

Microwave-assisted expeditious and efficient synthesis of novel quinolin-4-yl methoxychromen-2- and -4-ones catalyzed by YbCl₃ under solvent free one-pot three components domino reaction and their antimicrobial activity

Sumit Kumar,^aAlok Patel^b and Naseem Ahmed^{a,*}

^a*Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247 667, Uttarakhand, India.*

^b*Department of Biotechnology, Indian Institute of Technology Roorkee, Roorkee 247 667, Uttarakhand, India.*

E-mail address: nasemfcy@iitr.ac.in

SUPPORTING INFORMATION

Table of Contents

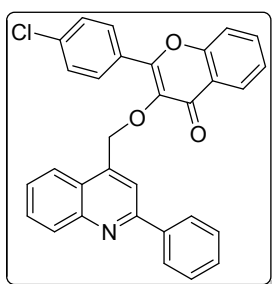
General Information	S2
Characterization Data	S2-S13
¹H and ¹³C Spectra	S14-S35

General Information

Unless otherwise noted, chemicals were purchased from commercial suppliers at the highest purity grade available and were used without further purification. Solvents were distilled by standard methods. Thin layer chromatography was performed on Merck precoated 0.25 mm silica gel plates (60F-254) using UV light as visualizing agent and/or iodine as developing agent. Silica gel (100-200 mesh) was used for column chromatography. IR spectra were recorded on FT-IR spectrometer and expressed as wave numbers (cm^{-1}). ^1H and ^{13}C NMR spectra were recorded on a BrukerAvance500&Jeol Resonance ECX 400 spectrometer. Spectra were referenced internally to the residual proton resonance in CDCl_3 (δ 7.26 ppm) or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to CDCl_3 (δ 77.23 ppm, the middle peak). Spectra were processed using Bruker Topspin[®] 3.0.b.8. Coupling constants are expressed in Hz. The following abbreviations are used to explain the multiplicities: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet, br = broad. High-resolution mass spectra (HRMS) were obtained on a Bruker micrOTOF[™]-Q II mass spectrometer (ESIMS).

Characterization Data

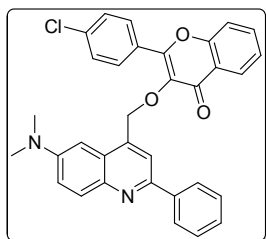
2-(4-chlorophenyl)-3-((2-phenylquinolin-4-yl)methoxy)-4H-chromen-4-one (4a)



Yield: 95% as pale yellow liquid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.11 (d, $J = 11$ Hz, 1H), 7.89-7.87 (m, 3H), 7.71-7.68 (m, 1H), 7.65-7.60 (m, 2H), 7.53 (d, $J = 9.5$ Hz, 3H), 7.52-7.49 (m, 1H), 7.48-7.46 (m, 1H), 7.44-7.39 (m, 1H), 7.24-7.20 (m, 2H), 6.91-6.87 (m, 3H), 4.98 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.4, 158.5, 156.2, 155.3, 140.6, 138.7, 137.2, 136.3, 134.7, 134.1, 133.7, 130.4, 130.2, 129.9, 129.7, 129.3, 129.1, 128.8,

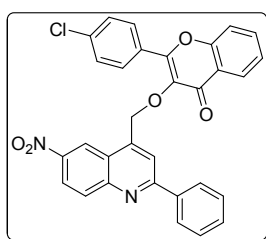
128.5, 125.9, 125.3, 123.8, 120.3, 118.2, 115.5, 86.3, 76.6. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1704, 1695, 1630, 1592, 1513, 1465, 1410, 1325, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{31}\text{H}_{20}\text{ClNNaO}_3$ $[\text{M}+\text{Na}]^+$: 512.1023, found: 512.1021.

2-(4-chlorophenyl)-3-((6-(dimethylamino)-2-phenylquinolin-4-yl)methoxy)-4H-chromen-4-one (4b)



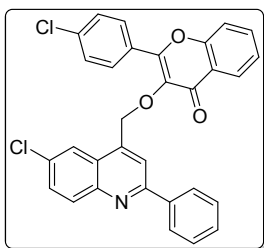
Yield: 94% as brownish semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.16 (dd, $J = 2, 10$ Hz, 1H), 8.06 (d, $J = 11$ Hz, 2H), 7.93 (dd, $J = 1.5, 10$ Hz, 2H), 7.73 (dd, $J = 2, 10.5$ Hz, 2H), 7.64-7.62 (m, 3H), 7.46 (d, $J = 10$ Hz, 1H), 7.39 (d, $J = 11$ Hz, 4H), 7.34-7.30 (m, 1H), 7.18 (s, 1H), 4.96 (s, 2H), 2.98 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 174.2, 160.4, 155.1, 155.0, 154.3, 152.5, 143.1, 141.5, 138.4, 136.7, 133.5, 131.5, 130.0, 129.8, 129.7, 129.0, 128.5, 125.5, 125.2, 124.8, 123.7, 118.0, 111.1, 110.8, 110.5, 86.3, 76.5, 42.1. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3090, 3072, 2949, 2915, 1705, 1692, 1625, 1594, 1515, 1460, 1412, 1303, 1244, 1176, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{33}\text{H}_{25}\text{ClN}_2\text{NaO}_3$ $[\text{M}+\text{Na}]^+$: 555.1445, found: 555.1432.

2-(4-chlorophenyl)-3-((6-nitro-2-phenylquinolin-4-yl)methoxy)-4H-chromen-4-one (4c)



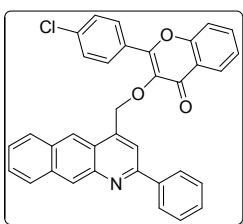
Yield: 91% as yellow semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.35 (d, $J = 11$ Hz, 2H), 8.15 (dd, $J = 1.5, 10$ Hz, 2H), 8.09-8.05 (m, 4H), 7.99 (d, $J = 10$ Hz, 1H), 7.78 (dd, $J = 1.5, 10.5$ Hz, 1H), 7.69-7.64 (m, 2H), 7.50-7.39 (m, 3H), 7.23-7.22 (m, 2H), 4.98 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.1, 160.5, 155.8, 155.5, 151.2, 146.2, 141.3, 140.2, 138.6, 136.8, 133.2, 133.6, 130.5, 130.2, 129.4, 129.0, 128.5, 125.6, 125.5, 125.1, 124.4, 123.9, 121.2, 118.3, 115.2, 86.3, 76.5. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3095, 3077, 2953, 2915, 1702, 1685, 1628, 1598, 1517, 1490, 1455, 1410, 1360, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{31}\text{H}_{19}\text{ClN}_2\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 557.0874, found: 557.0871.

3-((6-chloro-2-phenylquinolin-4-yl)methoxy)-2-(4-chlorophenyl)-4H-chromen-4-one (4d)



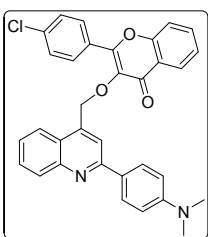
Yield: 89% as brownish semi-solid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 8.25 (dd, $J = 2, 10$ Hz, 1H), 8.11 (d, $J = 10.5$ Hz, 2H), 7.87 (d, $J = 9$ Hz, 2H), 7.70-7.41 (m, 6H), 7.28 (d, $J = 3$ Hz, 2H), 7.10 (dd, $J = 3.5, 11$ Hz, 2H), 6.95 (d, $J = 11$ Hz, 2H), 4.96 (s, 2H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3 , ppm): δ 175.5, 161.4, 156.4, 155.3, 150.6, 138.7, 137.3, 136.2, 134.7, 134.1, 130.4, 130.2, 129.9, 129.2, 129.1, 128.8, 128.5, 128.4, 125.9, 125.4, 125.3, 123.7, 120.7, 118.1, 117.3, 86.5, 76.6. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1701, 1695, 1629, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI $^+$): m/z calcd. for $\text{C}_{31}\text{H}_{19}\text{Cl}_2\text{NNaO}_3$ $[\text{M}+\text{Na}]^+$: 546.0634, found: 546.0635.

2-(4-chlorophenyl)-3-((2-phenylbenzo[g]quinolin-4-yl)methoxy)-4H-chromen-4-one (4e)



Yield: 86% as brownish semi-solid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 8.1-7.0 (m, 20 H), 4.83 (s, 2H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3 , ppm): δ 175.7, 159.4, 156.5, 155.3, 153.9, 138.7, 137.3, 136.1, 134.8, 134.2, 133.7, 130.4, 130.2, 130.0, 129.7, 129.3, 129.1, 128.8, 128.5, 127.8, 126.5, 126.4, 125.8, 125.4, 123.4, 118.1, 109.5, 86.1, 76.8. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3098, 3055, 2955, 2919, 1701, 1686, 1627, 1594, 1517, 1462, 1410, 1247, 1174, 1029. HRMS (ESI $^+$): m/z calcd. for $\text{C}_{35}\text{H}_{22}\text{ClNNaO}_3$ $[\text{M}+\text{Na}]^+$: 562.1180, found: 562.1169.

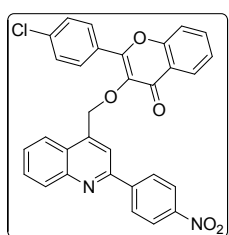
2-(4-chlorophenyl)-3-((2-(4-(dimethylamino)phenyl)quinolin-4-yl)methoxy)-4H-chromen-4-one (4f)



Yield: 84% as pale yellow semi-solid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 8.14 (dd, $J = 2, 10$ Hz, 1H), 8.04 (d, $J = 11$ Hz, 1H), 7.91 (dd, $J = 1.5, 10$ Hz, 1H), 7.72 (dd, $J = 2, 10.5$ Hz, 1H), 7.64-7.62 (m, 6H), 7.46 (d, $J = 10$ Hz, 1H), 7.39 (d, $J = 11$ Hz, 1H), 7.34-7.30 (m, 1H), 7.18-7.14 (m, 2H),

6.59 (d, $J = 10$ Hz, 2H), 4.94 (s, 2H), 2.96 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 174.6, 160.3, 155.2, 155.0, 154.2, 152.7, 143.2, 141.7, 138.5, 136.7, 133.7, 133.4, 131.8, 130.1, 129.2, 129.0, 128.5, 125.5, 125.2, 124.8, 123.7, 118.0, 111.1, 110.8, 110.5, 86.0, 76.5, 39.9. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1703, 1695, 1630, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{33}\text{H}_{25}\text{ClN}_2\text{NaO}_3$ $[\text{M}+\text{Na}]^+$: 555.1445, found: 555.1441.

2-(4-chlorophenyl)-3-((2-(4-nitrophenyl)quinolin-4-yl)methoxy)-4H-chromen-4-one (4g)

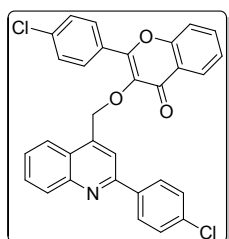


Yield: 95% as yellow semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.34 (d, $J = 11$ Hz, 2H), 8.17 (dd, $J = 1.5, 10$ Hz, 2H), 8.08-8.03 (m, 4H), 7.98 (d, $J = 10$ Hz, 1H), 7.79 (dd, $J = 1.5, 10.5$ Hz, 1H), 7.67-7.65 (m, 2H), 7.52-7.35 (m, 3H), 7.25-7.21 (m, 2H), 4.96 (s, 2H). ^{13}C NMR (100

MHz, CDCl_3 , ppm): δ 174.8, 160.9, 155.5, 155.2, 151.1, 146.5, 141.9, 140.0, 138.6, 136.9, 133.9, 133.5, 130.5, 130.3, 129.3, 129.1, 128.7, 125.7, 125.4, 125.0, 124.3, 123.9, 121.1, 118.1, 115.3, 86.2, 76.5. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3095, 3077, 2953, 2915, 1700, 1685, 1627, 1598, 1517, 1490, 1455, 1410, 1360, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{31}\text{H}_{19}\text{ClN}_2\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 557.0874, found: 557.0865.

2-(4-chlorophenyl)-3-((2-(4-chlorophenyl)quinolin-4-yl)methoxy)-4H-chromen-4-one

(4h)



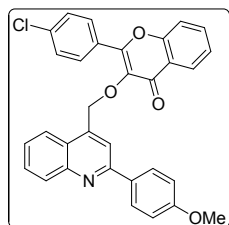
Yield: 88% as brownish semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.16 (d, $J = 10$ Hz, 1H), 8.05 (d, $J = 11$ Hz, 1H), 7.94 (d, $J = 9.5$ Hz, 1H), 7.77-7.72 (m, 5H), 7.65-7.61 (m, 1H), 7.43-7.40 (m, 6H), 7.34 (t, $J = 9.5$ Hz, 1H), 7.21-7.17 (m, 1H), 4.96 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3 ,

ppm): δ 174.7, 161.4, 155.4, 155.1, 152.8, 144.8, 141.8, 140.8, 138.6, 136.8, 134.6, 133.8, 133.4, 130.8, 130.2, 129.4, 129.3, 129.0, 128.6, 125.6, 125.3, 124.9, 123.8, 121.1, 118.0, 86.2, 76.5. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1699, 1695, 1627, 1592, 1513,

1465, 1410, 1247, 1174, 1029. HRMS (ESI+): m/z calcd. for $C_{31}H_{19}Cl_2NNaO_3$ $[M+Na]^+$: 546.0634, found: 546.0634.

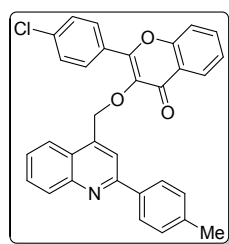
2-(4-chlorophenyl)-3-((2-(4-methoxyphenyl)quinolin-4-yl)methoxy)-4H-chromen-4-one

(4i)



Yield: 86% as brownish semi-solid; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.22 (dd, $J = 1.5, 11.5$ Hz, 1H), 8.09 (dd, $J = 2.5, 8.5$ Hz, 2H), 8.00 (dd, $J = 1.5, 9.5$ Hz, 1H), 7.82-7.79 (m, 5H), 7.71-7.67 (m, 1H), 7.52 (d, $J = 10.5$ Hz, 1H), 7.47-7.44 (m, 3H), 7.41-7.39 (m, 1H), 7.27-7.23 (m, 1H), 6.98 (s, 1H), 4.98 (s, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 174.9, 164.7, 155.6, 155.3, 153.0, 151.0, 145.9, 142.0, 138.7, 137.0, 133.9, 133.5, 132.1, 130.4, 130.0, 129.5, 129.1, 128.8, 125.9, 125.5, 125.1, 124.0, 120.4, 118.1, 114.4, 86.3, 76.5, 55.7. FTIR (KBr, $\nu = cm^{-1}$): 3089, 3067, 2950, 2916, 1702, 1695, 1629, 1592, 1513, 1425, 1410, 1246, 1174, 1029. HRMS (ESI+): m/z calcd. for $C_{32}H_{22}ClNNaO_4$ $[M+Na]^+$: 542.1129, found: 542.1118.

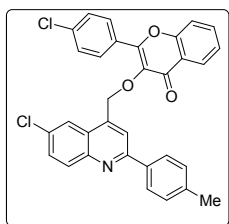
2-(4-chlorophenyl)-3-((2-(p-tolyl)quinolin-4-yl)methoxy)-4H-chromen-4-one (4j)



Yield: 90% as brownish semi-solid; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.23 (dd, $J = 1.5, 10$ Hz, 2H), 8.09 (d, $J = 11$ Hz, 1H), 8.00 (dd, $J = 1.5, 10$ Hz, 1H), 7.81 (dd, $J = 1.5$ Hz, 10 Hz, 2H), 7.74 (d, $J = 10.5$ Hz, 1H), 7.48-7.44 (m, 3H), 7.39 (t, $J = 1.5$ Hz, 1H), 7.29 (d, $J = 10$ Hz, 2H), 7.25-7.22 (m, 2H), 4.99 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 174.8, 158.5, 155.5, 155.2, 153.0, 148.1, 145.6, 143.4, 141.9, 138.7, 136.9, 134.2, 133.8, 133.5, 130.3, 129.9, 129.8, 129.4, 129.1, 128.7, 125.8, 125.4, 125.0, 123.9, 118.1, 86.3, 76.5, 21.9. FTIR (KBr, $\nu = cm^{-1}$): 3092, 3075, 2953, 2917, 1705, 1695, 1630, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI+): m/z calcd. for $C_{32}H_{22}ClNNaO_3$ $[M+Na]^+$: 526.1180, found: 526.1183.

3-((6-chloro-2-(p-tolyl)quinolin-4-yl)methoxy)-2-(4-chlorophenyl)-4H-chromen-4-one

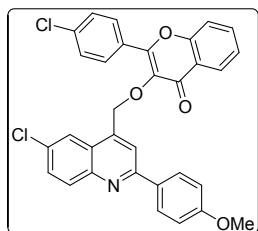
(4k)



Yield: 89% as brownish semi-solid; ^1H NMR (500 MHz, CDCl_3 , ppm): δ 8.17 (m, 3H), 7.75 (d, $J = 7.5$ Hz, 2H), 7.69 (t, $J = 7$ Hz, 1H), 7.54-7.46 (m, 3H), 7.40 (t, $J = 7.5$ Hz, 1H), 7.31-7.28 (m, 2H), 7.09 (d, $J = 8$ Hz, 2H), 6.95 (d, $J = 8.5$ Hz, 2H), 4.98 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (100

MHz, CDCl_3 , ppm): δ 175.2, 156.0, 155.4, 150.8, 149.0, 145.9, 141.5, 138.8, 137.2, 134.2, 134.0, 130.4, 130.0, 129.8, 129.4, 129.0, 128.8, 128.3, 125.9, 125.3, 125.2, 123.9, 120.8, 118.2, 117.4, 86.4, 76.6, 22.0. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3096, 3075, 2959, 2915, 1698, 1695, 1630, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{32}\text{H}_{21}\text{Cl}_2\text{NNaO}_3$ [$\text{M}+\text{Na}$]⁺: 560.0790, found: 560.0785.

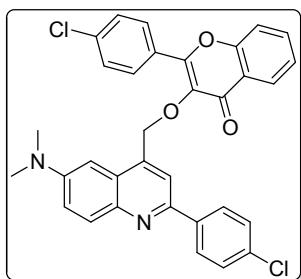
3-((6-chloro-2-(4-methoxyphenyl)quinolin-4-yl)methoxy)-2-(4-chlorophenyl)-4H-chromen-4-one (4l)



Yield: 85% as pale yellow semi-solid; ^1H NMR (500 MHz, CDCl_3 , ppm): δ 8.22-8.08 (m, 2H), 7.81-7.66 (m, 4H), 7.53-7.37 (m, 3H), 7.25 (s, 1H), 7.07 (d, $J = 8$ Hz, 1H), 6.97-6.93 (m, 5H), 4.96 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.1, 164.8, 155.9,

155.3, 150.8, 145.7, 141.7, 138.7, 137.1, 135.6, 134.0, 132.2, 130.3, 129.8, 129.3, 129.0, 128.8, 128.2, 125.8, 125.2, 123.8, 120.8, 118.1, 117.4, 114.4, 87.0, 76.6, 55.6. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1701, 1695, 1628, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{32}\text{H}_{21}\text{Cl}_2\text{NNaO}_4$ [$\text{M}+\text{Na}$]⁺: 576.0739, found: 576.0735.

