

Ixora coccinea flowers derived green luminescent carbon quantum dots for Fe³⁺ recognition and preparation of Pd nanoparticles for the Suzuki-Miyaura coupling and cyanation process

Namrata Priyadarshini Hota and Sathiyarayanan Kulathu Iyer*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632 014, India. *E-mail: sathiyarayanank@vit.ac.in

Table of Contents:

1. Quantum Yield Measurement -----	S1
2. HRTEM Images of NCQD -----	Figure S1
3. Different wavelength and PH of NCQD -----	Figure S2
4. Preparation of Blood sample -----	S2
5. Time response and Calibration plot of NCQD with Fe ³⁺ -----	Figure S3
6. Quenching mechanism of NCQD upon addition of Fe ³⁺ -----	Figure S4
7. Comparison Table of different sensors for Fe ³⁺ detection -----	Table S1
8. Plausible mechanism for Suzuki and Cyanation Reaction -----	Figure S5
9. Optimization Table for Suzuki-Miyaura Reactions -----	Table S2
10. Optimization Table for Aryl Cyanation Reactions -----	Table S3
11 Comparison table of PdNPs for Suzuki-Miyaura reaction -----	Table S4
12. Comparison table of PdNPs for Aryl Cyanation reaction -----	Table S5
13. Recyclability of PdNPs -----	S3
14. Recyclability of PdNPs 3 cycle -----	Figure S6
15. H ¹ NMR analysis of Suzuki-Miyaura Reaction -----	S4
16. H ¹ NMR analysis of Aryl Cyanation Reaction -----	S5
17. H ¹ NMR spectra (400 MHz) of the products -----	S6

S1 Quantum Yield Measurement:

Using quinine sulfate ($\phi = 0.54$ in $0.1\text{M H}_2\text{SO}_4$) as a standard reference, we determined the quantum yield of carbon dots. Using the following formula, the quantum yield was determined.

$$\Phi_{\text{CQD}} = \Phi_{\text{R}} \times \frac{I_{\text{CQD}}}{I_{\text{R}}} \times \frac{A_{\text{R}}}{A_{\text{CQD}}} \times \frac{n_{\text{R}}^2}{n_{\text{CQD}}^2}$$

The carbon dot and reference are denoted by CQD and R, respectively, in the equation above. " n " indicates the refractive index of the solvent medium (ethanol has a refractive index of 1.37), " I " stands for the integrated fluorescence intensity, and " A " for the absorbance value at the exciting wavelength. After calculating every value, the quantum Yield was found to be **43.5%**.

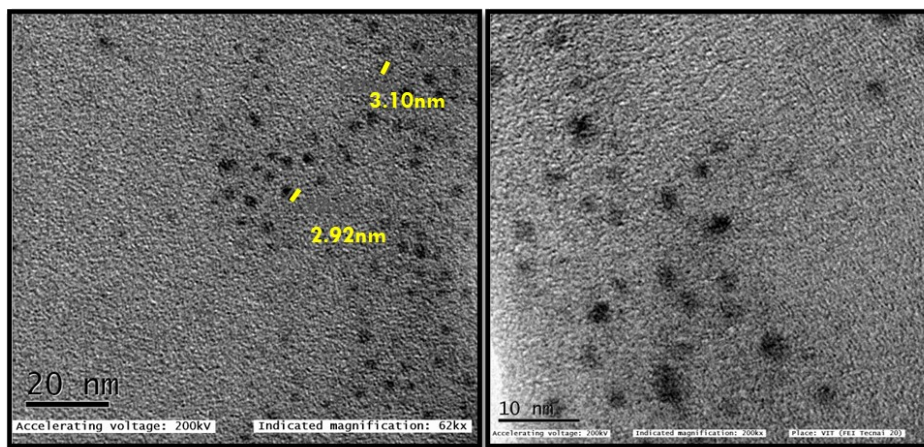


Figure S1. HRTEM Images of NCQD

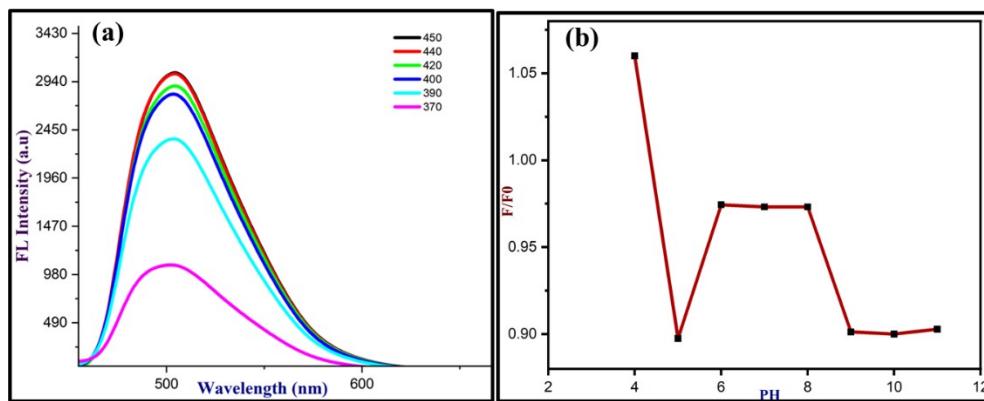


Figure S2. (a) NCQD at different excitation wavelengths, (b) PH study of NCQD

S2 Preparation of Blood sample for real-time application:

A healthy donor's blood was collected. To the blood sample, the same amount of 20% of ascorbic acid was added. The ascorbic acid's function in the blood sample changes Fe^{2+} to Fe^{3+} . Following a 15-minute heating period at 90 degrees Celsius, the solution was centrifuged at 4000 RPM after reaching

room temperature. To obtain the precise value, the supernatant was treated with buffer solution (pH=7) and then exposed to the real-time application to detect Fe³⁺.

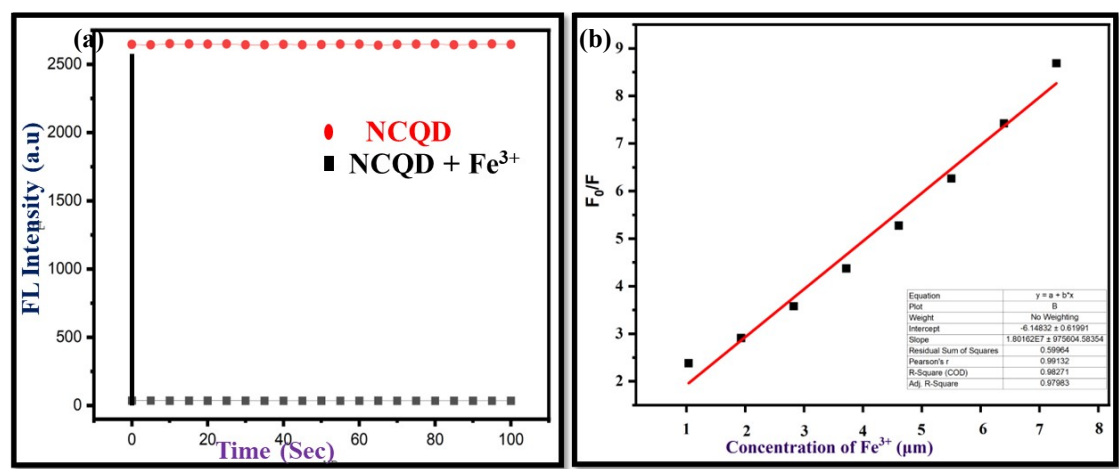


Figure S3. (a)Time response of NCQD with Fe³⁺ (b) Calibration plot of NCQD with different concentrations of Fe³⁺ (0-8 μm).

