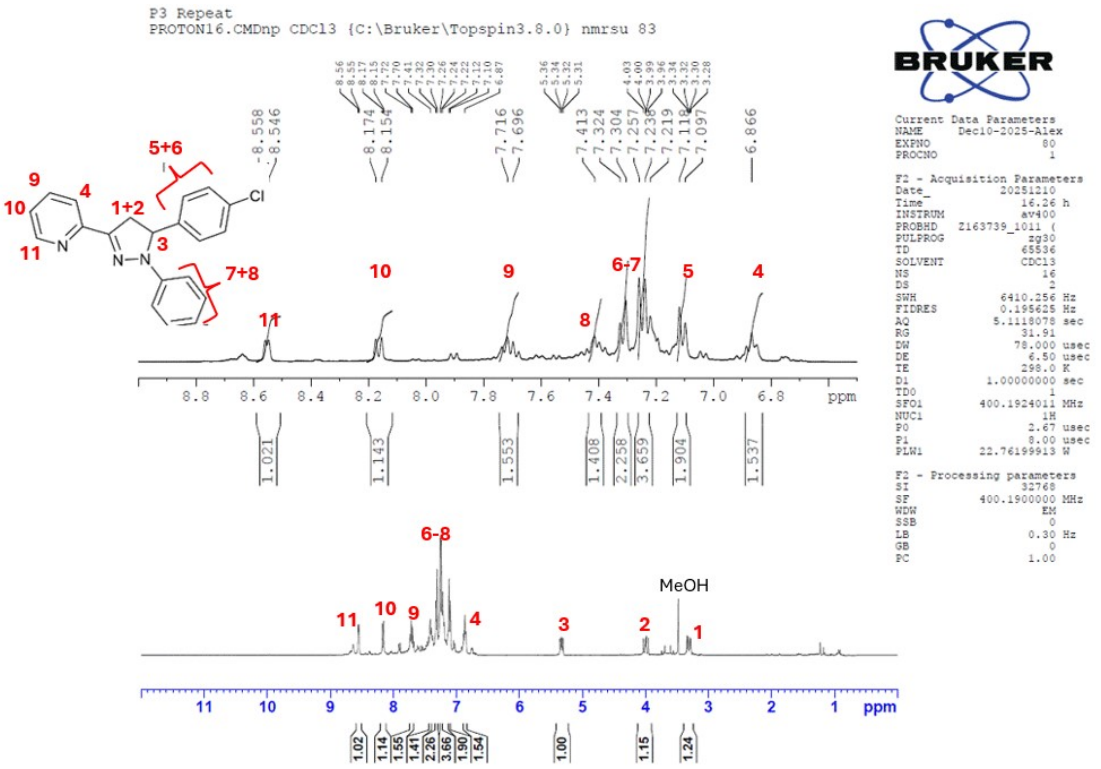
Current Data Parameters
NAME Oct10-2025-Alex
EXPNO 50
PROCNO 1

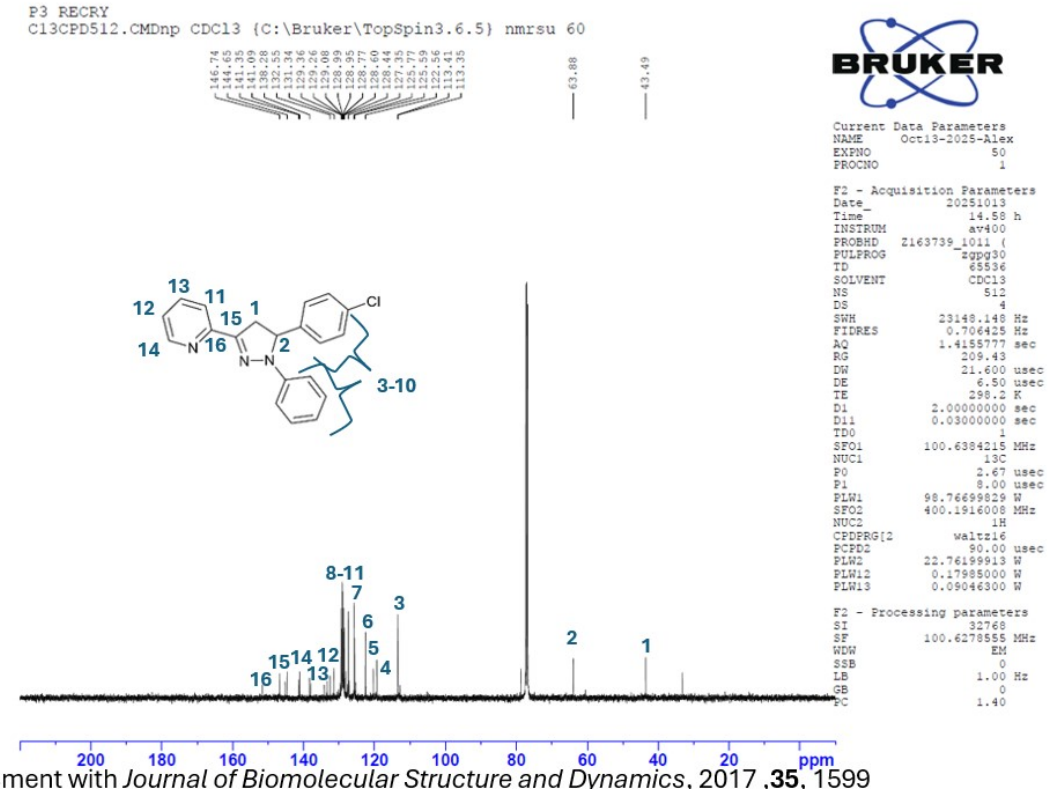
F2 - Acquisition Parameters
Date_ 20251010
Time 23.15 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900435 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

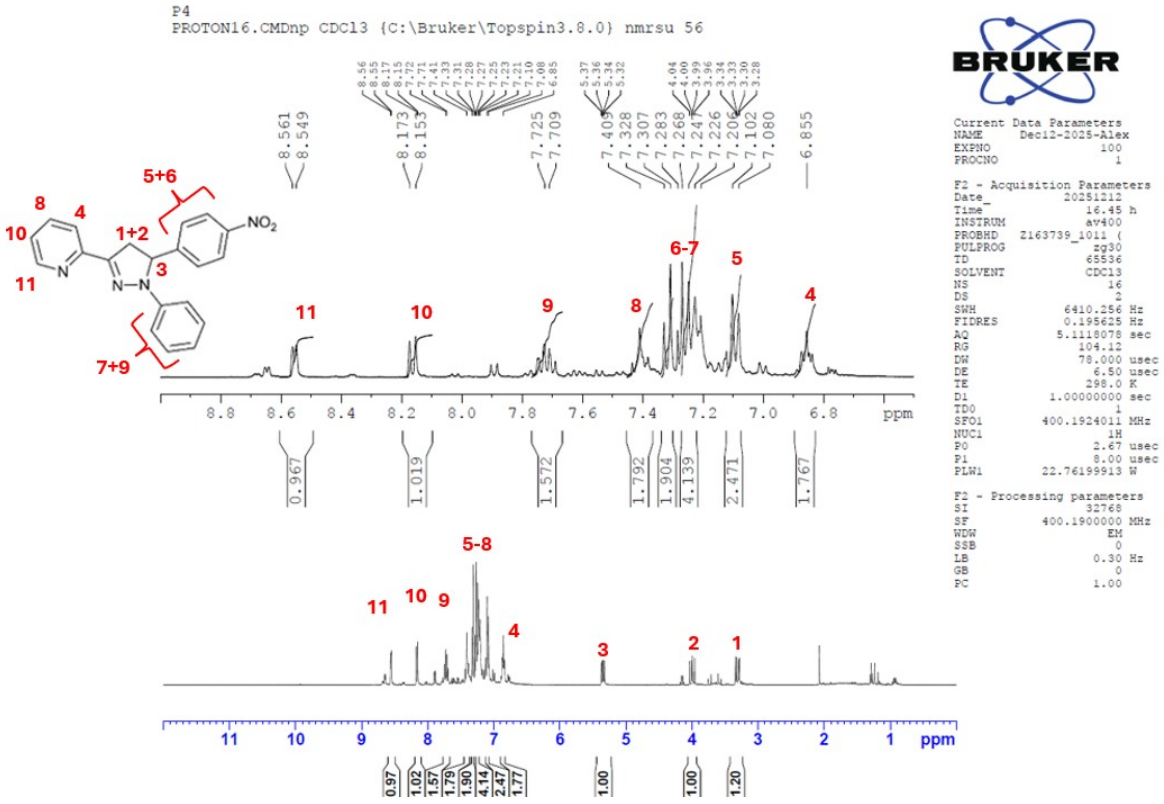


In agreement with *Journal of Biomolecular Structure and Dynamics*, 2017 ,**35**, 1599

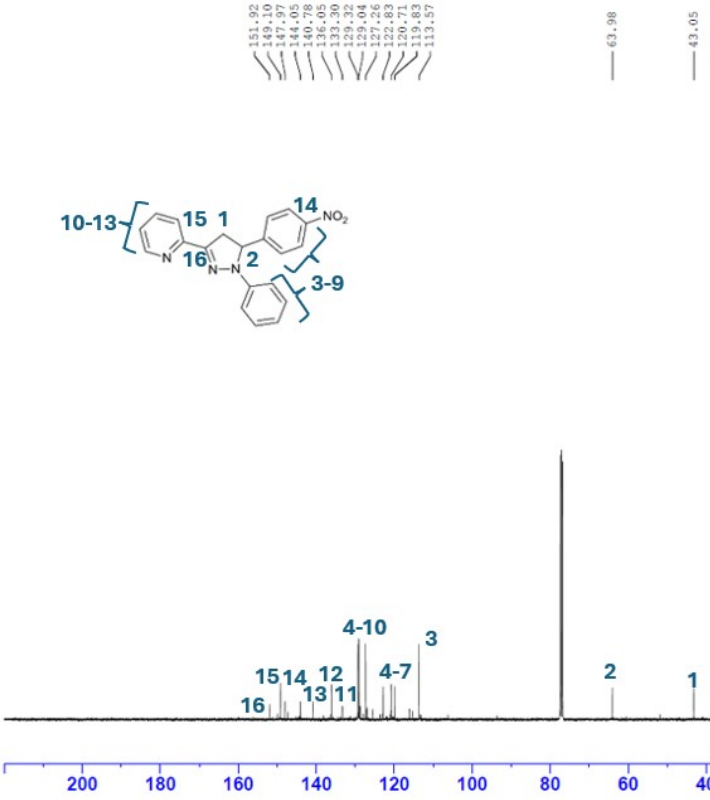




In agreement with *Journal of Biomolecular Structure and Dynamics*, 2017 ,**35**, 1599