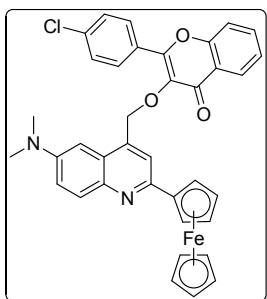
2-(4-chlorophenyl)-3-((2-(4-chlorophenyl)-6-(dimethylamino)quinolin-4-yl)methoxy)-4H-chromen-4-one (4m)



Yield: 90% as brownish semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.21-8.09 (m, 2H), 7.69-7.67 (m, 4H), 7.52-7.37 (m, 3H),

7.05-6.94 (m, 3H), 6.62 (d, $J = 10$ Hz, 4H), 4.96 (s, 2H), 3.01 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.1, 155.9, 155.1, 154.5, 151.2, 145.2, 141.5, 138.6, 137.0, 134.0, 132.3, 130.3, 129.2, 129.0, 128.7, 128.0, 125.6, 125.1, 124.7, 124.5, 123.7, 121.0, 118.1, 117.4, 111.0, 86.3, 76.6, 39.9. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1701, 1695, 1629, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{33}\text{H}_{24}\text{Cl}_2\text{N}_2\text{NaO}_3$ $[\text{M}+\text{Na}]^+$: 589.1056, found: 589.1051.

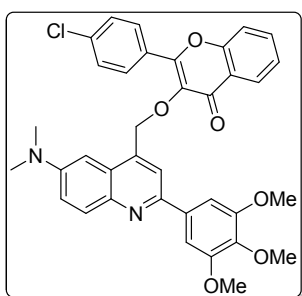
3-((6-dimethylamino-2-(ferrocenyl)quinolin-4-yl)methoxy)-2-(4-chlorophenyl)-4H-chromen-4-one (4n)



Yield: 85% as blackish semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.23 (dd, $J = 1.5, 10$ Hz, 1H), 8.10 (dd, $J = 2.5, 9$ Hz, 2H), 7.69-7.67 (m, 1H), 7.53 (d, $J = 10.5$ Hz, 1H), 7.48-7.45 (m, 2H), 7.42-7.38 (m, 1H), 7.28 (d, $J = 3$ Hz, 1H), 7.09 (dd, $J = 3, 11$ Hz, 2H), 6.96 (s, 1H), 4.96 (s, 2H), 4.79 (t, $J = 2.5$ Hz, 2H), 4.62 (t, $J = 2.5$ Hz, 2H), 4.25 (s,

5H), 3.01 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.4, 156.2, 155.3, 150.8, 146.1, 142.3, 138.7, 137.2, 134.1, 130.4, 129.3, 128.9, 128.8, 128.3, 125.8, 125.3, 125.2, 123.8, 120.8, 118.1, 117.4, 87.2, 78.4, 76.9, 73.8, 70.0, 69.9, 42.5. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3102, 3092, 3078, 2956, 2915, 1703, 1695, 1630, 1592, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{37}\text{H}_{29}\text{ClFeN}_2\text{NaO}_3$ $[\text{M}+\text{Na}]^+$: 663.1108, found: 663.1102.

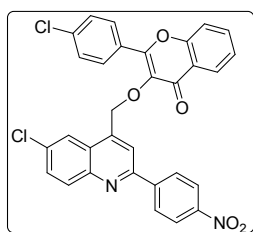
2-(4-chlorophenyl)-3-((6-(dimethylamino)-2-(3,4,5-trimethoxyphenyl)quinolin-4-yl)methoxy)-4H-chromen-4-one (4o)



Yield: 86% as brownish semi-solid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.09 (dd, $J = 3, 10$ Hz, 2H), 7.68-7.65 (m, 4H), 7.51-7.37 (m, 3H), 7.32-7.28 (m, 3H), 7.25 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.3, 156.2, 155.1, 151.0, 150.4, 147.1, 142.6, 140.0, 138.7, 137.3, 134.2, 132.4, 130.6, 130.4, 129.3, 128.8,

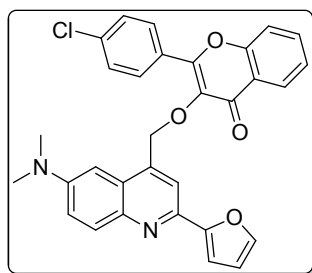
128.1, 125.7, 125.3, 125.1, 124.5, 123.5, 120.8, 118.1, 102.2, 86.5, 76.6, 61.0, 56.3, 42.2.
FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1699, 1695, 1627, 1592, 1513, 1465,
1410, 1346, 1247, 1174, 1030. HRMS (ESI⁺): m/z calcd. for $\text{C}_{36}\text{H}_{31}\text{ClN}_2\text{NaO}_6$ $[\text{M}+\text{Na}]^+$:
645.1762, found: 645.1756.

3-((6-chloro-2-(4-nitrophenyl)quinolin-4-yl)methoxy)-2-(4-chlorophenyl)-4H-chromen-4-one (4p)



Yield: 94% as yellow liquid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.33 (dd, $J = 2, 10.5$ Hz, 2H), 8.21 (d, $J = 10.5$ Hz, 1H), 8.09-8.01 (m, 2H), 8.03-8.01 (m, 2H), 7.70-7.66 (m, 1H), 7.53 (d, $J = 10.5$ Hz, 1H), 7.45 (dd, $J = 3, 11$ Hz, 2H), 7.41-7.37 (m, 1H), 7.25-7.24 (m, 2H), 7.09-7.07 (m, 1H), 6.93 (d, $J = 3$ Hz, 1H), 4.93 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.5, 156.4, 155.4, 151.2, 150.6, 147.0, 142.6, 140.0, 138.7, 137.3, 134.2, 132.4, 130.6, 130.4, 129.3, 128.8, 128.4, 125.9, 125.4, 125.3, 124.4, 123.7, 120.7, 118.2, 117.4, 87.6, 76.7. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1695, 1624, 1592, 1513, 1455, 1418, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{31}\text{H}_{18}\text{Cl}_2\text{N}_2\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 591.0484, found: 591.0475.

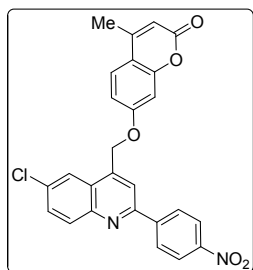
2-(4-chlorophenyl)-3-((6-(dimethylamino)-2-(furan-2-yl)quinolin-4-yl)methoxy)-4H-chromen-4-one (4q)



Yield: 87% as black-brown liquid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 8.21 (d, $J = 10$ Hz, 1H), 8.09 (d, $J = 10.5$ Hz, 1H), 7.69-7.67 (m, 2H), 7.53 (d, $J = 10.5$ Hz, 1H), 7.45 (d, $J = 10$ Hz, 1H), 7.41-7.37 (m, 1H), 7.26-7.25 (m, 3H), 7.08-7.05 (m, 2H), 6.93 (dd, $J = 1, 11$ Hz, 2H), 6.58 (s, 1H), 4.94 (s, 2H), 3.01 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 175.3, 160.9, 156.2, 155.3, 152.9, 150.8, 148.5, 143.2, 138.7, 137.2, 134.1, 132.1, 130.4, 129.2, 128.9, 128.8, 128.2, 125.8, 125.3, 125.2, 123.7, 121.8, 120.8, 118.1, 117.4, 112.8, 76.7, 41.8. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3092, 3075, 2953, 2917, 1701, 1695, 1628, 1592,

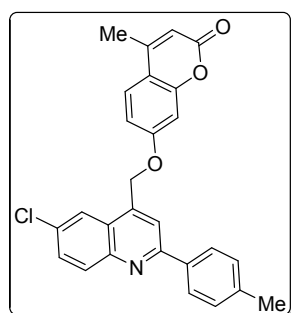
1513, 1465, 1410,1348, 1321, 1247, 1174, 1042. HRMS (ESI+): m/z calcd. for $C_{31}H_{23}ClN_2NaO_4$ $[M+Na]^+$: 545.1238, found: 545.1229.

7-((6-chloro-2-(4-nitrophenyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5a)



Yield: 94% as brown liquid; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.38 (d, $J = 11$ Hz, 3H), 8.07 (d, $J = 10.5$ Hz, 3H), 7.52 (d, $J = 11.5$ Hz, 1H), 7.30 (d, $J = 3$ Hz, 1H), 7.12 (dd, $J = 3, 11$ Hz, 2H), 6.92 (d, $J = 4$ Hz, 1H), 6.16 (s, 1H), 4.75 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 163.4, 161.7, 160.5, 155.1, 153.0, 151.2, 150.5, 140.1, 136.1, 130.7, 128.8, 128.6, 125.8, 125.6, 124.4, 120.6, 117.3, 114.4, 113.0, 112.4, 102.2, 86.1, 72.4, 18.8. FTIR (KBr, $\nu = cm^{-1}$): 3105, 3078, 2958, 2917, 1720, 1628, 1599, 1513, 1475, 1410, 1247, 1174, 1029. HRMS (ESI+): m/z calcd. for $C_{26}H_{17}ClN_2NaO_5$ $[M+Na]^+$: 495.0718, found: 495.0712.

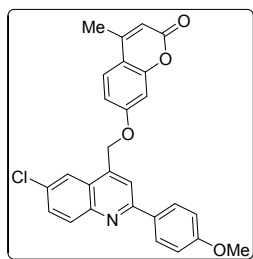
7-((6-chloro-2-(p-tolyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5b)



Yield: 91% as brown liquid; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.78 (d, $J = 10$ Hz, 2H), 7.53 (d, $J = 7.53, J = 10.5$ Hz, 1H), 7.34-7.30 (m, 4H), 7.12 (dd, $J = 10, 18$ Hz, 2H), 6.97-6.93 (m, 2H), 6.18 (s, 1H), 4.76 (s, 2H), 2.44 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 162.7, 161.6, 160.3, 154.7, 152.9, 150.4, 145.6, 135.8, 133.9, 129.8, 129.6, 128.6, 128.2, 125.5, 125.1, 120.5, 117.1, 114.1, 112.8, 112.0, 101.9, 86.6, 72.4, 21.7, 18.5. FTIR (KBr, $\nu = cm^{-1}$): 3105, 3078, 2958, 2917, 1725, 1627, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI+): m/z calcd. for $C_{27}H_{20}ClN_2NaO_3$ $[M+Na]^+$: 464.1023, found: 464.1019.

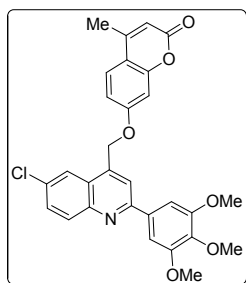
7-((6-chloro-2-(4-methoxyphenyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one

(5c)



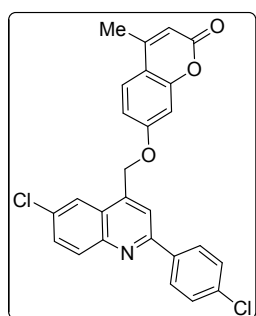
Yield: 89% as light yellow liquid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 7.85 (d, $J = 11$ Hz, 2H), 7.54 (d, $J = 11.5$ Hz, 1H), 7.32 (d, $J = 3$ Hz, 1H), 7.14 (dd, $J = 3, 10.5$ Hz, 2H), 7.01 (d, $J = 11$ Hz, 2H), 6.97-6.94 (m, 3H), 6.19 (s, 1H), 4.84 (s, 2H), 3.90 (s, 3H), 2.41 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3 , ppm): δ 164.9, 161.9, 160.6, 155.1, 153.1, 150.6, 134.4, 132.3, 129.9, 128.8, 128.5, 125.8, 125.5, 123.5, 120.7, 117.3, 114.5, 114.4, 113.1, 112.4, 102.2, 86.8, 76.7, 55.7, 18.8. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3105, 3078, 2958, 2917, 1723, 1629, 1592, 1513, 1465, 1410, 1245, 1173, 1024. HRMS (ESI⁺): m/z calcd. for $\text{C}_{27}\text{H}_{20}\text{ClNNaO}_4$ $[\text{M}+\text{Na}]^+$: 480.0973, found: 480.0965.

7-((6-chloro-2-(3,4,5-trimethoxyphenyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5d)



Yield: 85% as brown liquid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 8.02 (d, $J = 10.5$ Hz, 1H), 7.79 (d, $J = 3$ Hz, 1H), 7.63 (s, 3H), 7.60 (dd, $J = 3, 11$ Hz, 1H), 7.45-7.41 (m, 3H), 6.65 (s, 1H), 5.26 (s, 2H), 3.80 (s, 9H), 2.4 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3 , ppm): δ 162.5, 161.5, 160.5, 155.0, 153.7, 152.9, 150.7, 143.6, 137.9, 131.7, 128.9, 128.2, 125.7, 125.2, 120.7, 117.3, 114.3, 112.9, 112.3, 106.8, 102.2, 86.3, 76.6, 61.0, 56.3, 18.7. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3105, 3078, 2958, 2917, 1726, 1627, 1593, 1513, 1468, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for $\text{C}_{29}\text{H}_{24}\text{ClNNaO}_6$ $[\text{M}+\text{Na}]^+$: 540.1184, found: 540.1186.

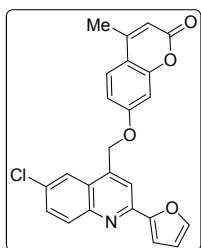
7-((6-chloro-2-(4-chlorophenyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5e)



Yield: 86% as brown liquid; $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 8.33-8.32 (m, 3H), 8.01-7.99 (m, 4H), 7.62-7.59 (m, 1H), 7.46-7.43 (m, 3H), 6.66 (s, 1H), 5.26 (s, 2H), 2.42 (s, 3H). $^{13}\text{C NMR}$ (100 MHz,

CDCl₃, ppm): δ 162.5, 161.5, 160.5, 155.0, 152.8, 150.7, 141.1, 137.7, 134.7, 131.0, 129.5, 128.9, 128.3, 125.8, 125.3, 120.7, 117.3, 114.3, 112.9, 112.4, 102.2, 86.5, 76.6, 18.7. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3102, 3078, 2958, 2917, 1722, 1629, 1595, 1513, 1465, 1410, 1247, 1174, 1029. HRMS (ESI⁺): m/z calcd. for C₂₆H₁₇Cl₂NNaO₃ [M+Na]⁺: 484.0477, found: 484.0469.

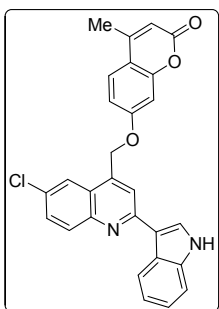
7-((6-chloro-2-(furan-2-yl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5f)



Yield: 88% as brown liquid; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.75 (t, $J = 1\text{ Hz}$, 1H), 7.58 (dd, $J = 3, 9\text{ Hz}$, 1H), 7.35 (d, $J = 3\text{ Hz}$, 2H), 7.31 (dd, $J = 0.5, 3\text{ Hz}$, 1H), 7.16 (dd, $J = 3.5, 11\text{ Hz}$, 2H), 7.01-6.97 (m, 2H), 6.66-6.65 (m, 1H), 6.21 (s, 1H), 4.85 (s, 2H), 2.44 (s, 3H). ¹³C NMR (100 MHz,

CDCl₃, ppm): δ 162.9, 161.6, 160.5, 155.0, 153.0, 152.9, 150.7, 148.3, 136.1, 128.9, 128.4, 125.8, 125.3, 121.5, 120.7, 117.4, 114.3, 112.9, 112.8, 112.4, 102.2, 86.3, 76.6, 18.8. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3107, 3075, 2953, 2915, 1725, 1630, 1595, 1513, 1465, 1410, 1247, 1174, 1024. HRMS (ESI⁺): m/z calcd. for C₂₄H₁₆ClNNaO₄ [M+Na]⁺: 440.0660, found: 440.0664.

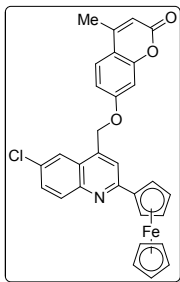
7-((6-chloro-2-(1H-indol-3-yl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5g)



Yield: 85% as brown liquid; ¹H NMR (500 MHz, CDCl₃, ppm): δ 8.17 (br, s, 1H, D₂O exchangeable), 7.75 (d, $J = 8\text{ Hz}$, 1H), 7.42-7.37 (m, 3H), 7.29 (t, $J = 7\text{ Hz}$, 1H), 7.22 (t, $J = 7\text{ Hz}$, 1H), 7.18-7.16 (m, 3H), 6.99 (m, 2H), 6.63 (s, 1H), 6.20 (s, 1H), 4.74 (s, 2H), 2.35 (s, 3H). ¹³C NMR (100 MHz, CDCl₃, ppm): δ 162.6, 160.6, 160.2, 155.7, 154.1, 152.5, 144.8,

136.3, 132.5, 131.0, 130.7, 128.4, 125.6, 124.3, 123.2, 121.4, 121.2, 120.9, 119.6, 114.0, 112.3, 111.5, 110.8, 110.2, 102, 86.4, 76.6, 18.5. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3307, 3114, 3075, 2958, 2917, 1723, 1628, 1599, 1515, 1463, 1410, 1247, 1174, 1024. HRMS (ESI⁺): m/z calcd. for C₂₈H₁₉ClN₂NaO₃ [M+Na]⁺: 489.0976, found: 489.0968.