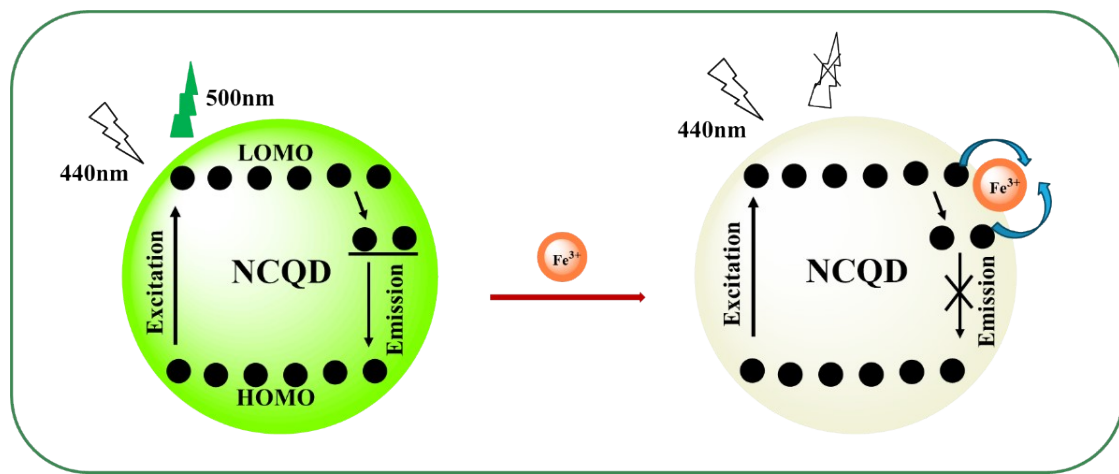


Figure S4. Schematic representation of the Quenching mechanism of NCQD upon the addition of Fe³⁺ ions

Table S1: Comparison Table of different sensors for Fe³⁺ detection:

Sensing Probe for Fe ³⁺	Linear range (μm)	Lod (μm)	Ref.
Mint leaf-derived Carbon quantum dots	0-50	0.37	[RSC advances, 2019, 9, 12070-12077]
CQD from Pear juice	0-0.38	1.27	[Scientific reports, 2019, 9, 15084]

Catharanthus roseus leaves CQD	1-6	0.8	[Sustainable materials and technologies, 2020, 23, e00138]
Nitrogen-doped Tea Leaves CQD	0.1-400	0.079	[Nanomaterials, 2022, 12, 986]
Nitrogen-doped Ixora coccinea flowers CQD	1-8	0.06	This work

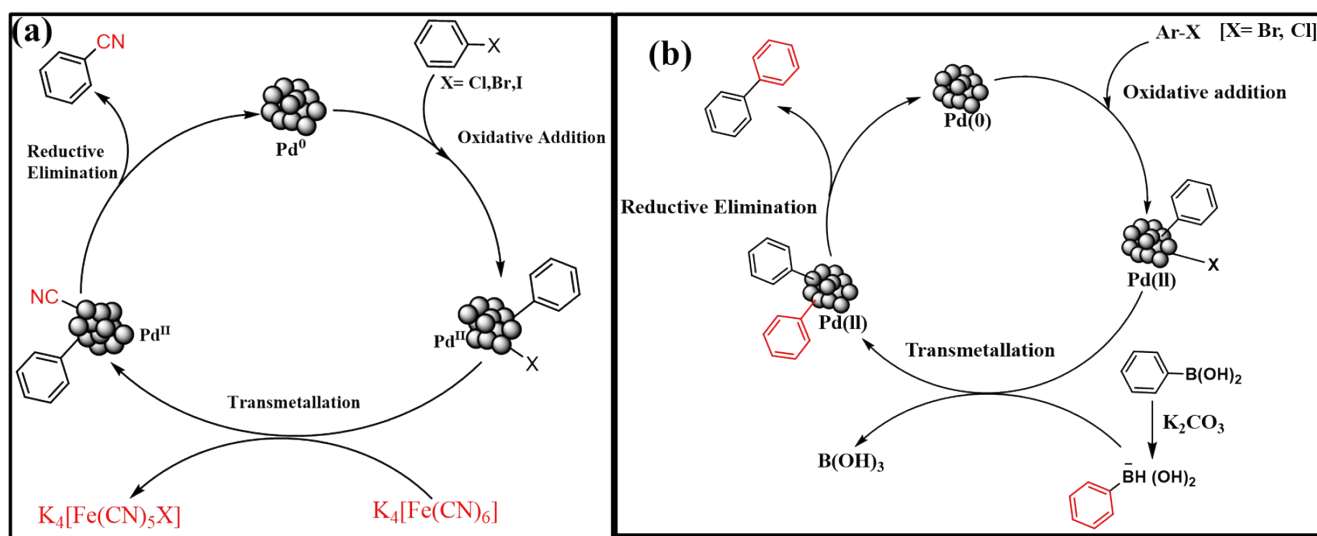


Figure S5. (a) Plausible mechanism of Aryl Cyanide Reactions and (b) Plausible mechanism of PdNPs catalyzed Suzuki-Miyaura coupling reactions

Table S2: Optimization table for Suzuki Miyaura coupling reactions:

Sl. No	Solvent	Base	Temp (°C)	Pd(mol%)	Time(h)	Yield (%)
1	H ₂ O	K ₂ CO ₃	50	0.3	2	30
2	DMF	K ₂ CO ₃	50	0.3	2	25
3	Acetone	K ₂ CO ₃	50	0.3	2	Trace
4	Acetonitrile	K ₂ CO ₃	50	0.3	2	Trace
5	Toluene	K ₂ CO ₃	50	0.3	2	20
6	1,4-Dioxane	K ₂ CO ₃	50	0.3	2	30
7	EtOH	K ₂ CO ₃	50	0.3	2	51
8	THF	K ₂ CO ₃	50	0.3	2	Trace
9	1,4-Dioxane: H ₂ O	K ₂ CO ₃	50	0.3	2	45
10	EtOH: H ₂ O: Toluene	K ₂ CO ₃	50	0.3	2	60
11	EtOH: H ₂ O	K ₂ CO ₃	50	-	2	NR
12	EtOH: H ₂ O	-	40	0.3	2	Trace
13	EtOH: H ₂ O	KOH	50	0.3	2	90
14	EtOH: H ₂ O	NaOH	50	0.3	2	89
15	EtOH: H ₂ O	Na ₂ CO ₃	40	0.3	2	90
16	EtOH: H ₂ O	K ₂ CO ₃	50	0.3	2	95
17	EtOH: H₂O	K₂CO₃	40	0.3	1.5	94
18	EtOH: H ₂ O	K ₂ CO ₃	40	0.5	1.5	94

Reaction conditions: Aryl halide (1 eq), boronic acid (1.15 eq), base (2 eq), PdNPs (0.3 mol% respect to the aryl halide), solvent (EtOH: H₂O (1:1) (5ml)) in a Nitrogen atmosphere. NR= No Reaction, **Yield (%)**- Isolated yield after separation by column chromatography

Table S3: Optimization table for aryl halide cyanation reactions:

Sl. No	Solvent	Base	Temp (°C)	Pd(mol%)	Time(h)	Yield (%)
1	H ₂ O	Na ₂ CO ₃	110	0.5	5	50
2	DMF: H ₂ O	Na ₂ CO ₃	110	0.5	5	55
3	Acetone	Na ₂ CO ₃	50	0.5	5	Trace
4	Acetonitrile	Na ₂ CO ₃	90	0.5	5	40
5	Toluene	Na ₂ CO ₃	110	0.5	5	20
6	EtOH: H ₂ O	Na ₂ CO ₃	110	0.5	5	25
7	EtOH	Na ₂ CO ₃	70	0.5	5	Trace
8	THF	Na ₂ CO ₃	110	0.5	5	20
9	DMF	K ₂ CO ₃	110	0.5	5	75
10	DMF	-	110	0.5	5	Trace
11	DMF	K ₂ CO ₃	110	-	5	NR
12	DMF	Na ₂ CO ₃	110	-	5	NR
13	DMF	NaOH	110	0.5	5	70
14	DMF	KOH	110	0.5	5	65
15	DMF	Na ₂ CO ₃	110	0.5	4	94
16	DMF	Na₂CO₃	110	0.5	3.5	93

Reaction conditions: Aryl halide (1 eq), K₄[Fe (CN)₆].3H₂O (0.18 eq.), Na₂CO₃ (1.5 eq.) PdNPs (0.3 mol% respect to the aryl halide), solvent (DMF (6ml)) in a Nitrogen atmosphere, **Yield (%)**- Isolated yield after separation by column chromatography.

