

Supporting Documents

Unveiling the Photocatalytic Activity of Carbon Dots/g-C₃N₄ Nanocomposite for the O-Arylation of 2-Chloroquinoline-3-carbaldehydes

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Text S1. Materials details

All of the analytical-grade chemicals were procured from Sigma-Aldrich, India, and Alpha-Aldrich and used as such. Avra Synthesis Pvt. Ltd. in India supplied the ethanol and other solvents. All reagents used were of analytical grade (AR) and used without further purification, and deionized water was made in our lab.

Text S2. Characterization details

All samples' X-ray diffraction patterns were obtained using the Bruker D8 Advance X-ray diffraction technique with CuK α radiation ($\lambda = 0.154$ nm) in the range of 2θ from 10° to 90° at a scan speed of 2° min^{-1} . The surface chemical composition was confirmed using X-ray photoelectron spectra (XPS) (TPHI 5000 Versa Probe III) with an Al K X-ray source. With the aid of KBr pellets, the FT-IR spectra were determined on a Shimadzu spectrophotometer. For each sample, 48 scans were logged with a resolution of 2 cm^{-1} in the $4000\text{--}400 \text{ cm}^{-1}$ range. The compositional and morphological examination of the synthesized samples was investigated using transmission electron microscopy (Tecnai G2-20 twin field emission microscope). Quantachrome analyzer was used to assess the materials' specific surface areas, and a zeta potential (HORIBA SZ-100) was used to measure the surface charge and stability of the built-up materials. In the Zeta potential analysis condition, the electrode was filled with synthesized materials dispersed in distilled water, and the parameters were adjusted to 3.4 V electrode voltage, 25°C temperature, a 10 min data capture period, and a pH of 7. HR-MS was conducted by Ultimate 3000 UHPLC-Q Exactive (Thermo Scientific, US) to determine the mass of the compound. The Jasco V-670 spectrometer and Shimadzu (RF-700) spectrometer systems were used to record UV Vis-DRS and photoluminescence spectra.

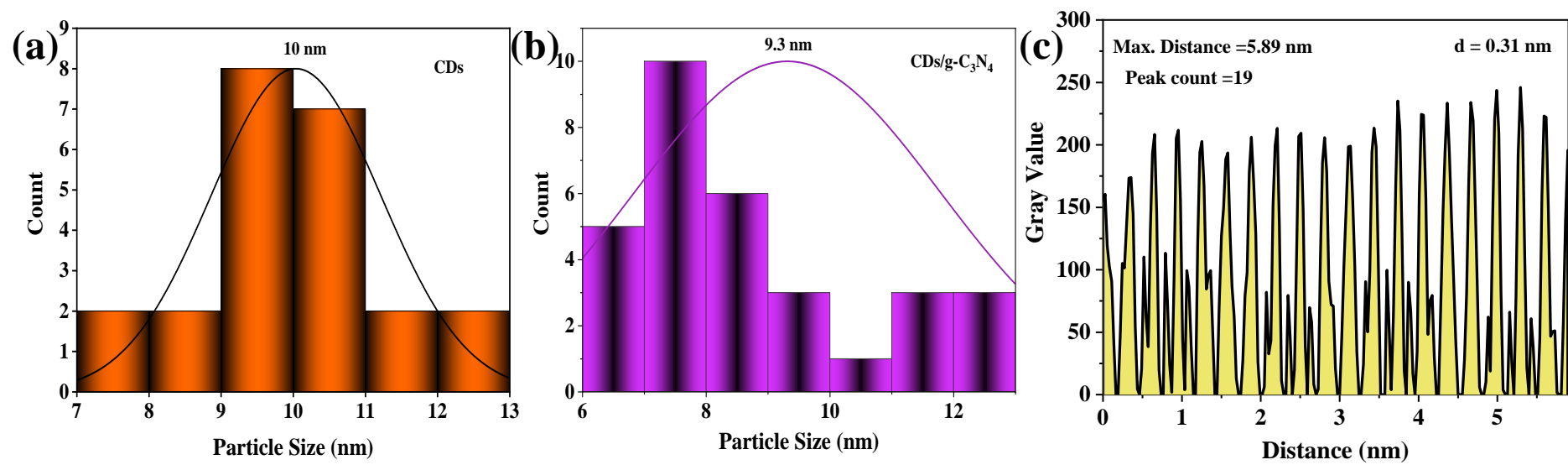
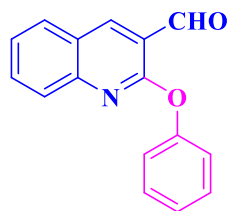
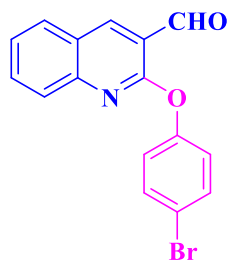


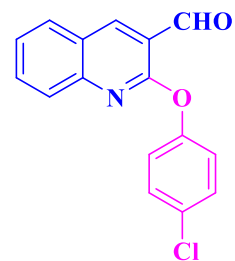
Figure S1. Particle size histogram of a) CDs, b) 3CDCN, and c) HRTEM d-spacing value of 3CDCN calculation



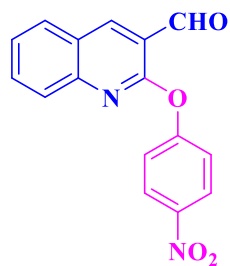
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3.1



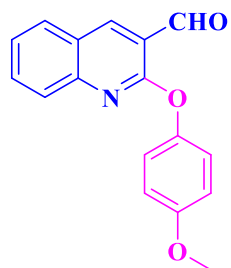
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Exact Mass: 326.99
3.2



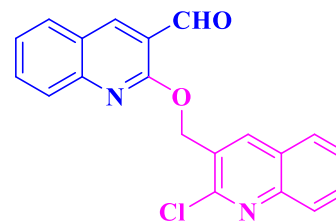
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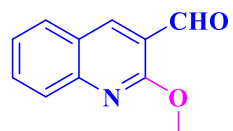
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3.4



C₁₇H₁₃NO₃
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3.5

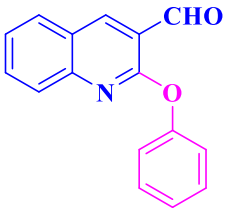
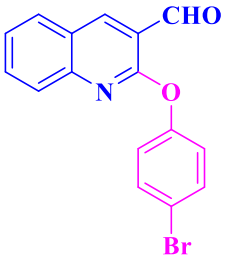


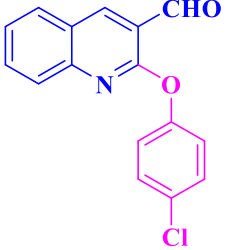
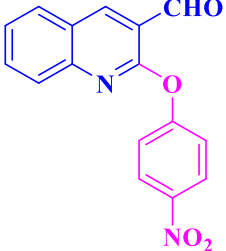
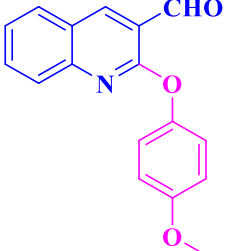
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3.6

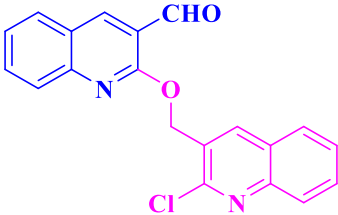
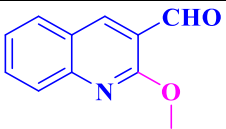


C₁₁H₉NO₂
Exact Mass: 187.06
3.7

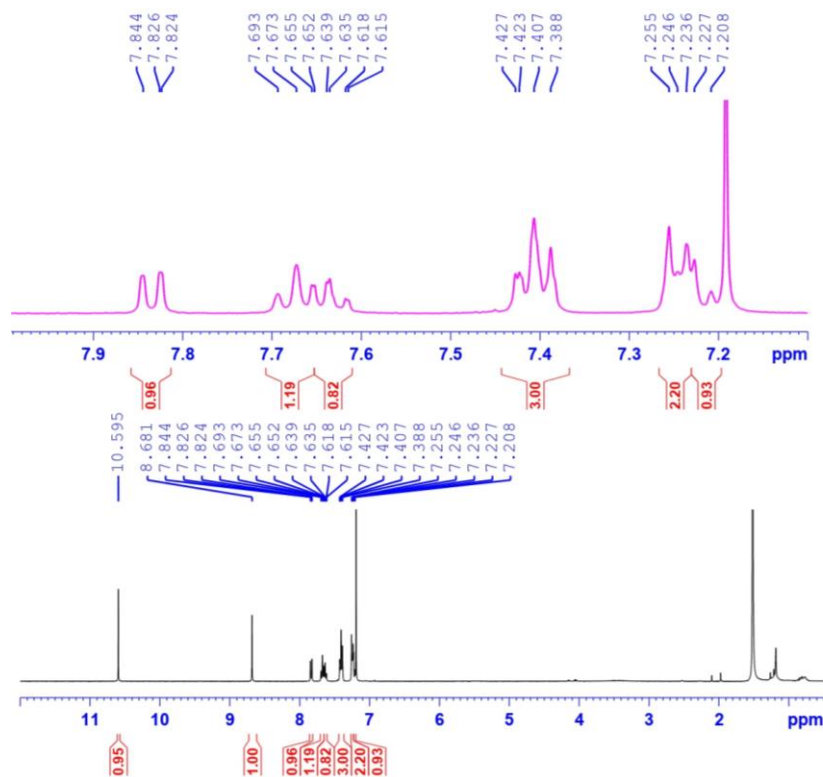
Characterization data of organic compounds:

S.No.	Structure of the compound	Name of the compound & Molecular formula	Appearance & Melting point (°C)	FT-IR, v/cm ⁻¹	¹ H-NMR (400 MHz, CDCl ₃ , Me ₄ Si) (ppm):	¹³ C-NMR (100 MHz, CDCl ₃ , Me ₄ Si) (ppm):	HRMS [M+H] ⁺
3.1.		2-phenoxyquinoline-3- carbaldehyde & C ₁₆ H ₁₁ NO ₂	Colourless crystals & 126 °C	2959, 1688, 1257, 893, 754, 682	δ 10.60 (s, 1H), 8.68 (s, 1H), 7.84 (t, 1H), 7.69 (t, 1H), 7.65 (d, 1H), 7.43 (m, 3H), 7.26 (d, 2H), 7.22 (d, 1H)	δ 187.96, 159.49, 152.06, 147.61, 139.53, 131.69, 128.61, 128.51, 126.85, 124.77, 124.19, 124.15, 120.78, 119.21	250.0872
3.2.		2-(4- bromophenoxy)quinoline-3- carbaldehyde & C ₁₆ H ₁₀ BrNO ₂	White solid & 148 °C	2959, 1689, 1206, 1011, 900, 806	δ 10.56 (s, 1H), 8.68 (s, 1H), 7.85 (d, 1H), 7.69 (d, 1H), 7.66 (t, 1H), 7.52 (d, 2H), 7.44 (m, 1H), 7.15 (d, 2H)	δ 188.60, 160.01, 152.02, 148.39, 140.81, 132.89, 132.51, 129.65, 127.75, 125.99, 125.22, 123.72, 120.02, 118.10	327.9975