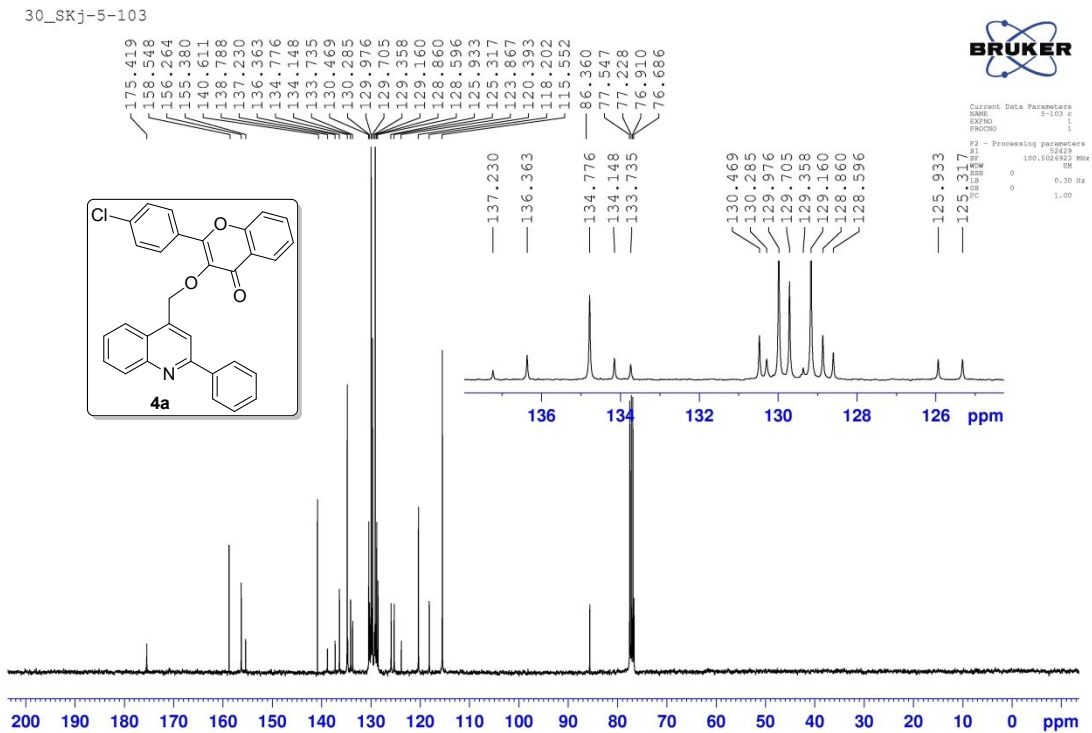
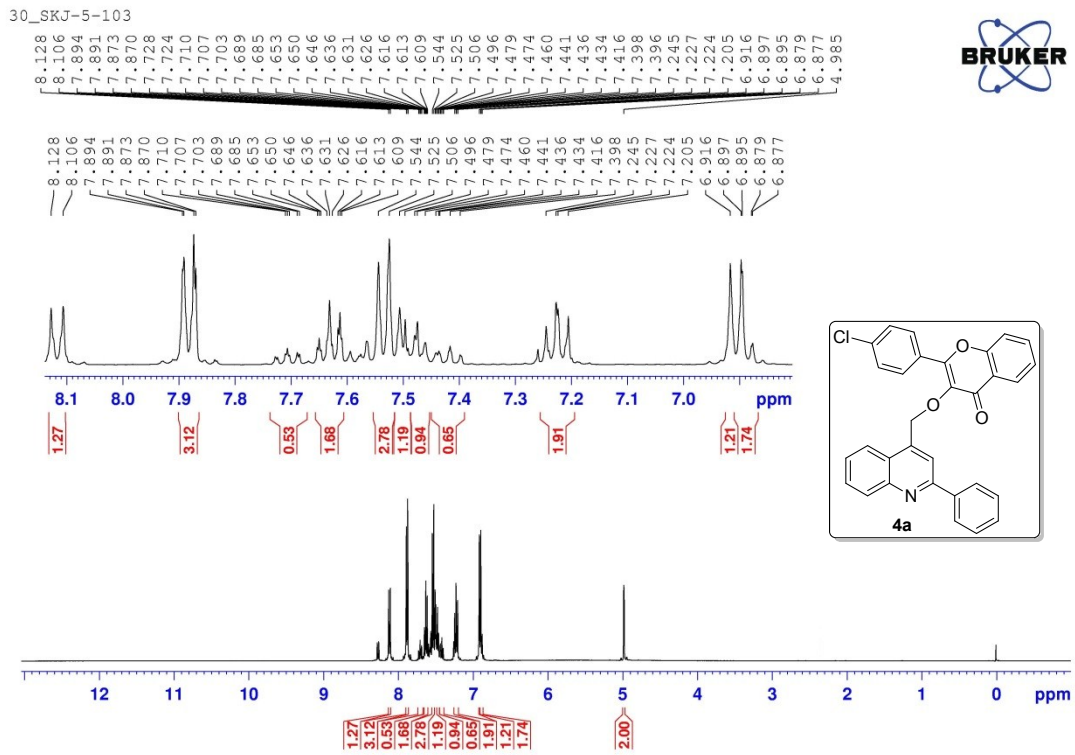
7-((6-chloro-2-(ferrocenyl)quinolin-4-yl)methoxy)-4-methyl-2H-chromen-2-one (5h)

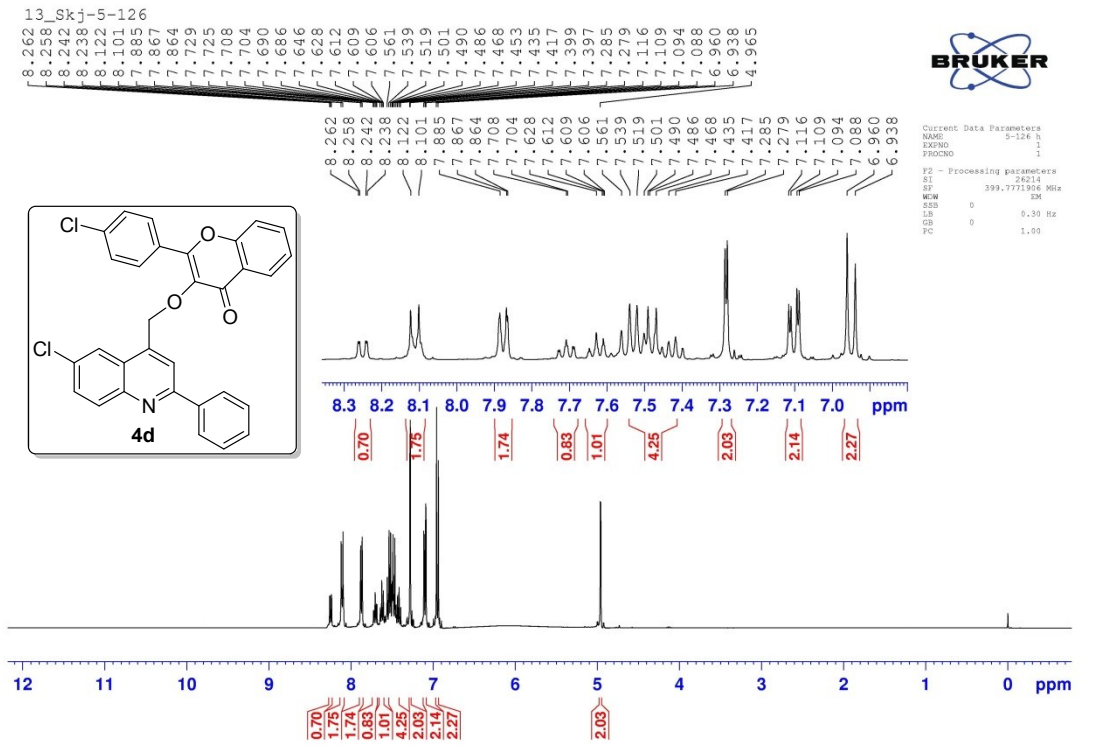
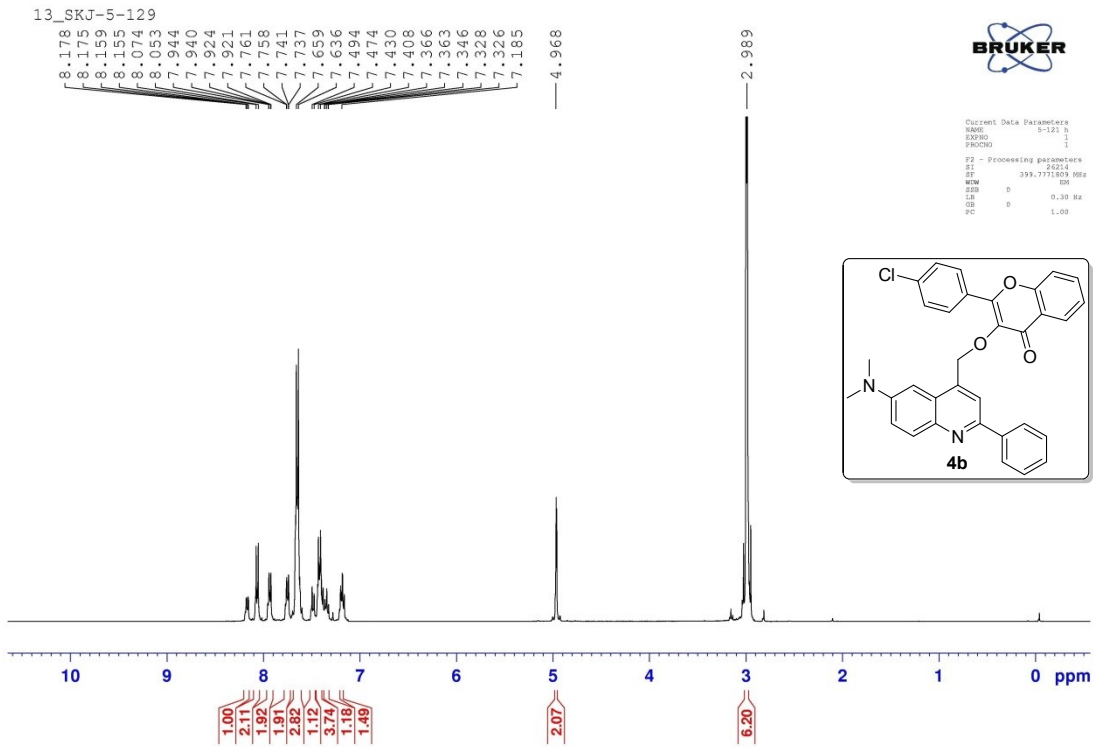


Yield: 80% as black liquid; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 7.50 (d, $J = 10.5$ Hz, 1H), 7.29 (s, 1H), 7.10 (d, $J = 3.5$ Hz, 2H), 6.91 (d, $J = 11$ Hz, 3H), 6.15 (s, 1H), 4.78 (s, 2H), 4.73 (s, 2H), 4.61 (s, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 161.9, 160.5, 155.0, 153.2, 150.8, 147.6, 133.5, 128.9, 128.4, 125.8, 125.3, 120.8, 117.4, 114.3, 113.0, 112.3, 102.2, 86.5,

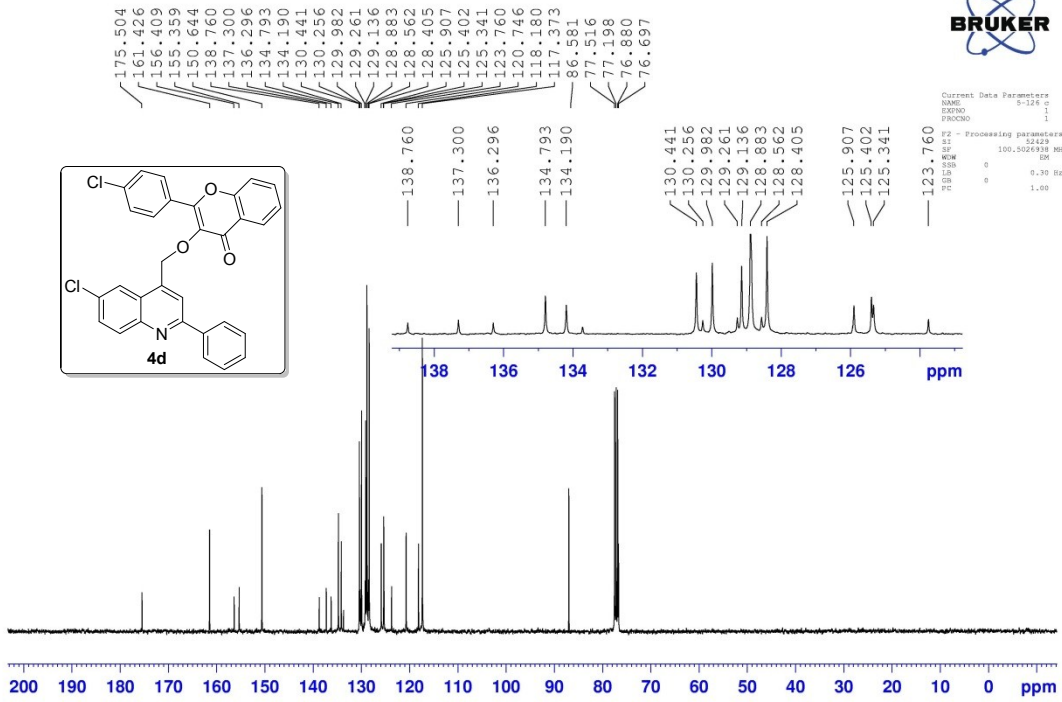
79.1, 76.7, 73.7, 69.9, 69.9, 18.8. FTIR (KBr, $\nu = \text{cm}^{-1}$): 3102, 3077, 2952, 2915, 1720, 1629, 1594, 1515, 1465, 1412, 1247, 1174, 1029. HRMS (ESI $^+$): m/z calcd. for $\text{C}_{30}\text{H}_{22}\text{ClFeNNaO}_3$ $[\text{M}+\text{Na}]^+$: 558.0529, found: 558.0518.

¹H and ¹³C Spectra

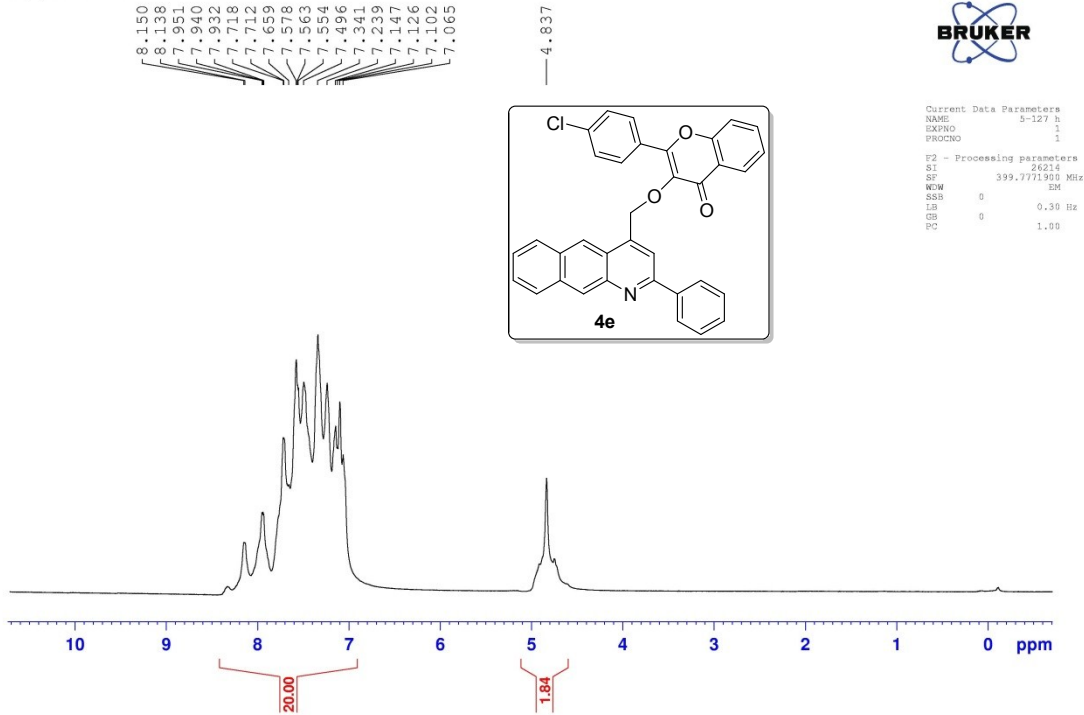


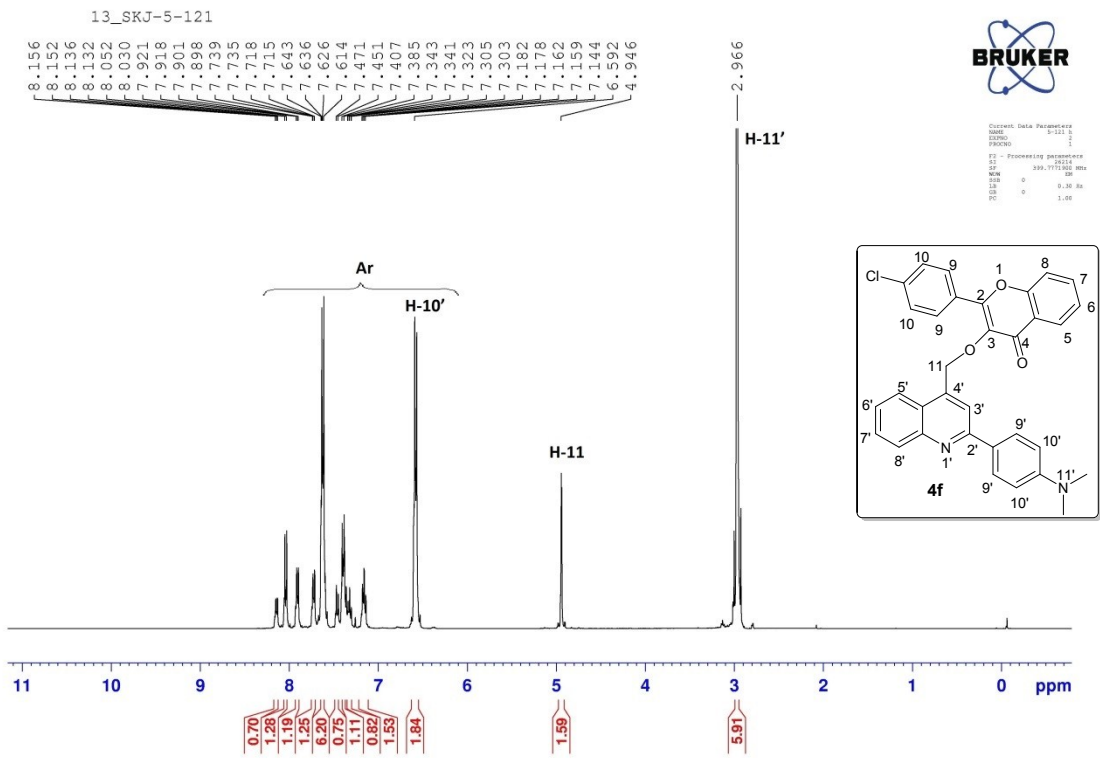
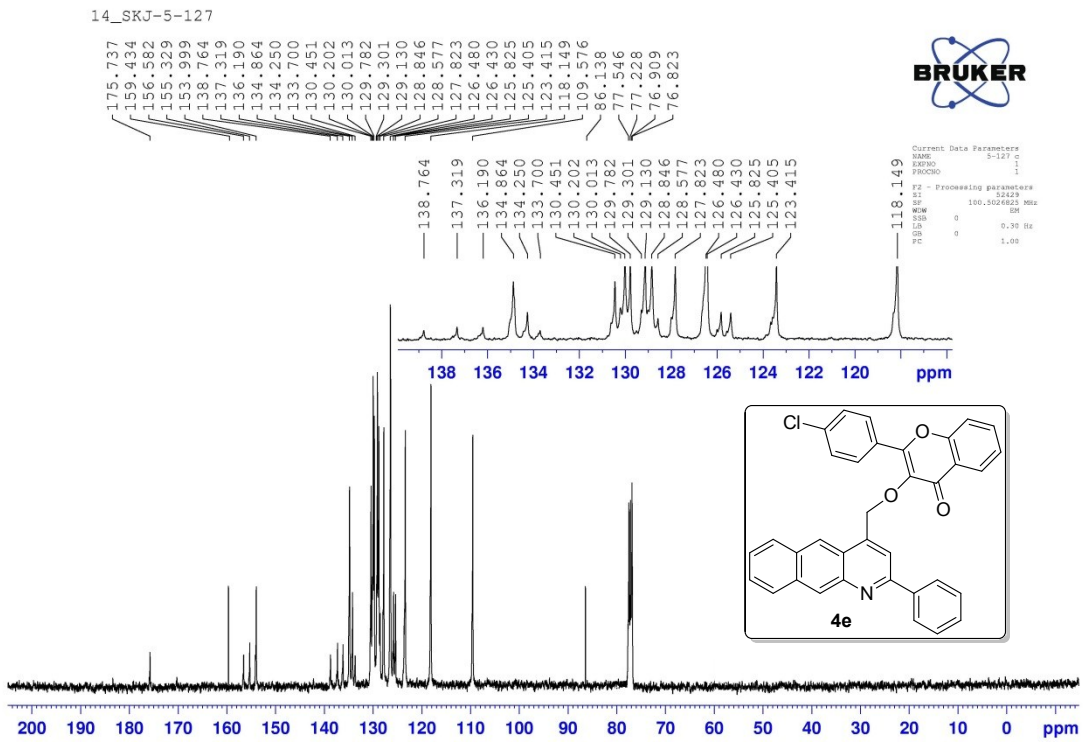


