Supporting Information

Bimetallic Copper/Cobalt cocatalyzed double aerobic oxidative [3+2] cycloaddition toward π-extended benzofuro[2,3-b]indoles as electron donors for electroluminescence

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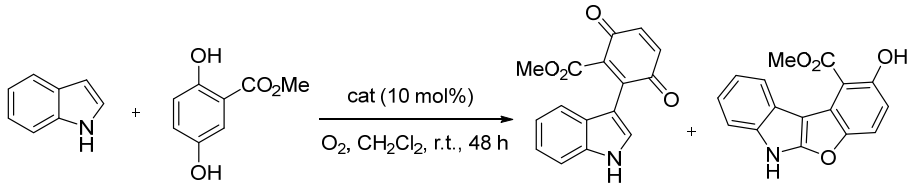
(A) General information

Chemicals and solvents were purchased from commercial suppliers and used as received unless noted. All products were purified by flash chromatography on silica gel. The chemical yields referred are isolated products. ^{1}H NMR and ^{13}C NMR spectra were recorded on 400 MHz or 600 MHz Bruker spectrometers. Chemical shifts of ^{1}H NMR were reported in part per million relatives to the $CDCl_3$ residual peak (δ 7.26). Chemical shifts of ^{13}C NMR were reported relative to $CDCl_3$ (δ 77.16) or CD_3OD (δ 49.00). The used abbreviations are as follows: s (singlet), d (doublet), t (triplet), quart. (quartet), quint. (quintet), m (multiplet), br (broad). Multiplets which arise from accidental equality of coupling constants of magnetically non-equivalent protons are marked as virtual (*virt.*). High resolution mass spectra (HRMS) data were measured on a ESI-microTOF II. Melting points were measured on a SGW® X-4B and are not corrected. Reactions were monitored by TLC analysis using silica gel 60 Å F-254 thin layer plates and compounds were visualized with a UV light at 254 nm or 365 nm. Further visualization was achieved by staining with iodine, or $KMnO_4$ followed by heating on a hot plate. Flash column chromatography was performed on silica gel 60 Å, 10-40 μm.

(B) Optimization of reaction conditions

Table S1 The effect of different catalysts[a]

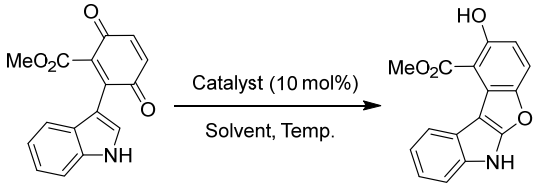


1a **2a** **3a** **4a**

entry	Cat.	Yield (%, 3a)[b]	Yield (%, 4a)[b]
1	$Cu(OTf)_2$	24	0
2	$[Cu(CH_3CN)_4][PF_6]$	60	10
3	$CuBr_2$	0	0
4	$CuCl_2$	0	0
5	$Cu(OAc)_2$	<10	0
6	$FeCl_3$	0	0
7	$Fe(OTf)_3$	0	0
8	$Fe(acac)_3$	0	0
9	$CoCl_2$	0	0

[a] Reactions were performed with **1a** (0.2 mmol, 23.43 mg, 1 equiv.), **2a** (0.2 mmol, 33.60 mg, 1 equiv.), and cat (10 mol%) in 4.0 mL of CH_2Cl_2 at room temperature. [b] Isolated yield.

Table S2. The effect of different solvents on the cyclization of 3a[a]

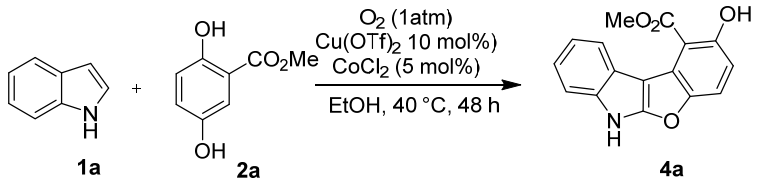


3a **4a**

Entry	Solvent	Catalyst	T(°C)	Time	Yield (%)[b]
1	DCM	$Cu(OTf)_2$	r.t.	overnight	>99
2	DCM	$[Cu(CH_3CN)_4][PF_6]$	r.t.	overnight	>99
3	DCM	$Fe(acac)_3$	r.t.	overnight	0
4	DCM	$Fe(OTf)_2$	r.t.	overnight	>99
5	DCM	$Fe(OTf)_3$	r.t.	5 min	>99
6	EtOH	$Cu(OTf)_2$	40	20 h	95
7	EtOH	$[Cu(CH_3CN)_4][PF_6]$	40	20 h	80
8	EtOH	$Fe(OTf)_2$	40	20 h	84
9	EtOH	$Fe(OTf)_3$	r.t.	20h	0
10	EtOH	$Fe(OTf)_3$	40	5 min	81
11	EtOH	$Sc(OTf)_3$	r.t.	20 h	>95
12	EtOH	$Bi(OTf)_3$	40	20 h	<10
13	ETOH	/	40	48 h	0

[a]Reaction was performed with **3a** (0.2 mmol) and catalyst (10 mol%) in solvent (4.0 m). [b]Isolated yield.

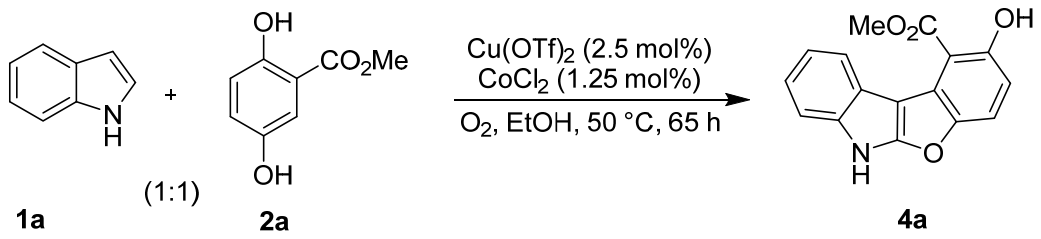
(C) General procedure for catalytic oxidative [3+2] cycloaddition



1a **2a** **4a**

To an oven dried 25 mL round bottom flask was added indole **1a** (0.2 mmol, 1.0 eq), methyl 2,5-dihydroxybenzoate **2a** (0.2 mmol, 1.0 equiv), $Cu(OTf)_2$ (7.3 mg, 10 mol%), and $CoCl_2$ (1.3 mg, 5 mol%) under 1 atm O_2 by using a balloon. EtOH (4 mL) was added via syringe, and the reaction mixture was stirred under O_2 at 40 °C for 48 h. It was quenched by introducing water (15 mL) and then extracted with CH_2Cl_2 (3*10 mL). The combined organic fractions were then dried over MgSO4, filtered, and concentrated in vacuum. Purification of crude product was performed by column chromatography using hexane/EtOAc (100:3 to 100:5) to afford product **4a** as a pale-yellow solid.

(D) Gram-scale synthesis of compound 4a

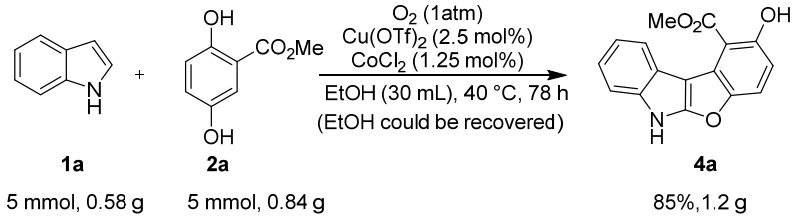


An oven dried 100 mL round bottom flask was charged with 1H-indole **1a** (5 mmol, 0.58 g, 1.0 equiv), methyl 2,5-dihydroxybenzoate **2a** (5 mmol, 0.84 g, 1.0 equiv), and $Cu(OTf)_2$ (45.2 mg, 2.5 mol%), and $CoCl_2$ (8 mg, 1.25 mol%) then caped with rubber septum, sealed by parafilm, under the constant pressure of O_2 (1 atm), the reaction was vented 3 times for 10 sec. to remove air then 20 mL EtOH was added *via* syringe a dramatic color change was observed within 2 min, resulting in a purple reaction mixture. The reaction mixture was stirred under O_2 at 50 °C for 60 h, after the reaction completed checked by TLC metal catalysts were removed by a short pad of silica eluted by 20 mL CH_2Cl_2 the reaction concentrated *in vacuo* the purification of crude product was performed by recrystallization using *n*-hexane (10 mL) and CH_2Cl_2 and to afford methyl 2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate **4a** (85% 1.2 g)

(E) Green metrics calculation

E-factor, atom economy, atom efficiency, carbon efficiency and reaction mass efficiency were calculated based on the scale-up synthesis of compound **4a**.

The E-factor is calculated under the optimized conditions for this reaction conducted on the model substrate. For comparison, the E factors for literature known procedures are also calculated. The calculation is based on the equation: **E-factor = m(waste)/m(product)**. All chemicals used, including solvents and water for work-up procedures, are considered. The purification step is neglected due to a lack of information (amounts of solvents used, etc.).



$$\boldsymbol{E-factor} = \frac{0.0452\ g\ \ Cu(OTf)2 + 0.0081\ g\ \ CoCl2 + 0.18\ \ gH2O}{1.2g\ \ (4a)}$$

$$= 0.194\ \ kg\ \ waste\ \ per\ \ 1k\ \ product$$

$$\boldsymbol{Atom\ \ economy}\ (\%) = \frac{molecular\ \ mass\ \ of\ \ desire\ \ product}{molecular\ \ mass\ \ of\ \ all\ \ reactants} \times 100$$

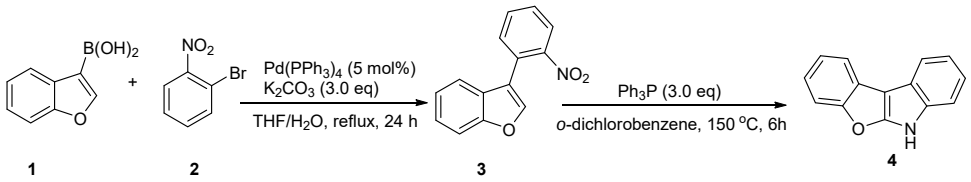
$$= \frac{281.06}{293.29\ \ (1a + 2b + O2)} = \ \ 95.8\ \ \%$$

Atom efficiency *= 85% × 95.8%= 81.4%*

$$\textbf{\textit{Carbon efficiency}} = \frac{14}{14} = 100\ \ \%$$

$$\textbf{Reaction mass efficiency (\%)} = \frac{mass\ of\ desired\ product}{mass\ of\ all\ reactants} \times 100\% = \frac{1.2}{0.58+0.84+0.16} = 75.9\%$$

In Comparison with recent work (*J. Mater. Chem. C, 2019, 7, 13912; Chem. – Asian J., 2019, 14, 2251.*)



1 Mw: 161.9, 28 mmol, 5.0 g

2 Mw: 202.01 g/mol, 42.1 mmol, 8.1 g

3 Mw: 239.2 g/mol, 5.0 g, 80% yield

4 Mw: 207.2 g/mol, 4.0 g, 81%

$$\boldsymbol{E-factor}$$

$$= \frac{benzofuranylboronic\ acid\ 5g + 8.4\ g\ Nitrobenzene + 1.6g\ Pd(Ph3)4 + K2CO3\ 11.6g + H2O\ 66mL + 34mL\ THF + PPh3\ 17.2g + 20\ mL\ oDCB}{4g\ Final\ Product}$$

$$= \mathbf{41.49\ kg\ waste\ per\ 1k\ product}$$

$$Atom\ economy = \frac{molecular\ mass\ of\ desire\ product}{molecular\ mass\ of\ all\ reactants} \times 100\% = \frac{207.23}{161.9+202.1} = 56.9\ \%$$

$$Atom\ efficiency = 80\% \times 81\% \times 56.9\% = 36.9\%$$

$$Reaction\ mass\ efficiency\ (\%) = \frac{mass\ of\ desired\ product}{mass\ of\ all\ reactants} \times 100\% = \frac{4}{5+8.1} = 30.5\%$$

Table S3 EcoScale calculation for the synthesis of **4a**

	parameters	Penalty points
1 Yield	(100-%)/2=(100-85)/2=7.5	7.5
2 Price of reaction components	(To obtained 10 mmol end product) 1. indole = 0.5 g = $ 3.47 2. methyl 2,5-dihydroxybenzoate$ 2 3. $Cu(OTf)_2$ =$ 0.2 4. $CoCl_2$ =$ 0.1 5. EtOH 20 mL =$ 1.1 Total price = $ 6.7 Thus inexpensive (<$10)	0
3 Safety EtOH (Toxic) Flammable		 5 5
4 Temperature and time 50 °C and 60 hours		2
5 Workup and purification Removal of solvent less than <150 °C Classical chromatography purification		0 0
Total Penalty points		19.5
EcoScale		80.5

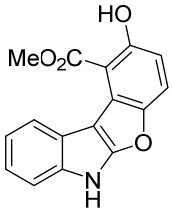
EcoScale = 100 - Sum of individual penalties

Scores on EcoScale: >75, Excellent; >50, Acceptable<50, inadequate

(Ref. Van Aken, K.; Strekowski, L.; Patiny, L. *Beilstein J. Org. Chem.* **2006**, *2*, doi:10.1186/1860-5397-2-3)

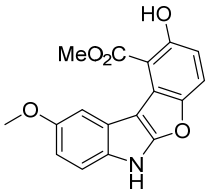
(F) Analytical data of cylcoadducts

Methyl 2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4a



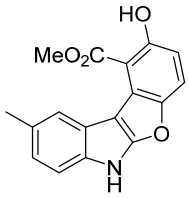
A pale yellow solid, 53 mg, 91% yield.
m.p.: 188-190 °C.
TLC: R_f = 0.69 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 7.72 – 7.64 (m, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.10 – 7.02 (m, 2H), 6.61 (d, *J* = 8.8 Hz, 1H), 3.95 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 157.6, 157.4, 149.0, 136.4, 124.2, 120.7, 120.4, 119.9, 119.4, 117.0, 111.2, 107.9, 102.6, 98.3, 51.7.
IR (ATR/cm^{-1}) 3242.5, 1648.8, 1566.9, 1284.4, 1020.84, 745.9.
HRMS (ESI): $C_{16}H_{12}NO_4^+$ [$(M+H)^+$]: calcd.: 282.0761; found: 282.0762.