P4
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 56



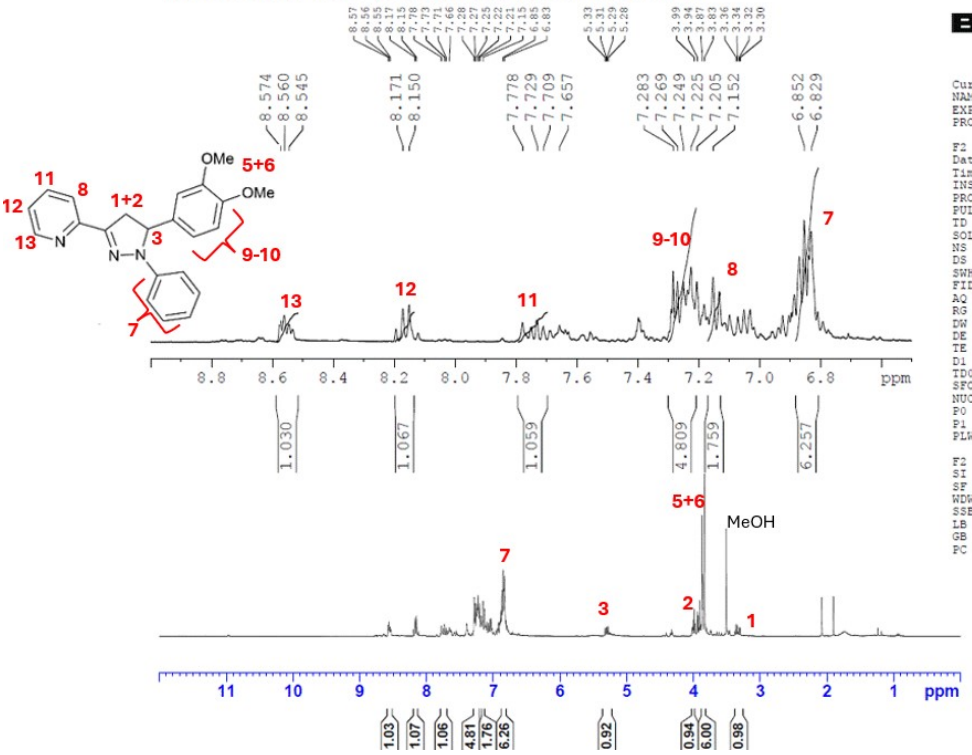
BRUKER

```
Current Data Parameters
NAME      Dec12-2025-Alex
EXPNO                140
PROCNO                 1

F2 - Acquisition Parameters
Date_              20251212
Time                 23.26 h
INSTRUM              av400
PROBHD   Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES             0.706425 Hz
AQ                 1.4155777 sec
RG                   209.43
DW                  21.600 usec
DE                   6.50 usec
TE                  298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           100.6384215 MHz
NUC1                  13C
P0                   2.67 usec
P1                   8.00 usec
PLW1           98.76699829 W
SFO2           400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           22.76199913 W
PLW12           0.17985000 W
PLW13           0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

P6
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 60



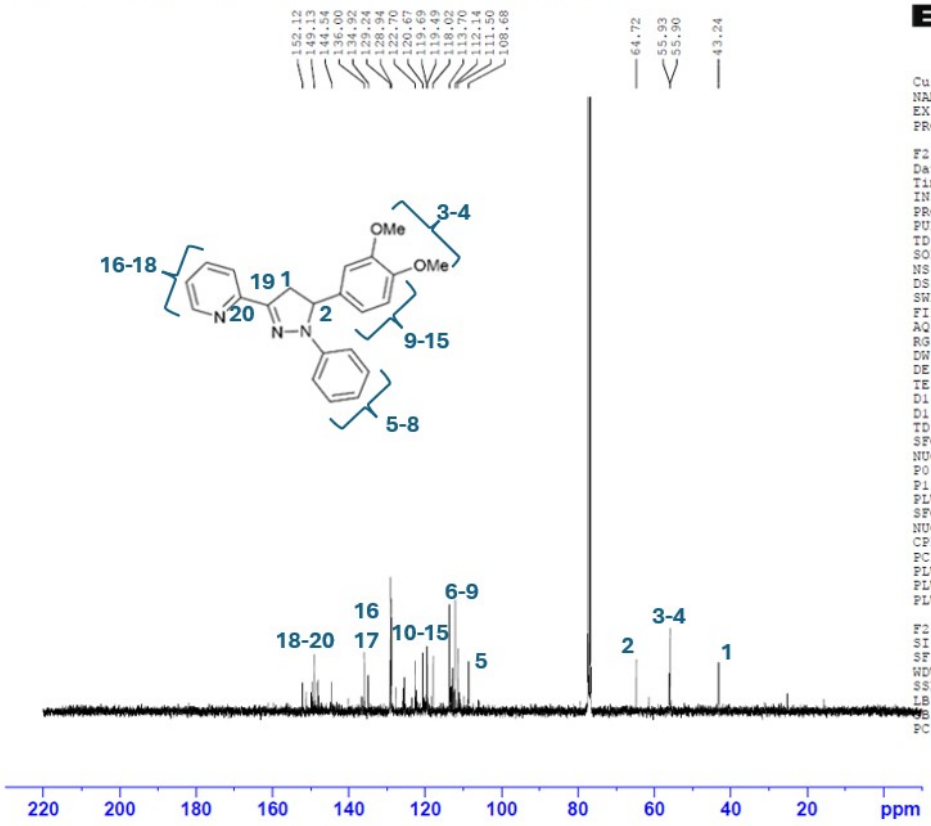
BRUKER

```
Current Data Parameters
NAME      Dec10-2025-Alex
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_              20251210
Time                 13.39 h
INSTRUM              av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES             0.195625 Hz
AQ                 5.1118078 sec
RG                   104.12
DW                  78.000 usec
DE                   6.50 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                    1
SFO1           400.1924011 MHz
NUC1                  1H
P0                   2.67 usec
P1                   8.00 usec
PLW1           22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

P6
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 92



Current Data Parameters

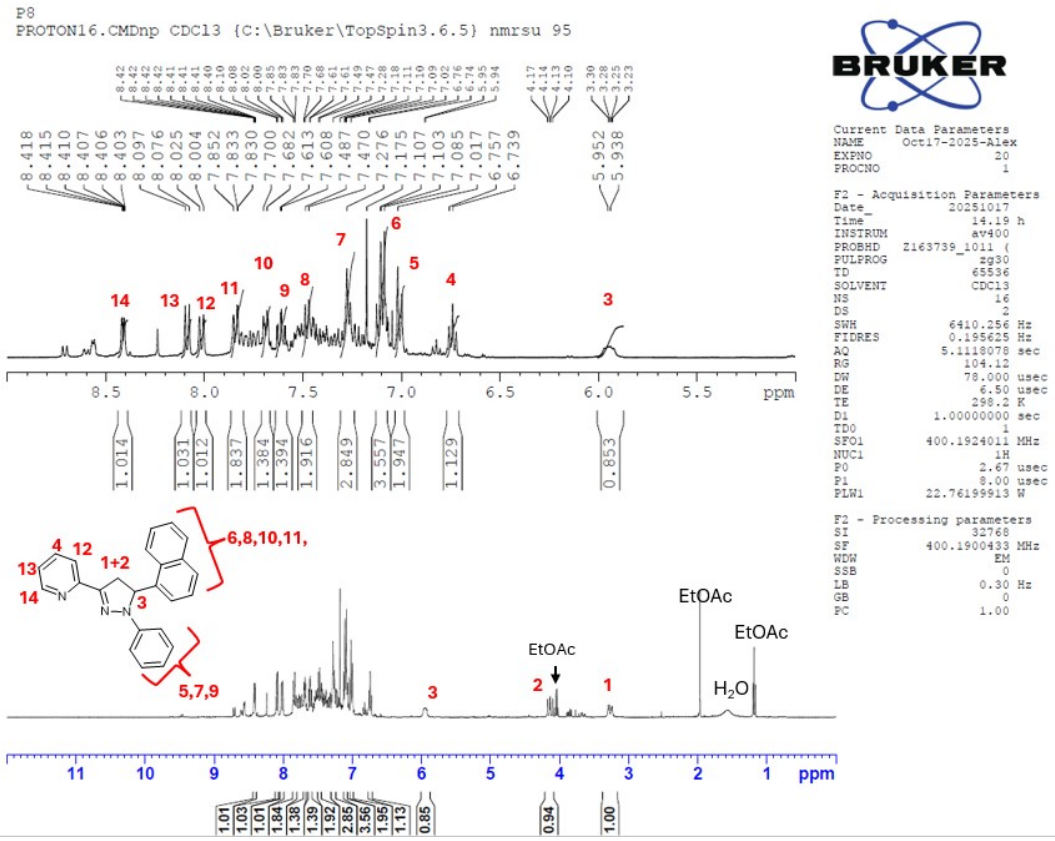
NAME	Dec13-2025-Alex
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20251213	
Time	10.35	h
INSTRUM	av400	
PROBHD	Z163739_1011 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	512	
DS	4	
SWH	23148.148	Hz
FIDRES	0.706425	Hz
AQ	1.4155777	sec
RG	209.43	
DW	21.600	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
SFO1	100.6384215	MHz
NUC1	13C	
P0	2.67	usec
P1	8.00	usec
PLW1	98.76699829	W
SFO2	400.1916008	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	usec
PLW2	22.76199913	W
PLW12	0.17985000	W
PLW13	0.09046300	W