13_skj-5-126

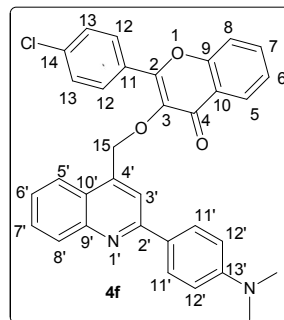
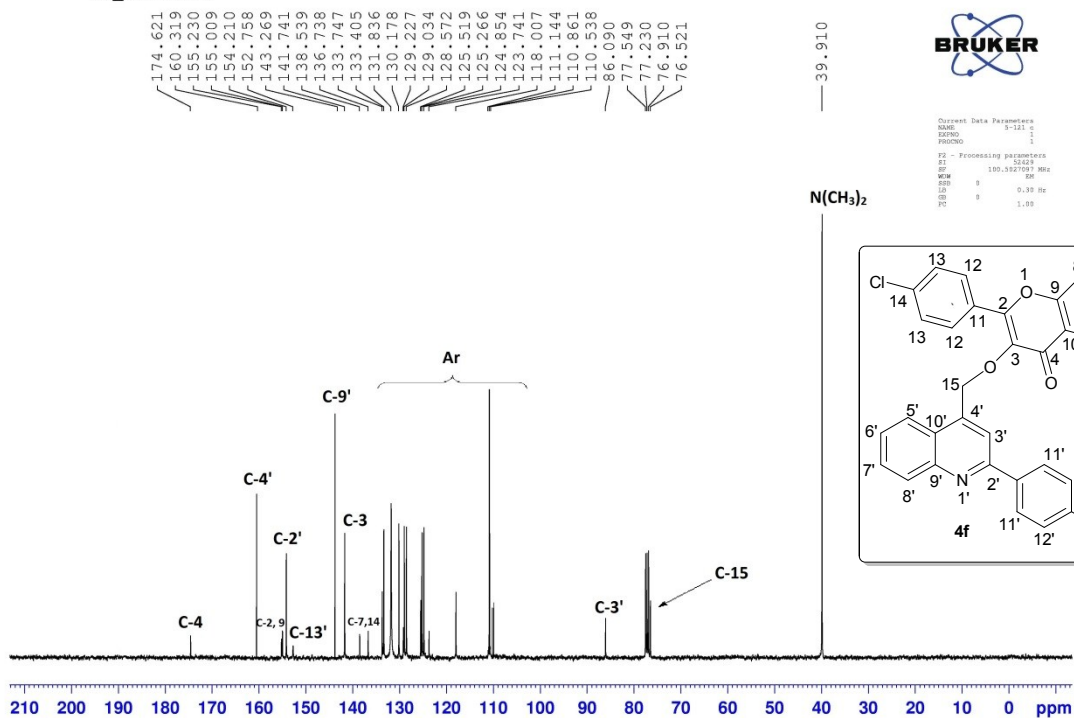


14_SKJ-5-127

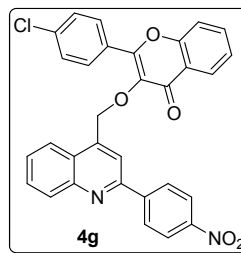
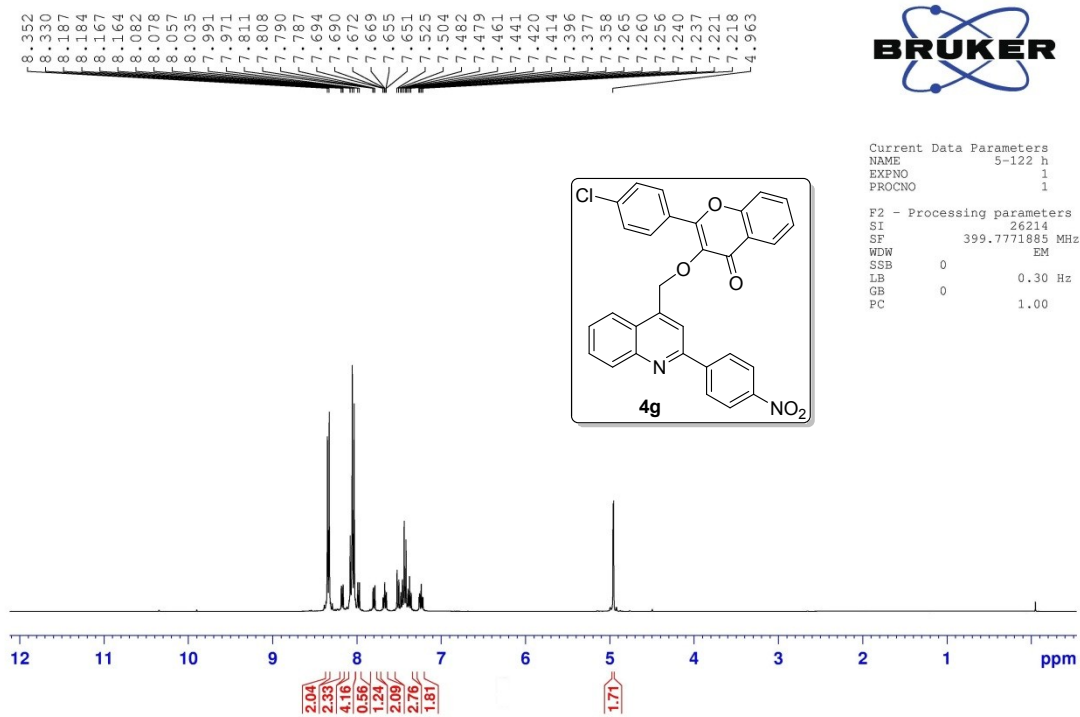




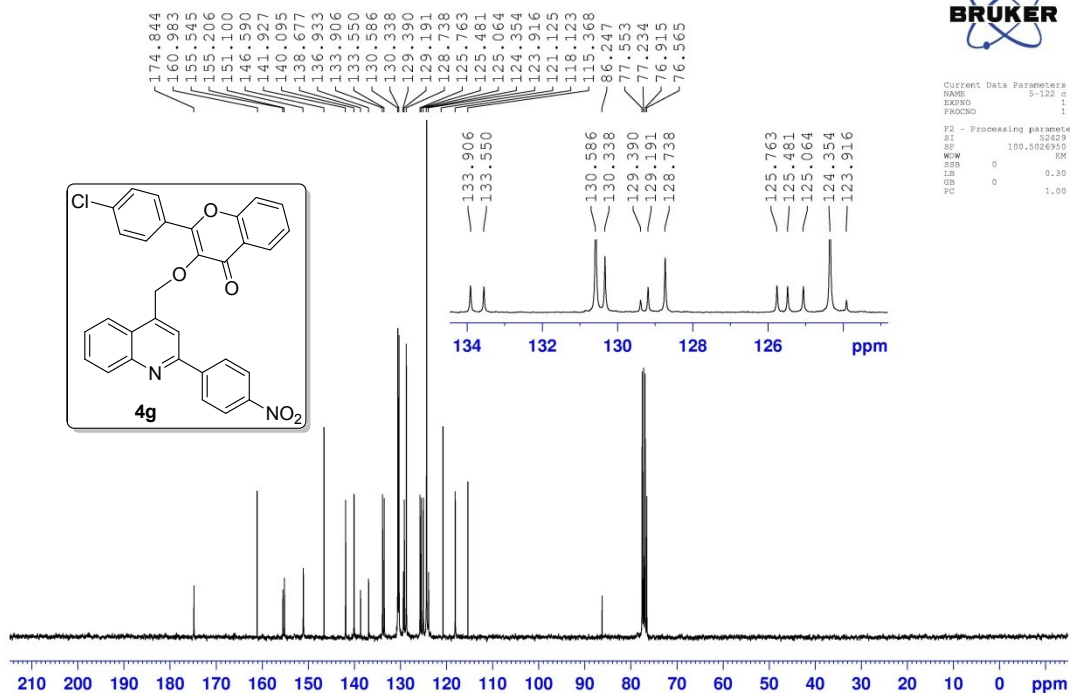
13_SKJ-5-121



13_SKJ-5-122

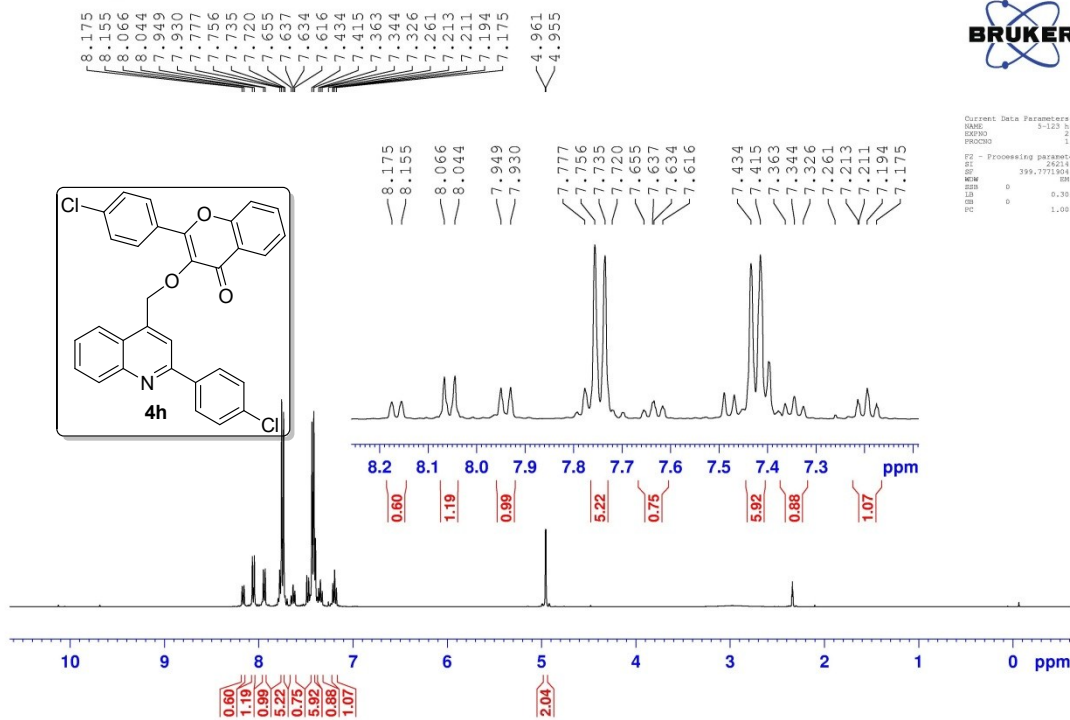


13_SKJ-5-122



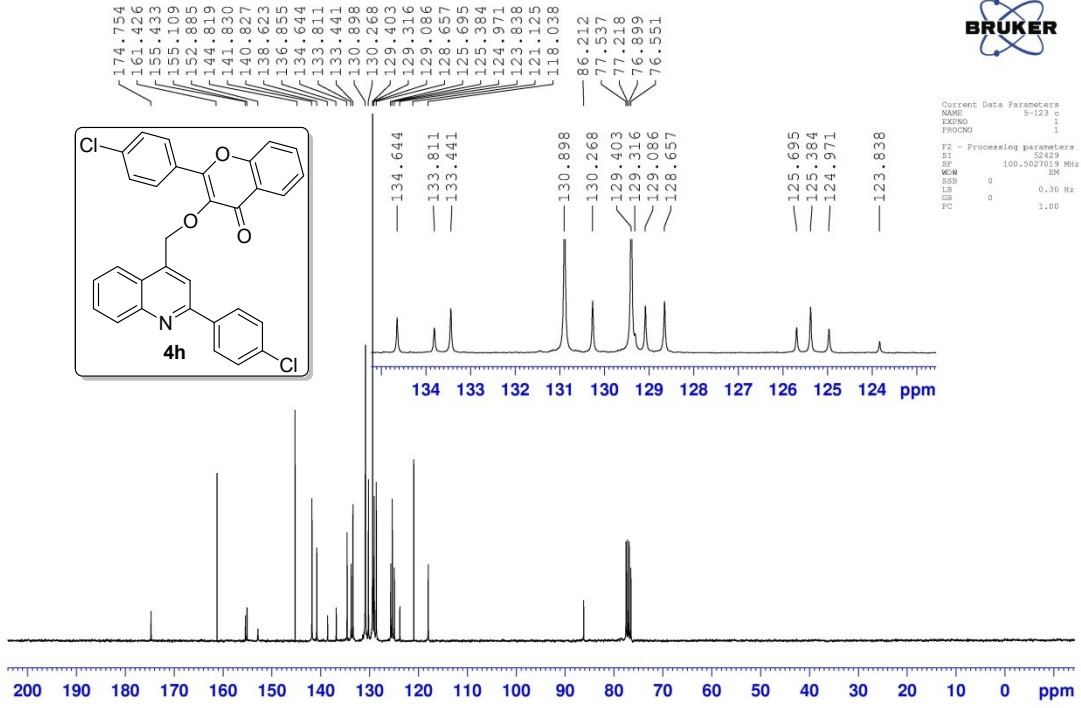
Current Data Parameters
 NAME: 5-122.c
 EXPNO: 1
 PROCNO: 1
 F2 - Processing parameters
 SI: 32429
 SF: 100.5026950 MHz
 WVM: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