Methyl 2-hydroxy-9-methoxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4b



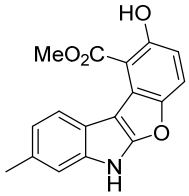
A yellow solid, 56 mg, 94% yield.
m.p.: 161–163 °C
TLC: R_f = 0.76 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (600 MHz, DMSO) δ 12.24 (s, 1H), 10.31 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.38 – 7.32 (m, 2H), 6.83 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.11 (s, 3H), 3.84 (s, 3H).
^{13}C NMR (151 MHz, DMSO) δ 169.1, 158.5, 155.1, 154.0, 149.2, 131.7, 124.7, 121.4, 116.5, 112.9, 109.6, 108.9, 106.4, 104.4, 97.8, 55.3, 52.6.
IR (ATR/cm^{-1}) 2953.61, 1620.65, 1539.8, 1523.18, 1091.07, 823.22.
HRMS (ESI): $C_{17}H_{14}NO_5^+$ [$(M+H)^+$]: calcd.: 312.0866; found: 312.0868.

Methyl 2-hydroxy-9-methyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4c



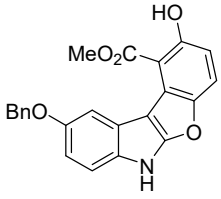
A pale yellow solid, 54 mg, 91.2 % yield.
m.p.: 198-200 °C.
TLC: R_f = 0.46 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.53 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.34 – 7.31 (m, 1H), 7.10 – 7.04 (m, 1H), 6.78 – 6.71 (m, 1H), 4.24 (s, 3H), 2.53 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 158.8, 158.3, 149.9, 135.5, 129.4, 125.2, 122.4, 121.6, 121.1, 117.8, 111.7, 108.6, 103.5, 98.91, 52.5, 21.6.
IR (ATR/cm^{-1}) 3261.7, 1649.1, 2854.5, 1564.4, 1241.0, 1024.6, 646.1.
HRMS (ESI): $C_{17}H_{14}NO_4^+$ [$(M+H)^+$]: calcd.: 296.0917; found: 296.0918.

Methyl 2-hydroxy-8-methyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4d



A pale yellow solid, 54.5 mg, 92% yield.
m.p.: 207–209 °C.
TLC: R_f = 0.48 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, DMSO) δ 12.29 (s, 1H), 10.34 (s, 1H), 7.74 – 7.59 (m, 2H), 7.26 (s, 1H), 7.09 – 6.95 (m, 1H), 6.72 (d, *J* = 8.8 Hz, 1H), 4.08 (s, 3H), 2.43 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 158.4, 149.9, 137.7, 131.2, 125.2, 121.8, 120.5, 119.3, 117.9, 112.4, 108.6, 103.5, 99.1, 52.7, 21.4.
IR (ATR/cm^{-1}) 3262.2, 1640.84, 1230.83, 1129.53, 857.88.
HRMS (ESI): $C_{17}H_{14}NO_4^+$ [$(M+H)^+$]: calcd.: 296.0917; found: 296.0918.

Methyl 9-(benzyloxy)-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4e



A yellow solid, 63 mg, 86% yield.

m.p.: 170– 172 °C.

TLC: R_f = 0.50 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

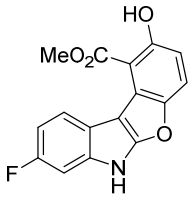
^{1}H NMR (400 MHz, DMSO) δ 10.29 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.42 (s, 1H), 7.42 – 7.36 (m, 3H), 7.34 (d, *J* = 7.5 Hz, 1H), 6.94 – 6.89 (m, 1H), 6.72 (d, *J* = 8.8 Hz, 1H), 5.17 (s, 2H), 4.05 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 159.1, 158.4, 153.8, 149.9, 137.5, 132.5, 128.5, 127.9, 127.5, 125.2, 122.4, 118.0, 112.5, 110.7, 109.0, 107.5, 103.7, 99.5, 71.5, 52.7.

IR (**ATR/cm^{-1}**) 3316.7, 1640.3, 1386.5, 1286.5, 822.0, 799, 741.2, 627.2.

HRMS (ESI): $C_{23}H_{18}NO_5^+$ [$(M+H)^+$]: calcd.: 388.1179; found: 388.1180.

Methyl 8-fluoro-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4f



A pale yellow solid, 44 mg, 74% yield.

m.p.: 242– 244 °C.

TLC: R_f = 0.72 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

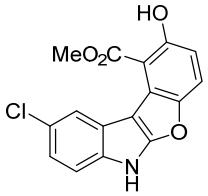
^{1}H NMR (400 MHz, DMSO**)** δ 10.31 (s, 1H), 7.84 – 7.76 (m, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.28 (dd, *J* = 9.7, 2.5 Hz, 1H), 7.09 – 7.01 (m, 1H), 6.74 (d, *J* = 8.8 Hz, 1H), 4.07 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 169.0, 158.9, 158.1, 157.4, 155.4, 149.2, 137.1 (d, *J* = 12.3 Hz), 124.5, 121.5 (d, *J* = 23.0 Hz), 117.6, 116.8, 109.4, 107.9 (d, *J* = 9.4 Hz), 106.3, 99.1 (d, *J* = 26.3.0 Hz), 97.5, 52.6.

IR (**ATR/cm^{-1}**) 3282.6, 1644.6, 1513.3, 1289.3, 1058.9, 786.6.

HRMS (ESI): $C_{16}H_{11}FNO_4^+$ [$(M+H)^+$]: calcd.: 300.0667; found: 300.0667.

Methyl 9-chloro-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4g



A pale yellow solid, 45.5 mg, 72% yield.

m.p.: 244– 246 °C.

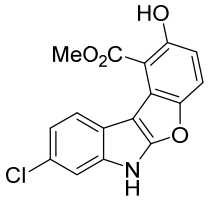
TLC: R_f = 0.80 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

^{1}H NMR (400 MHz, DMSO) δ 10.25 (s, 1H), 7.87 (d, *J* = 2.1 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.22 (dd, *J* = 8.6, 2.2 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 4.07 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 168.8, 159.0, 155.3, 149.46, 124.7, 124.6, 122.0, 120.9, 120.1, 116.9, 114.0, 109.8, 106.6, 97.5, 52.6.

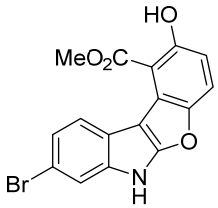
IR (ATR/cm^{-1}) 3238.4, 1651.0, 1565.1, 1462.0, 1126.2, 973.0, 878.0.
HRMS (ESI): $C_{16}H_{11}ClNO_4^+$ [$(M+H)^+$]: calcd.: 316.0371; found: 316.0371.

Methyl 8-chloro-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4h



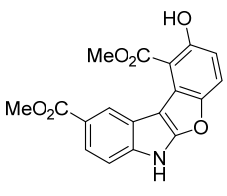
A yellow solid, 47.5 mg, 77% yield.
m.p.: 235– 237 °C.
TLC: R_f = 0.76 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.6 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.44 (d, *J* = 2.1 Hz, 1H), 7.23 – 7.18 (m, 1H), 6.76 (d, *J* = 8.8 Hz, 1H), 4.21 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.7, 158.7, 158.3, 149.9, 137.8, 126.6, 124.7, 121.5, 120.6, 120.1, 118.0, 112.1, 109.2, 103.6, 98.9, 52.6.
IR (**ATR/cm^{-1}**) 3269.9, 2438.0, 1737.7, 1456.1, 1317.9, 826.0.
HRMS (ESI): $C_{16}H_{11}ClNO_4^+$ [$(M+H)^+$]: calcd.: 316.0371; found: 316.0370.

Methyl 8-bromo-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4i



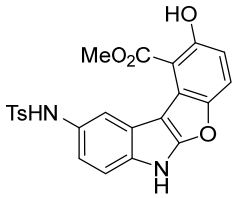
Pale yellow solid, 52 mg, 75% yield.
m.p.: 229– 231 °C.
TLC: R_f = 0.50 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.6 Hz, 1H), 7.60 – 7.51 (m, 2H), 7.38 – 7.32 (m, 1H), 6.78 (d, *J* = 8.8 Hz, 1H), 4.20 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.4, 167.7, 164.9, 158.9, 147.4, 133.9, 132.7, 131.8, 129.5, 126.4, 124.5, 122.8, 119.3, 116.1, 107.2, 62.2.
IR (**ATR/cm^{-1}**) 2953.7, 1643.8, 1466.8, 1332.9, 1185.8, 847.6, 798.1.
HRMS (ESI): $C_{16}H_{11}{}^{79}BrNO_4^+$ [$(M+H)^+$]: calcd.: 359.9866; found: 359.9866.

Dimethyl 2-hydroxy-6H-benzofuro[2,3-b]indole-1,9-dicarboxylate 4j



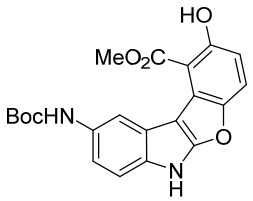
A yellow solid, 41 mg, 60 % yield.
m.p.: 269 – 271 °C.
TLC: R_f = 0.41 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, DMSO) δ 10.62 (s, 1H), 8.57 (d, *J* = 1.7 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 6.80 (d, *J* = 8.9 Hz, 1H), 4.16 (s, 3H), 3.89 (s, 3H).
^{13}C NMR (101 MHz, DMSO) δ 169.3, 167.1, 158.7, 156.4, 149.4, 139.9, 124.0, 122.6, 122.2, 121.5, 120.4, 117.5, 112.3, 109.9, 105.6, 98.3, 52.7, 51.8.
IR (**ATR/cm^{-1}**) 3190.3 2919.1, 1664.3, 1526.3, 1497.3, 1287.5, 1126.7, 1090.2.
HRMS (ESI): $C_{18}H_{14}NO_6^+$ [$(M+H)^+$]: calcd.: 340.0816; found: 340.0816.

Methyl 2-hydroxy-9-((4-methylphenyl)sulfonamido)-6H-benzofuro[2,3-b]indole-1-carboxylate 4k



A yellow solid, 74 mg, 82 % yield.
m.p.: 275– 277 °C.
TLC: R_f = 0.25 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, DMSO) δ 12.43 (s, 1H), 10.41 (s, 1H), 9.92 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.50 (d, *J* = 2.1 Hz, 1H), 7.30 (dd, *J* = 8.4, 7.0 Hz, 3H), 6.92 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.04 (s, 3H), 2.30 (s, 3H).
^{13}C NMR (101 MHz, DMSO) δ 169.1, 158.4, 155.2, 149.2, 142.7, 136.7, 134.6, 130.3, 129.4, 126.8, 124.2, 120.8, 117.1, 116.6, 115.1, 112.6, 109.2, 106.4, 97.7, 52.7, 20.8.
IR (**ATR/cm^{-1}**) 3271.4, 2952.2, 1651.0, 1485.3, 1245.2, 1106.5, 847.4.
HRMS (ESI): $C_{23}H_{19}N_2O_6S^+$ [$(M+H)^+$]: calcd.: 451.0958; found: 451.0966.

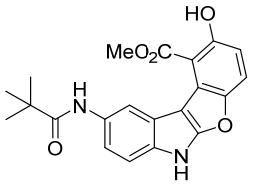
Methyl 9-((tert-butoxycarbonyl)amino)-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4l



A pale yellow solid, 70 mg, 88 % yield.
m.p.: 212– 214 °C.
TLC: R_f = 0.54 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

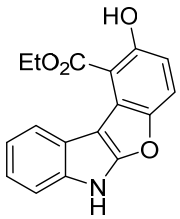
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.55 – 7.48 (m, 1H), 7.30 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.12 – 7.02 (m, 1H), 6.77 – 6.68 (m, 1H), 4.30 (s, 3H), 1.56 (s, 9H).
^{13}C NMR (101 MHz, DMSO) δ 169.4, 158.4, 155.2, 153.2, 149.2, 133.0, 132.6, 124.4, 120.7, 116.4, 112.1, 108.8, 106.4, 97.7, 78.4, 52.9, 28.2
IR (**ATR/cm^{-1}**) 2998.0, 1703.1, 1587.1, 1442.0, 1174.4, 1055.9, 1443.5, 926.8.
HRMS (ESI): $C_{21}H_{21}N_2O_6^+$ [$(M+H)^+$]: calcd.: 397.1394; found: 397.1394.

