

Exploring Metal/Base-Free Porphyrin Involving Carboxyl Functionalized Pyridine Moiety for Photocatalytic N-Arylation of Benzamide Validated by RSM

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Signature SIF VIT VELLORE
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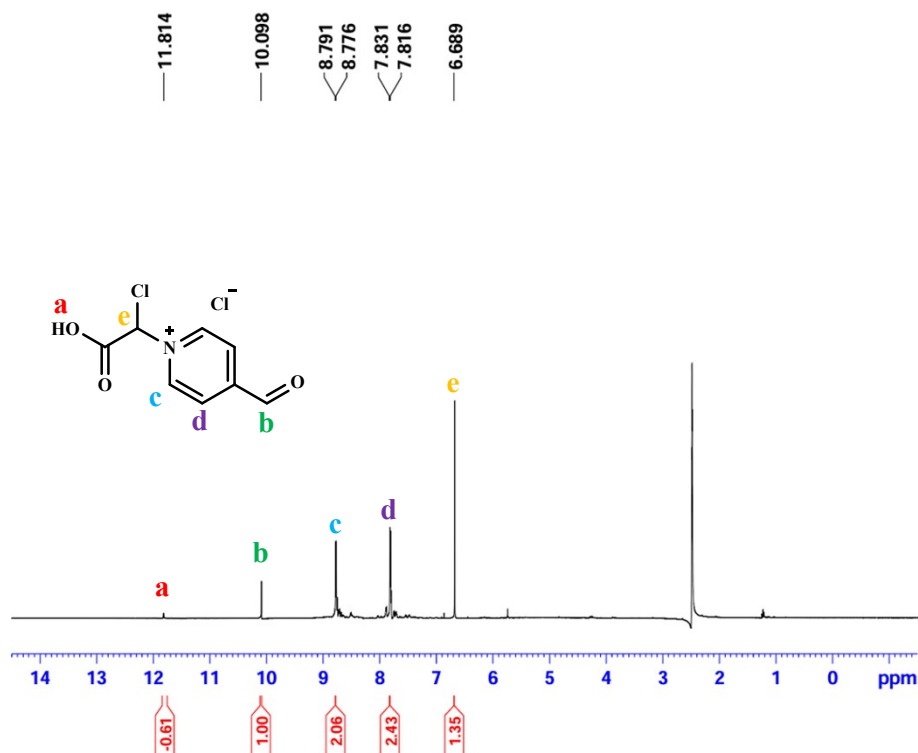


Fig S1. ¹H NMR spectrum of 1-(carboxychloromethyl)-4-formyl-pyridin-1-ium chloride [1A]

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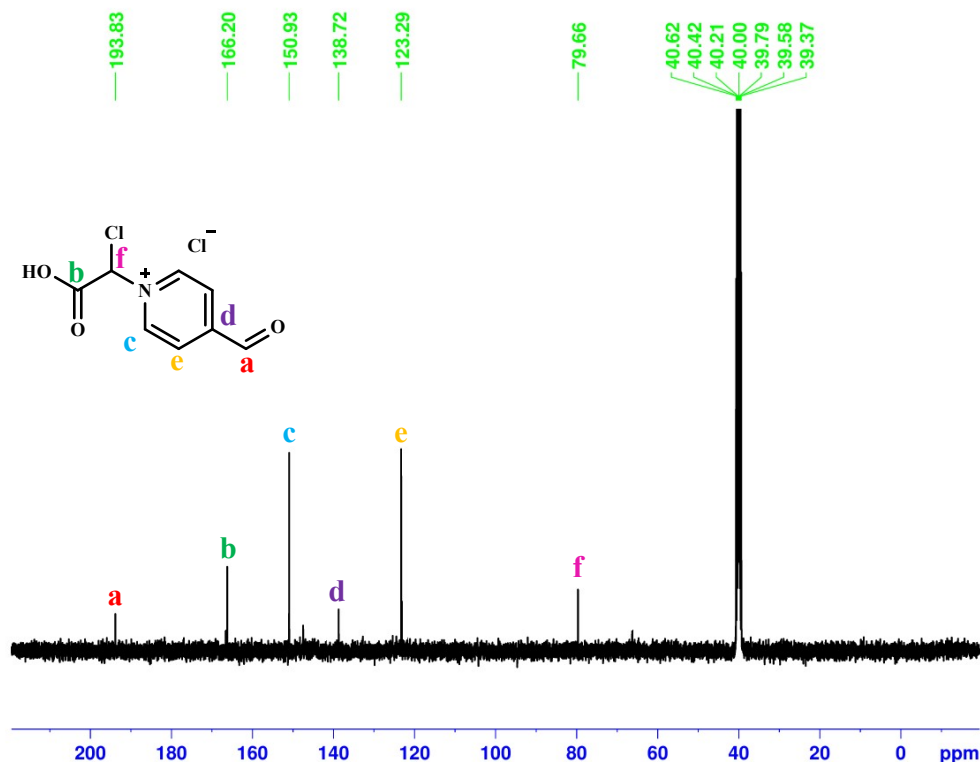


Fig S2. ¹³C NMR spectrum of 1-(carboxychloromethyl)-4-formyl-pyridin-1-ium chloride [1A]

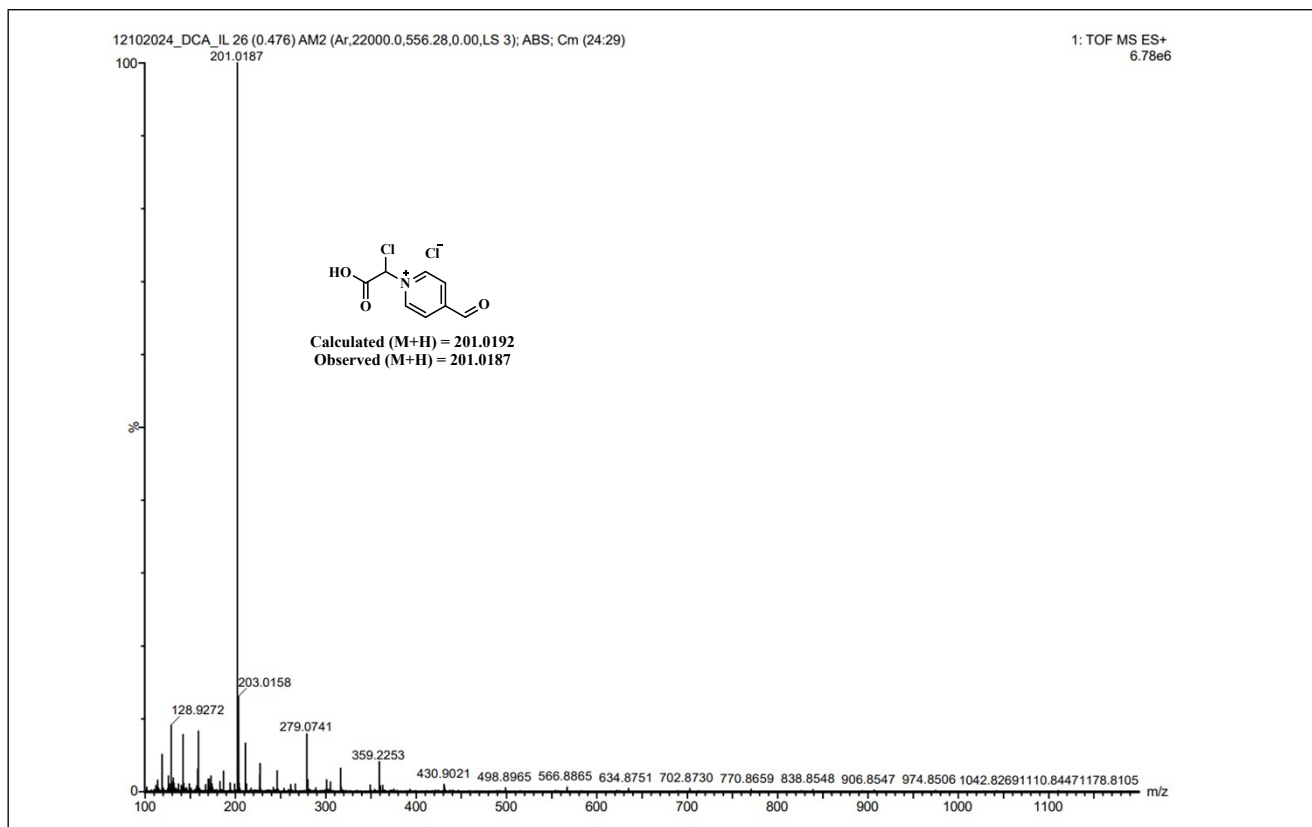


Fig S3. TOF MS ES +Ve mode of 1-(carboxychloromethyl)-4-formyl-pyridin-1-ium chloride [1A]

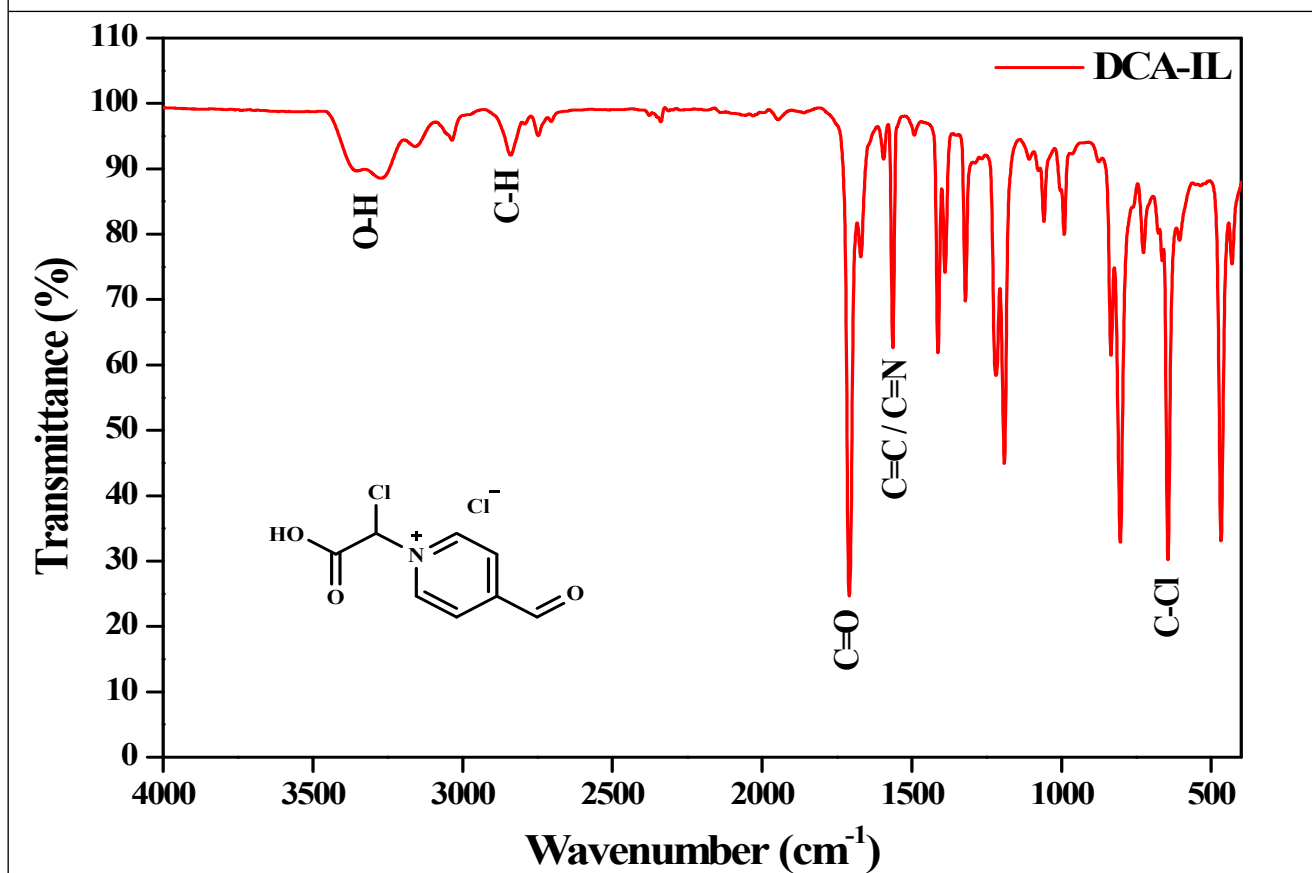


Fig S4. FT-IR spectrum of 1-(carboxychloromethyl)-4-formyl-pyridin-1-ium chloride [1A]

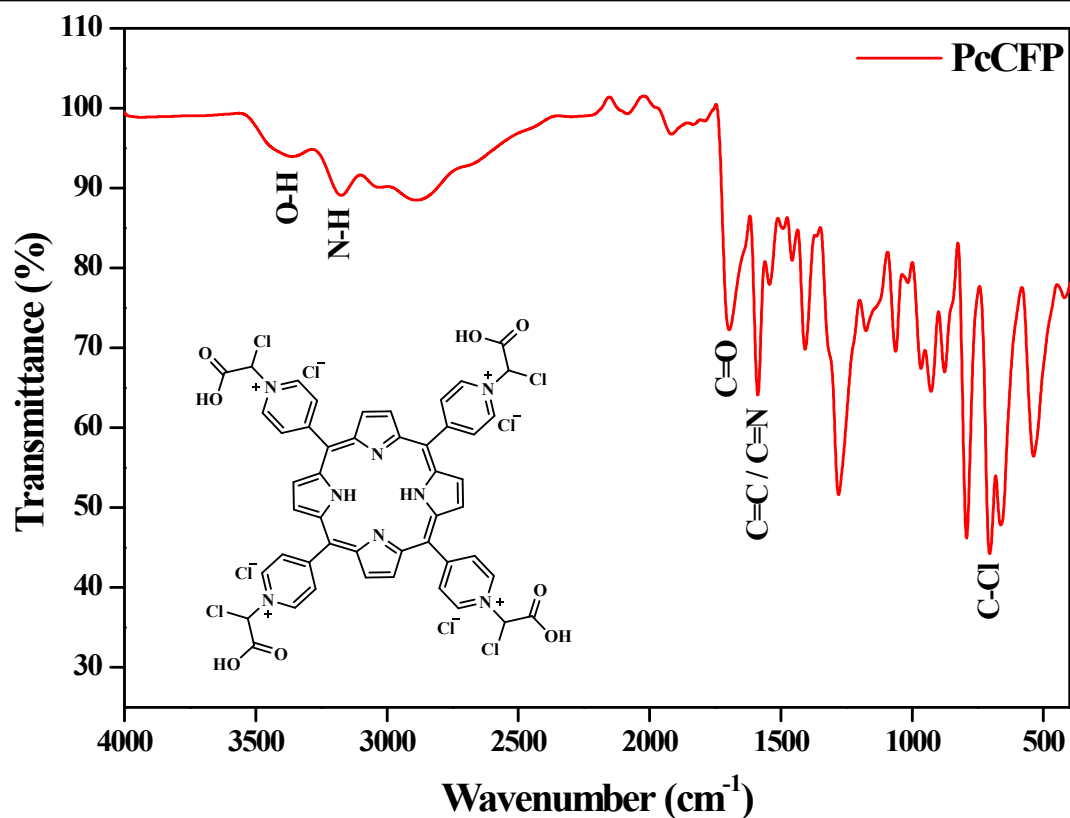


Fig S5. FT-IR Spectrum of PcCFP Photocatalyst

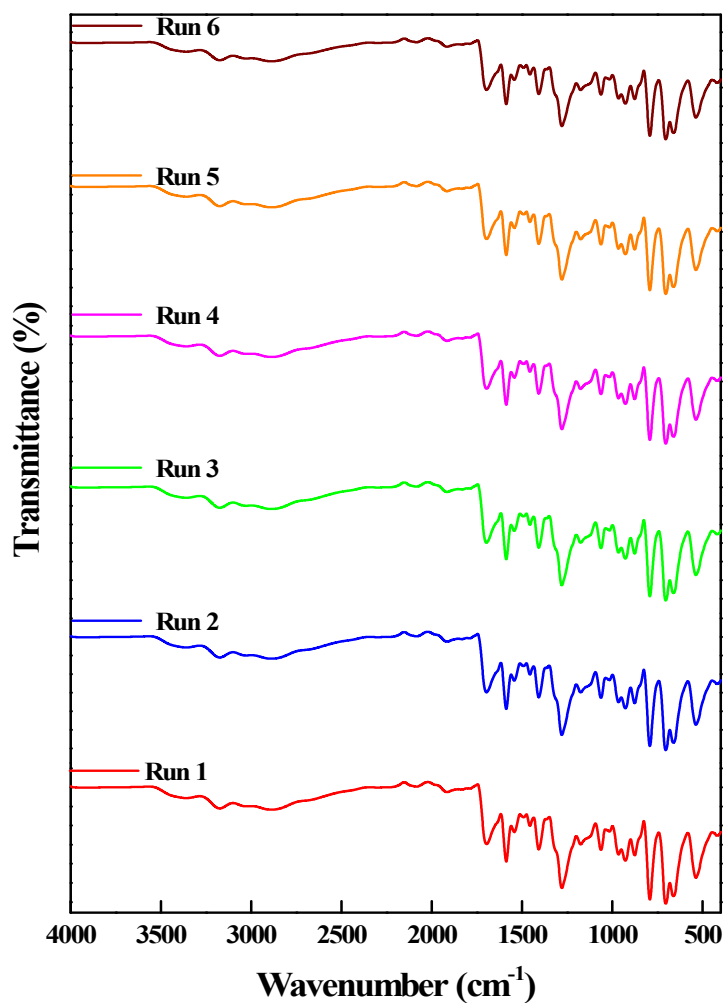
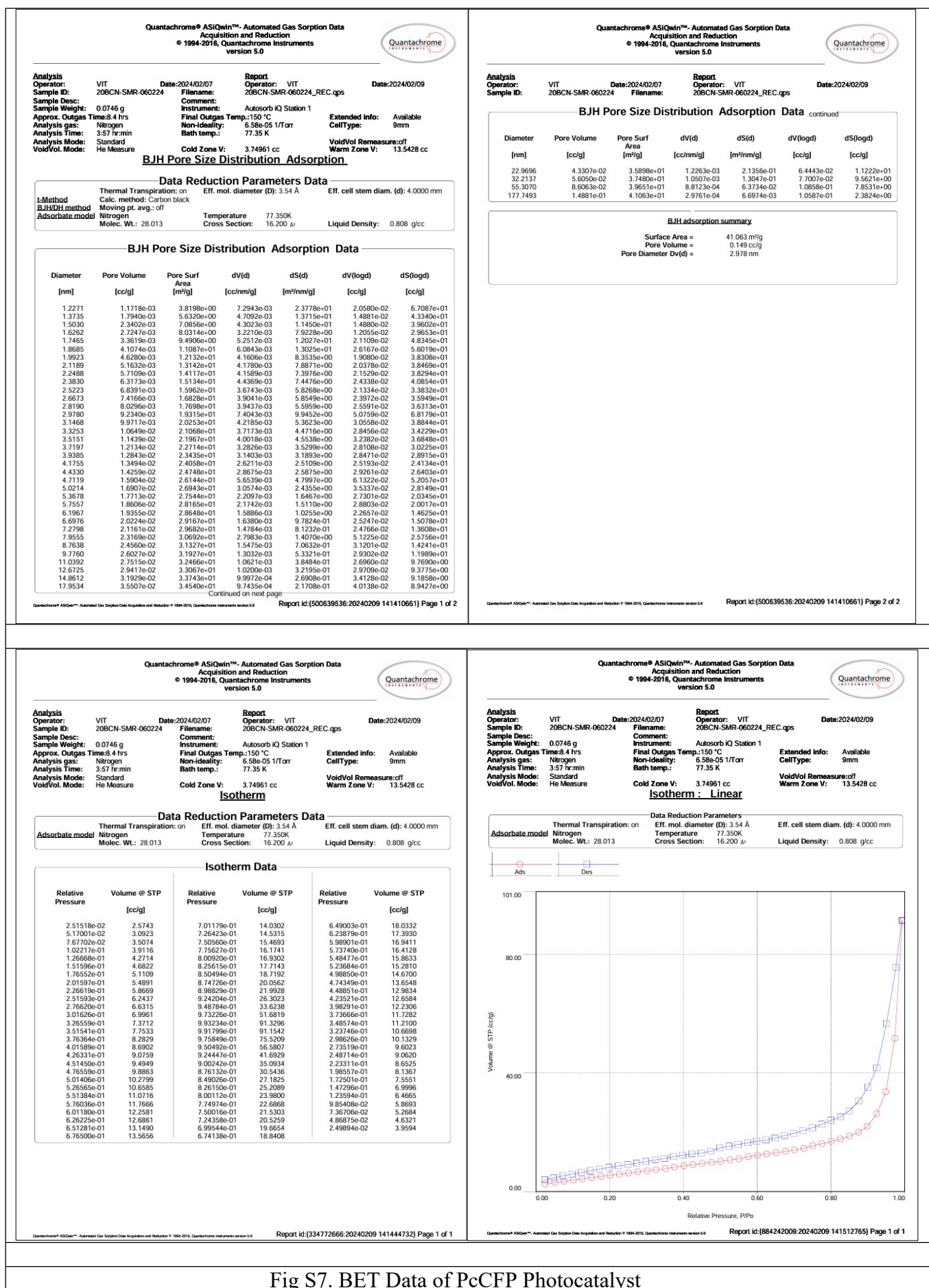


Fig S6. Comparative FT-IR Spectra of PcCFP Photocatalyst recycled upto 6th Run



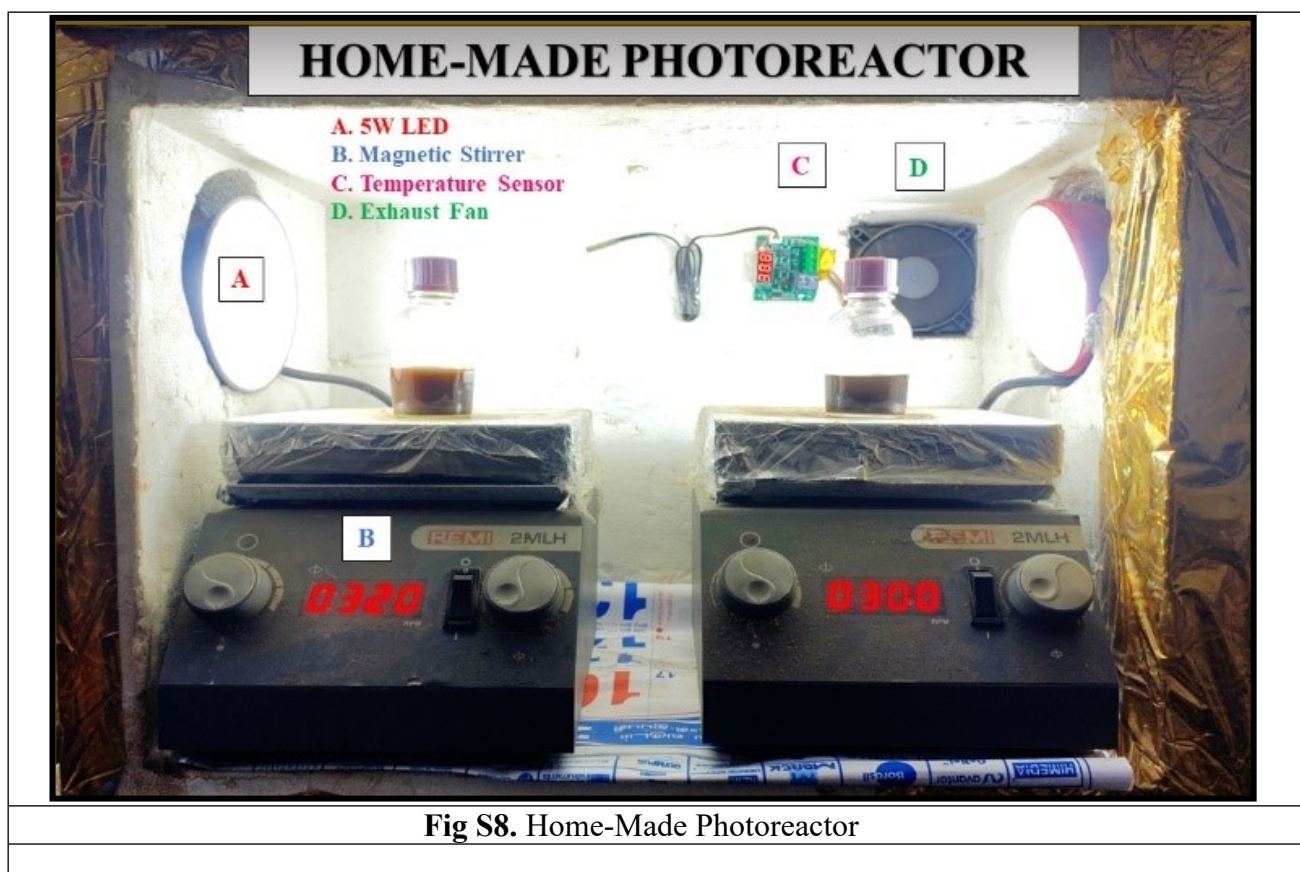


Fig S8. Home-Made Photoreactor

Explanation of Normal Distribution Plots:

The use of normal probability plots allows for a comparison between expected and residual responses, facilitating a visual assessment of the normality of these residuals, as depicted in Figure S9. Evaluating the model's adequacy necessitates a comparison between predicted values and experimental data. It is vital to ascertain whether the residuals exhibit a normal distribution to ensure an optimal distribution of data. This analysis plays a significant role in validating the reliability of the outputs generated by the predictive model. Additionally, the configuration of data points in relation to the fitted line can be employed to evaluate which model aligns most closely with the data. The plot of normal probability against externally studentized residuals (Fig S9. a) exhibited a linear association, though with some deviations, suggesting that data points conforming to the principles of normal distribution would yield superior model performance. Therefore, linearity in the data would be evident if the connecting line forms a 45° angle.

To determine the adequacy of the models used for the conversion of Benzamide to N-Aryl Amides through the photocatalytic process, we assessed both residuals and the distribution plot. The alignment of the plotted points with the theoretical normality line was analyzed to evaluate the model's suitability and significance (Fig S9. b). Likewise, Fig S9.c adeptly showcases the random characteristics of the residuals concerning the predicted response, highlighting the absence of any noticeable patterns or trends in the experimental data. This scatter plot confirms the lack of systematic variation, reinforcing the unpredictable nature of the residuals. Additionally, a plot of residuals plotted against the run number displays a random and scattered distribution (Fig S9. d). Such results are pivotal in affirming the adequacy and credibility of the model utilized.

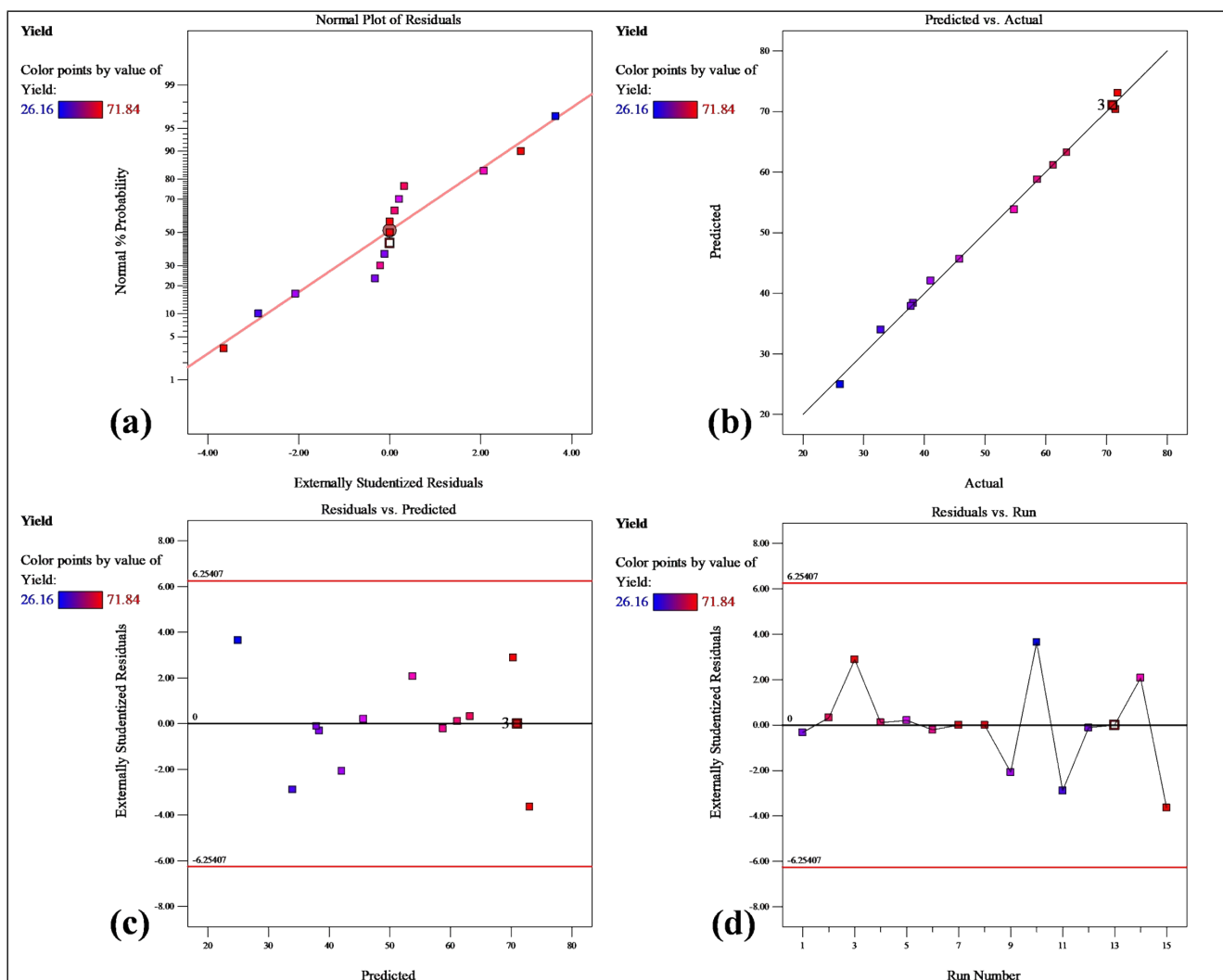


Fig S9. Plot illustrating the normal distribution of Linear models **a.** depicting the efficiency of PcCFP Photocatalyst for the N-Arylation of Benzamide. **b.** Comparison between the observed and predicted results for photocatalytic N-Arylation of Benzamide. Normal probability plots of residual for photo-transesterification of UFO to Biofuel as a function of **c.** Predicted Response and **d.** Run Number

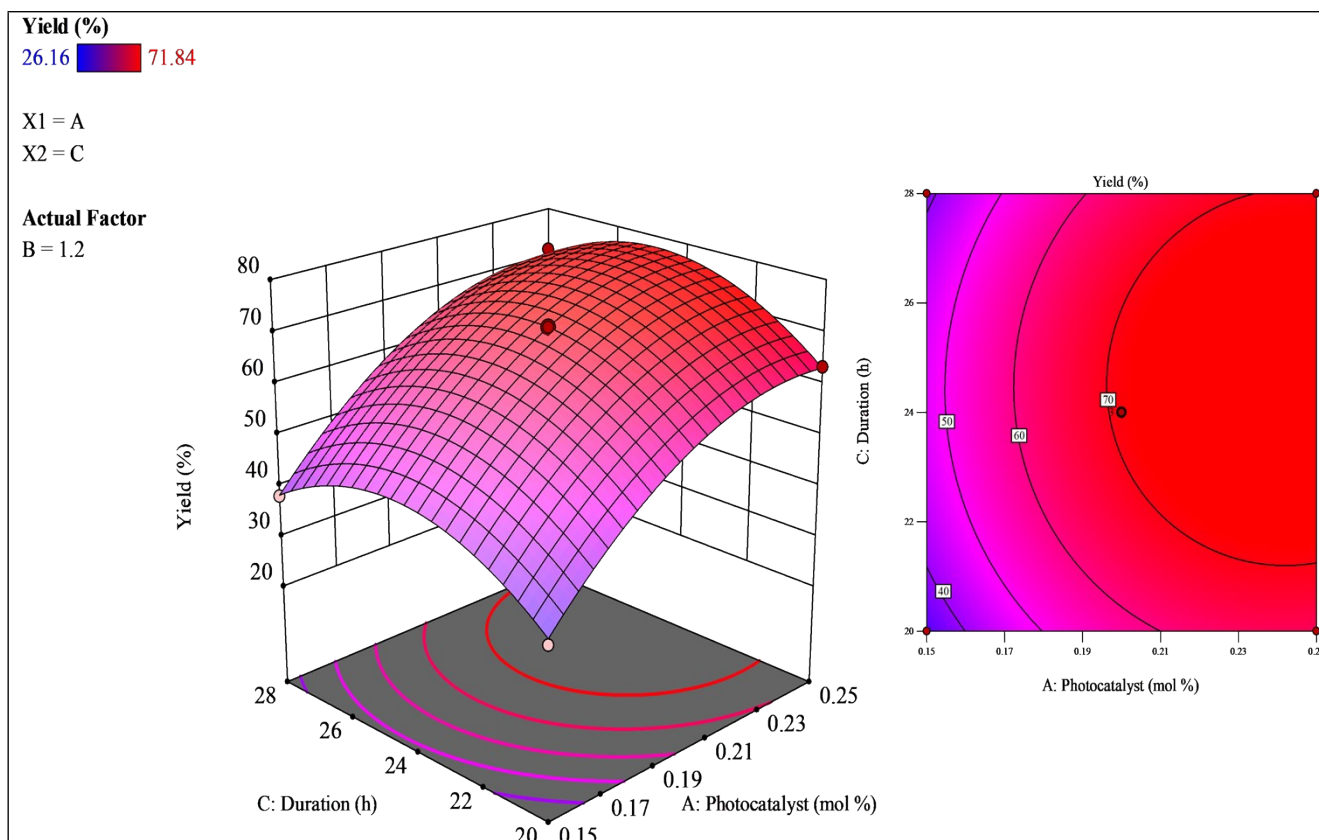


Fig S10. 3-D Surface and Contour Plot of N-arylation of Benzamide highlighting the relationship between the amount of PcCFP Photocatalyst (A) and duration of reaction (C) with constant molar ratio of reactants (B)

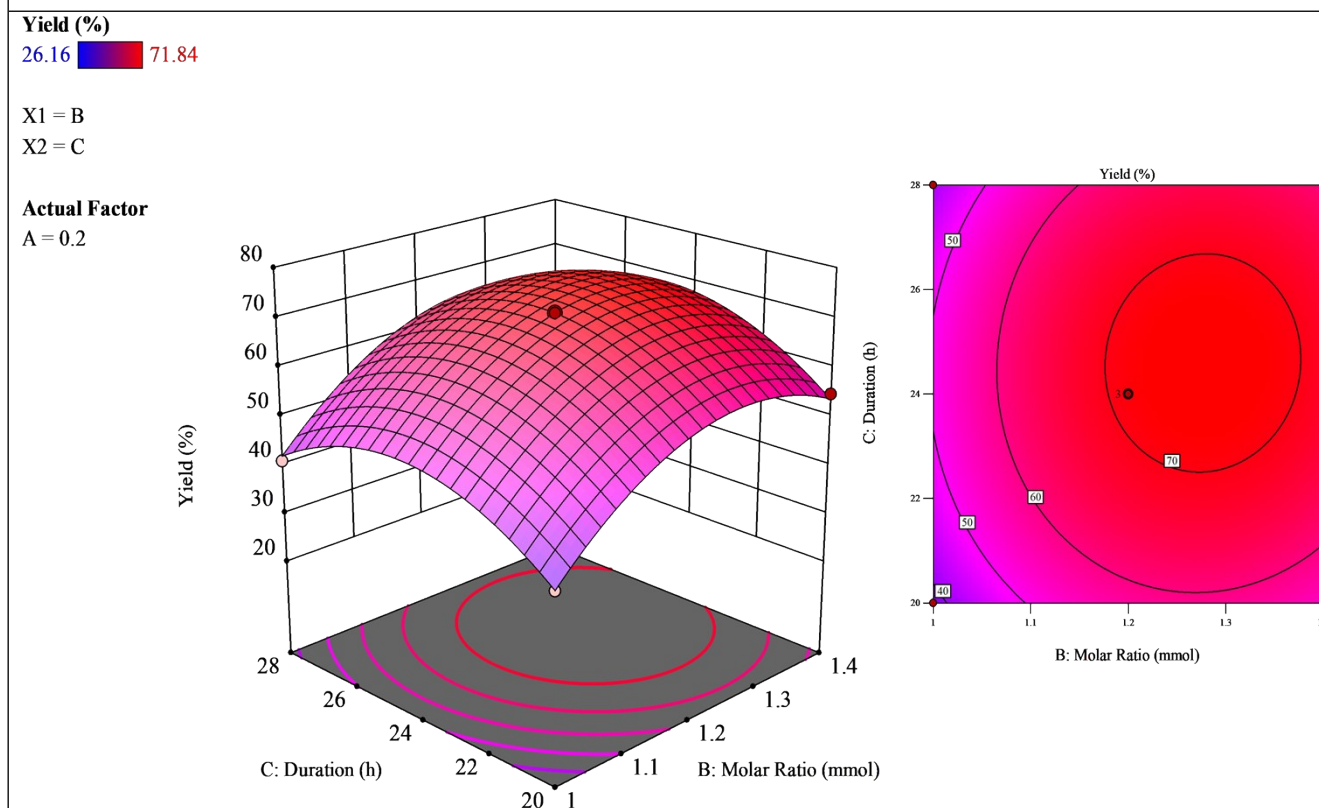


Fig S11. 3-D Surface and Contour Plot of N-arylation of Benzamide highlighting the relationship between the molar ratio of reactants (B) and duration of reaction (C) with constant amount of PcCFP Photocatalyst (A)

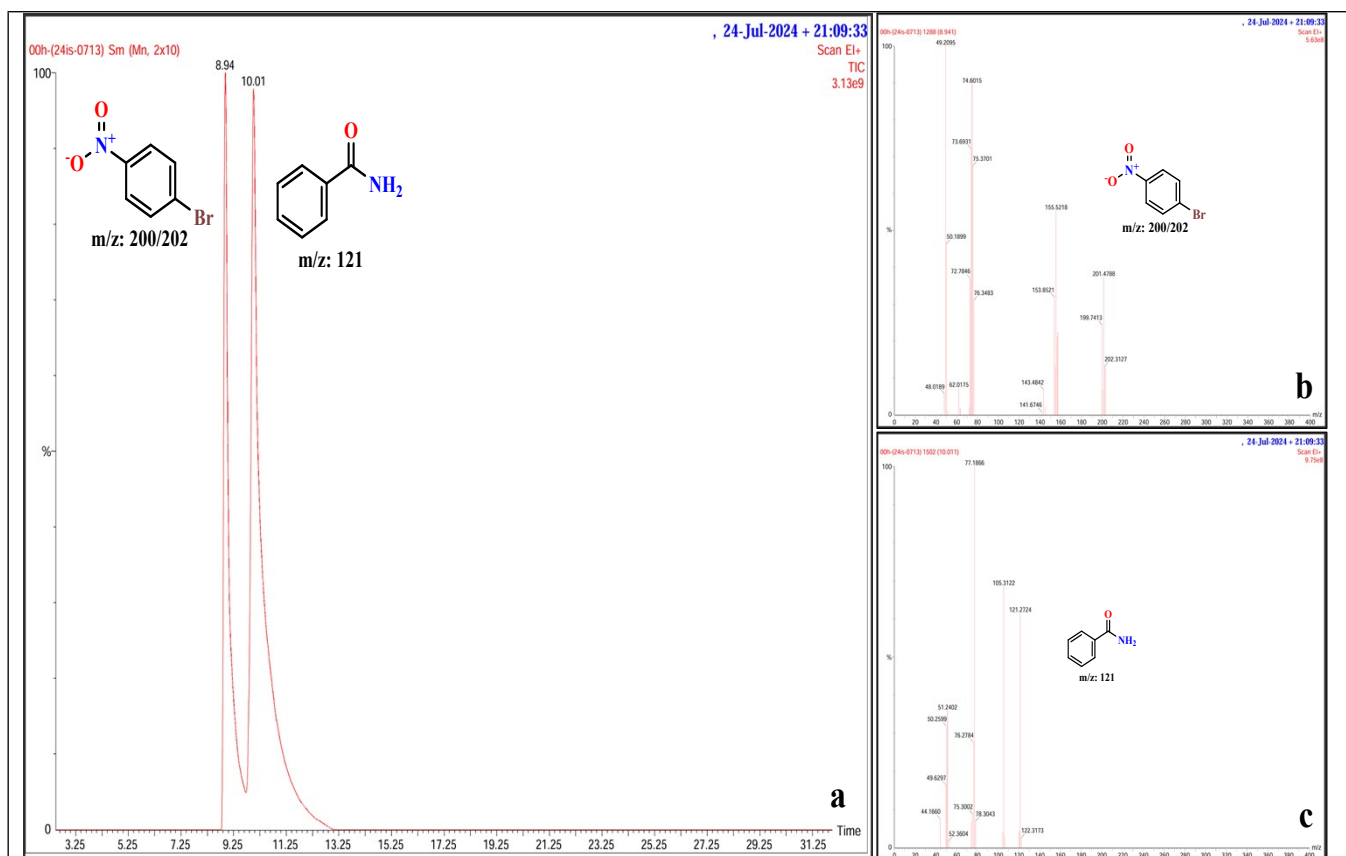


Fig S12. a. GC-MS Chromatogram of sample taken initially at 0 hour of reaction time. **b.** m/z of Ar-Br obtained at 8.94 RT in chromatogram. **c.** m/z of benzamide obtained at 10.01 RT in chromatogram.

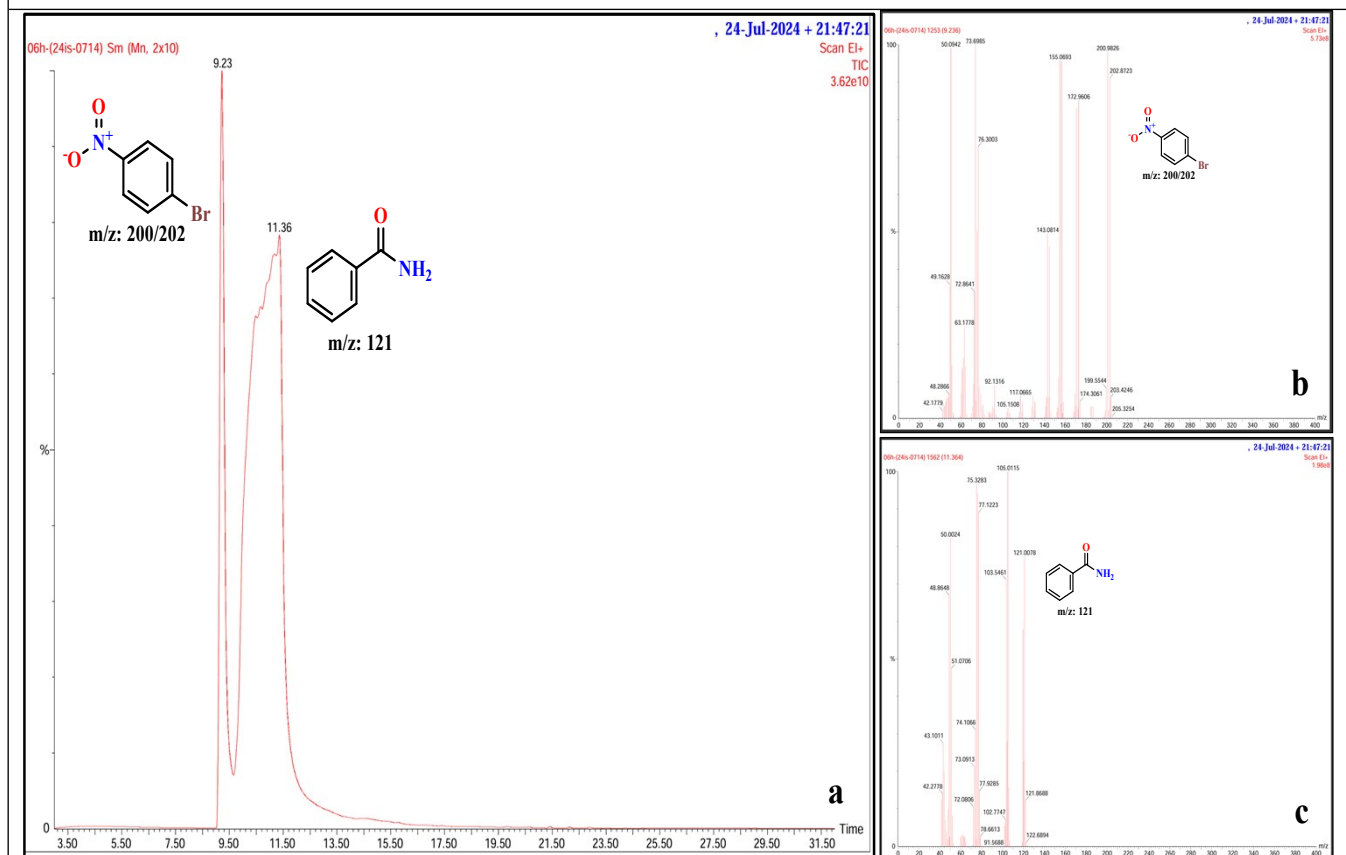


Fig S13. a. GC-MS Chromatogram of sample taken initially at 6 hour of reaction time. **b.** m/z of Ar-Br obtained at 9.23 RT in chromatogram. **c.** m/z of benzamide obtained at 11.36 RT in chromatogram.