Table S4 Comparison table of catalytic activity of PdNPs for Suzuki-Miyaura coupling reaction:

Sl. No	Catalyst	Solvent	Temperature (°C)	Time	Yield (%)	References
1	PdNPs@CAP	Solvent-free	MW, 400 W	6 min	92	[<i>International journal of biological macromolecules</i> , 2020, 148, 565-573.]
2	Pd@C-dots	H ₂ O	60	6h	93	[<i>Dalton Transactions</i> , 2013, 42, 13821-13825]
3	Cellulose@NHC-Pd	EtOH: H ₂ O	Room Temp.	30 min	95	[<i>Cellulose</i> , 2023, 30, 7551-7573]
4	PdNPs/TMC	H ₂ O	80	14h	99	[<i>RSC Advances</i> , 2015, 5, 27533-27539]

5	Pd NPs	EtOH: H ₂ O	Room Temp.	3h	93	[<i>Applied Organometallic Chemistry</i> , 2019, 33, e4758]
6	PdNPs	EtOH: H ₂ O	40	1.5 h	94	This Work

Table S5 Comparison table of catalytic activity of PdNPs for Aryl Cyanation reaction:

Sl. No	Catalyst	Solvent	Temperature (°C)	Time (h)	Yield (%)	References
	Pd					
1	NPs@Fe ₃ O ₄ /lignin/chitosan	DMF	MW, 400 W	6	92	[<i>International journal of biological macromolecules</i> , 2020, 155, 814-822]
2	Pd@CC ²	DMF	140	15	90	[<i>Journal of the American Chemical Society</i> , 2016, 138, 1709-1716]
3	Pd NPs	DMF	120	7	85	[<i>Catalysis Letters</i> , 2018, 148, 1562-1578.]
4	TZ-IL@Pd NPs	DMF	120	24	88	[<i>Journal of Organometallic Chemistry</i> , 2022, 970, 122359]
5	Pd@CuFe ₂ O ₄	DMF	120	7	97	[<i>Journal of Molecular Catalysis A: Chemical</i> , 2015, 397, 106-113]
6	PdNPs	DMF	110	3.5	93	This Work

S3 Recyclability of PdNPs:

The reaction mixture was transferred to a centrifuge tube once the reaction was finished and allowed to cool to room temperature. The PDNPS that had sunk to the bottom of the reaction mixture was then repeatedly cleaned with water, ethanol, and acetone after the reaction mixture had been centrifuged for 10 minutes at 4000 RPM. following which it was ground into a fine powder and let it to dry in an oven. Thereafter, the catalyst was utilized for the reactions once more.

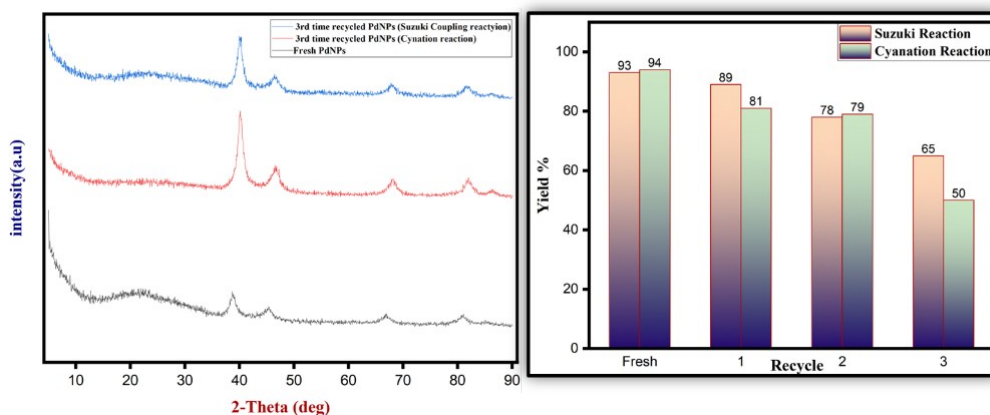


Figure S6. Recyclability of PdNPs, 3rd time recycled after Suzuki-Miyaura and Aryl Cyanation Reaction

S4 ¹H NMR analysis result of Suzuki-Miyaura coupling Reaction:

1. *Biphenyl* (Table 3, SI No. 1 and 2): Colourless Crystals. ¹H NMR (400 MHz, CDCl₃), δ (PPM) = 7.60 (d, J =8Hz, 4H), 7.44 (t, J = 7.2Hz, 4H), 7.35 (t, J =7.5 Hz, 2H).

2. *4-Phenylbenzaldehyde* (Table 3, SI No. 3 and 4): Light yellow Crystals. ¹H NMR (400 MHz, CDCl₃), δ (PPM)= 9.99 (s, 1H), 7.89 (d, J = 8.4Hz, 2H), 7.70 (d, J = 8.4Hz, 2H), 7.58 (d, J = 7.2Hz, 2H), 7.43 (t, J =7.2Hz, 2H), 7.36 (t, J =7.2, 1H).

3. *4-Cyanobiphenyl* (Table 3, SI No. 5): white crystalline Powder. ¹H NMR (400 MHz, CDCl₃), δ (PPM)= 7.74 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8Hz, 2H), 7.60 (d, J =7.2 Hz, 2H), 7.50 (t, J = 7.2 Hz, 2H), 7.44 (m, 1H).

4. *4-Cyanophenyl benzaldehyde* (Table 3, SI No. 6): White Powder. ¹H NMR (400 MHz, CDCl₃), δ (PPM)= 10.09 (s, 1H), 8.01 (d, J = 8Hz, 2H), 7.77 (m, 6H).

5. *4-Acetylbiphenyl* (Table 3, SI No. 7, 8): White powder. ¹H NMR (400 MHz, CDCl₃), δ (PPM)= 8.03 (d, J = 8.0 Hz, 2H), 7.68 (d, J = 8.0 Hz, 2H), 7.63 (d, J = 7.6 Hz, 2H), 7.48 (m, 2H), 7.41 (m, 1H), 2.62 (s, 3H).

6. *4-phenyl-1,8-naphthalic anhydride* (Table 3, SI No. 9): White powder. ¹H NMR (400 MHz, CDCl₃), δ (PPM)= 8.69 (t, J = 7.6 Hz, 2H), 8.38 (d, J = 7.6Hz, 1H), 7.78 (t, J = 7.6 Hz, 2H), 7.58 (m, 3H), 7.52 (m, 2H).

7. *1,1'-biphenyl]-4-yl(phenyl)methanone* (Table 3, SI No. 10): Off White powder. ^1H NMR (400 MHz, CDCl_3), δ (PPM)= 7.91 (d, J = 8.4Hz, 2H), 7.85 (d, J = 7.2Hz, 2H), 7.72 (d, J = 8Hz, 2H), 7.66 (d, J = 7.6Hz, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.50 (m, 4H), 7.42 (t, J = 7.2Hz, 1H).

8. *4'-hydroxy-[1,1'-biphenyl]-4-yl) (phenyl)methanone* (Table 3, SI No. 11): White powder. ^1H NMR (400 MHz, DMSO), δ (PPM)= 9.77 (s, 1H), 7.79 (t, J = 8.4Hz, 6H), 7.71 (t, J = 7.2Hz, 2H), 7.63 (m, 4H), 6.69 (d, J = 8.4Hz, 2H).

9. *4'-benzoyl-[1,1'-biphenyl]-4-carbaldehyde* (Table 3, SI No. 12): White powder. ^1H NMR (400 MHz, CDCl_3), δ (PPM)= 10.09 (s, 1H), 8.01 (d, J = 8Hz, 2H), 7.94 (d, J = 8Hz, 2H), 7.85 (m, 4H), 7.64 (t, J = 7.6Hz, 1H), 7.53 (t, J = 7.6Hz, 2H).