3.3.		2-(4-chlorophenoxy)quinoline-3-carbaldehyde & $C_{16}H_{10}ClNO_2$	White solid & 165 °C	3054, 2862, 1685, 1212, 1079, 691	δ 10.57 (s, 1H), 8.68 (s, 1H), 7.85 (d, 1H), 7.69 (d, 2H), 7.44 (t, 1H), 7.39 (d, 2H), 7.22 (d, 1H), 7.20 (d, 1H)	δ 187.67, 159.13, 150.44, 147.42, 139.79, 131.87, 129.48, 128.65, 128.55, 126.76, 124.96, 124.21, 122.27, 119.03	284.0478
3.4.		2-(4-nitrophenoxy)quinoline-3-carbaldehyde & $C_{16}H_{10}N_2O_4$	White solid & 134 °C	3126, 2854, 1695, 1509, 846, 752	δ 10.56 (s, 1H), 8.74 (s, 1H), 8.31 (d, 2H), 7.90 (d, 1H), 7.71 (d, 1H), 7.70 (d, 1H), 7.50 (m, 1H), 7.45 (d, 2H)	δ 188.70, 140.81, 132.90, 130.50, 129.67, 129.57, 127.78, 125.98, 123.29	295.0727
3.5.		2-(4-methoxyphenoxy)quinoline-3-carbaldehyde & $C_{17}H_{13}NO_3$	White solid & 120 °C	2953, 1692, 1500, 1200, 758, 556	δ 10.59 (s, 1H), 8.66 (s, 1H), 7.83 (d, 1H), 7.60 (d, 1H), 7.64 (d, 1H), 7.40 (t, 1H), 7.18 (d, 2H), 6.93 (d, 2H), 3.80 (s, 3H)	δ 189.11, 160.85, 140.48, 132.66, 129.63, 127.84, 125.66, 125.08, 122.74, 120.15, 114.56, 55.66	280.0978

3.6.		2-((2-chloroquinolin-3-yl)methoxy)quinoline-3-carbaldehyde & C ₂₀ H ₁₃ ClN ₂ O ₂	White solid & 180 °C	1600, 1328, 1018, 753, 492	δ 10.53 (s, 1H), 8.60 (s, 1H), 8.00 (d, 1H), 8.35 (s, 1H) 7.86 (d, 1H), 7.81 (d, 1H), 7.80 (d, 1H), 7.73 (d, 1H), 7.67 (d, 1H), 7.53 (t, 1H), 7.43 (t, 1H), 5.85 (s, 2H)	δ 187.77, 158.90, 147.67, 146.22, 139.79, 136.81, 131.85, 129.62, 128.74, 127.71, 127.33, 126.64, 126.43, 126.32, 126.10, 124.49, 123.68, 118.94, 63.81, 28.68	349.0744
3.7.		2-methoxyquinoline-3-carbaldehyde & C ₁₁ H ₉ NO ₂	White solid & 109 °C	3350, 2870, 1594, 1337, 1003, 759, 471	δ 10.40 (s, 1H), 8.52 (s, 1H), 7.82 (t, 2H), 7.69 (td, 1H), 7.38 (t, 1H), 4.12 (s, 3H)	δ 189.35, 161.26, 148.96, 140.06, 132.59, 129.75, 127.28, 125.06, 124.41, 120.09, 53.88	187.0712

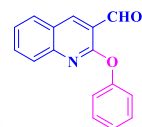
Signature SIF VIT VELLORE
Phenol



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EXPNO 13
PROCNO 1

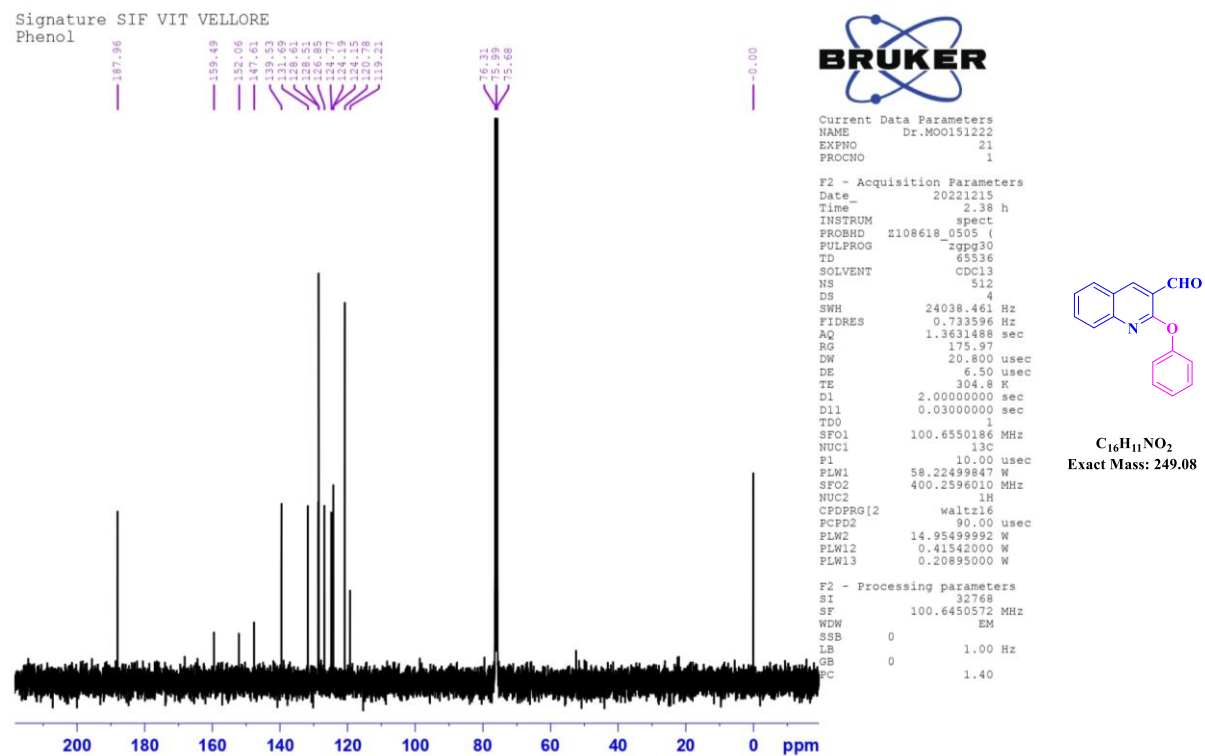
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FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 305.1 K
D1 1.00000000 sec
TDO 1
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NUC1 1H
F1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580370 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



$C_{16}H_{11}NO_2$
Exact Mass: 249.08

Figure S2. 1H NMR spectrum of 2-phenoxyquinoline-3-carbaldehyde (3.1)



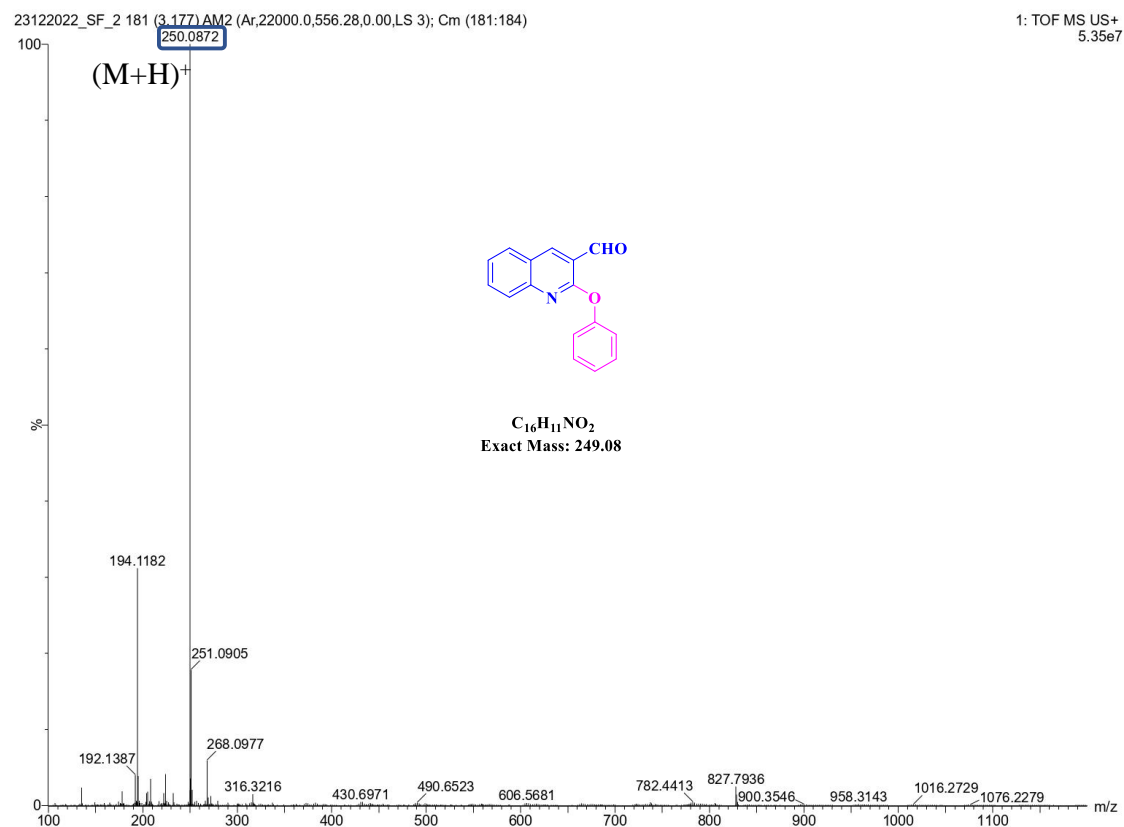


Figure S4. HRMS spectrum of 2-phenoxyquinoline-3-carbaldehyde (**3.1**)