F2 - Processing parameters

SI	32768	
SF	100.6278555	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

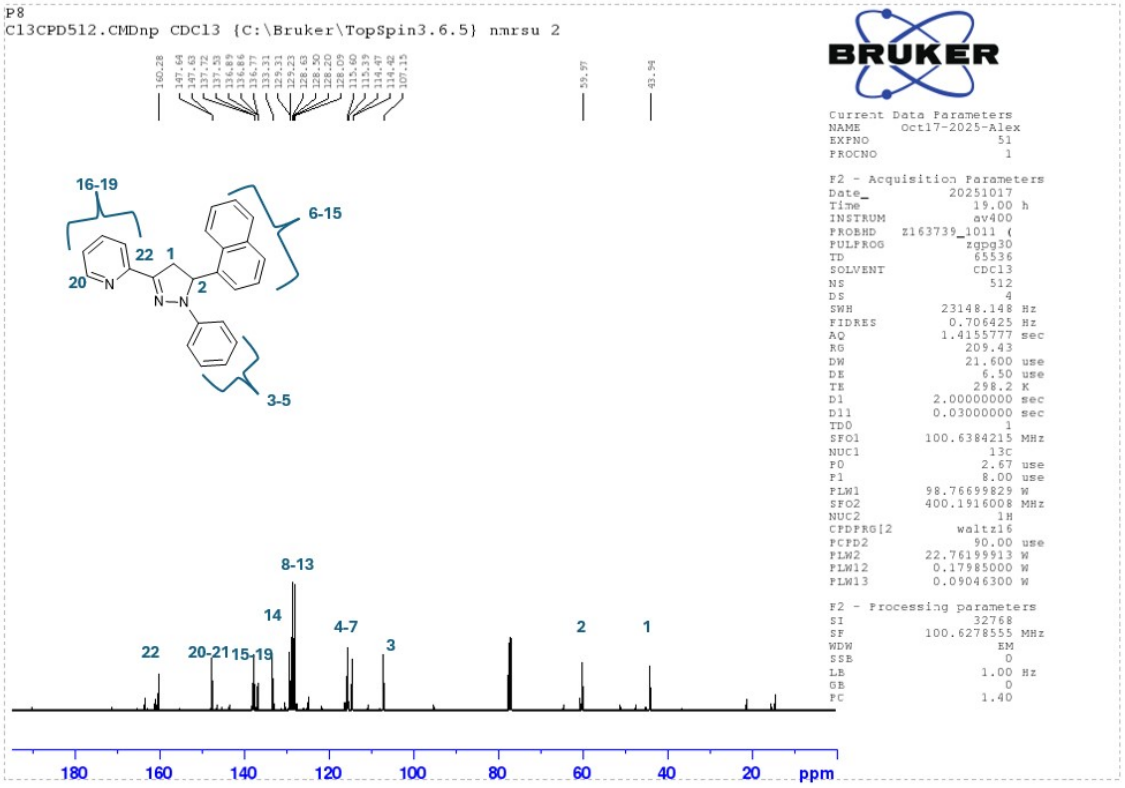


BRUKER

```
Current Data Parameters
NAME      Oct17-2025-Alex
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251017
Time              14.19 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              5.1118076 sec
RG                104.12
DW                78.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1924011 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          22.76199913 W

F2 - Processing parameters
SI                 32768
SF            400.1900433 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

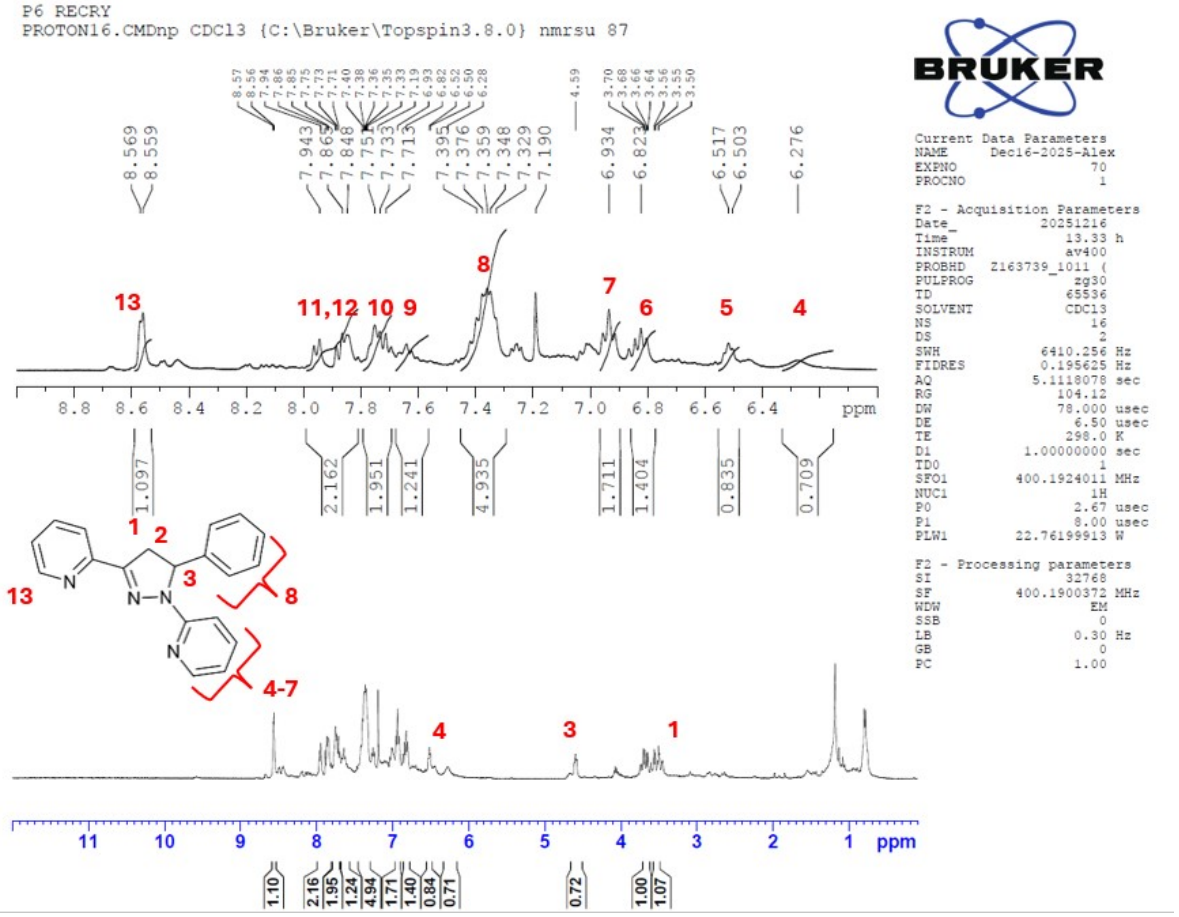


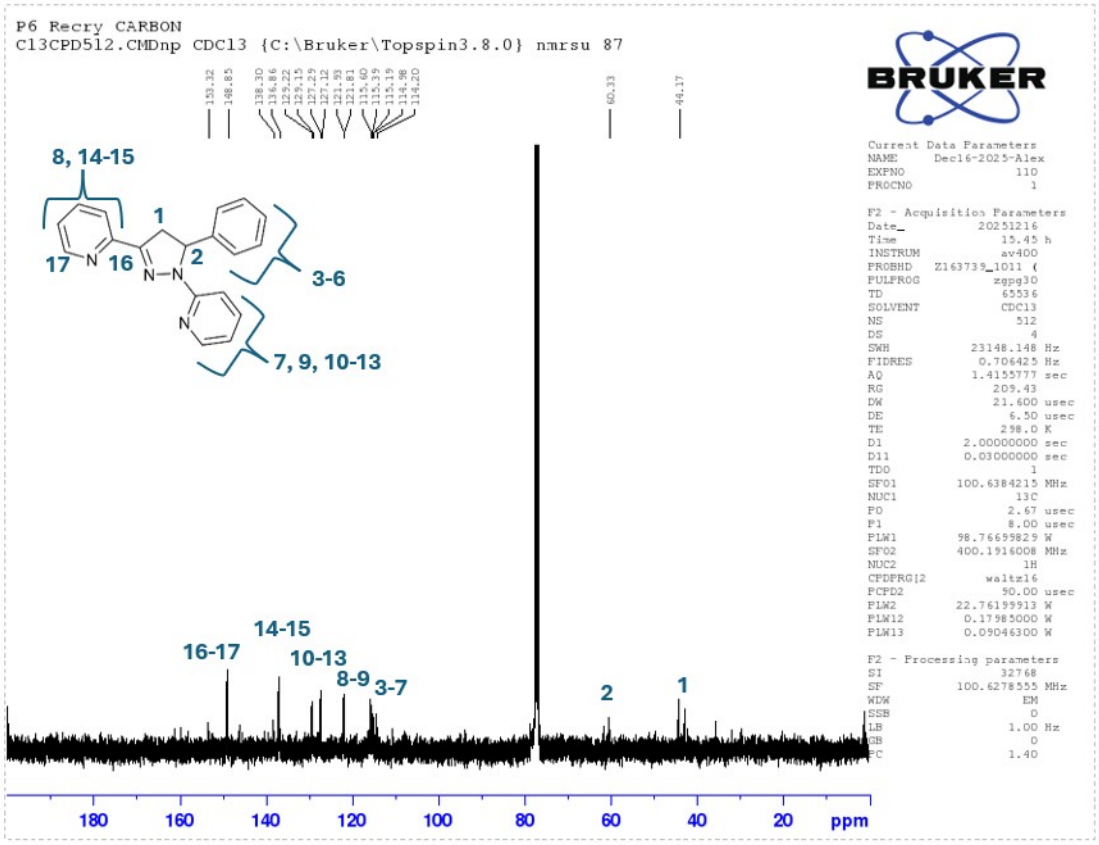
BRUKER

```
Current Data Parameters
NAME      Oct17-2025-Alex
EXPNO                 51
PROCNO                 1

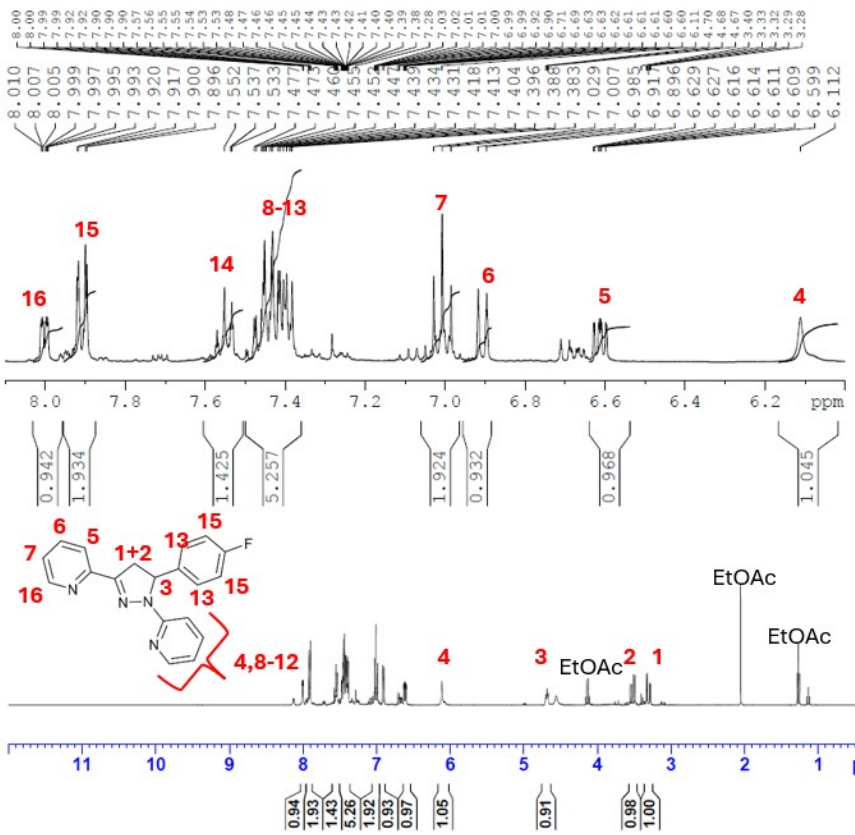
F2 - Acquisition Parameters
Date_           20251017
Time              19.00 h
INSTRUM             av400
PROBHD   Z163739_1011 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              1.4155777 sec
RG                209.43
DW                21.600 use
DE                 6.50 use
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6384215 MHz
NUC1                  13c
P0                 2.67 use
P1                 8.00 use
PLW1          98.76699829 W
SFO2          400.1916008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 use
PLW2          22.76199913 W
PLW12          0.17985000 W
PLW13          0.09046300 W

F2 - Processing parameters
SI                 32768
SF            100.6278555 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


P6 RECRY
PROTON16.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 87
8.569
8.559
7.943
7.863
7.848
7.752
7.733
7.715
7.395
7.376
7.359
7.348
7.329
7.190
6.934
6.823
6.517
6.503
6.276
13
11,12
10
9
8
7
6
5
4
ppm
1.097
2.162
1.951
1.241
4.935
1.711
1.404
0.835
0.709
1
2
3
13
8
4-7
4
3
1
11
10
9
8
7
6
5
4
3
2
1
ppm
1.10
2.16
1.95
1.24
4.94
1.71
1.40
0.84
0.71
0.72
1.00
1.07
Current Data Parameters
NAME Dec16-2025-Alex
EXPNO 70
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251216
Time 13.33 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 104.12
DW 78.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W
F2 - Processing parameters
SI 32768
SF 400.1900372 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


P6 Recry CARBON
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 87
153.32
148.85
138.30
136.86
129.22
129.15
127.29
127.12
121.93
121.81
115.60
115.53
115.19
114.98
114.20
60.33
44.17
8, 14-15
17
16
1
2
3-6
7, 9, 10-13
16-17
14-15
10-13
8-9
3-7
2
1
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Dec16-2025-Alex
EXPNO 110
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251216
Time 15.45 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76695829 W
SF02 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W
F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P11 RECRY
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 93

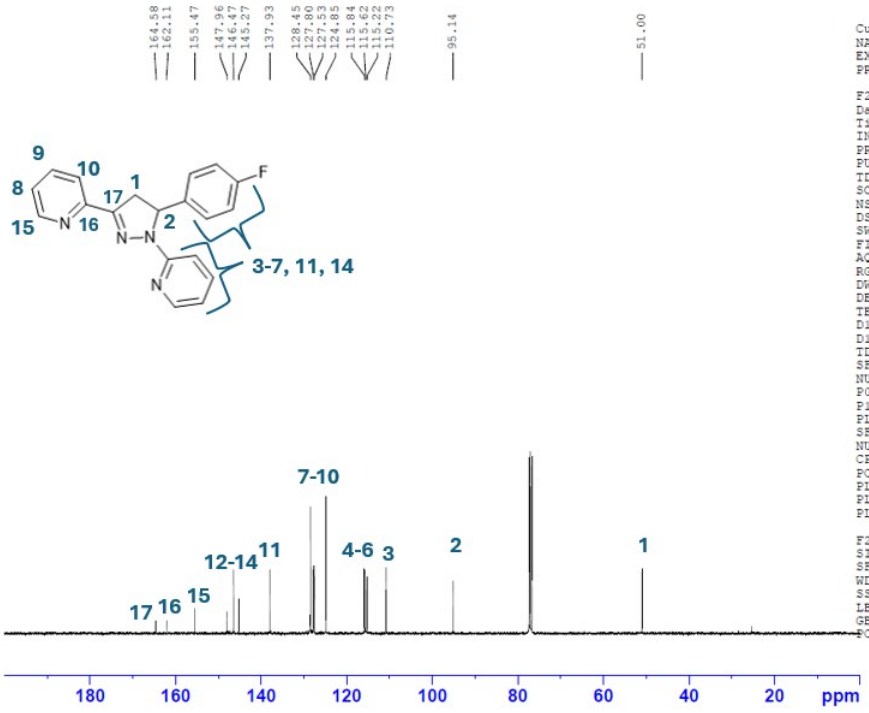


Current Data Parameters
NAME Oct14-2025-Alex
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251014
Time 8.26 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 5.1118078 sec
RG 35.24
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1924011 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.76199913 W

F2 - Processing parameters
SI 32768
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P11 Recry
C13CPD512.CMDnp CDCl3 {C:\Bruker\Topspin3.8.0} nmrsu 62

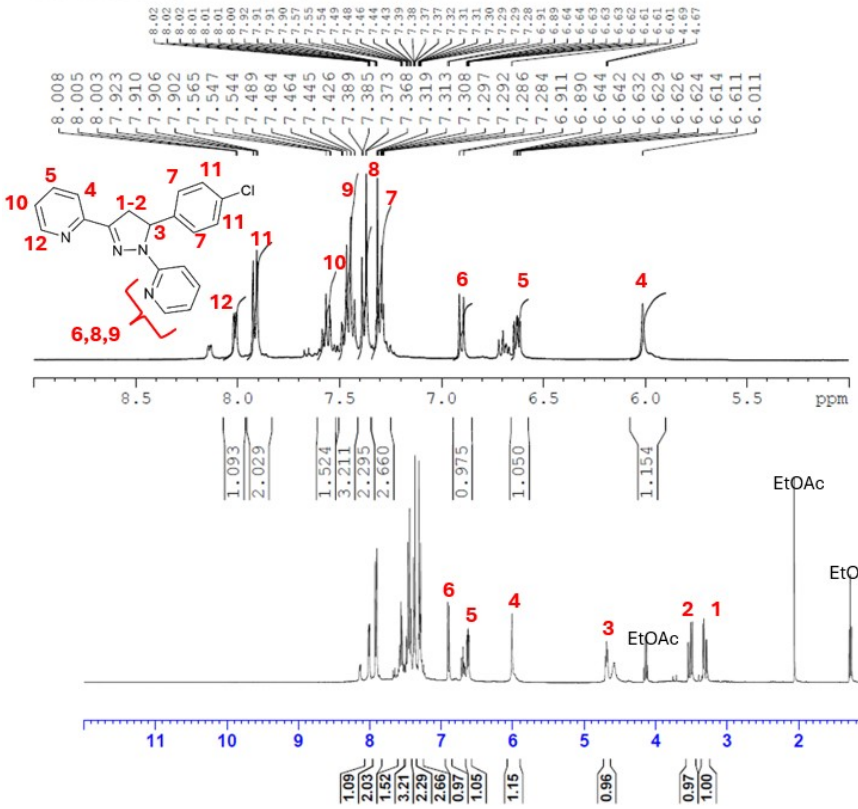


Current Data Parameters
NAME Dec15-2025-Alex
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251215
Time 16.54 h
INSTRUM av400
PROBHD Z163739_1011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 1.4155777 sec
RG 209.43
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 98.76699829 W
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 22.76199913 W
PLW12 0.17985000 W
PLW13 0.09046300 W