Methyl 2-hydroxy-9-pivalamido-6H-benzofuro[2,3-b]indole-1-carboxylate 4m



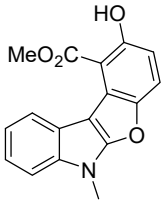
A pale yellow solid, 68 mg, 89% yield.
m.p.: 229– 231 °C.
TLC: R_f = 0.20 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (400 MHz, DMSO) δ 10.51 (s, 1H), 9.15 (s, 1H), 8.04 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.25 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.17 (s, 3H), 1.27 (s, 9H).
^{13}C NMR (101 MHz, DMSO) δ 176.1, 169.4, 158.4, 155.5, 149.2, 133.7, 132.2, 124.3, 120.5, 116.7, 116.3, 114.1, 111.8, 108.9, 106.1, 97.8, 52.9, 27.4.
IR (**ATR/cm^{-1}**) 3448.3, 1660.6, 1551.2, 1453.4, 1396.0, 1166.1, 931.7.
HRMS (ESI): $C_{21}H_{21}N_2O_5^+$ [$(M+H)^+$]: calcd.: 381.1445; found: 381.1443.

Ethyl 2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4n



A yellow solid, 51.3 mg, 87% yield.
m.p.: 128– 130 °C.
TLC: R_f = 0.24 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].
^{1}H NMR (600 MHz, DMSO-d_6) δ 12.42 (s, 1H), 10.09 (s, 1H), 7.84 – 7.79 (m, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.23 – 7.17 (m, 2H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.59 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (101 MHz, DMSO) δ 168.4, 158.0, 154.3, 149.4, 137.1, 124.6, 121.2, 120.8, 120.5, 120.3, 116.0, 112.4, 109.1, 107.7, 97.6, 61.3, 14.3.
IR (ATR/cm^{-1}) 3287.0, 1647.0, 1452.4, 1201.9, 1125.0, 851.6, 740.1.
HRMS (ESI): $C_{17}H_{14}NO_4^+$ [$(M+H)^+$]: calcd.: 296.0917; found: 296.0917.

Methyl 2-hydroxy-6-methyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4o



A yellow solid, 58 mg, 85% yield.

m.p.: 197–199 °C

TLC: R_f = 0.60 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

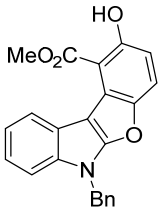
^{1}H NMR (400 MHz, DMSO) δ 10.36 (s, 1H), 7.86 – 7.80 (m, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.29 – 7.21 (m, 2H), 6.74 (d, *J* = 8.8 Hz, 1H), 4.07 (s, 3H), 3.88 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 168.9, 158.0, 155.3, 149.3, 137.9, 124.9, 121.1, 120.7, 120.6, 120.3, 116.7, 110.5, 109.1, 106.5, 96.7, 52.6, 29.0.

IR (ATR/cm^{-1}) 2943.8, 1650.0, 1313.78, 1136.7, 1047.9, 750.5.

HRMS (ESI): $C_{17}H_{14}NO_4^+$ [$(M+H)^+$]: calcd.: 296.0917; found: 296.0917.

Methyl 6-benzyl-2-hydroxy-6H-benzofuro[2,3-b]indole-1-carboxylate 4p



A pale yellow, 53 mg, 71% yield.

m.p.: 147– 149 °C.

TLC: R_f = 0.32 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

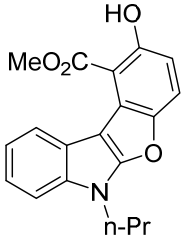
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.7 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 1H), 7.36 – 7.16 (m, 9H), 6.75 (d, *J* = 8.8 Hz, 1H), 5.46 (s, 2H), 4.21 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 158.8, 158.7, 150.3, 138.0, 136.1, 129.1, 128.1, 127.1, 125.5, 121.84, 121.5, 121.1, 118.5, 110.7, 109.5, 104.0, 53.0, 46.8.

IR (**ATR/cm^{-1}**) 3026.8, 1650.0, 1507.1203.6, 1074.8, 789.0, 728.6.

HRMS (ESI): $C_{23}H_{18}NO_4^+$ [$(M+H)^+$]: calcd.: 372.1230; found: 372.1231.

Methyl 2-hydroxy-6-propyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4q



A pale yellow, 57mg, 89% yield.

m.p.: 125– 127 °C.

TLC: R_f = 0.59 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

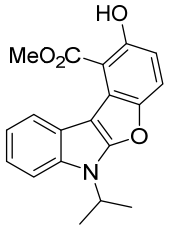
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 – 7.82 (m, 1H), 7.58 – 7.50 (m, 1H), 7.42 – 7.33 (m, 1H), 7.28 – 7.21 (m, 2H), 6.73 (d, *J* = 8.7 Hz, 1H), 4.22 (t, *J* = 7.0 Hz, 2H), 4.20 (s, 3H), 3.10 (s, 4H), 1.95 (q, *J* = 7.3 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 159.3, 159.1, 150.7, 138.4, 125.9, 121.9, 121.1, 118.5, 110.6, 109.5, 104.3, 98.7, 53.1, 45.2, 23.1, 11.6.

IR (**ATR/cm^{-1}**) 2916.6, 2847.2, 1661.0, 1488.6, 1295.8, 924.3.

HRMS (ESI): $C_{19}H_{18}NO_4^+$ [$(M+H)^+$]: calcd.: 324.1230; found: 324.1229.

Methyl 2-hydroxy-6-isopropyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4r



Pale yellow solid, 55 mg, 88% yield

m.p.: 119– 121 °C.

TLC: R_f = 0.89 (Hexane/EtOAc = 50:1) [UV, $KMnO_4$].

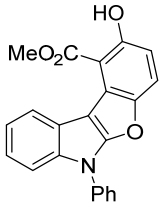
^{1}H NMR (600 MHz, $CDCl_3$) δ 11.07 (s, 1H), 7.98 – 7.93 (m, 1H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.34 – 7.29 (m, 2H), 6.80 (d, *J* = 8.8 Hz, 1H), 5.06 – 4.74 (m, 1H), 4.26 (s, 3H), 1.75 (s, 3H), 1.73 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.4, 158.8, 158.7, 150.7, 137.7, 125.2, 121.7, 121.6, 121.6, 120.8, 118.4, 110.6, 109.4, 104.1, 99.6, 53.0, 47.8, 21.6.

IR (**ATR/cm^{-1}**) 2982.6, 1655.2, 1503.1, 1311.1, 1137.2, 841.0.

HRMS (ESI): $C_{19}H_{18}NO_4^+$ [$(M+H)^+$]: calcd.: 324.1230; found: 324.1230.

Methyl 2-hydroxy-6-phenyl-6H-benzofuro[2,3-b]indole-1-carboxylate 4s



A pale yellow solid, 53 mg, 75 % yield.

m.p.: 152– 154 °C.

TLC: R_f = 0.35 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

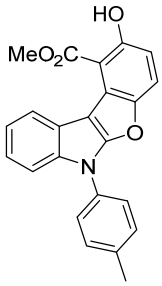
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.64 – 7.60 (m, 2H), 7.58 – 7.55 (m, 2H), 7.48 (t, 1H), 7.34 (t, *J* = 1.1 Hz, 1H), 7.28 (t, 2H), 6.81 (d, *J* = 8.8 Hz, 1H), 4.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 170.3, 158.5, 158.3, 156.9, 149.2, 149.1, 137.4, 134.4, 129.3, 127.2, 124.5, 124.2, 121.4, 121.1, 121.1, 120.8, 117.9, 117.9, 110.5, 109.6, 109.5, 103.5, 99.2, 52.3.

IR (**ATR/cm^{-1}**) 2917.4, 1657.8, 1540.4, 1323.5, 1096.7, 833.6.

HRMS (ESI): $C_{22}H_{16}NO_4^+$ [$(M+H)^+$]: calcd.: 358.1074; found: 358.1074.

Methyl 2-hydroxy-6-(p-tolyl)-6H-benzofuro[2,3-b]indole-1-carboxylate 4t



A pale yellow solid, 57.2 mg, 77 % yield.

m.p.: 160– 162 °C.

TLC: R_f = 0.52 (Hexane/EtOAc = 10:1) [UV, $KMnO_4$].

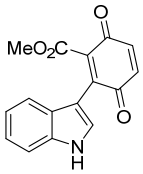
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.9 Hz, 1H), 7.60 – 7.51 (m, 4H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.38 – 7.24 (m, 2H), 6.86 – 6.75 (m, 1H), 4.26 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$)δ 170.8, 158.6, 157.5, 149.7, 138.0, 137.8, 132.1, 130.3, 124.9, 124.8, 121.8, 121.4, 121.4, 121.2, 118.3, 110.9, 109.7, 103.9, 99.4, 95.9, 52.7, 21.0.

IR (**ATR/cm^{-1}**) 2918.6, 1650.6, 1541.1, 1710.5, 1186.9, 1024.7.

HRMS (ESI): $C_{23}H_{18}NO_4^+$ [$(M+H)^+$]: calcd.: 372.1230; found: 372.1228.

Methyl 2-(1H-indol-3-yl)-3,6-dioxocyclohexa-1,4-diene-1-carboxylate 3a



A blue solid, 52 mg, 92 % yield.

m.p.: 185-187 °C.

TLC: R_f = 0.21 (Hexane/EtOAc = 3:1) [UV, $KMnO_4$].

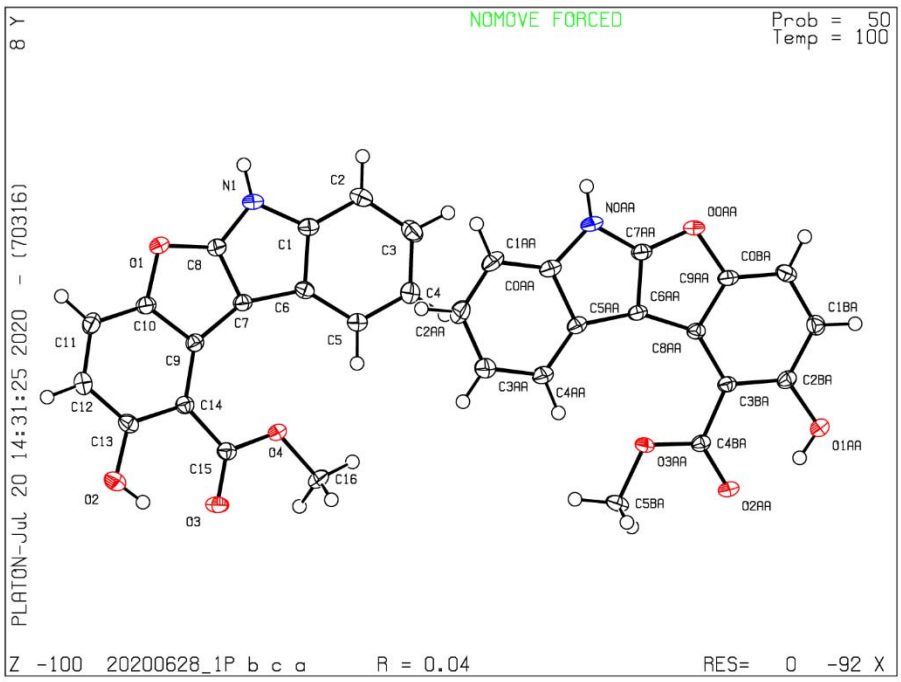
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.54 – 7.50 (m, 1H), 7.46 (d, *J* = 2.9 Hz, 1H), 7.40 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.27 – 7.16 (m, 2H), 6.98 – 6.87 (m, 2H), 3.70 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 186.6, 184.2, 165.6, 138.2, 136.7, 136.3, 133.8, 128.9, 126.1, 123.4, 121.4, 120.5, 111.8, 107.9, 53.0.