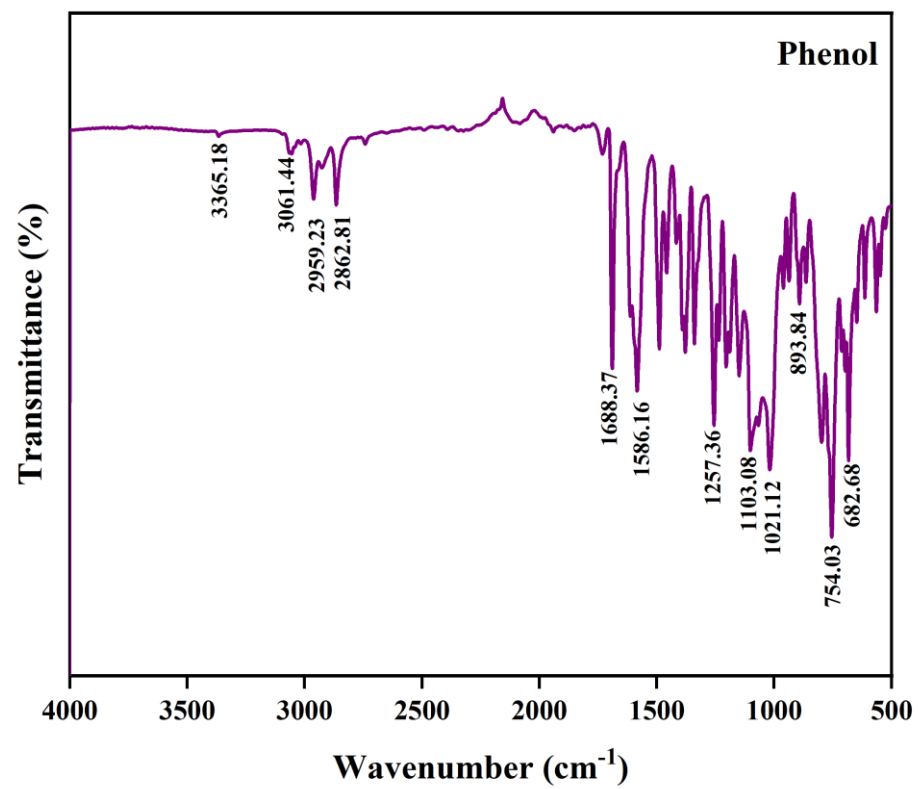
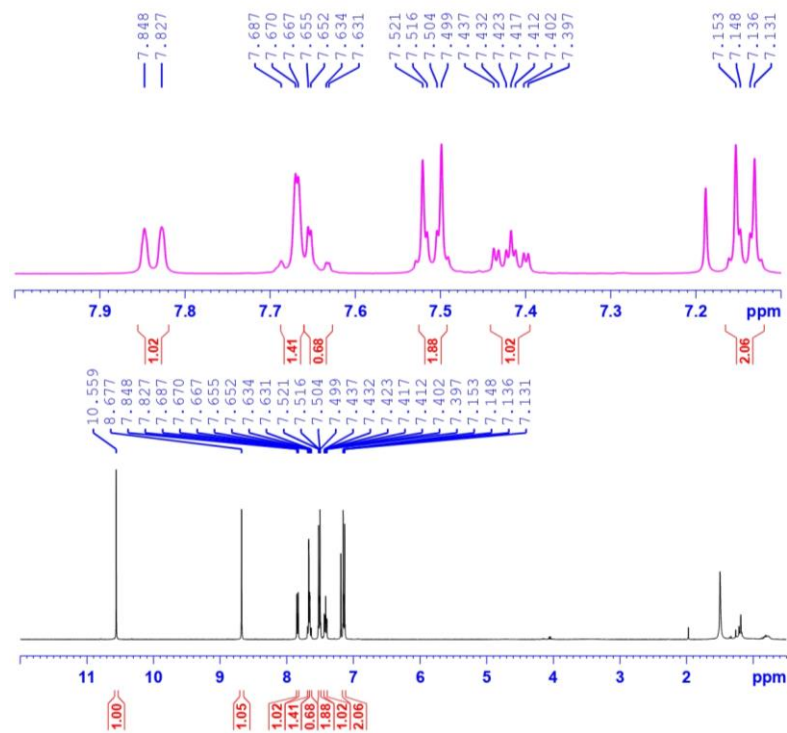


Figure S5. FTIR spectrum of 2-phenoxyquinoline-3-carbaldehyde (3.1)

Signature SIF VIT VELLORE
Bromo



Current Data Parameters
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EXPNO 5
PROCNO 1

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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 305.1 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PL1 14.95499992 W
F2 - Processing parameters
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SF 400.2580382 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

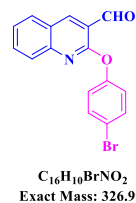
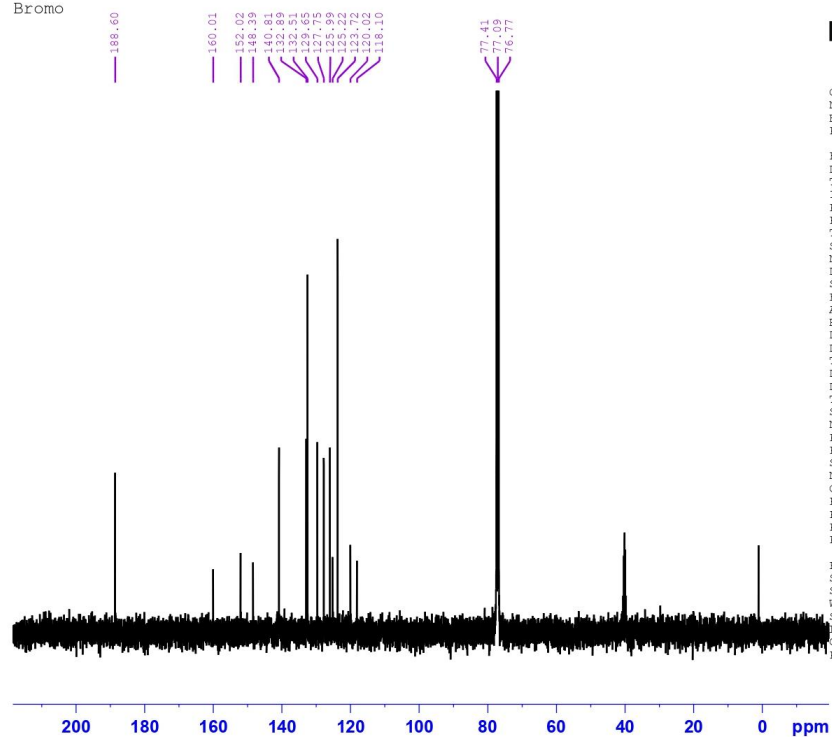


Figure S6. ¹H NMR spectrum of 2-(4-bromophenoxy)quinoline-3-carbaldehyde (3.2)

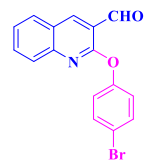
Signature SIF VIT VELLORE
Bromo



Current Data Parameters
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EXPNO 7
PROCNO 1

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TD 65536
SOLVENT CDCl3
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 306.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



$C_{16}H_{10}BrNO_2$
Exact Mass: 326.99

Figure S7. ^{13}C NMR spectrum of 2-(4-bromophenoxy)quinoline-3-carbaldehyde (3.2)

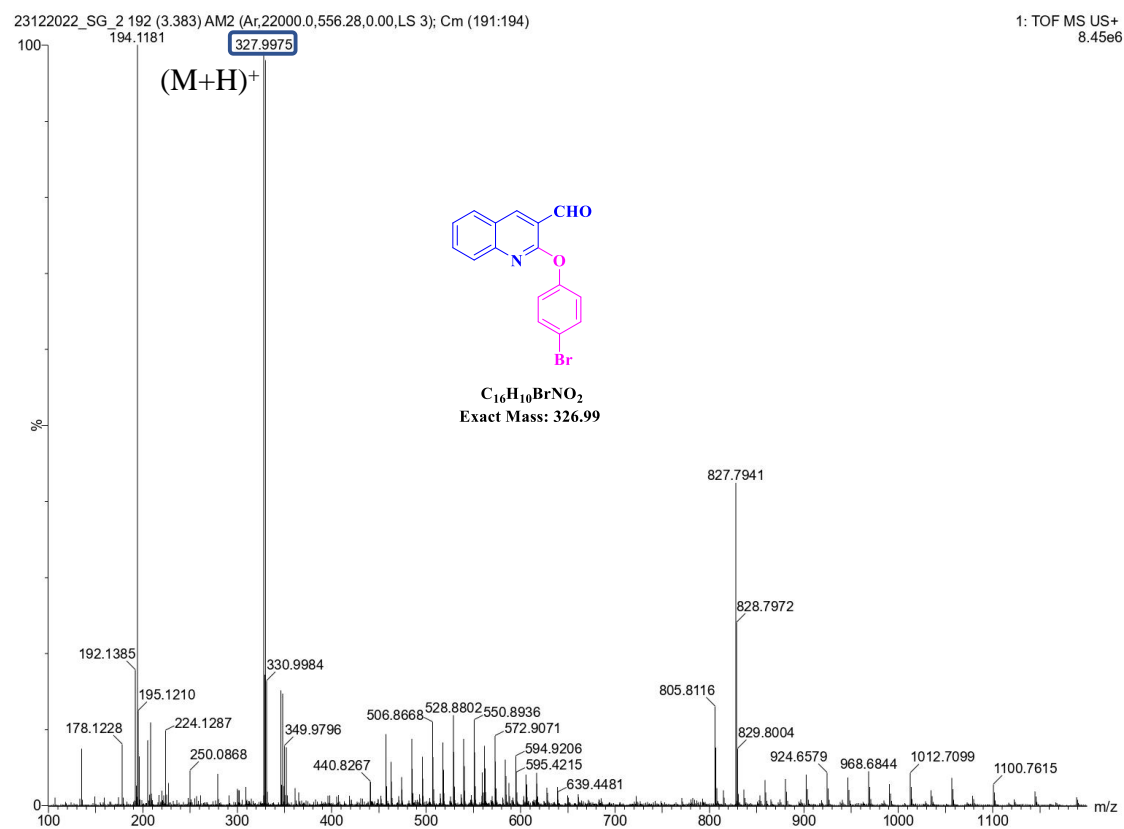


Figure S8. HRMS spectrum of 2-(4-bromophenoxy)quinoline-3-carbaldehyde (3.2)

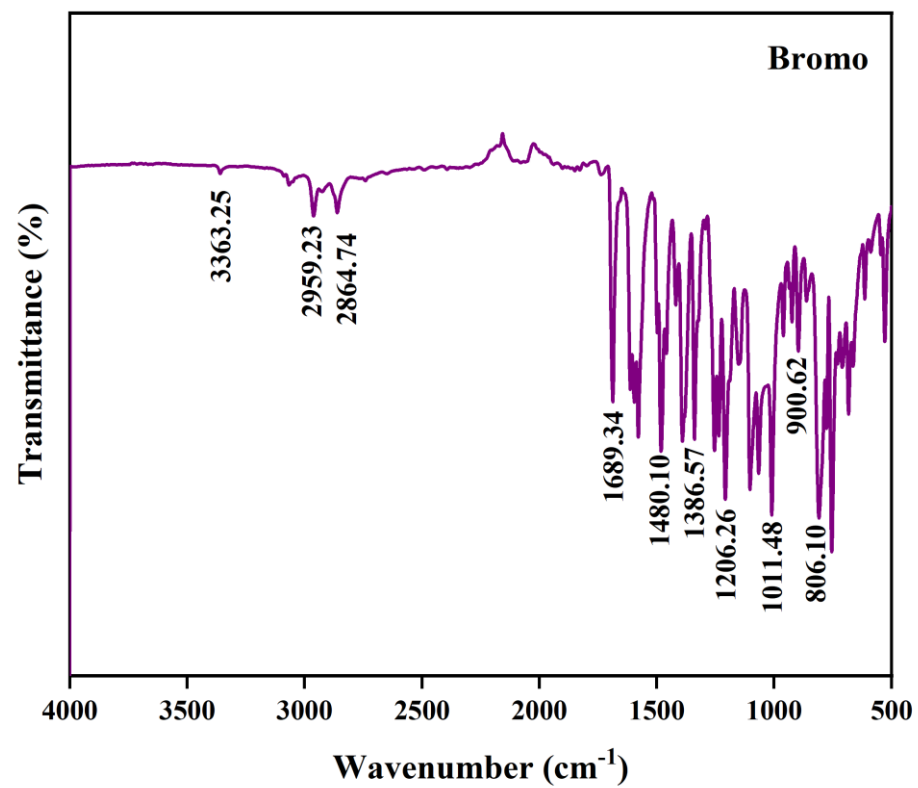
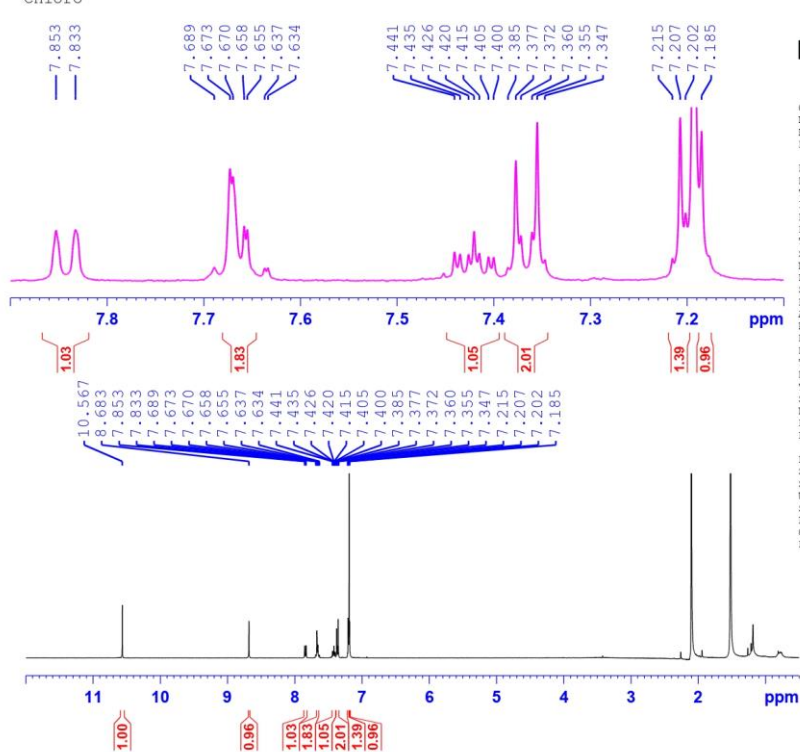