S.5 ^1H NMR analysis result of Cyanation Reaction:

1. *Benzonitrile* (Table 4, SI No. 1, 2): Colourless liquid. ^1H NMR (400 MHz, CDCl_3), δ (PPM)= 7.59 (m, 3H), 7.44 (t, J = 7.6Hz, 2H).

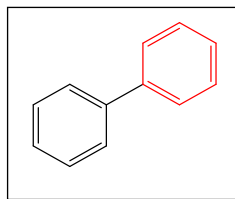
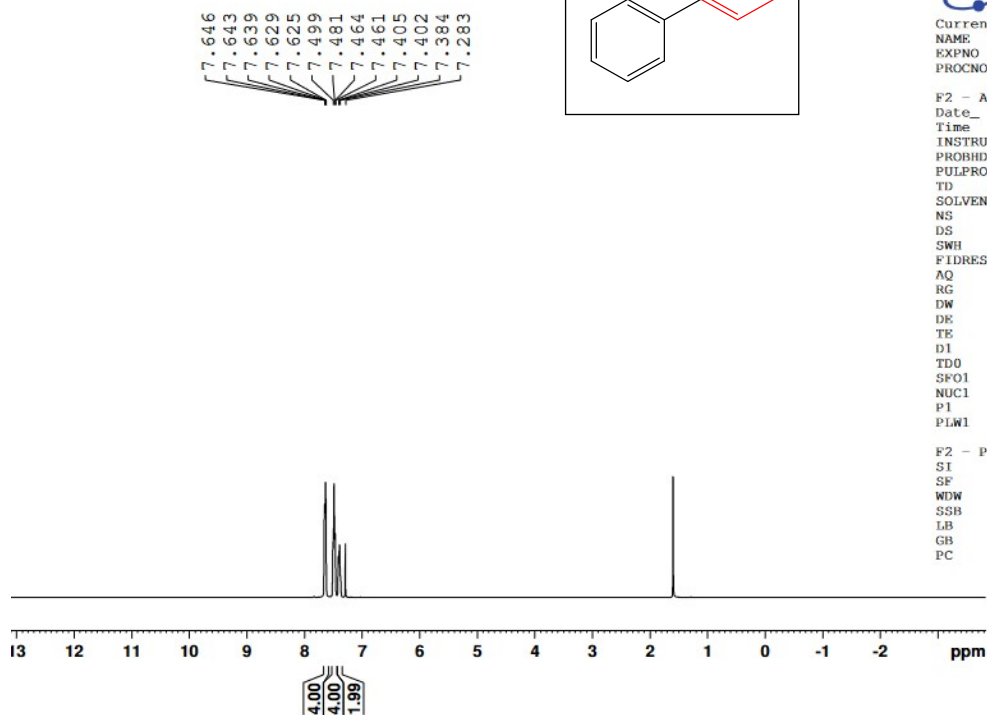
2. *4-Formylbenzonitrile* (Table 4, SI No. 3, 4): White crystal. ^1H NMR (400 MHz, CDCl_3), δ (PPM)= 10.01 (s, 1H), 8.01 (m, 2H), 7.87 (t, J = 8Hz, 2H).

3. *4-benzoyl benzonitrile* (Table 4, SI No. 5): Off-white Powder. ^1H NMR (400 MHz, CDCl_3), δ (PPM)= 7.89 (d, J = 8.4Hz, 2H), 7.80 (m, 4H), 7.66 (t, J = 7.6Hz, 1H), 7.58 (t, J = 7.6Hz, 2H).

5. *1,4-Dicyanobenzene* (Table 4, SI No. 6): Off-white crystals. ^1H NMR (400 MHz, CDCl_3): δ (ppm)= 7.97 (s, 4H)

6. *4-Aminobenzonitrile* (Table 4, SI No. 7): Light brown crystal. ^1H NMR (400 MHz, CDCl_3), δ (ppm)= 7.39 (d, J = 8Hz, 2H), 6.61 (d, J = 8Hz, 2H), 6.14 (s, 2H).

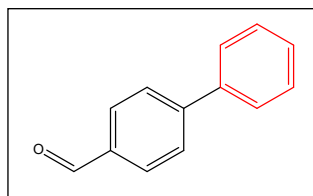
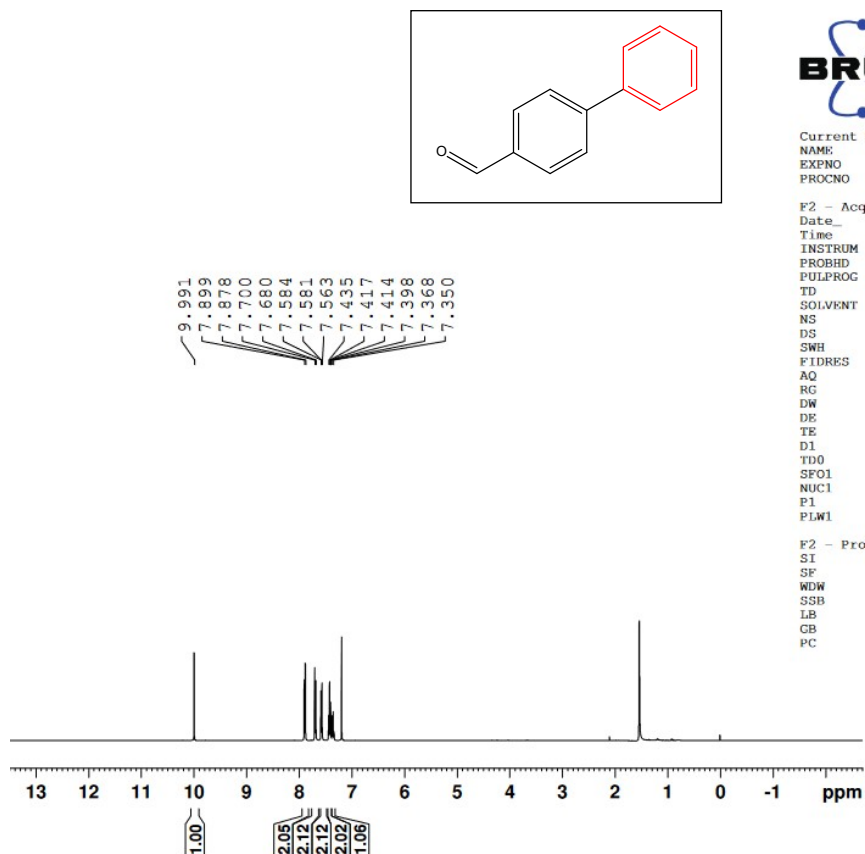
7. *4-Acetylbenzonitrile* (Table 4, SI No. 8,9): Off White Crystal. ^1H NMR (400 MHz, CDCl_3), δ (ppm)= 8.05 (d, J = 8, 2H), 7.79 (d, J = 8, 2H), 2.65 (s, 3H).