13_SKJ-5-123

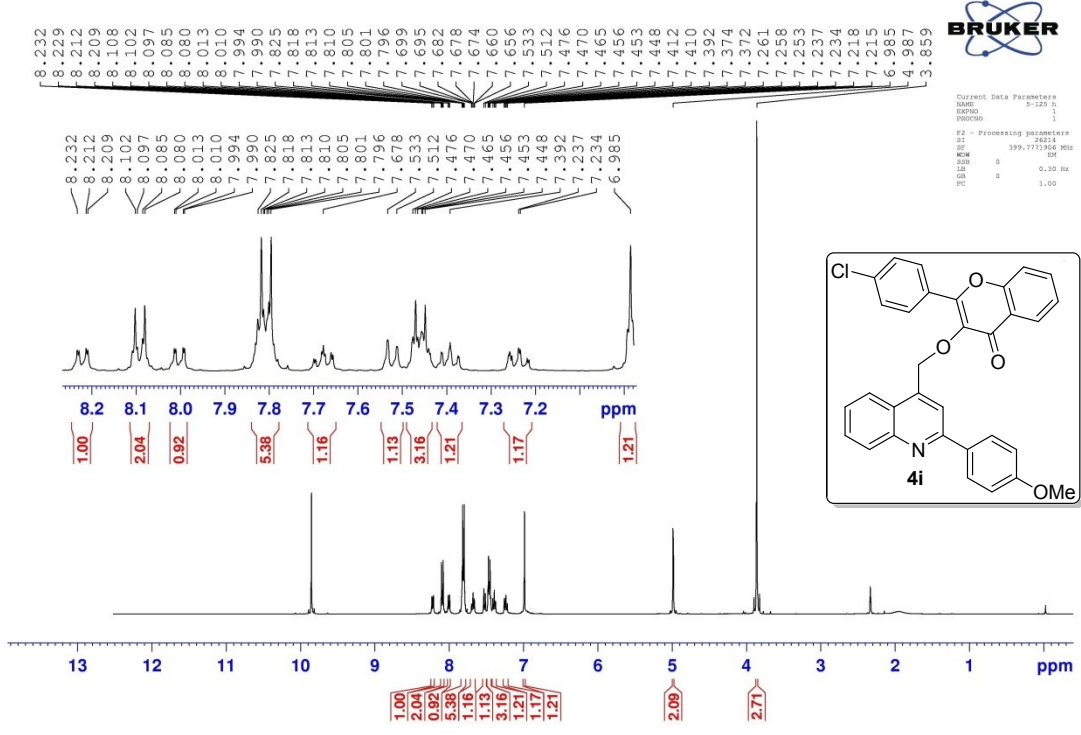


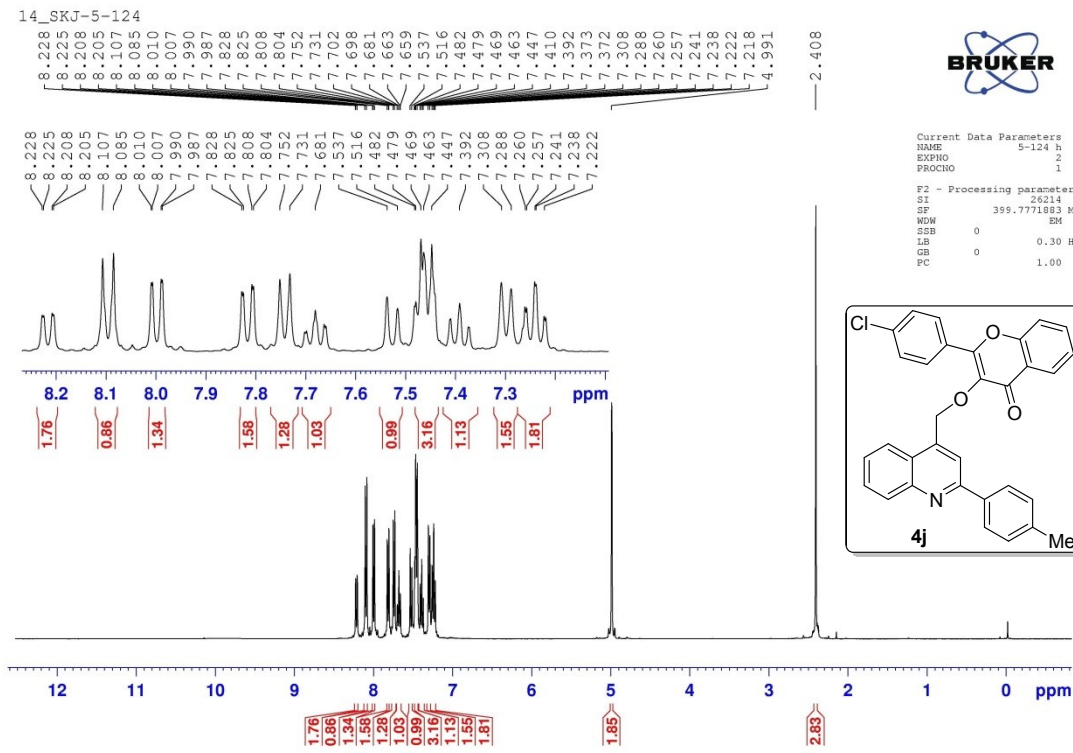
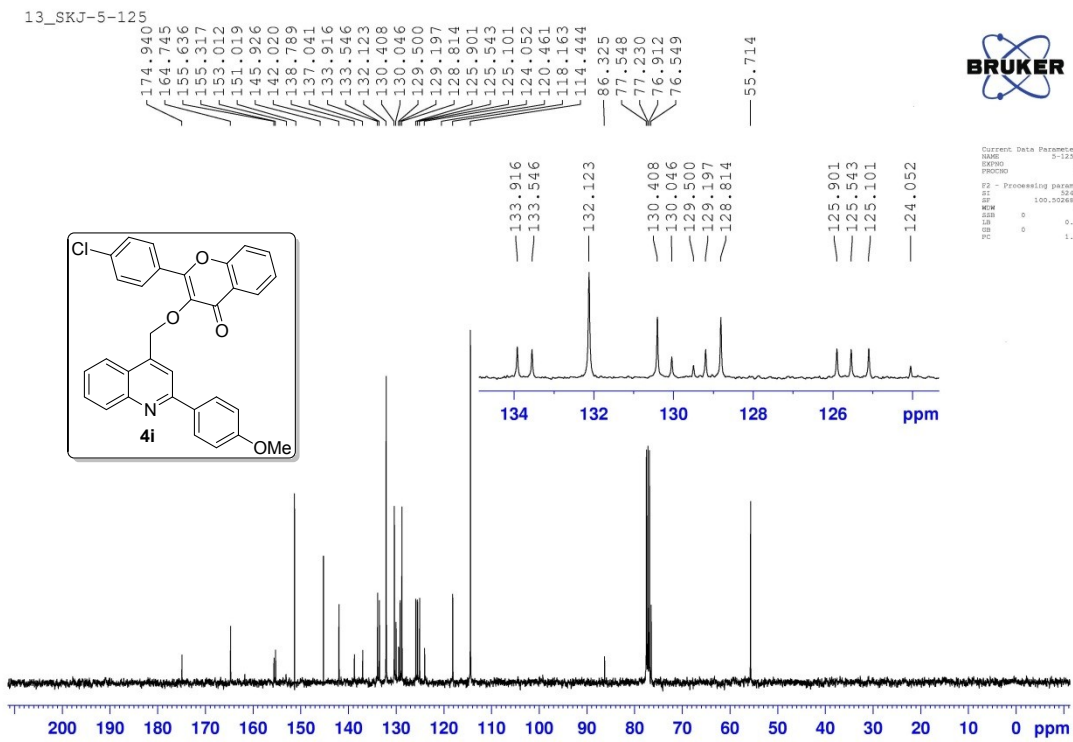
Current Data Parameters
 NAME: 5-123.c
 EXPNO: 2
 PROCNO: 1
 F2 - Processing parameters
 SI: 24214
 SF: 399.771504 MHz
 WVM: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

13_SKJ-5-123

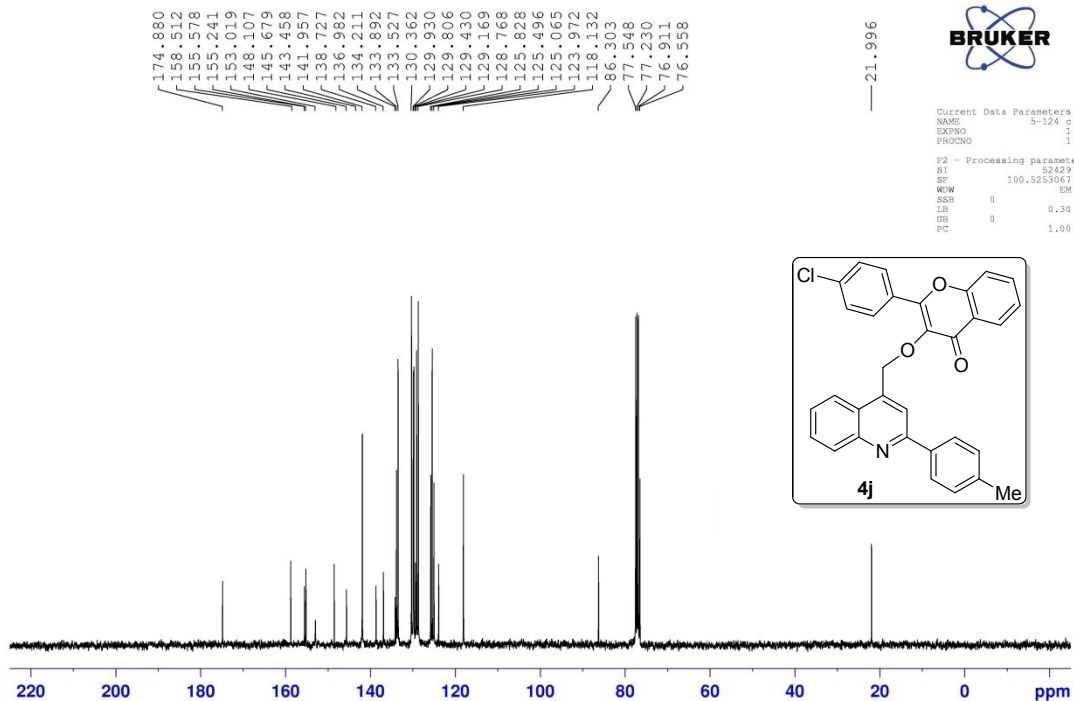


13_SKJ-5-125





14_SKJ-5-124

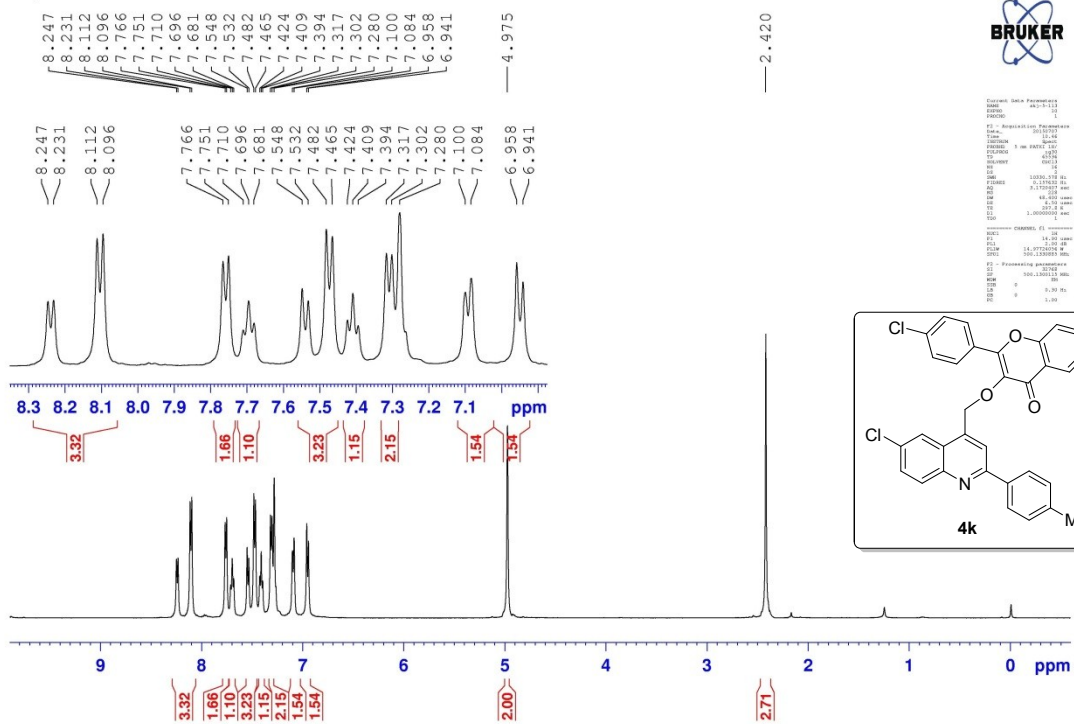


BRUKER

Current Data Parameters
 NAME 5-124 c
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 S1 52429
 SF 100.625067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

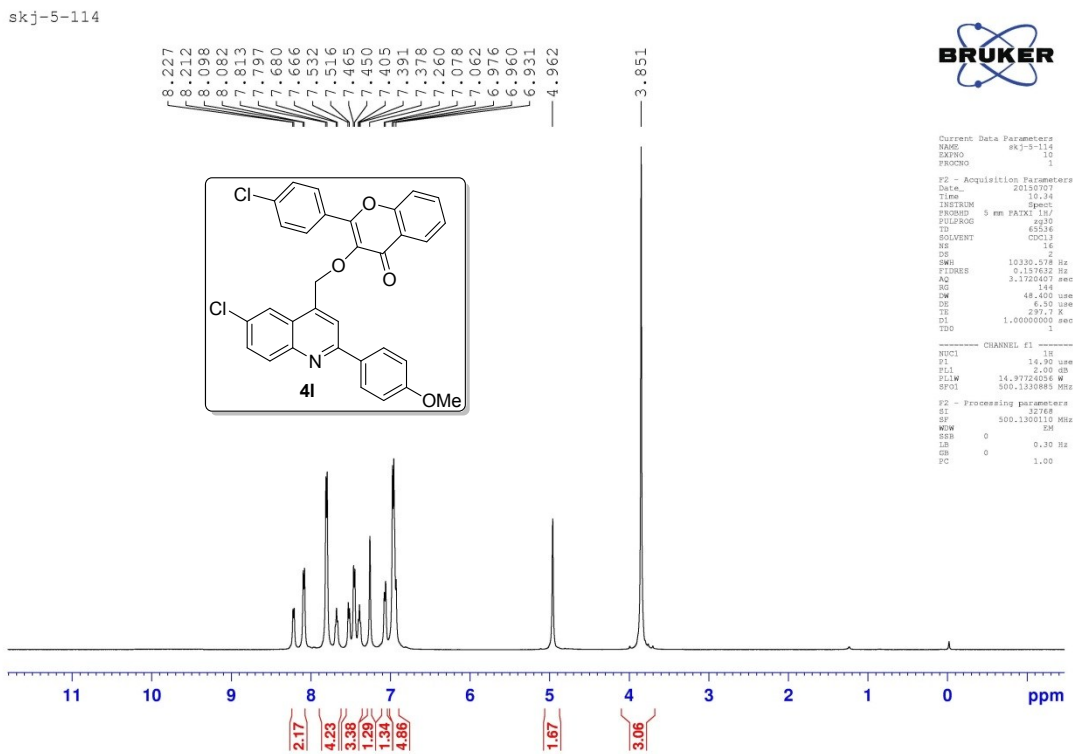
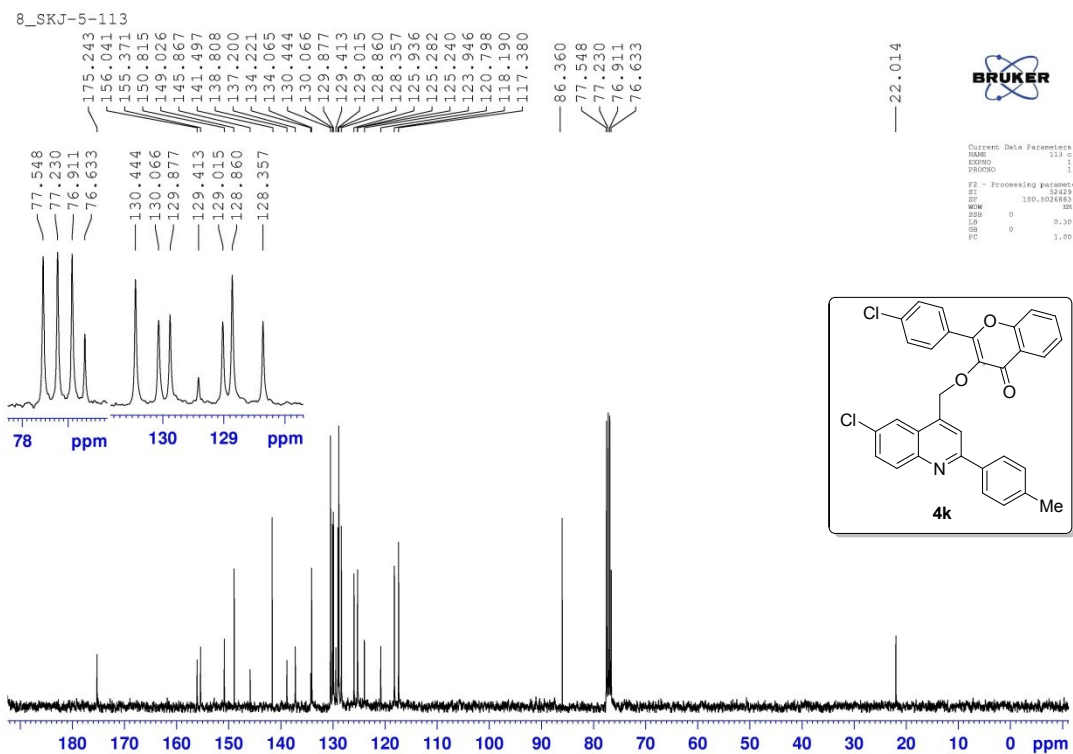
skj-5-113

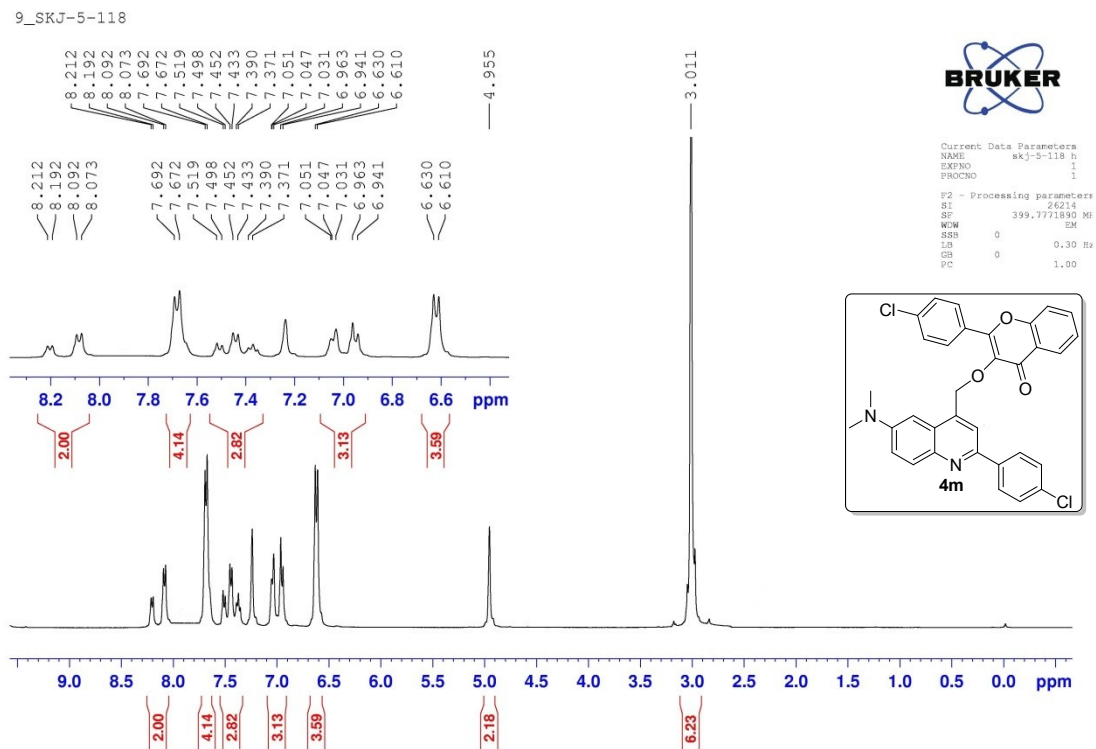
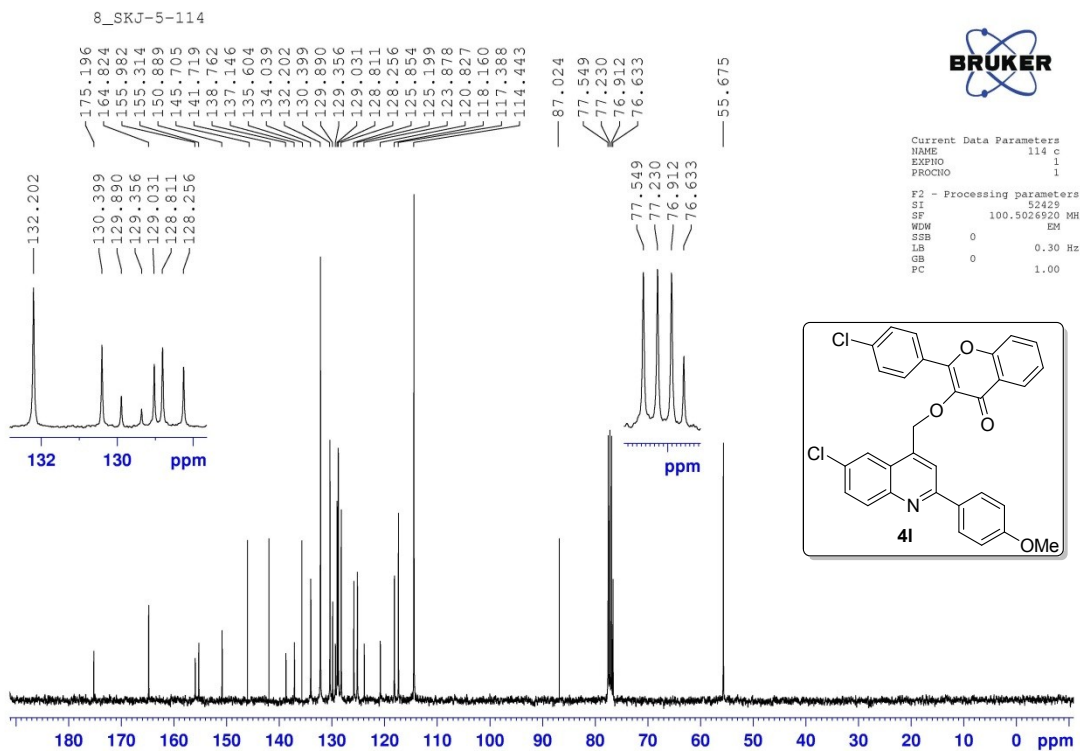