Figure S9. FTIR spectrum of 2-(4-bromophenoxy)quinoline-3-carbaldehyde (3.2)

Signature SIF VIT VELLORE
Chloro



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EXPNO 3
PROCNO 1

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SOLVENT CDC13
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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 303.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLWL 14.95499992 W

F2 - Processing parameters
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GB 0
FC 1.00

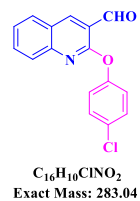
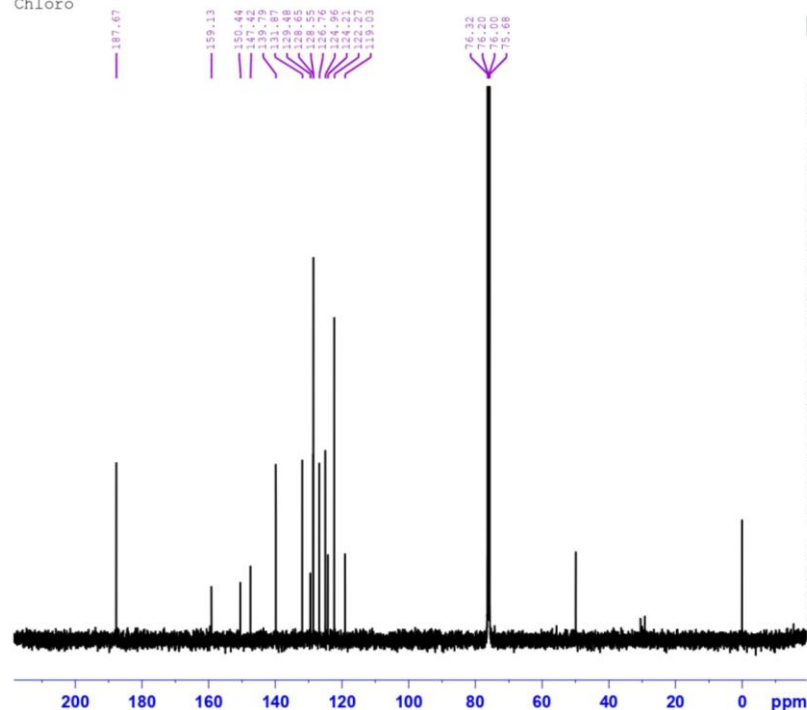


Figure S10. ¹H NMR spectrum of 2-(4-chlorophenoxy)quinoline-3-carbaldehyde (3.3)

Signature SIF VIT VELLORE
Chloro



Current Data Parameters
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EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
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Time_ 19.08 h
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SOLVENT CDCl3
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 305.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

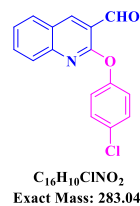


Figure S11. ^{13}C NMR spectrum of 2-(4-chlorophenoxy)quinoline-3-carbaldehyde (**3.3**)

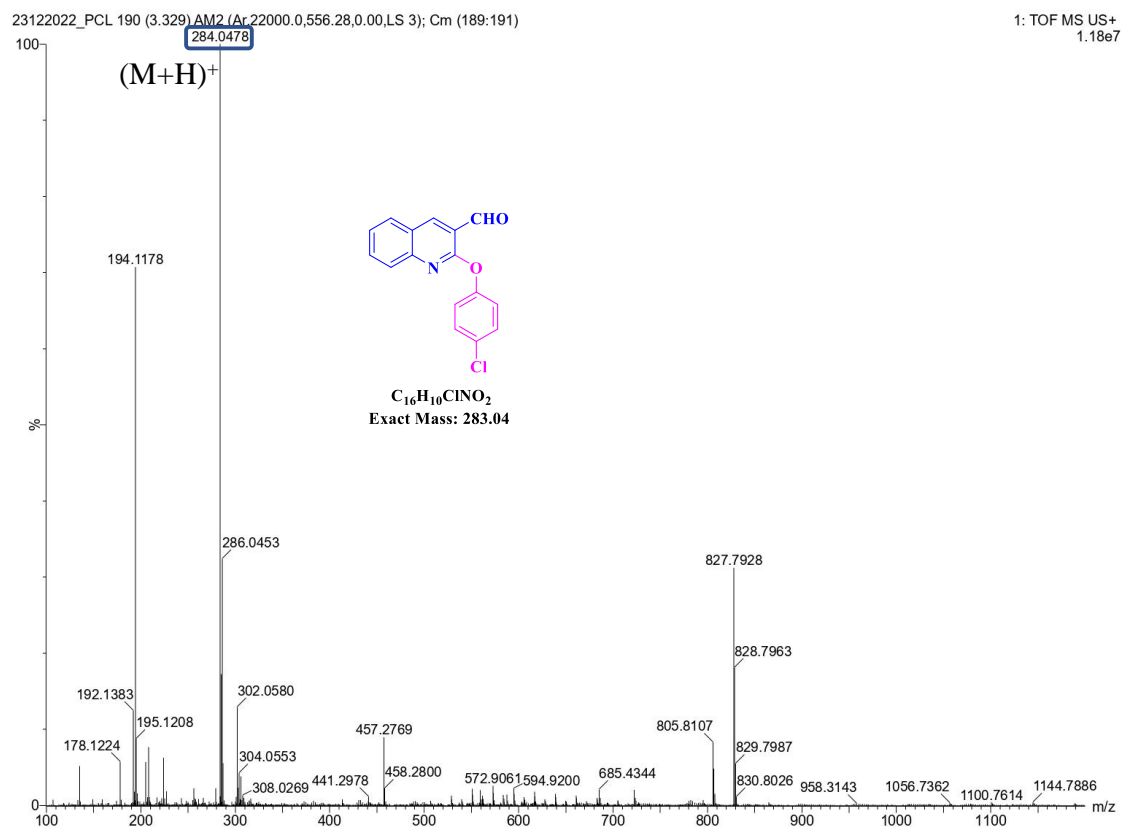


Figure S12. HRMS spectrum of 2-(4-chlorophenoxy)quinoline-3-carbaldehyde (**3.3**)

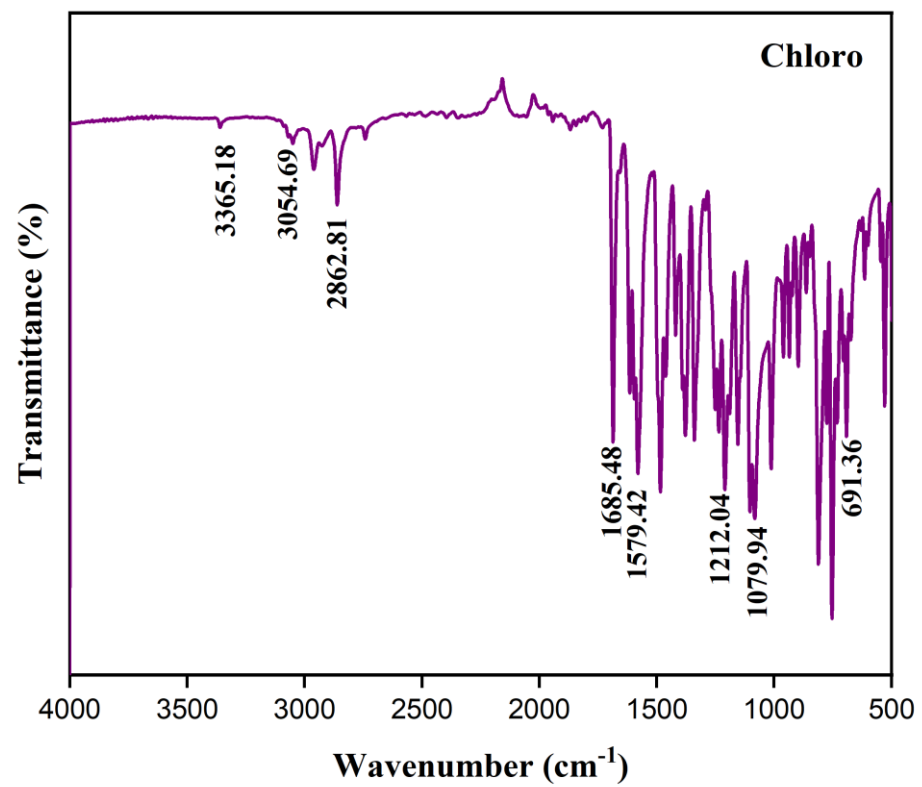
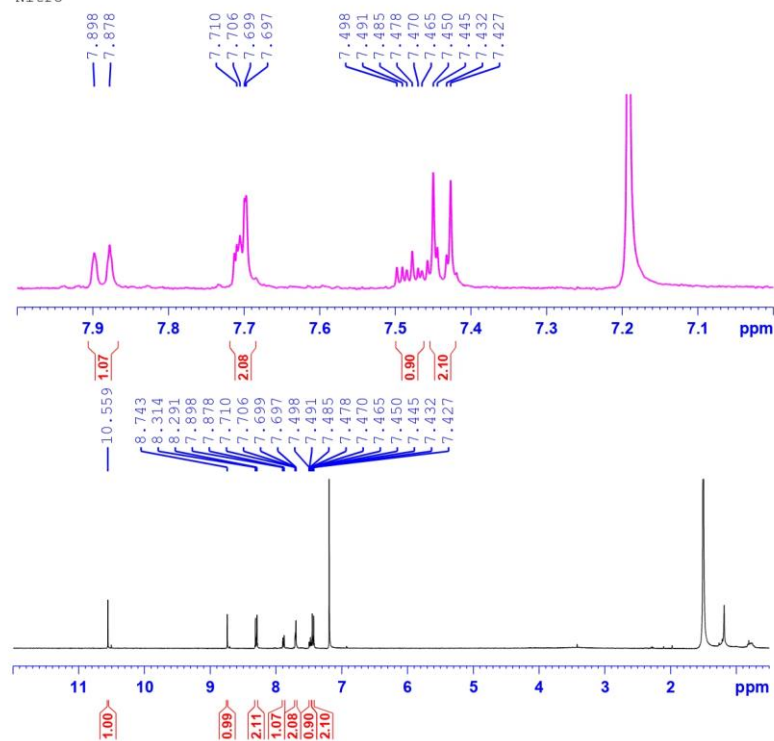