F2 - Processing parameters
SI 32768
SF 100.6278555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P12 Recry
PROTON16.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 94



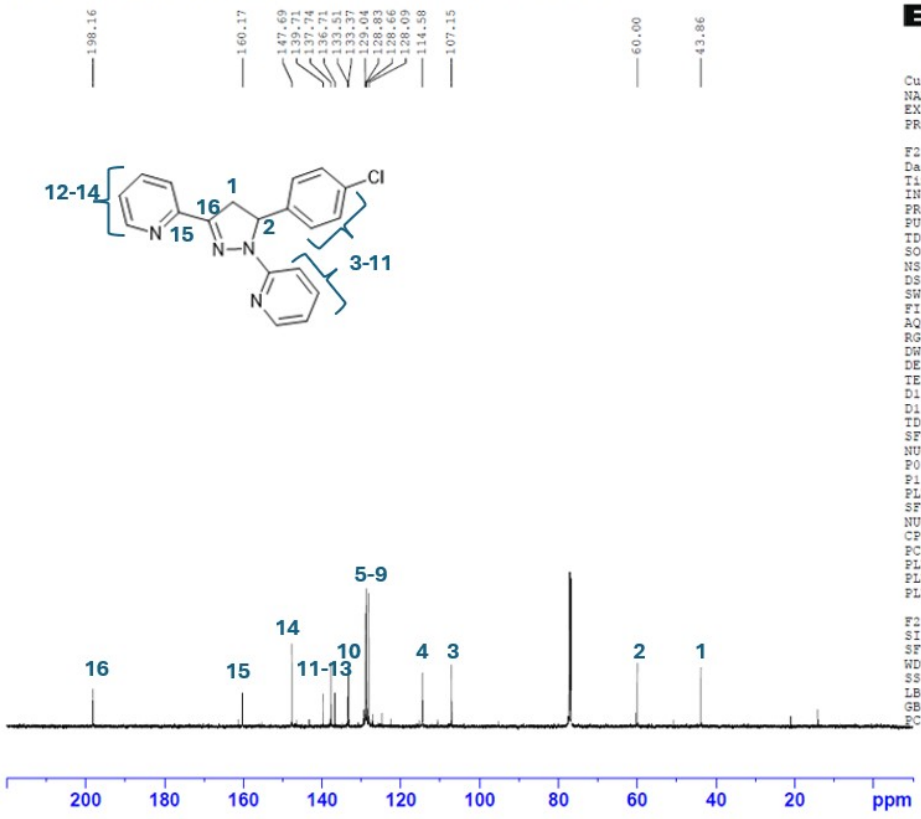
BRUKER

```
Current Data Parameters
NAME      Oct14-2025-Alex
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251014
Time              8.34 h
INSTRUM           av400
PROBHD    Z163739_1011 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           6410.256 Hz
FIDRES        0.195625 Hz
AQ            5.1118078 sec
RG                55.93
DW               78.000 usec
DE                6.50 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1
SFO1        400.1924011 MHz
NUC1                 1H
P0                2.67 usec
P1                8.00 usec
PLW1         22.76199913 W

F2 - Processing parameters
SI                32768
SF        400.1900000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

P12
C13CPD512.CMDnp CDCl3 {C:\Bruker\TopSpin3.6.5} nmrsu 3



BRUKER

```
Current Data Parameters
NAME      Oct17-2025-Alex
EXPNO                 61
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251017
Time             19.35 h
INSTRUM           av400
PROBHD    Z163739_1011 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH          23148.148 Hz
FIDRES        0.706425 Hz
AQ            1.4155777 sec
RG                209.43
DW               21.600 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
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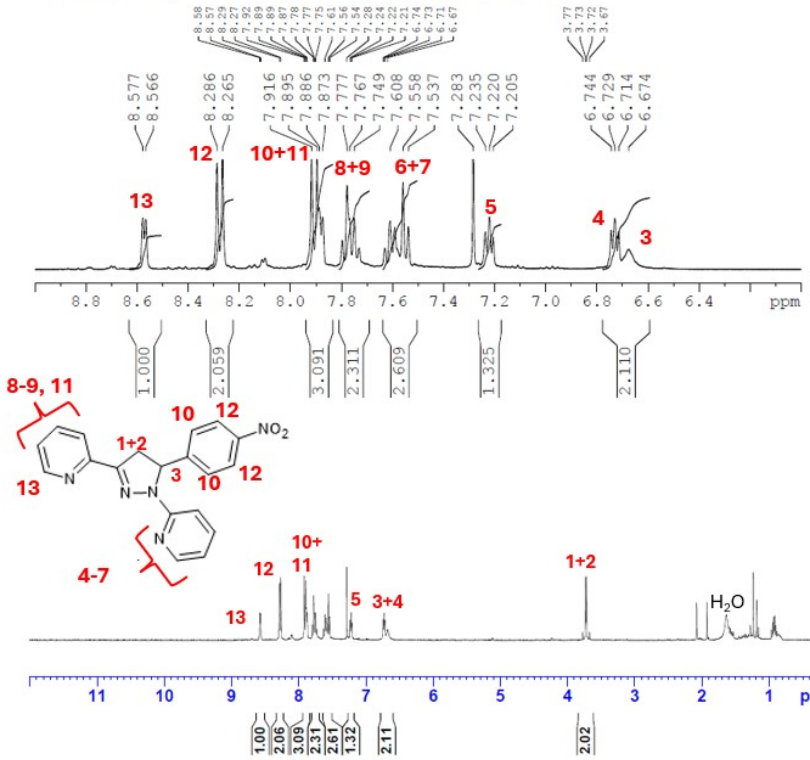

BRUKER

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F2 - Processing parameters
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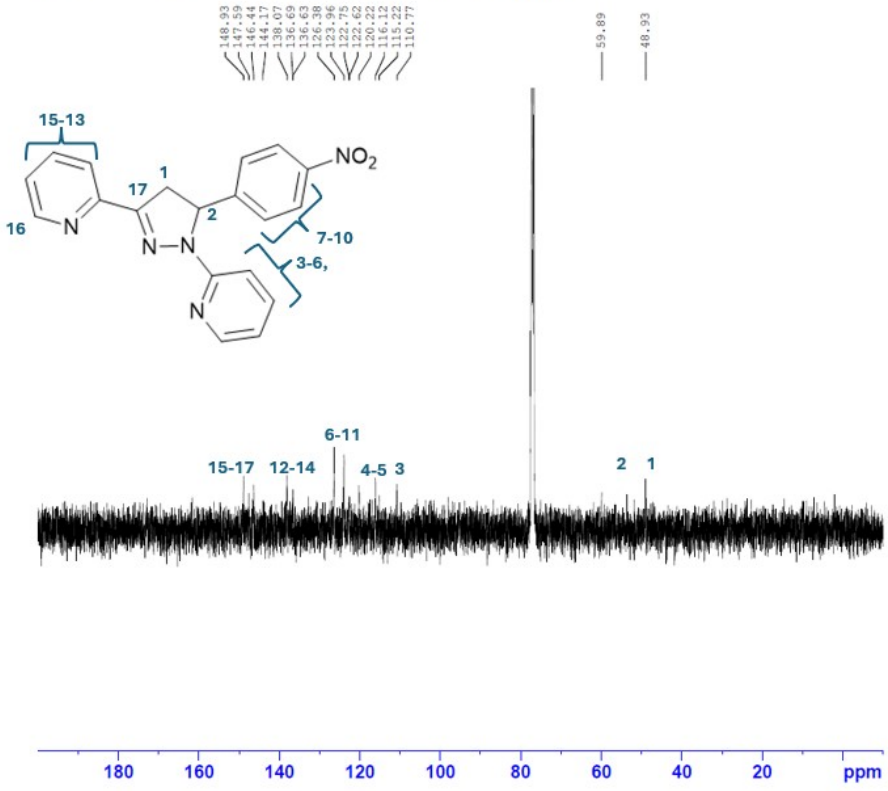

BRUKER

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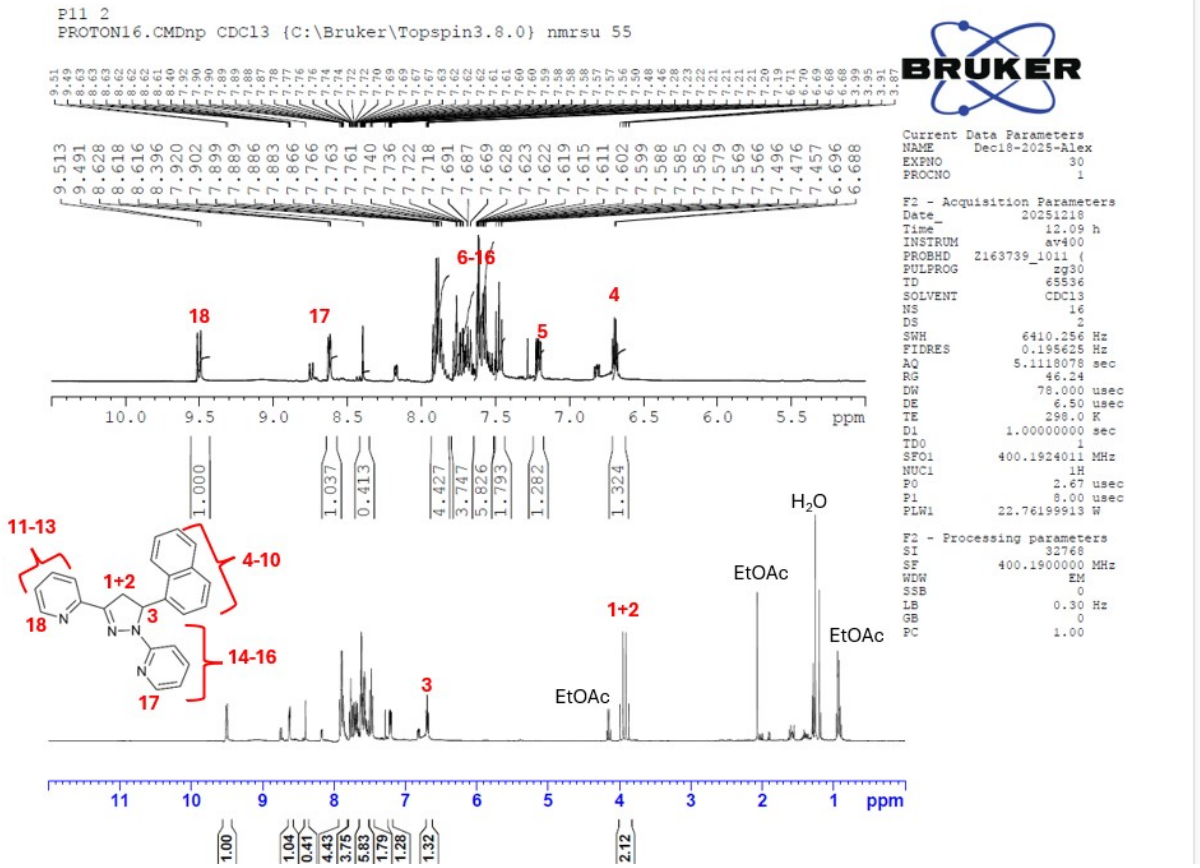
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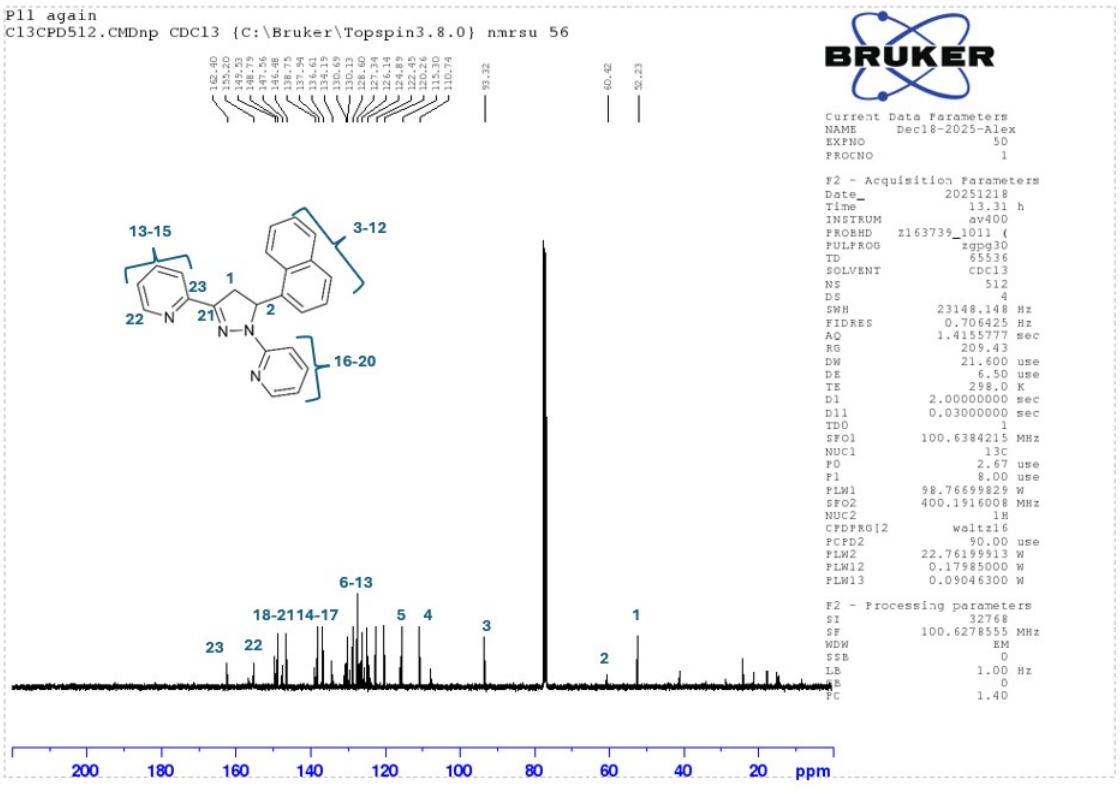
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BRUKER
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PROCNO 1
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AQ 1.4155777 sec
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DE 6.50 use
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D1 2.00000000 sec
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SFO1 100.6384215 MHz
NUC1 13C
P0 2.67 use
P1 8.00 use
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SFO2 400.1916008 MHz
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23
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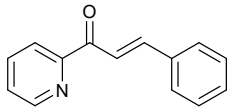
Chalcone Characterisation (S8)