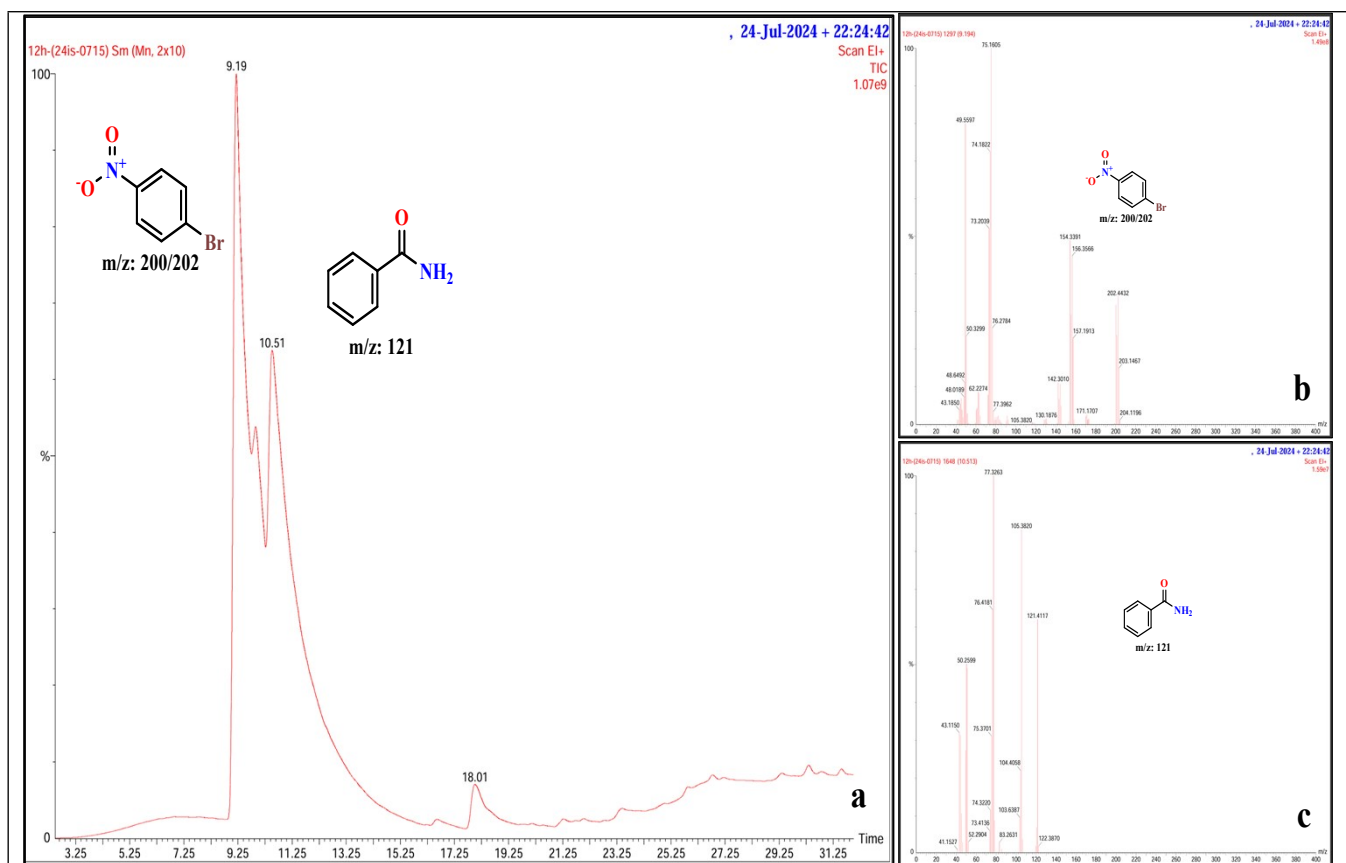


Fig S14. a. GC-MS Chromatogram of sample taken initially at 12 hour of reaction time. **b.** m/z of Ar-Br obtained at 9.19 RT in chromatogram. **c.** m/z of benzamide obtained at 10.51 RT in chromatogram.

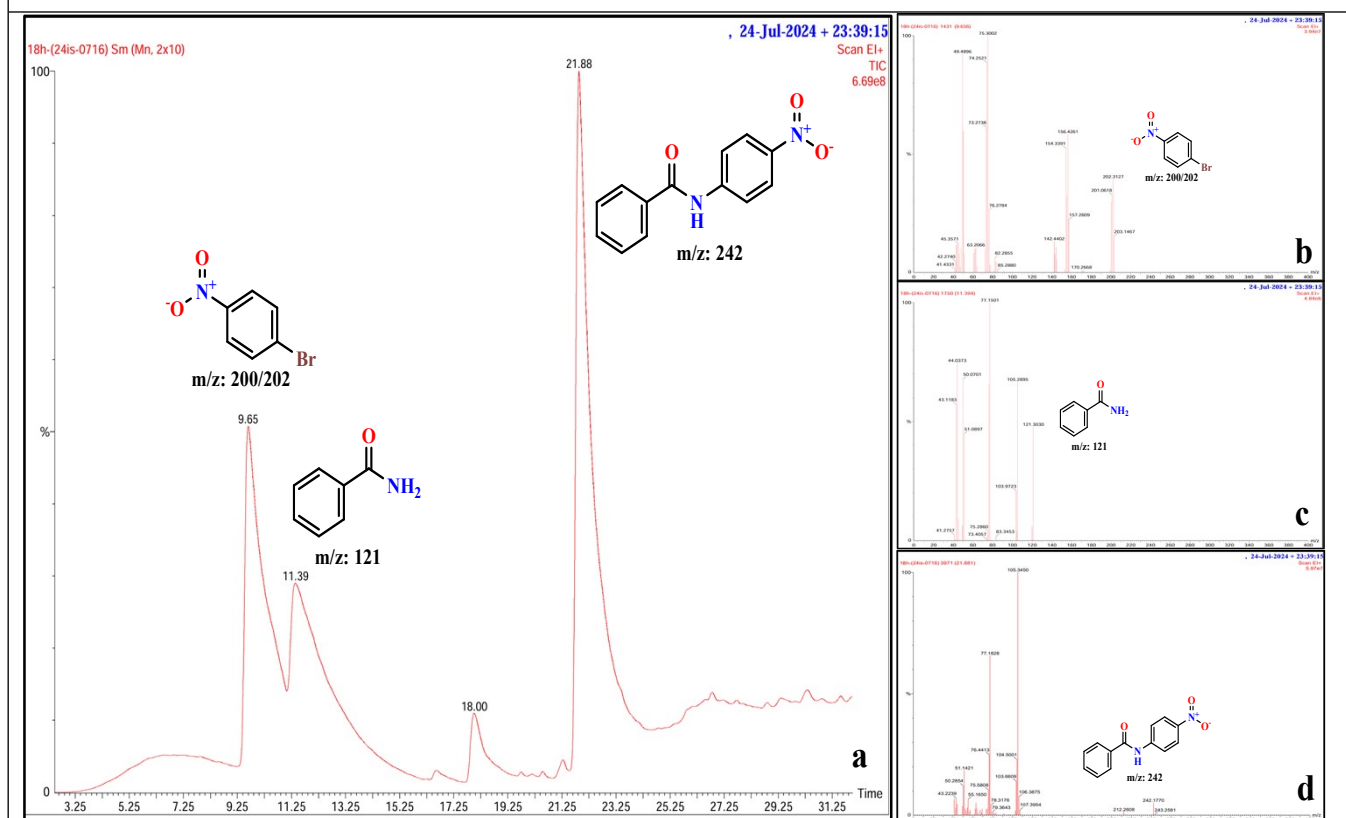


Fig S15. a. GC-MS Chromatogram of sample taken initially at 18 hour of reaction time. **b.** m/z of Ar-Br obtained at 9.65 RT in chromatogram. **c.** m/z of benzamide obtained at 11.39 RT in chromatogram. **d.** m/z of product obtained at 21.88 RT in chromatogram.

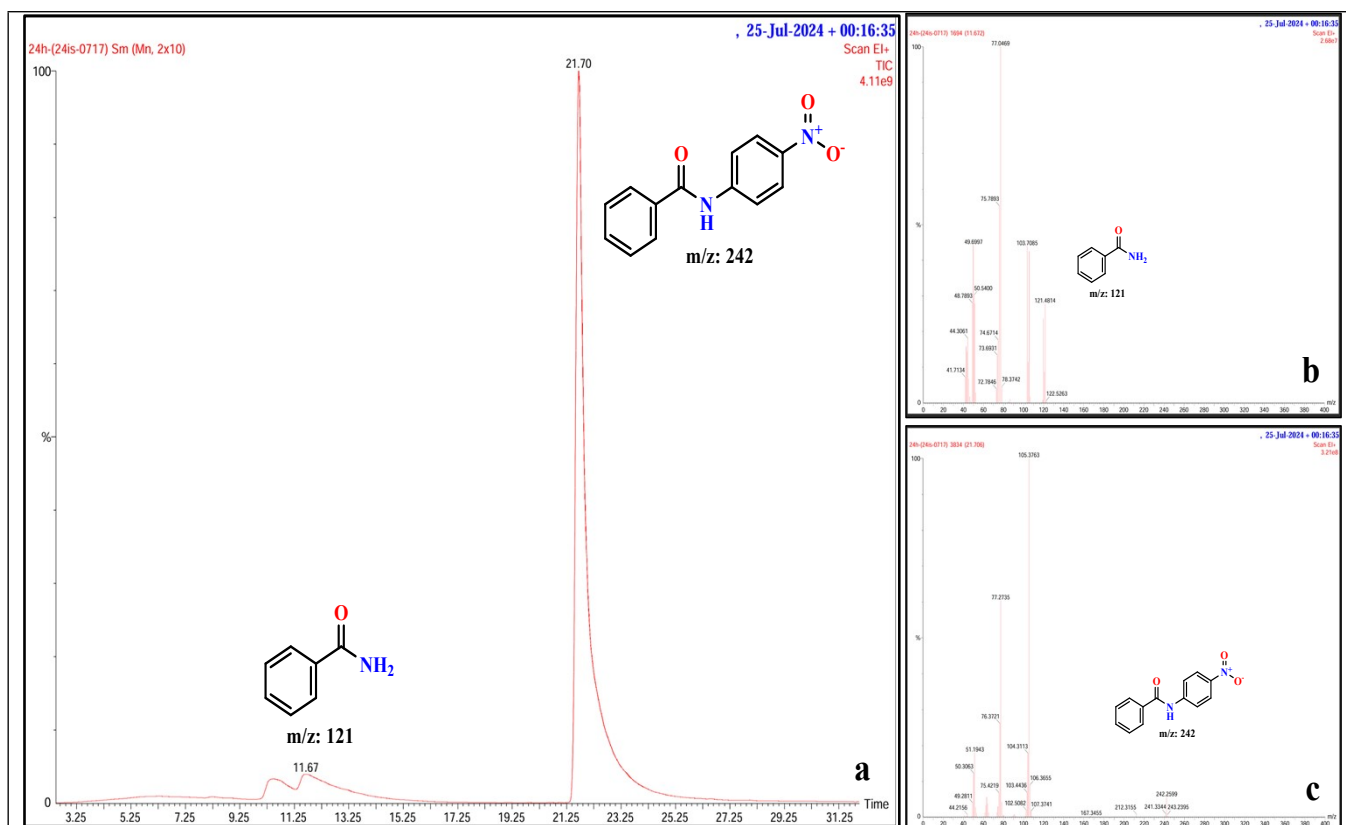


Fig S16. a. GC-MS Chromatogram of sample taken initially at 24 hour of reaction time. **b.** m/z of benzamide traces obtained at 11.67 RT in chromatogram. **c.** m/z of product obtained at 21.70 RT in chromatogram.

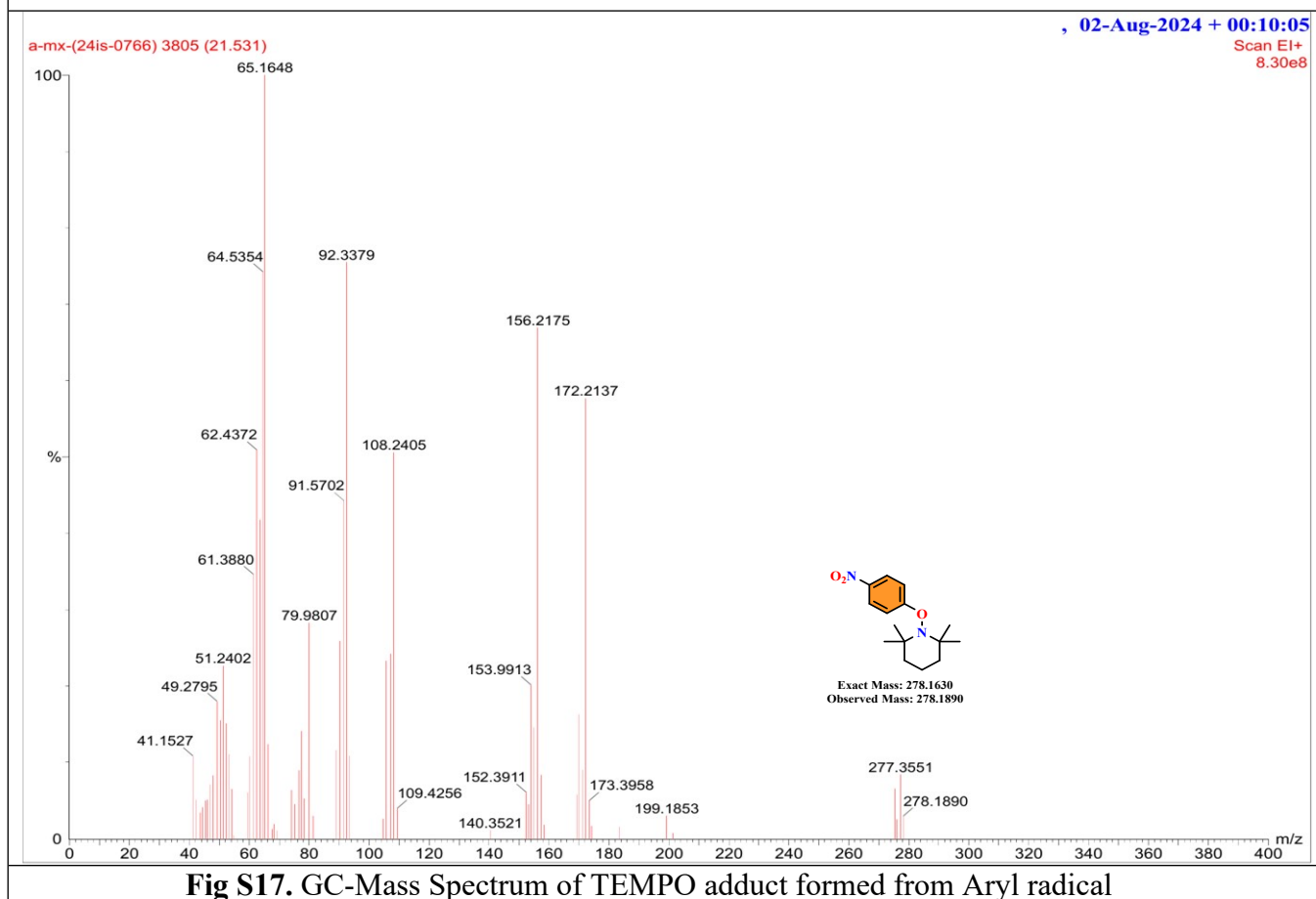
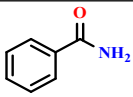
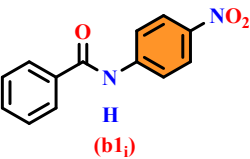
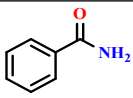
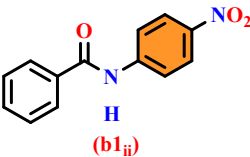
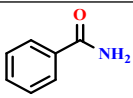
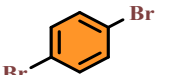
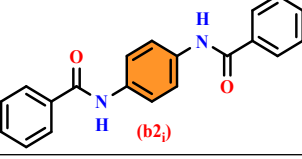
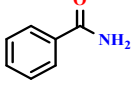
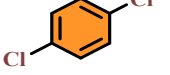
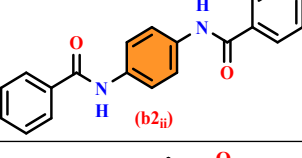
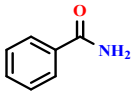
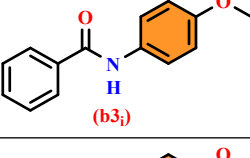
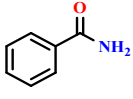
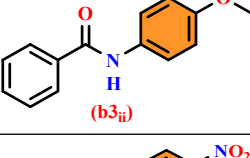
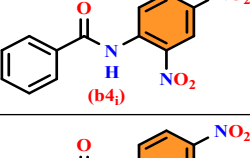
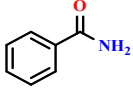
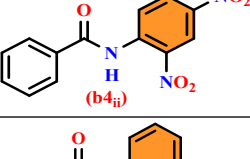
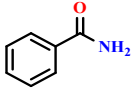
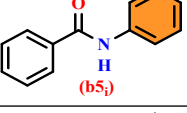
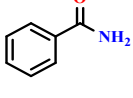
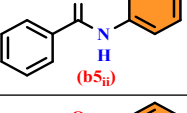
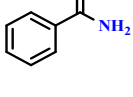
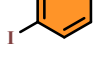
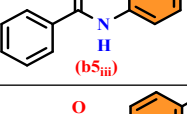
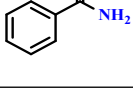
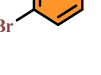
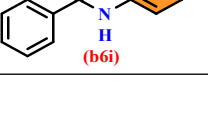
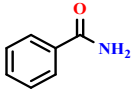
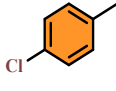
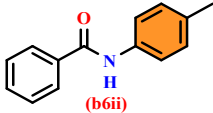
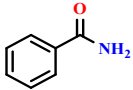
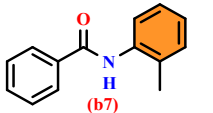
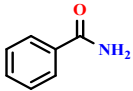
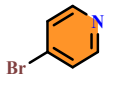
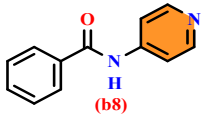
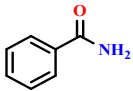
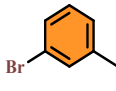
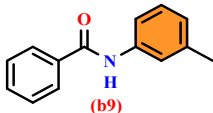
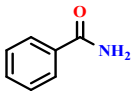
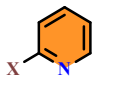
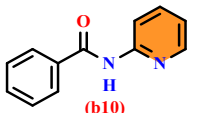
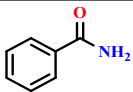
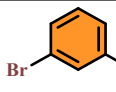
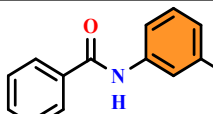
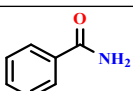
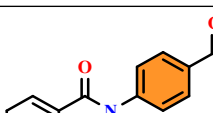
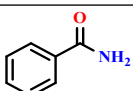
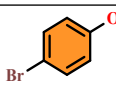
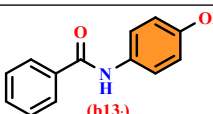
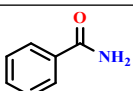
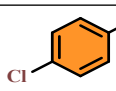
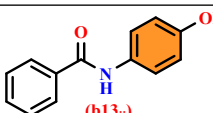
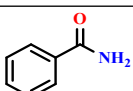
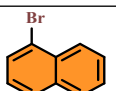
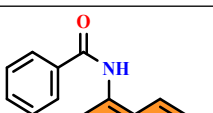
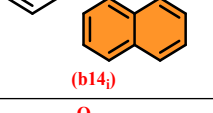
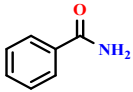
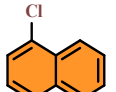
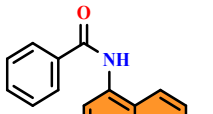
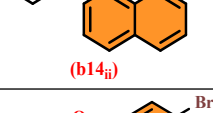
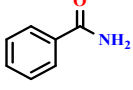
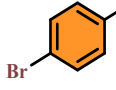
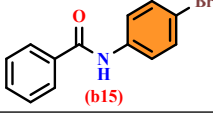
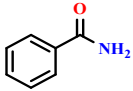
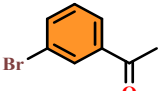
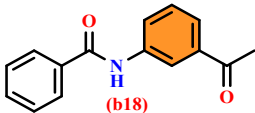
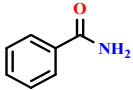
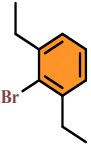
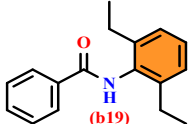
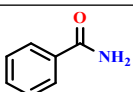
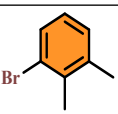
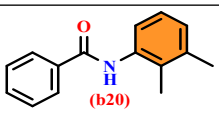
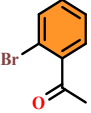
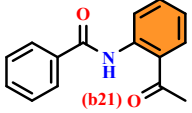
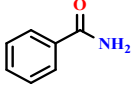
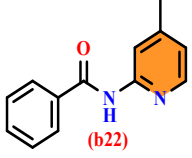
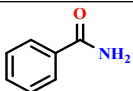
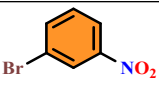
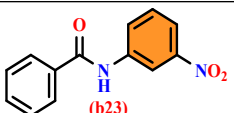
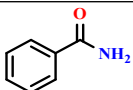
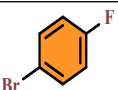
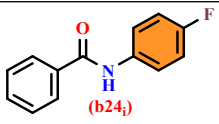
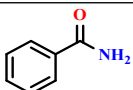
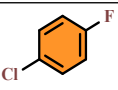
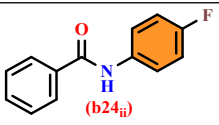
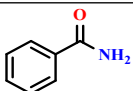
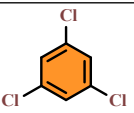
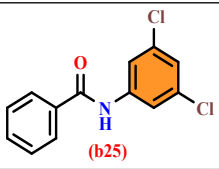


Fig S17. GC-Mass Spectrum of TEMPO adduct formed from Aryl radical

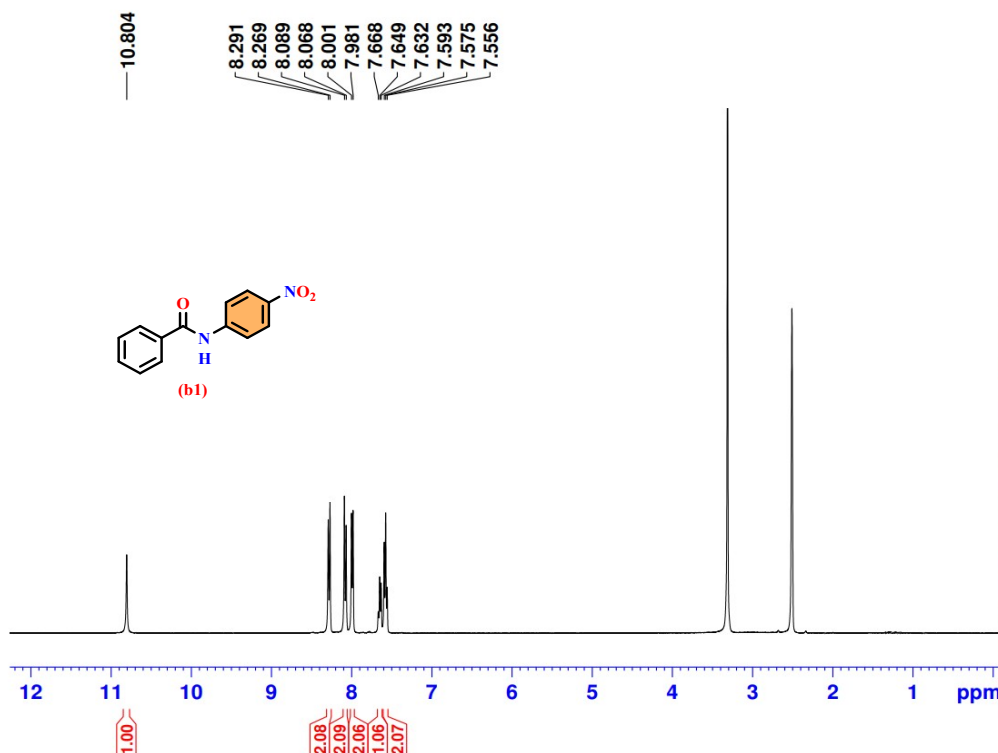
Table S1. Precursor with respective halogens and its Product obtained via N-arylation of Benzamide

Sr. No	Product Code	Reactant R1	Reactants R2	Product	Yield (%)
1.	b1 _i			 (b1 _i)	71%
2.	b1 _{ii}			 (b1 _{ii})	29%
3.	b2 _i			 (b2 _i)	64%
4.	b2 _{ii}			 (b2 _{ii})	27%
5.	b3 _i			 (b3 _i)	61%
6.	b3 _{ii}			 (b3 _{ii})	22%
7.	b4 _i			 (b4 _i)	73%
8.	b4 _{ii}			 (b4 _{ii})	35%
9.	b5 _i			 (b5 _i)	63%
10.	b5 _{ii}			 (b5 _{ii})	30%
11.	b5 _{iii}			 (b5 _{iii})	72%
12.	b6 _i			 (b6 _i)	58%

13.	b6 _{ii}			 (b6ii)	21%
14.	b7			 (b7)	54%
15.	b8			 (b8)	67%
16.	b9			 (b9)	60%
17.	b10			 (b10)	62%
18.	b11			 (b11)	61%
19.	b12			 (b12)	73%
20.	b13 _i			 (b13 _i)	59%
21.	b13 _{ii}			 (b13 _{ii})	22%
22.	b14 _i			 (b14 _i)	60%
23.	b14 _{ii}			 (b14 _{ii})	26%
24.	b15			 (b15)	68%
25.	b16			 (b16)	51%
26.	b17			 (b17)	60%

27.	b18				63%
28.	b19				53%
29.	b20				55%
30.	b21				61%
31.	b22				28%
32.	b23				69%
33.	b24 _i				70%
34.	b24 _{ii}				28%
35.	b25				31%

Signature SIF VIT VELLORE
Bz-01-Br



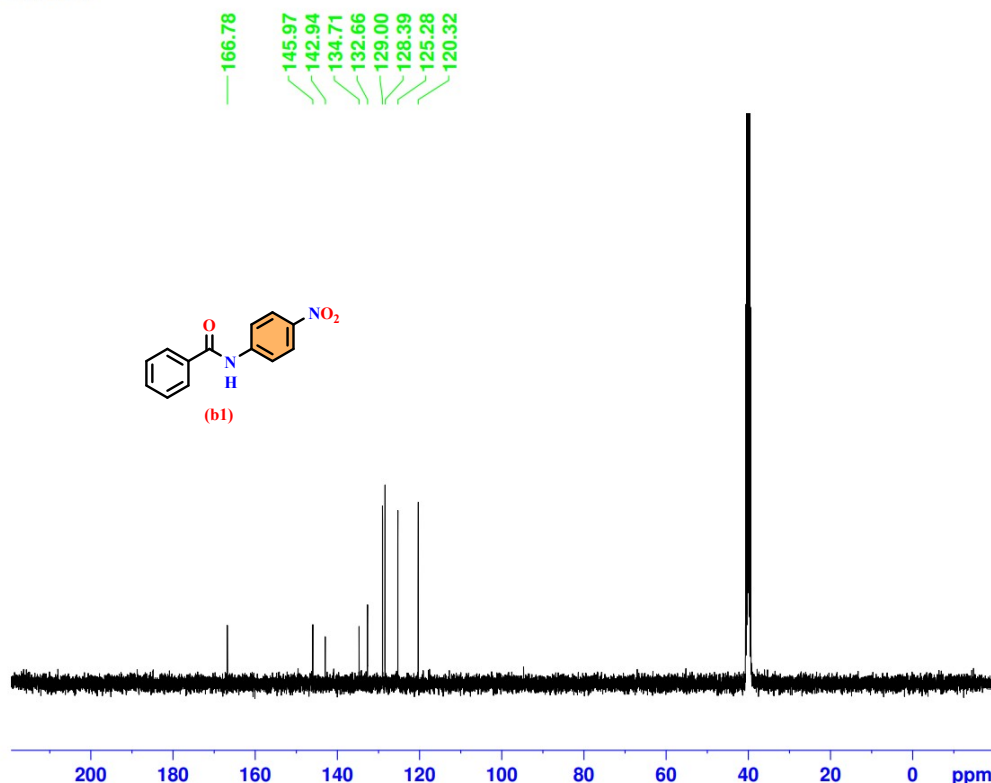
Current Data Parameters
NAME Dr.PDK040524
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240504
Time 15.00 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 307.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S18. ¹H NMR spectrum of *N*-(4-nitrophenyl)benzamide (b1)

Signature SIF VIT VELLORE
Bz-01-Br



Current Data Parameters
NAME Dr.PDK090524
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240509
Time 22.41 h
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S19. ¹³C NMR spectrum of *N*-(4-nitrophenyl)benzamide (b1)

bz-01-(23es-01540) 4033 (21.171)

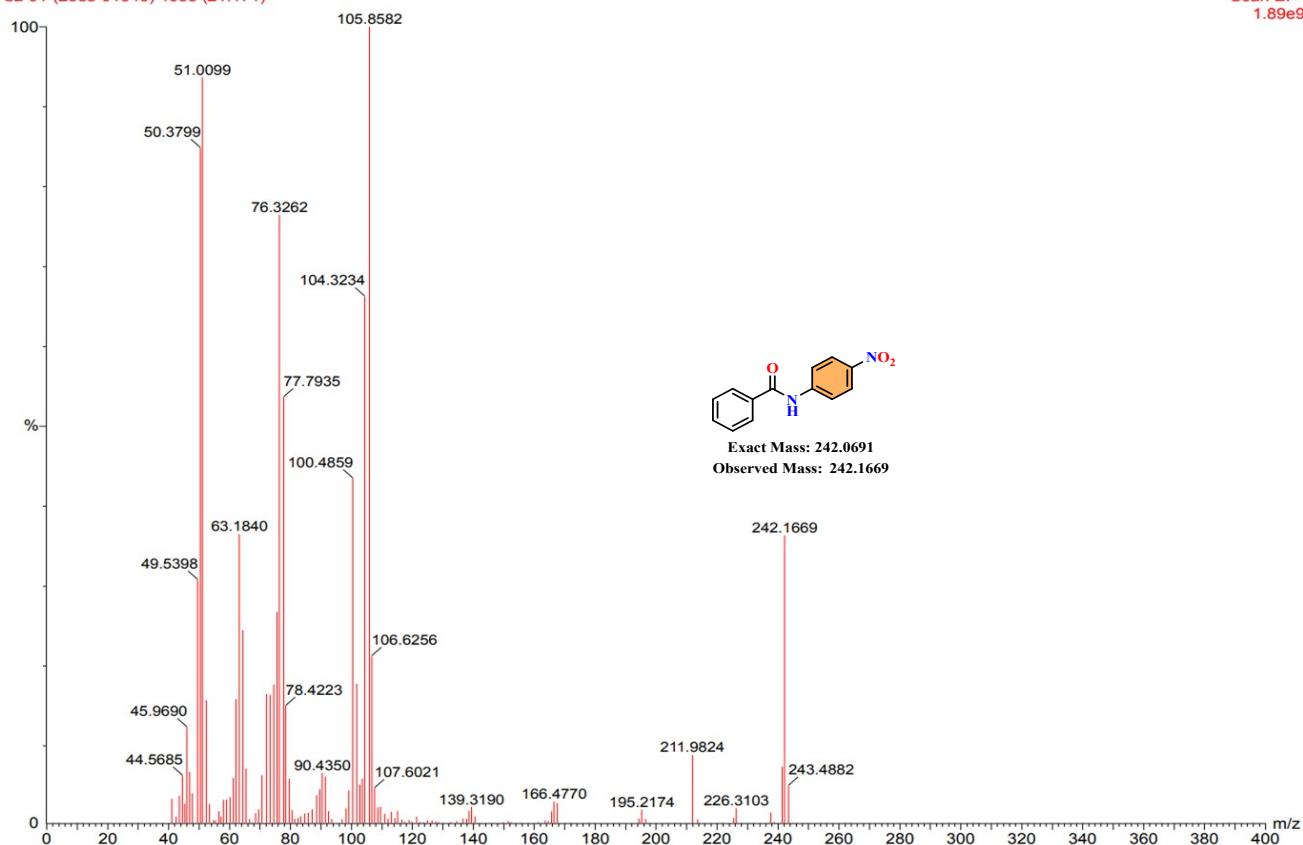
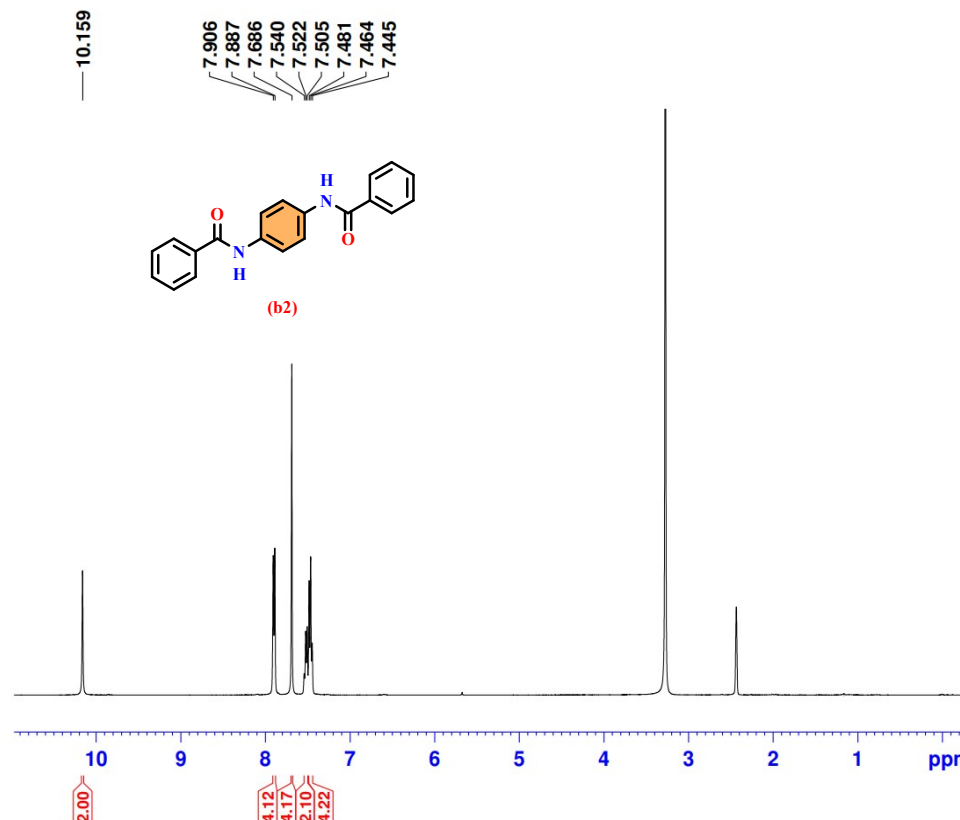


Fig S20. GC-Mass spectrum (m/z) of *N*-(4-nitrophenyl)benzamide (b1j)

Signature SIF VIT VELLORE
BZ-02-Br



Current Data Parameters
NAME Dr.PDK090424
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240410
Time 2.53 h
INSTRUM spect
PROBHD Z108618_0505 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 308.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580303 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S21. ¹H NMR spectrum of *N,N'*-(1,4-phenylene)dibenzamide (b2j)

Signature SIF VIT VELLORE
BZ-02-Br



Current Data Parameters
NAME Dr.PDK090424
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240410
Time 3.24 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

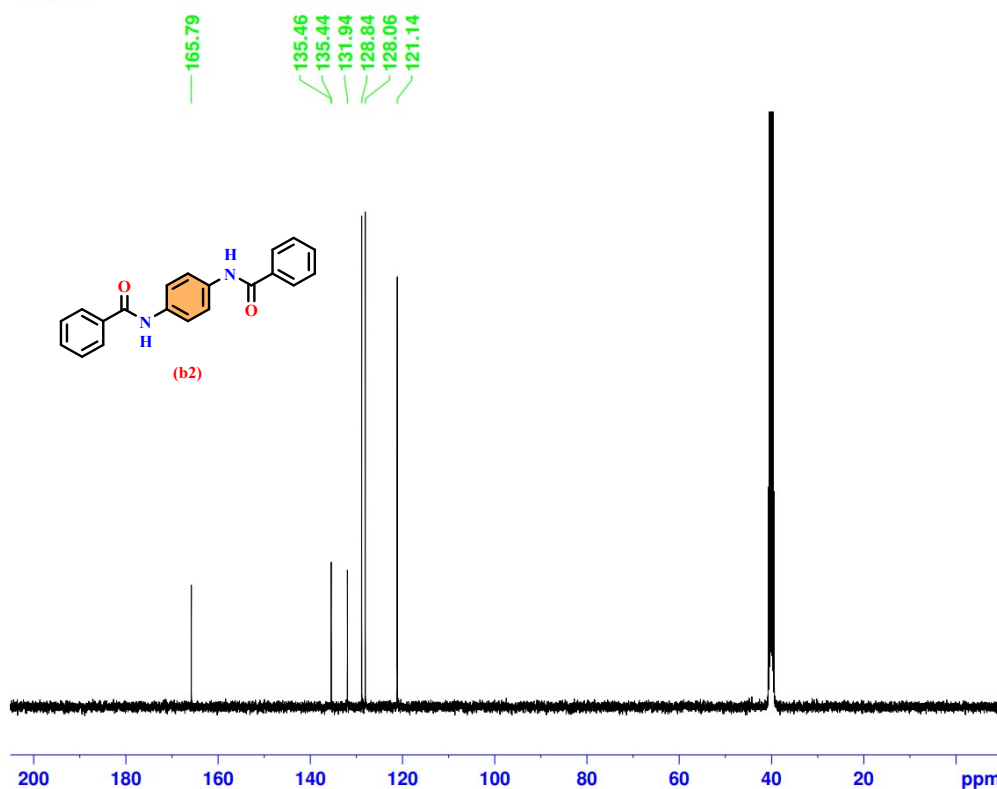


Fig S22. ¹³C NMR spectrum of *N,N'*-(1,4-phenylene)dibenzamide (b2)

bz-02-(23is-01541) 5698 (29.500)

, 14-Dec-2023 + 03:56:44

Scan EI+
3.82e8

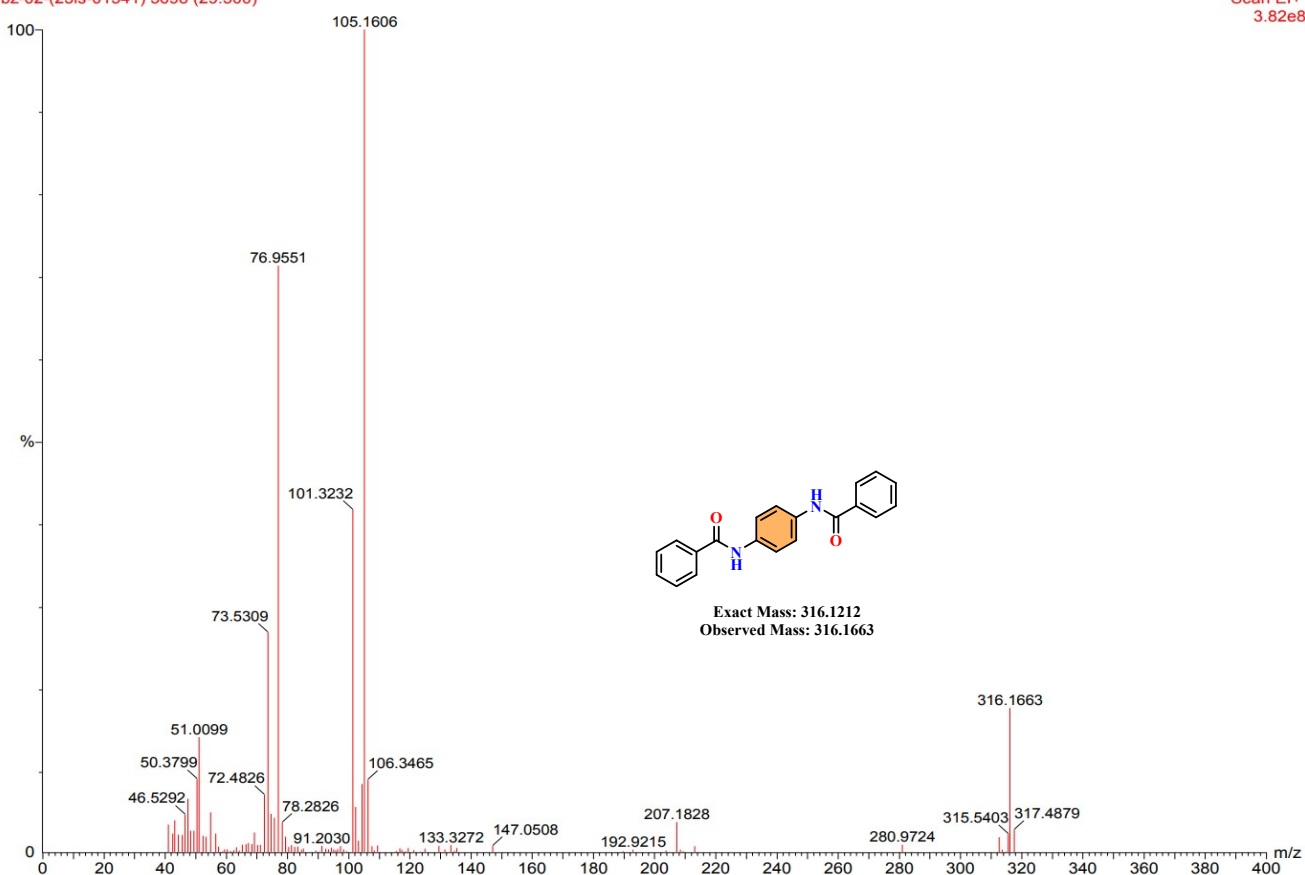


Fig S23. GC-Mass spectrum (m/z) of *N,N'*-(1,4-phenylene)dibenzamide (b2)

Signature SIF VIT VELLORE
Bz-03-Br



Current Data Parameters
NAME Dr.AKT020424
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240402
Time 23.00 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 306.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580299 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

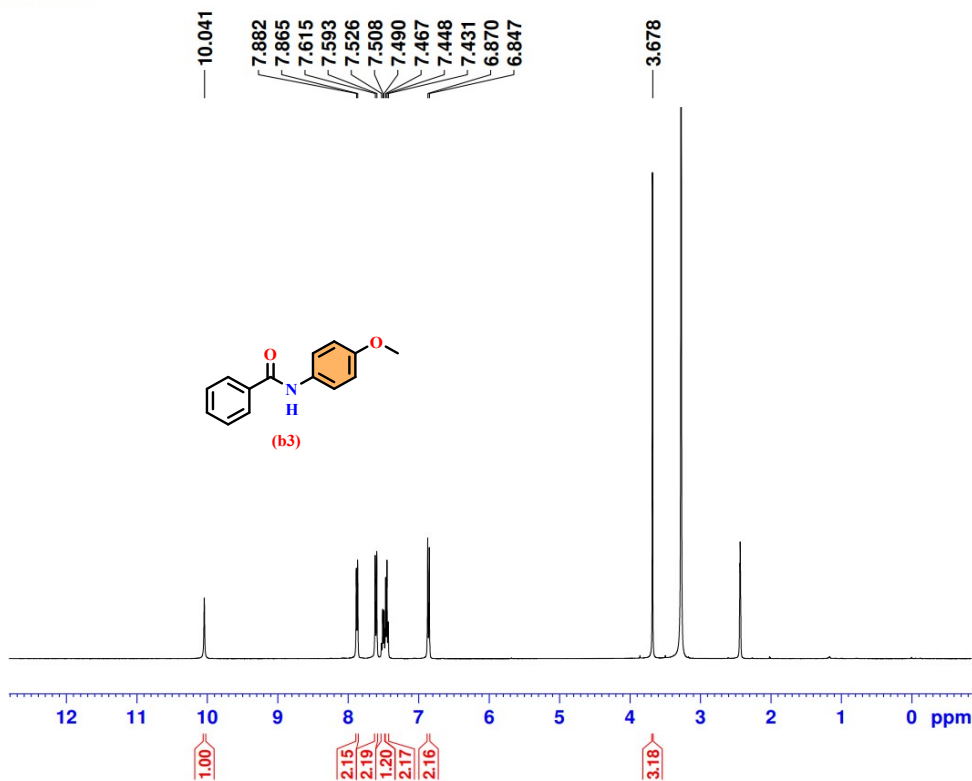


Fig S24. ¹H NMR spectrum of *N*-(4-methoxyphenyl)benzamide (*b3j*)