Figure S13. FTIR spectrum of 2-(4-chlorophenoxy)quinoline-3-carbaldehyde (**3.3**)

Signature SIF VIT VELLORE
Nitro



Current Data Parameters
NAME Dr.M00121222
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT CDC13
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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 304.3 K
DL 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
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SF 400.2580369 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

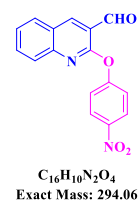
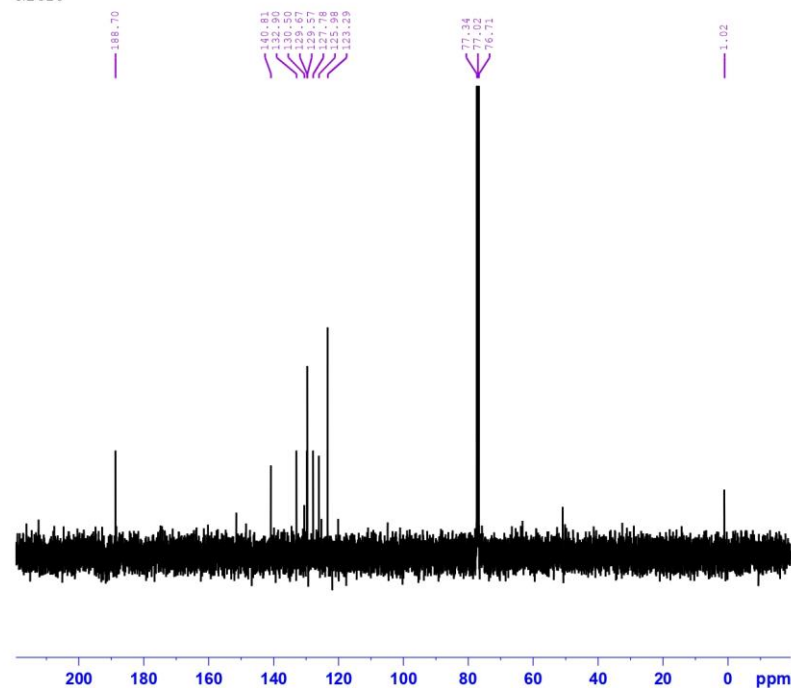


Figure S14. 1H NMR spectrum of 2-(4-nitrophenoxy)quinoline-3-carbaldehyde (3.4)

Signature SIF VIT VELLORE
Nitro



Current Data Parameters
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EXPNO 29
PROCNO 1

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SOLVENT cdcl3
NS 35
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DM 20.800 usec
DE 6.50 usec
TE 305.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

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



$C_{16}H_{10}N_2O_4$
Exact Mass: 294.06

Figure S15. ^{13}C NMR spectrum of 2-(4-nitrophenoxy)quinoline-3-carbaldehyde (3.4)

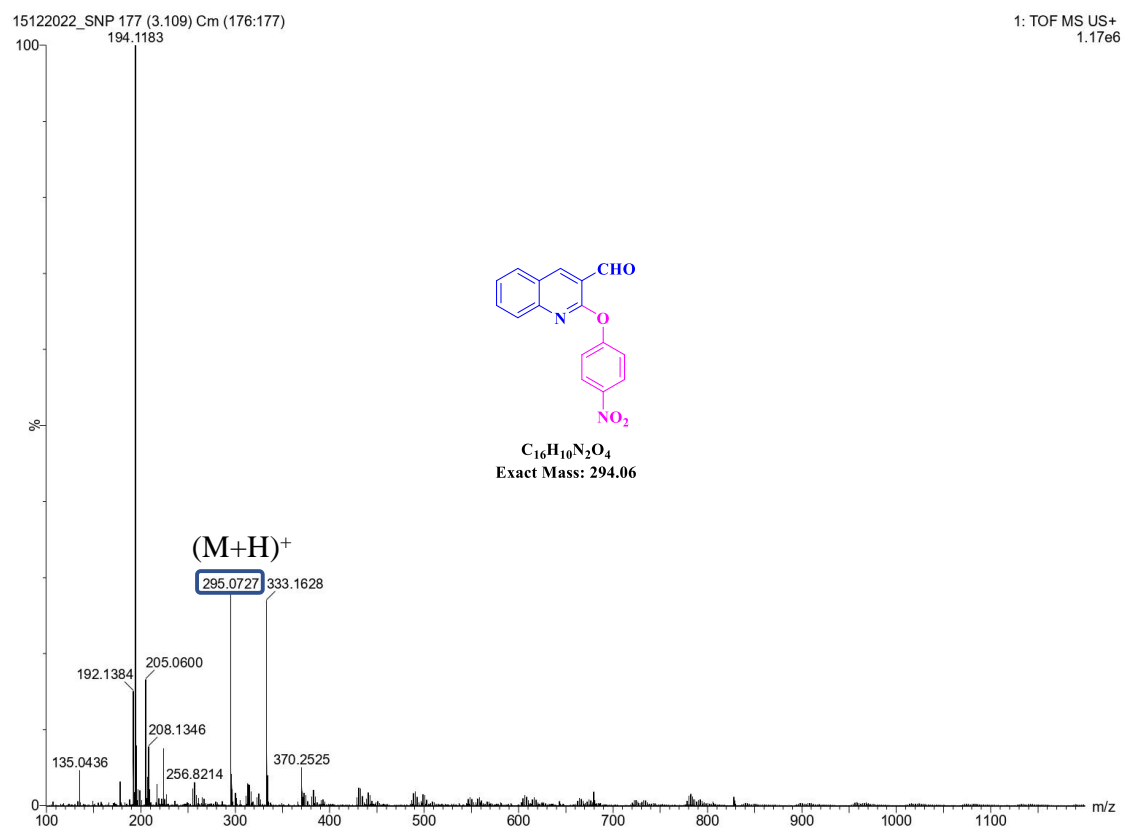


Figure S16. HRMS spectrum of 2-(4-nitrophenoxy)quinoline-3-carbaldehyde (**3.4**)

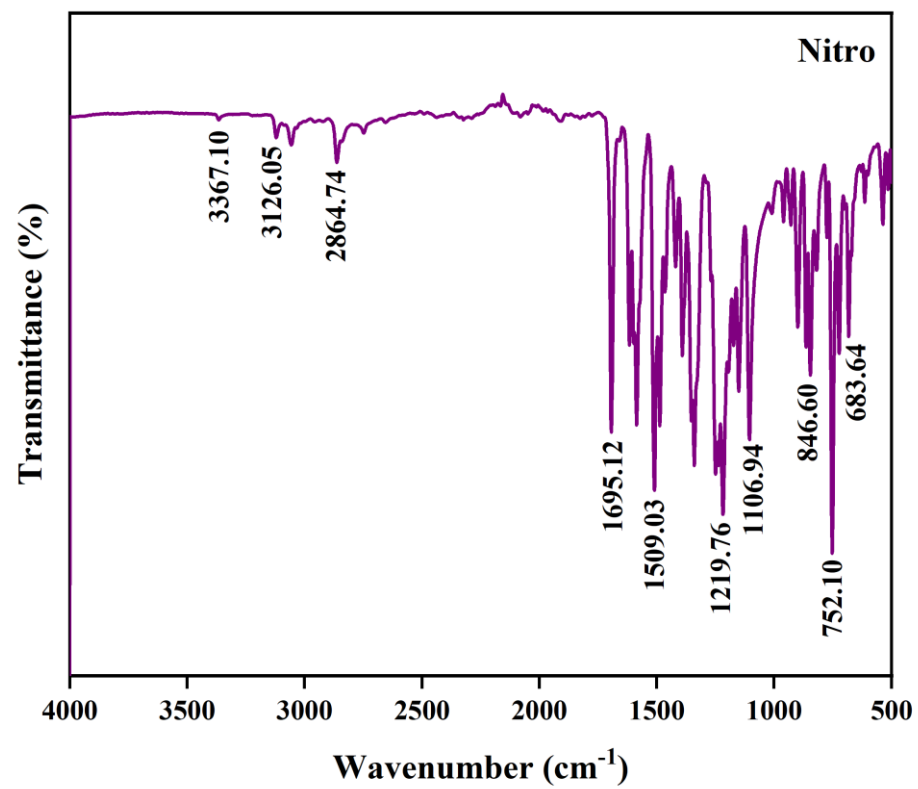


Figure S17. FTIR spectrum of 2-(4-nitrophenoxy)quinoline-3-carbaldehyde (3.4)