C1



Yield (83%)

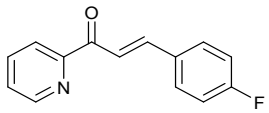
^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.43-7.44 (3 H, m, CH), 7.50-7.51 (1 H, m, CH), 7.75-7.76 (2 H, m, CH), 7.80-7.92 (1 H, m, CH), 7.95- 7.99 (1 H, d, CH, *J* = 16.0 Hz, CH=CH), 8.20-8.22 (1 H, m, CH), 8.31- 8.35 (1H, d, *J* = 16.0 Hz, CH=CH) and 8.76-8.77 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 120.1, 122.9, 126.9, 128.8, 128.9, 130.6, 135.2, 137.0, 144.8, 148.9, 154.2 and 189.5;

Above in agreement with previous data from *J. Am. Chem. Soc.,* 1996, **118**, 33, 7702

and *Org. Biomol. Chem*., 2012,**10**, 8753.

C2



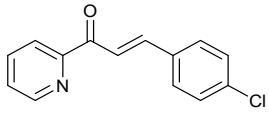
Yield (72%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.10-7.14 (2 H, m, CH), 7.49-7.53 (1 H, m, CH), 7.72-7.75 (2 H, m, CH), 7.89- 7.94 (2 H, m, CH and CH=CH), 8.20-8.27 (2 H, m, CH and CH=CH) and 8.74- 8.76 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 115.9, 116.1, 120.6, 122.9, 126.9, 127.0, 130.7, 136.8, 137.1, 143.4, 148.8 and 189.3;

Above in agreement with previous data from *Inorg. Chem*. 2019, **58**, 19, 12547 and *New J. Chem.,* 2024,**48**, 13900.

C3



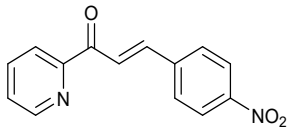
Yield (86%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.28-7.40 (2 H, m, CH), 7.48-7.51 (1 H, m, CH), 7.63- 7.64 (2H, m, CH), 7.82-7.90 (2 H, m, CH and CH=CH), 8.18-8.20 (1 H, m, CH), 8.27-8.31 (1H, d, J = 16.0 Hz, CH=CH), 8.73-8.76 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 121.4, 122.9, 127.0, 129.2, 130.0, 133.7, 136.4, 137.1, 143.2, 148.9 and 189.3;

Above in agreement with previous data from *Inorg. Chem*. 2019, **58**, 19, 12547 and *New J. Chem.,* 2024,**48**, 13900.

C4



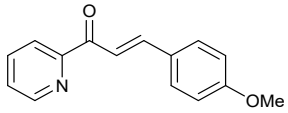
Yield (60%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.55-7.57 (1 H, m, CH), 7.87-7.96 (4 H, m, CH), 8.21-8.30 (3 H, m, CH), 8.42-8.47 (1 H, m, CH), 8.42-8.47 (1 H, m, CH) and 8.77-8.78 (1 H, m, CH;

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.1, 124.1, 124.8, 127.4, 229.3, 137.2, 141.3, 141.3, 148.6, 149.0 153.6 and 188.9;

Above in agreement with previous data from *Inorg. Chem*. 2019, **58**, 19, 12547 and *New J. Chem.,* 2024,**48**, 13900.

C5



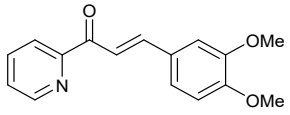
Yield (75%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.44-7.46 (3 H, m, CH), 7.54-7.59 (2 H, m, CH and CH=CH), 7.66- 7.68 (2 H, m, CH), 7.83-7.87 (1 H, d, J = 16 Hz, CH=CH) and 8.04-8.07 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 122.1, 128.5, 128.5, 128.7, 129.0, 130.6, 132.8, 134.9, 138.2, 144.9 and 190.6;

Above in agreement with previous data from *Inorg. Chem*. 2019, **58**, 19, 12547 and *New J. Chem.,* 2024,**48**, 13900.

C6



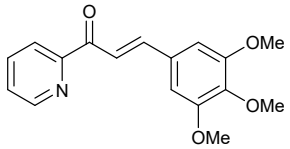
Yield (89%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.95 (3 H, s, CH_3), 3.99 (3 H, s, CH_3), 6.90-6.93 (1 H, d, *J* = 12.0 Hz, CH), 7.28-7.32 (2 H, m, CH), 7.48-7.52 (1 H, m, CH), 7.87-7.95 (2 H, m, CH and CH=CH), 8.14-8.22 (2 H, m, CH and CH=CH) and 8.75-8.77 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.0, 56.1, 110.2, 111.0, 118.6, 122.9, 124.0, 126.8, 128.2, 137.1, 145.1, 148.8, 149.2, 151.5, 154.5 and 189.3;

Above in agreement with previous data from *Inorg. Chem*. 2019, **58**, 19, 12547 and *New J. Chem.,* 2024,**48**, 13900.

C7



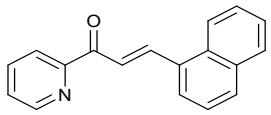
Yield (87%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.91-3.94 (9 H, m, CH_3), 6.96 (2 H, s, CH), 7.49-7.52 (1 H, m, CH), 7.86-7.89 (2 H, m, CH and CH=CH), 8.16-8.20 (2 H, m, CH and CH=CH) and 8.75-8.76 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.3, 61.0, 106.1, 119.6, 122.9, 126.9, 130.6, 137.1, 140.5, 145.1, 148.8, 153.4, 154.3 and 189.3;

Above in agreement with previous data from *Med. Chem. Commun*., 2013, **4**, 956.

C8



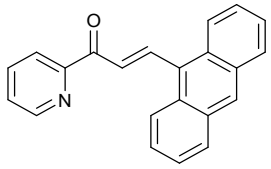
Yield (92%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.53- 7.63 (4H, m, CH), 7.90-7.96 (3 H, m, CH), 8.07-8.09 (1 H, m, CH), 8.25-7.27 (1 H, m, CH), 8.35-8.36 (1 H, m, CH), 8.41-8.45 (1 H, d, *J* = 16.0 Hz, CH=CH), 8.78-8.79 (1 H, m, CH) and 8.83-8.87 (1 H, d, *J*= 16.0 Hz, CH=CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.0, 123.3, 123.5, 125.5, 125.6, 126.2, 126.9, 128.8, 130.9, 132.0, 132.4, 133.8, 137.1, 141.4, 148.9, 154.3 and 189.4;

Above in agreement with previous data from *Research on Chemical Intermediates,* 2023, **49**, 469.

C9



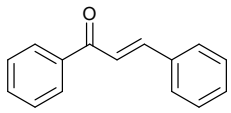
Yield (77%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.52-7.55 (5 H, m, CH), 7.93-7.94 (1 H, m, CH), 8.04-6.06 (2 H, m, CH), 8.29- 8.49 (5 H, m, CH), 8.71-8.72 (1 H, m, CH) and 8.94-8.97 (1 H, d, *J* = 12.0 Hz, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.1, 125.4, 125.5, 126.4, 126.9, 128.5, 128.9, 129.9, 130.2, 131.3, 137.0, 141.8, 149.1, 154.2 and 189.2;

Above in agreement with previous data from *Research on Chemical Intermediates,* 2023, **49**, 469.

C10



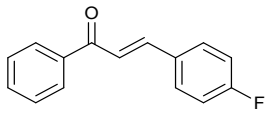
Yield (72%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.44-7.46 (3 H, m, CH), 7.54-7.59 (3 H, m, CH and CH=CH), 7.58-7.90 (1 H, m, CH), 7.66-7.68 (2 H, m, CH), 7.83-7.87 (1 H, d, *J* = 16.0 Hz, CH=CH), 8.04-8.07 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 122.1, 128.5, 128.5, 128.7, 129.0, 130.6, 132.8, 134.9, 138.2, 144.9 and 190.6;

Above in agreement with previous data from *Dalton Trans*., 2023, **52**, 12368.

C11



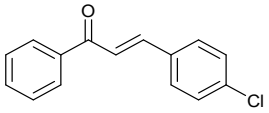
Yield (73%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.11-7.16 (2 H, m, CH), 7.47-7.55 (3 H, m, CH), 7.62-7.68 (3 H, m, CH), 7.78-7.82 (1 H, d, *J* = 16.0 Hz, CH=CH), 8.03-8.05 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 116.1, 116.3, 121.8, 128.5, 128.7, 130.3, 130.4, 132.9, 138.2, 143.5 and 190.3;

Above in agreement with previous data from *Chem. Commun*., 2019, **55**, 2348.

C12



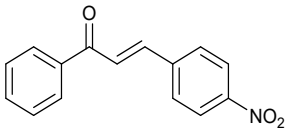
Yield (77%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.40-7.42 (2 H, m, CH), 7.51-7.55 (3 H, m, CH), 7.86-7.62 (3 H, m, CH), 7.76-7.80 (1 H, d, *J* = 16.0 H, CH=CH), 8.03-6.05 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 122.5, 128.5, 128.7, 129.3, 129.6, 132.9, 133.4, 136.5, 138.0, 143.3 and 190.3;

Above in agreement with previous data from *Dalton Trans*., 2023, **52**, 12368.

C13



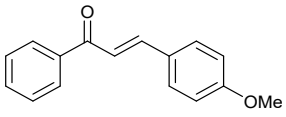
Yield (84%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.53-7.57 (2 H, m, CH), 7.63-7.67 (2 H, m, CH), 7.80-7.86 (3 H, m, CH), 8.05-8.07 (2 H, m, CH) and 8.28-8.30 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 124.3, 125.7, 128.6, 128.8, 129.0, 133.4, 137.6, 141.1, 141.5, 148.6 and 189.7;

Above in agreement with previous data from *Tett. Lett*., 2017, **58**, 3984.