Signature SIF VIT VELLORE
BZ-03-Br



Current Data Parameters
NAME Dr.AKT020424
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240402
Time 23.30 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 307.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

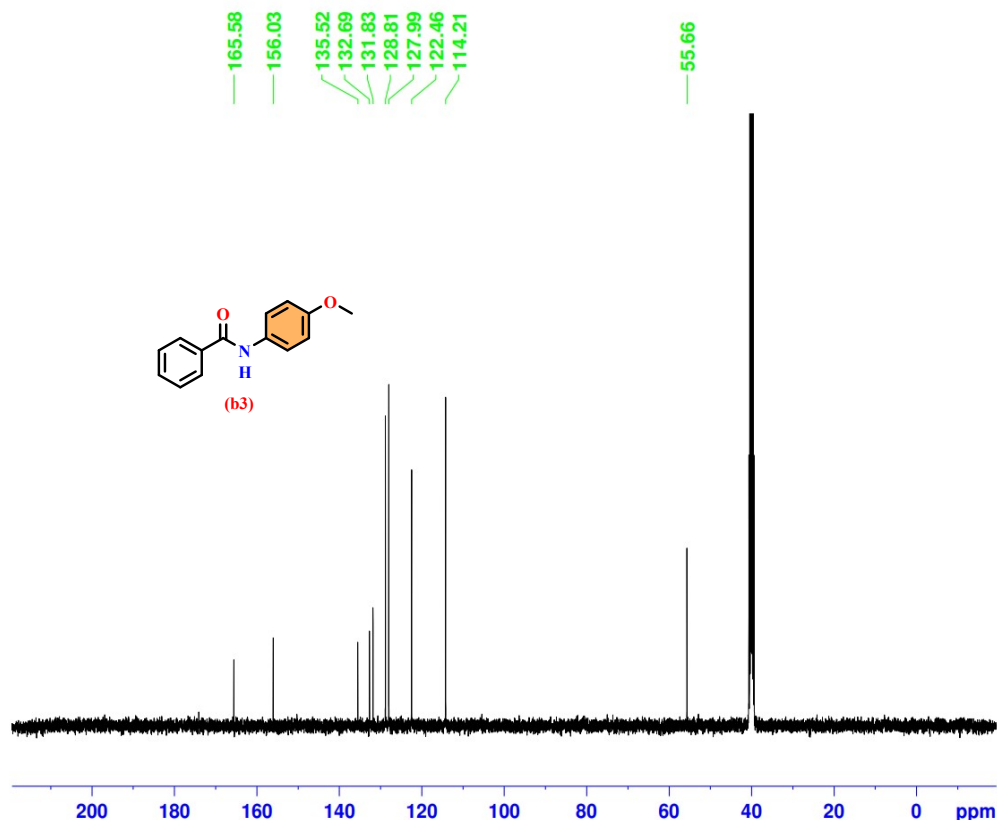
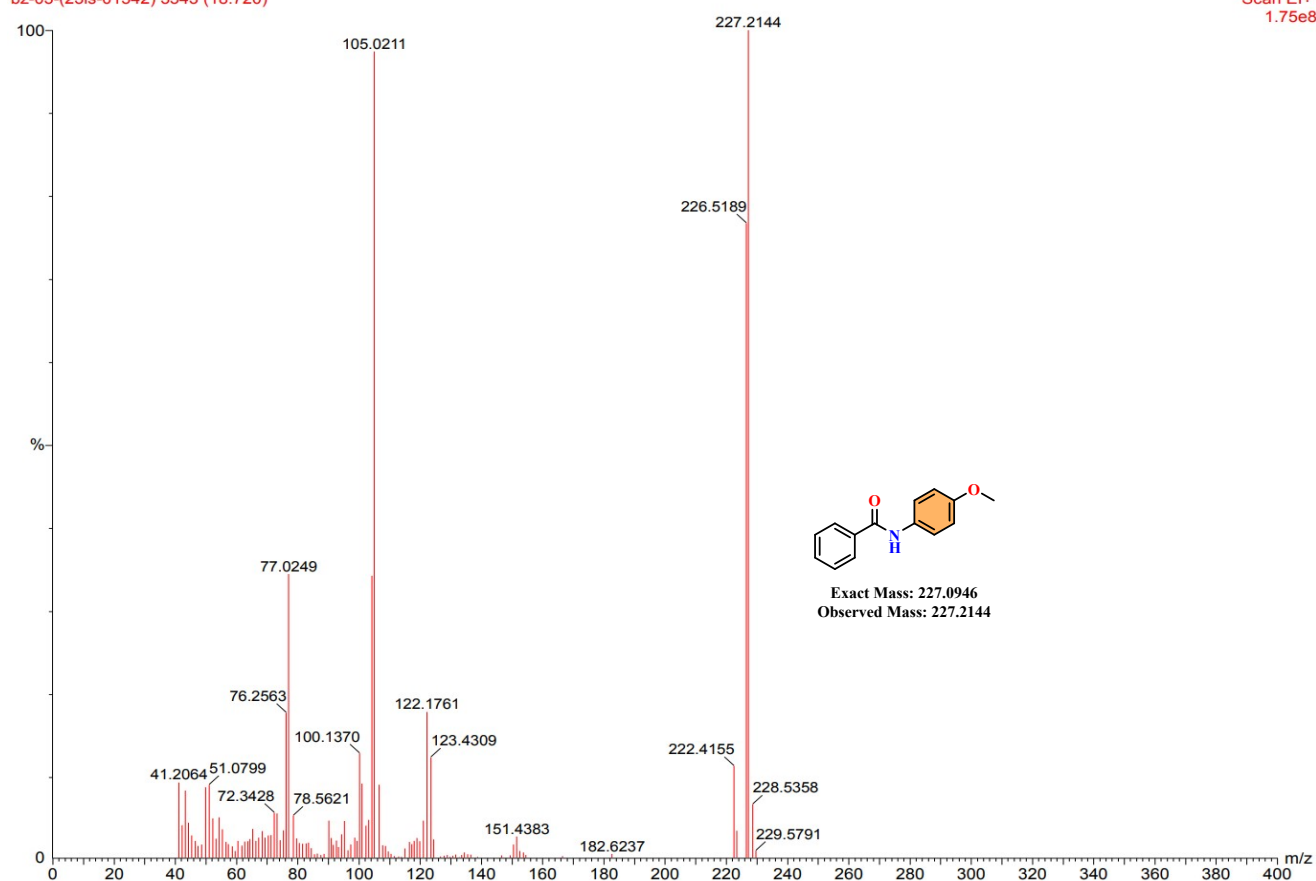


Fig S25. ¹³C NMR spectrum of *N*-(4-methoxyphenyl)benzamide (*b3j*)

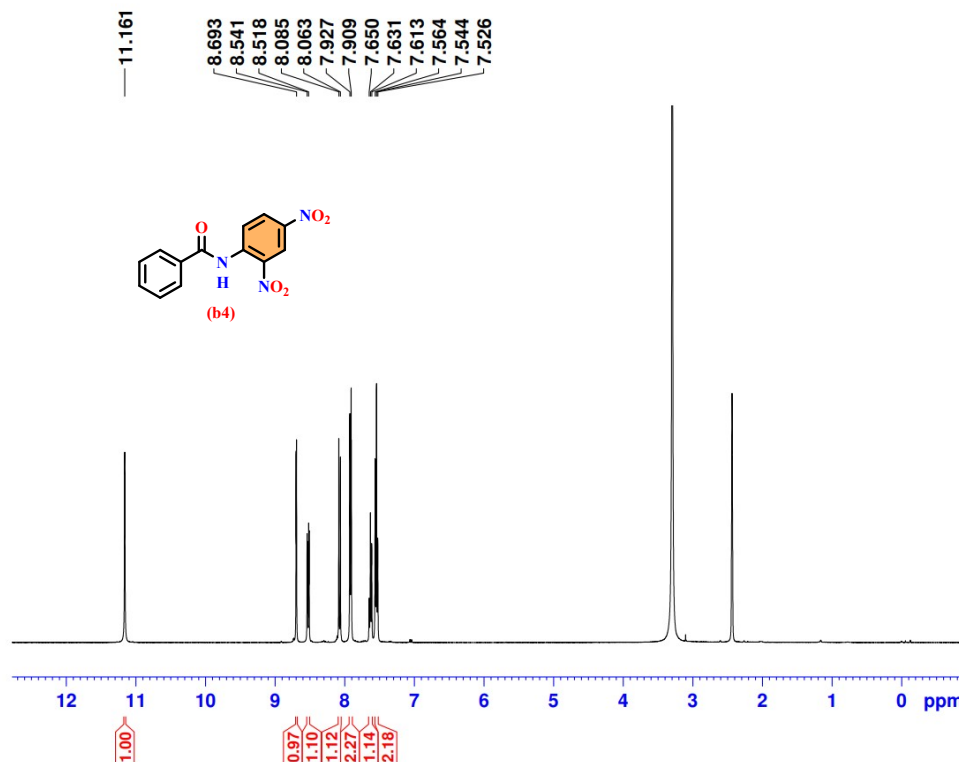
Fig S26. GC-Mass spectrum (m/z) of *N*-(4-methoxyphenyl)benzamide (*b3j*)Signature SIF VIT VELLORE
Bz-04-BrCurrent Data Parameters
NAME Dr.PDK160424
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters

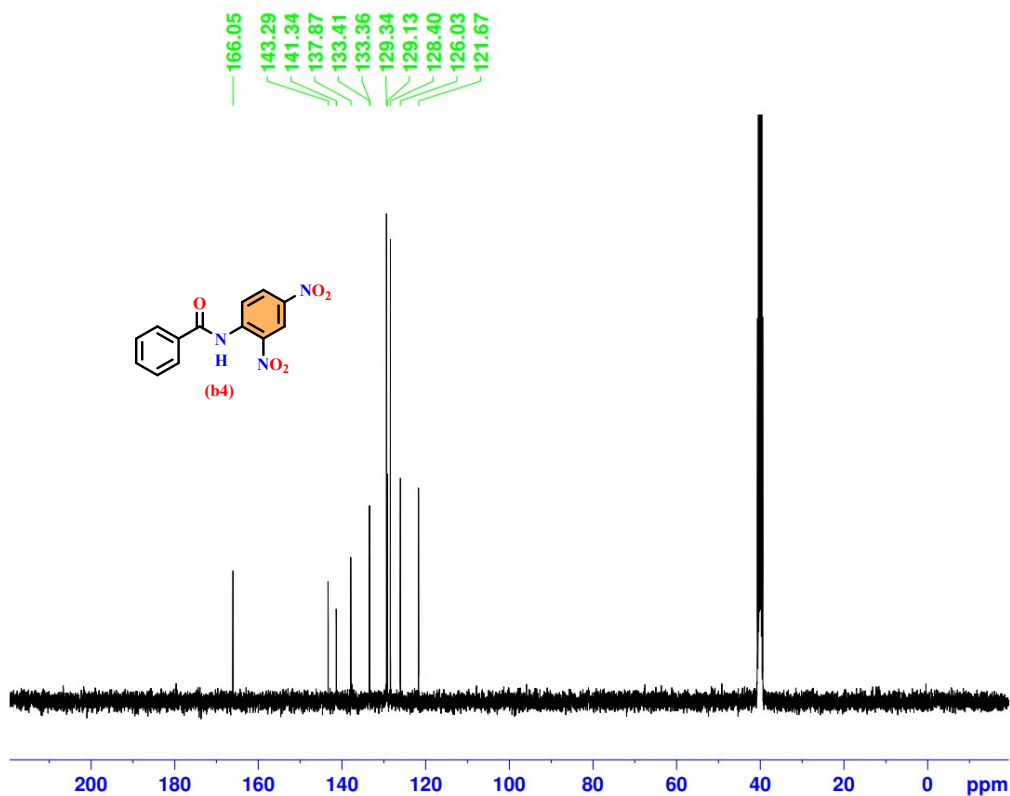
Date_ 20240416
Time 20.04 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 304.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters

SI 65536
SF 400.2580287 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S27. ¹H NMR spectrum of *N*-(2,4-dinitrophenyl)benzamide (*b4j*)

Signature SIF VIT VELLORE
BZ-04-Br



Current Data Parameters
NAME Dr.PDK100424
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240411
Time 9.05 h
INSTRUM spect
PROBHD Z108618_0505 (zpgp30)
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 310.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

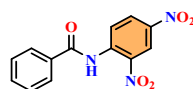
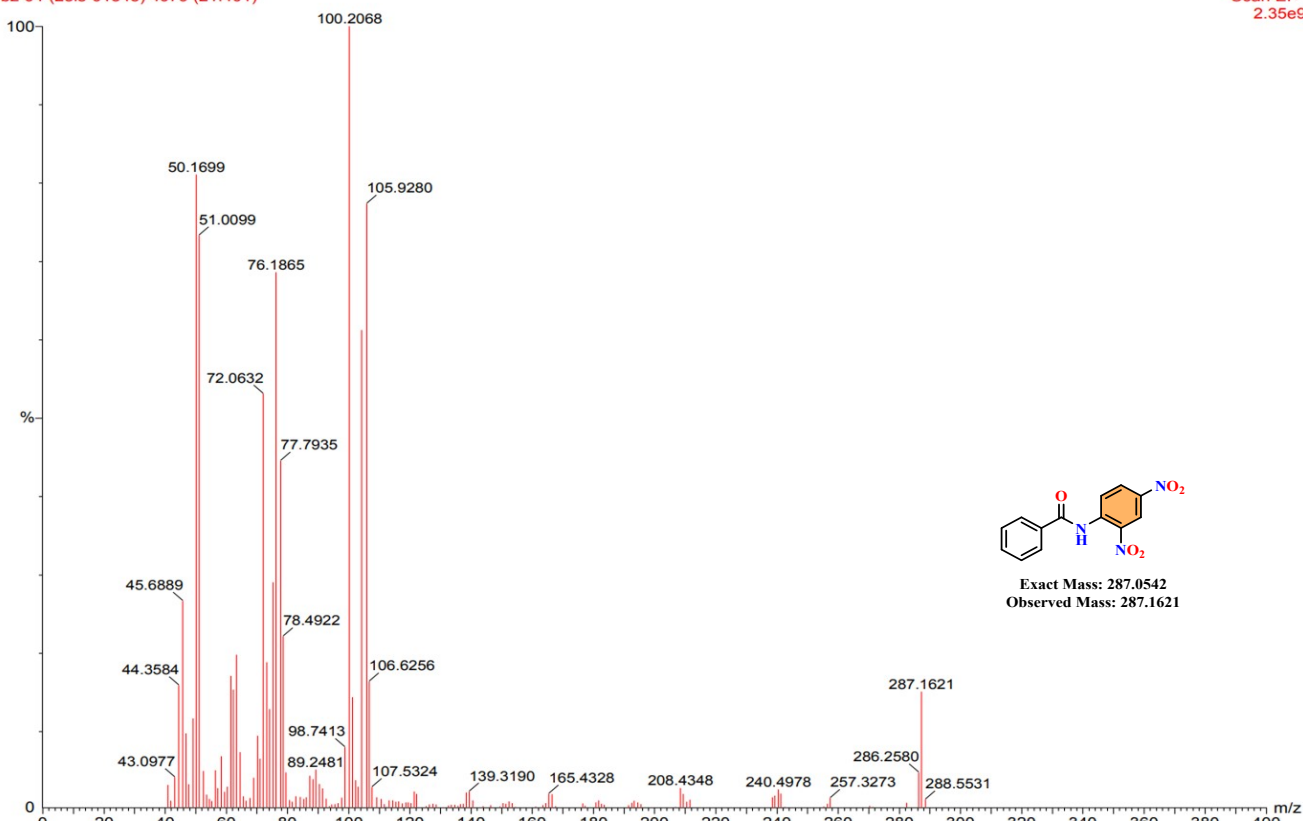
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S28. ¹³C NMR spectrum of *N*-(2,4-dinitrophenyl)benzamide (b4j)

bz-04-(23is-01543) 4079 (21.401)

, 14-Dec-2023 + 05:09:04

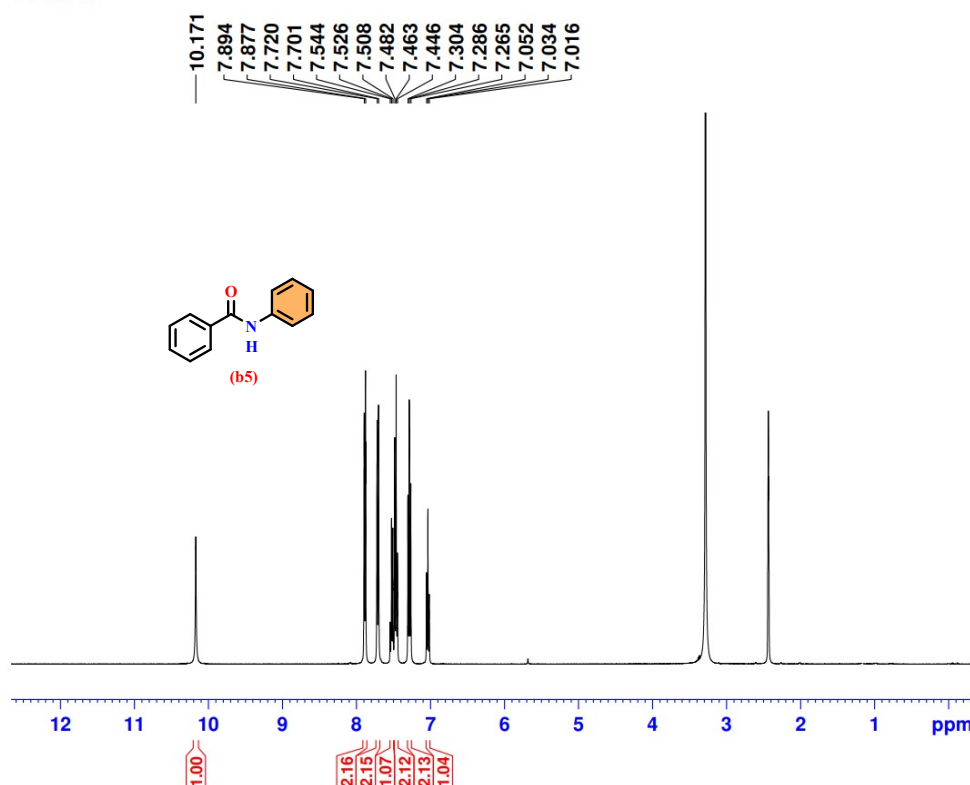
Scan EI+
2.35e9



Exact Mass: 287.0542
Observed Mass: 287.1621

Fig S29. GC-Mass spectrum (m/z) of *N*-(2,4-dinitrophenyl)benzamide (b4j)

Signature SIF VIT VELLORE
BZ-05-Br



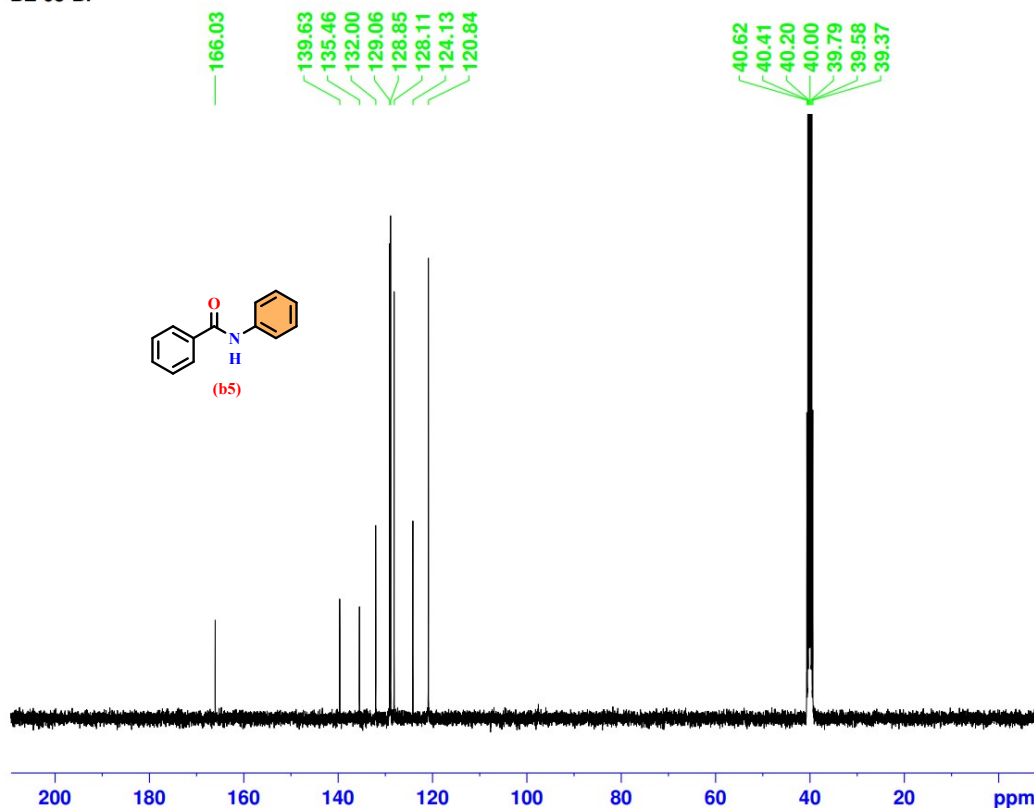
Current Data Parameters
NAME Dr.PDK060424
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240406
Time 10.20 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 304.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580299 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S30. ¹H NMR spectrum of *N*-phenylbenzamide (b5j)

Signature SIF VIT VELLORE
BZ-05-Br



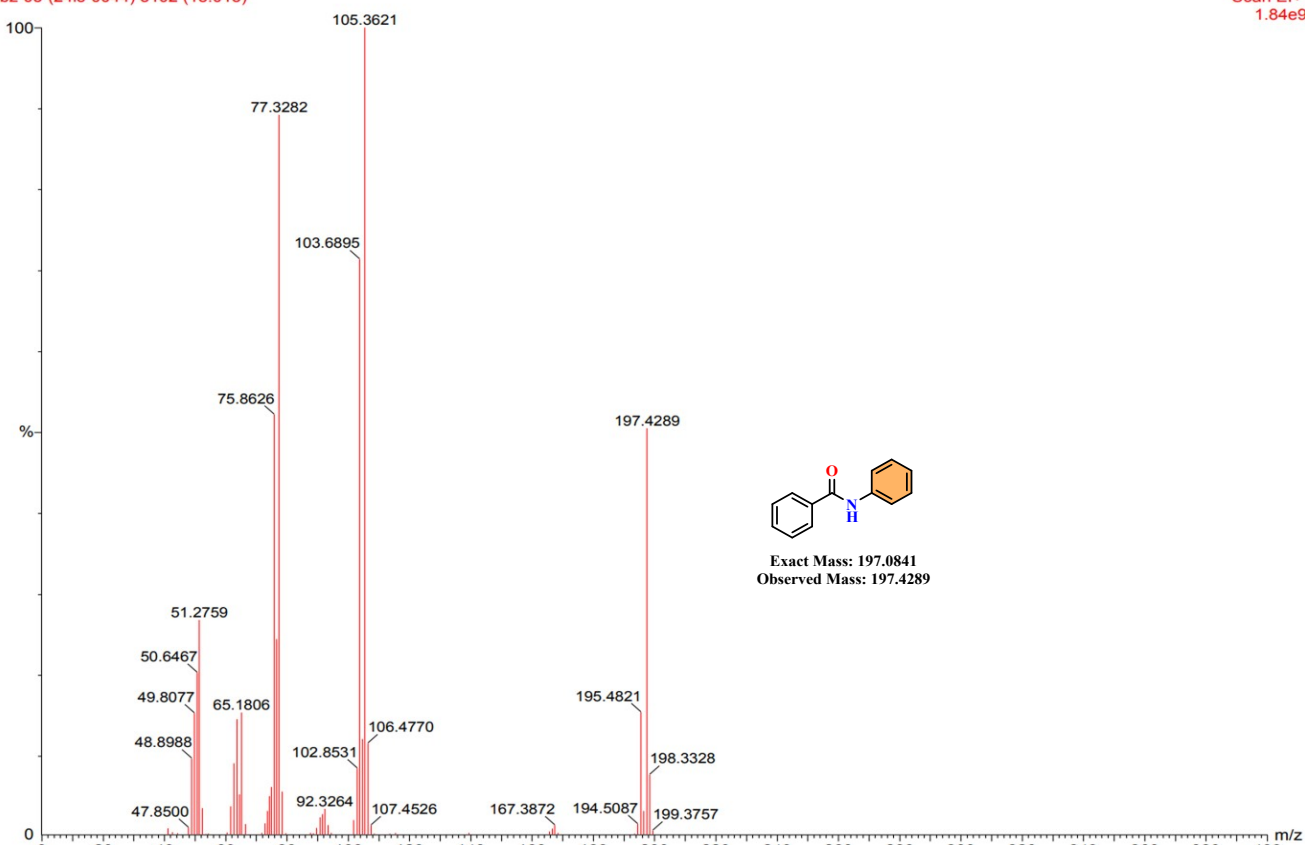
Current Data Parameters
NAME Dr.AKT030424
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240404
Time 6.04 h
INSTRUM spect
PROBHD Z108618_0505 (Zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S31. ¹³C NMR spectrum of *N*-phenylbenzamide (b5j)

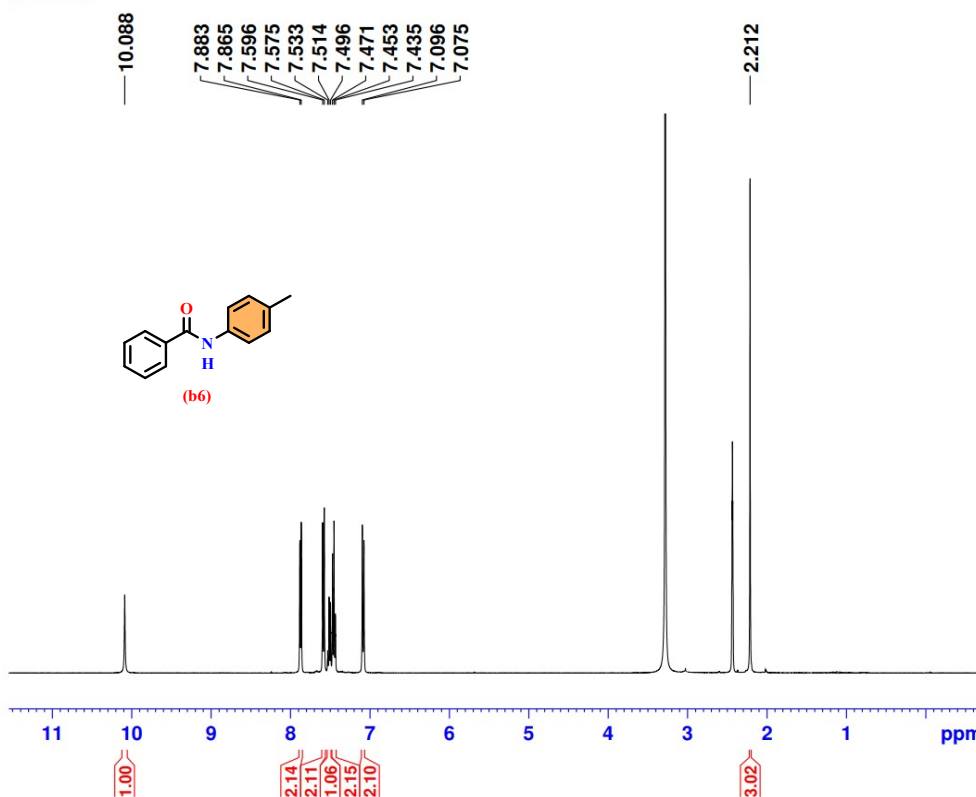
bz-05-(24is-0044) 3102 (18.015)

Fig S32. GC-Mass spectrum (m/z) of *N*-phenylbenzamide (*b5*)Signature SIF VIT VELLORE
BZ-06-Br

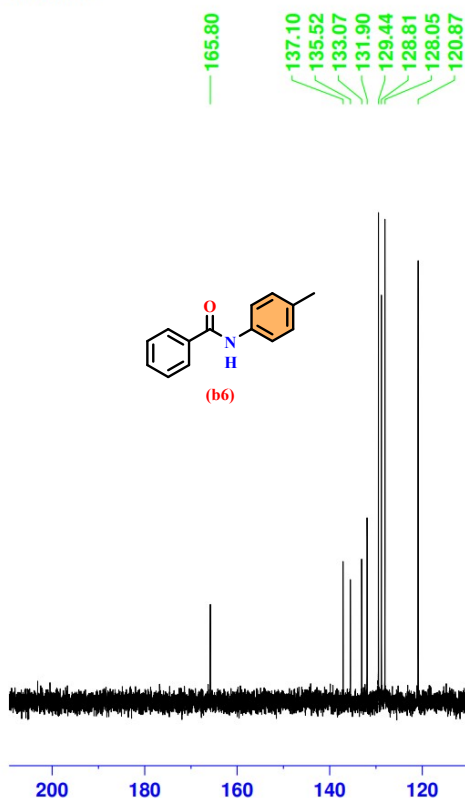
Current Data Parameters
NAME Dr.PDK060424
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240406
Time 10.25 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 304.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580295 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S33. ¹H NMR spectrum of *N*-(*p*-tolyl)benzamide (*b6*)

Signature SIF VIT VELLORE
BZ-06-Br



Current Data Parameters
NAME Dr.CM030424
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date 20240404
Time 7.12 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 307.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S34. ^{13}C NMR spectrum of *N*-(*p*-tolyl)benzamide (b6j)

bz-06-(24is-0045) 3176 (18.385)

, 07-Mar-2024 + 21:16:12

Scan EI+
9.49e8

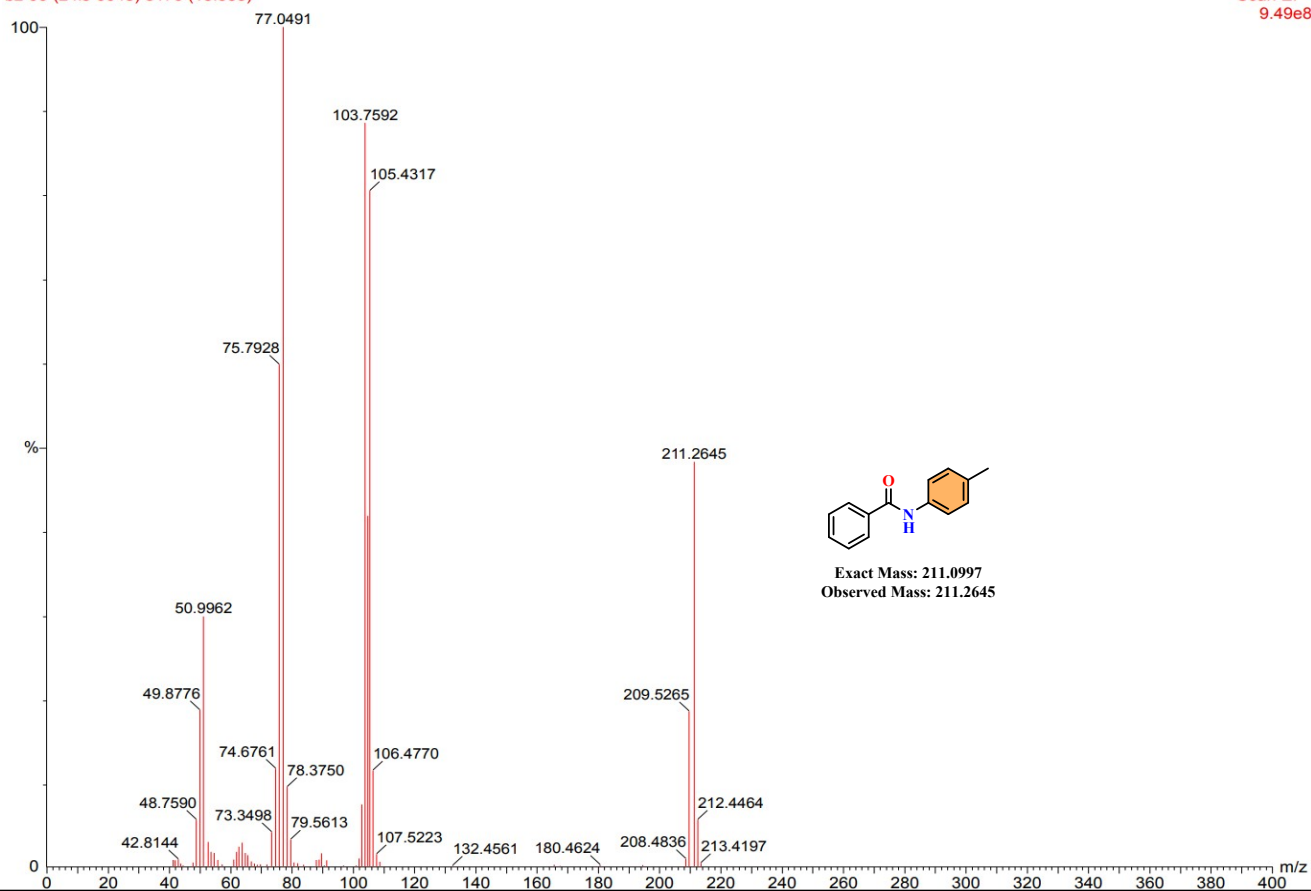
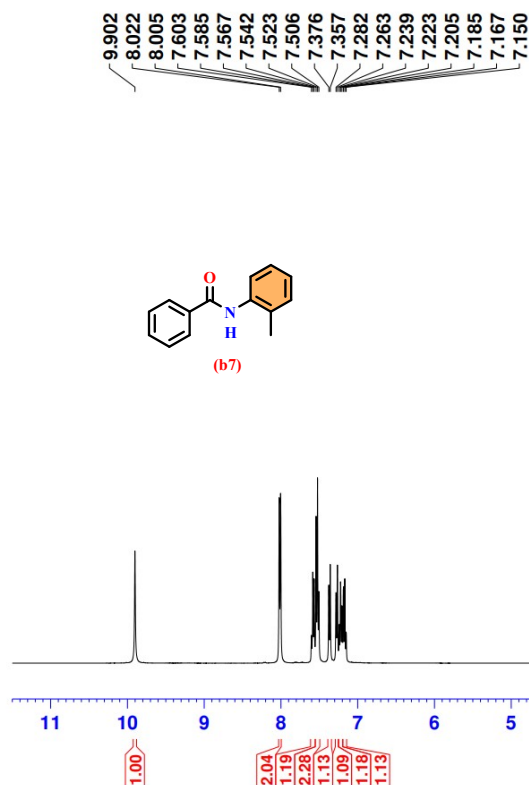


Fig S35. GC-Mass spectrum (m/z) of *N*-(*p*-tolyl)benzamide (b6j)

Signature SIF VIT VELLORE
Bz-07-Br



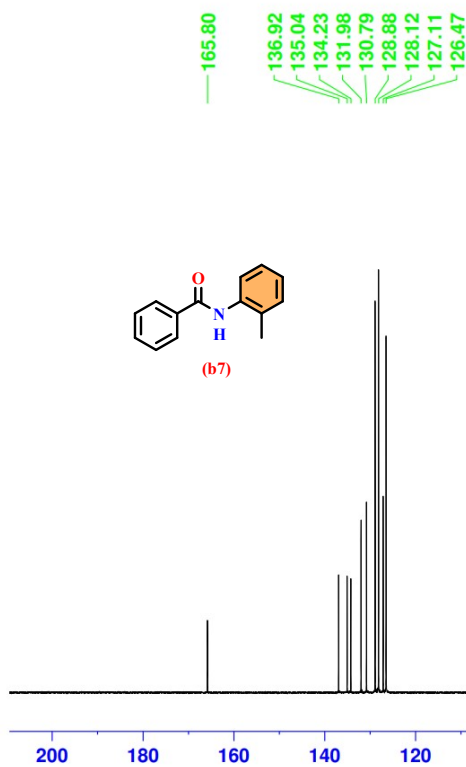
Current Data Parameters
NAME Dr.PDK020424
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240402
Time 21.12 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 304.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S36. ¹H NMR spectrum of *N*-(*o*-tolyl)benzamide (b7)

Signature SIF VIT VELLORE
Bz-07-Br

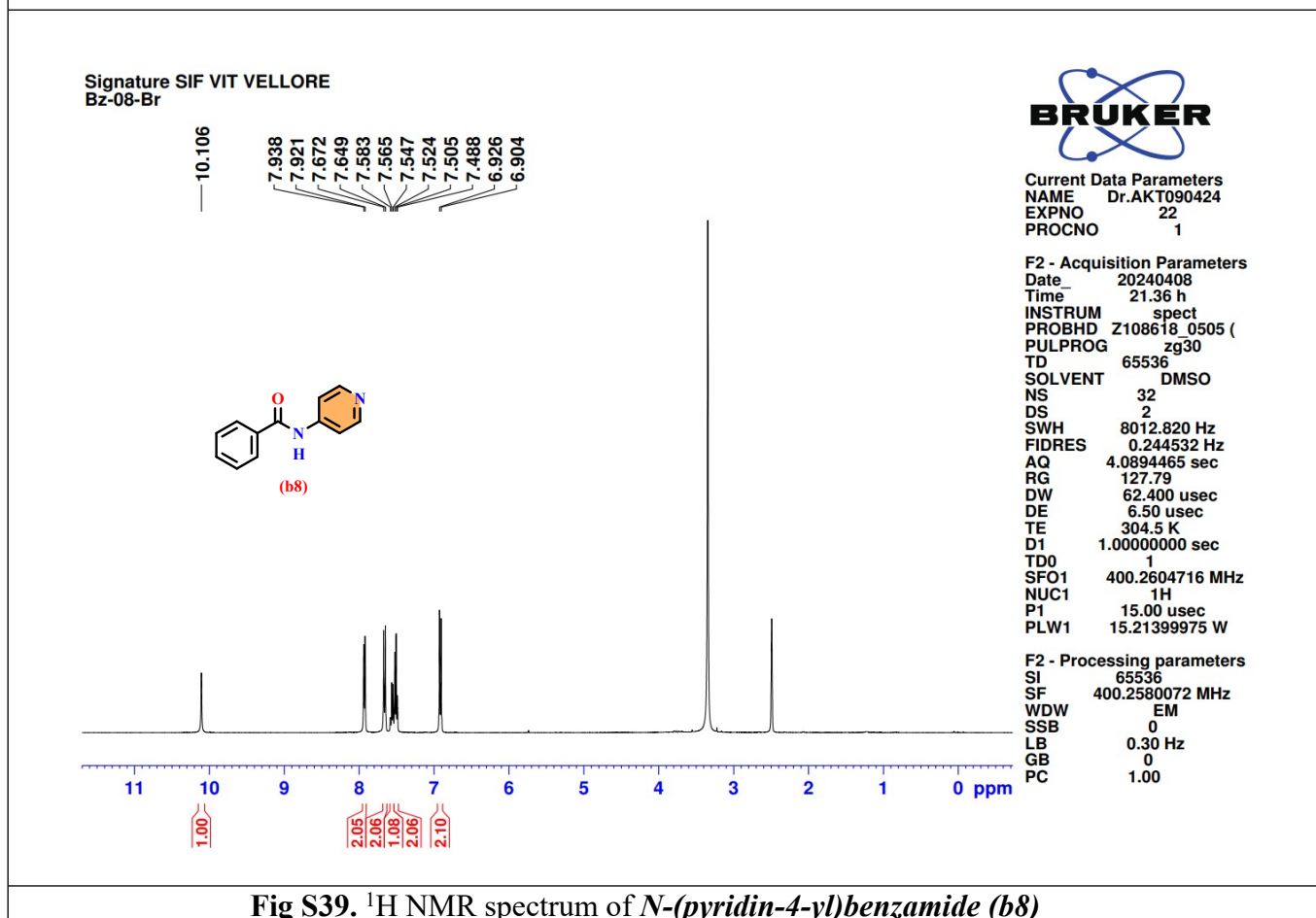
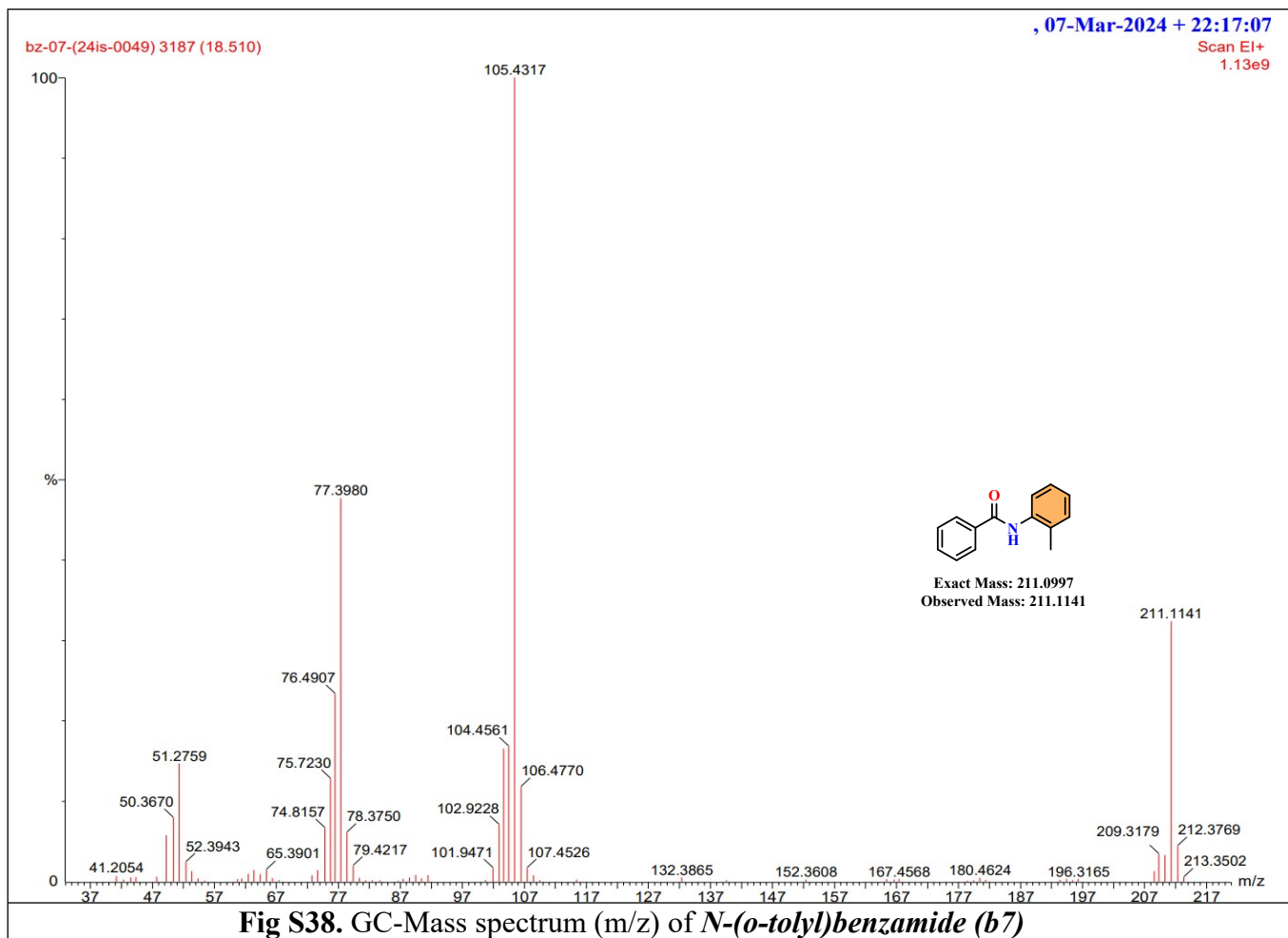


Current Data Parameters
NAME Dr.CM300324
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240330
Time 21.04 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW13 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S37. ¹³C NMR spectrum of *N*-(*o*-tolyl)benzamide (b7)



Signature SIF VIT VELLORE
Bz-08-Br



Current Data Parameters
NAME Dr.AKT090424
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240408
Time 22.07 h
INSTRUM spect
PROBHD Z108618_0505 (Z108618_0505)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