Signature SIF VIT VELLORE
OMe

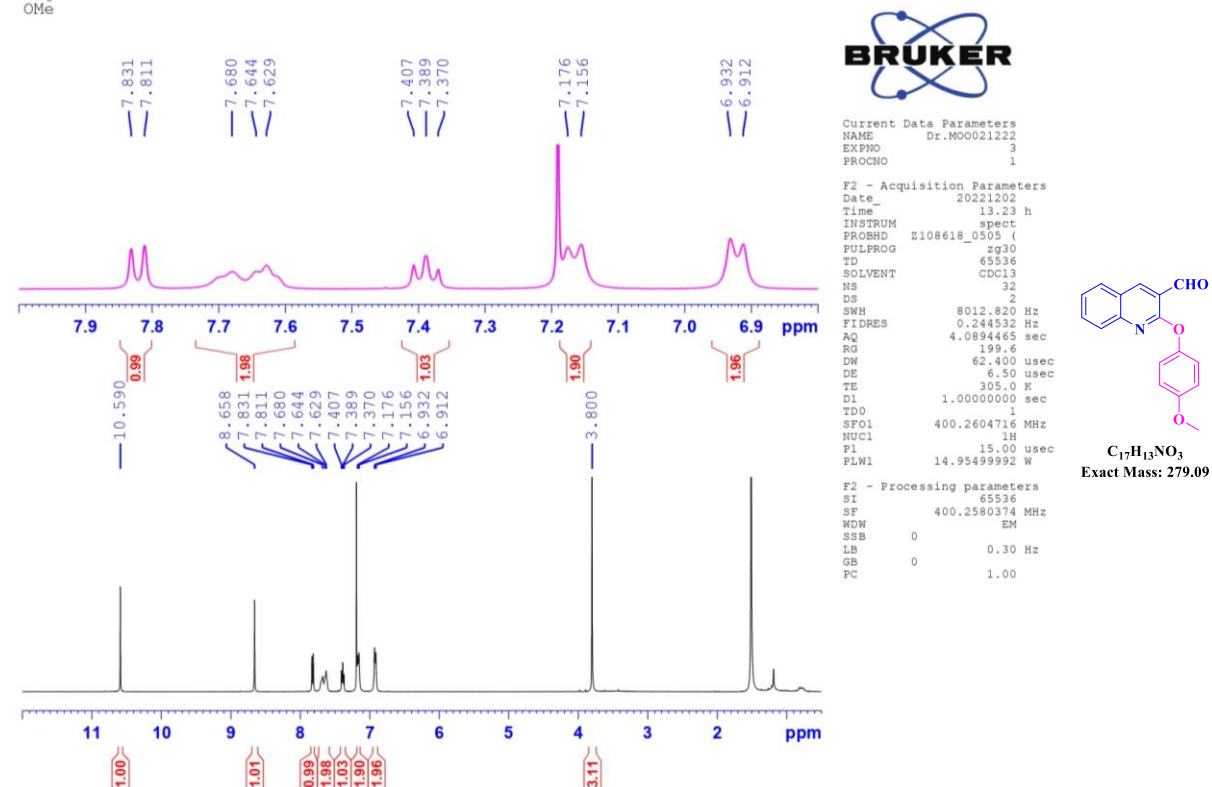
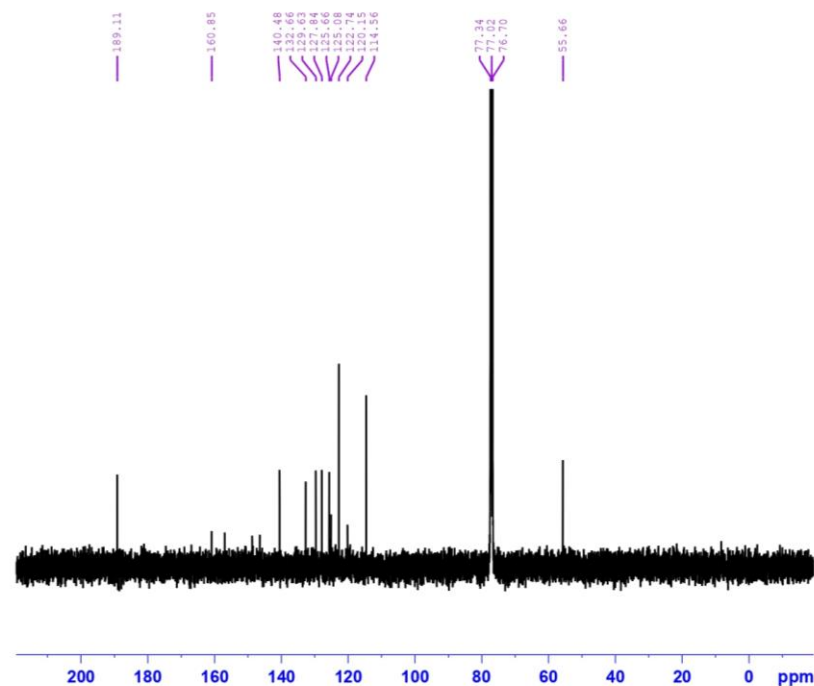