BRUKER

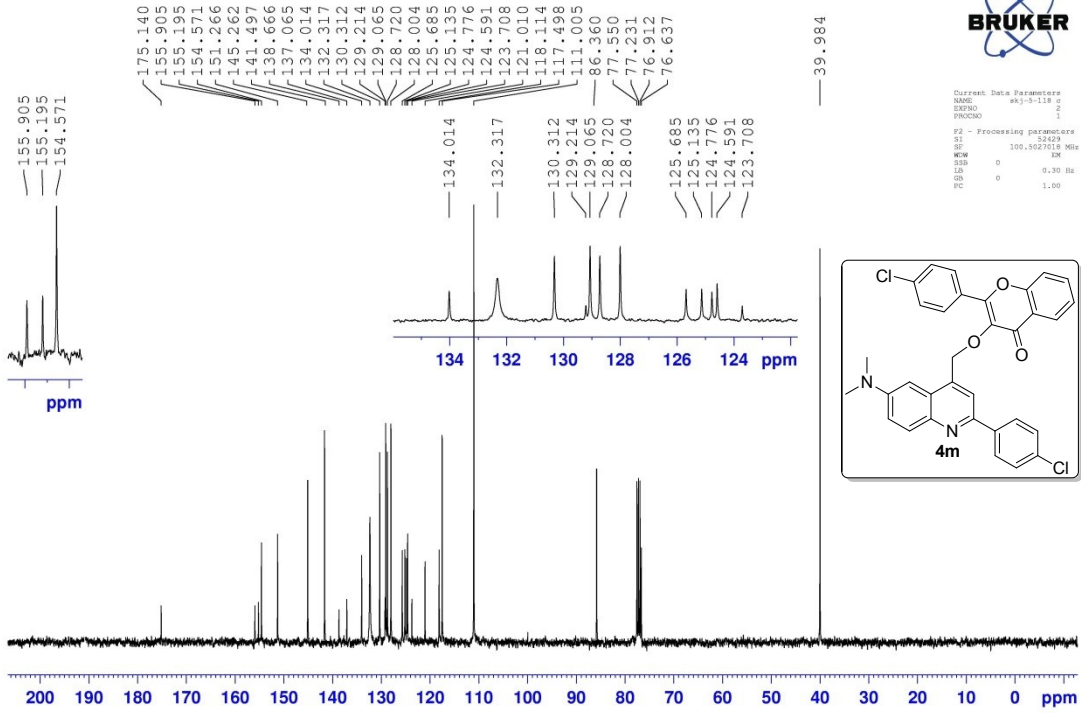
Current Data Parameters
 NAME skj-5-113
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 S1 52429
 SF 100.625067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

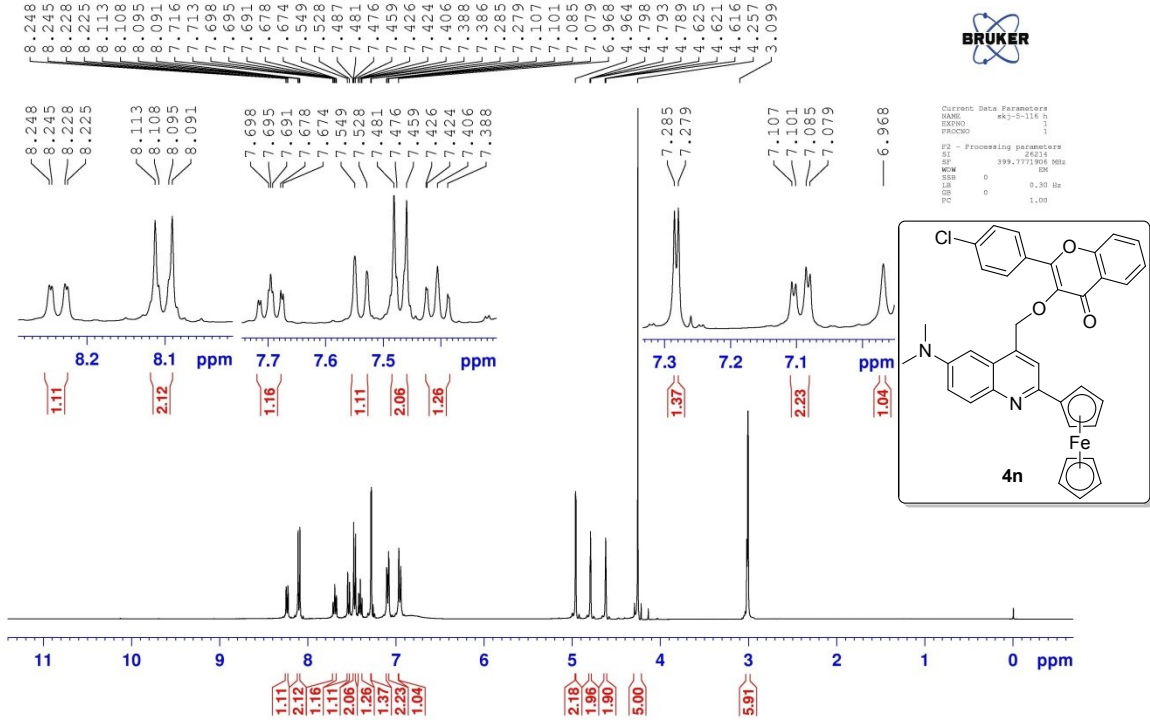




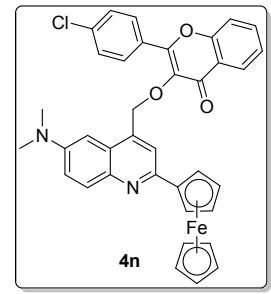
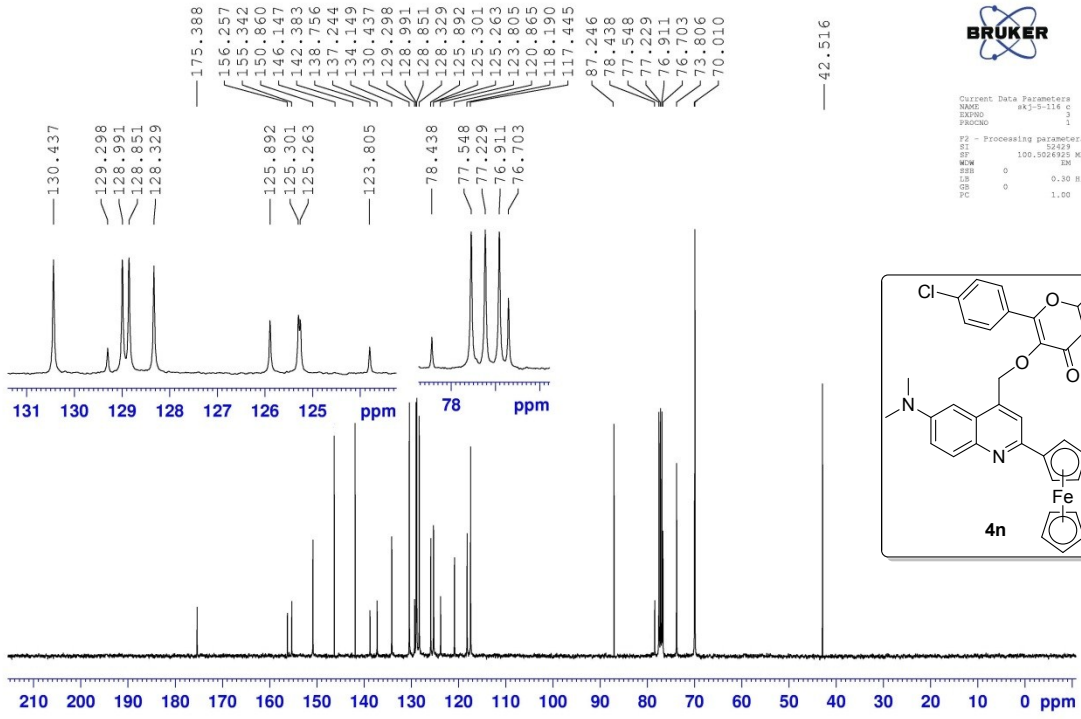
9_SKJ-5-118



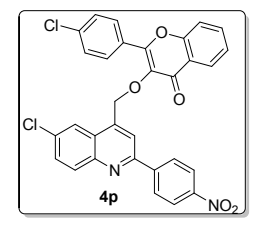
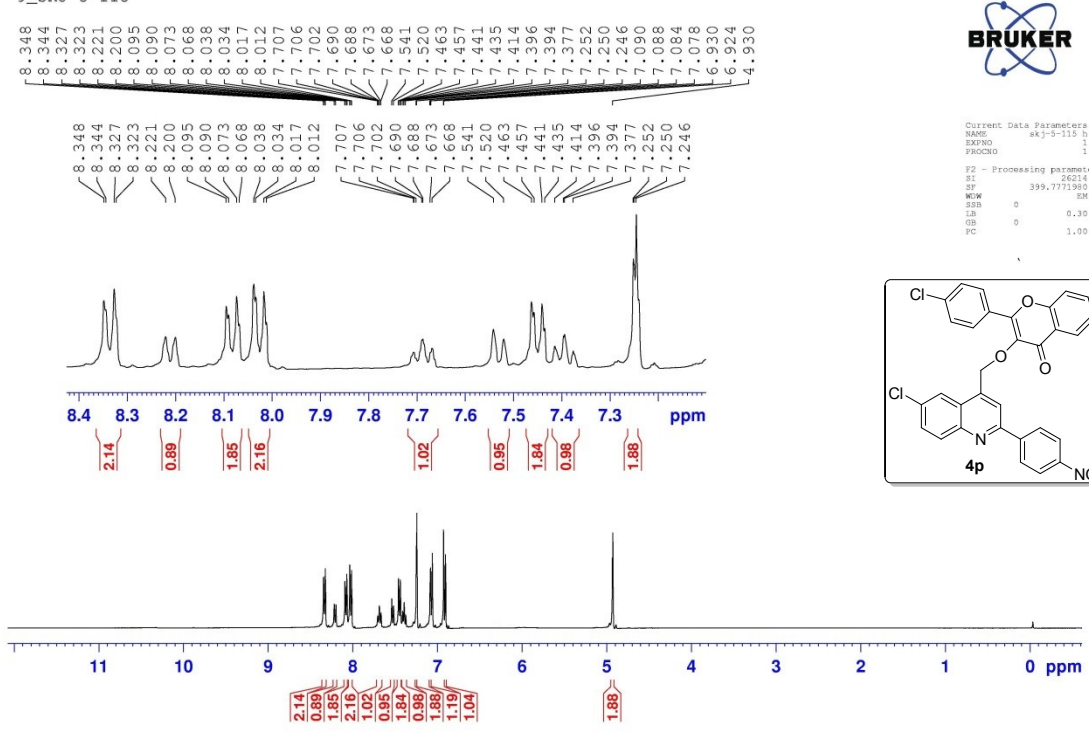
9_SKJ-5-116

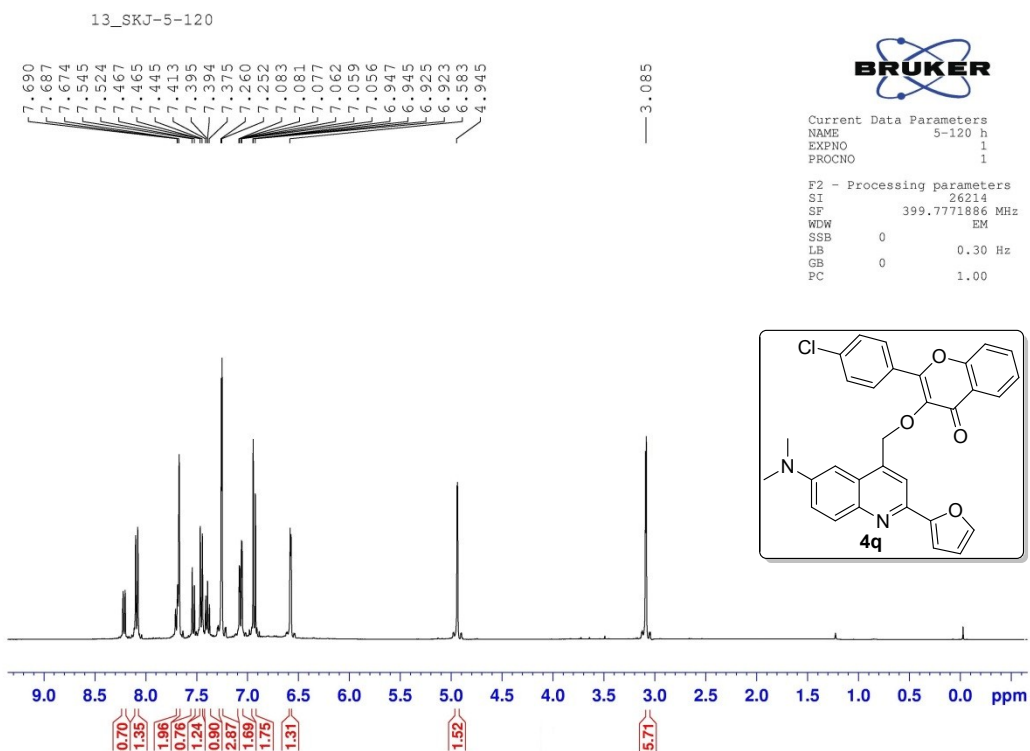
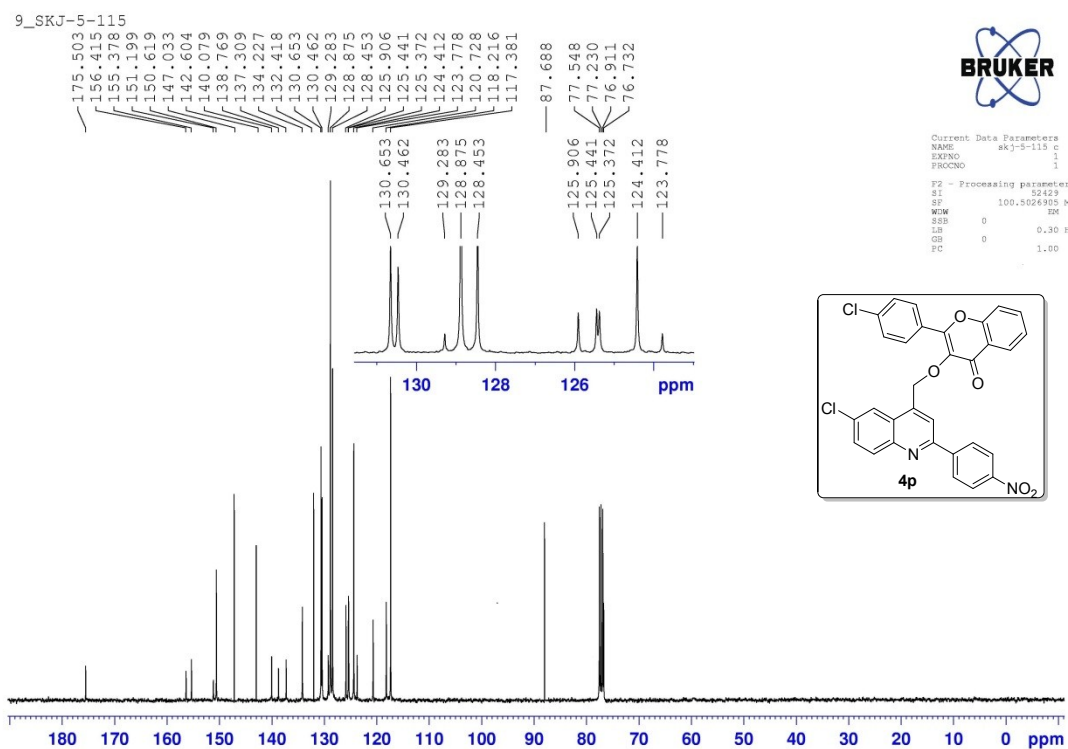