IR (ATR/cm^{-1}) 3289.4, 1661.5, 1535.4, 1416.1, 1264.7, 1101.5, 882.7

HRMS (ESI): $C_{16}H_{12}NO_4^+$ [$(M+H)^+$]: calcd.: 282.0761; found: 282.0761

(G) X-Ray crystallographic analysis of 4a



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Temperature:			
Reported			
Volume			
Space group	4905.05(10)		
Hall group			
P b c a			
-P 2ac 2ab			
C16 H11 N O4			
C16 H11 N O4			
Moiety formula C16 H11 N O4			
Sum formula	C16 H11 N O4		
Mr	281.26		
Dx,g cm-3	1.523		
Z	16		
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F000’	2343.95
h,k,lmax	23,8,47
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Tmin’	
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16	
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2336.0	
22,8,47	
4810	
0.400,1.000	
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wR2(reflections)=	
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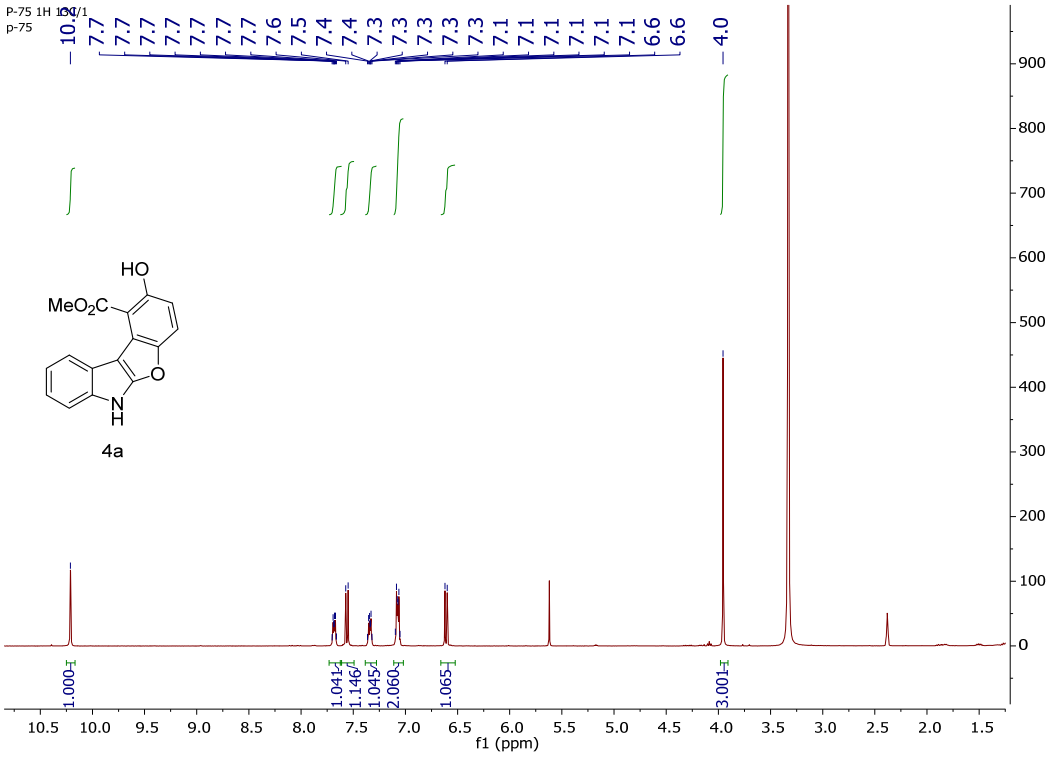
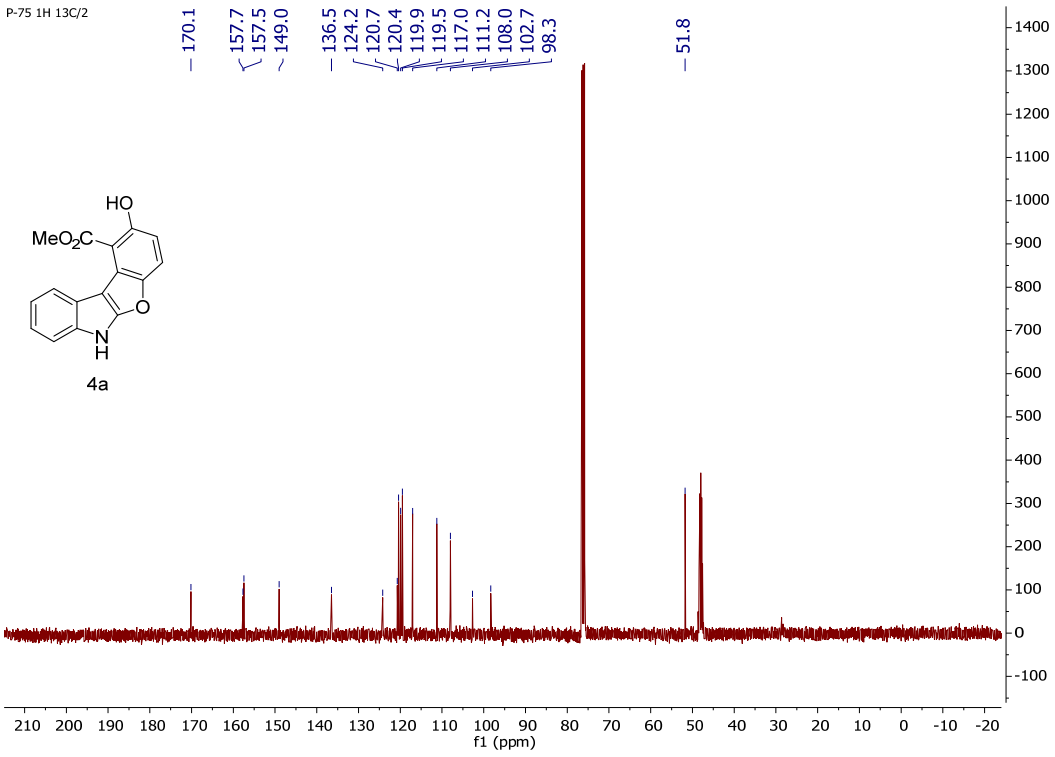
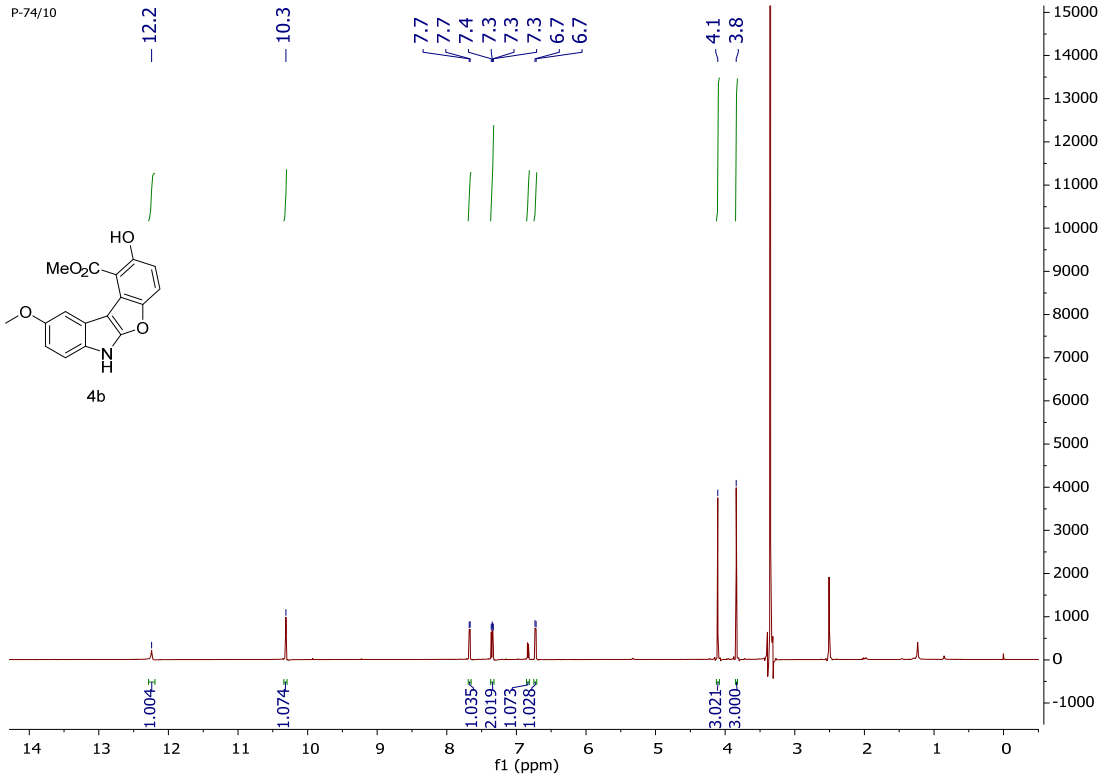
(H) NMR spectra of cycloadducts