Figure S18. ¹H NMR spectrum of 2-(4-methoxyphenoxy)quinoline-3-carbaldehyde (**3.5**)



```

Current Data Parameters
NAME          Dr.MMG051222
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
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PROBHD        Z108618
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG            143.73 Hz
SW            20.800 usec
DE            6.50 usec
TE            305.9 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SF01          100.6550186 MHz
NUC1          13C
P1            10.00 usec
PL1           58.22499847 W
SF02          400.2596010 MHz
NUC2          1H
CPDPRG2       waltz12
PCPD2         90.00 usec
PL2           14.95499992 W
PLM12         0.41542000 W
PLM13         0.20895000 W

F2 - Processing parameters
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SF            100.64499542 MHz
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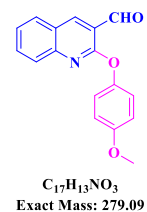


Figure S19. ¹³C NMR spectrum of 2-(4-methoxyphenoxy)quinoline-3-carbaldehyde (**3.5**)

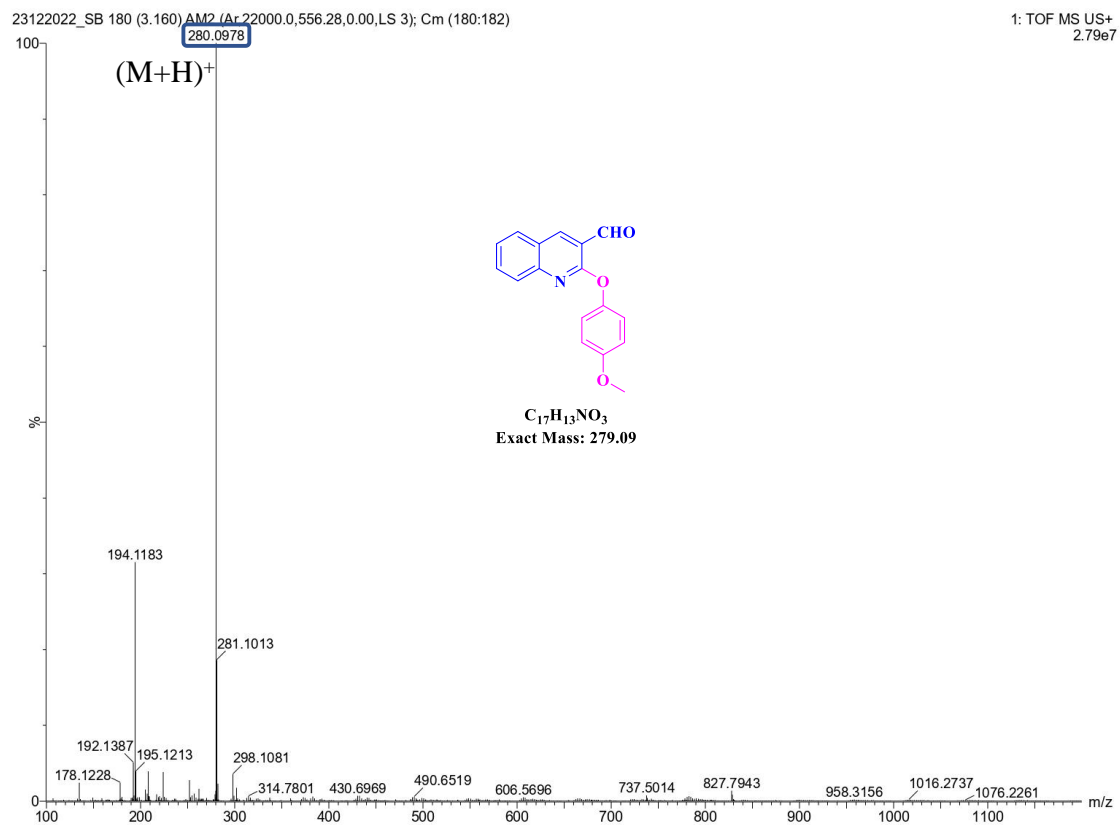


Figure S20. HRMS spectrum of 2-(4-methoxyphenoxy)quinoline-3-carbaldehyde (**3.5**)

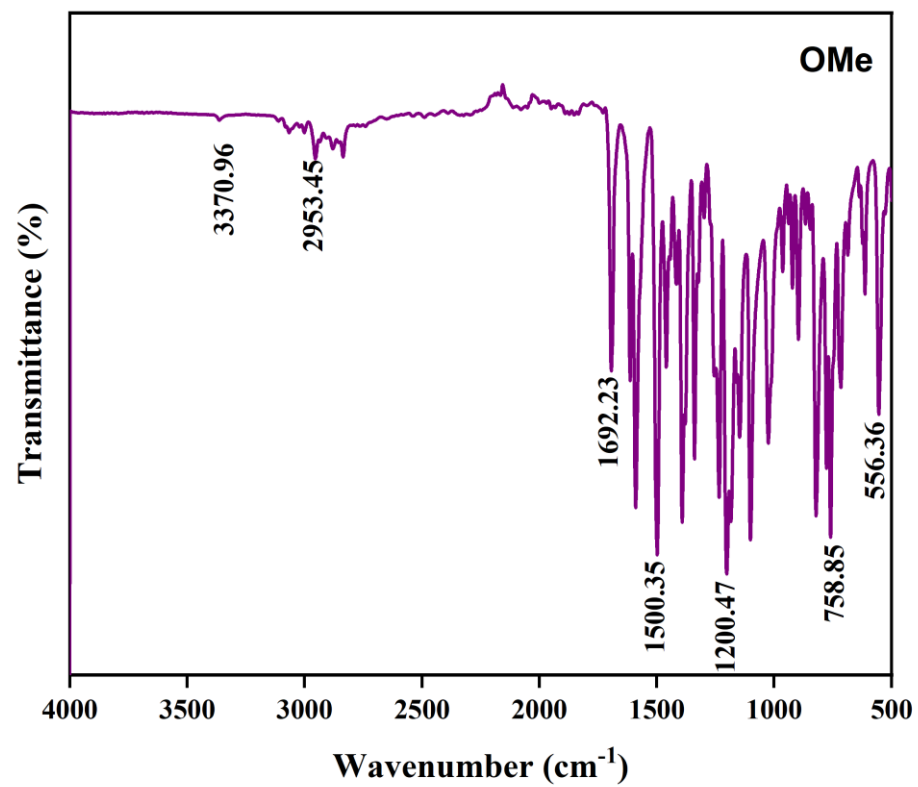


Figure S21. FTIR spectrum of 2-(4-methoxyphenoxy)quinoline-3-carbaldehyde (3.5)

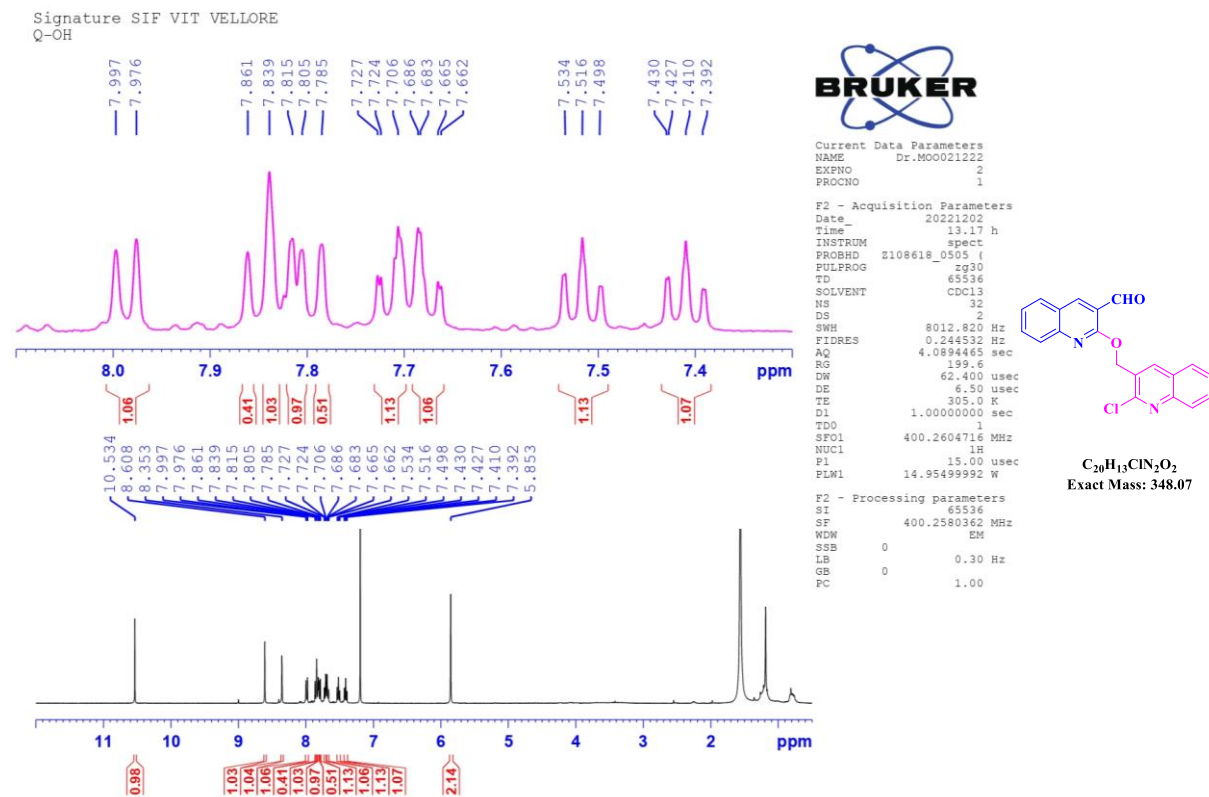


Figure S22. ¹H NMR spectrum of 2-((2-chloroquinolin-3-yl)methoxy)quinoline-3-carbaldehyde (3.6)

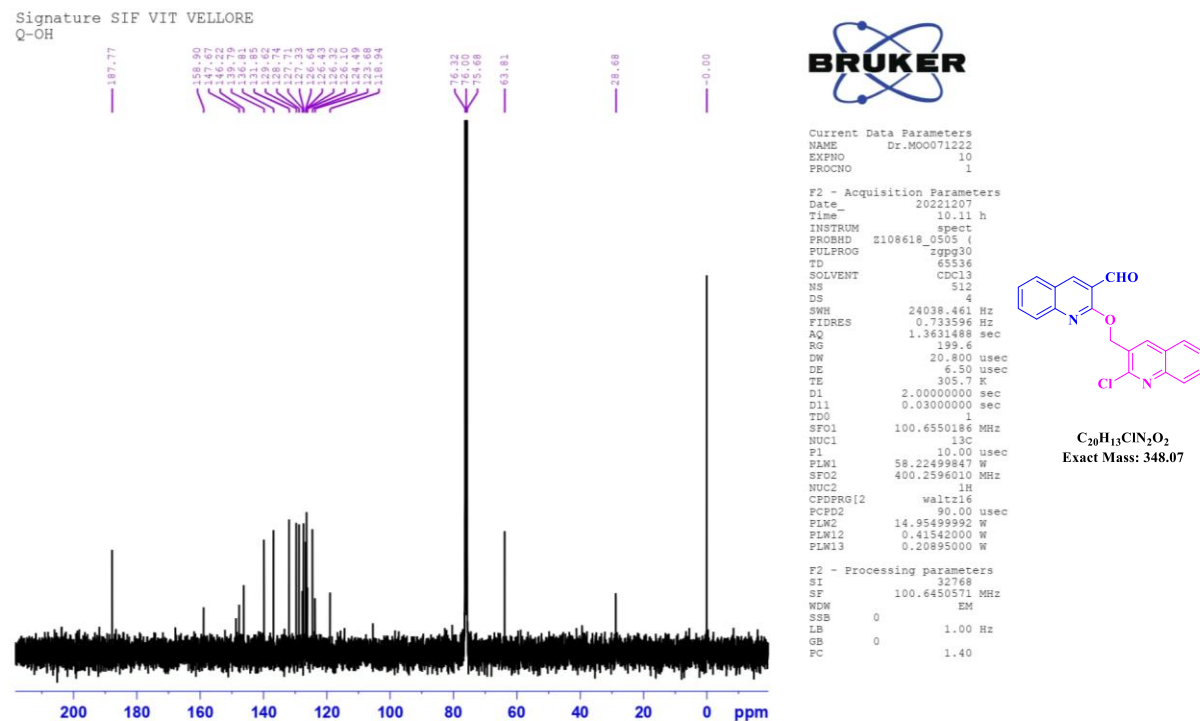


Figure S23. NMR spectrum of 2-((2-chloroquinolin-3-yl)methoxy)quinoline-3-carbaldehyde (**3.6**)

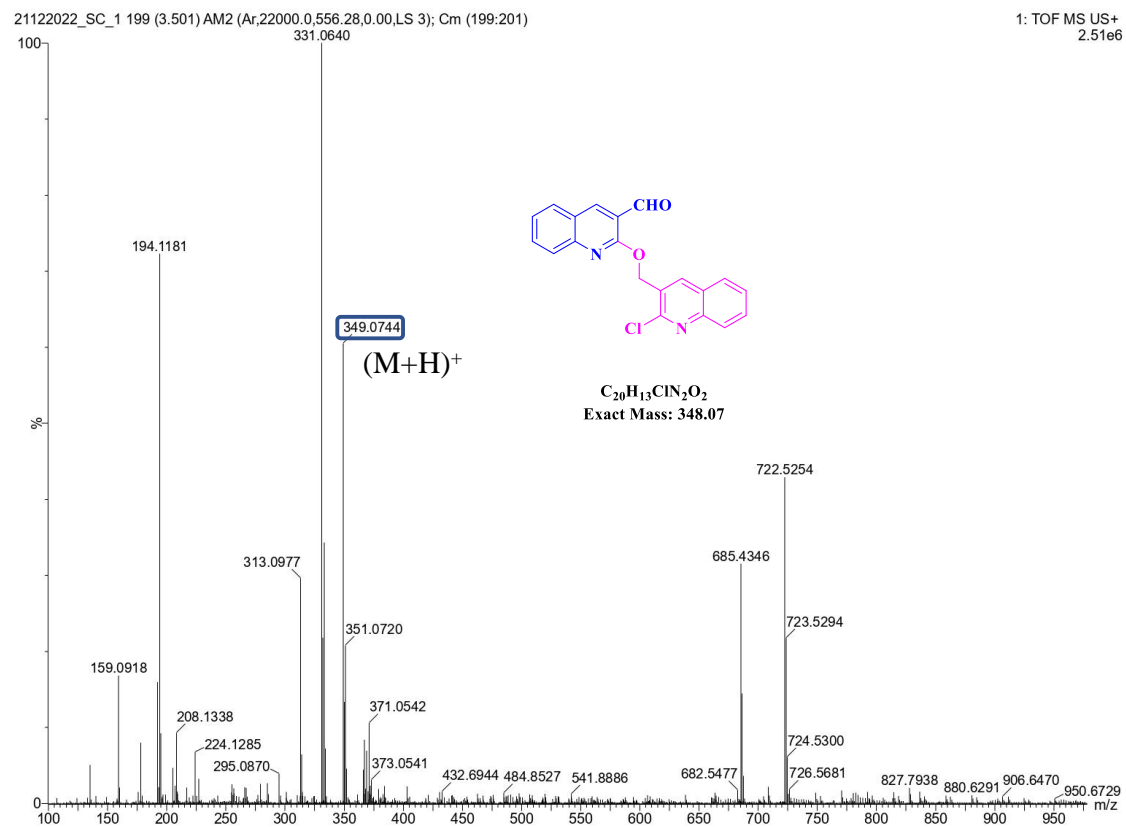


Figure S24. HRMS spectrum of 2-((2-chloroquinolin-3-yl)methoxy)quinoline-3-carbaldehyde (**3.6**)