Current Data Parameters
NAME Dr.SYN290124
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240129
Time 18.31 h
INSTRUM spect
PROBHD z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDC13
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 300.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

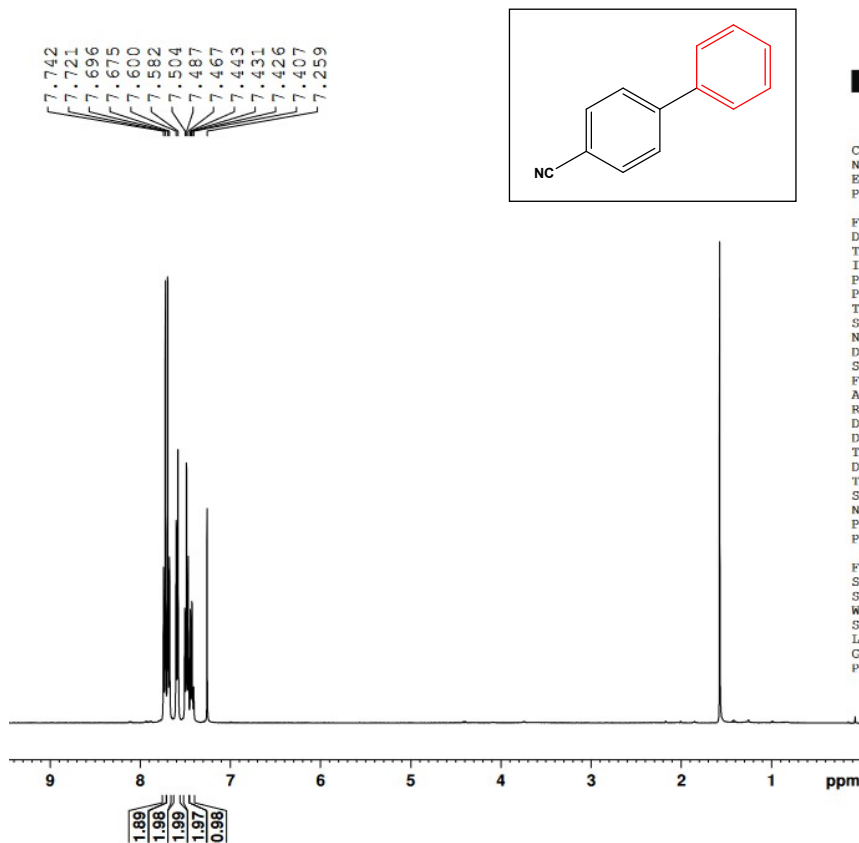
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Dr.SYN030224
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240203
Time 12.59 h
INSTRUM spect
PROBHD z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDC13
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

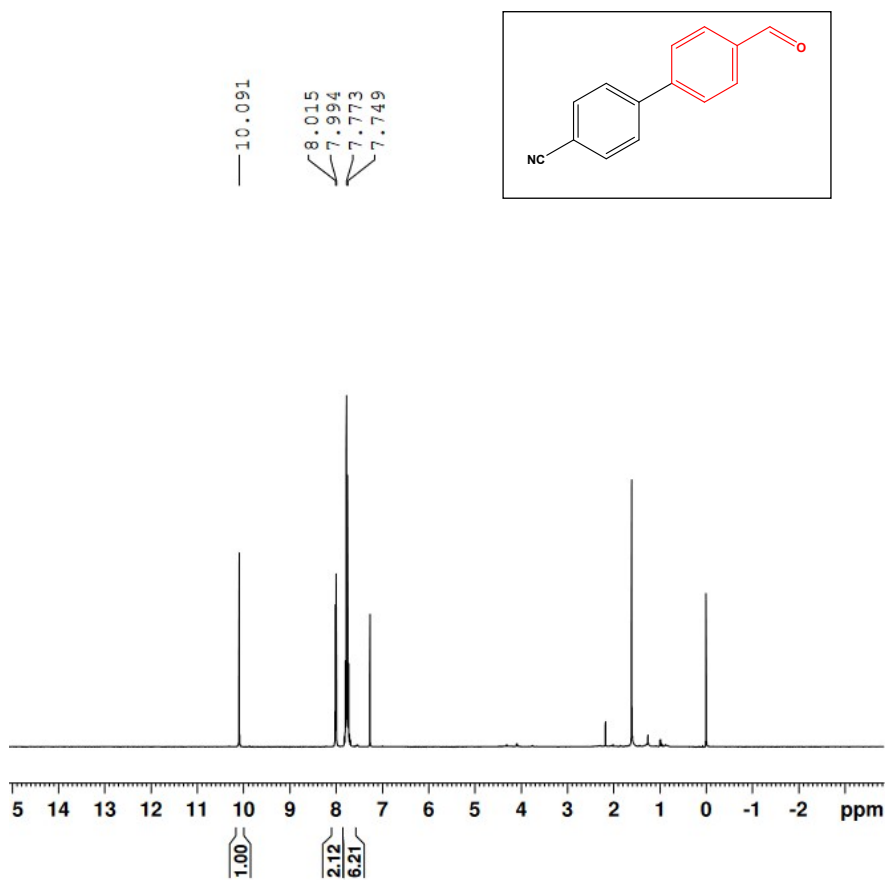
F2 - Processing parameters
SI 65536
SF 400.2580378 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME Dr.SYN110324
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240311
 Time 12.48 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 156.91
 DW 62.400 usec
 DE 6.50 usec
 TE 302.8 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

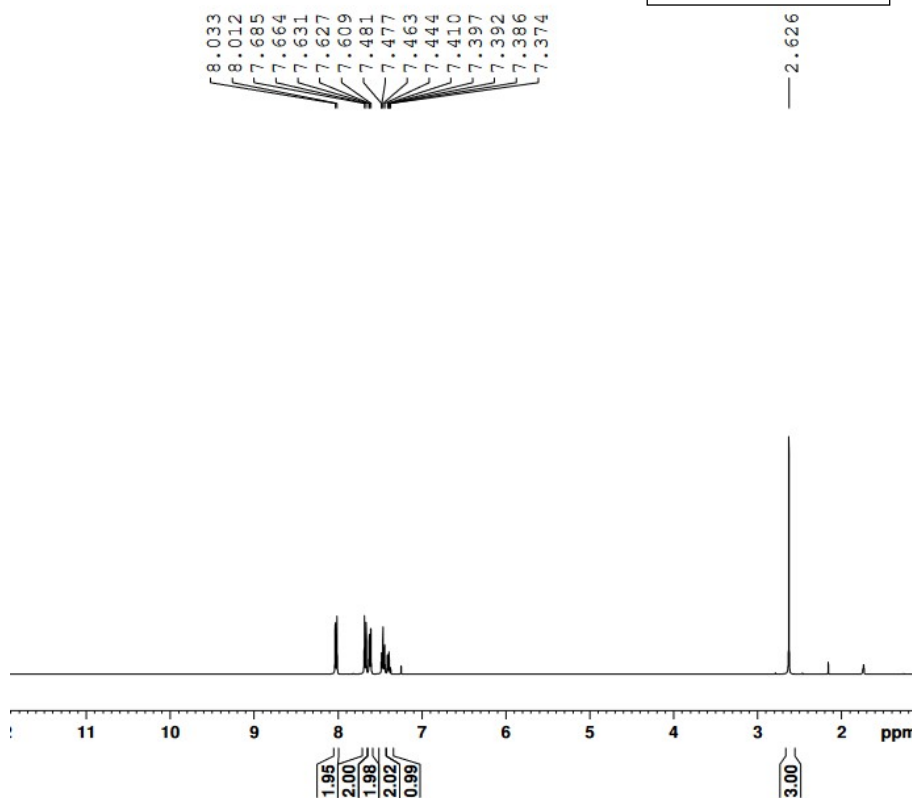
F2 - Processing parameters
 SI 65536
 SF 400.2580103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN220324
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240322
 Time 15.32 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 304.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