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7.7
7.4
7.3
7.3
7.3
6.7
6.7
4.1
3.8
HO
MeO2C
O
O
N
H
4b
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1.035
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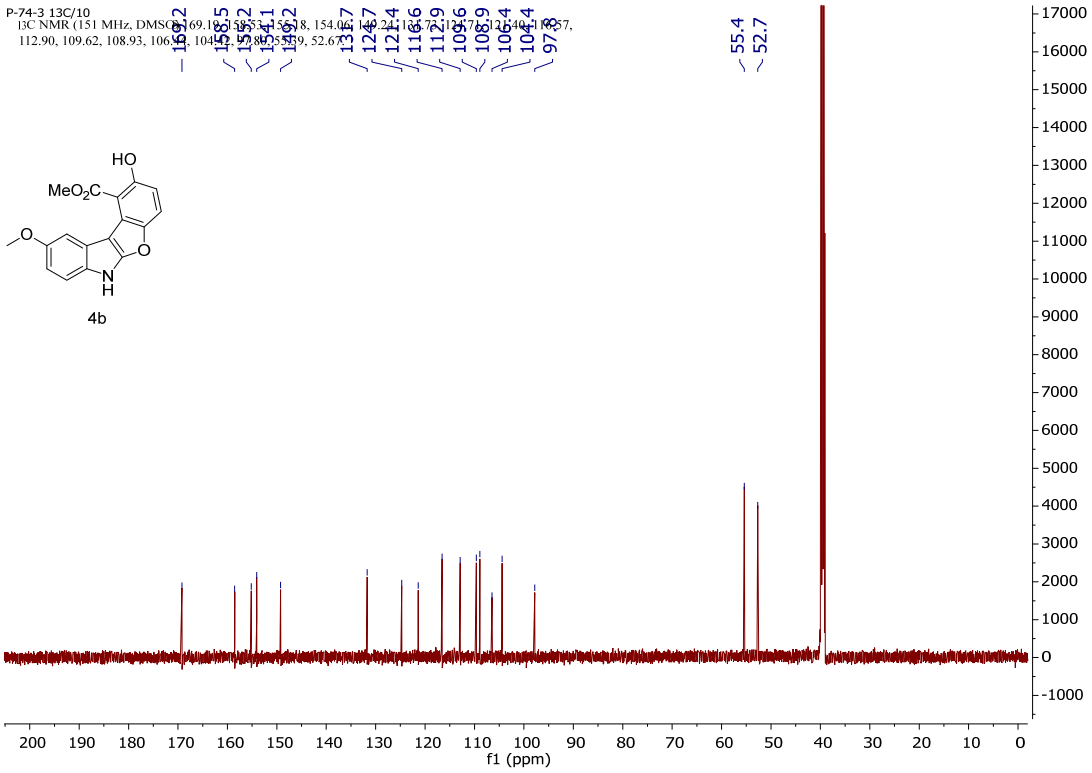
3.021
3.000
f1 (ppm)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HO
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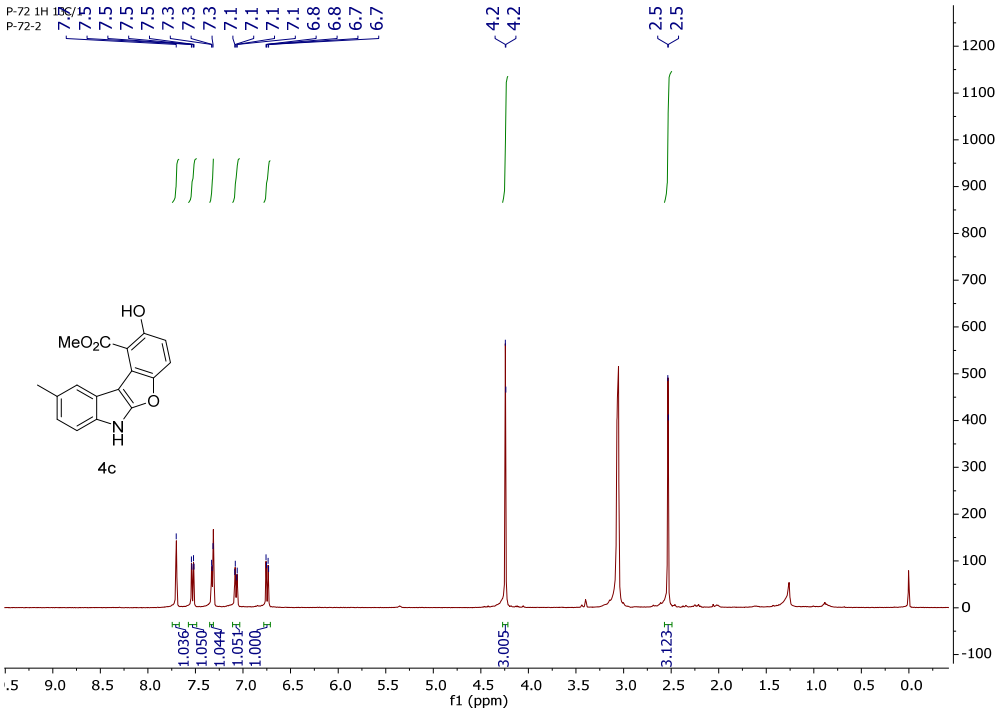
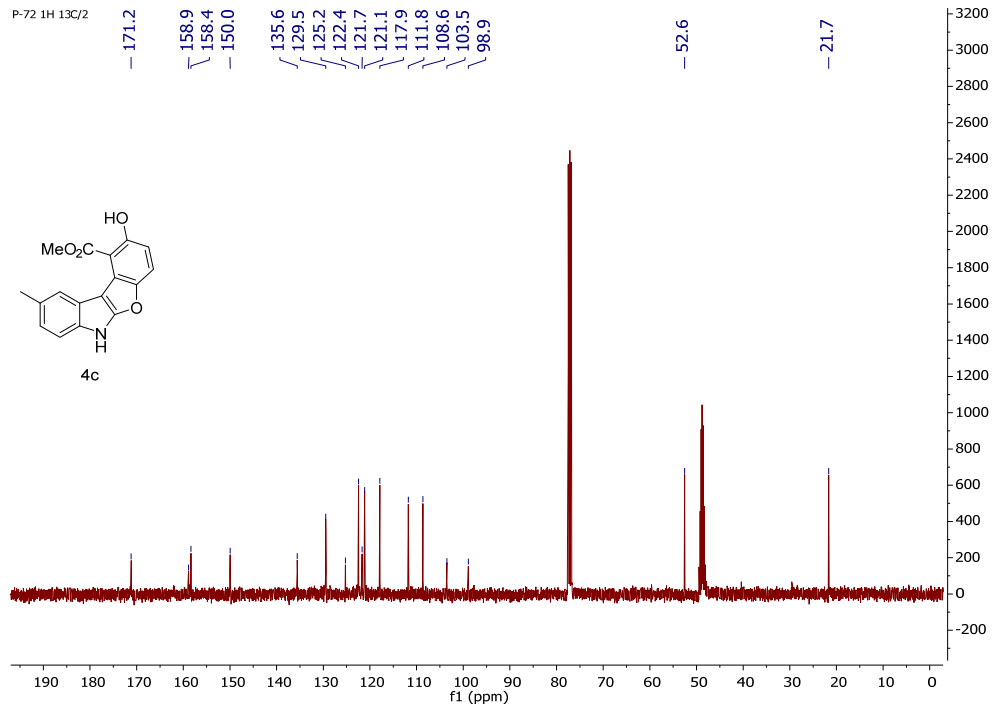
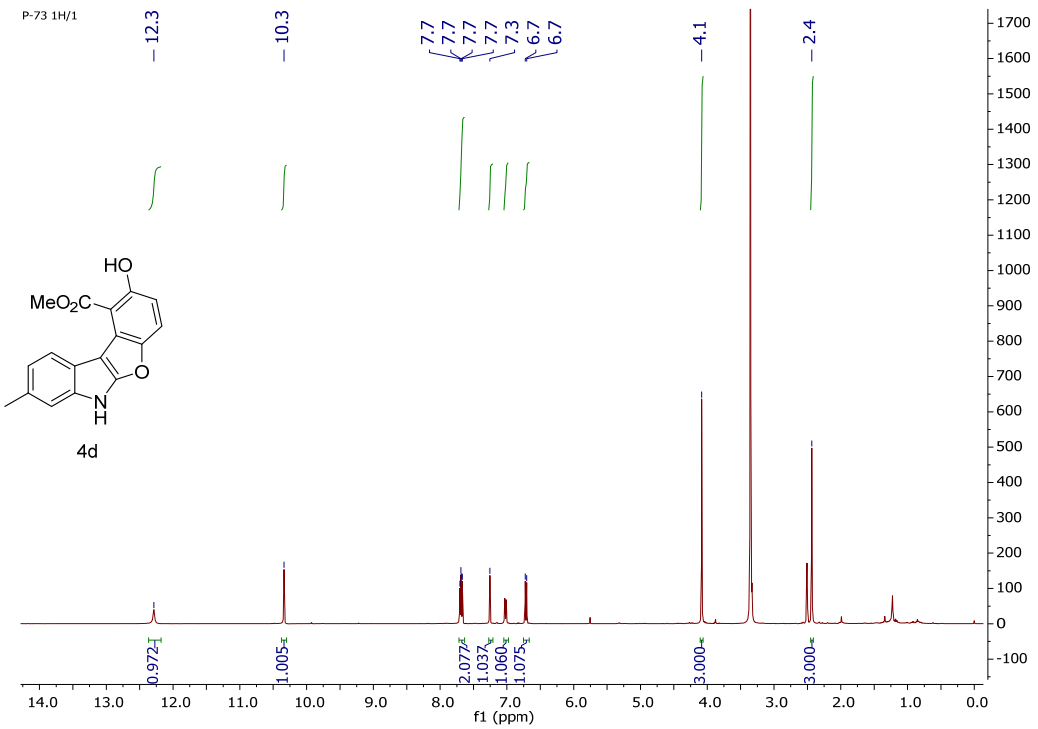
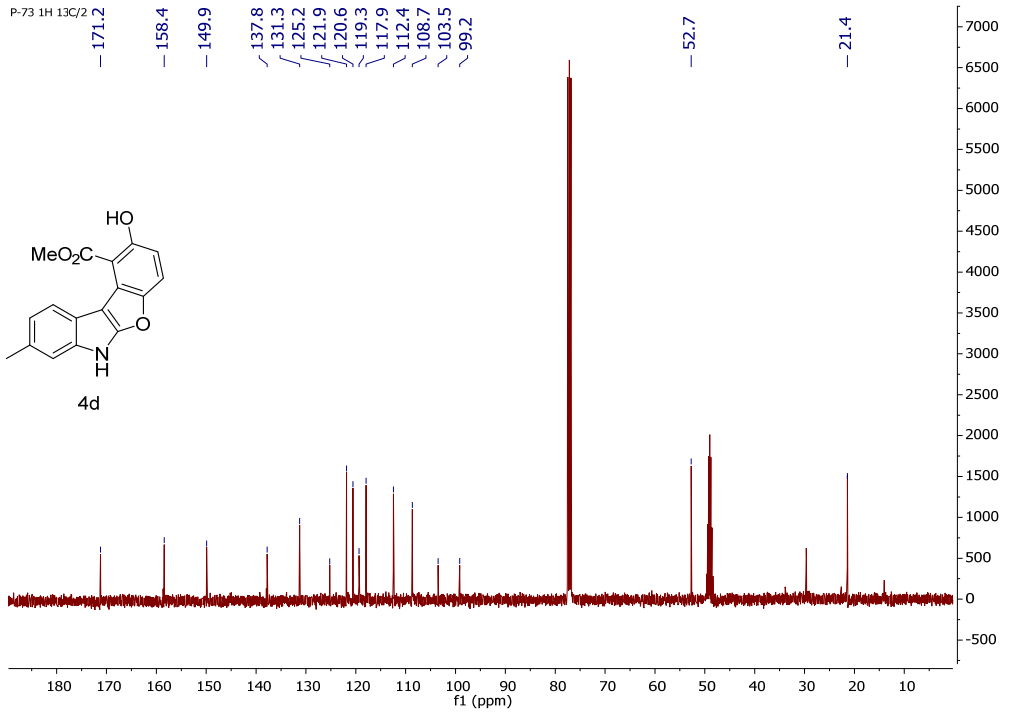
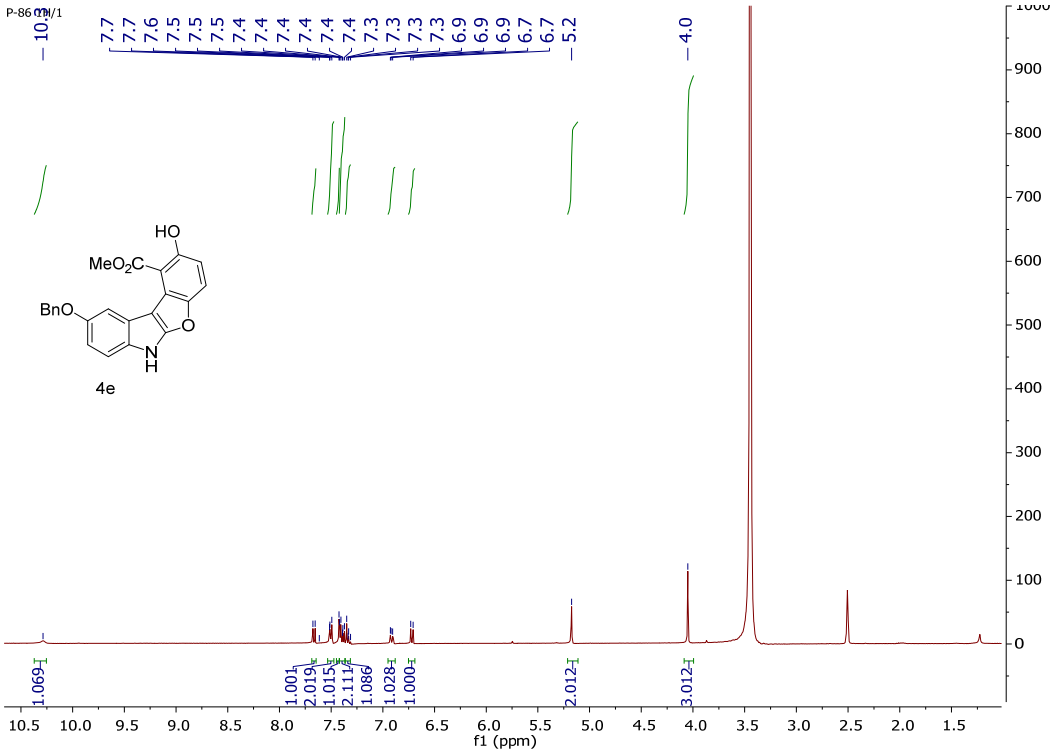
O
N
H
4b
f1 (ppm)

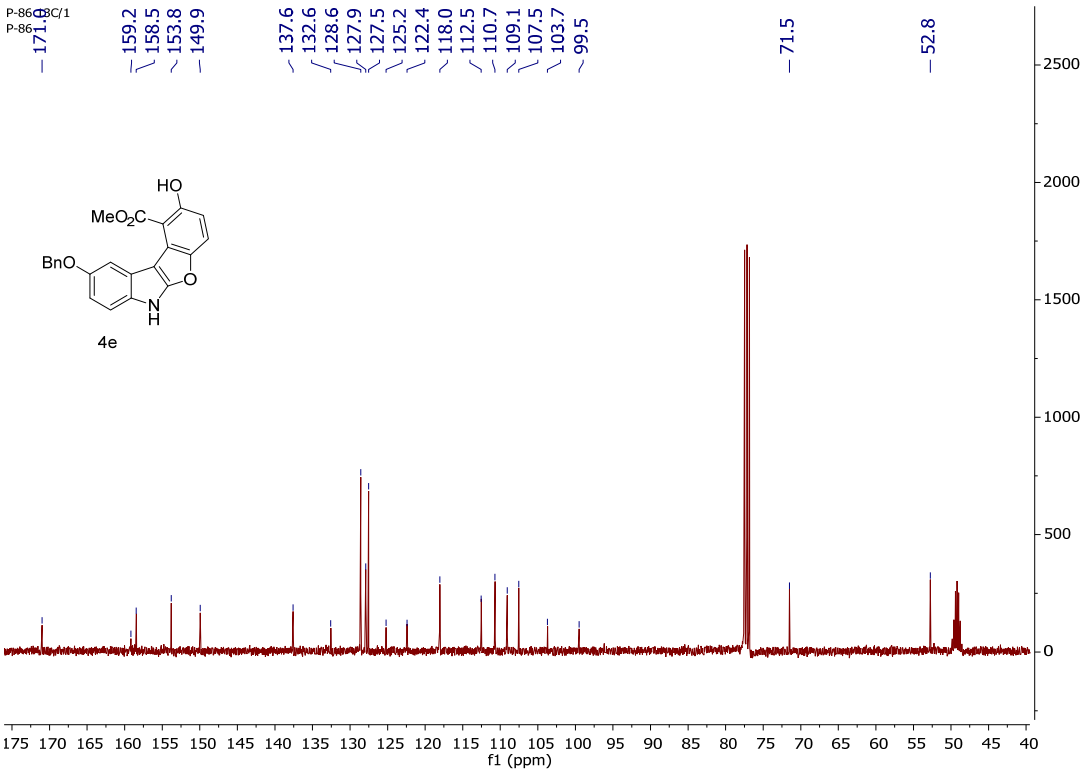

P-72 1H 13C/1
P-72-2
7.5
7.5
7.5
7.5
7.5
7.3
7.3
7.3
7.1
7.1
7.1
7.1
6.8
6.8
6.7
6.7
4.2
4.2
2.5
2.5
HO
MeO2C
O
N
H
4c
1.036
1.050
1.044
1.051
1.000
3.005
3.123
f1 (ppm)