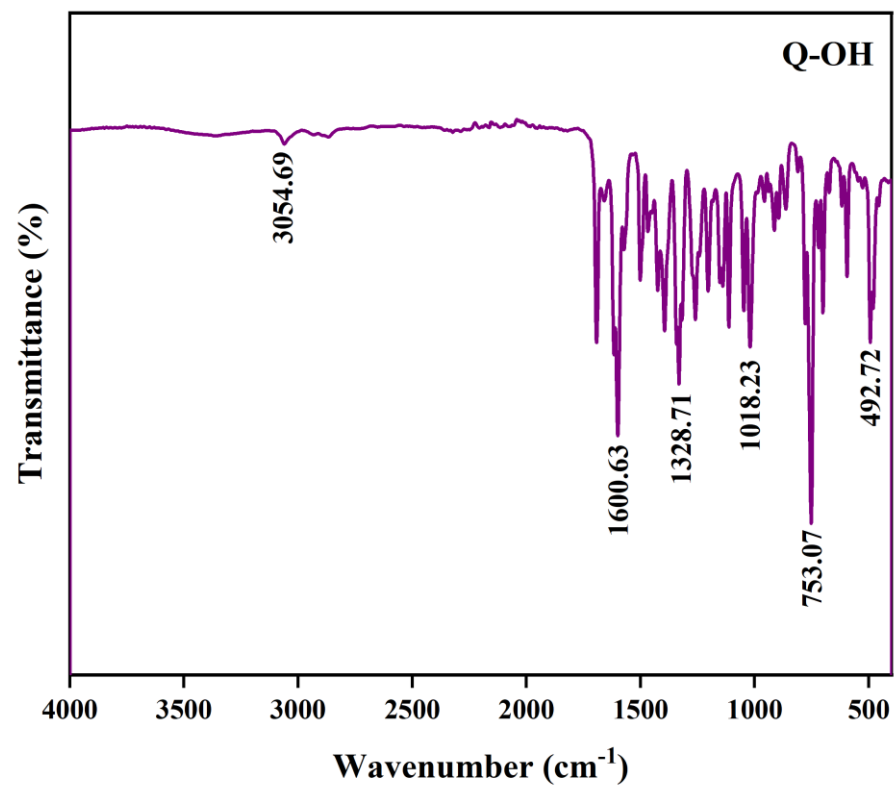


Figure S25. FTIR spectrum of 2-((2-chloroquinolin-3-yl)methoxy)quinoline-3-carbaldehyde (**3.6**)

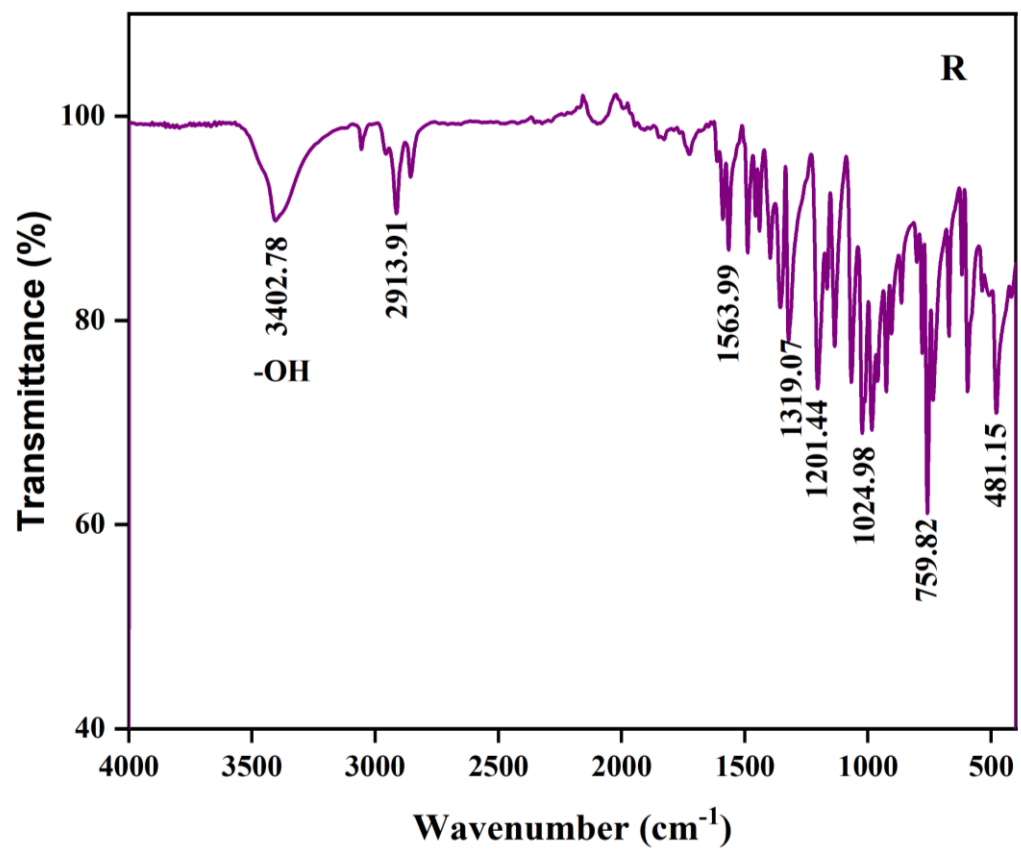
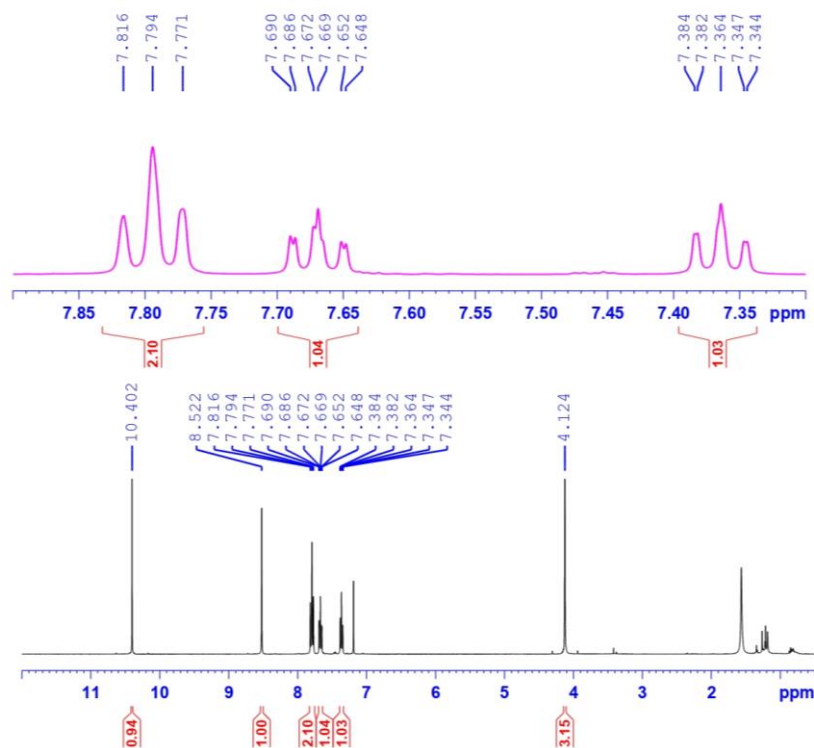


Figure S26. FTIR spectrum of (2-chloroquinolin-3-yl)methanol

Signature SIF VIT VELLORE
MeOH



Current Data Parameters
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EXPNO 30
PROCNO 1

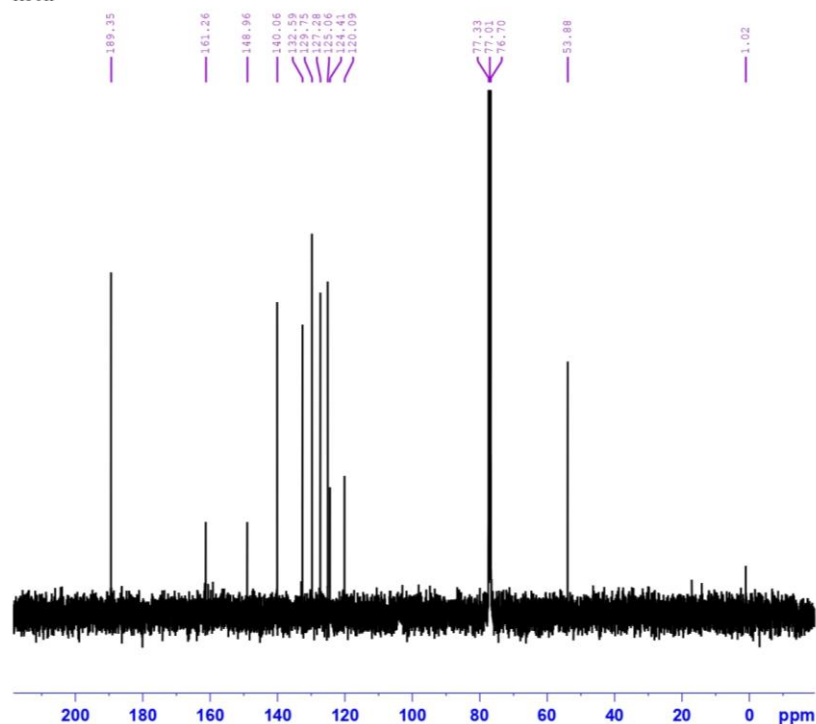
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 304.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580376 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Figure S27. 1H NMR spectrum of 2-methoxyquinoline-3-carbaldehyde (3.7)

Signature SIF VIT VELLORE
MeOH



Current Data Parameters
NAME MeOH C13
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
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SOLVENT CDC13
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SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DM 20.800 usec
DE 6.50 usec
TE 305.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLN1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLN2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

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

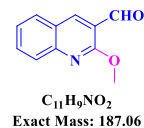


Figure S28. ¹³C NMR spectrum of 2-methoxyquinoline-3-carbaldehyde (**3.7**)

23122022_SMH 166 (2,923) AM2 (Ar,22000.0,556.28,0.00,LS 3); Cm (166:169)

1: TOF MS US+
5.53e7

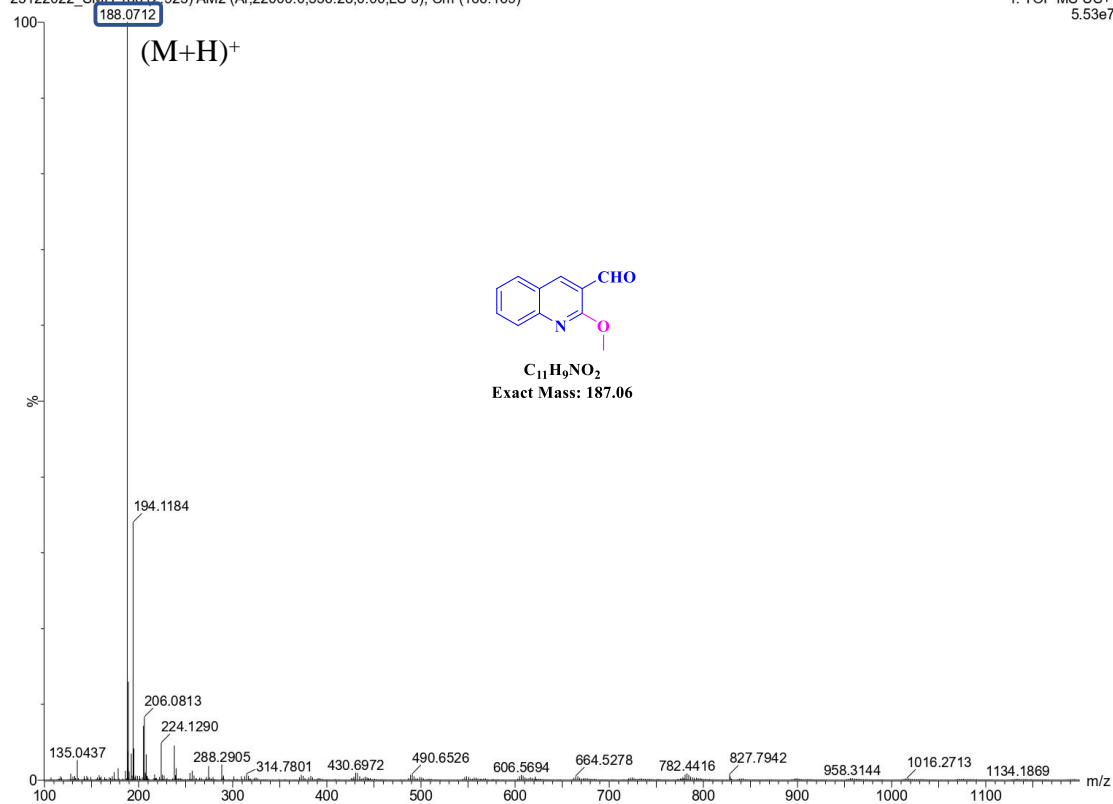


Figure S29. HRMS spectrum of 2-methoxyquinoline-3-carbaldehyde (**3.7**)

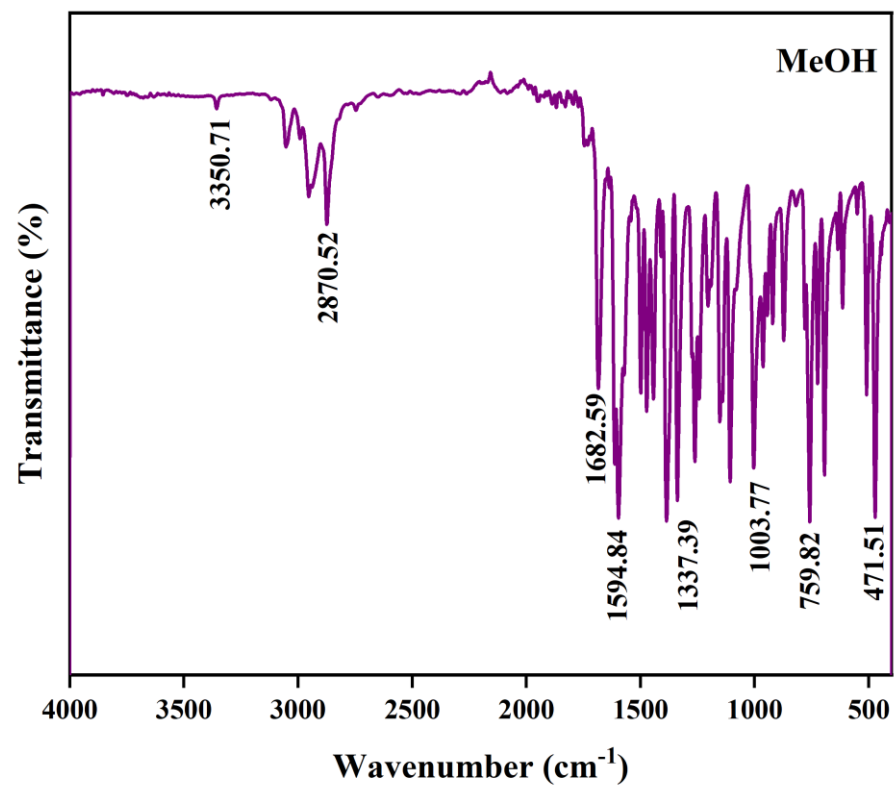


Figure S30. FTIR spectrum of 2-methoxyquinoline-3-carbaldehyde (3.7)