9_SKJ-5-116

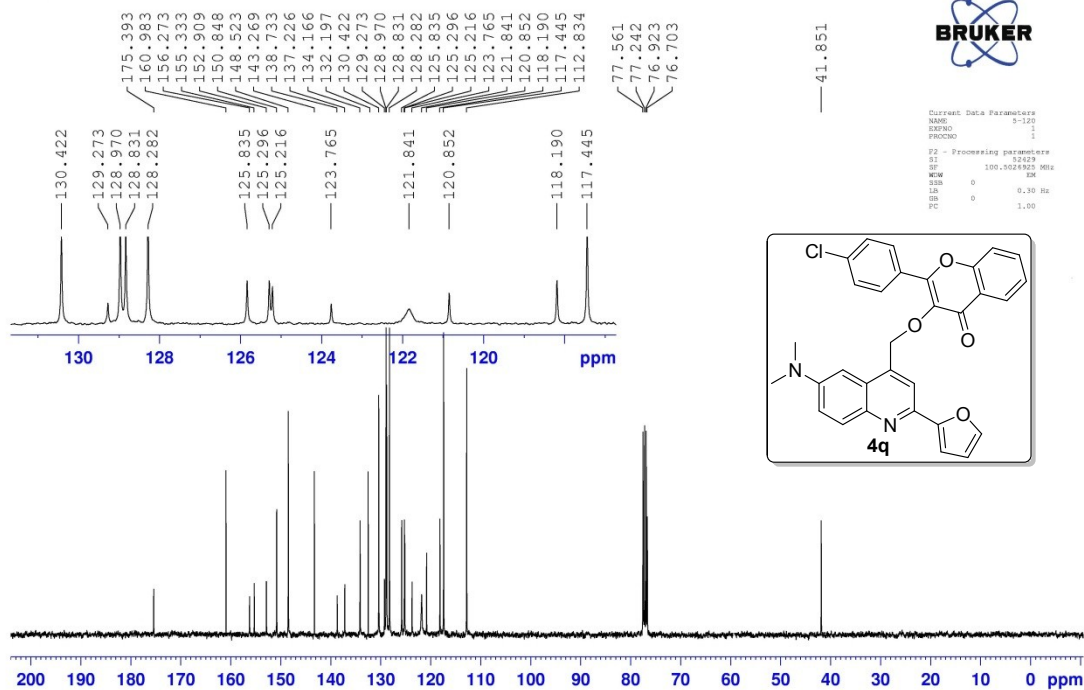


9_SKJ-5-115

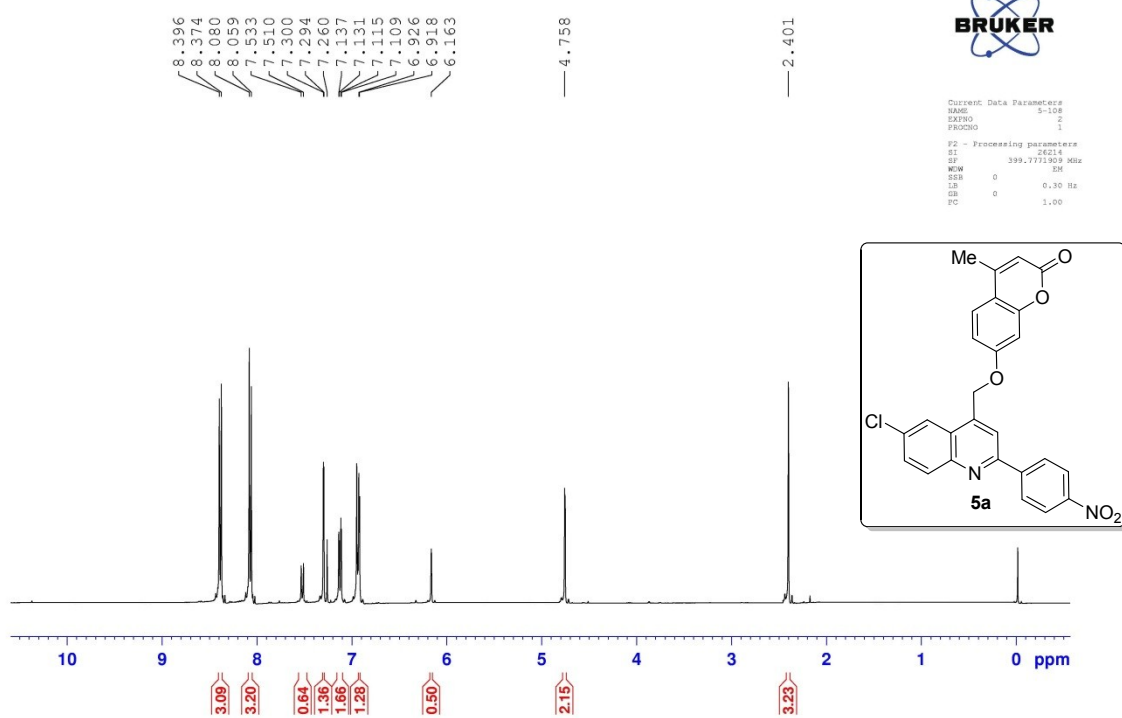




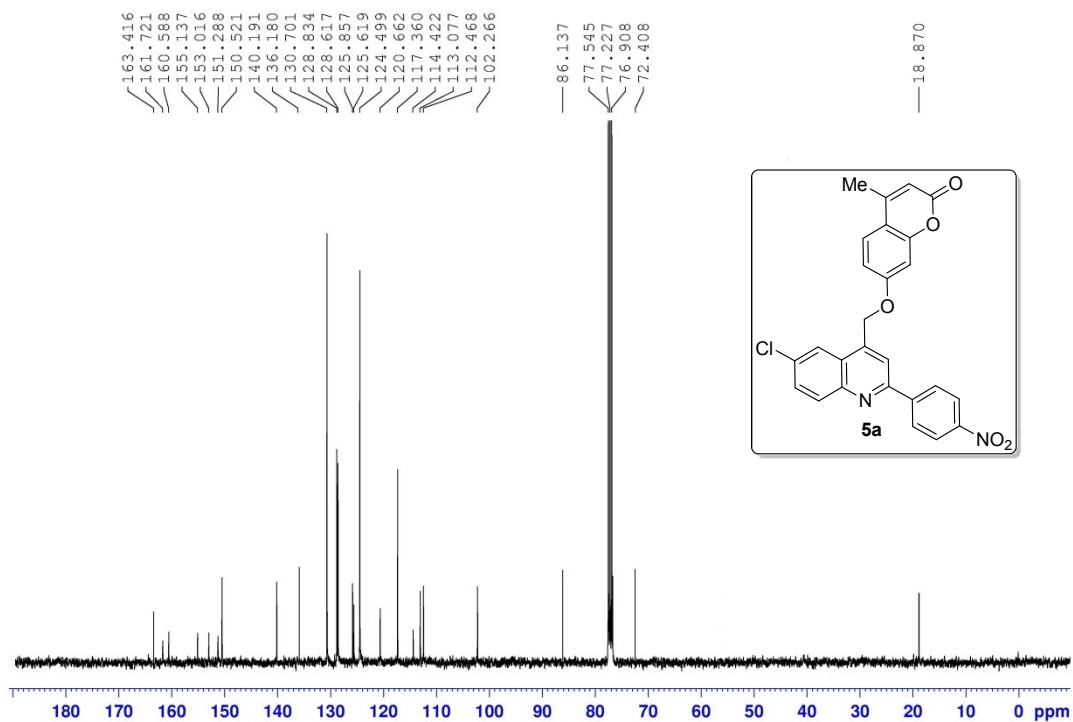
13_SKJ-5-120



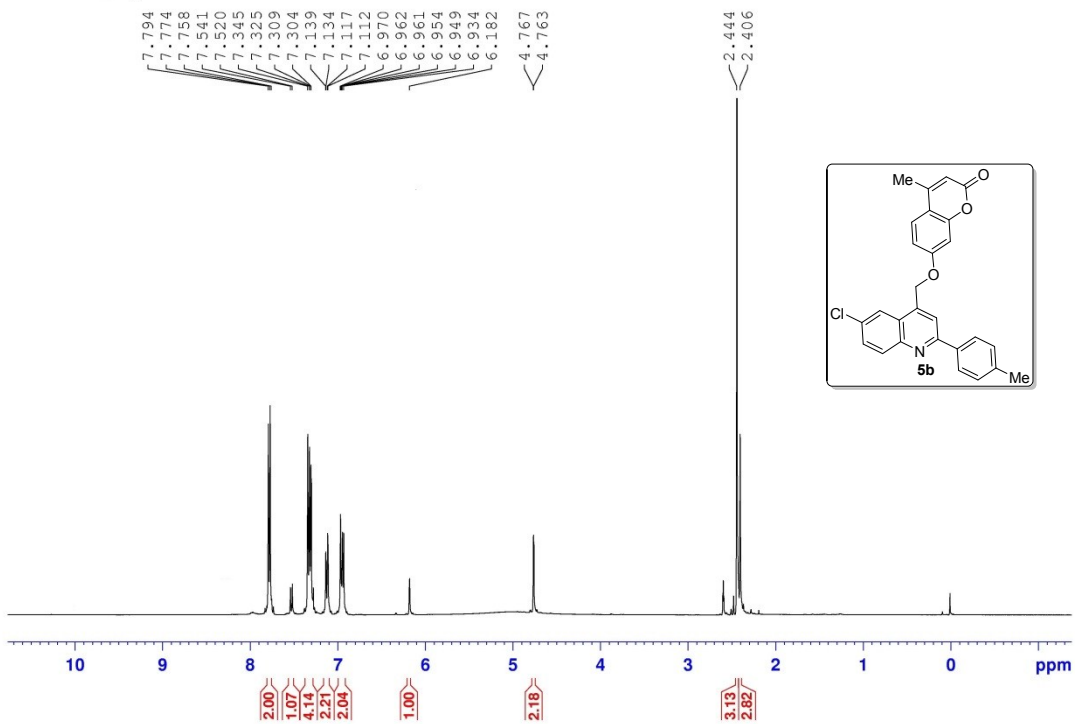
2_SKJ-5-108



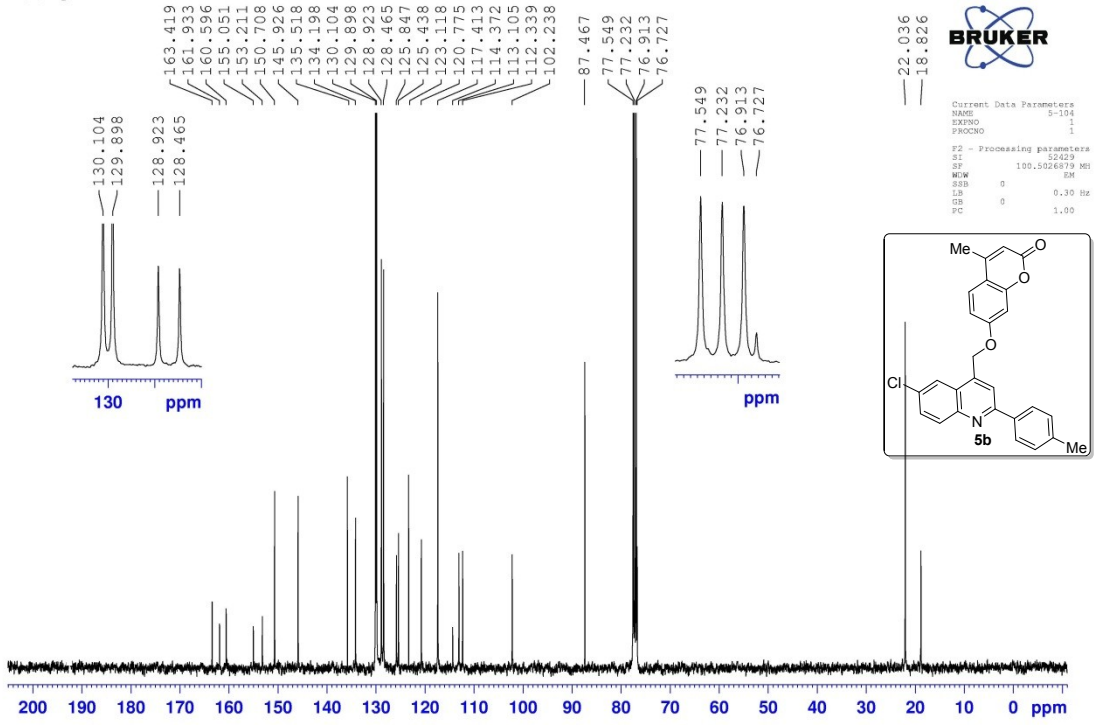
2_SKJ-5-108



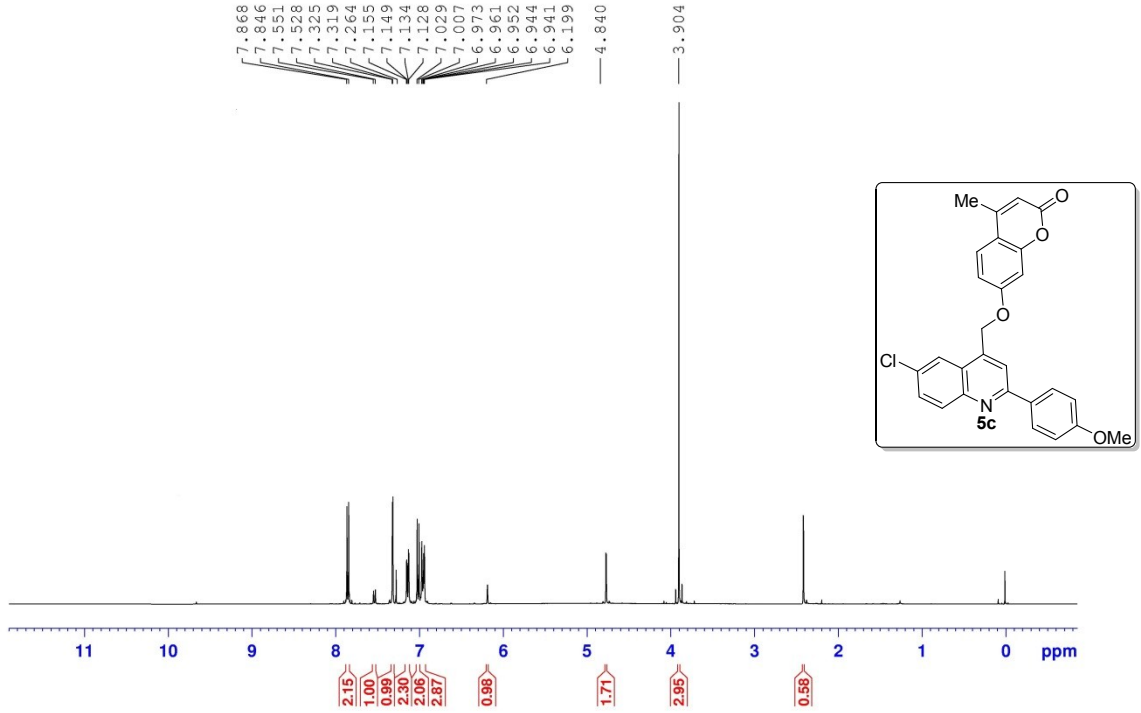
2_skj-5-104



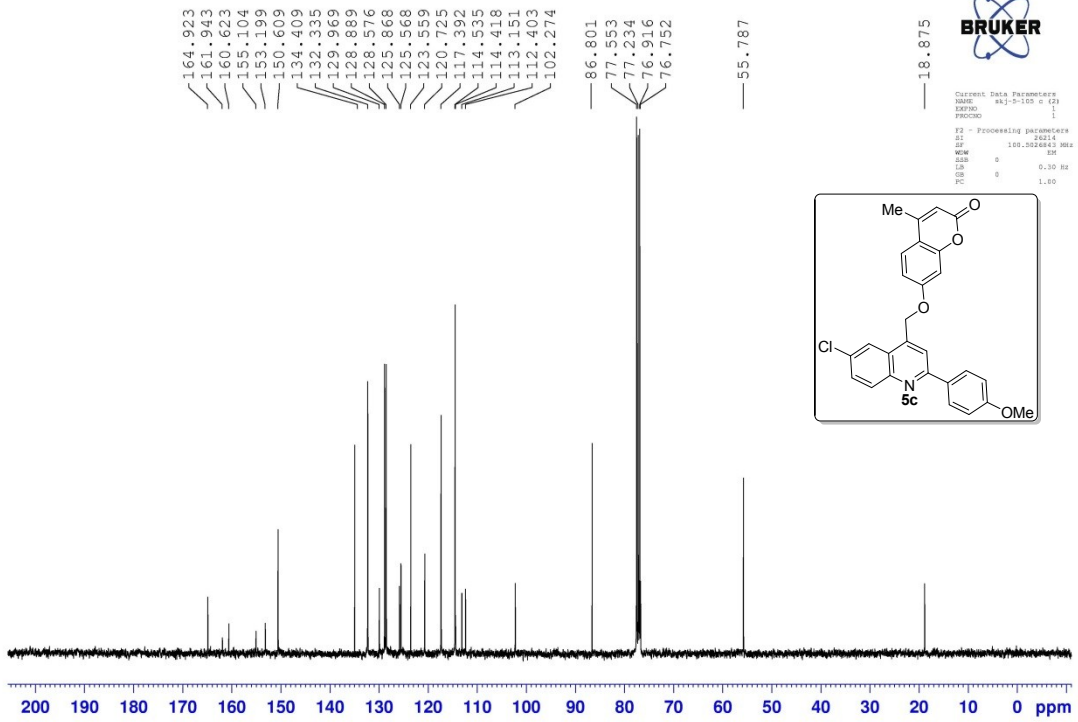
2_skj-5-104



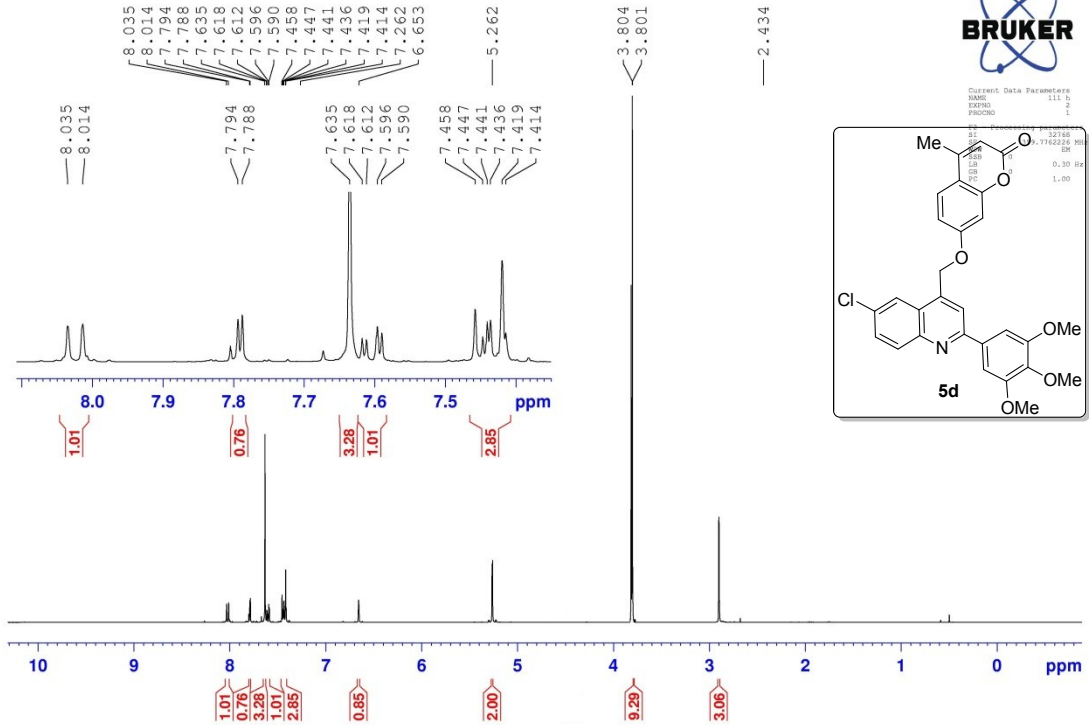