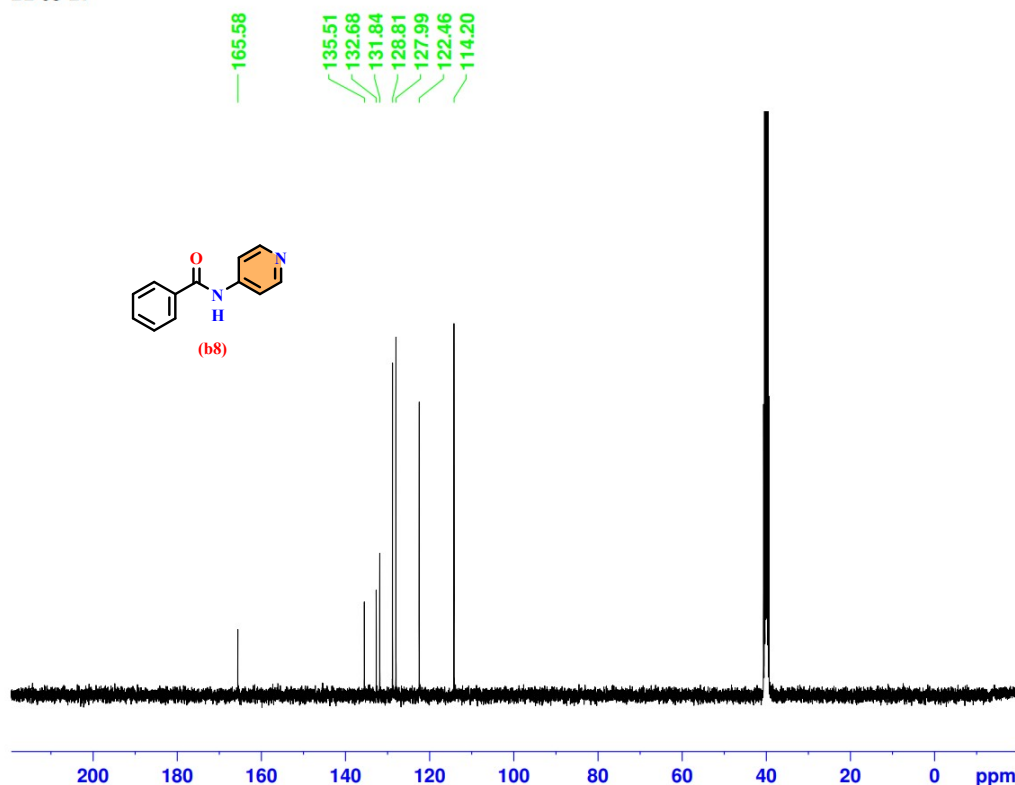


Fig S40. ^{13}C NMR spectrum of *N*-(pyridin-4-yl)benzamide (b8)

bz-08-(24is-0046) 3397 (19.490)

, 07-Mar-2024 + 21:53:41

Scan EI+
2.83e9

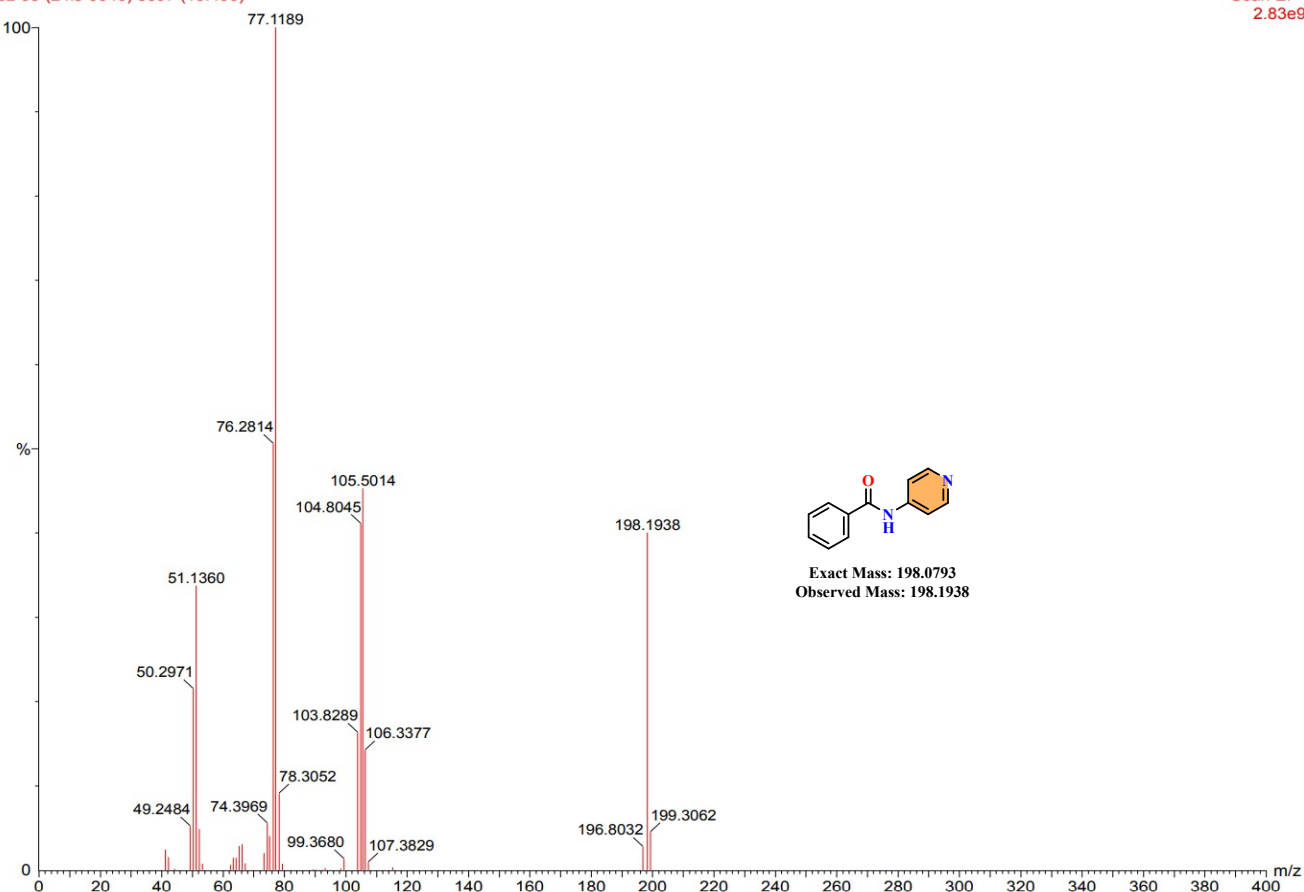
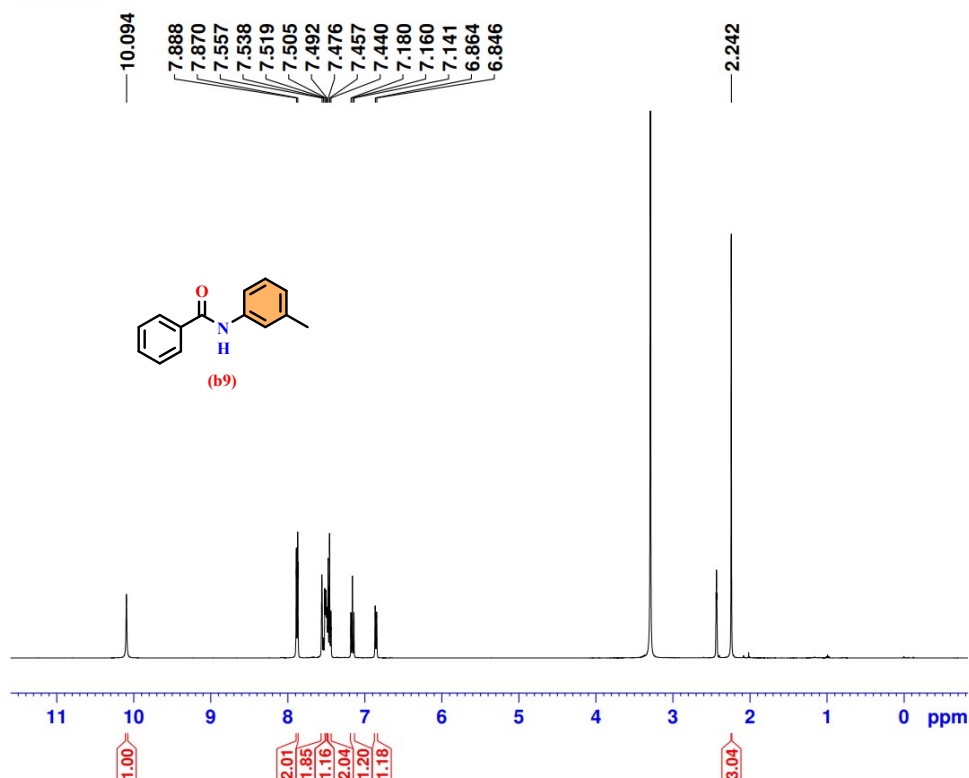


Fig S41. GC-Mass spectrum (m/z) of *N*-(pyridin-4-yl)benzamide (b8)

Signature SIF VIT VELLORE
BZ-09-Br



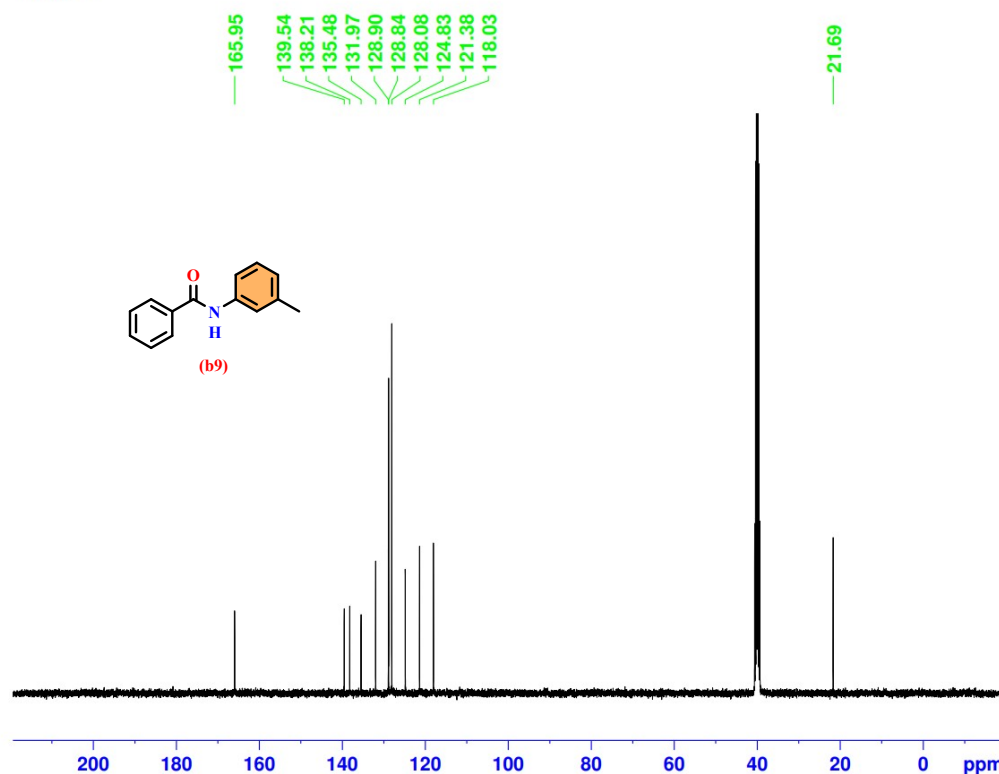
Current Data Parameters
NAME Dr.PDK090424
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240409
Time 20.10 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 303.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580299 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S42. ¹H NMR spectrum of *N*-(*m*-tolyl)benzamide (b9)

Signature SIF VIT VELLORE
Bz-09-Br



Current Data Parameters
NAME Dr.CM130424
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240414
Time 2.33 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 304.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S43. ¹³C NMR spectrum of *N*-(*m*-tolyl)benzamide (b9)

bz-09-(24is-0288) 3368 (18.845)

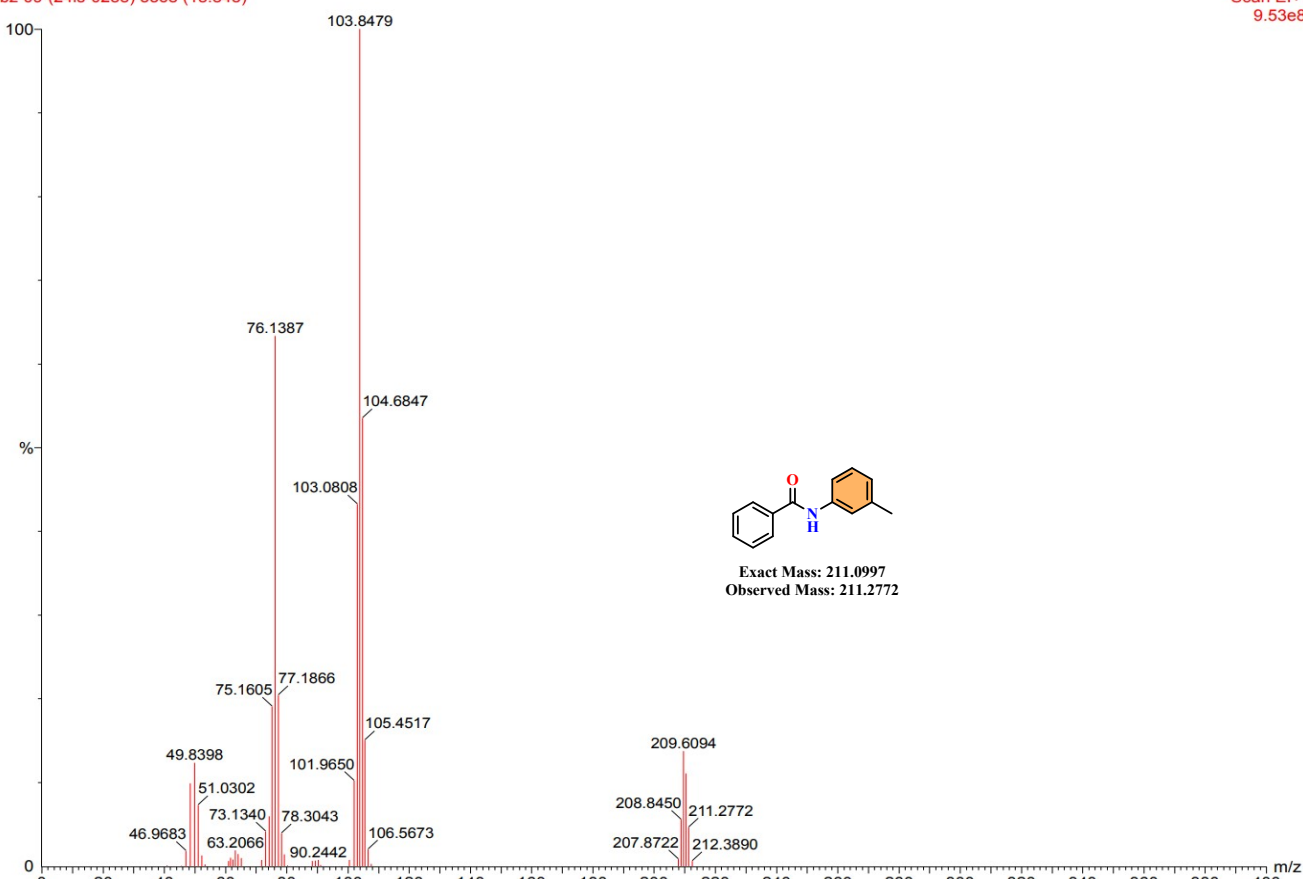
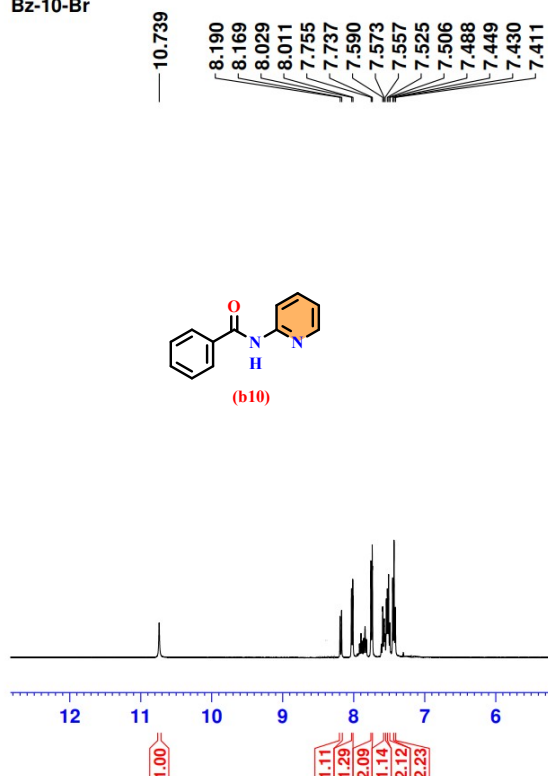


Fig S44. GC-Mass spectrum (m/z) of *N*-(*m*-tolyl)benzamide (b9)

Signature SIF VIT VELLORE
Bz-10-Br



Current Data Parameters
NAME Dr.PDK200424
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240421
Time 7.31 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S45. ¹H NMR spectrum of *N*-(pyridin-2-yl)benzamide (b10)

Signature SIF VIT VELLORE
BZ-10-Br



Current Data Parameters
NAME Dr.PDK200424
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240421
Time 8.03 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

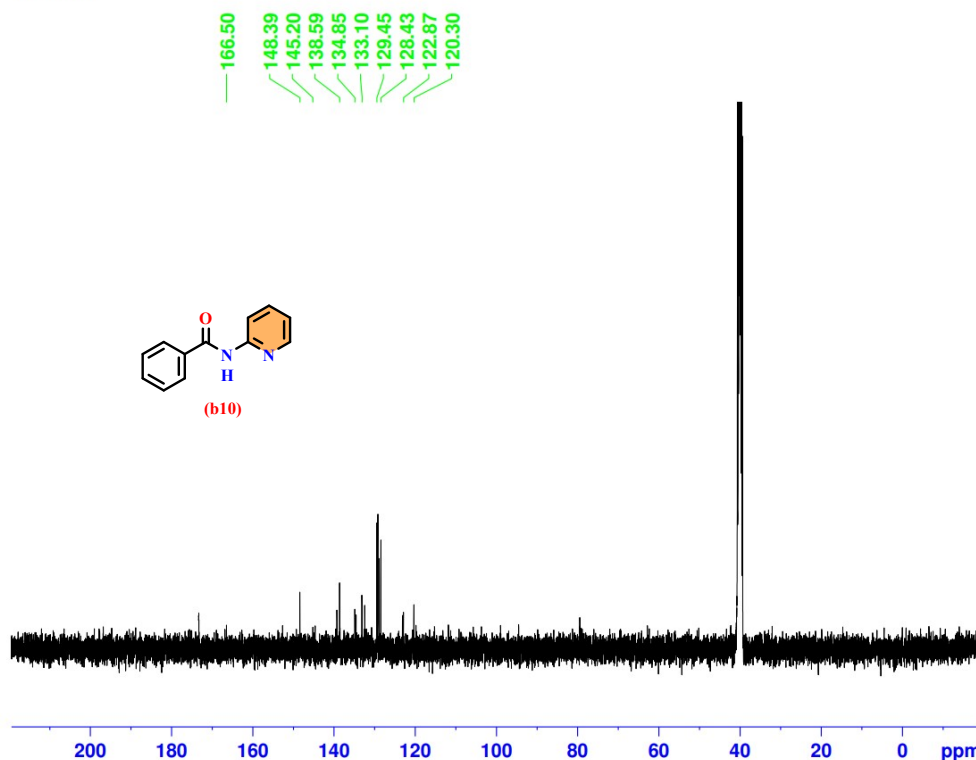


Fig S46. ^{13}C NMR spectrum of *N*-(pyridin-2-yl)benzamide (b10)

bz-10-(24is-0246) 3387 (19.440)

, 18-Apr-2024 + 02:21:32

Scan EI+
7.02e9

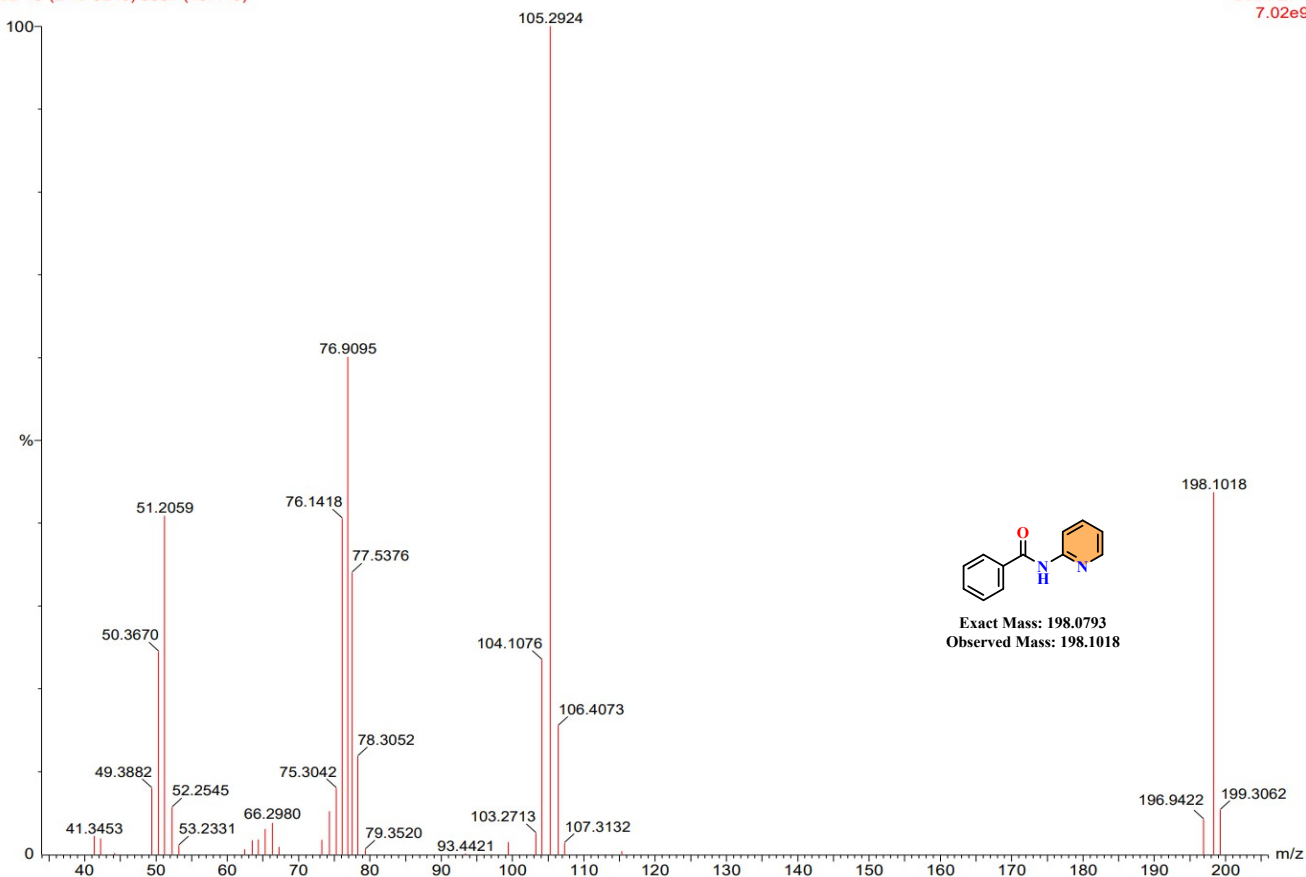
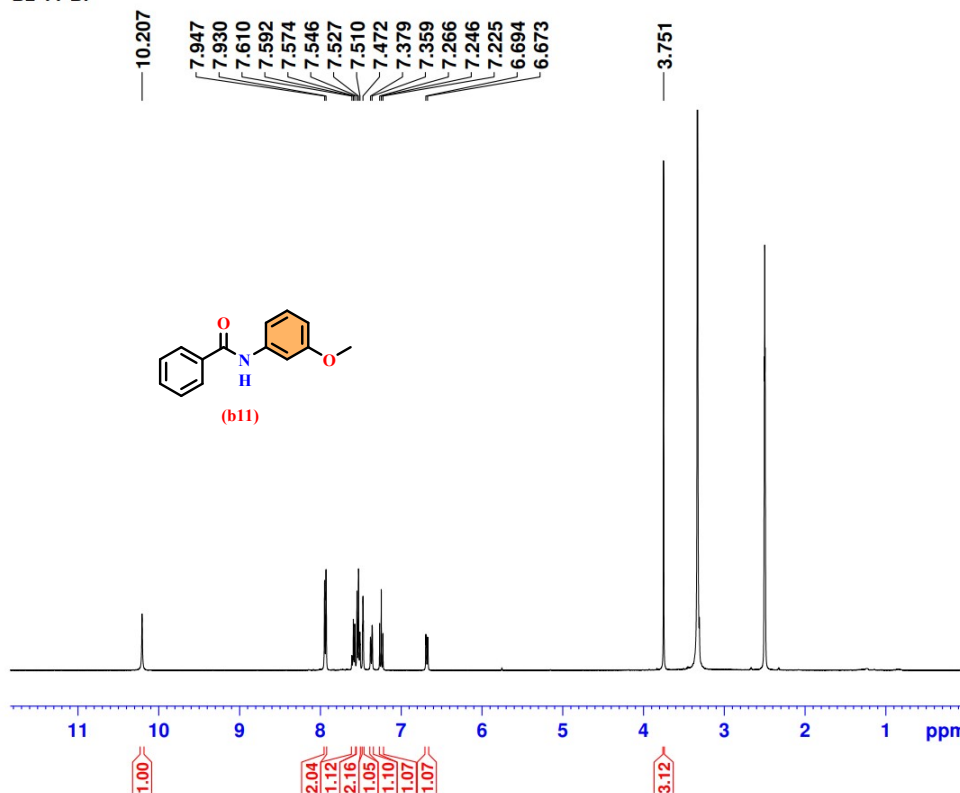


Fig S47. GC-Mass spectrum (m/z) of *N*-(pyridin-2-yl)benzamide (b10)

Signature SIF VIT VELLORE
Bz-11-Br



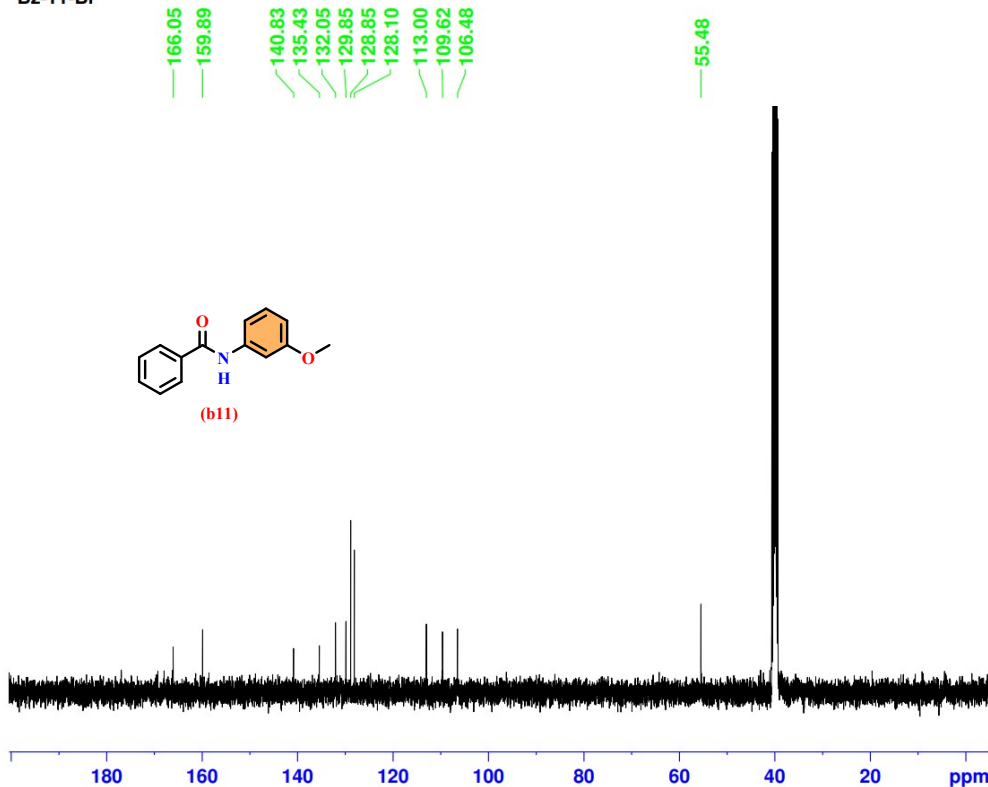
Current Data Parameters
NAME Dr.PDK180524
EXPNO 56
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240518
Time 17.45 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 303.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S48. ¹H NMR spectrum of *N*-(3-methoxyphenyl)benzamide (b11)

Signature SIF VIT VELLORE
Bz-11-Br

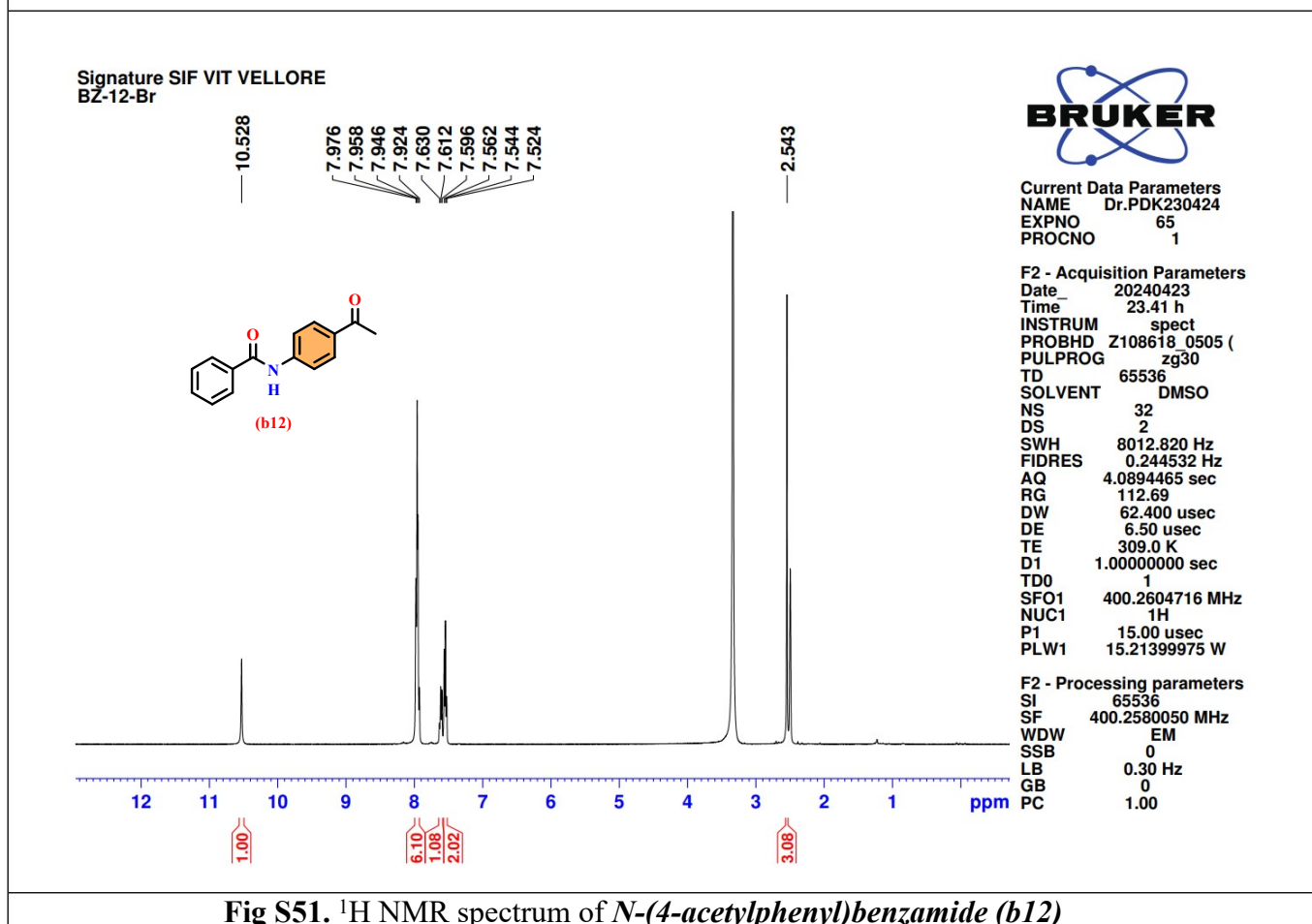
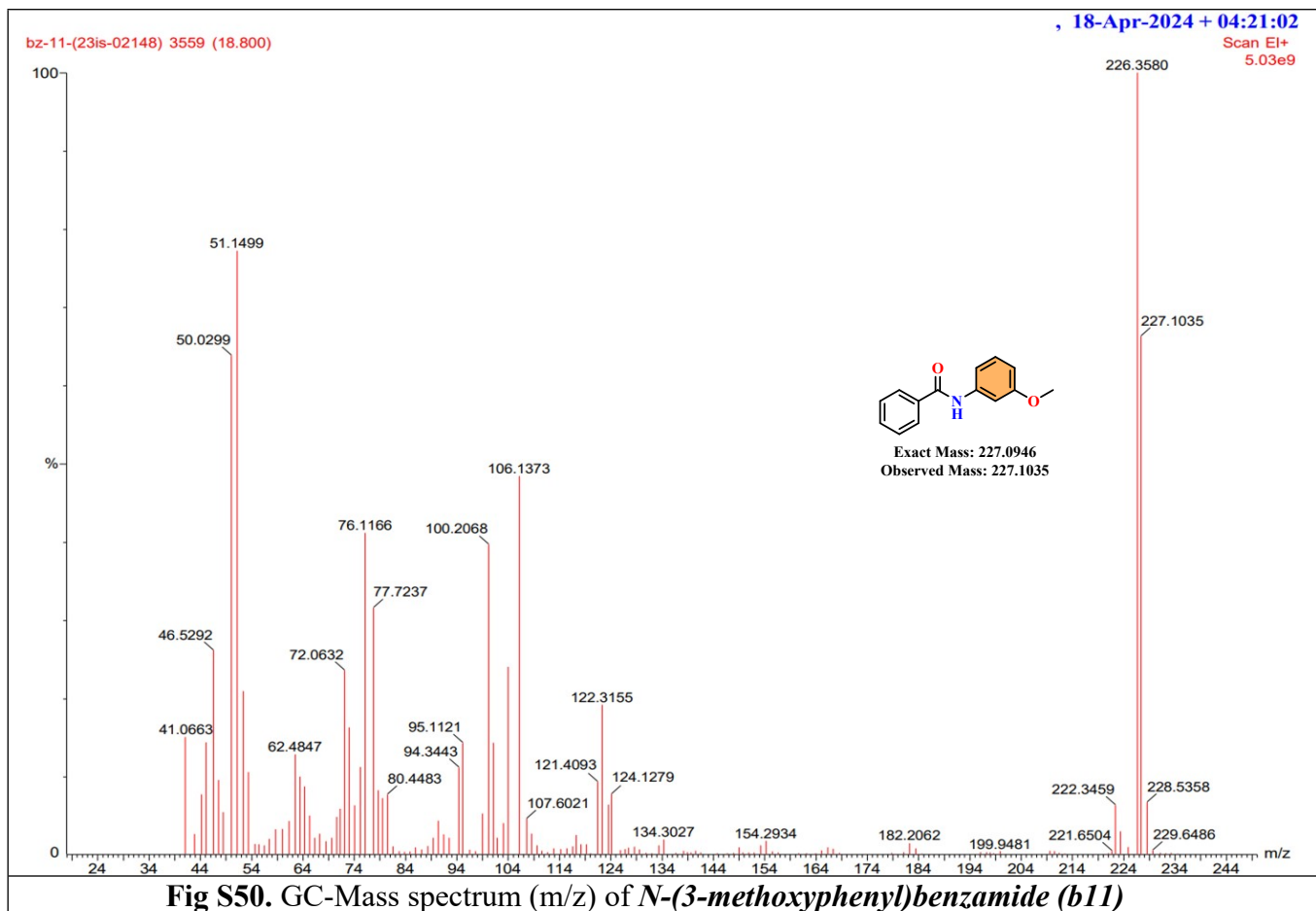


Current Data Parameters
NAME Dr.PDK180524
EXPNO 57
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240518
Time 18.15 h
INSTRUM spect
PROBHD Z108618_0505 (Zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S49. ¹³C NMR spectrum of *N*-(3-methoxyphenyl)benzamide (b11)



Signature SIF VIT VELLORE
BZ-12-Br

197.09
166.48
144.06
135.05
132.54
132.36
129.74
128.92
128.26
119.95



Current Data Parameters
NAME Dr.PDK230424
EXPNO 66
PROCNO 1

F2 - Acquisition Parameters
Date 20240424
Time 0.12 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

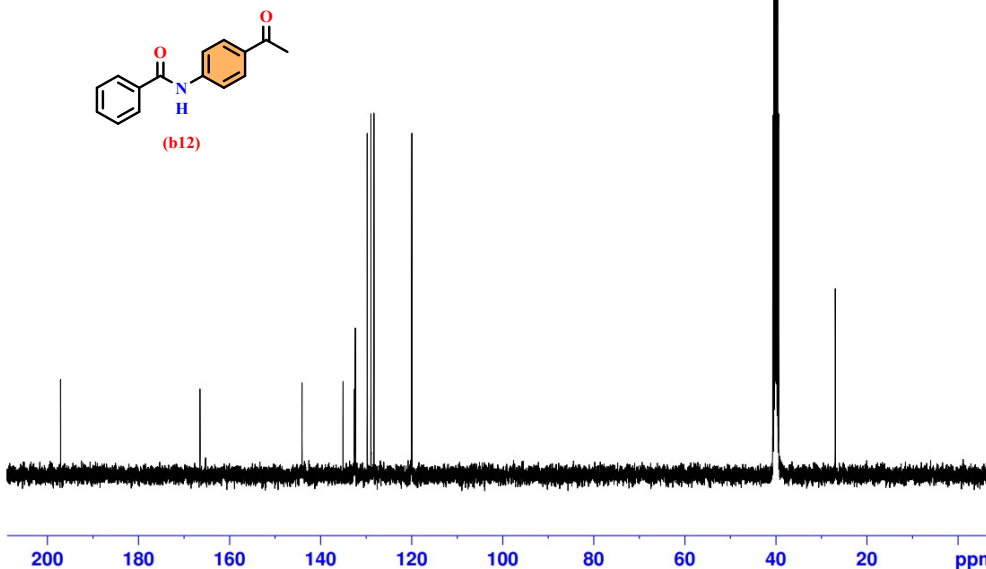


Fig S52. ^{13}C NMR spectrum of *N*-(4-acetylphenyl)benzamide (b12)

bz-12-(24is-0284) 4042 (22.217)

, 18-Apr-2024 + 01:13:17

Scan EI+
3.82e8

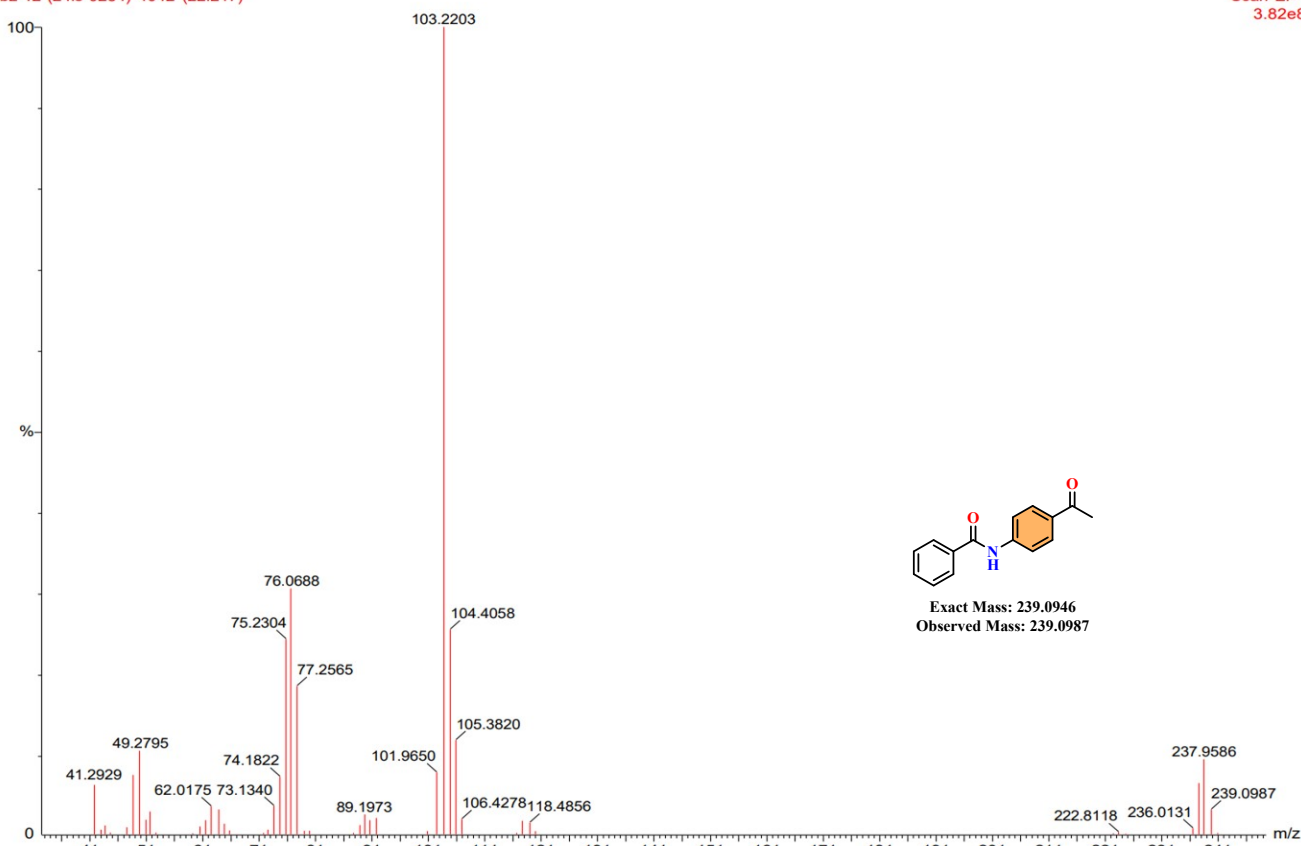
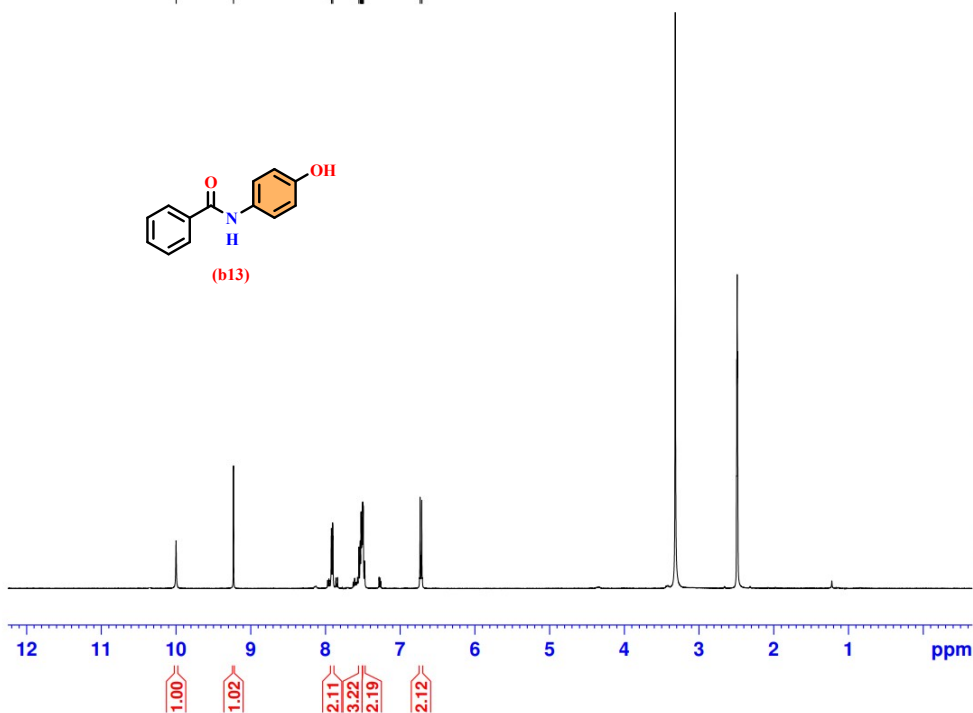
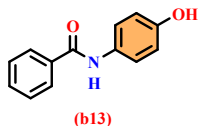


Fig S53. GC-Mass spectrum (m/z) of *N*-(4-acetylphenyl)benzamide (b12)

Signature SIF VIT VELLORE
Bz-13-Br

9.999
9.231
7.920
7.902
7.552
7.534
7.523
7.518
7.512
7.508
7.501
7.493
6.732
6.710