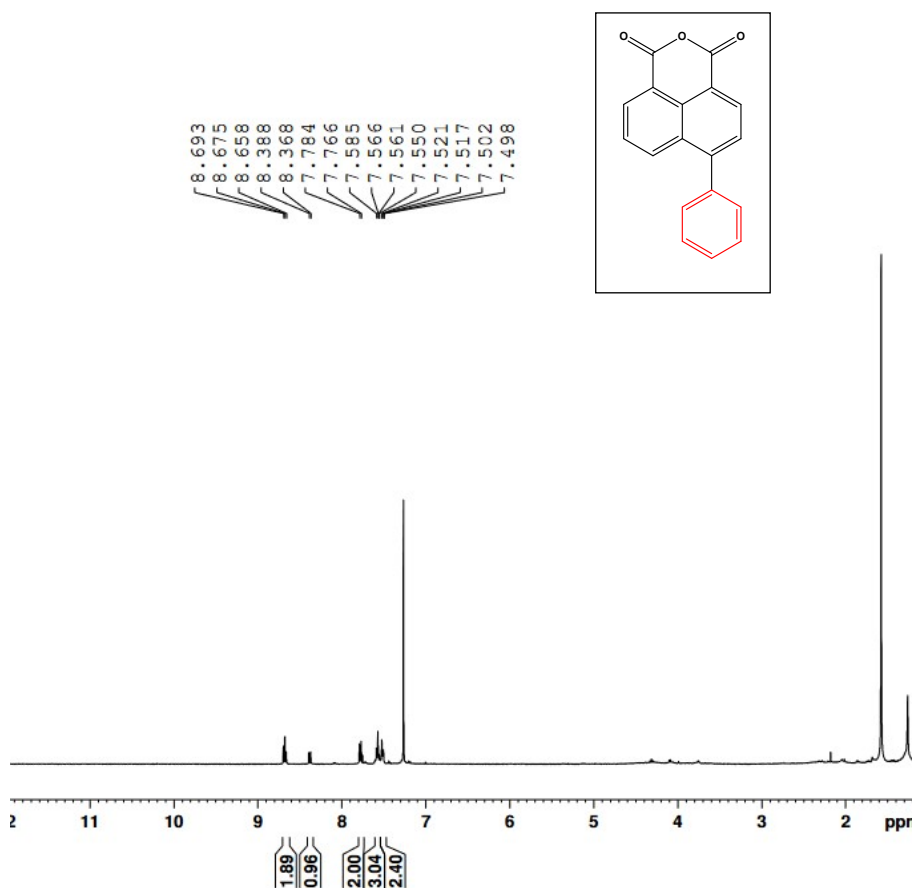
F2 - Processing parameters
 SI 65536
 SF 400.2580076 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN030424
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240403
 Time 20.24 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 77.73
 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

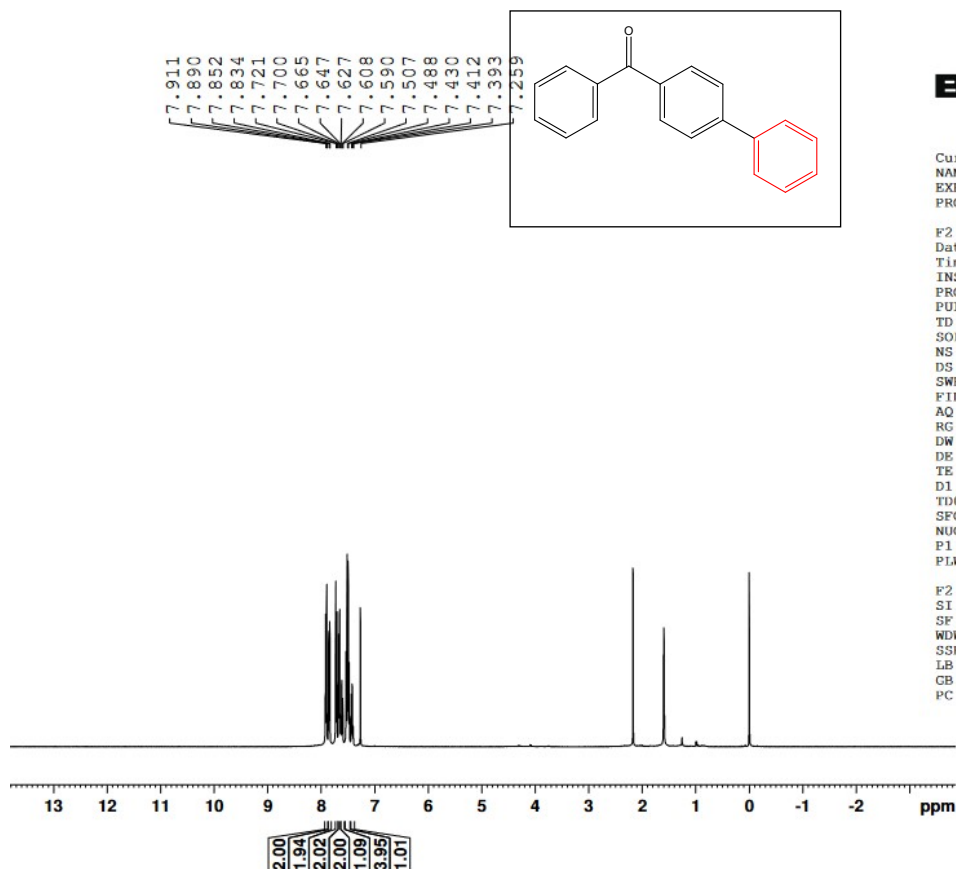
F2 - Processing parameters
 SI 65536
 SF 400.2580146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN130324
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240313
 Time 13.18 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 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

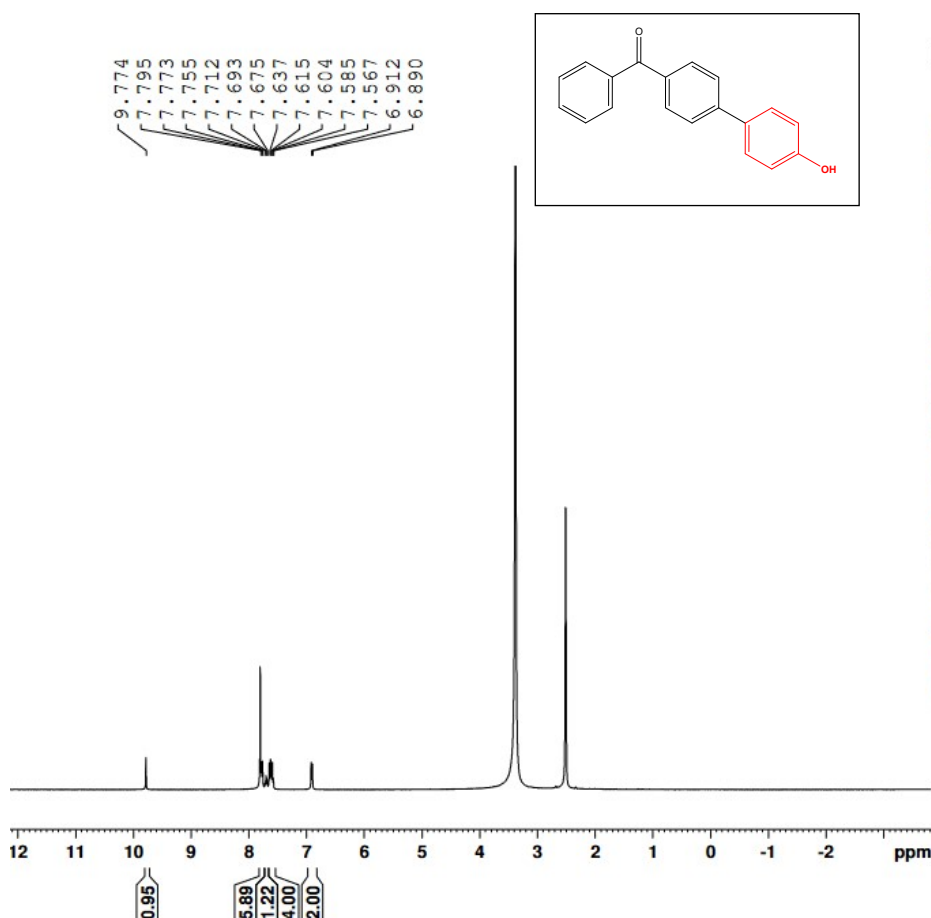
F2 - Processing parameters
 SI 65536
 SF 400.2580090 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN080224
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240208
 Time 16.58 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 156.91
 DW 62.400 usec
 DE 6.50 usec
 TE 300.6 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