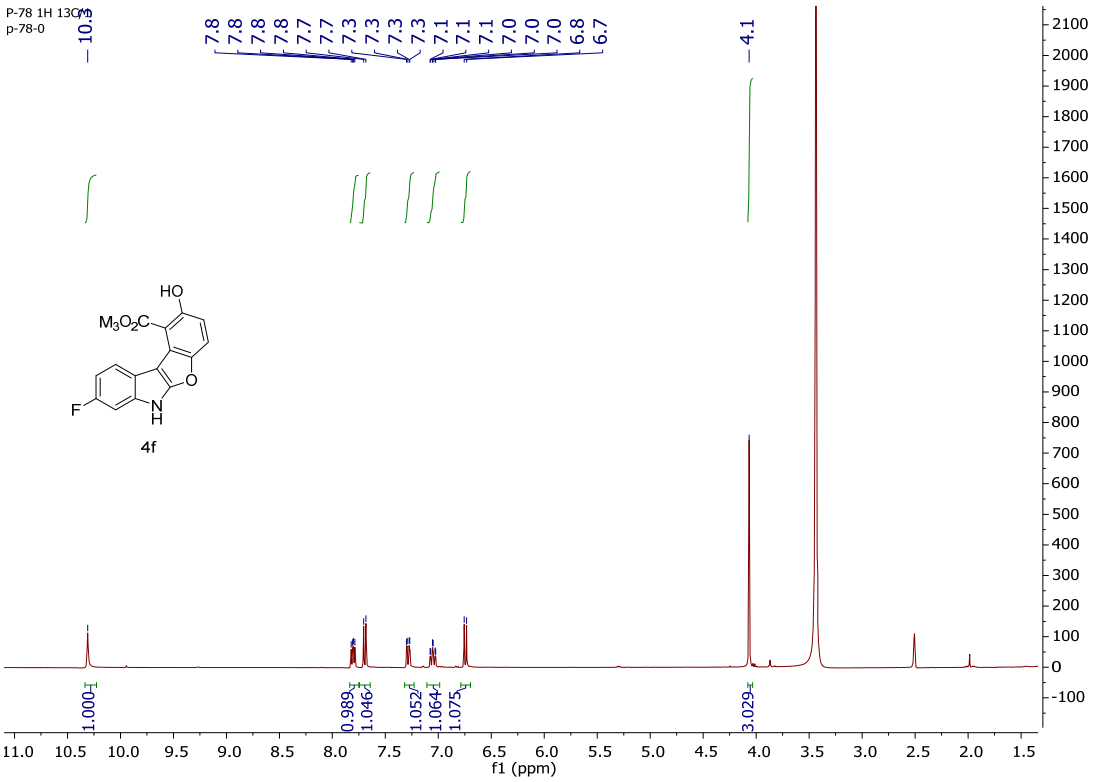

P-72 1H 13C/2
171.2
158.9
158.4
150.0
135.6
129.5
125.2
122.4
121.7
121.1
117.9
111.8
108.6
103.5
98.9
52.6
21.7
HO
MeO2C
O
N
H
4c
f1 (ppm)

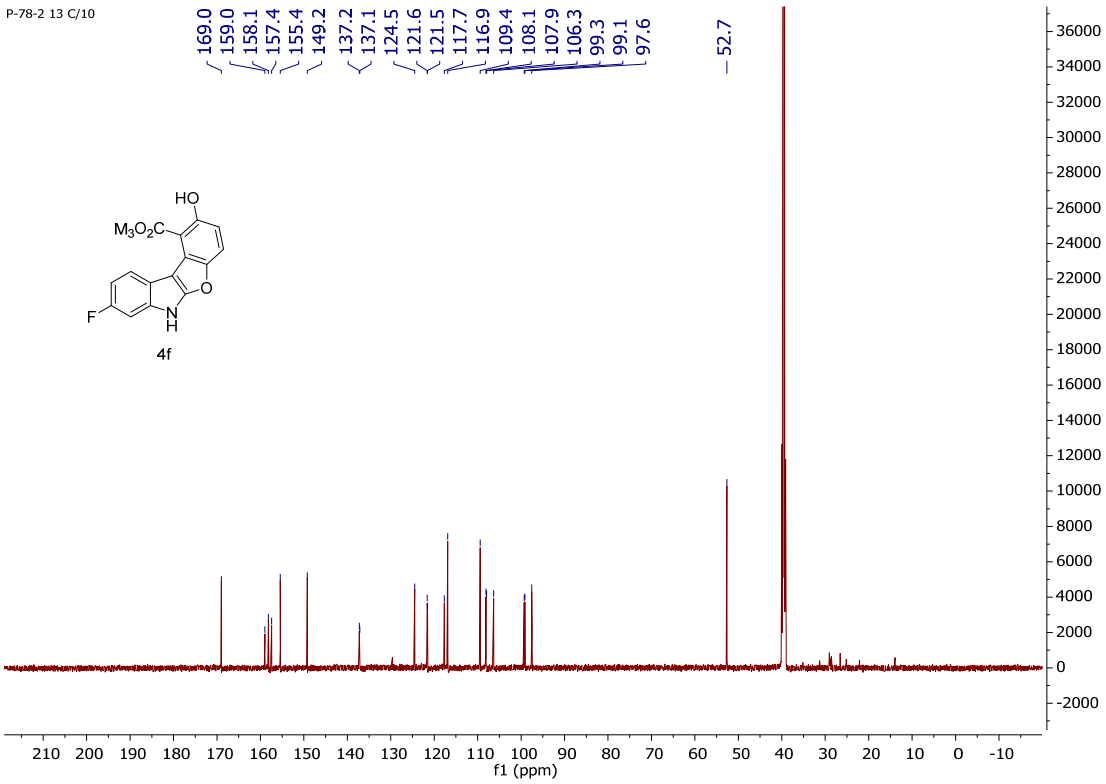

P-73 1H/1
12.3
10.3
7.7
7.7
7.7
7.7
7.3
6.7
6.7
4.1
2.4
HO
MeO2C
O
N
H
4d
0.972
1.005
2.077
1.037
1.060
1.075
3.000
3.000
f1 (ppm)

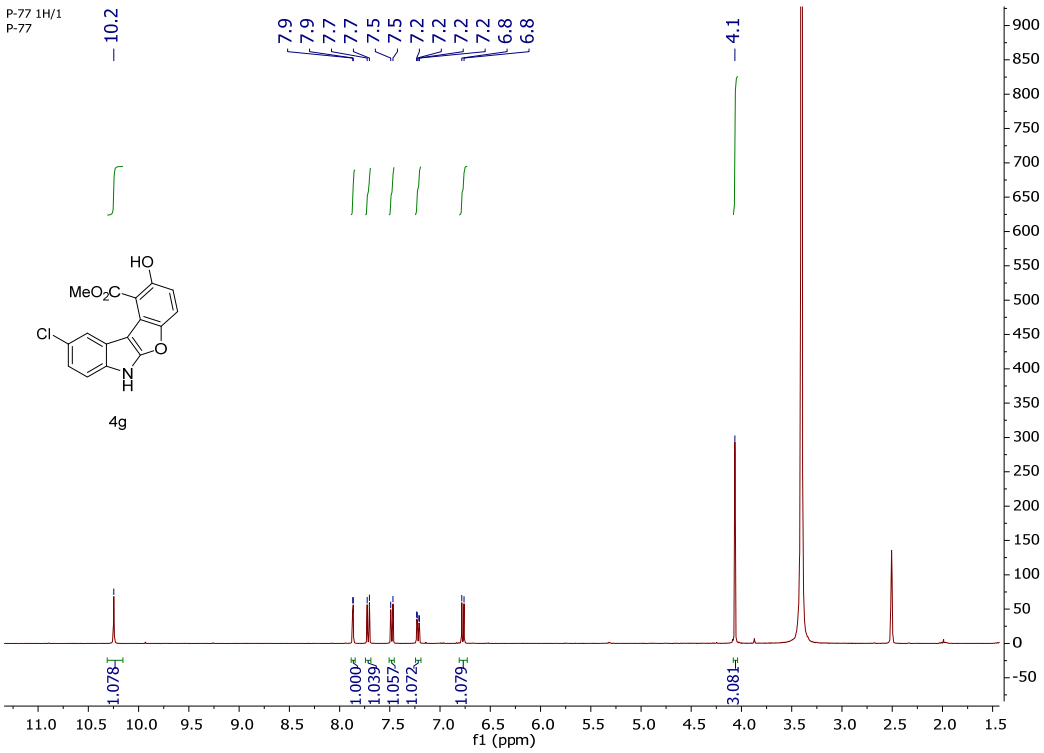

P-73 1H 13C/2
171.2
158.4
149.9
137.8
131.3
125.2
121.9
120.6
119.3
117.9
112.4
108.7
103.5
99.2
52.7
21.4
HO
MeO2C
O
N
H
4d
f1 (ppm)

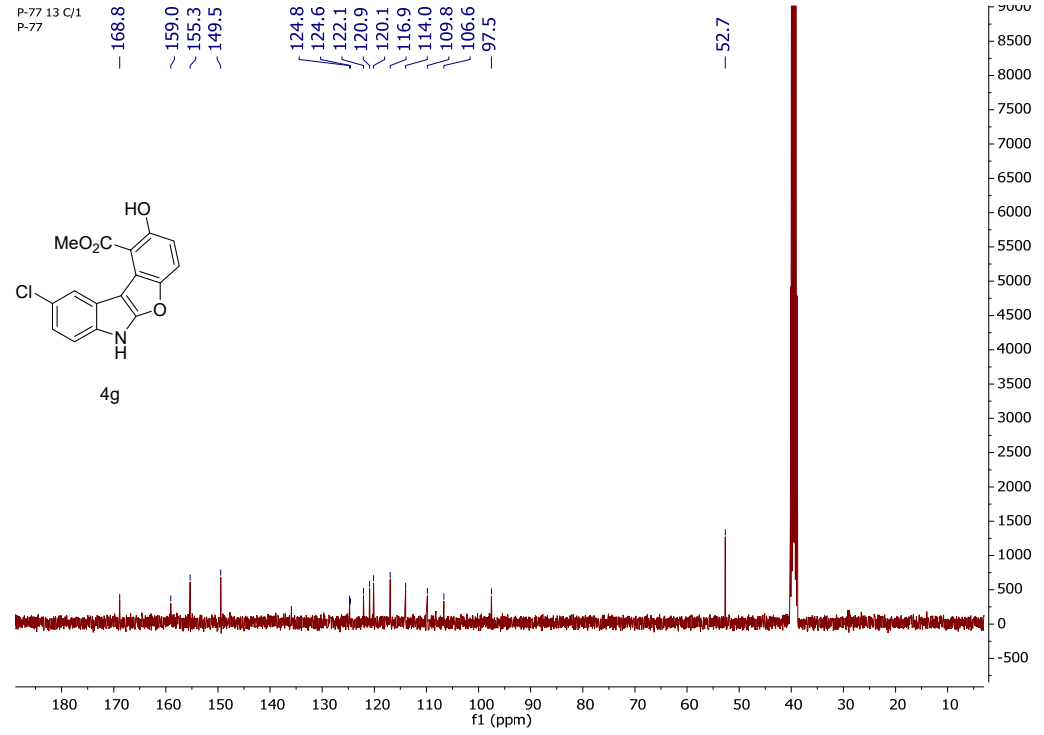

10.2
7.7
7.7
7.6
7.5
7.5
7.5
7.4
7.4
7.4
7.4
7.4
7.4
7.3
7.3
7.3
6.9
6.9
6.9
6.7
6.7
5.2
4.0
HO
MeO2C
BnO
O
N
H
4e
1.069
1.001
2.019
1.015
2.111
1.086
1.028
1.000
2.012
3.012
f1 (ppm)

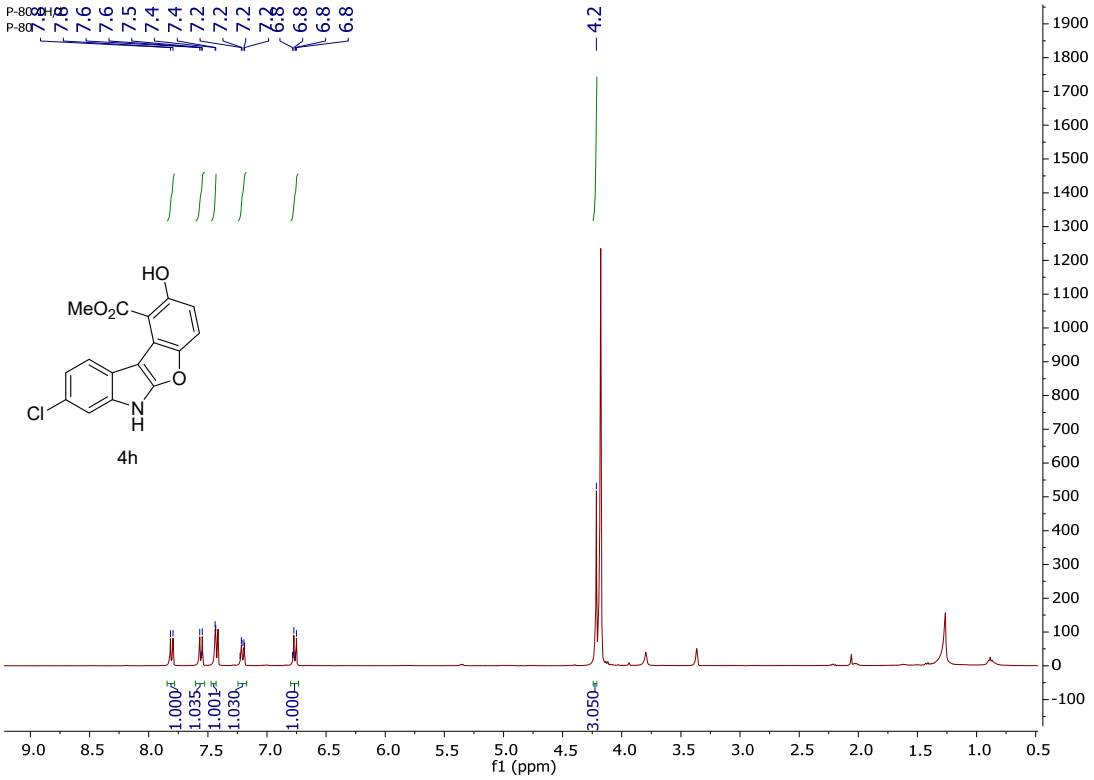

171.8
159.2
158.5
153.8
149.9
137.6
132.6
128.6
127.9
127.5
125.2
122.4
118.0
112.5
110.7
109.1
107.5
103.7
99.5
71.5
52.8
HO
MeO2C
BnO
O
N
H
4e
f1 (ppm)