Current Data Parameters
NAME Dr.AKT090524
EXPNO 7
PROCNO 1

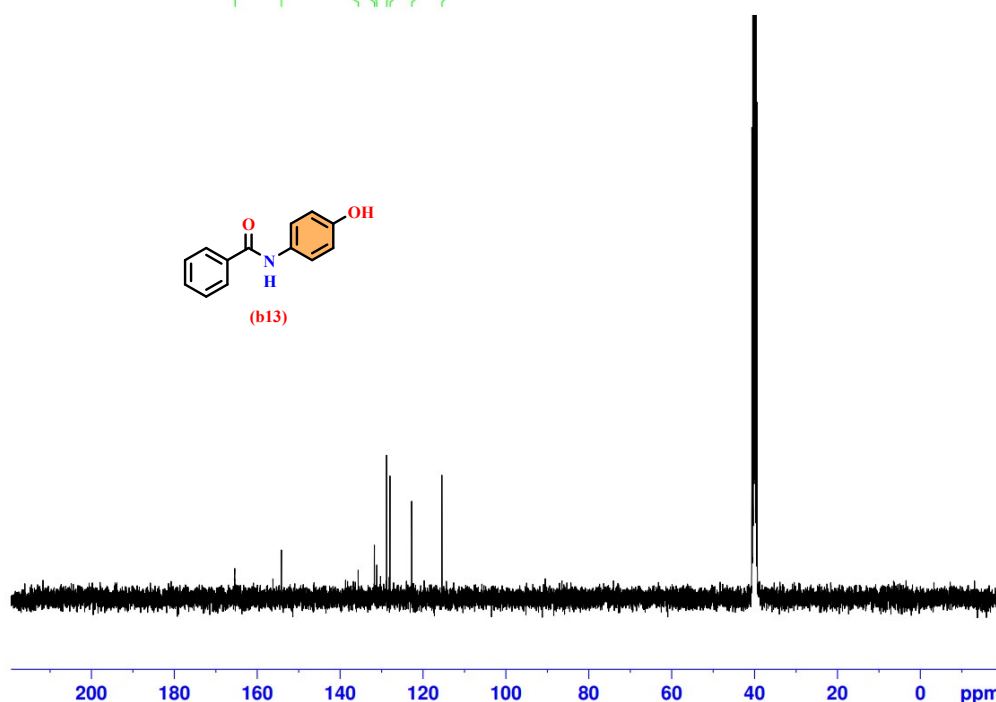
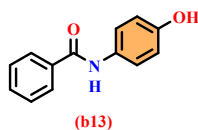
F2 - Acquisition Parameters
Date_ 20240509
Time 23.28 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 303.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S54. ¹H NMR spectrum of *N*-(4-hydroxyphenyl)benzamide (b13)

Signature SIF VIT VELLORE
Bz-13-Br

165.32
154.16
135.63
131.73
131.15
128.78
127.95
122.72
115.42



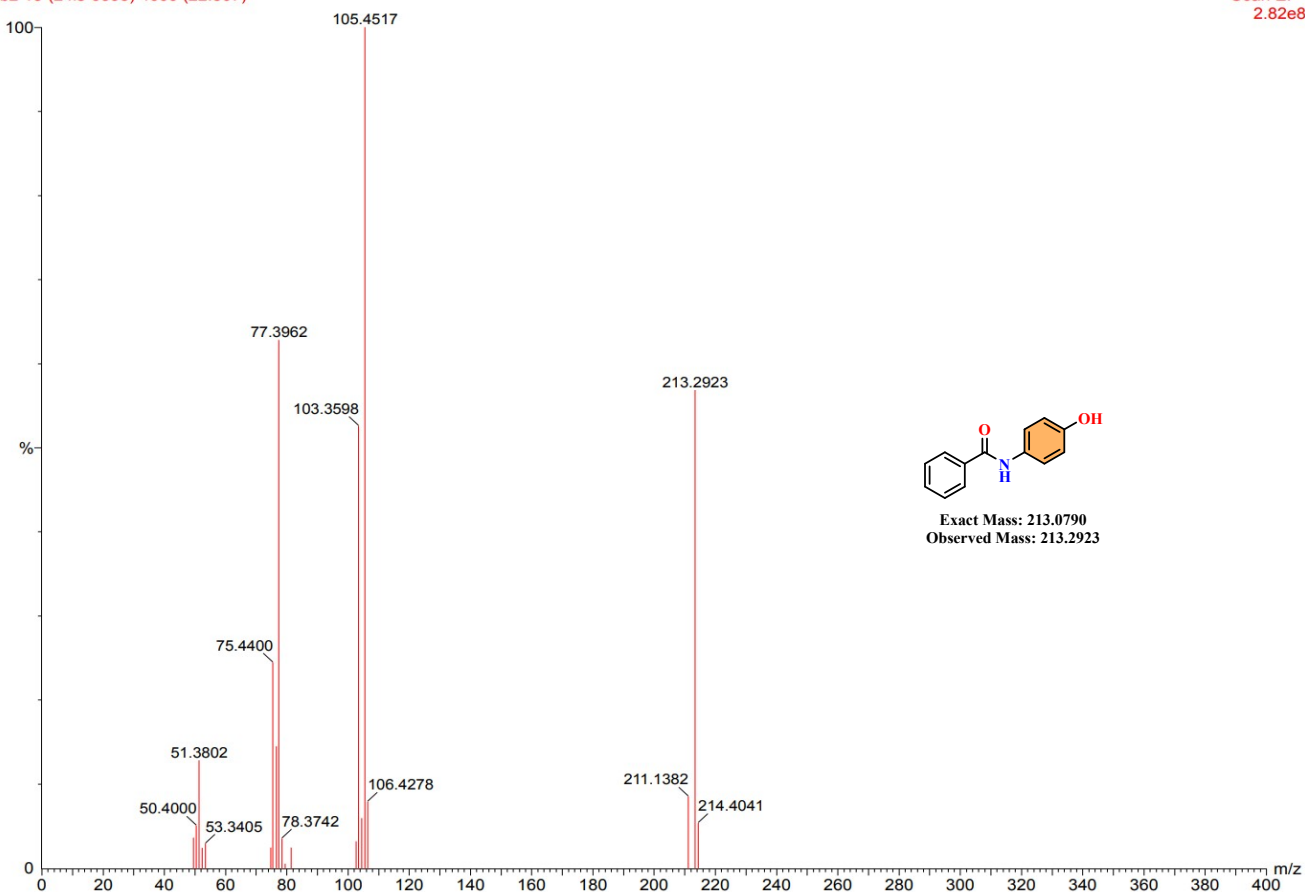
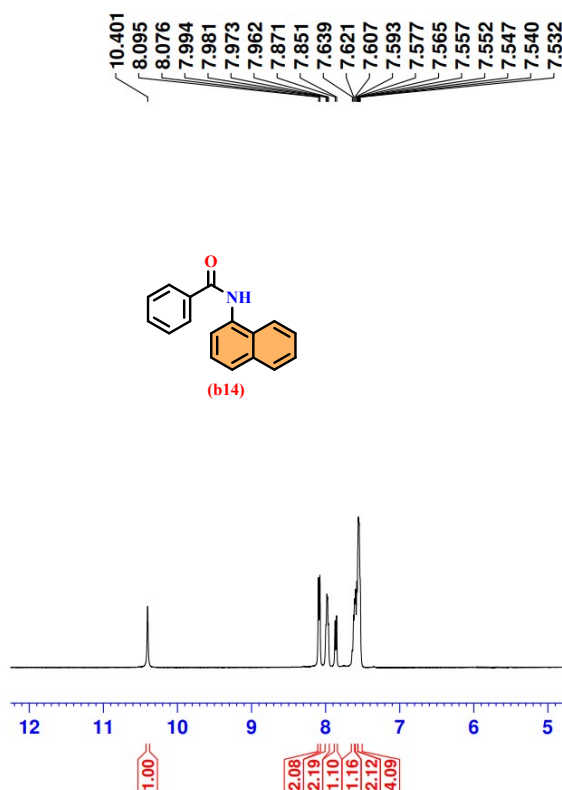
Current Data Parameters
NAME Dr.AKT090524
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240509
Time 23.59 h
INSTRUM spect
PROBHD Z108618_0505 (Zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631468 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S55. ¹³C NMR spectrum of *N*-(4-hydroxyphenyl)benzamide (b13)

bz-13-(24is-0395) 4060 (22.307)

Fig S56. GC-Mass spectrum (m/z) of *N*-(4-hydroxyphenyl)benzamide (b13)Signature SIF VIT VELLORE
BZ-14-Br

Current Data Parameters

NAME Dr.CM200424
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters

Date_ 20240420
Time 9.52 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 309.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters

SI 65536
SF 400.2580062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S57. ¹H NMR spectrum of *N*-(naphthalen-1-yl)benzamide (b14)

Signature SIF VIT VELLORE
BZ-14-Br



Current Data Parameters
NAME Dr.AKT230424
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240424
Time 9.05 h
INSTRUM spect
PROBHD Z108618_0505 (Zpgg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

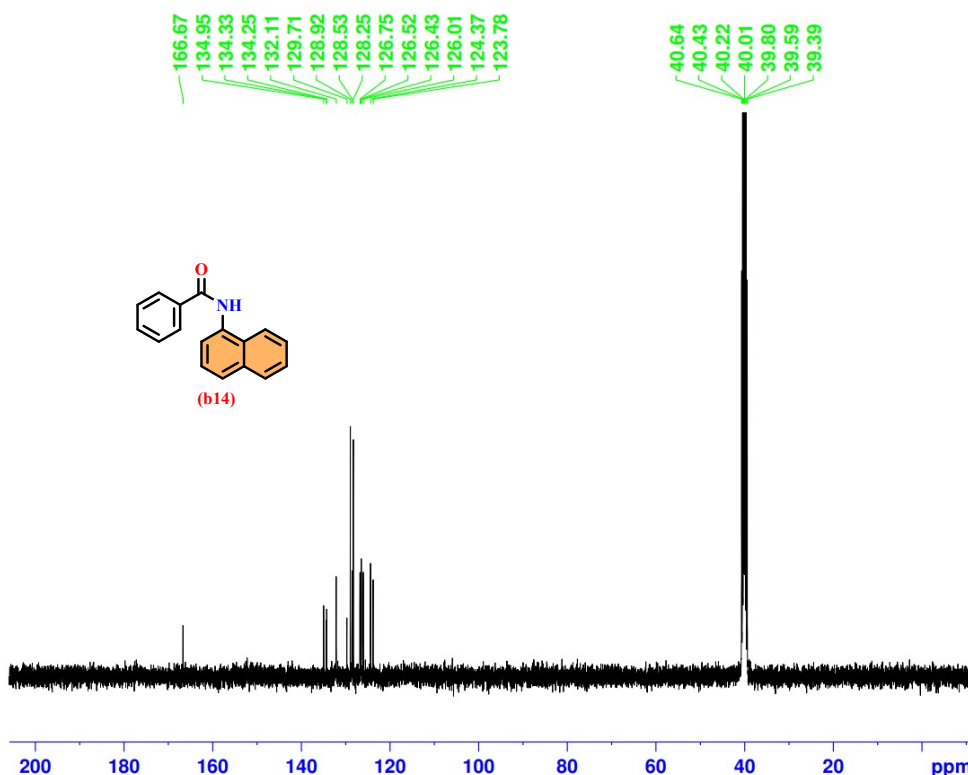


Fig S58. ^{13}C NMR spectrum of *N*-(naphthalen-1-yl)benzamide (b14)

, 03-May-2024 + 21:33:26
Scan EI+
2.38e8

bz-14-(24is-0396) 4258 (23.297)

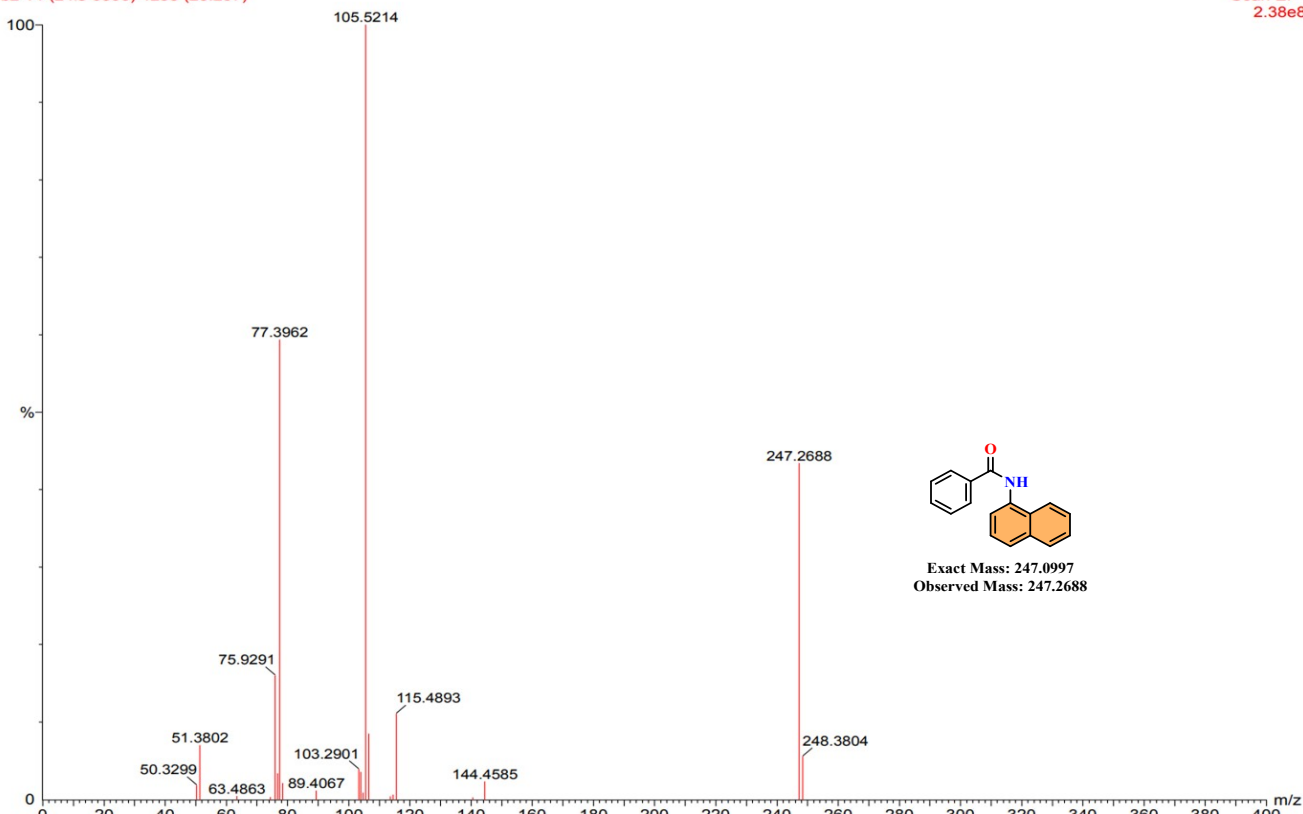
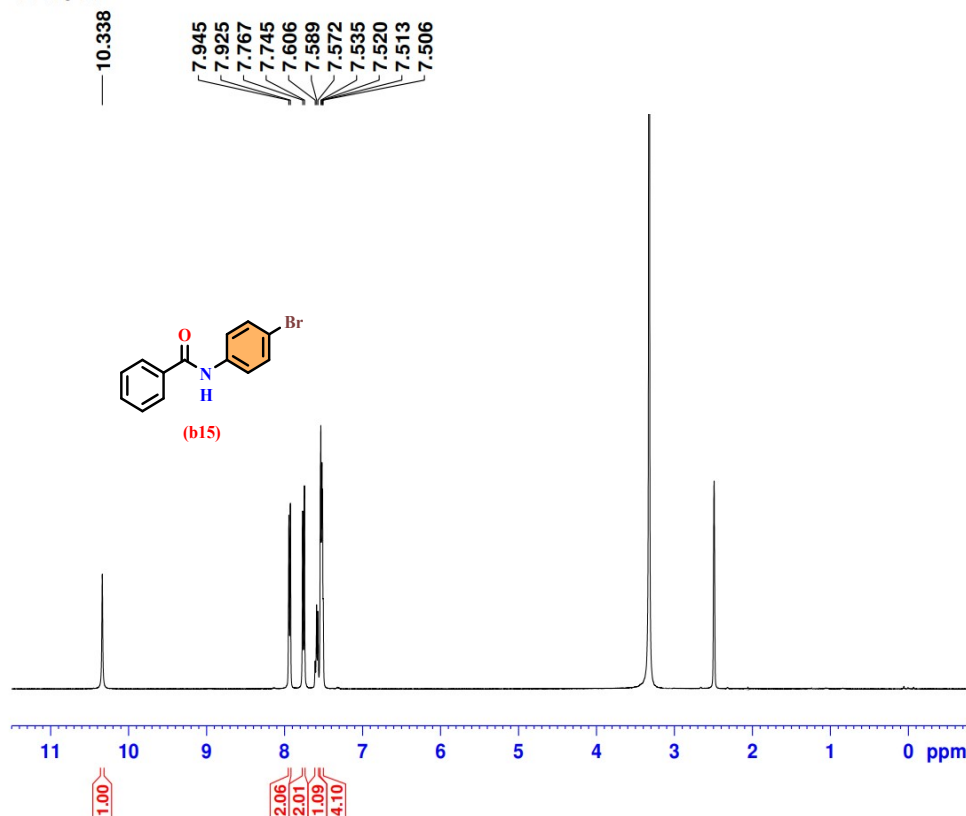


Fig S59. GC-Mass spectrum (m/z) of *N*-(naphthalen-1-yl)benzamide (b14)

Signature SIF VIT VELLORE
BZ-15-Br



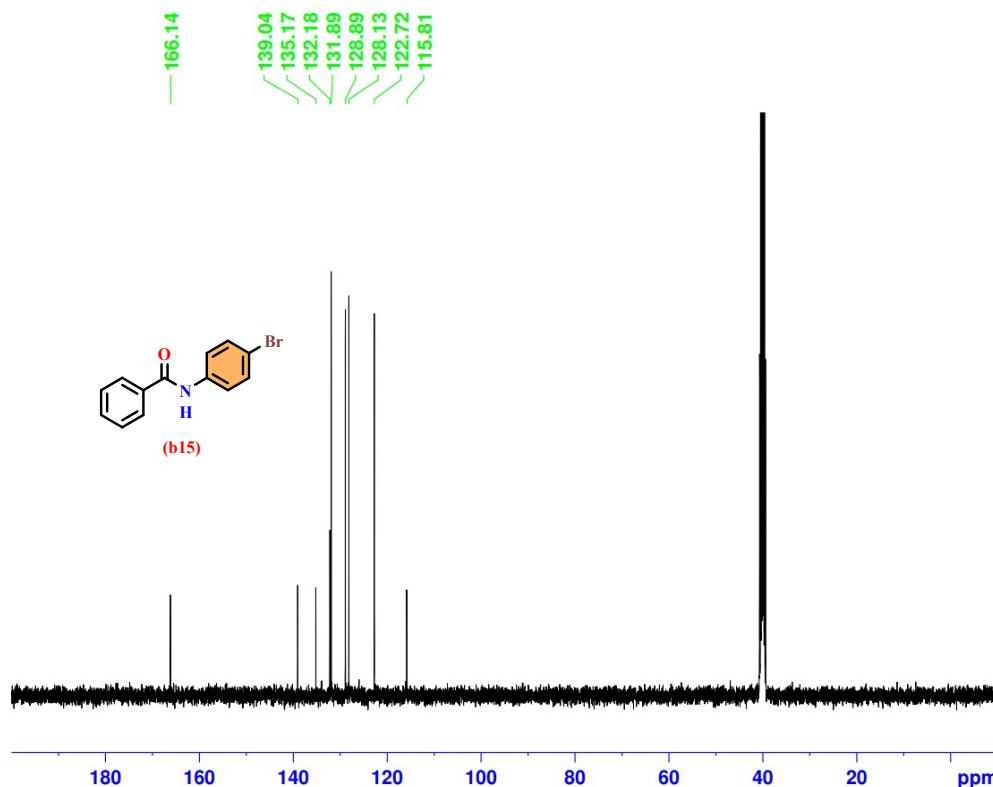
Current Data Parameters
NAME Dr.PDK200424
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240418
Time 21.35 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 308.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S60. ¹H NMR spectrum of *N*-(4-bromophenyl)benzamide (b15)

Signature SIF VIT VELLORE
BZ-15



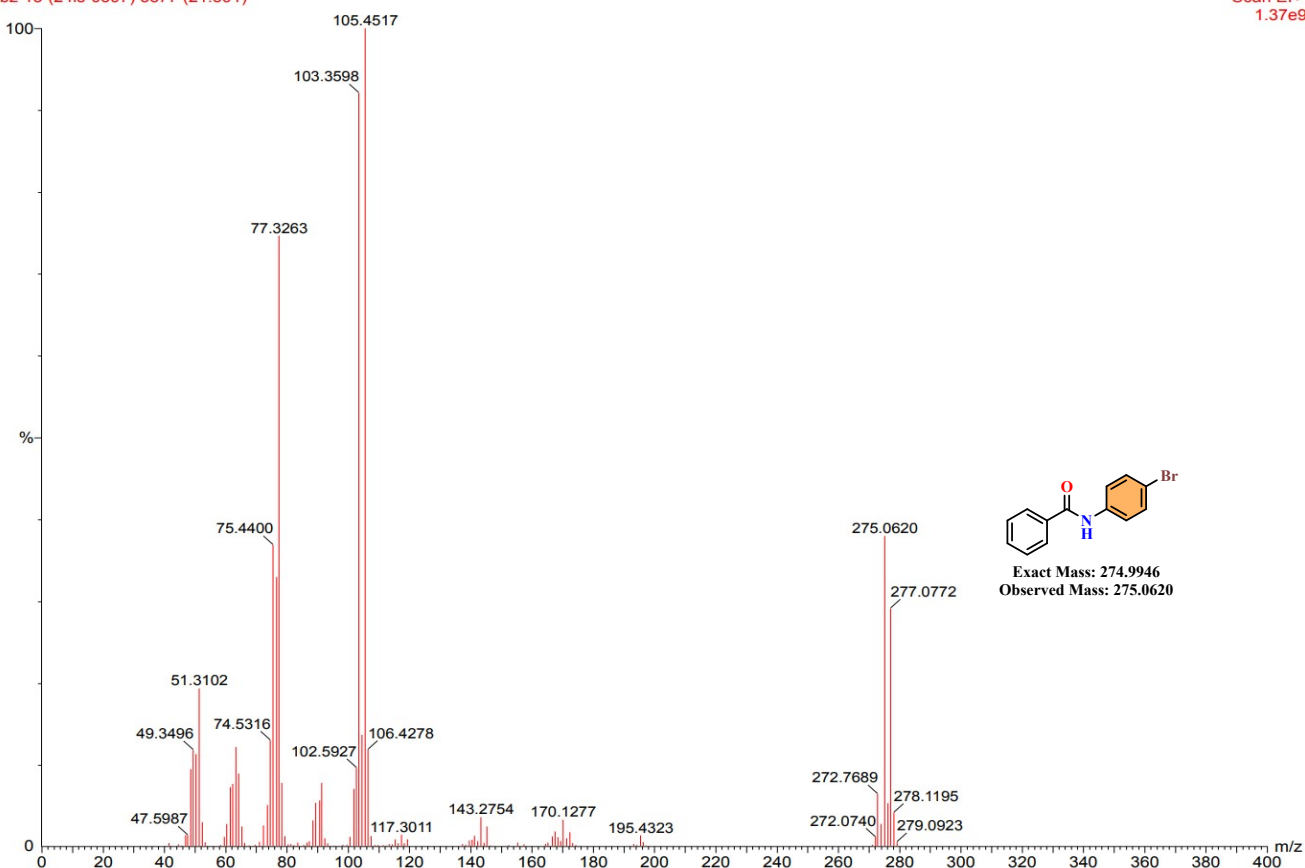
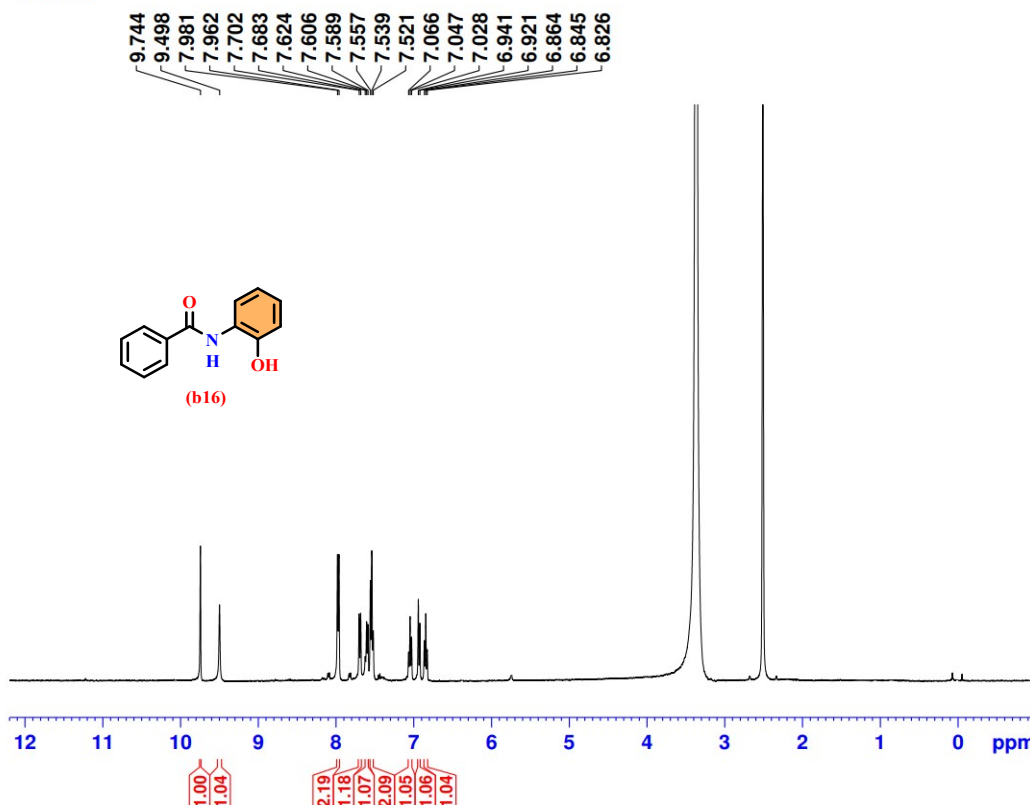
Current Data Parameters
NAME Dr.PDK200424
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240418
Time 22.06 h
INSTRUM spect
PROBHD Z108618_0505 (Zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S61. ¹³C NMR spectrum of *N*-(4-bromophenyl)benzamide (b15)

bz-15-(24is-0397) 3877 (21.391)

Fig S62. GC-Mass spectrum (m/z) of *N*-(4-bromophenyl)benzamide (b15)Signature SIF VIT VELLORE
Bz-16-Br

Current Data Parameters
NAME Dr.AKT020524
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240503
Time 11.24 h
INSTRUM spect
PROBHD Z108618_0505 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 309.0 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2579994 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S63. ¹H NMR spectrum of *N*-(2-hydroxyphenyl)benzamide (b16)

Signature SIF VIT VELLORE
Bz-16-Br



Current Data Parameters
NAME Dr.AKT020524
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240503
Time 11.55 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

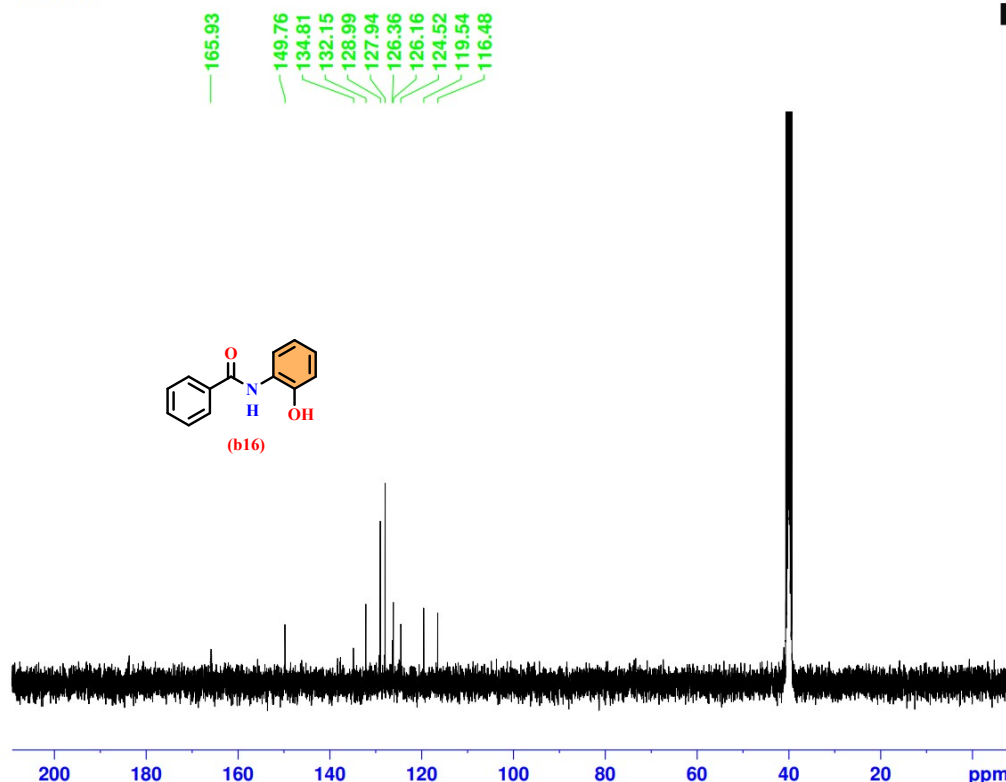


Fig S64. ^{13}C NMR spectrum of *N*-(2-hydroxyphenyl)benzamide (b16)

bz-16-(24is-0399) 4097 (22.412)

, 03-May-2024 + 21:33:11

Scan EI+
4.24e8

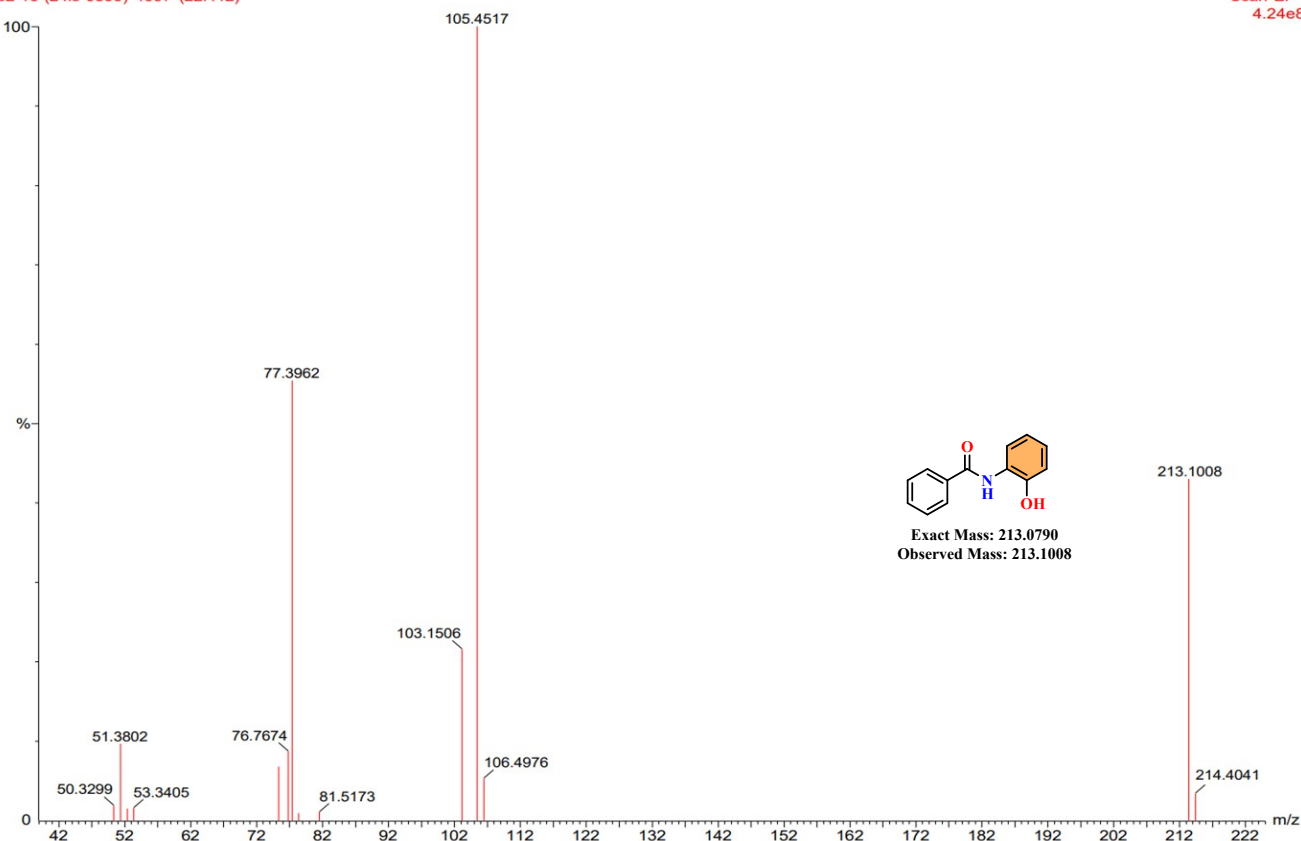
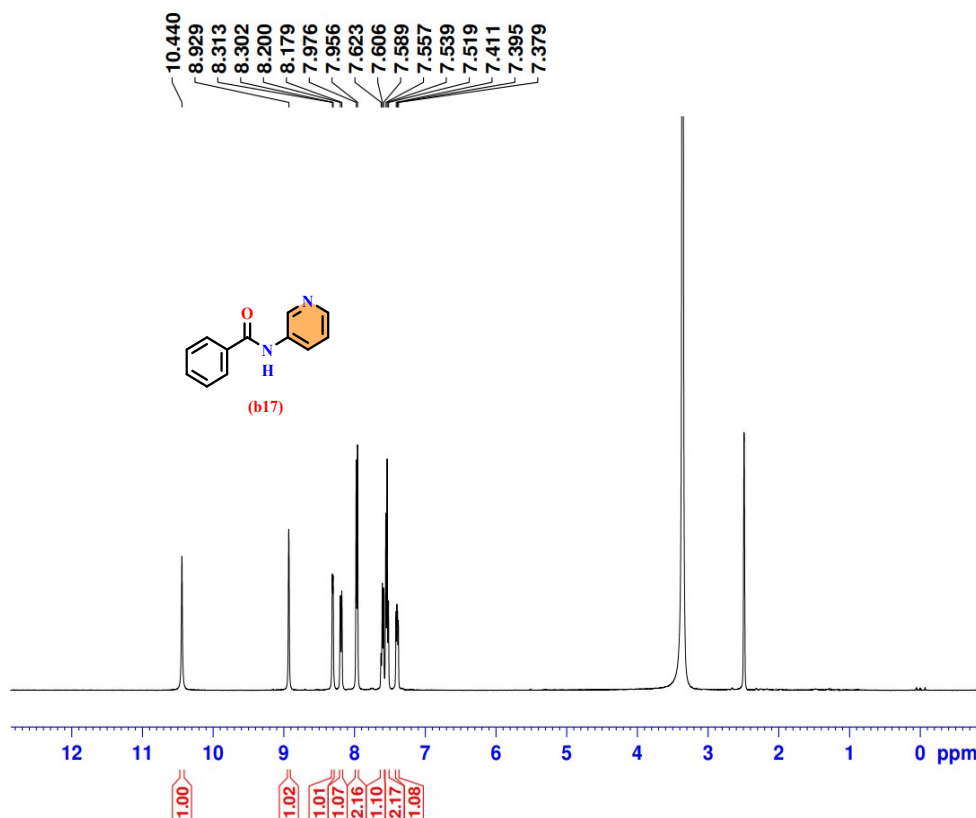


Fig S65. GC-Mass spectrum (m/z) of *N*-(2-hydroxyphenyl)benzamide (b16)

Signature SIF VIT VELLORE
Bz-17-Br



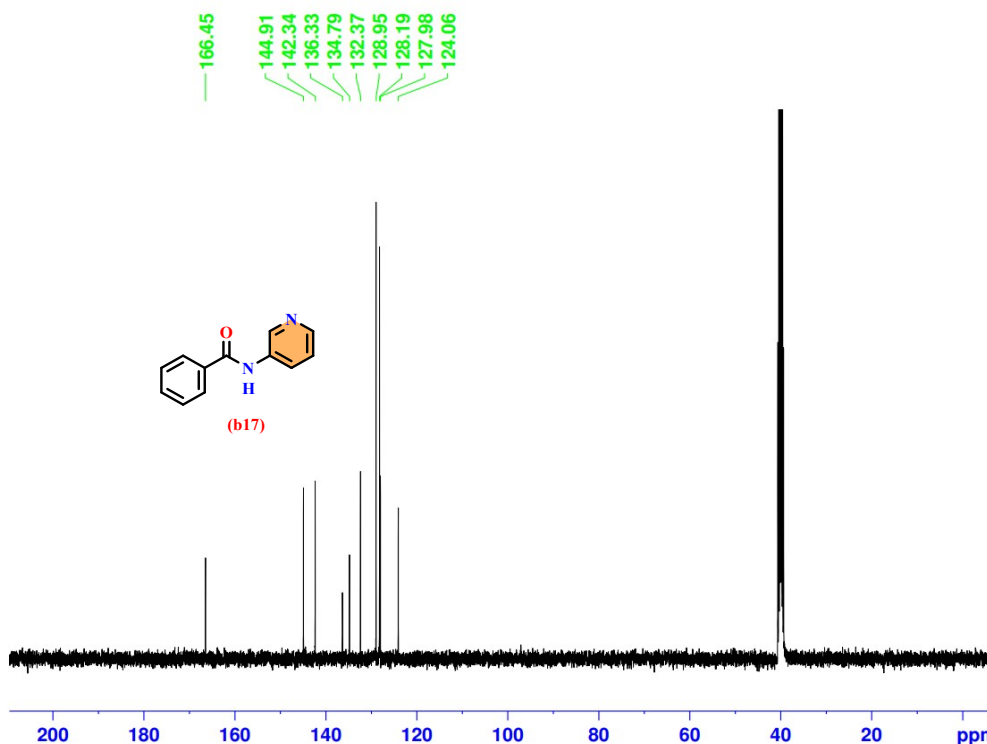
Current Data Parameters
NAME Dr.PDK070524
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240507
Time 19.58 h
INSTRUM spect
PROBHD Z108618_0505 (Z108618)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 308.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S66. ¹H NMR spectrum of *N*-(pyridin-3-yl)benzamide (b17)

Signature SIF VIT VELLORE
Bz-17-Br



Current Data Parameters
NAME Dr.PDK070524
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240507
Time 20.28 h
INSTRUM spect
PROBHD Z108618_0505 (Z108618)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 308.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 96.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S67. ¹³C NMR spectrum of *N*-(pyridin-3-yl)benzamide (b17)

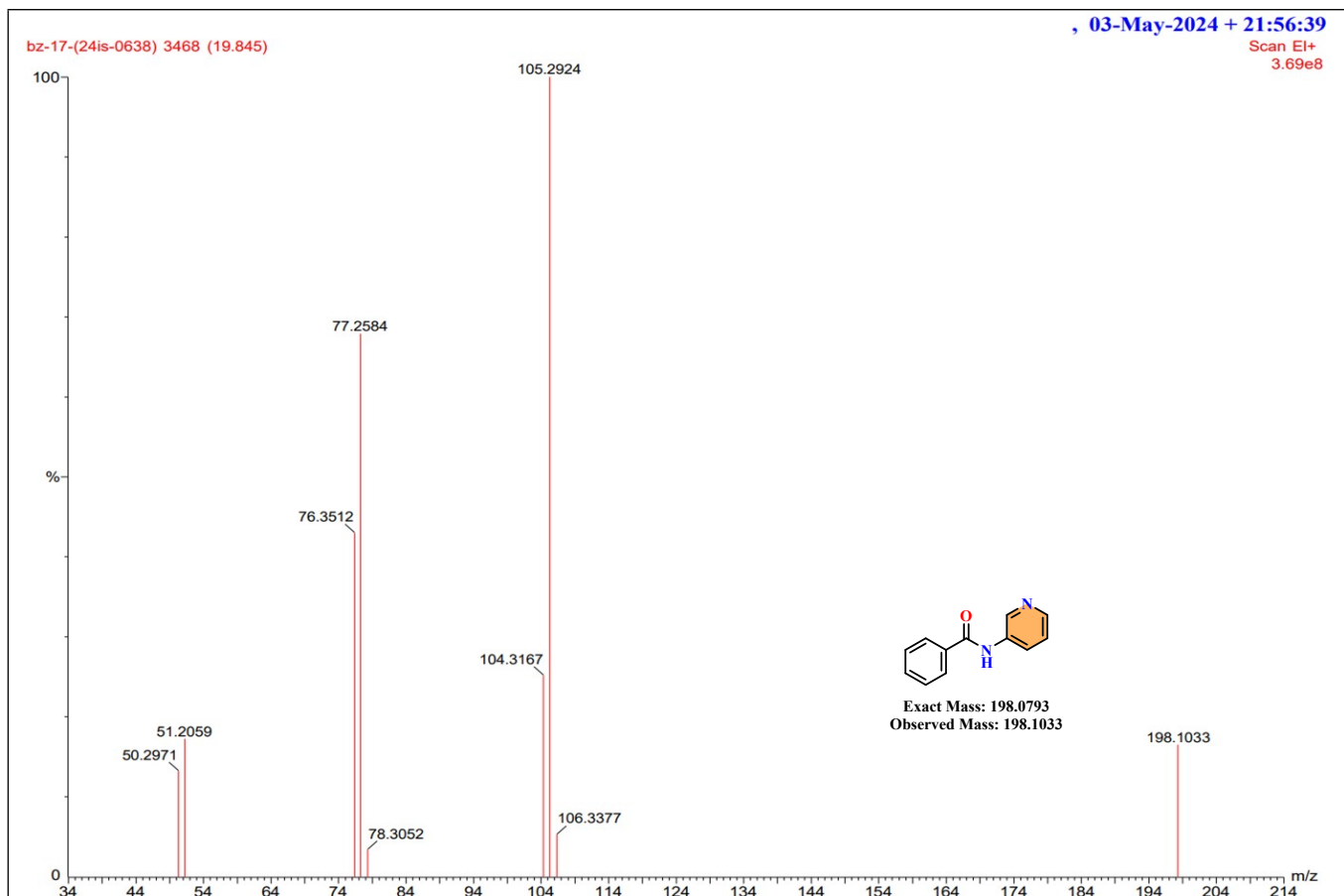


Fig S68. GC-Mass spectrum (m/z) of *N*-(pyridin-3-yl)benzamide (b17)

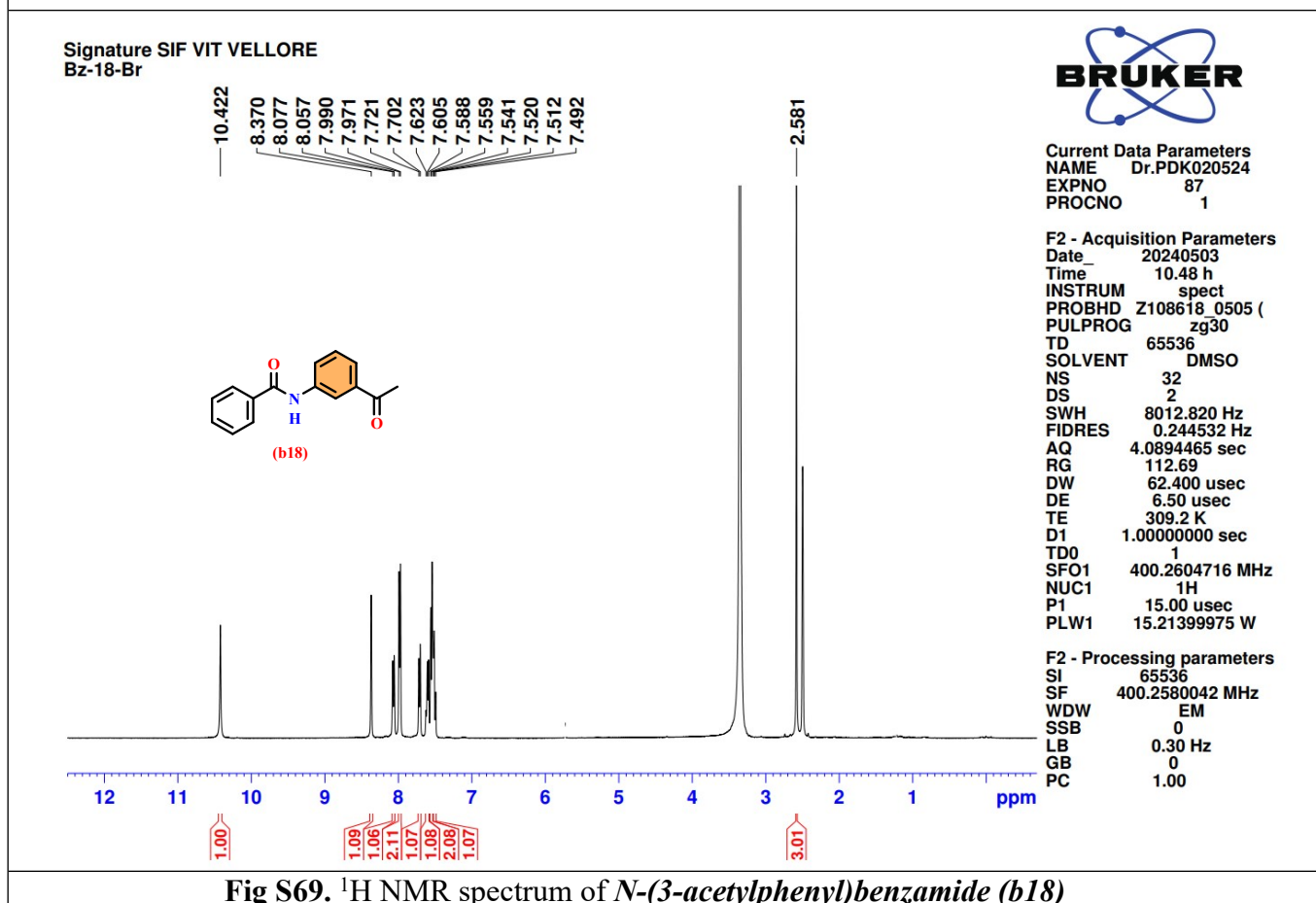


Fig S69. ¹H NMR spectrum of *N*-(3-acetylphenyl)benzamide (b18)