C14



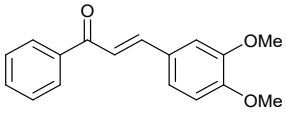
Yield (60%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.87 (3 H, s, CH_3), 6.94-6.97 (2 H, m, CH), 7.42-7.46 (1 H, d, *J* = 16.0 Hz, CH=CH), 7.49-7.51 (2 H, m, CH), 7.58-7.59 (1 H, m, CH), 7.61-7.63 (2 H, m, CH), 7.79-7.83 (1 H, d, *J* = 16.0 Hz, CH) and 8.02-8.05 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 55.4, 114.5, 119.8, 127.6, 128.4, 128.6, 130.3, 132.6, 138.5, 144.7, 161.8 and 190.6;

Above in agreement with previous data from *Chem. Commun*., 2019, **55**, 2348.

C15



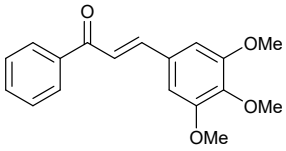
Yield (65%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.96-3.98 (6 H, m, CH_3), 6.93-6.98 (1 H, m, CH), 7.17-7.18 (1 H, m, CH), 7.24-7.28 (1 H, m, CH), 7.39-7.46 (2 , m, CH), 7.47-7.49 (2 H, m, CH), 7.50-7.57 (1 H, m, CH), 7.56-7.59 (1 H, m, CH) and 7.75-7.79 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.0, 56.2, 110.4, 120.1, 123.2, 126.9, 128.3, 128.4, 128.6, 132.6, 133.1, 138.5, 145.1, 149.3 and 190.9;

Above in agreement with previous data from *J. Org. Chem.* 2025, **90**, 16, 5343.

C16



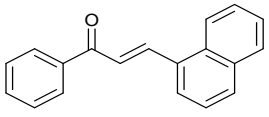
Yield (74%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.92-3.94 (9 H, m, CH3), 6.88 (2 H, s, CH), 7.40-7.44 (1 H, m, CH), 7.51-7.55 (2 H, m, CH), 7.56-7.61 (1 H, m, CH), 7.12-7.76 (1 H, m, CH) and 8.02-8.03 (2 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.2, 61.0, 105.7, 106.7, 121.5, 128.6, 130.4, 132.7, 138.3, 140.5, 145.1, 153.4 and 190.6;

Above in agreement with previous data from *Arch. Pharm*., 2020, **353**, 2000157.

C17



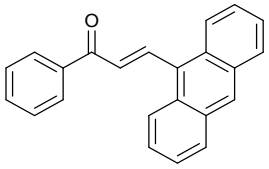
Yield (84%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.54-7.68 (7 H, m, CH), 7.91-7.70 (3 H, m, CH), 8.11-9.12 (2 H, m, CH), 8.27-8.29 (1 H, m, CH) and 8.69-8.73 (1 H, d, *J* = 16.0 Hz, CH=CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.5, 124.7, 125.1, 126.3, 127.0, 128.7, 128.8, 131.8, 132.4, 132.9, 133.8, 141.8 and 190.4;

Above in agreement with previous data from *J. Am. Chem. Soc.,* 2024, **146**, 25927.

C18



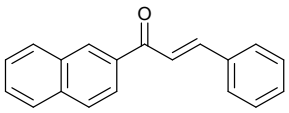
Yield (73%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.51- 7.71 (8 H, m, CH), 8.05-8.13 (4 H, m, CH), 8.32-8.34 (1 H, m, CH), 8.49-8.80 (2 H, m, CH) and 8.99-9.01 (1 H, d, *J*= 8.0 Hz, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.6, 125.3, 125.5, 125.7, 128.5, 128.9, 129.2, 129.7, 131.3, 135.3, 141.9 and 193.0;

Above in agreement with previous data from *RSC Adv*., 2015, **5**, 72764.

C19



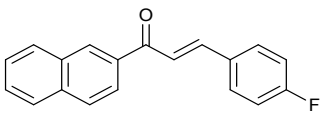
Yield (72%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.46-7.60 (3 H, m, CH), 7.62-7.65 (2 H, m, CH), 7.71-7.75 (3 H, m, CH), 7.89-7.98 (4 H, m, CH) and 8.12-8.15 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 122.1, 124.5, 126.8, 127.9, 128.4, 128.5, 128.6, 129.0, 129.6, 130.0, 130.6, 135.0, 135.5, 135.6, 144.8 and 190.4;

Above in agreement with previous data from *Dalton Trans***.**, 2022, **51**, 16181.

C20

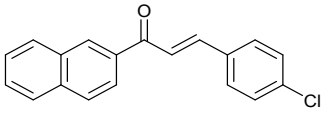


Yield (76%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.14-7.18 (2 H, m, CH), 7.61-7.72 (5 H, m, CH), 7.85-8.01 (4 H, m, CH), 8.11-8.13 (1 H, m, CH) and 8.56 (1 H, s, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 76.7, 77.4, 116.1, 124.5, 126.9, 128.6, 129.6, 130.0, 130.5, 131.2, 132.6, 135.5, 135.5, 143.5, 190.1;

C21

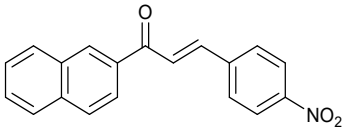


Yield (79%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.41-7.59 (2 H, m, CH), 7.59-7.71 (5 H, m, CH), 7.82-7.86 (1 H, m, CH), 7.91-8.01 (4 H, m, CH), 8.03-8.13 (1 H, m, CH) and 8.55 (1 H, s, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 122.5, 123.5, 126.9, 127.0, 127.2, 127.8, 128.5, 128.7, 128.9, 129.3, 129.6, 129.7, 130.0, 130.2, 132.4, 132.6, 133.8, 135.6, 135.8, 136.5, 141.5, 143.3 and 190;

C22



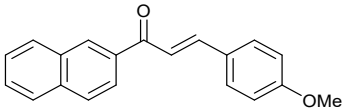
Yield (72%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.62-7.67 (2 H, m, CH), 7.81-8.07 (8 H, m, CH), 8.05-8.14 (1 H, m, CH), 8.30-8.32 (2 H, m, CH) and 8.57 (1 H, s, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.9, 124.3, 124.3, 125.7, 126.6, 127.1, 127.9, 128.8, 128.9, 129.0, 129.6, 130.3, 132.5, 134.9, 135.7, 141.1, 141.5, 148.6 and 189.4;

Above in agreement with previous data from *J. Mol. Struc.,* 2025, **1340**, 42526.

C23

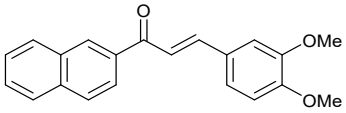


Yield (70%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.89 (3 H, s, CH_3), 6.96-6.99 (2 H, m, CH), 7.58-7.86 (2 H, m, CH), 7.87-8.13 (10 H, m, CH) and 8.48-8.55 (1 H, m, CH;

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.6, 124.6, 124.8, 125.2, 125.5, 126.4, 126.9, 127.0, 127.9, 128.5, 128.7, 128.8, 129.6, 130.1, 130.9, 135.6 and 141.6;

C24

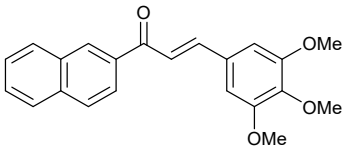


Yield (89%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.96-3.99 (6 H, m, CH_3), 6.96-6.95 (1 H, m, CH), 7.22-7.28 (2 H, m, CH), 7.43-7.43 (2 H, m, CH), 7.55-7.60 (4 H, m, CH), 7.83-7.95 (8 H, m, CH) and 8.04-8.10 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.0, 56.2, 108.9, 110.3, 110.4, 111.2, 120.1, 123.2, 123.9, 124.6, 126.8, 126.9, 127.8, 128.0, 128.3, 128.4, 128.5, 129.5, 129.6, 149.3, 190.39;

C25



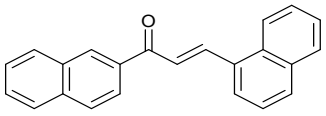
Yield (95%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.94-3.97 (9 H, m, CH3), 6.91-6.92 (2 H, s, CH), 7.15 (1 H, s, CH), 7.58-7.65 (3 H, m, CH), 7.8-7.82 (1 H, m, CH), 7.91-8.11 (5 H, m, CH) and 8.55 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 56.3, 61.0, 105.8, 106.7, 121.6, 124.6, 126.8, 127.9, 128.4, 128.6, 129.5, 129.9, 130.5, 132.6, 135.5, 145.1, 153.4 and 191.1;

Above in agreement with previous data from *Chem. Biol. Drug. Des*., 2013, **82**, 732.

C26



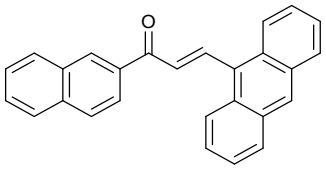
Yield (76%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.56-7.66 (6 H, m, CH), 7.80-7.84 (1 H, m, CH), 7.92-8.00 (7 H, m, CH), 8.18-8.20 (1 H, m, CH), 8.31-8.32 (1H, m, CH), 8.62-8.63 (1 H, m, CH) and 8.75-8.78 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 123.6, 124.6, 124.8, 125.2, 125.5, 126.4, 126.9, 127.0, 127.9, 128.5, 128.7, 128.8, 129.6, 130.1, 130.9, 135.6, 141.7 and 190.1;

Above in agreement with previous data from *Eur. J. Med. Chem*., 2013, **64**, 35.

C27



Yield (75%)

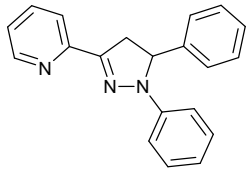
^{1}H NMR δ_H (400 MHz; $CDCl_3$) 7.54-7.59 (6 H, m, CH), 7.74-7.78 (1 H, m, CH), 7.92-8.09 (5 H, m, CH), 8.22-8.23 (1 H, m, CH), 8.37-8.39 (2 H, m, CH), 8.51-8.57 (2 H, m, CH), 8.87-8.91 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 124.5, 125.4, 125.5, 126.5, 126.9, 127.9, 128.5, 128.8,129.0, 129.6, 129.7, 130.3, 131.1, 131.4, 132.6, 135.3, 135.6, 141.9 and 189.5;

Above in agreement with previous data from *New J. Chem***.**, 2018,**42**, 1037.

Pyrazoline Characterisation (S9)

P1



Yield (75%)

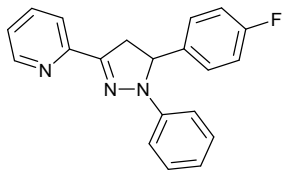
^{1}H NMR δ_H (400 MHz; $CDCl_3$) 2.37-2.43 (1 H, m, CH), 2.86-2.91 (1 H, m, CH), 4.93-4.97 (1 H, m, CH), 6.08 (1H, m, CH), 6.68-6.91 (1 H, m, CH), 6.91-6.93 (2 H, m, CH), 7.07-7.08 (2 H, m, CH), 7.18-7.19 (2 H, m, CH), 7.27-7.31 (2 H, m, CH), 7.42-7.43 (2 H, m, CH), 7.67-7.75 (2 H, m, CH) and 8.49-8.50 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 64.4, 113.6, 119.6, 120.6, 125.8, 127.5, 127.7, 129.0, 129.1, 135.9, 137.1, 142.3, 144.3, 148.0, 148.1 and 152.2;

HRMS m/z Found 300.1500 ($M+H^+$). $C_{20}H_{18}N_3$ requires 300.1501.

Above in agreement with previous data from Med. Chem. Commun., 2013 ,**4**, 956.

P2



Yield (38%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.00-3.06 (1 H, m, CH), 3.72-3.79 (1 H, m, CH), 5.16-5.21 (1 H, m, CH), 6.69-7.33 (10 H, m, CH) and 7.63-7.65 (3 H, m, CH);

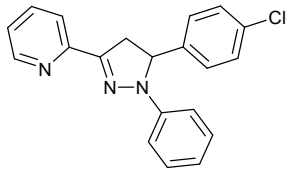
^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.6, 63.8, 113.4, 115.9, 116.2, 119.3, 122.6, 125.8, 127.5, 127.6, 128.6, 128.9, 129.1, 131.3, 132.6 and 146.7;

HRMS m/z Found 318.1465 ($M+H^+$). $C_{20}H_{17}FN_3$ requires 318.1407.

Above in agreement with previous data from Journal of biomolecular structure and dynamics, 2017,

35, 1599.