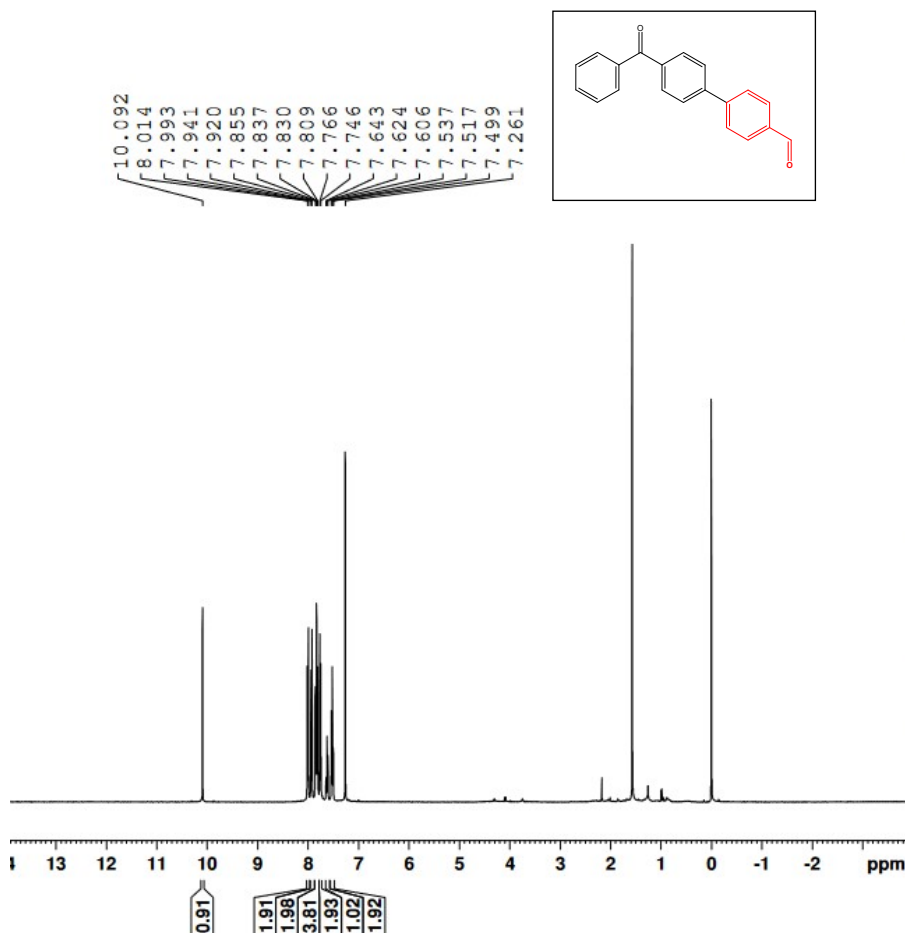
F2 - Processing parameters
 SI 65536
 SF 400.2580104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 CB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN130324
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240313
 Time 13.23 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 303.4 K
 D1 1.00000000 sec
 TDO 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
 CB 0
 PC 1.00

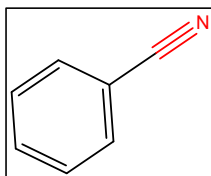


Current Data Parameters
 NAME: Dr.SYN160324
 EXPNO: 14
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240316
 Time: 14.01 h
 INSTRUM: spect
 PROBHD: Z108618_0505 (
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 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: 304.1 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: 400.2580096 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

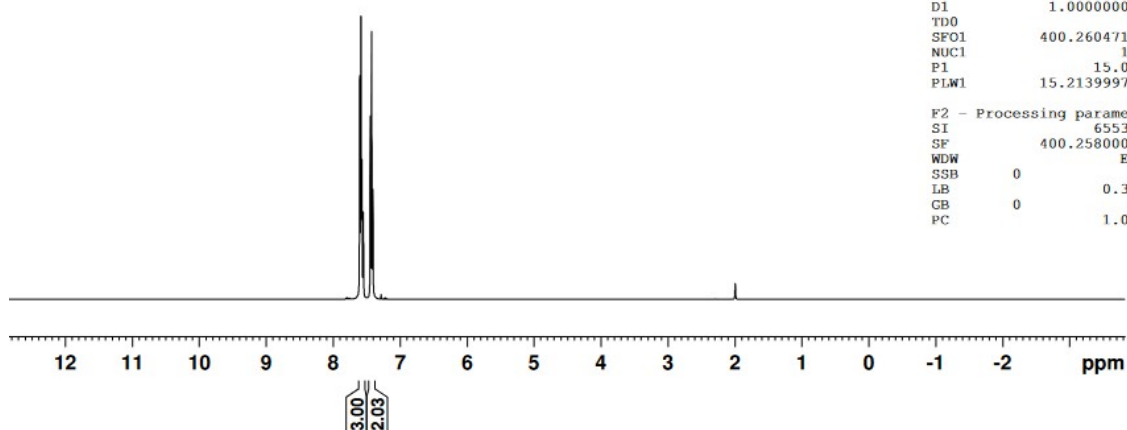
7.596
7.578
7.563
7.544
7.445
7.425
7.406



Current Data Parameters
NAME Dr.SYN310124
EXPNO 54
PROCNO 1

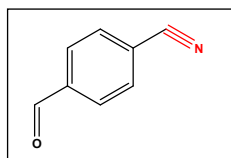
F2 - Acquisition Parameters
Date_ 20240131
Time 19.49 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 300.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

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



— 10.107

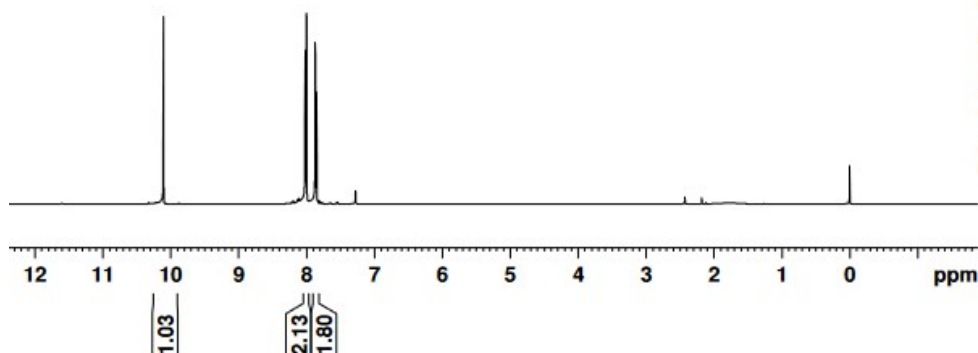
8.019
8.015
8.003
7.998
7.871
7.867
7.850

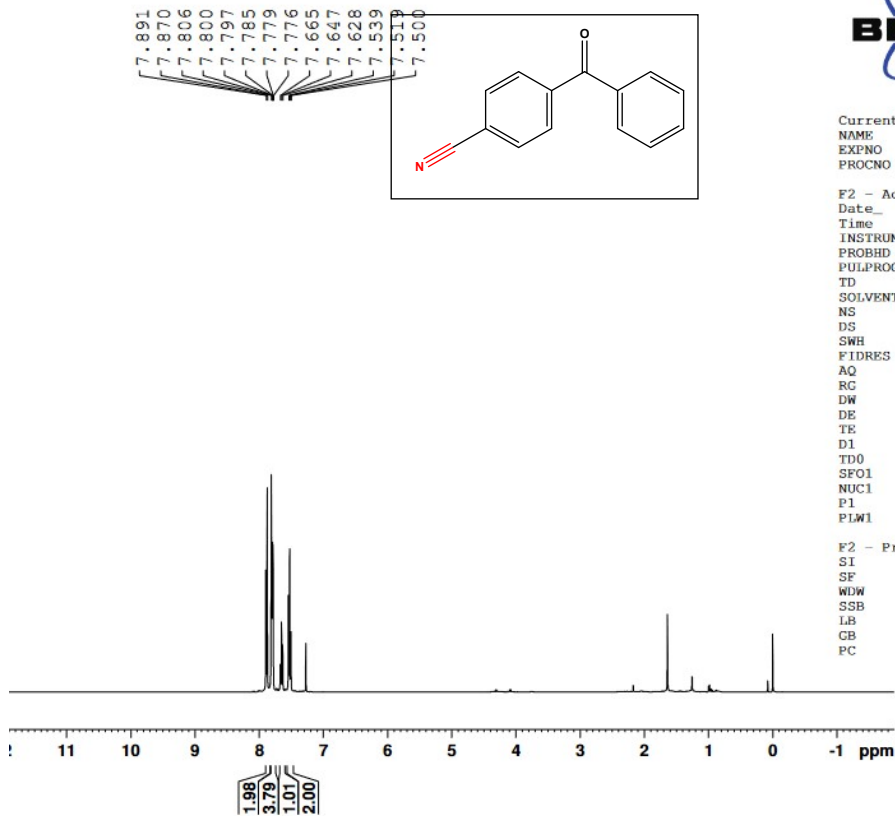


Current Data Parameters
NAME Dr.SYN160324
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240316
Time 13.54 h
INSTRUM spect
PROBHD z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDC13
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 304.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