Signature SIF VIT VELLORE
Bz-18-Br



Current Data Parameters
NAME Dr.PDK020524
EXPNO 88
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240503
Time 11.19 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 309.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449832 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

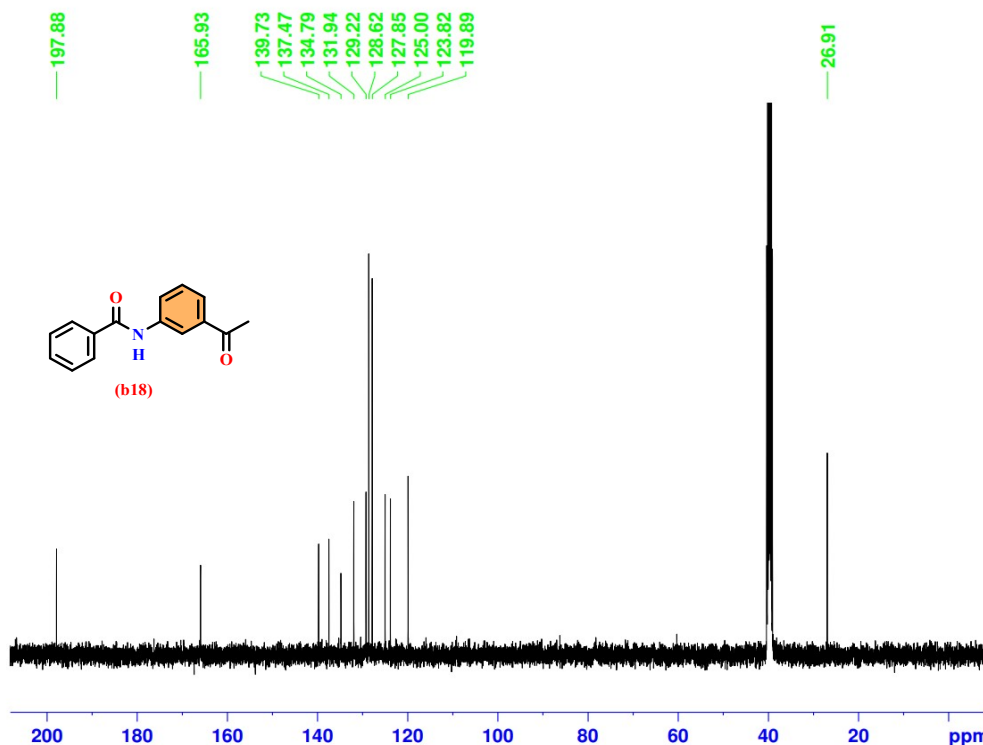


Fig S70. ^{13}C NMR spectrum of *N*-(3-acetylphenyl)benzamide (b18)

, 03-May-2024 + 22:23:19

Scan El+
3.91e7

bz-18-(24is-1984) 4165 (22.832)

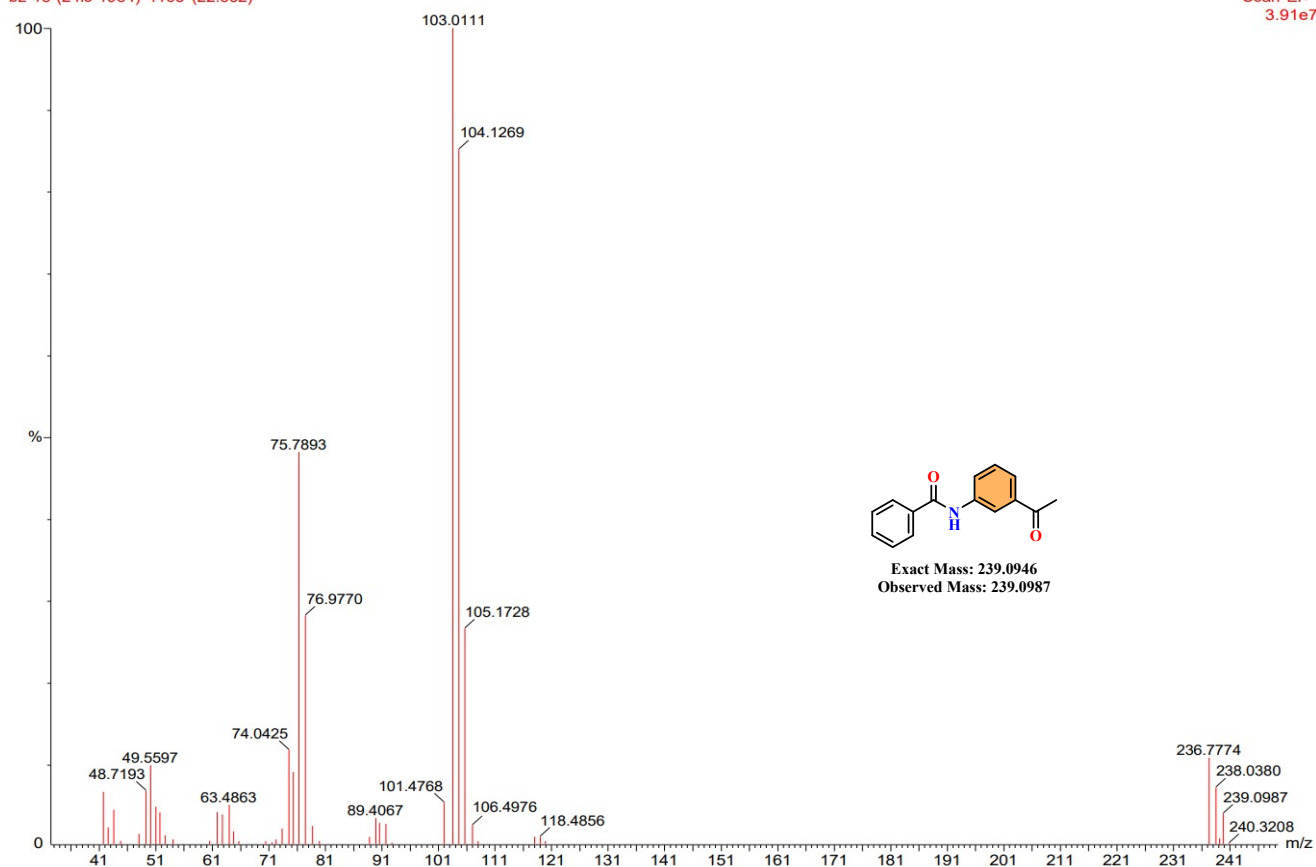
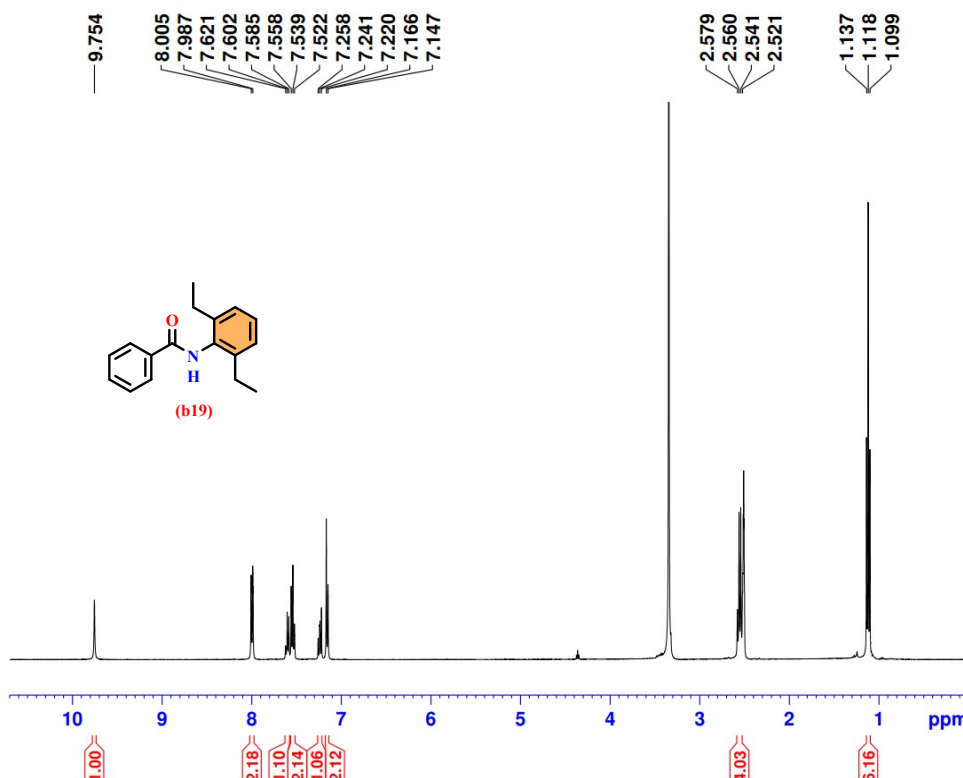


Fig S71. GC-Mass spectrum (m/z) of *N*-(3-acetylphenyl)benzamide (b18)

Signature SIF VIT VELLORE
Bz-19-Br



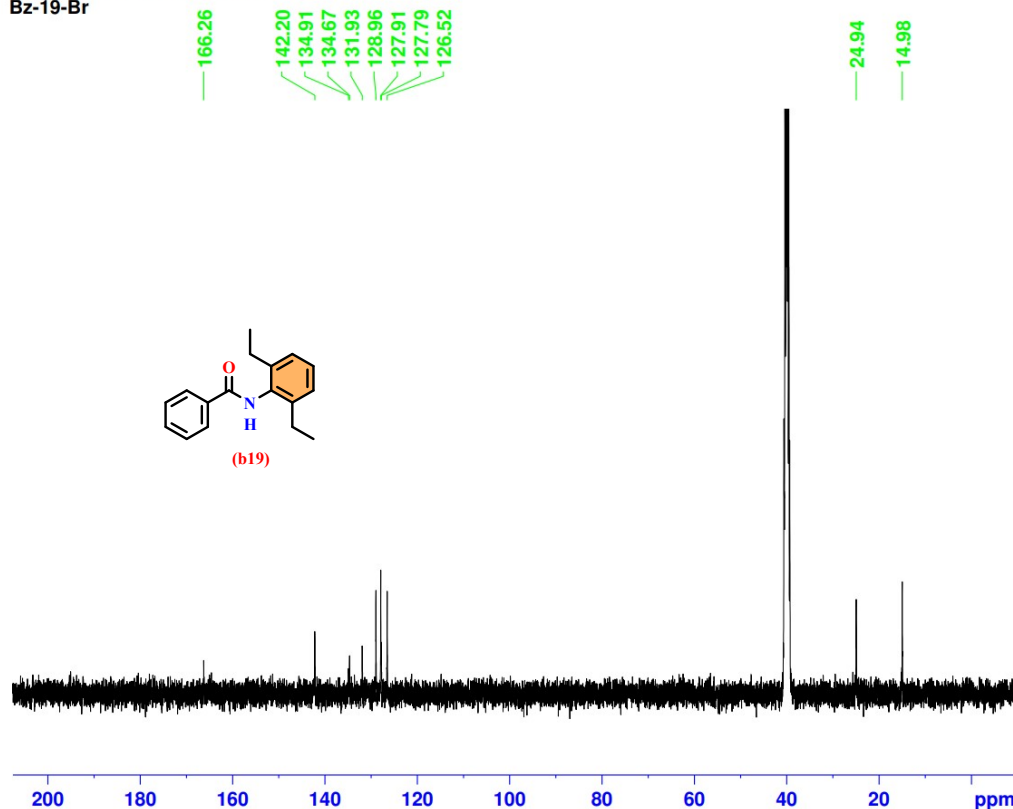
Current Data Parameters
NAME Dr.PDK250524
EXPNO 92
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240525
Time 15.06 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 304.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S72. ¹H NMR spectrum of *N*-(2,6-diethylphenyl)benzamide (b19)

Signature SIF VIT VELLORE
Bz-19-Br

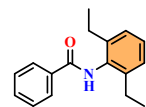
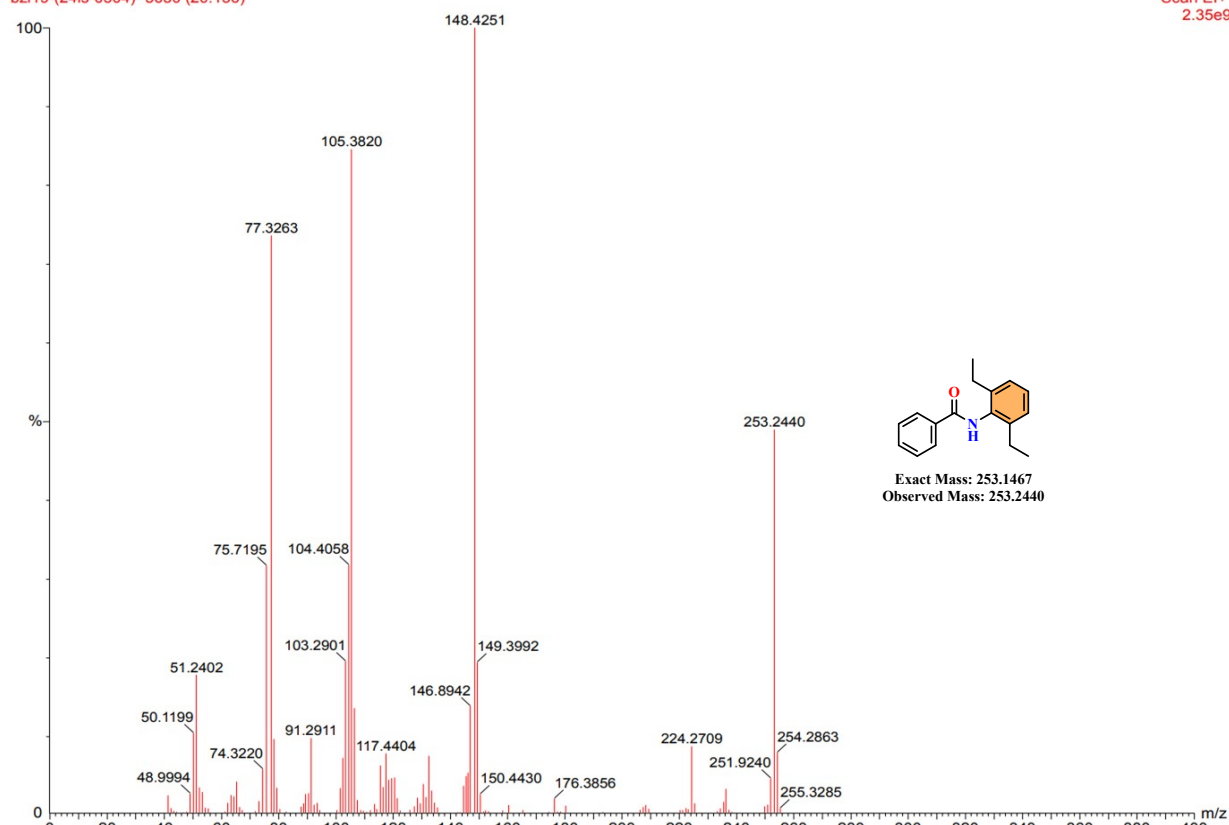


Current Data Parameters
NAME Dr.AKT230524
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240524
Time 8.01 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 302.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

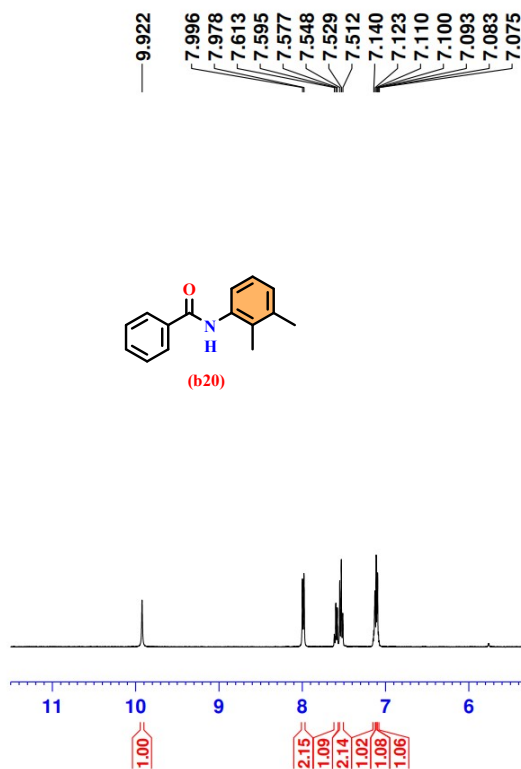
Fig S73. ¹³C NMR spectrum of *N*-(2,6-diethylphenyl)benzamide (b19)



Exact Mass: 253.1467
Observed Mass: 253.2440

Fig S74. GC-Mass spectrum (m/z) of *N*-(2,6-diethylphenyl)benzamide (b19)

Signature SIF VIT VELLORE
Bz-20-Br



Current Data Parameters
NAME Dr.AKT290524
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240528
Time 17.10 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 304.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S75. ¹H NMR spectrum of *N*-(2,3-dimethylphenyl)benzamide (b20)

Signature SIF VIT VELLORE
Bz-20-Br



Current Data Parameters
NAME Dr.AKT290524
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240528
Time 17.41 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 305.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

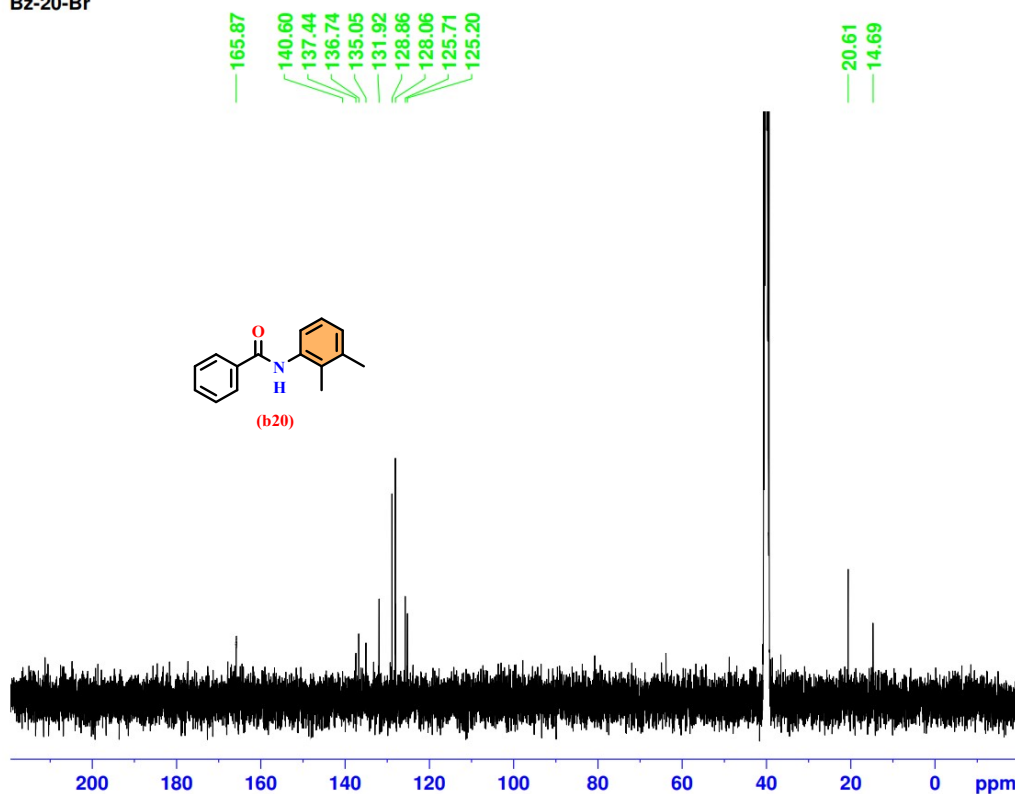


Fig S76. ¹³C NMR spectrum of *N*-(2,3-dimethylphenyl)benzamide (b20)

bz20-(24is-0505) 3947 (21.741)

, 23-May-2024 + 20:10:24

Scan EI+
3.93e7

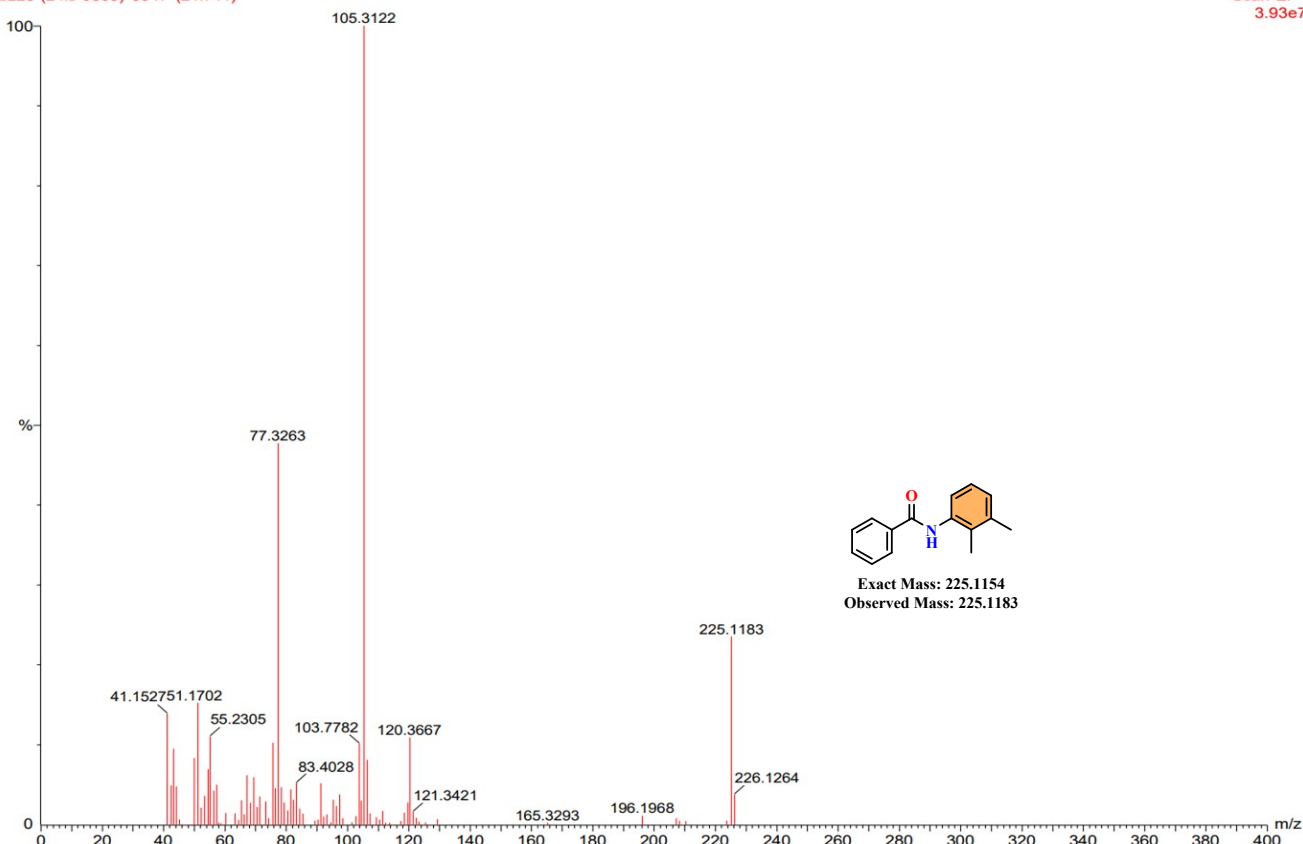
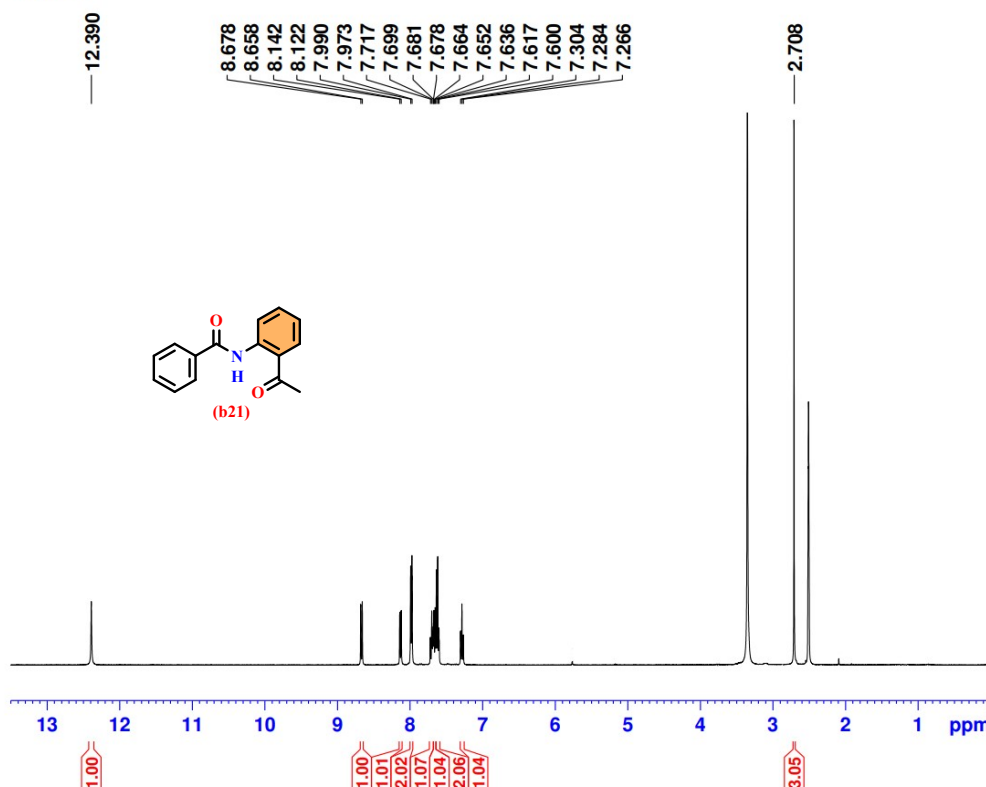


Fig S77. GC-Mass spectrum (m/z) of *N*-(2,3-dimethylphenyl)benzamide (b20)

Signature SIF VIT VELLORE
Bz-21-Br



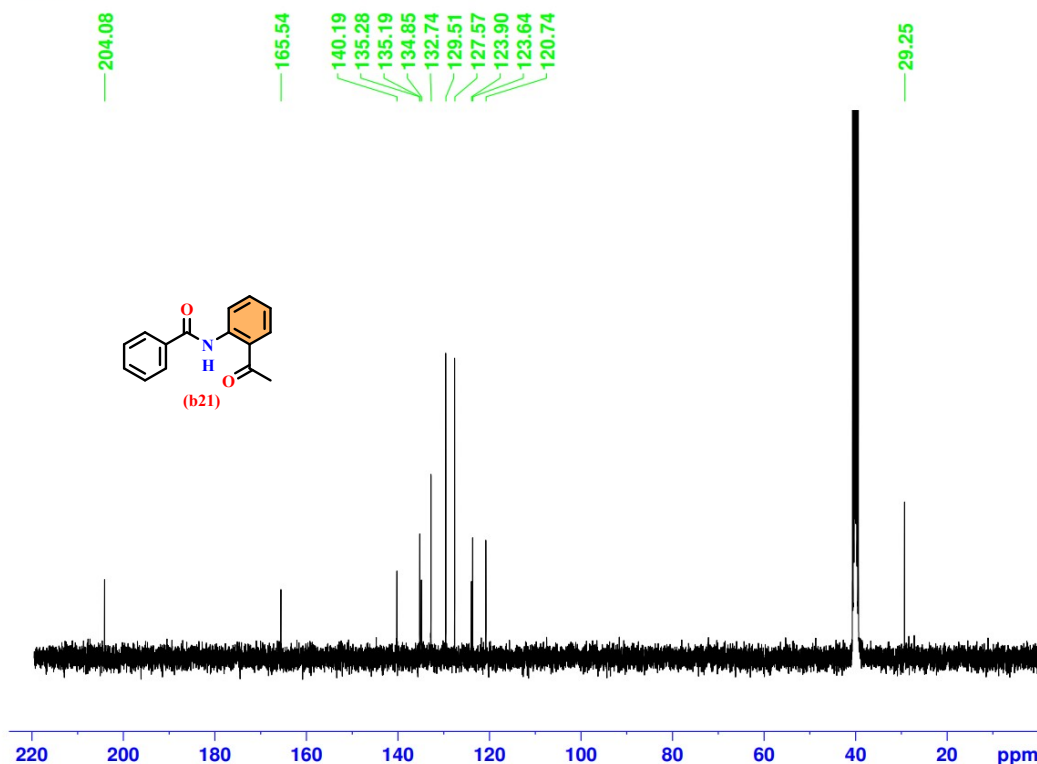
Current Data Parameters
NAME Dr.AKT290524
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240529
Time 4.43 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 302.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S78. ¹H NMR spectrum of *N*-(2-acetylphenyl)benzamide (b21)

Signature SIF VIT VELLORE
Bz-21-Br



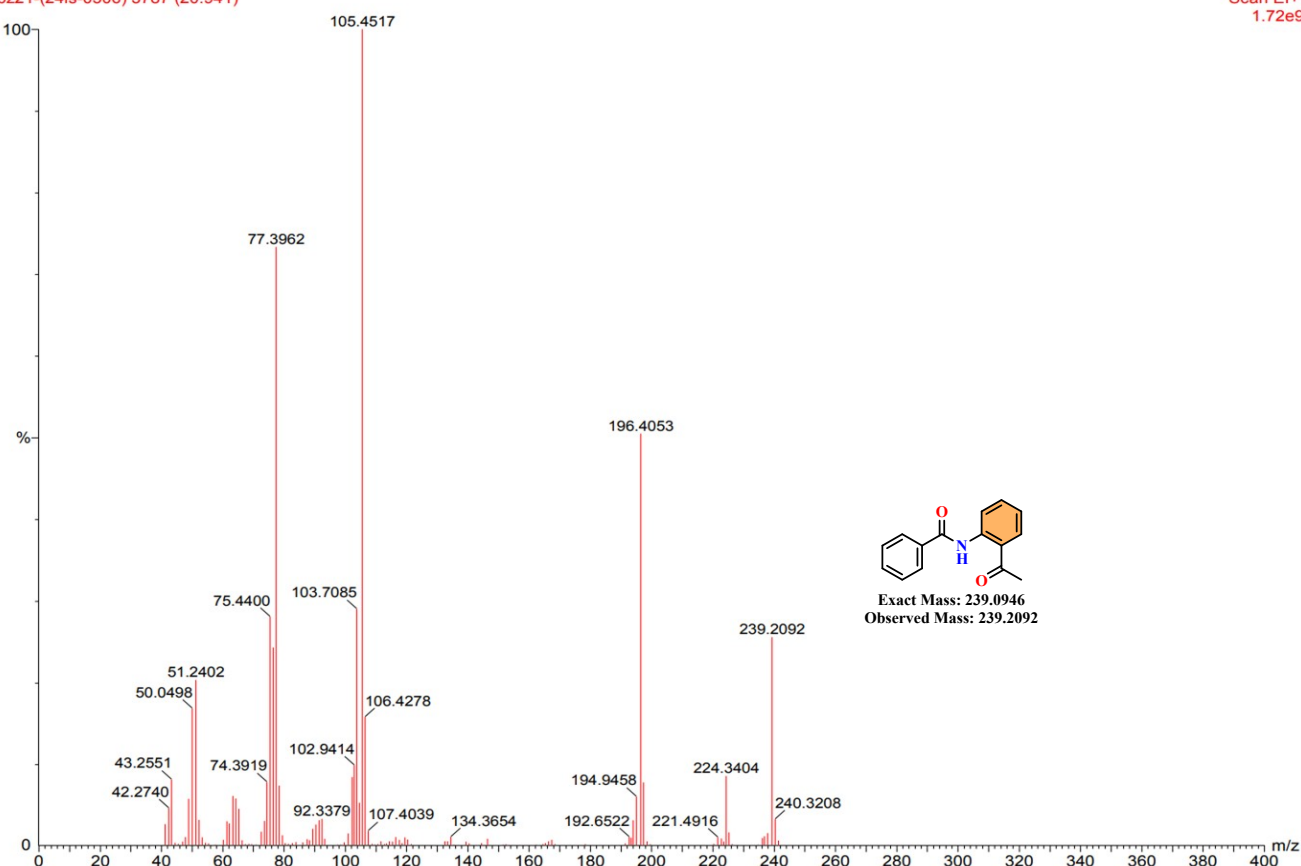
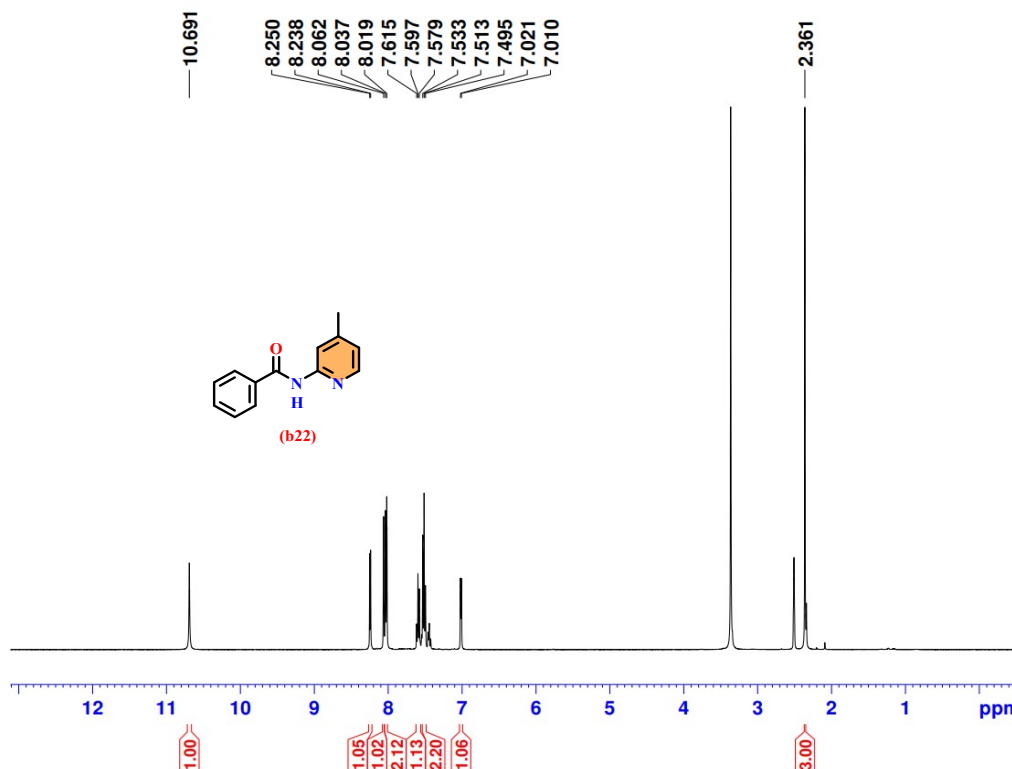
Current Data Parameters
NAME Dr.AKT290524
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240529
Time 5.14 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 302.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S79. ¹³C NMR spectrum of *N*-(2-acetylphenyl)benzamide (b21)

bz21-(24is-0506) 3787 (20.941)

Fig S80. GC-Mass spectrum (m/z) of *N*-(2-acetylphenyl)benzamide (b21)Signature SIF VIT VELLORE
Bz-22

Current Data Parameters
 NAME Dr.PDK050624
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240605
 Time 21.44 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 112.69
 DW 62.400 usec
 DE 6.50 usec
 TE 302.4 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 ¹H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Fig S81. ¹H NMR spectrum of *N*-(4-methylpyridin-2-yl)benzamide (b22)

Signature SIF VIT VELLORE
Bz-22



Current Data Parameters
NAME Dr.PDK050624
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date 20240605
Time 22.15 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 302.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

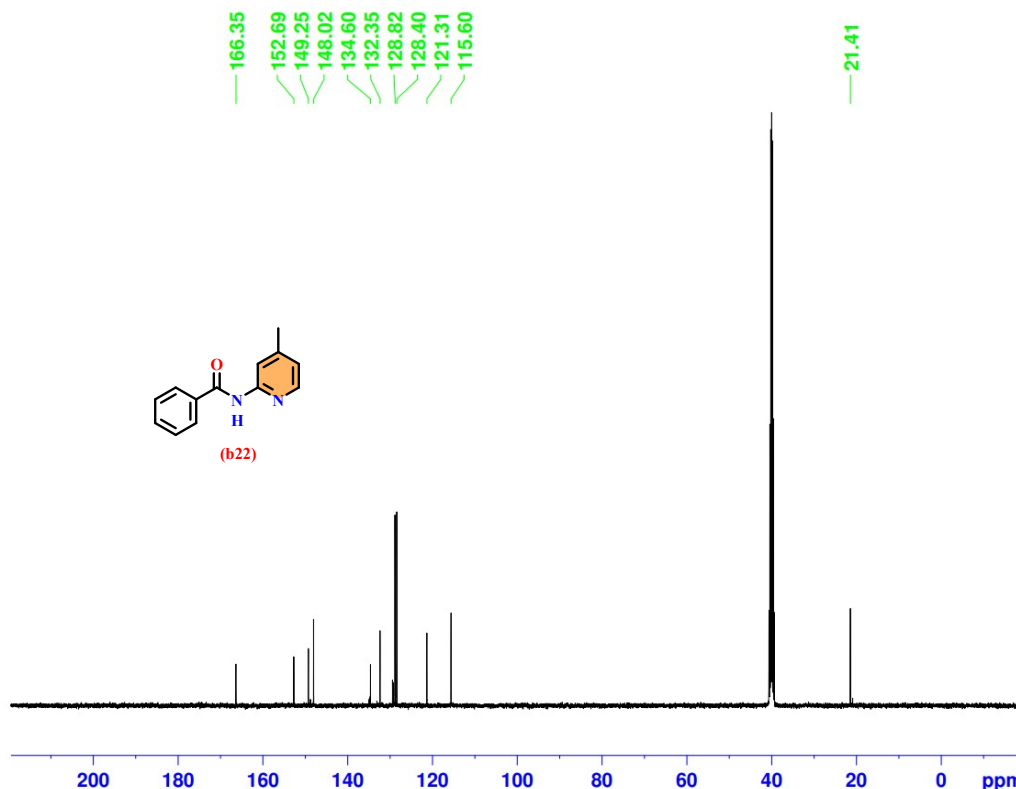


Fig S82. ^{13}C NMR spectrum of *N*-(4-methylpyridin-2-yl)benzamide (b22)

Bz-22-(24is-0703) 3606 (20.036)

, 15-Jul-2024 + 22:16:00

Scan EI+
1.22e9

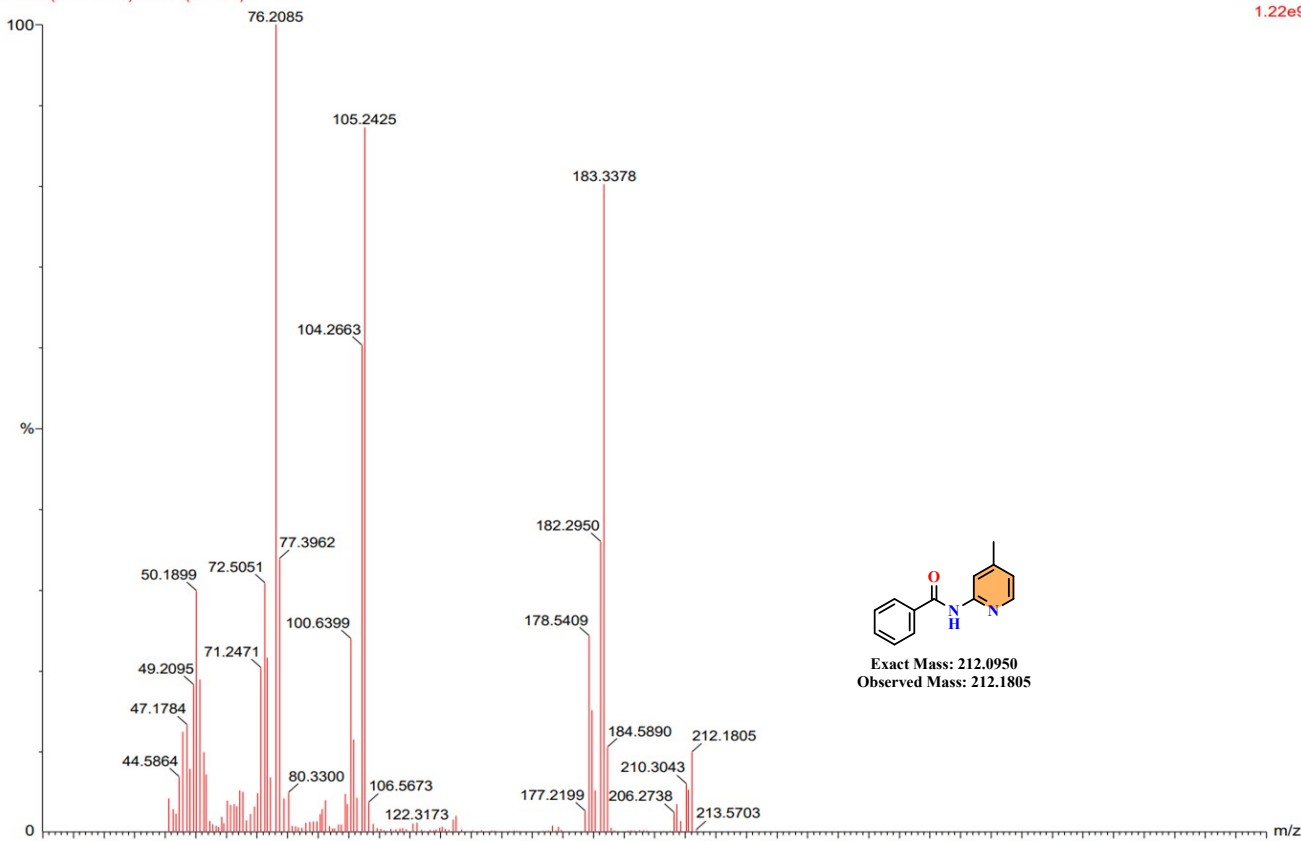
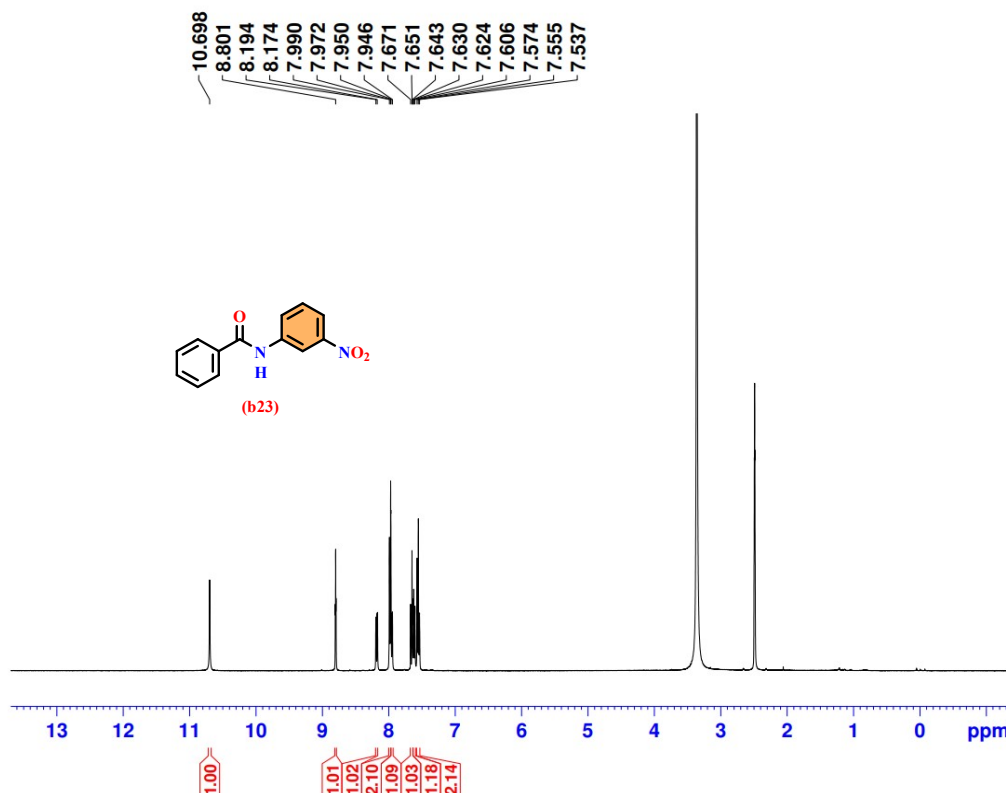