P3



Yield (94%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.28-3.34 (1 H, m, CH), 3.96-3.02 (1 H, m, CH), 5.31-5.36 (1 H, m, CH), 6.85-6.86 (1 H, m, CH), 7.22-7.26 (4 H, m, CH), 7.30-7.32 (2 H, m, CH), 7.40-7.41 (1H, m, CH), 7.69-7.72 (1 H, m, CH), 8.15-8.17 (1 H, m, CH) and 8.55-8.56 (1 H, m, CH);

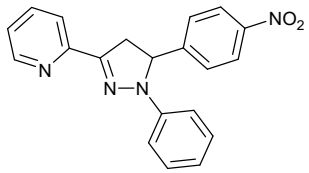
^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.5, 63.9, 113.4, 113.4, 122.6, 125.8, 127.4, 128.4, 128.6, 128.7, 129.3, 131.4, 138.3, 141.1, 141.4 and 146.7;

HRMS m/z Found 334.1080 ($M+H^+$). $C_{20}H_{17}ClN_3$ requires 334.1111.

Above in agreement with previous data from Journal of biomolecular structure and dynamics, 2017,

35, 1599.

P4



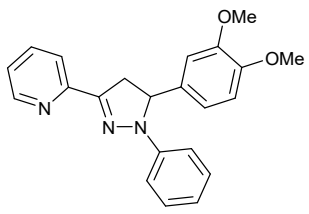
Yield (78%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.28-3.34 (1 H, m, CH), 3.96-4.04 (1 H, m, CH), 5.32-5.37 (1 H, m, CH), 6.84-6.86 (1 H, s, CH), 7.08-7.10 (2 H, m, CH), 7.21-7.33 (6 H, m, CH), 7.40-7.42 (2 H, m, CH), 7.71-7.73 (1 H, m, CH), 8.15-8.17 (1 H, m, CH) and 8.55-8.56 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.1, 63.9, 113.6, 119.8, 120.7, 122.8, 127.3, 129.0, 129.3, 133.3, 136.1, 140.8, 144.1, 147.9. 149.1 and 151.9;

HRMS m/z Found 345.1353 ($M+H^+$). $C_{20}H_{17}N_4O_2$ requires 345.1352.

P5



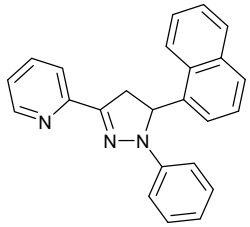
Yield (85%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.30-3.36 (1 H, m, CH), 3.83-3.99 (7 H, m, CH and CH_3), 5.28-5.33 (1 H, m, CH), 6.83-6.85 (4 H, m, CH), 7.15-7.28 (5 H, m, CH), 7.66-7.78 (1 H, m, CH), 8.15-8.17 (1 H, m, CH) and 8.55-8.57 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.2, 55.9, 56.0, 64.7, 108.7, 111.5, 112.1, 113.7, 118.0, 119.5, 119.7, 120.7, 129.2, 134.9, 136.0, 144.5, 149.1 and 152.1;

HRMS m/z Found 360.1724 ($M+H^+$). $C_{22}H_{22}N_3O_2$ requires 360.1712.

P6



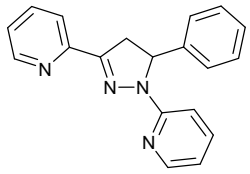
Yield (45%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.23-3.30 (1 H, m, CH), 4.10-4.17 (1 H, m, CH), 6.74-6.76 (1 H, m, CH), 7.01-7.70 (11 H, m, CH), 7.72-7.85 (5 H, m, CH), 8.00-8.07 (1 H, m, CH), 8.08-8.1 (1 H, m, CH) and 8.40-8.8.42 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.9, 59.9, 107.2, 114.4, 114.5, 115.4, 115.6, 128.1, 128.2, 128.5, 128.6, 129.2, 129.3, 133.3, 136.8, 136.9, 136.9, 137.5, 137.7, 147.6, 147.6 and 160.3;

HRMS m/z Found 350.1470 ($M+H^+$). $C_{24}H_{20}N_3$ requires 350.1657.

P7



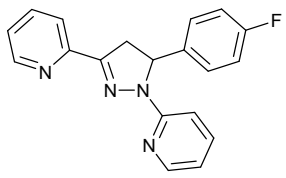
Yield (50%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.50-3.56 (1 H, m, CH), 3.64-3.70 (1 H, m, CH), 4.58-4.59 (1 H, m, CH), 6.50-6.52 (1 H, m, CH), 6.82-6.93 (2 H, m, CH), 7.33-7.40 (5 H, m, CH), 7.71-7.94 (4 H, m, CH) and 8.56-8.57 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 44.2, 60.3, 114.2, 114.6, 115.2, 115.4,115.6, 121.8, 121.9, 127.1, 127.3, 129.2, 136.8, 138.3, 148.8 and 153.3;

HRMS m/z Found 301.1459 ($M+H^+$). $C_{19}H_{17}N_4$ requires 301.1453.

P8



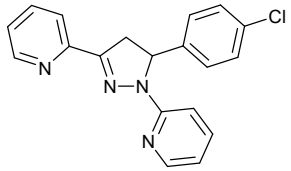
Yield (52%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.28-3.32 (1 H, m, CH), 3.33-3.4 (1 H, m, CH), 4.67-4.70 (1 H, m, CH), 6.11 (1 H, s, CH), 6.60-6.61 (1 H, m, CH), 6.89-6.82 (1 H, m, CH), 6.98-7.00 (2 H, m, CH), 7.38-7.47 (5 H, m, CH), 7.53-7.90 (2 H, m, CH) and 7.99-8.01 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 51.0, 95.1, 110.7, 115.2, 115.6, 115.8, 124.9, 127.5, 127.8, 128.5, 137.9, 145.3, 146.5, 147.9, 155.5, 162.1 and 164.6;

HRMS m/z Found 319.1410 ($M+H^+$). $C_{19}H_{16}FN_4$ requires 319.1359.

P9



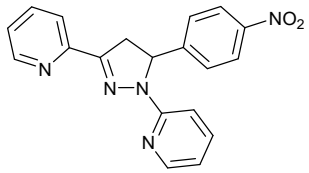
Yield (50%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.28-3.36 (1 H, m, CH), 3.48-3.54 (1 H, m, CH), 4.67-4.68 (1 H, m, CH), 6.01 (1 H, s, CH), 6.61-6.64 (1 H, m, CH), 6.89-6.91 (1 H, m, CH),7.28-7.32 (3 H, m, CH), 7.37-7.39 (2 H, m, CH), 7.46-7.46 (3 H, m, CH) and 7.54-7.56 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 43.9, 60.0, 107.2, 114.6, 128.1, 128.7, 128.8, 129.0, 133.4, 133.5, 136.7, 137.7, 139.7, 147.7, 160.2 and 198.2;

HRMS m/z Found 335.0941 ($M+H^+$). $C_{19}H_{16}ClN_4$ requires 335.1063.

P10



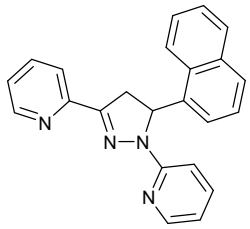
Yield (31%)

^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.67-3.77 (2 H, m, CH), 6.67-6.74 (2 H, m, CH), 7.20-7.23 (1 H, m, CH), 7.54-7.61(2 H, m, CH), 7.75-7.77 (2 H, m, CH), 7.87-7.92 (3 H, m, CH), 8.27-8.29 (2 H, m, CH), 8.57-8.58 (1 H, m, CH);

^{13}C NMR δ_c (100 MHz; $CDCl_3$) 48.9, 59.9, 110.8, 115.2, 116.2, 120.2, 122.6, 122.8, 123.9, 126.4, 136.6, 136.7, 138.1, 144.2, 146.4, 147.6, 148.9;

HRMS m/z Found 346.1279 ($M+H^+$). $C_{19}H_{16}N_5O_2$ requires 346.1304.

P11



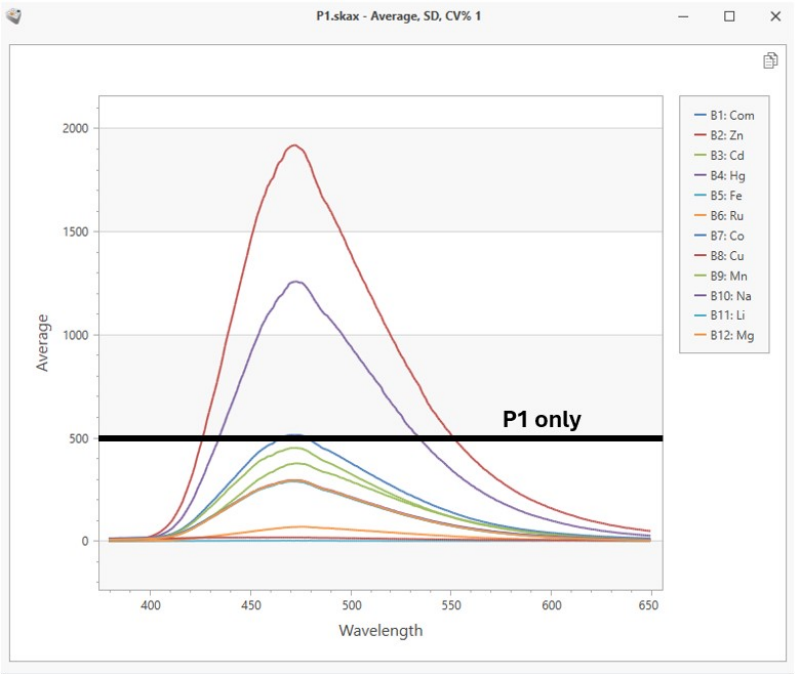
Yield (45%)

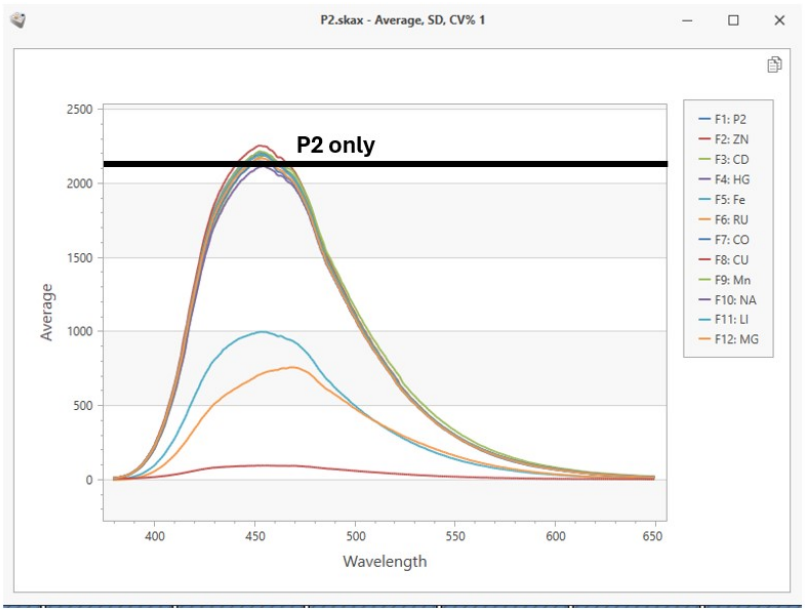
^{1}H NMR δ_H (400 MHz; $CDCl_3$) 3.87-3.99 (2 H, m, CH), 6.69-6.70 (1 H, m, CH), 7.19-7.23 (1 H, m, CH), 7.46-7.92 (12 H, m, CH), 8.39-8.62 (1 H, m, CH) and 9.49-9.51 (1 H, m, CH);

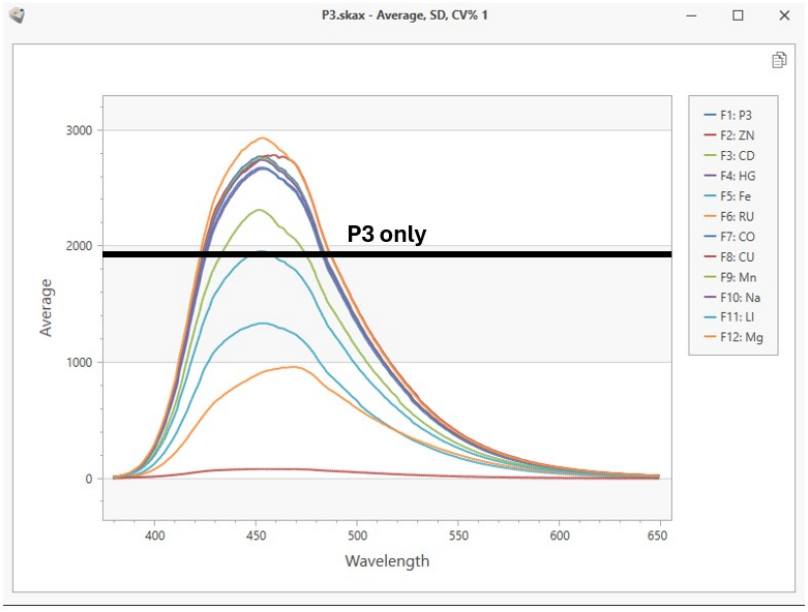
^{13}C NMR δ_c (100 MHz; $CDCl_3$) 42.7, 48.9, 95.2, 107.3, 110.8, 114.8, 116.1, 120.2, 122.0, 122.7, 123.5, 123.7, 123.9, 126.4, 127.5, 128.4, 128.7, 137.0, 138.1, 146.5, 147.6, 148.9 and 149.0;