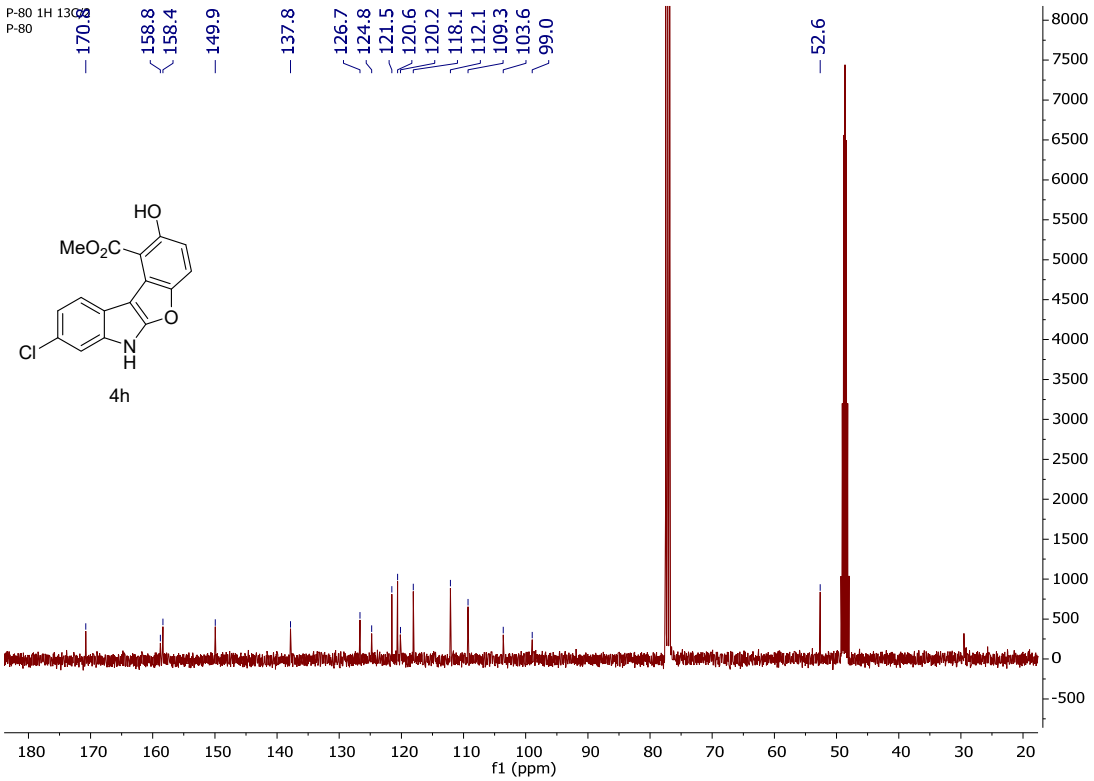

P-78 1H 13C/3
p-78-0
10.3
7.8
7.8
7.8
7.8
7.7
7.7
7.3
7.3
7.3
7.3
7.1
7.1
7.1
7.0
7.0
7.0
6.8
6.7
4.1
HO
M3O2C
F
O
N
H
4f
1.000
0.989
1.046
1.052
1.064
1.075
3.029
f1 (ppm)

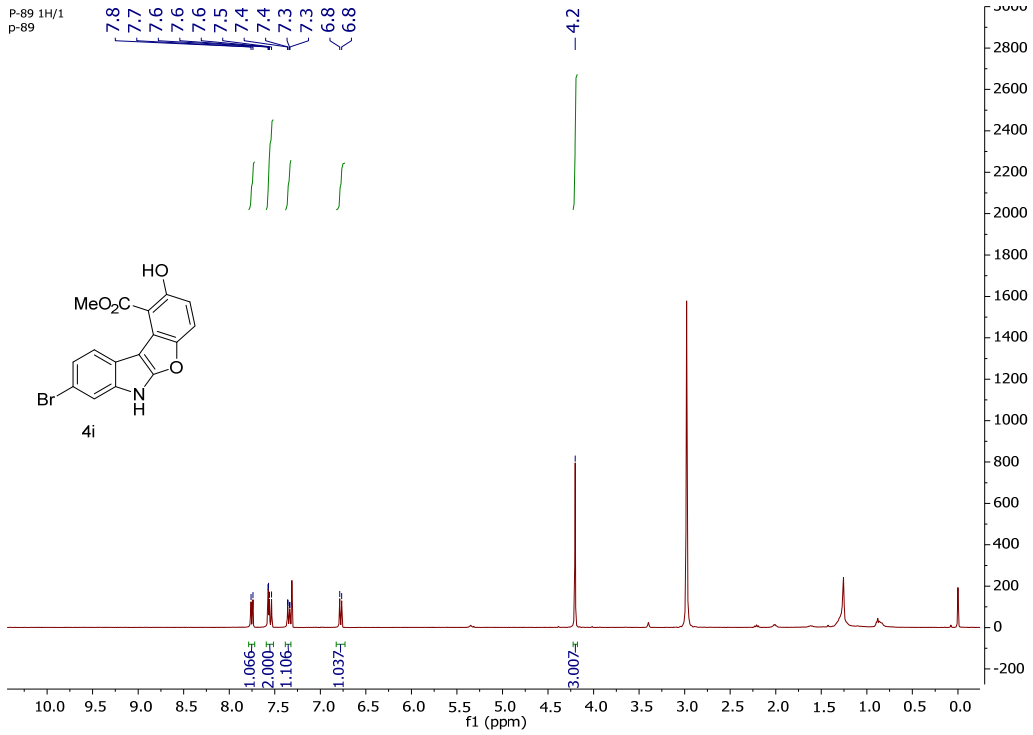

P-78-2 13 C/10
169.0
159.0
158.1
157.4
155.4
149.2
137.2
137.1
124.5
121.6
121.5
117.7
116.9
109.4
108.1
107.9
106.3
99.3
99.1
97.6
52.7
HO
M3O2C
F
O
N
H
4f
f1 (ppm)

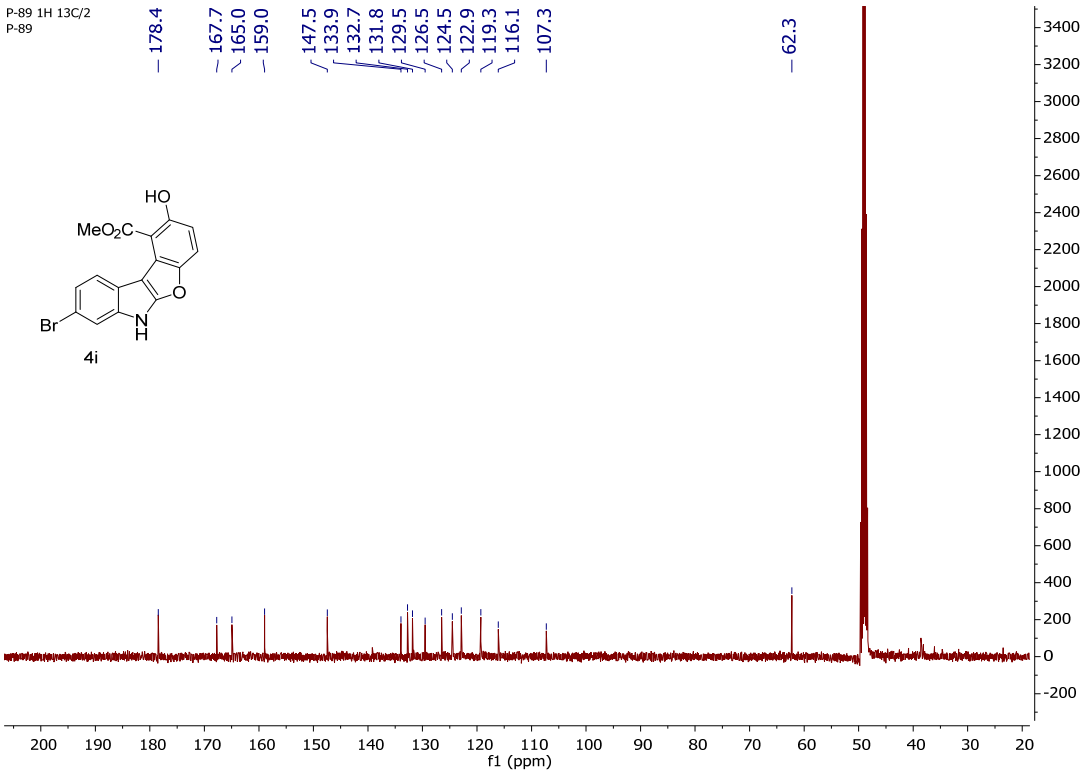

P-77 1H/1
P-77
10.2
7.9
7.9
7.7
7.7
7.5
7.5
7.2
7.2
7.2
7.2
6.8
6.8
4.1
HO
MeO2C
Cl
O
N
H
4g
1.078
1.000
1.039
1.057
1.072
1.079
3.081
f1 (ppm)

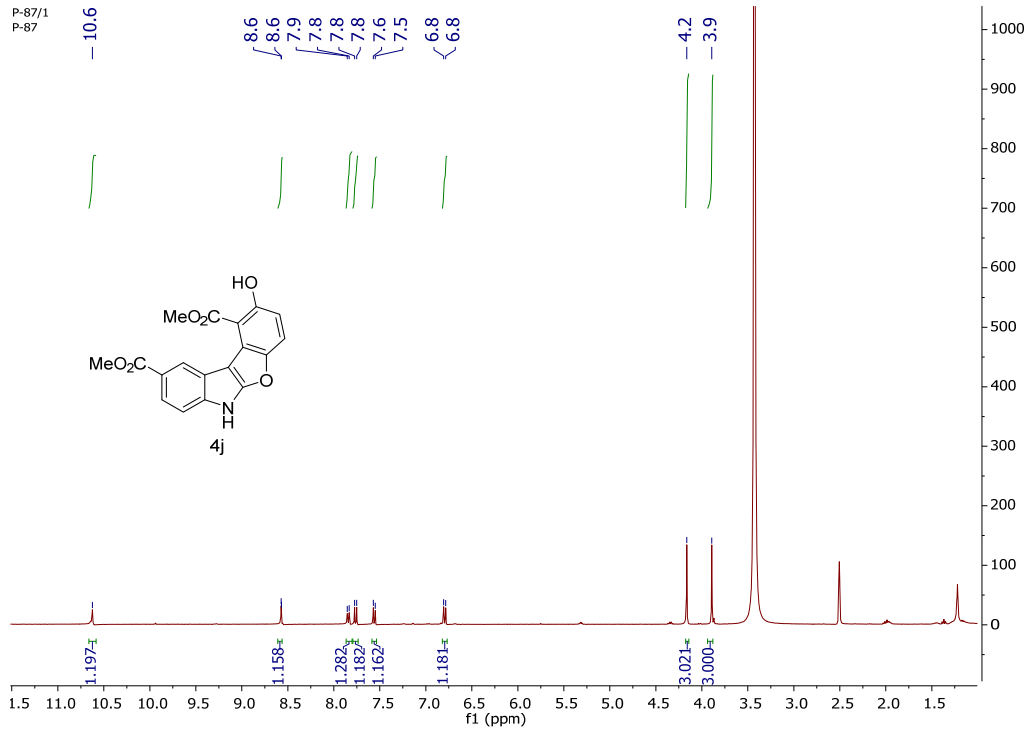

P-77 13 C/1
P-77
168.8
159.0
155.3
149.5
124.8
124.6
122.1
120.9
120.1
116.9
114.0
109.8
106.6
97.5
52.7
HO
MeO2C
Cl
O
N
H
4g
f1 (ppm)