Fig S83. GC-Mass spectrum (m/z) of *N*-(4-methylpyridin-2-yl)benzamide (b22)

Signature SIF VIT VELLORE
Bz-23



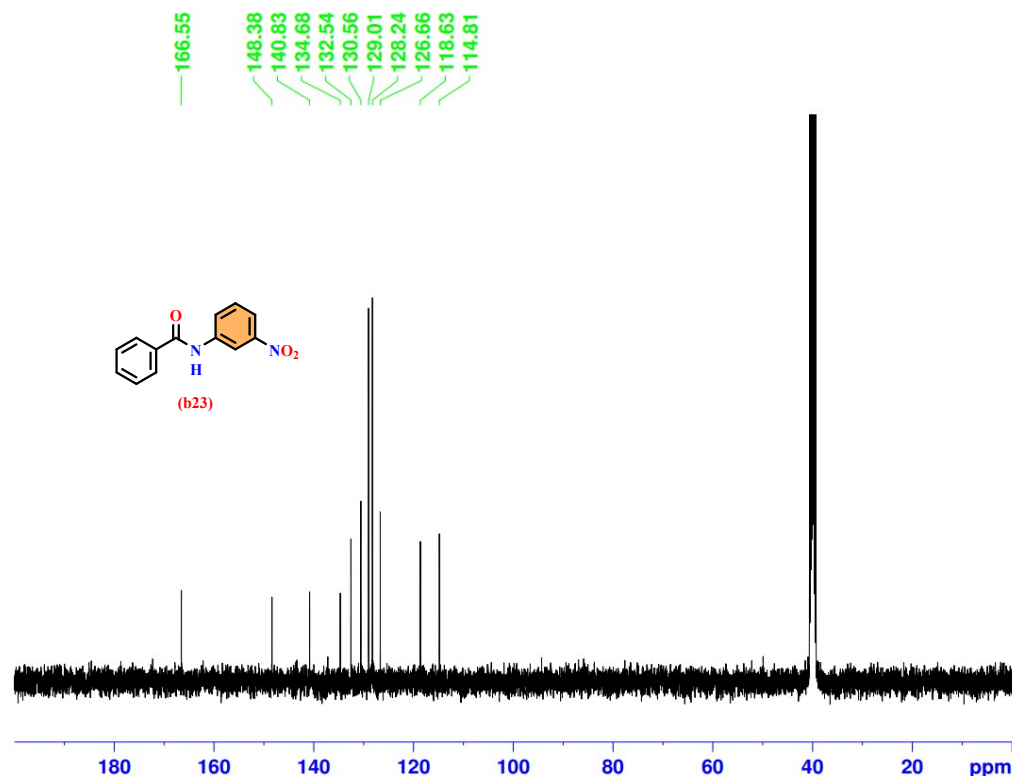
Current Data Parameters
NAME Dr.PDK150724
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240716
Time 14.04 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S84. ¹H NMR spectrum of *N*-(3-nitrophenyl)benzamide (b23)

Signature SIF VIT VELLORE
Bz-23



Current Data Parameters
NAME Dr.PDK150724
EXPNO 26
PROCNO 1

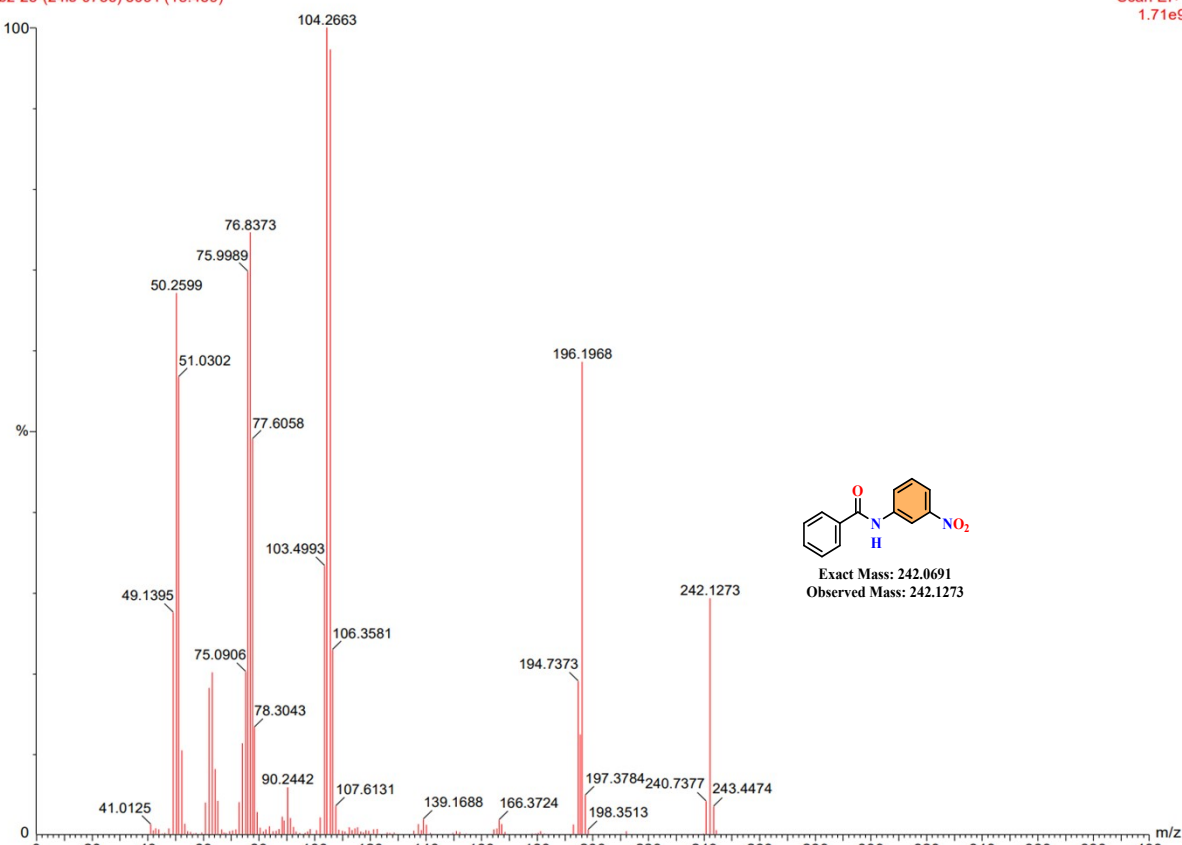
F2 - Acquisition Parameters
Date_ 20240716
Time 14.36 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig S85. ¹³C NMR spectrum of *N*-(3-nitrophenyl)benzamide (b23)

bz-23-(24is-0736) 3091 (18.459)

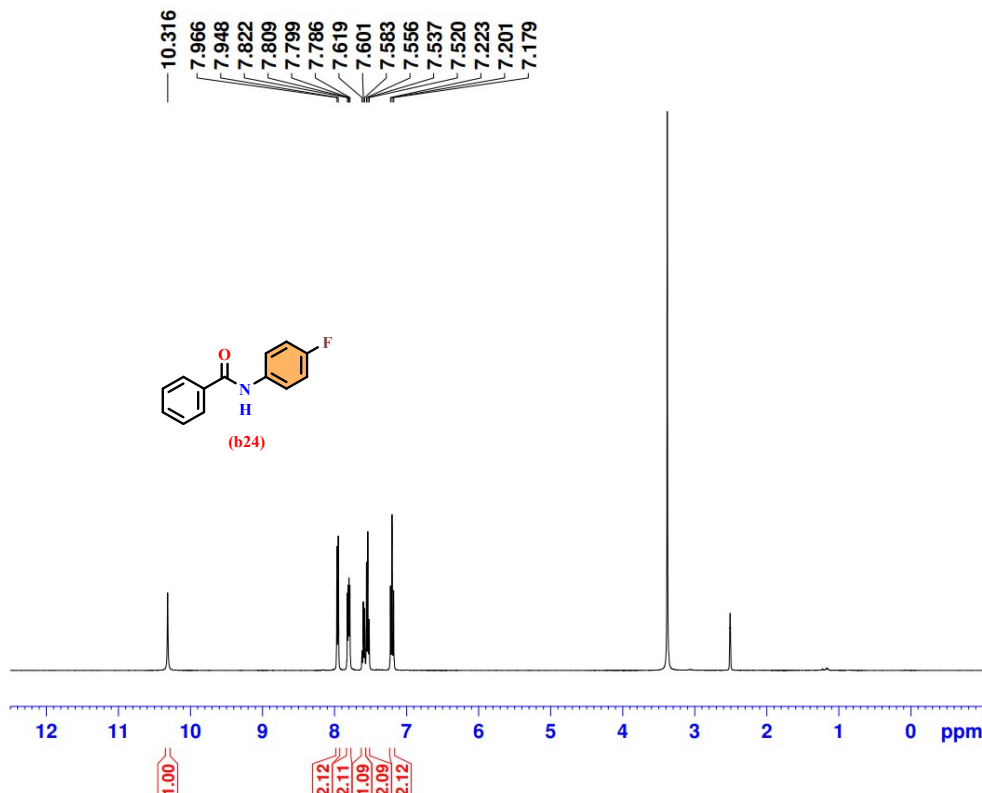
, 25-Jul-2024 + 22:53:21

Scan EI+
1.71e9Fig S86. GC-Mass spectrum (m/z) of *N*-(3-nitrophenyl)benzamide (b23)Signature SIF VIT VELLORE
Bz-24F

Current Data Parameters
NAME Dr.PDK090724
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date 20240709
Time 19.46 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 303.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S87. ¹H NMR spectrum of *N*-(4-fluorophenyl)benzamide (b24)

Signature SIF VIT VELLORE
Bz-24



Current Data Parameters
NAME Dr.PDK090724
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240709
Time 20.17 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

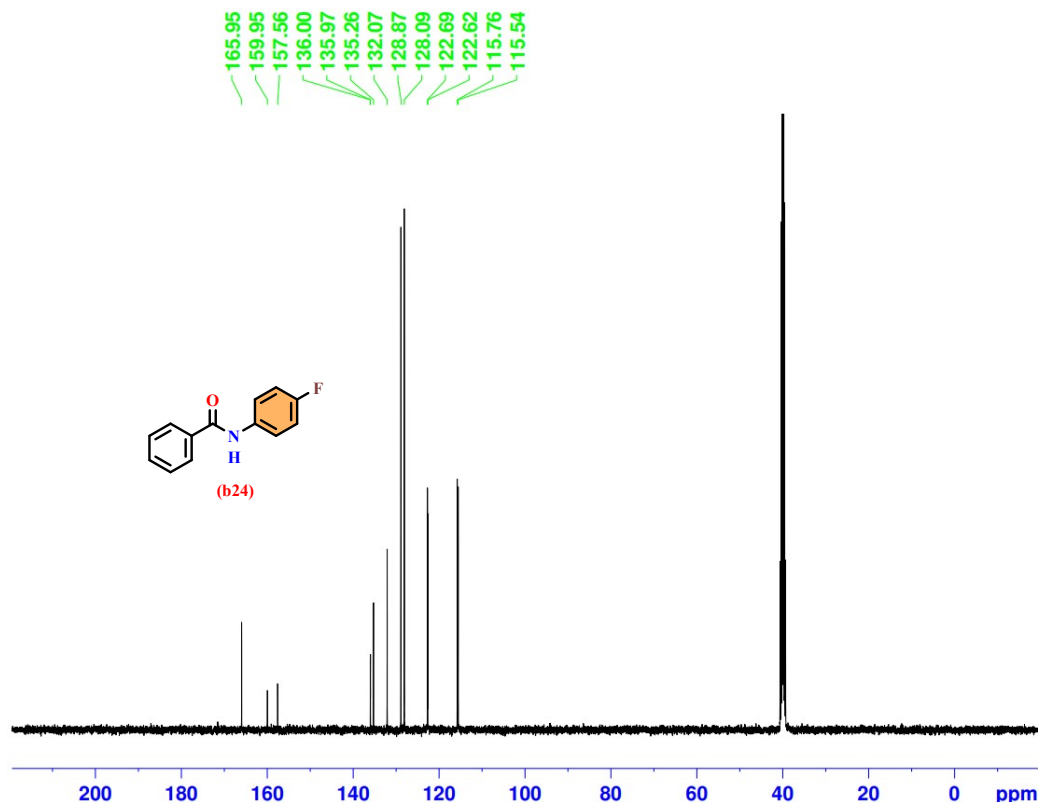


Fig S88. ^{13}C NMR spectrum of *N*-(4-fluorophenyl)benzamide (b24)

Signature SIF VIT VELLORE
Bz-24F



Current Data Parameters
NAME Dr.PDK090724
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240709
Time 20.19 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgfgqn
TD 131072
SOLVENT DMSO
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 199.6
DW 5.600 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TD0 1
SFO1 376.5811447 MHz
NUC1 19F
P1 15.00 usec
PLW1 20.11800003 W

F2 - Processing parameters
SI 65536
SF 376.6188065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

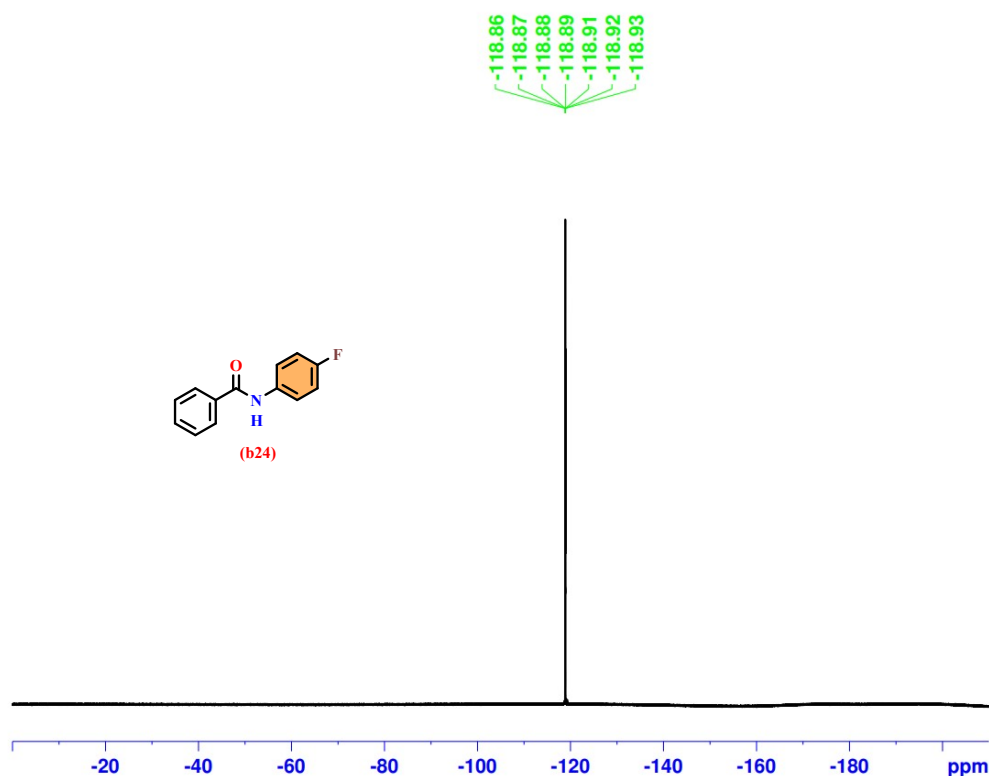


Fig S89. ^{19}F NMR spectrum of *N*-(4-fluorophenyl)benzamide (b24)

bz-f-(24is-0681) 3187 (17.940)

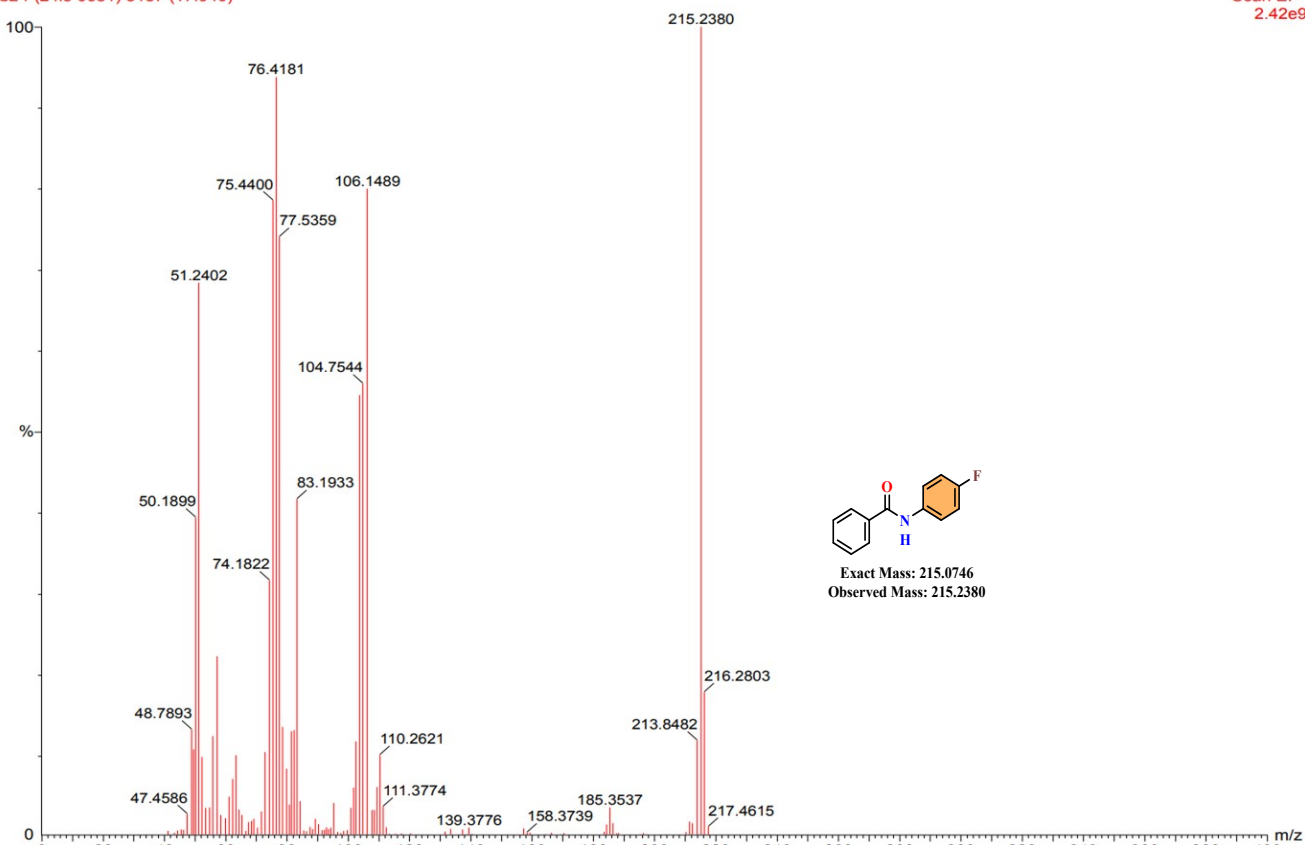
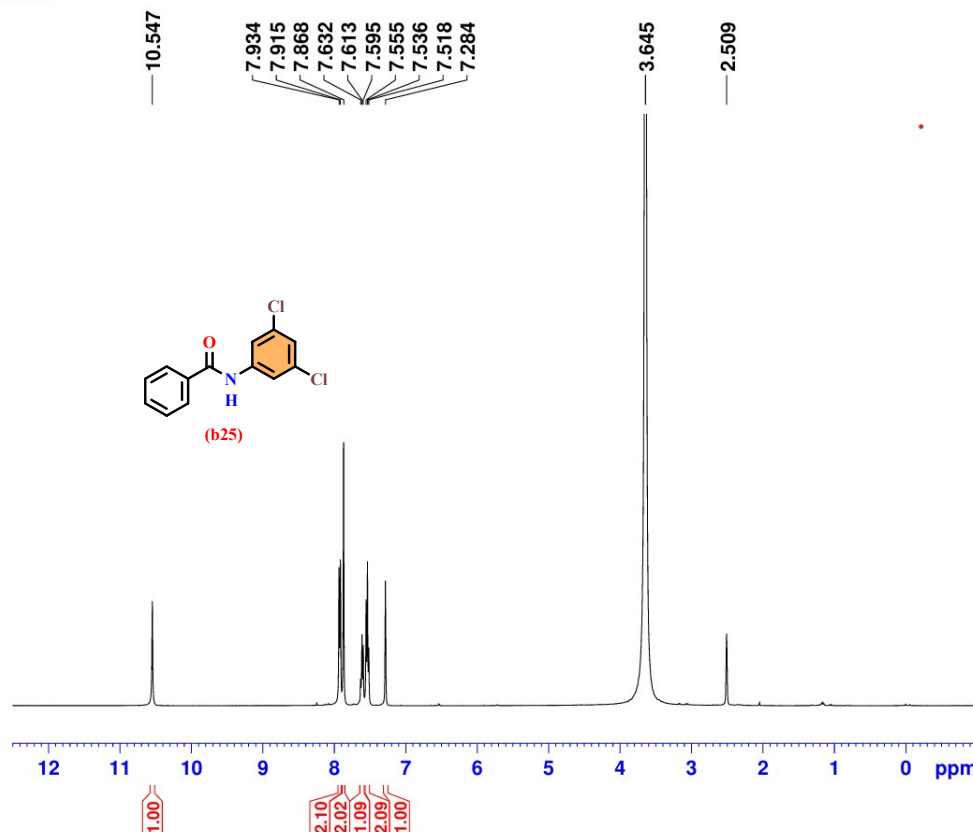


Fig S90. GC-Mass spectrum (m/z) of *N*-(4-fluorophenyl)benzamide (b24j)

Signature SIF VIT VELLORE
Bz-25



Current Data Parameters
NAME Dr.PDK031024
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241003
Time 20.42 h
INSTRUM spect
PROBHD Z108618_0505 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 302.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S91. ¹H NMR spectrum of *N*-(3,5-dichlorophenyl)benzamide (b25)

Signature SIF VIT VELLORE
Bz-25



Current Data Parameters
NAME Dr.PDK031024
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241003
Time 21.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

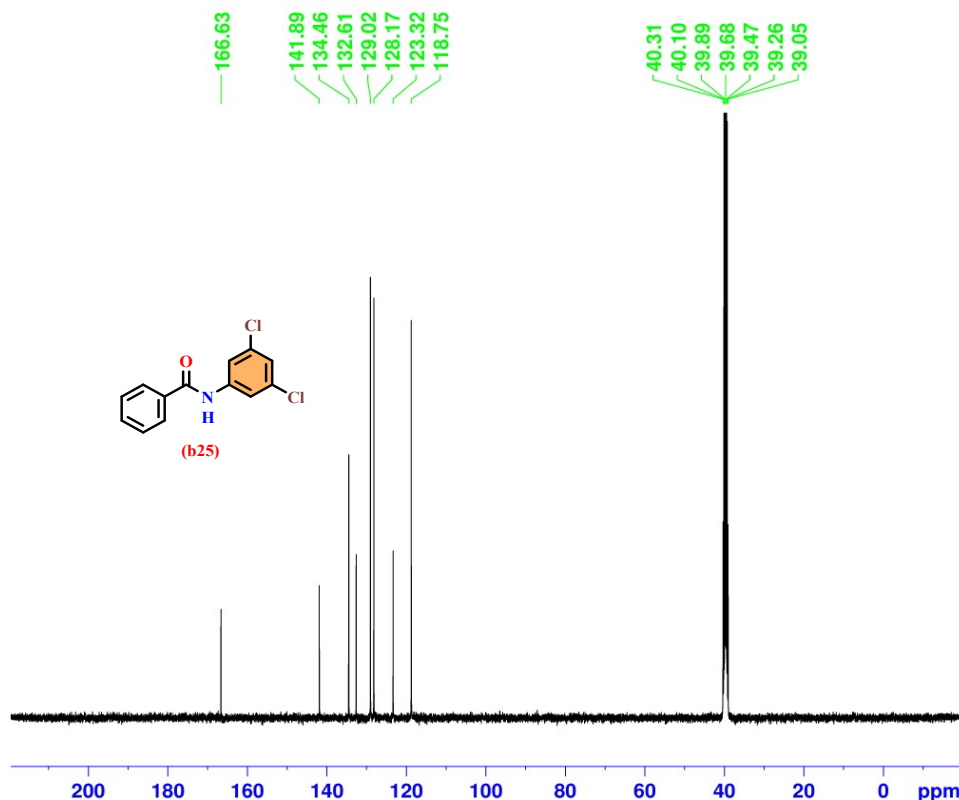


Fig S92. ^{13}C NMR spectrum of *N*-(3,5-dichlorophenyl)benzamide (b25)

bz-25-(24is-01072) 3514 (20.076)

, 04-Oct-2024 + 18:31:51

Scan EI+
1.67e9

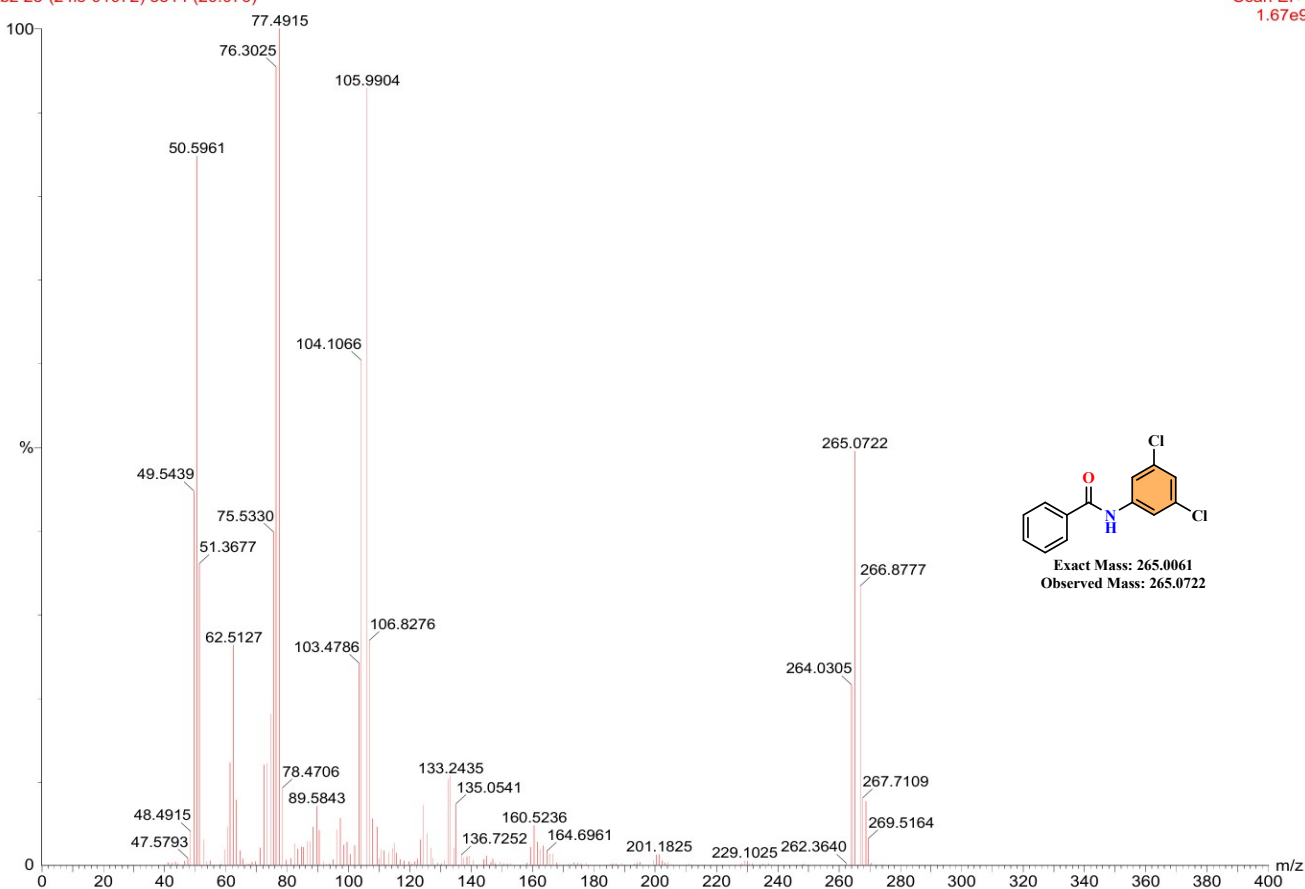


Fig S93. GC-Mass spectrum (m/z) of *N*-(3,5-dichlorophenyl)benzamide (b25)

Signature SIF VIT VELLORE
PcCFP

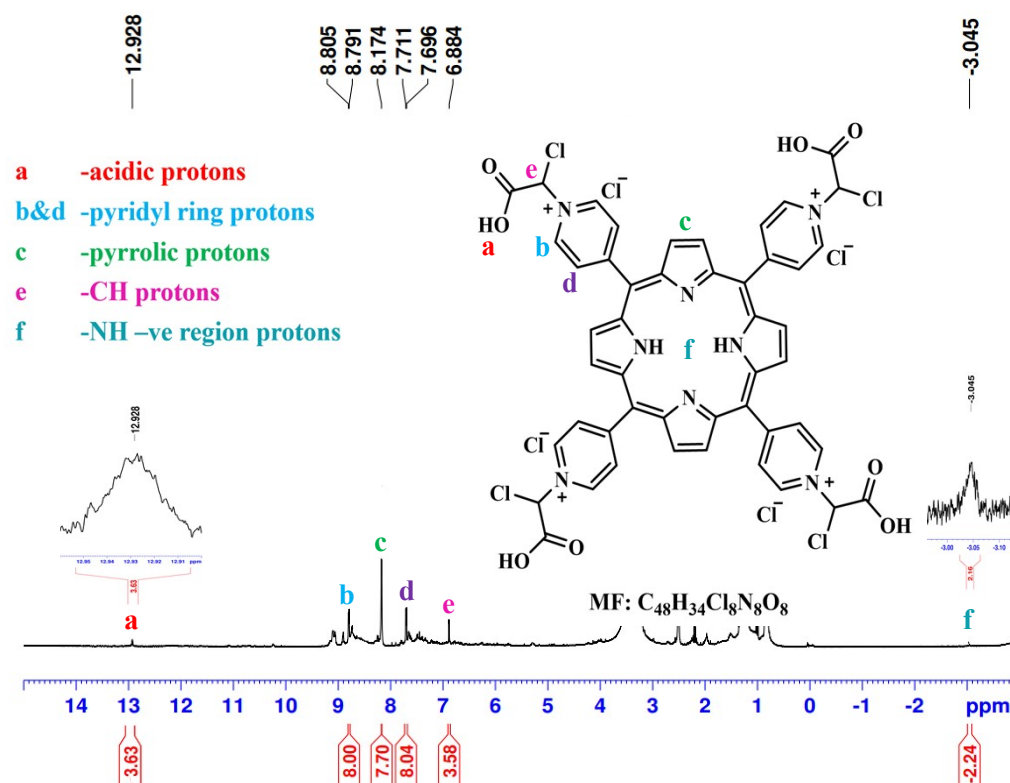


Fig S94. ¹H NMR spectrum of PcCFP Photocatalyst

Signature SIF VIT VELLORE
4-DCA-CT

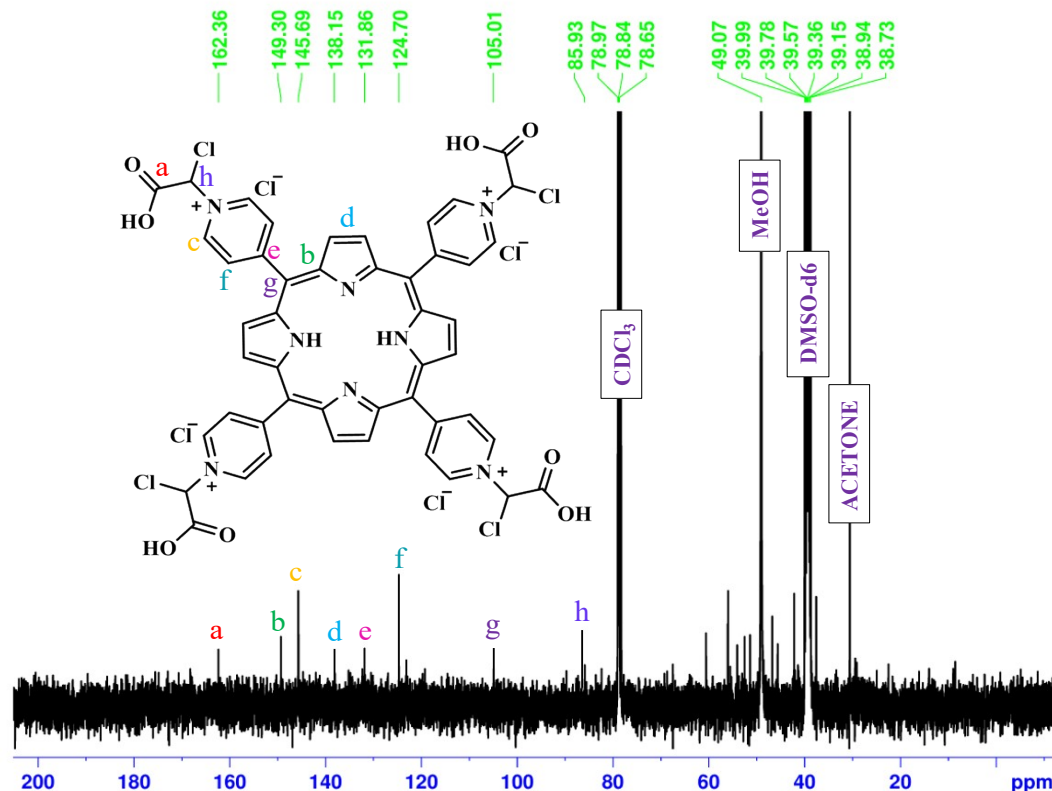


Fig S95. ¹³C NMR spectrum of PcCFP Photocatalyst

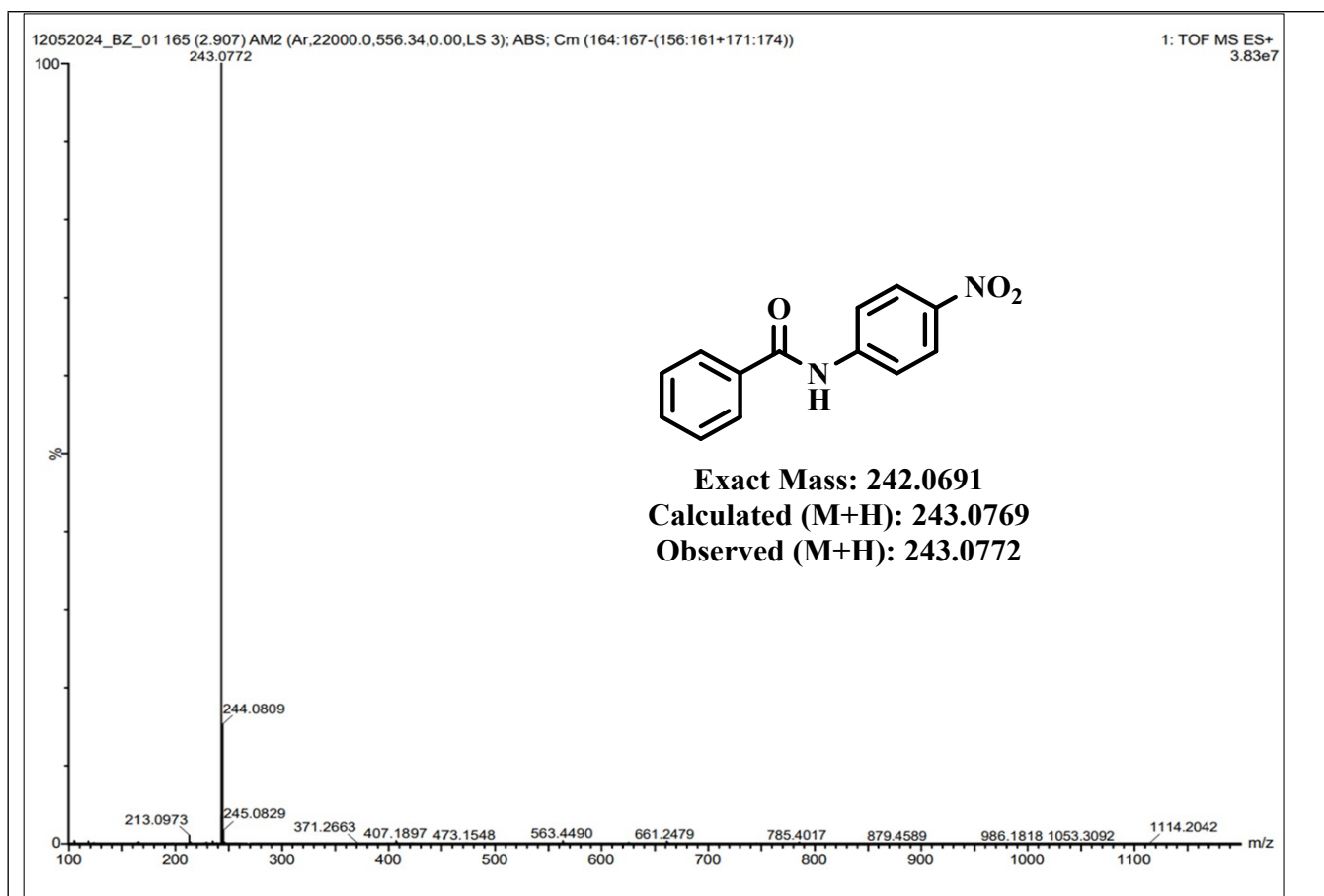


Fig S96. High Resolution Mass spectrum (m/z) of *N*-(4-nitrophenyl)benzamide (b1j)

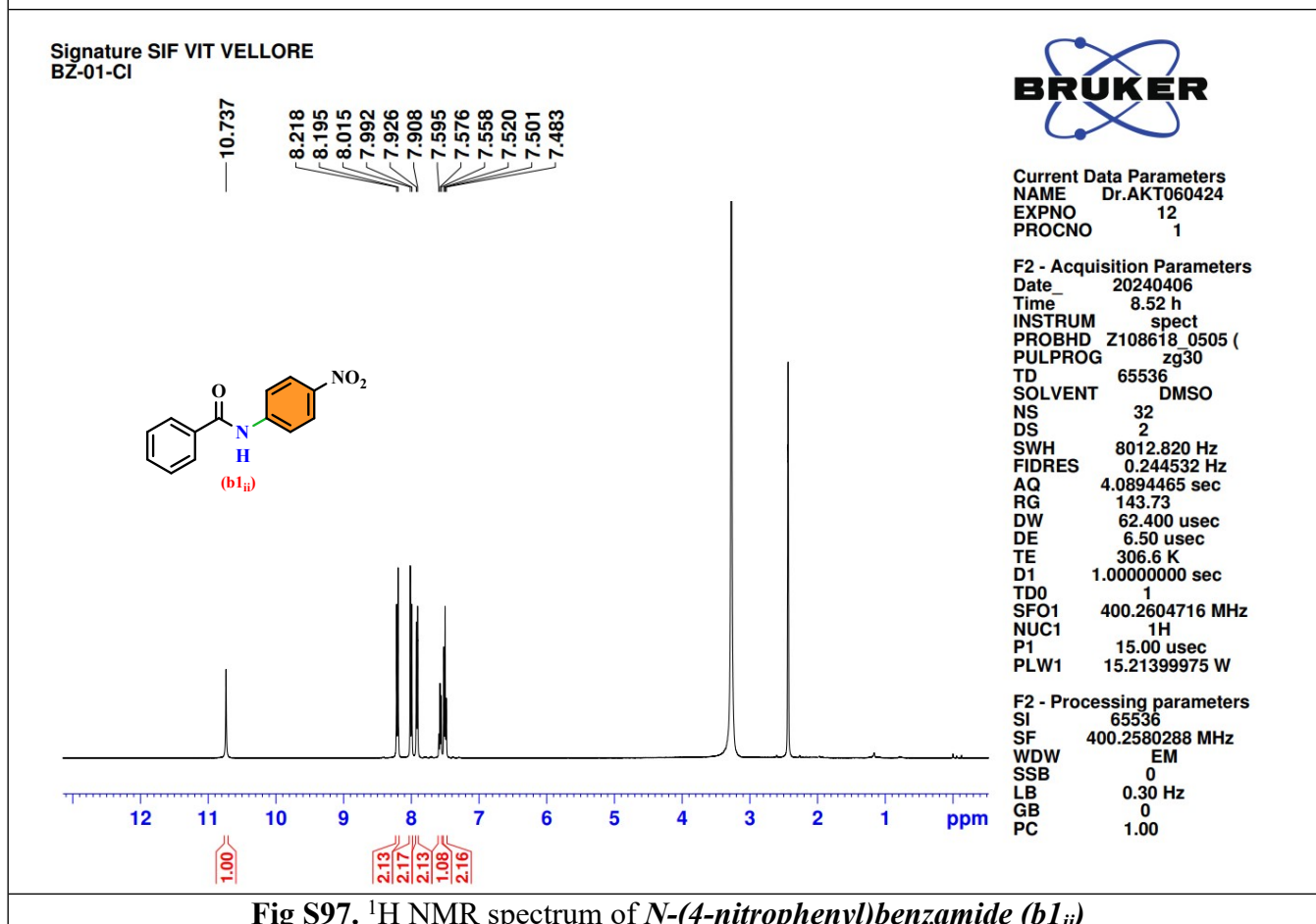
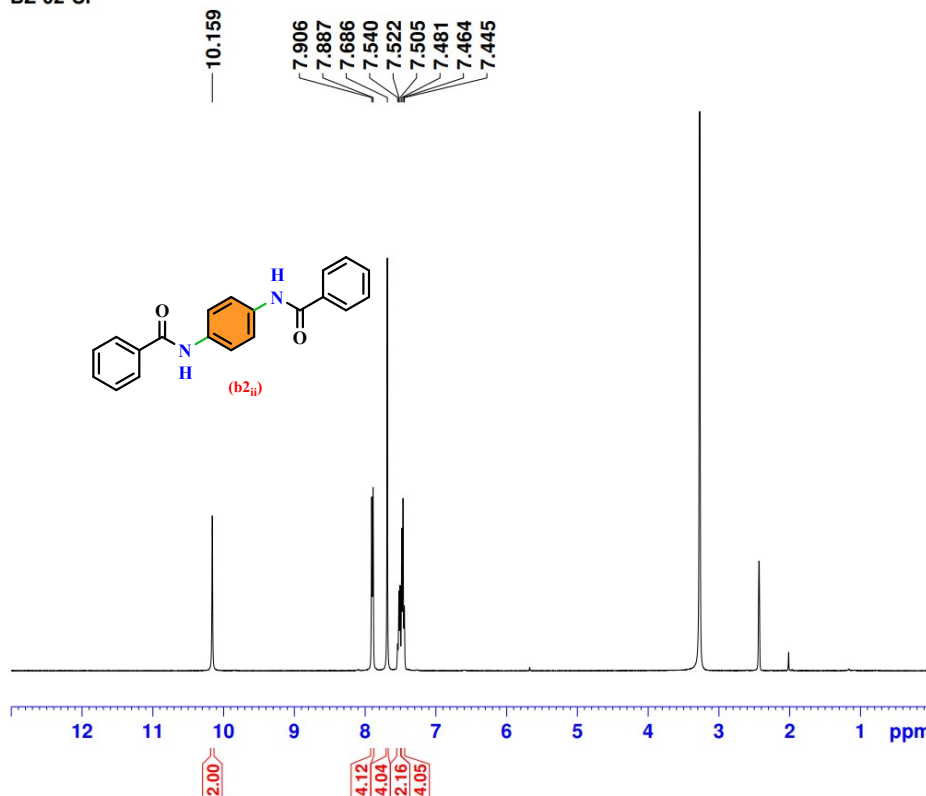


Fig S97. ¹H NMR spectrum of *N*-(4-nitrophenyl)benzamide (b1j)