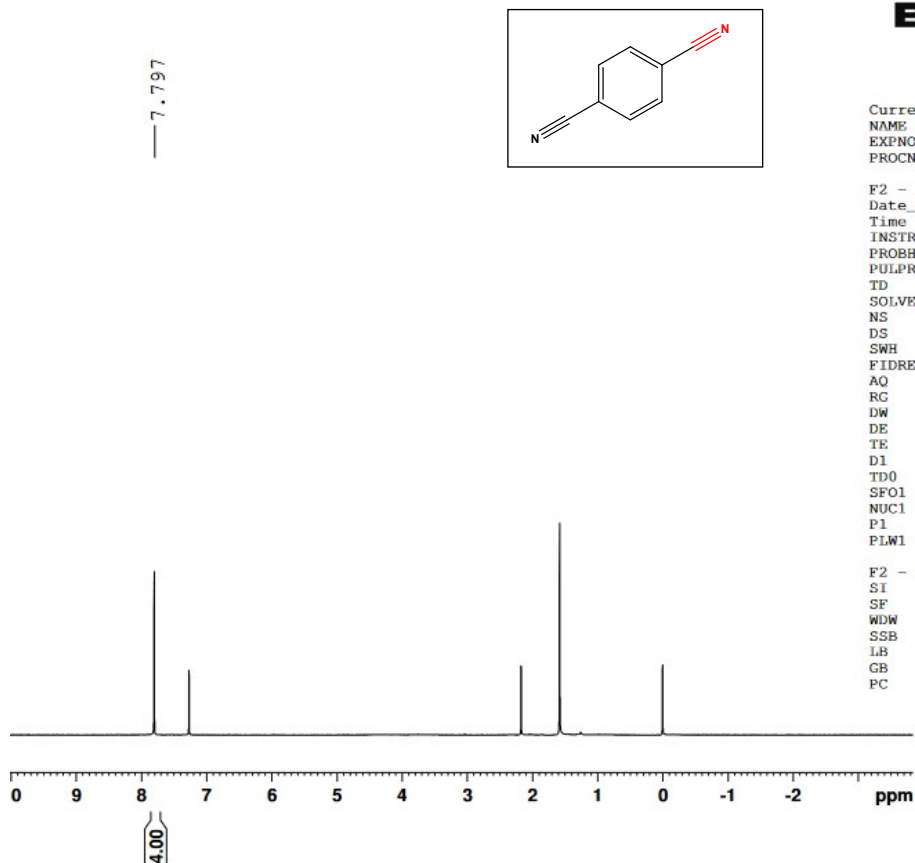




Current Data Parameters
 NAME Dr.SYN050324
 EXPNO 42
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240305
 Time 14.41 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 303.0 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 400.2580070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

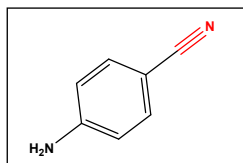


Current Data Parameters
 NAME Dr.SYN120424
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240412
 Time 14.16 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 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 400.2580085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

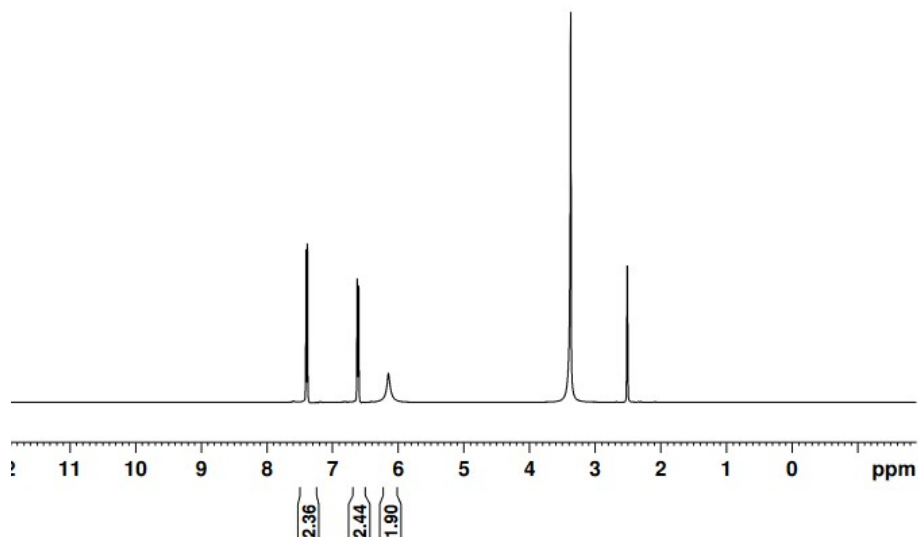
7.396
7.375
6.615
6.596
6.140

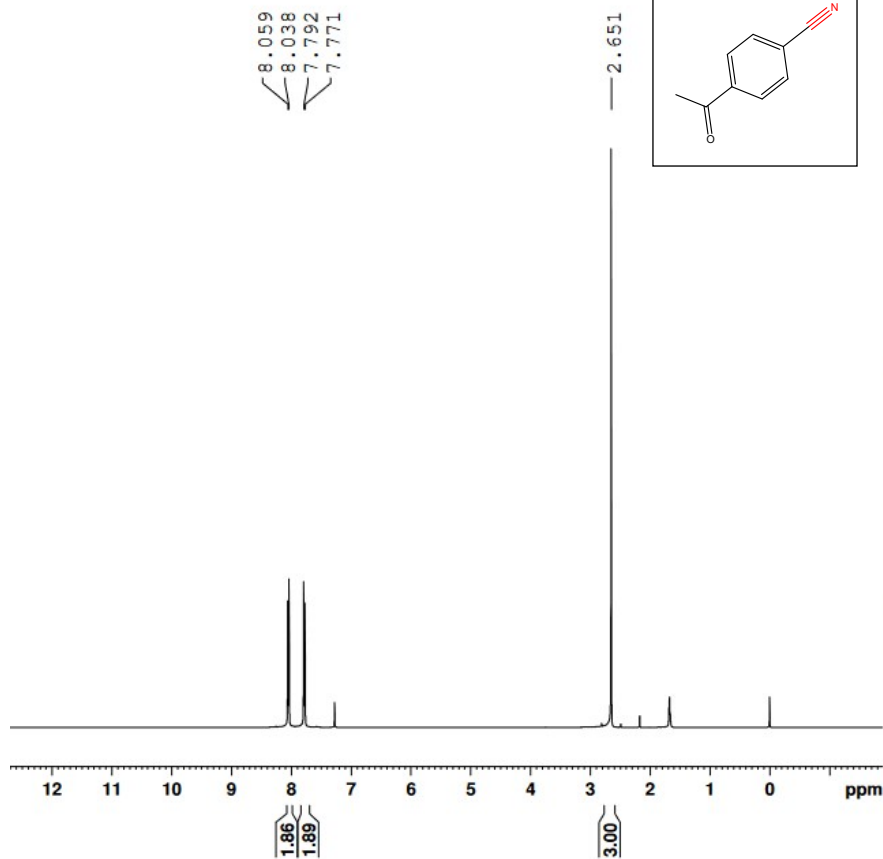


Current Data Parameters
NAME Dr.SYN310124
EXPNO 56
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240131
Time 20.24 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 300.9 K
D1 1.00000000 sec
TDO 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





Current Data Parameters
 NAME: Dr.SYN120424
 EXPNO 19
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240412
 Time 14.02 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 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 305.6 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 400.2580041 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00