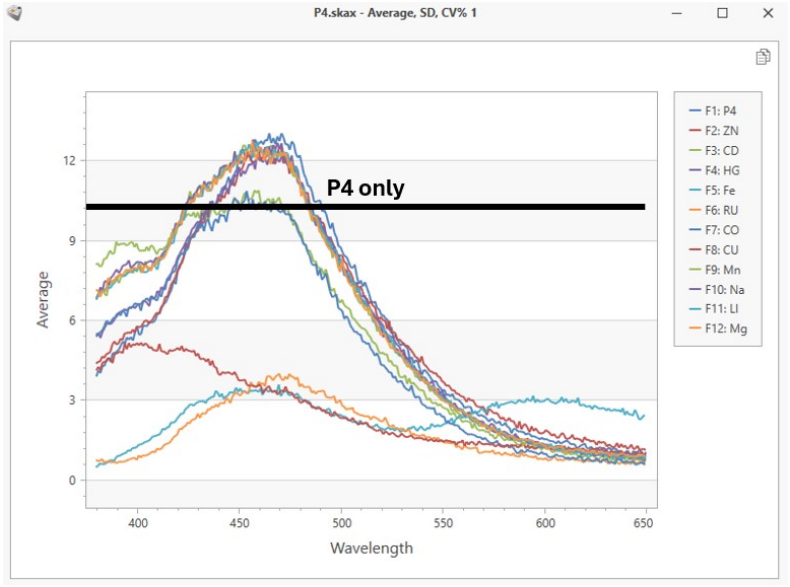
HRMS m/z Found 351.1540 ($M+H^+$). $C_{23}H_{19}N_4$ requires 351.1610.

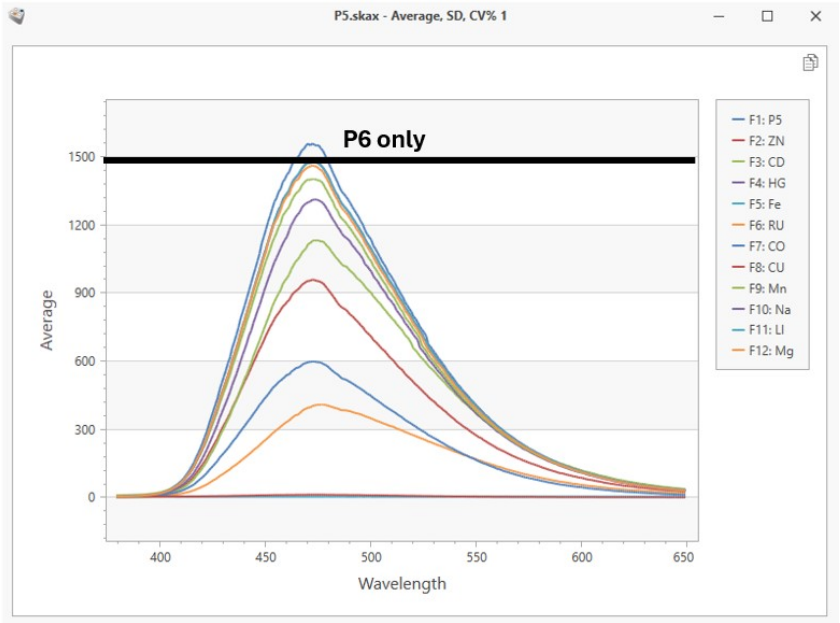
High throughput screening (S10)

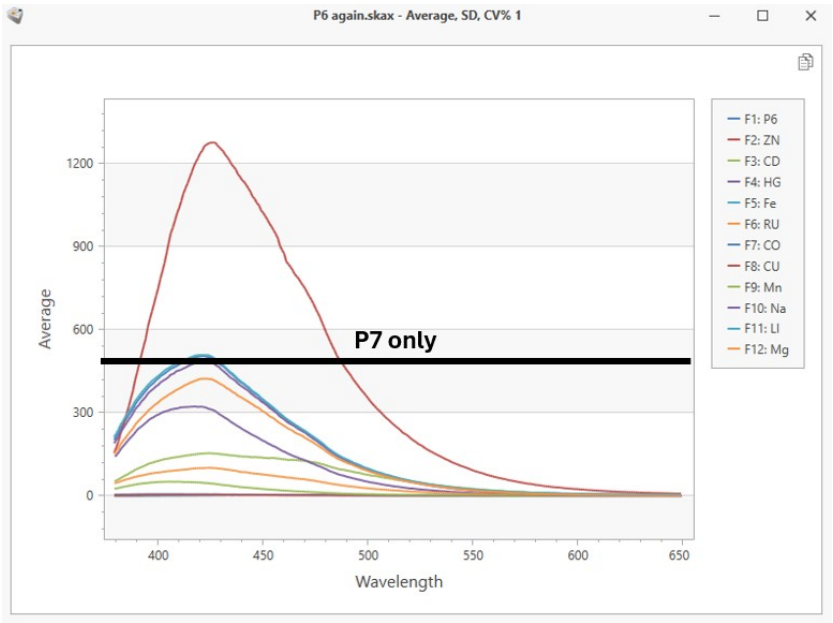


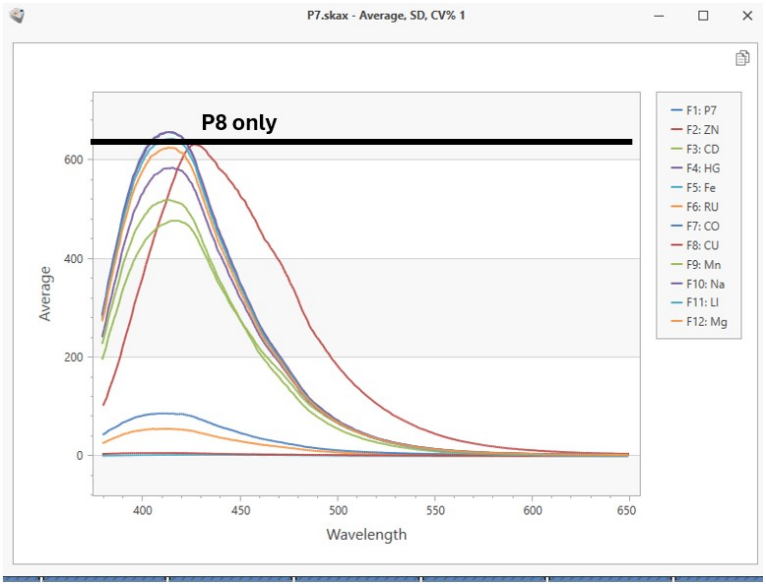

P2.skax - Average, SD, CV% 1
P2 only
Average
Wavelength
2500
2000
1500
1000
500
0
400
450
500
550
600
650
F1: P2
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: NA
F11: LI
F12: MG

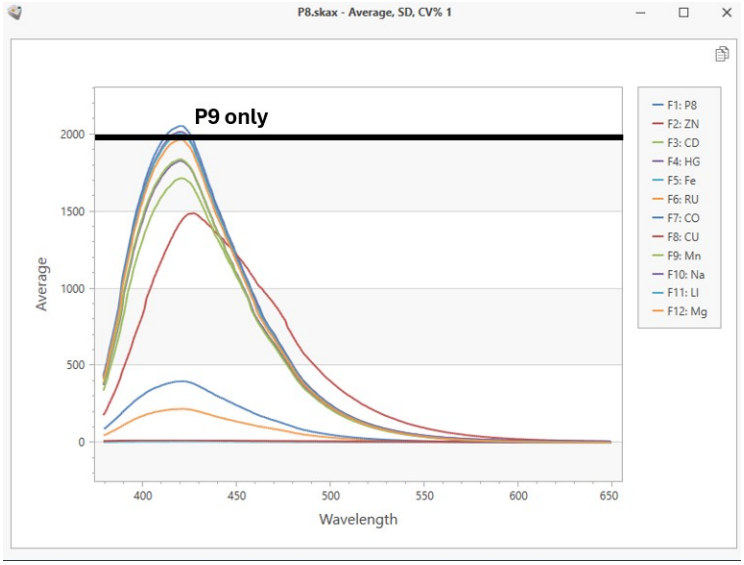

P3.skax - Average, SD, CV% 1
P3 only
Average
Wavelength
3000
2000
1000
0
400
450
500
550
600
650
F1: P3
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg

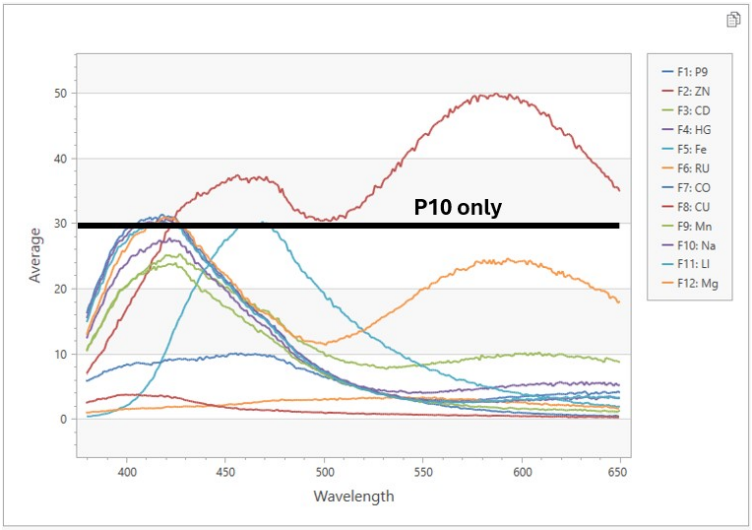

P4.skax - Average, SD, CV% 1
P4 only
Average
Wavelength
F1: P4
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg

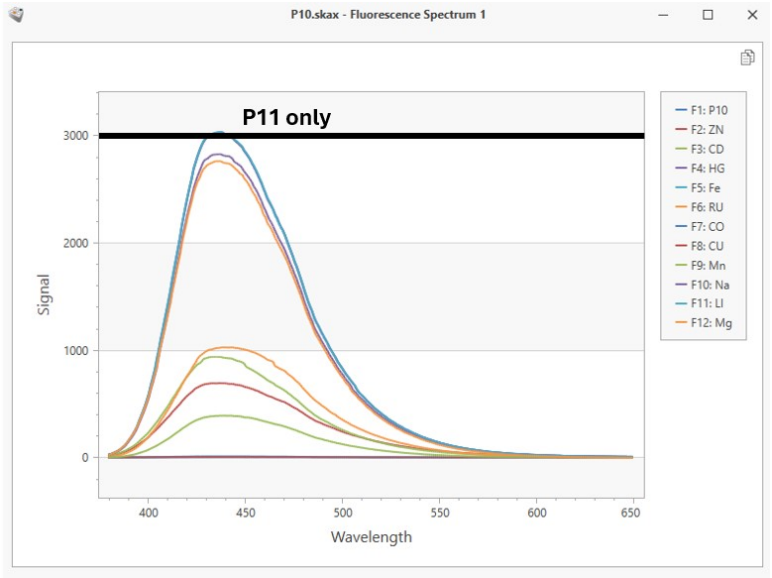

P5.skax - Average, SD, CV% 1
P6 only
Average
Wavelength
F1: P5
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg


P6 again.skax - Average, SD, CV% 1
P7 only
Average
Wavelength
1200
900
600
300
0
400
450
500
550
600
650
F1: P6
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg


P7.skax - Average, SD, CV% 1
P8 only
Average
Wavelength
600
400
200
0
400
450
500
550
600
650
F1: P7
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg


P8.skax - Average, SD, CV% 1
P9 only
Average
Wavelength
F1: P8
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg


P10 only
Average
Wavelength
F1: P9
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg


P10.skax - Fluorescence Spectrum 1
P11 only
Signal
Wavelength
3000
2000
1000
0
400
450
500
550
600
650
F1: P10
F2: ZN
F3: CD
F4: HG
F5: Fe
F6: RU
F7: CO
F8: CU
F9: Mn
F10: Na
F11: LI
F12: Mg