Signature SIF VIT VELLORE
BZ-02-Cl



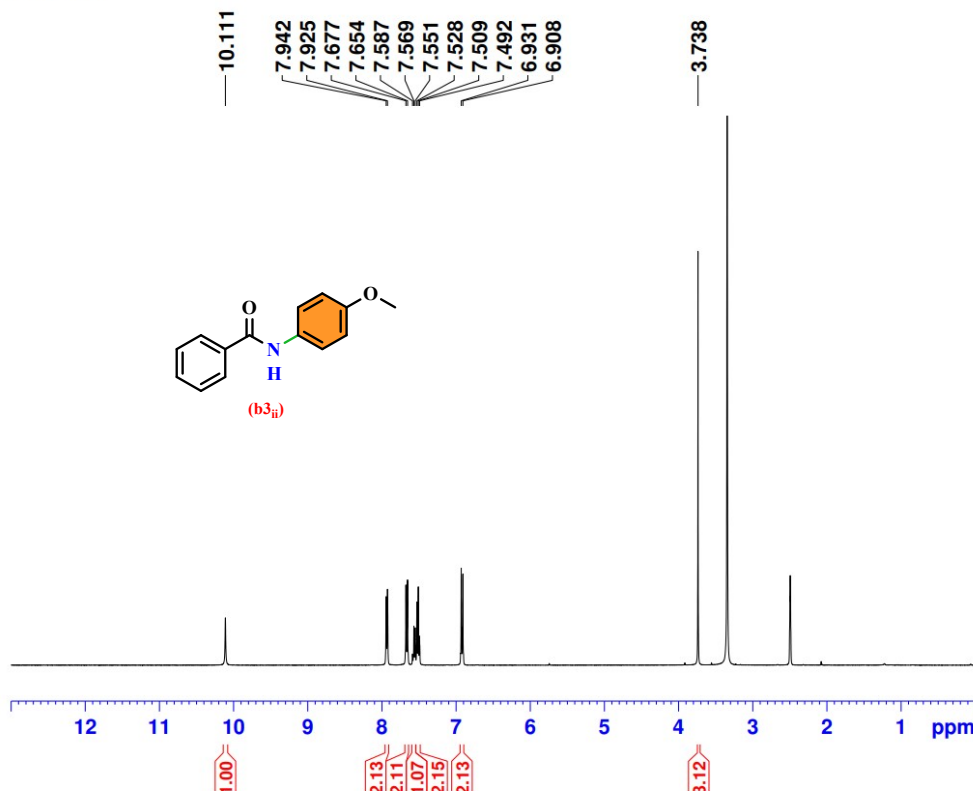
Current Data Parameters
NAME Dr.PDK090424
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
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Time 2.53 h
INSTRUM spect
PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 308.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580303 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S98. ¹H NMR spectrum of *N,N'*-(1,4-phenylene)dibenzamide (b_{2ii})

Signature SIF VIT VELLORE
BZ-03-Cl



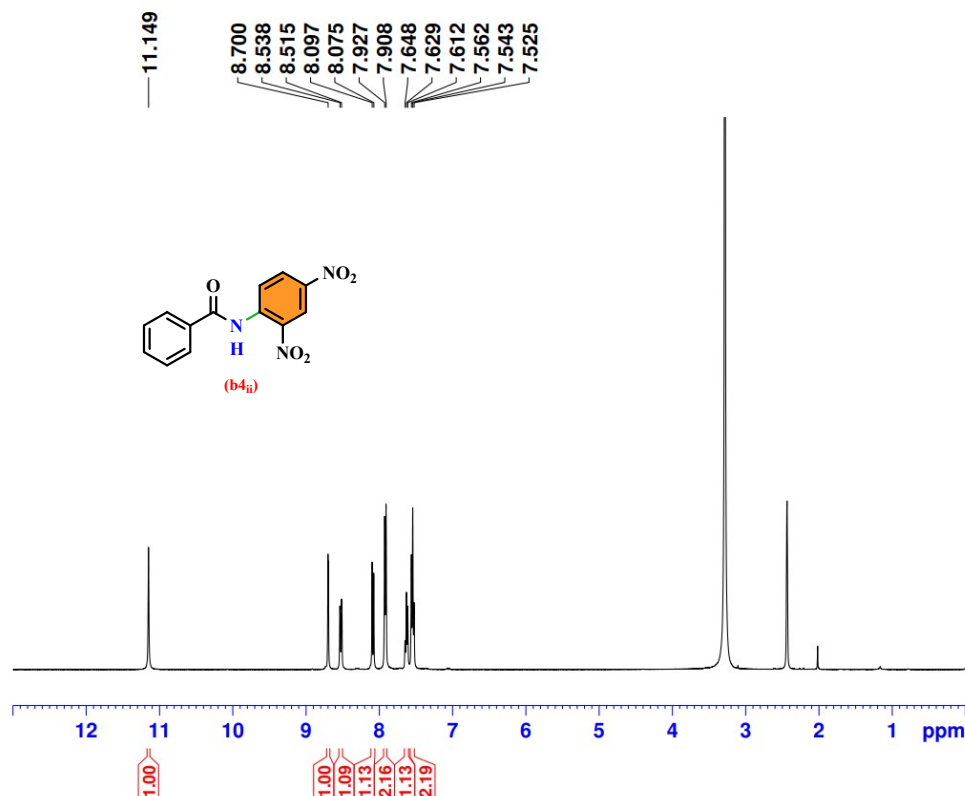
Current Data Parameters
NAME Dr.AKT040424
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240404
Time 15.41 h
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 304.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580057 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

Fig S99. ¹H NMR spectrum of *N*-(4-methoxyphenyl)benzamide (b_{3ii})

Signature SIF VIT VELLORE
BZ-04-Cl



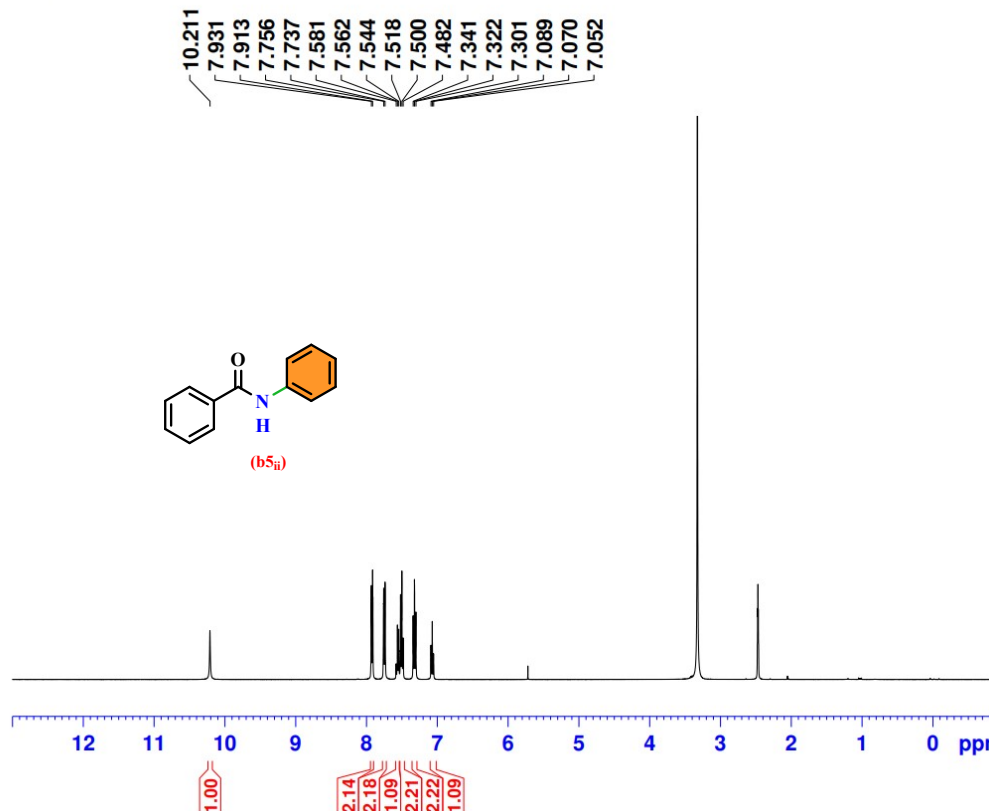
Current Data Parameters
NAME Dr.PDK200424
EXPNO 52
PROCNO 1

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PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 307.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580291 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S100. ¹H NMR spectrum of *N*-(2,4-dinitrophenyl)benzamide (b4_{ii})

Signature SIF VIT VELLORE
BZ-05-Cl



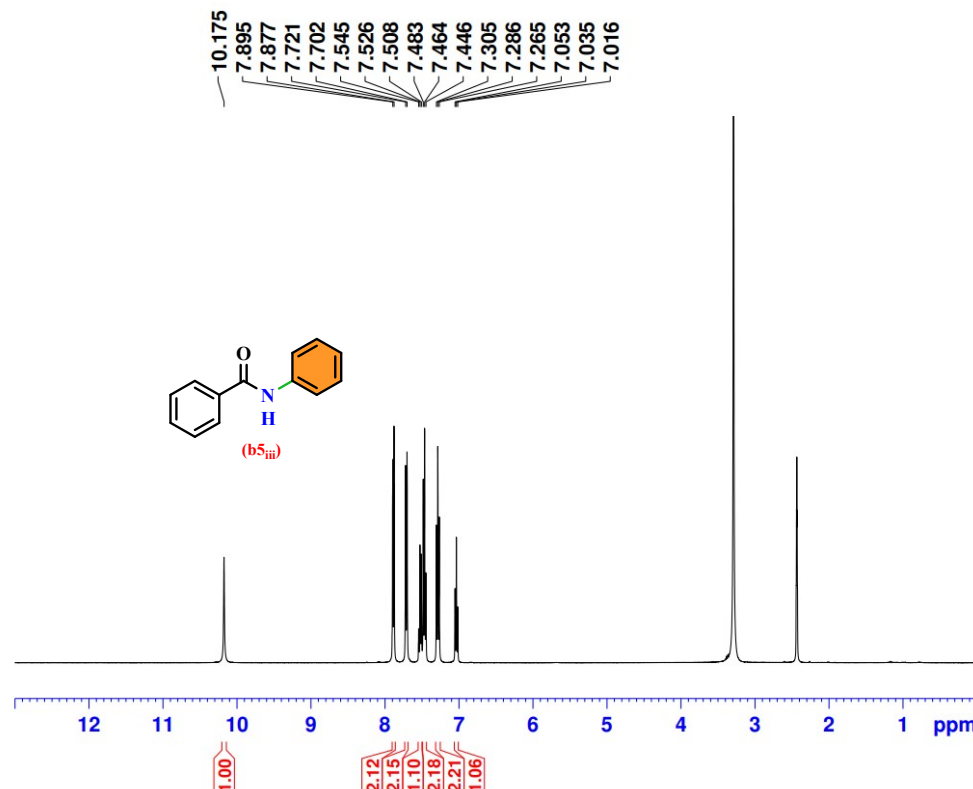
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EXPNO 21
PROCNO 1

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PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580297 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

Fig S101. ¹H NMR spectrum of *N*-phenylbenzamide (b5_{ii})

Signature SIF VIT VELLORE
BZ-05-I



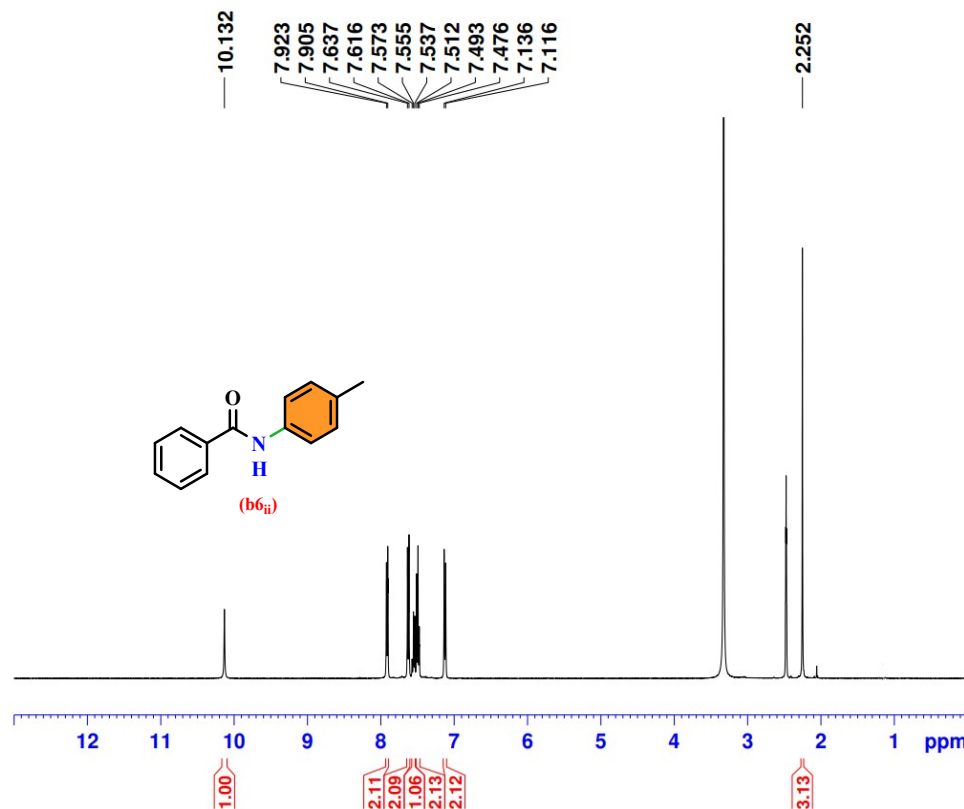
Current Data Parameters
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EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 307.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580291 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S102. ¹H NMR spectrum of *N*-phenylbenzamide (b5iii)

Signature SIF VIT VELLORE
BZ-06-CI



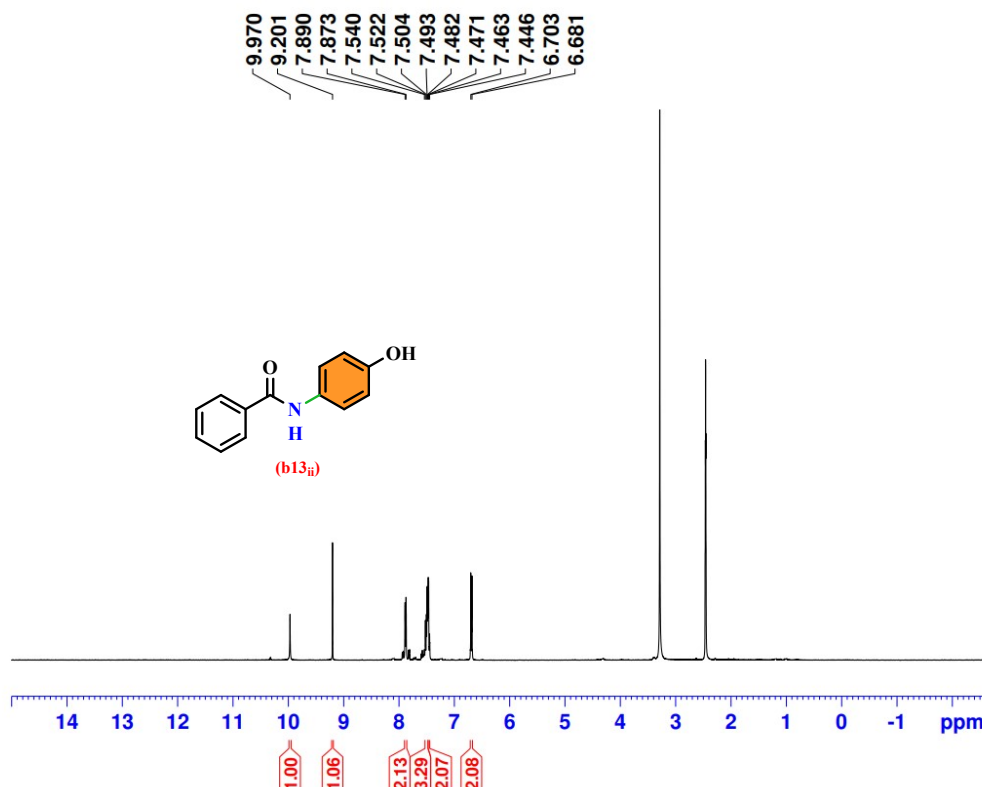
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NAME Dr.AKT080424
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240408
Time 16.00 h
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PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S103. ¹H NMR spectrum of *N*-(*p*-tolyl)benzamide (b6)

Signature SIF VIT VELLORE
BZ-13-Cl



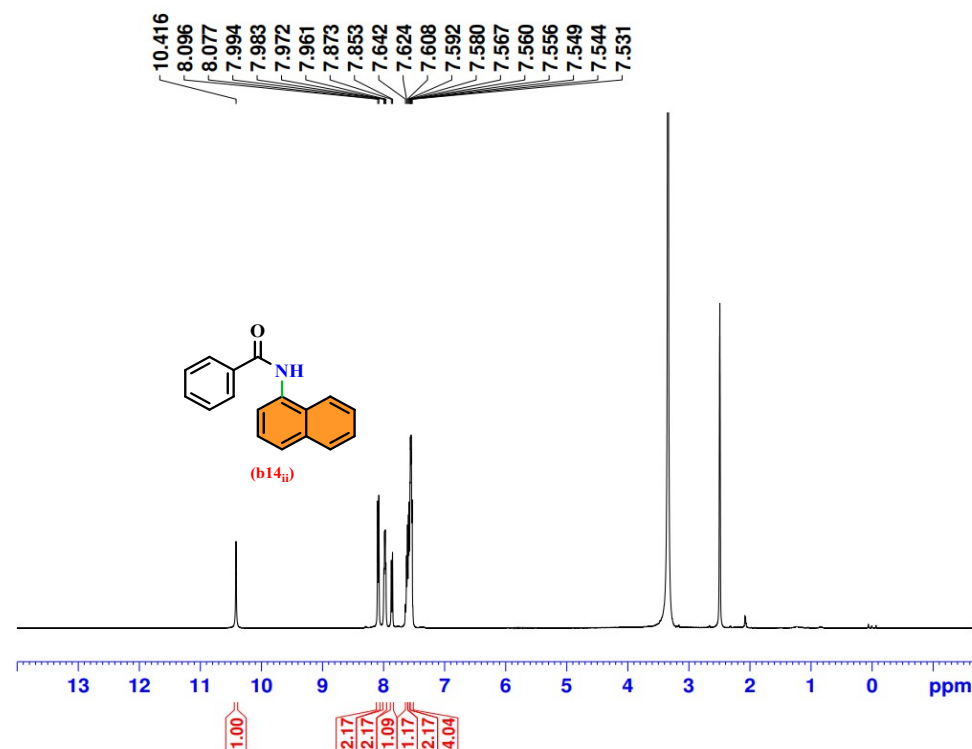
Current Data Parameters
NAME Dr.AKT090524
EXPNO 7
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 303.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580198 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S104. ¹H NMR spectrum of *N*-(4-hydroxyphenyl)benzamide (b13_{ii})

Signature SIF VIT VELLORE
BZ-14-Cl



Current Data Parameters
NAME Dr.ASK220424
EXPNO 63
PROCNO 1

F2 - Acquisition Parameters
Date 20240422
Time 15.28 h
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 305.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig S105. ¹H NMR spectrum of *N*-(naphthalen-1-yl)benzamide (b14_{ii})

Signature SIF VIT VELLORE
BZ-24-Cl



Current Data Parameters
NAME Dr.PDK250724
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
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Time 19.26 h
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
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SF 400.2580282 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

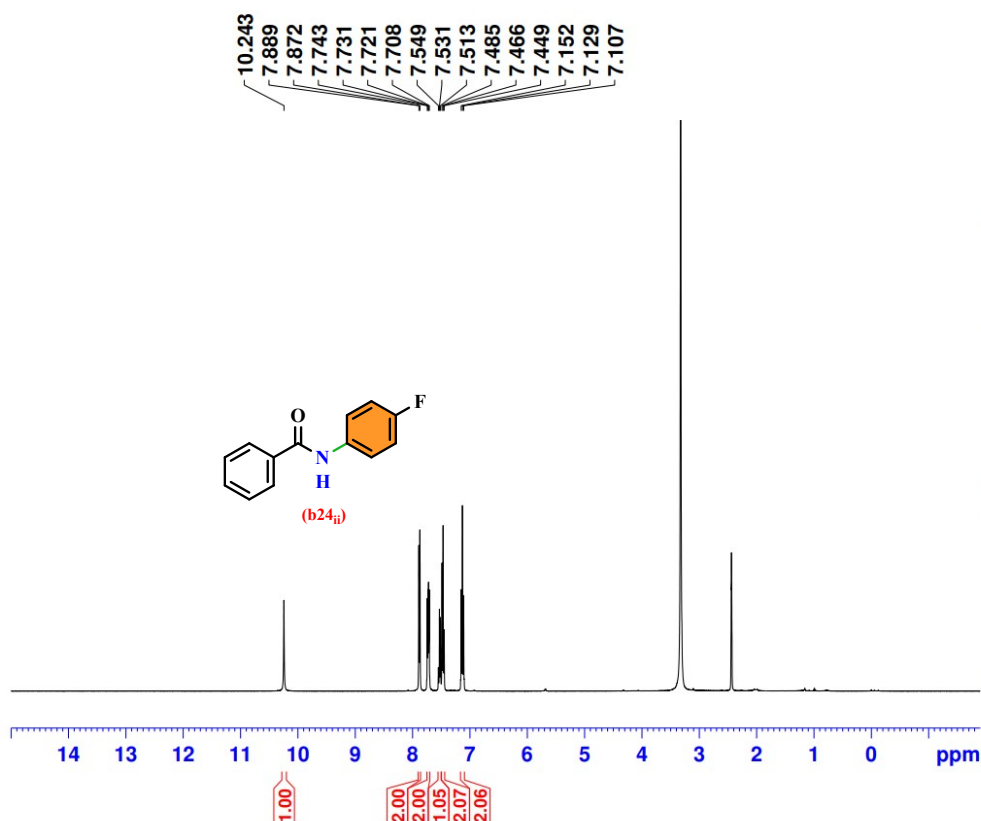
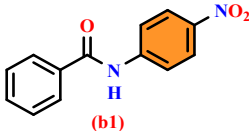
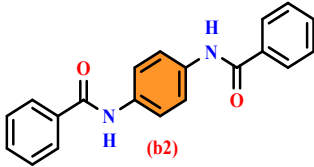
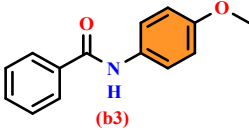
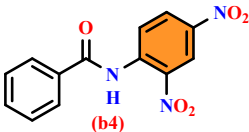
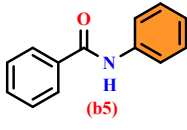
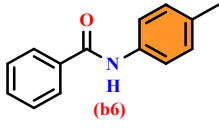
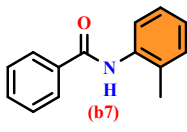
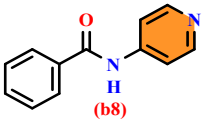
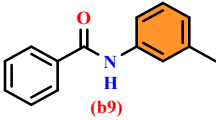
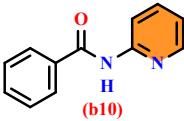
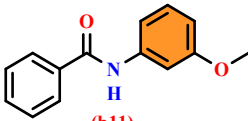
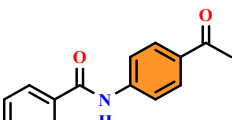
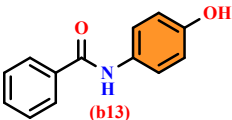
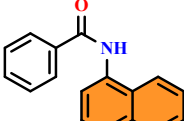
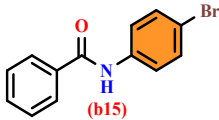
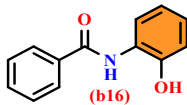
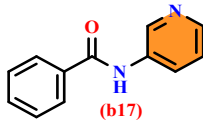
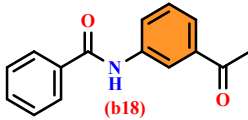
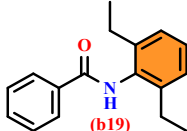
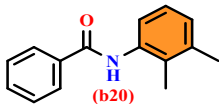
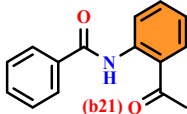


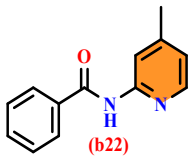
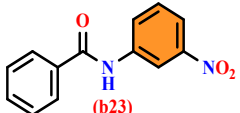
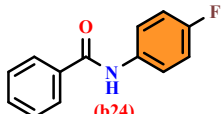
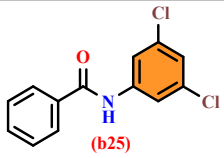
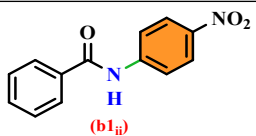
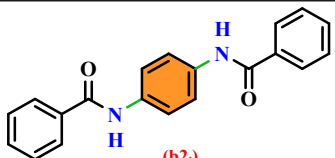
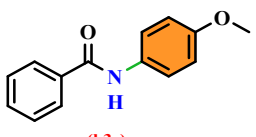
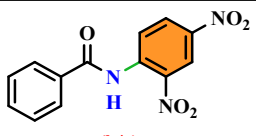
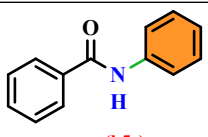
Fig S106. ¹H NMR spectrum of *N*-(4-fluorophenyl)benzamide (b24_{ii})

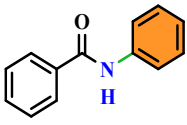
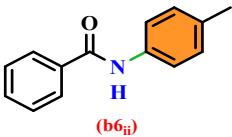
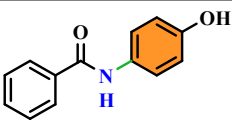
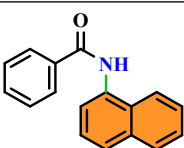
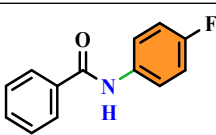
Table S2. Spectral data of Products

Sr. No	CODE	Characterization Data	Derivative Structure
1.	b1 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.80 (s, 1H), 8.28 (d, J = 8.80 Hz, 2H), 8.08 (d, J = 8.40 Hz, 2H), 7.99 (d, J = 8.00 Hz, 2H), 7.65 (t, J = 6.80 Hz, 1H), 7.58 (t, J = 7.60 Hz, 2H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.78, 145.97, 142.94, 134.71, 132.66, 129, 128.39, 125.28, 120.32. GCMS exact m/z ⁺ 242.0691 & observed m/z ⁺ 242.1669. HRMS calculated (M+H) 243.0691 & observed (M+H) 243.0772.	
2.	b2 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.16 (s, 2H), 7.90 (d, J = 7.60 Hz, 4H), 7.69 (s, 4H), 7.52 (t, J = 6.80 Hz, 2H), 7.46 (t, J = 7.60 Hz, 4H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.79, 135.46, 135.44, 131.94, 128.84, 128.06, 121.14. GCMS exact m/z 316.1212 & observed m/z is 316.1663.	
3.	b3 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.04 (s, 1H), 7.87 (d, J = 6.80 Hz, 2H), 7.60 (d, J = 8.80 Hz, 2H), 7.51 (t, J = 7.20 Hz, 1H), 7.45 (t, J = 6.80 Hz, 2H), 6.86 (d, J = 9.20 Hz, 2H), 3.68 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.58, 156.03, 135.52, 132.69, 131.83, 128.81, 127.99, 122.46, 114.21, 55.66. GCMS exact m/z 227.0946 & observed m/z is 227.2144.	
4.	b4 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 11.16 (s, 1H), 8.69 (s, 1H), 8.53 (d, J = 9.20 Hz, 1H), 8.07 (d, J = 8.80 Hz, 1H), 7.92 (d, J = 7.20 Hz, 2H), 7.63 (t, J = 7.20 Hz, 1H), 7.54 (t, J = 7.20 Hz, 1H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.05, 143.29, 141.34, 137.87, 133.41, 133.36, 129.34, 129.13, 128.40, 126.03, 121.67. GCMS exact m/z 287.0542 & observed m/z is 287.1621.	
5.	b5 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.17 (s, 1H), 7.89 (d, J = 6.80 Hz, 2H), 7.71 (d, J = 7.60 Hz, 2H), 7.53 (t, J = 7.20 Hz, 1H), 7.46 (t, J = 6.80 Hz, 2H), 7.29 (t, J = 8.40 Hz, 2H), 7.03 (t, J = 7.20 Hz, 1H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.03, 139.63, 135.46, 132.00, 129.06, 128.85, 128.11, 124.13, 120.84. GCMS exact m/z 197.0841 & observed m/z is 197.4289.	
6.	b6 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.09 (s, 1H), 7.87 (d, J = 7.20 Hz, 2H), 7.59 (d, J = 8.40 Hz, 2H), 7.51 (t, J = 7.20 Hz, 1H), 7.45 (t, J = 7.20 Hz, 2H), 7.09 (d, J = 8.40 Hz, 2H), 2.21 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.80, 137.10, 135.52, 133.07, 131.90, 129.44, 128.81, 128.05, 120.87, 20.96. GCMS exact m/z 211.0997 & observed m/z is 211.2645.	
7.	b7	¹ H NMR 400 MHz, DMSO-d ₆ : δ 9.90 (s, 1H), 8.01 (d, J = 6.80 Hz, 2H), 7.59 (t, J = 7.20 Hz, 1H), 7.52 (t, J = 6.80 Hz, 2H), 7.37 (d, J = 7.60 Hz, 1H), 7.27 (d, J = 7.60 Hz, 1H), 7.22 (t, J = 7.20 Hz, 1H), 7.17 (t, J = 6.80 Hz, 1H), 2.25 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.80, 136.92, 135.04, 134.23, 131.98, 130.79, 128.88, 128.12, 127.11, 126.47, 18.40. GCMS exact m/z 211.0997 &	

		observed m/z is 211.1141.	
8.	b8	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.11 (s, 1H), 7.93 (d, J = 6.80 Hz, 2H), 7.66 (d, J = 9.20 Hz, 2H), 7.57 (t, J = 7.20 Hz, 1H), 7.51 (t, J = 6.80 Hz, 2H), 6.92 (d, J = 8.80 Hz, 2H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.58, 135.51, 132.68, 131.84, 12881, 127.99, 122.46, 114.20. GCMS exact m/z 198.0793 & observed m/z is 198.1938.	 (b8)
9.	b9	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.09 (s, 1H), 7.88 (d, J = 7.20 Hz, 2H), 7.55 (d, J = 7.60 Hz, 2H), 7.51 (t, J = 5.20 Hz, 1H), 7.46 (t, J = 6.80 Hz, 2H), 7.16 (t, J = 7.60 Hz, 1H), 6.86 (d, J = 7.20 Hz, 1H), 2.24 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.95, 139.54, 138.21, 135.48, 131.97, 128.90, 128.84, 128.08, 124.83, 121.38, 118.03, 21.69. GCMS exact m/z 211.0977 & observed m/z is 211.2772.	 (b9)
10.	b10	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.74 (s, 1H), 8.18 (d, J = 8.40 Hz, 1H), 8.02 (d, J = 7.20 Hz, 1H), 7.75 (d, J = 7.20 Hz, 2H), 7.57 (t, J = 6.40 Hz, 1H), 7.51 (t, J = 7.20 Hz, 2H), 7.43 (t, J = 7.60 Hz, 2H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.50, 148.39, 145.20, 138.59, 134.85, 133.10, 129.45, 128.43, 122.87, 120.30. GCMS exact m/z 198.0793 & observed m/z is 198.1018.	 (b10)
11.	b11	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.21 (s, 1H), 7.94 (d, J = 6.80 Hz, 2H), 7.59 (t, J = 6.40 Hz, 1H), 7.53 (t, J = 6.80 Hz, 2H), 7.47 (s, 1H), 7.37 (d, J = 8.00 Hz, 1H), 7.25 (t, J = 8.40 Hz, 1H), 6.68 (d, J = 8.40 Hz, 1H), 3.75 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.05, 159.89, 140.83, 135.43, 132.05, 129.85, 128.85, 128.10, 113.00, 109.62, 106.48, 55.48. GCMS exact m/z 227.0946 & observed m/z is 227.1035.	 (b11)
12.	b12	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.53 (s, 1H), 7.92-7.95 (m, 6H), 7.61 (t, J = 6.40 Hz, 1H), 7.54 (t, J = 8.00 Hz, 2H), 2.54 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 197.09, 166.48, 144.06, 135.05, 132.54, 129.74, 128.92, 128.26, 119.95, 26.92. GCMS exact m/z 239.0946 & observed m/z is 239.0987.	 (b12)
13.	b13 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.00 (s, 1H), 9.23 (s, 1H), 7.91 (d, J = 7.20 Hz, 2H), 7.54 (d, J = 7.20 Hz, 2H), 7.52 (t, J = 2.40 Hz, 1H), 7.51 (t, J = 2.80 Hz, 2H), 6.72 (d, J = 8.80 Hz, 2H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.32, 154.16, 135.63, 131.73, 131.15, 128.78, 127.95, 122.72, 115.42. GCMS exact m/z 213.0790 & observed m/z is 213.2923.	 (b13)
14.	b14 _i	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.40 (s, 1H), 8.09 (d, J = 7.60 Hz, 2H), 7.96-7.97 (m, 2H), 7.86 (d, J = 8.00 Hz, 1H), 7.53-7.64 (m, 7H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.67, 134.95, 134.33, 134.25, 132.11, 129.71, 128.92, 128.53, 128.25, 126.75, 126.52, 126.43, 126.01, 124.37, 123.78. GCMS exact m/z 247.0997 & observed m/z is 247.2688.	 (b14)
15.	b15	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.34 (s, 1H), 7.94	

		(d, J = 8.00 Hz, 2H), 7.76 (d, J = 8.80 Hz, 2H), 7.59 (t, J = 6.80 Hz, 1H), 7.51-7.54 (m, 4H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.14, 139.04, 135.17, 132.18, 131.89, 128.89, 128.13, 122.72, 115.81. GCMS exact m/z 274.9946 & observed m/z is 275.0620.	
16.	b16	¹ H NMR 400 MHz, DMSO-d ₆ : δ 9.74 (s, 1H), 9.50 (s, 1H), 7.97 (d, J = 7.60 Hz, 2H), 7.69 (d, J = 7.60 Hz, 1H), 7.61 (t, J = 6.80 Hz, 1H), 7.54 (t, J = 7.20 Hz, 2H), 7.05 (t, J = 7.60 Hz, 1H), 6.93 (d, J = 8.00 Hz, 1H), 6.85 (t, J = 7.60 Hz, 1H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.93, 149.76, 134.81, 132.15, 128.99, 127.94, 126.36, 126.16, 124.52, 119.54, 116.48. GCMS exact m/z 213.0790 & observed m/z is 213.1008.	
17.	b17	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.44 (s, 1H), 8.93 (s, 1H), 8.31 (d, J = 4.40 Hz, 1H), 8.19 (d, J = 8.40 Hz, 1H), 7.97 (d, J = 8.00 Hz, 2H), 7.61 (t, J = 6.80 Hz, 1H), 7.54 (t, J = 8.00 Hz, 2H), 7.40 (t, J = 6.40 Hz, 1H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.45, 144.91, 142.34, 136.33, 134.79, 132.37, 128.95, 128.19, 127.98, 124.06. GCMS exact m/z 198.0793 & observed m/z is 198.1033.	
18.	b18	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.44 (s, 1H), 8.37 (s, 1H), 8.07 (d, J = 8.00 Hz, 1H), 7.98 (d, J = 7.60 Hz, 2H), 7.71 (d, J = 7.60 Hz, 1H), 7.61 (t, J = 6.80 Hz, 1H), 7.54 (t, J = 8.40 Hz, 2H), 7.50 (d, J = 8.00 Hz, 1H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 197.88, 165.93, 139.73, 137.47, 134.79, 131.94, 129.22, 128.62, 127.85, 125.00, 123.82, 119.89, 26.91. GCMS exact m/z 239.0946 & observed m/z is 239.0987.	
19.	b19	¹ H NMR 400 MHz, DMSO-d ₆ : δ 9.75 (s, 1H), 8.00 (s, 1H), 7.60 (t, J = 6.80 Hz, 1H), 7.54 (t, J = 6.80 Hz, 2H), 7.24 (t, J = 8.40 Hz, 1H), 7.16 (d, J = 7.60 Hz, 2H), 2.55 (q, J = 8.00 Hz, 4H), 1.12 (t, J = 7.60 Hz, 6H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 166.26, 142.20, 134.91, 134.67, 131.93, 128.96, 127.91, 127.79, 126.52, 24.94, 14.98. GCMS exact m/z 253.1467 & observed m/z 253.2440.	
20.	b20	¹ H NMR 400 MHz, DMSO-d ₆ : δ 9.92 (s, 1H), 7.99 (d, J = 7.20 Hz, 2H), 7.60 (t, J = 7.20 Hz, 1H), 7.53 (t, J = 6.80 Hz, 2H), 7.08-7.14 (m, 3H), 2.29 (s, 3H), 2.11 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 165.87, 140.60, 137.44, 136.74, 135.05, 131.92, 128.86, 128.06, 125.71, 125.20, 20.61, 14.69. GCMS exact m/z 225.1154 & observed m/z 225.1183.	
21.	b21	¹ H NMR 400 MHz, DMSO-d ₆ : δ 12.39 (s, 1H), 8.67 (d, J = 8.00 Hz, 1H), 8.13 (d, J = 8.00 Hz, 1H), 7.98 (d, J = 6.80 Hz, 2H), 7.70 (t, J = 7.20 Hz, 1H), 7.66 (t, J = 4.80 Hz, 1H), 7.62 (t, J = 6.80 Hz, 2H), 7.28 (t, J = 7.20 Hz, 1H), 2.71 (s, 3H). ¹³ C NMR 100 MHz, DMSO-d ₆ : δ 204.08, 165.54, 140.19, 135.28, 135.19, 134.85, 132.74, 129.51, 127.57, 123.90, 123.64, 120.74, 29.25. GCMS exact m/z 239.0946 & observed m/z 239.2092.	
22.	b22	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.69 (s, 1H), 8.24	

		(d, J = 4.80 Hz, 1H), 8.06 (s, 1H), 8.03 (d, J = 7.20 Hz, 2H), 7.60 (t, J = 7.20 Hz, 1H), 7.51 (t, J = 7.20 Hz, 2H), 7.02 (d, J = 4.40 Hz, 1H), 2.36 (s, 3H). ¹³C NMR 100 MHz, DMSO-d₆: δ 166.35, 152.69, 149.25, 148.02, 134.60, 132.35, 128.82, 128.40, 121.31, 115.60, 21.41. GCMS exact m/z 212.0950 & observed m/z 212.1805.	 (b22)
23.	b23	¹H NMR 400 MHz, DMSO-d₆: δ 10.70 (s, 1H), 8.80 (s, 1H), 8.18 (d, J = 8.00 Hz, 1H), 7.98 (d, J = 7.20 Hz, 2H), 7.95 (d, J = 1.60 Hz, 1H), 7.66 (t, J = 3.20 Hz, 1H), 7.62 (t, J = 7.20 Hz, 1H), 7.56 (t, J = 7.20 Hz, 2H). ¹³C NMR 100 MHz, DMSO-d₆: δ 166.55, 148.38, 140.83, 134.68, 132.54, 130.56, 129.01, 128.24, 126.66, 118.63, 114.81. GCMS exact m/z 242.0691 & observed m/z 242.1273.	 (b23)
24.	b24 _i	¹H NMR 400 MHz, DMSO-d₆: δ 10.32 (s, 1H), 7.96 (d, J = 7.20 Hz, 2H), 7.79-7.80 (m, 2H), 7.60 (t, J = 7.20 Hz, 1H), 7.54 (t, J = 6.80 Hz, 2H), 7.20 (t, J = 8.80 Hz, 2H). ¹³C NMR 100 MHz, DMSO-d₆: δ 165.95, 159.95, 157.56, 136.00, 135.97, 135.26, 132.07, 128.87, 128.09, 122.69, 122.62, 115.76, 115.54. ¹⁹F NMR 377 MHz, DMSO-d₆: δ – (118.93-118.86, m, 1F). GCMS exact m/z 215.0746 & observed m/z 215.2380.	 (b24)
25.	b25	¹H NMR 400 MHz, DMSO-d₆: δ 7.92 (d, J = 7.60 Hz, 2H), 7.87 (s, 2H), 7.61 (t, J = 7.20 Hz, 1H), 7.54 (t, J = 6.80 Hz, 2H), 7.28 (s, 1H). ¹³C NMR 100 MHz, DMSO-d₆: δ 166.63, 141.89, 134.46, 132.61, 129.02, 128.17, 123.32, 118.75. GCMS exact m/z 265.0061 & observed m/z 265.0722.	 (b25)
26.	b1 _{ii}	¹H NMR 400 MHz, DMSO-d₆: δ 10.74 (s, 1H), 8.20 (d, J = 8.80 Hz, 2H), 8.00 (d, J = 8.40 Hz, 2H), 7.91 (d, J = 8.00 Hz, 2H), 7.57 (t, J = 6.80 Hz, 1H), 7.5 (t, J = 7.60 Hz, 2H).	 (b1ii)
27.	b2 _{ii}	¹H NMR 400 MHz, DMSO-d₆: δ 10.16 (s, 2H), 7.90 (d, J = 7.60 Hz, 4H), 7.69 (s, 4H), 7.52 (t, J = 6.80 Hz, 2H), 7.46 (t, J = 7.60 Hz, 4H).	 (b2i)
28.	b3 _{ii}	¹H NMR 400 MHz, DMSO-d₆: δ 10.11 (s, 1H), 7.93 (d, J = 6.80 Hz, 2H), 7.66 (d, J = 8.80 Hz, 2H), 7.57 (t, J = 7.20 Hz, 1H), 7.5 (t, J = 6.80 Hz, 2H), 6.92 (d, J = 9.20 Hz, 2H), 3.73 (s, 3H).	 (b3ii)
29.	b4 _{ii}	¹H NMR 400 MHz, DMSO-d₆: δ 11.15 (s, 1H), 8.7 (s, 1H), 8.52 (d, J = 9.20 Hz, 1H), 8.08 (d, J = 8.80 Hz, 1H), 7.92 (d, J = 7.20 Hz, 2H), 7.63 (t, J = 7.20 Hz, 1H), 7.53 (t, J = 7.20 Hz, 1H).	 (b4ii)
30.	b5 _{ii}	¹H NMR 400 MHz, DMSO-d₆: δ 10.21 (s, 1H), 7.92 (d, J = 6.80 Hz, 2H), 7.74 (d, J = 7.60 Hz, 2H), 7.56 (t, J = 7.20 Hz, 1H), 7.49 (t, J = 6.80 Hz, 2H), 7.32 (t, J = 8.40 Hz, 2H), 7.06 (t, J = 7.20 Hz, 1H).	 (b5ii)

31.	b5 _{iii}	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.18 (s, 1H), 7.89 (d, J = 6.80 Hz, 2H), 7.71 (d, J = 7.60 Hz, 2H), 7.52 (t, J = 7.20 Hz, 1H), 7.46 (t, J = 6.80 Hz, 2H), 7.29 (t, J = 8.40 Hz, 2H), 7.02 (t, J = 7.20 Hz, 1H).	 (b5 _{iii})
32.	b6 _{ii}	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.13 (s, 1H), 7.91 (d, J = 7.20 Hz, 2H), 7.62 (d, J = 8.40 Hz, 2H), 7.55 (t, J = 7.20 Hz, 1H), 7.49 (t, J = 7.20 Hz, 2H), 7.12 (d, J = 8.40 Hz, 2H), 2.25(s, 3H).	 (b6 _{ii})
33.	b13 _{ii}	¹ H NMR 400 MHz, DMSO-d ₆ : δ 9.97 (s, 1H), 9.2 (s, 1H), 7.88 (d, J = 7.20 Hz, 2H), 7.52 (d, J = 7.20 Hz, 2H), 7.49 (t, J = 2.40 Hz, 1H), 7.46 (t, J = 2.80 Hz, 2H), 6.69 (d, J = 8.80 Hz, 2H).	 (b13 _{ii})
34.	b14 _{ii}	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.42 (s, 1H), 8.09 (d, J = 7.60 Hz, 2H), 7.96-7.99 (m, 2H), 7.86 (d, J = 8.00 Hz, 1H), 7.53-7.64 (m, 7H).	 (b14 _{ii})
35.	b24 _{ii}	¹ H NMR 400 MHz, DMSO-d ₆ : δ 10.24 (s, 1H), 7.88 (d, J = 7.20 Hz, 2H), 7.71-7.74 (m, 2H), 7.53 (t, J = 7.20 Hz, 1H), 7.47 (t, J = 6.80 Hz, 2H), 7.13 (t, J = 8.80 Hz, 2H).	 (b24 _{ii})

ICP-MS of PcCFP Photocatalyst

A quantity of 1 mg of PC was dissolved in 4 mL of aqua regia within a borosilicate glass beaker until complete dissolution was achieved. The resulting transparent solution was subsequently transferred to a 100 mL volumetric flask, where double distilled water was added to bring the total volume to 100 mL. This final volume corresponds to a 10ppm solution of the photocatalyst. From this 100 mL solution, 0.5 mL was extracted using a pipette and added to a 10 mL volumetric flask, which was then filled with double distilled water to achieve a total volume of 10 mL. This preparation results in a concentration of 0.5 ppm, equivalent to 500 ppb, necessary for the sample preparation.

The ICP-MS analysis was carried out by using 500ppb of solution and the metals are detected in Below Detection Limit (BDL)

Table S3. Metal detection in Photocatalyst by ICP-MS

Sample ID	Cu 63 (ppb)	Fe 57 (ppb)	Ni 60 (ppb)	Zn 66 (ppb)	Pd 106 (ppb)	Ir 193 (ppb)
Standard 1	2.000	2.000	2.000	2.000	2.000	2.000
Standard 2	9.960	9.270	9.992	9.555	9.999	9.924
Standard 3	49.949	47.653	49.998	49.613	50.056	52.032
Standard 4	100.069	95.294	100.367	99.412	109.008	110.906
Standard 5	215.366	192.887	200.236	199.040		
PcCFP	4.947	9.401	0.898	20.488	0.033	0.007