2_skj-5-105



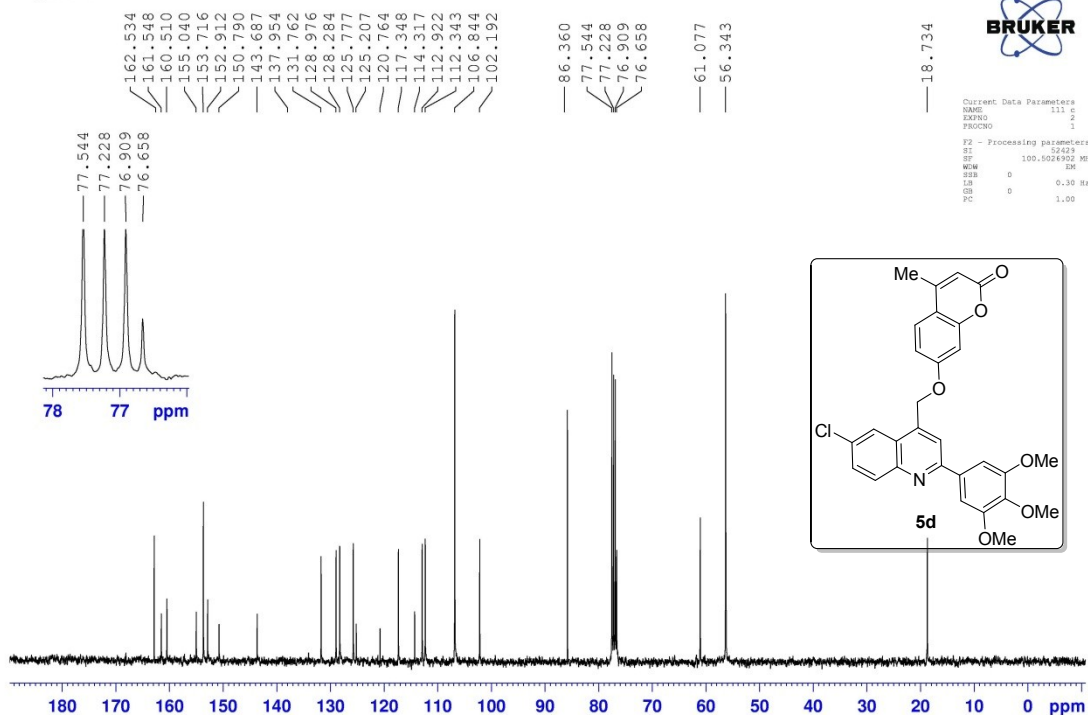
2_skj-5-105



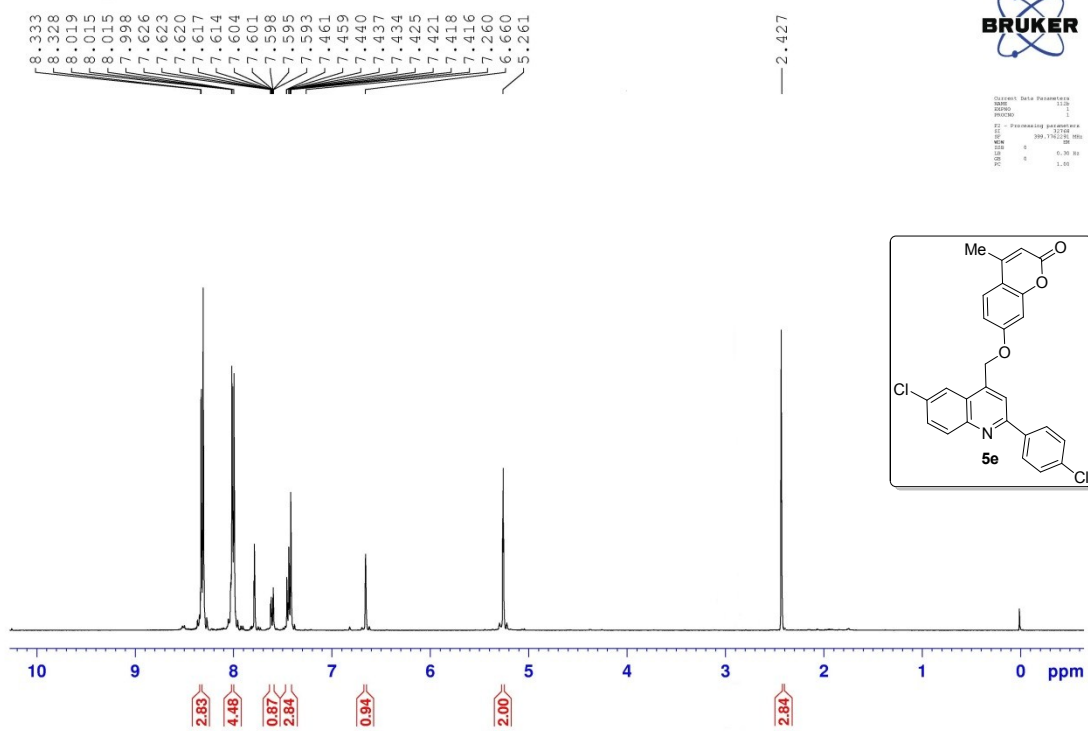
8_SKJ-5-111

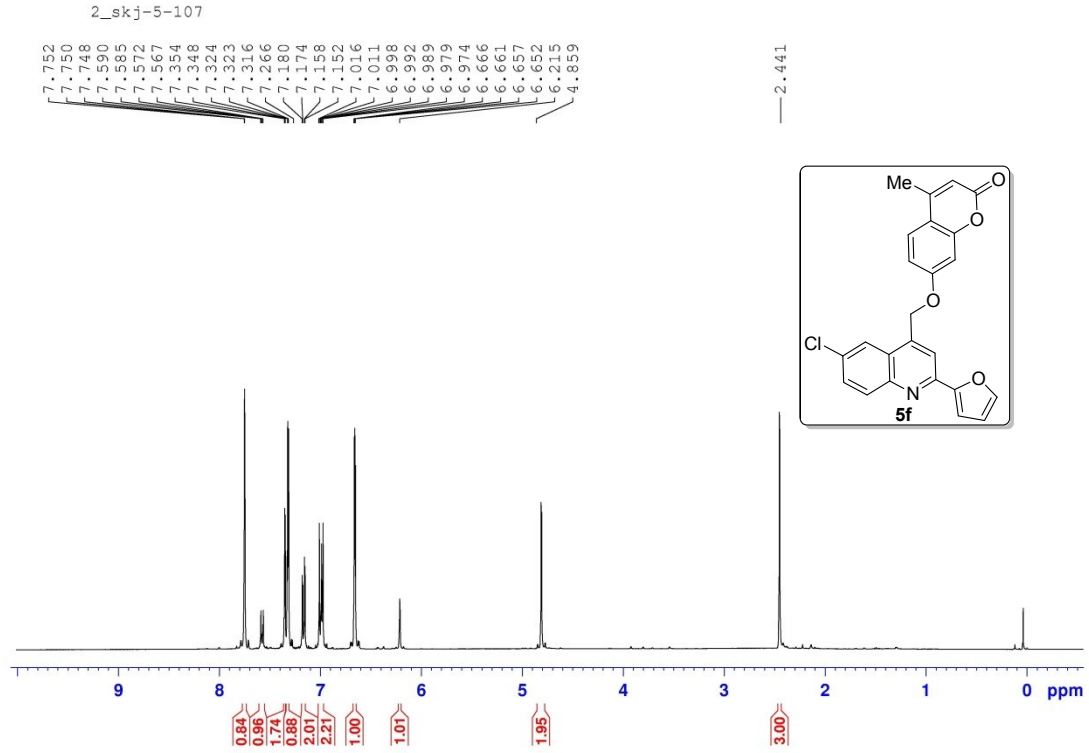
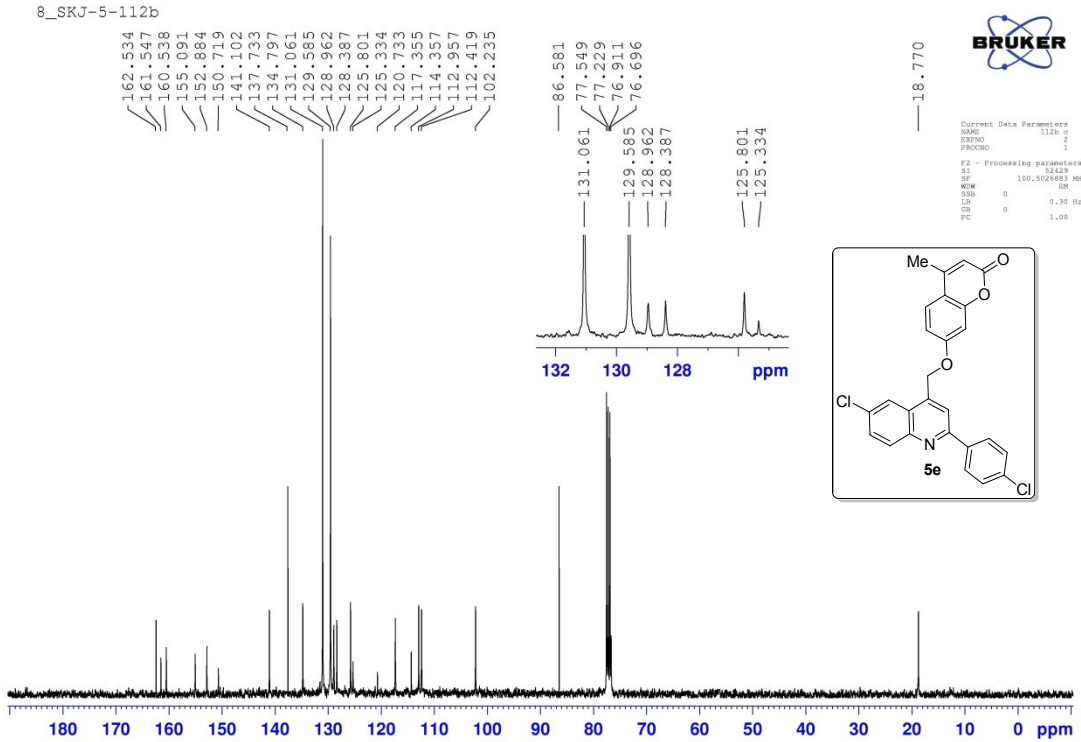


8_SKJ-5-111

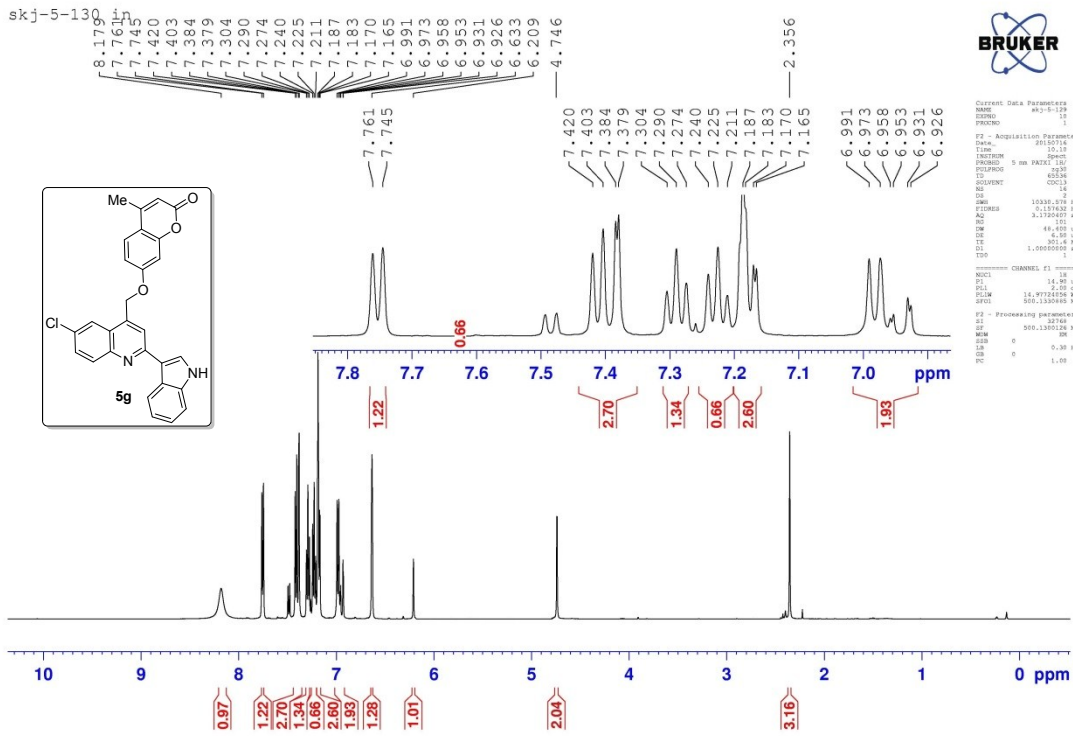
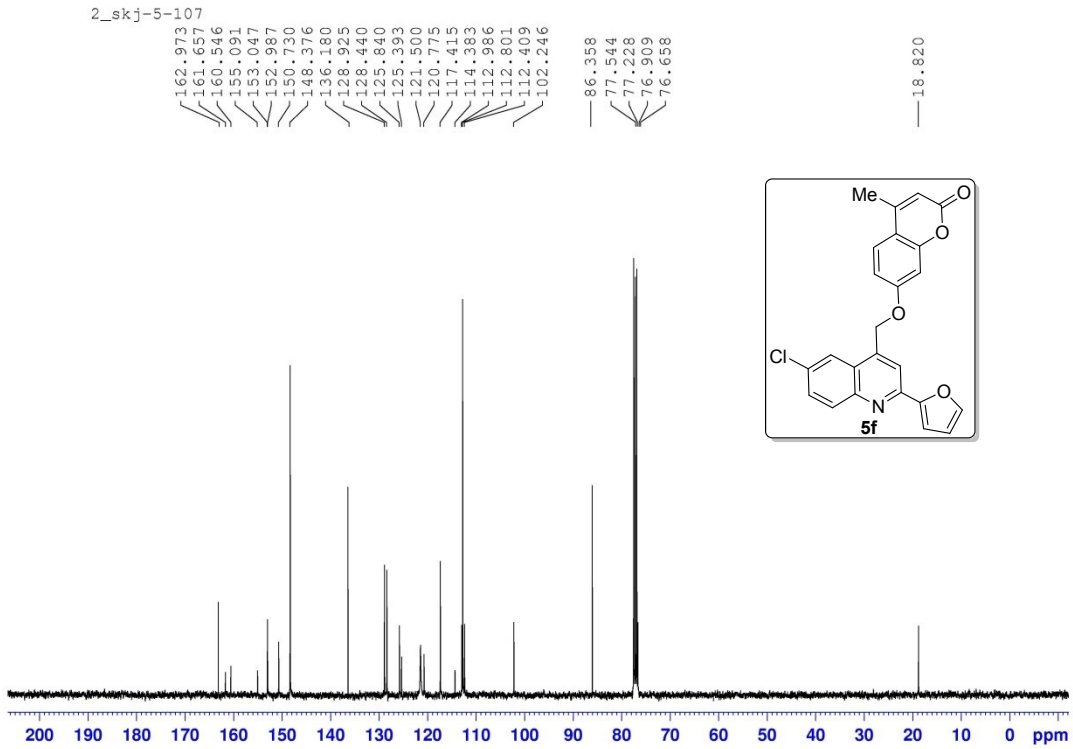


8_SKJ-5-112b

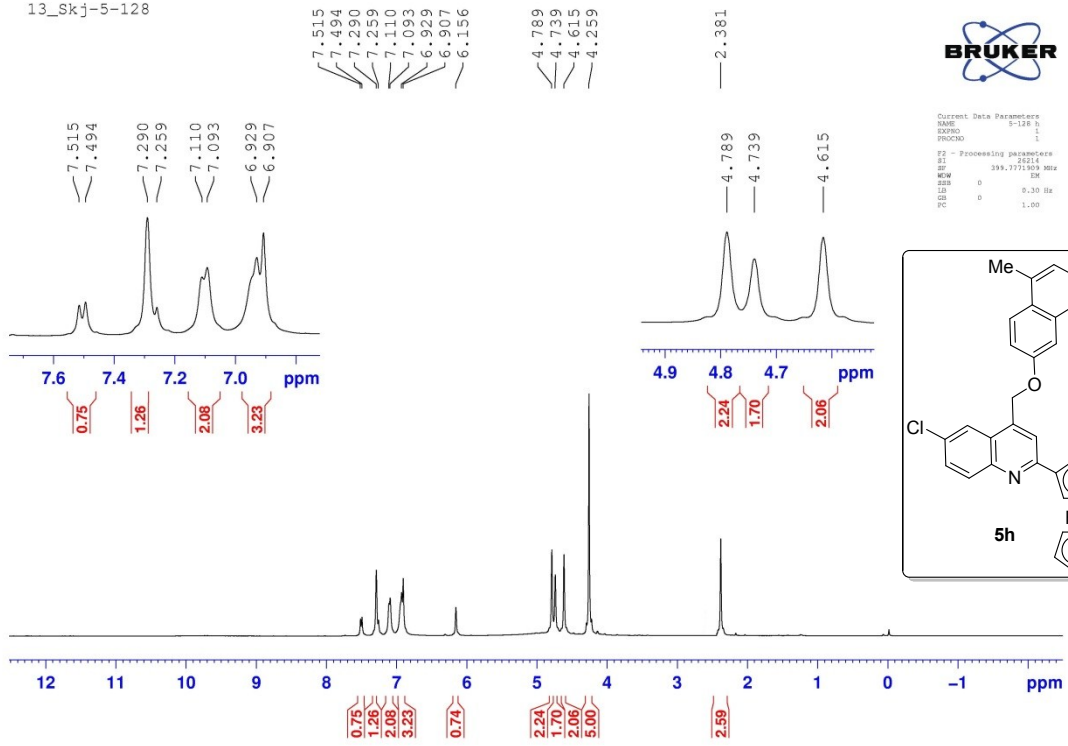




2_skj-5-107



13_Skj-5-128



13_Skj-5-128