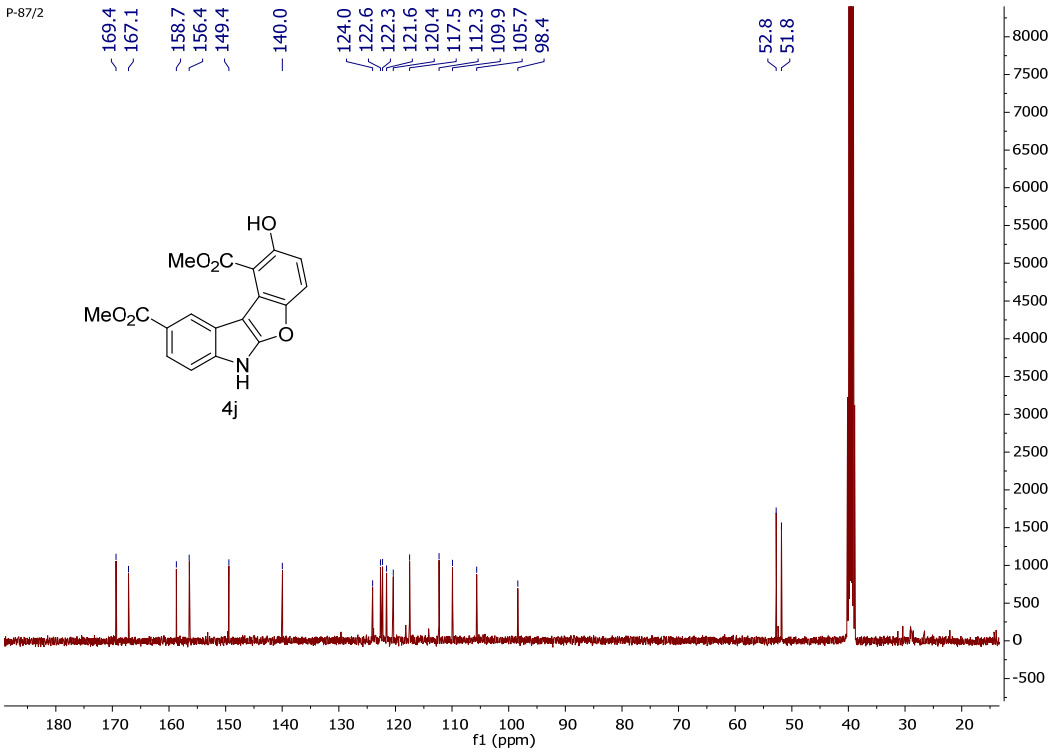

P-80
7.8
7.6
7.6
7.5
7.4
7.4
7.2
7.2
7.2
6.8
6.8
6.8
4.2
HO
MeO2C
O
Cl
N
H
4h
1.000
1.035
1.001
1.030
1.000
3.050
f1 (ppm)

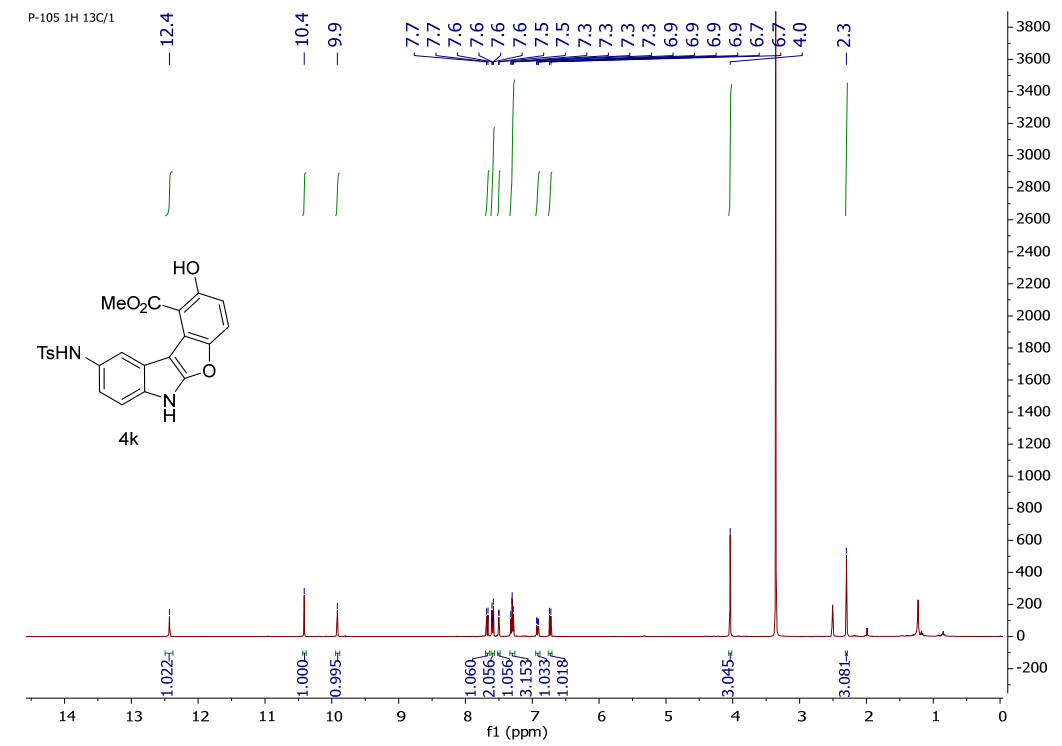

P-80 1H 13C
P-80
170.8
158.8
158.4
149.9
137.8
126.7
124.8
121.5
120.6
120.2
118.1
112.1
109.3
103.6
99.0
52.6
HO
MeO2C
O
Cl
N
H
4h
f1 (ppm)

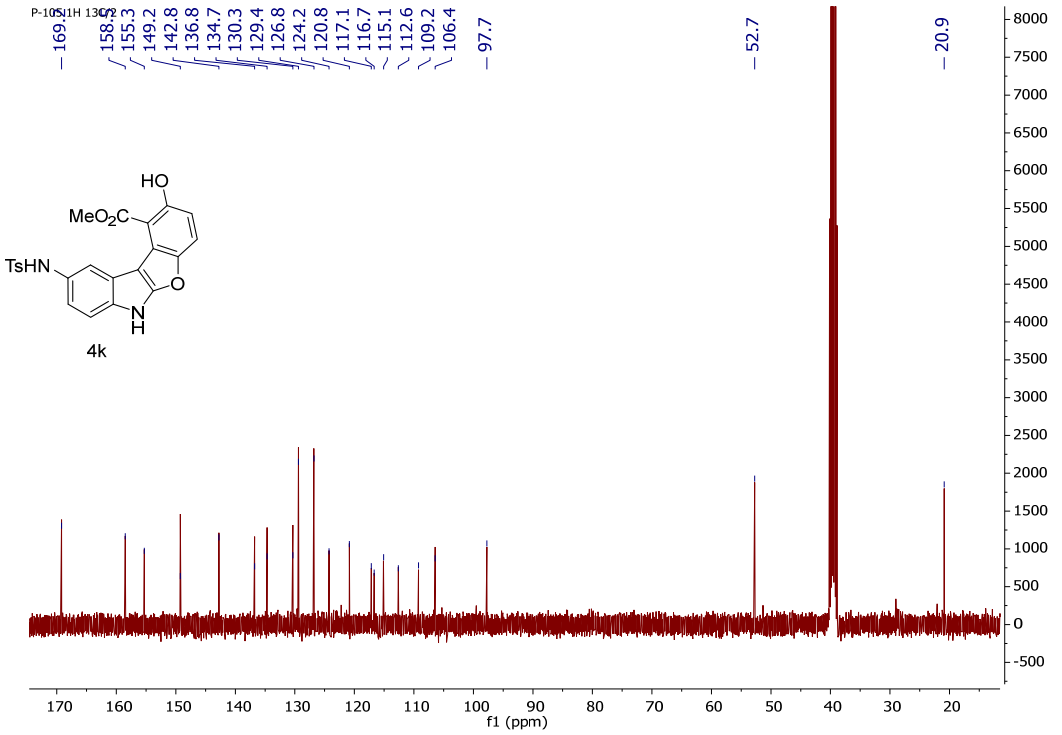

P-89 1H/1
p-89
7.8
7.7
7.6
7.6
7.6
7.5
7.4
7.4
7.3
7.3
6.8
6.8
4.2
HO
MeO2C
O
Br
N
H
4i
1.066
2.000
1.106
1.037
3.007
f1 (ppm)

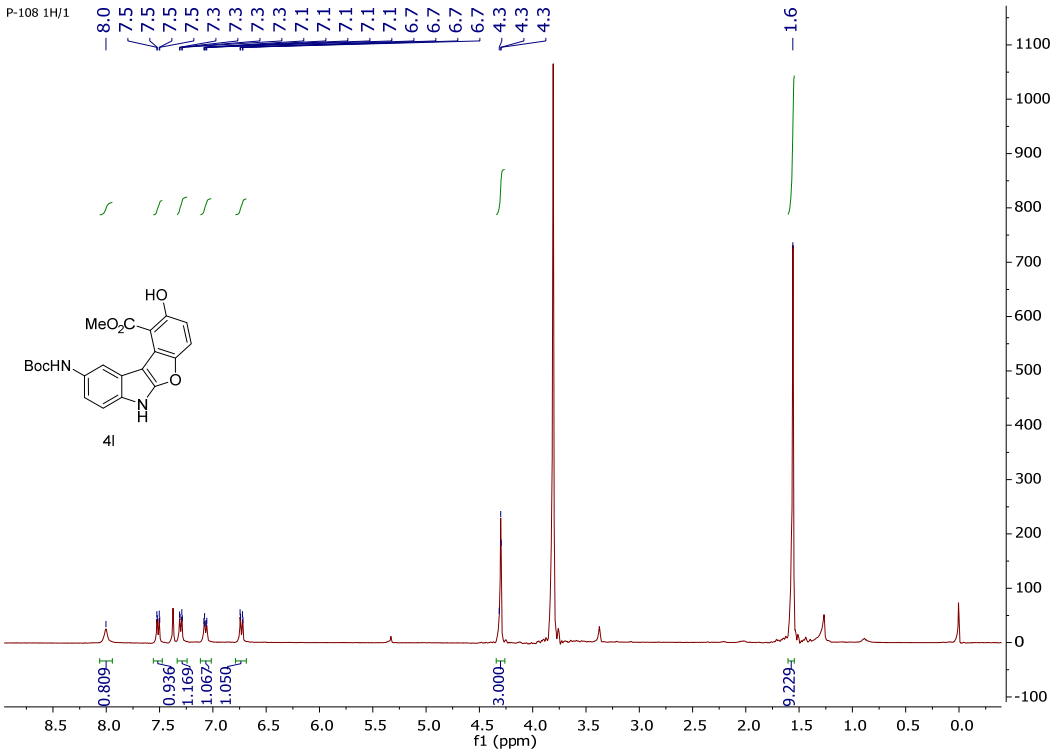

P-89 1H 13C/2
P-89
178.4
167.7
165.0
159.0
147.5
133.9
132.7
131.8
129.5
126.5
124.5
122.9
119.3
116.1
107.3
62.3
HO
MeO2C
O
Br
N
H
4i
f1 (ppm)

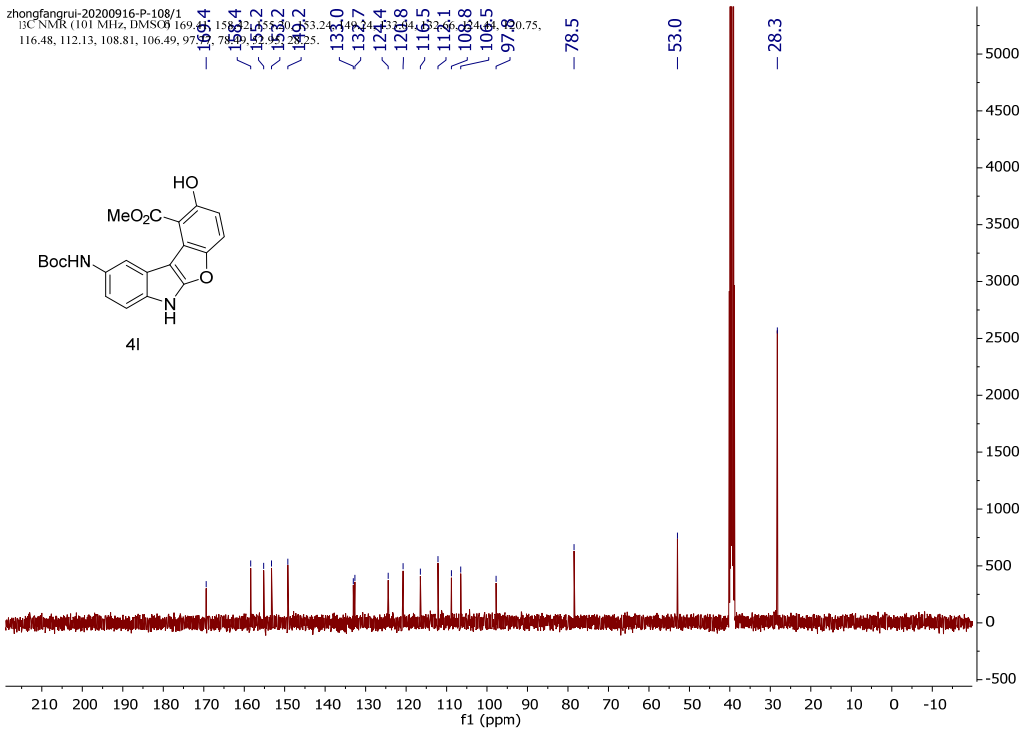

P-87/1
P-87
10.6
8.6
8.6
7.9
7.8
7.8
7.8
7.6
7.5
6.8
6.8
4.2
3.9
HO
MeO2C
MeO2C
O
N
H
4j
1.197
1.158
1.282
1.182
1.162
1.181
3.021
3.000
f1 (ppm)

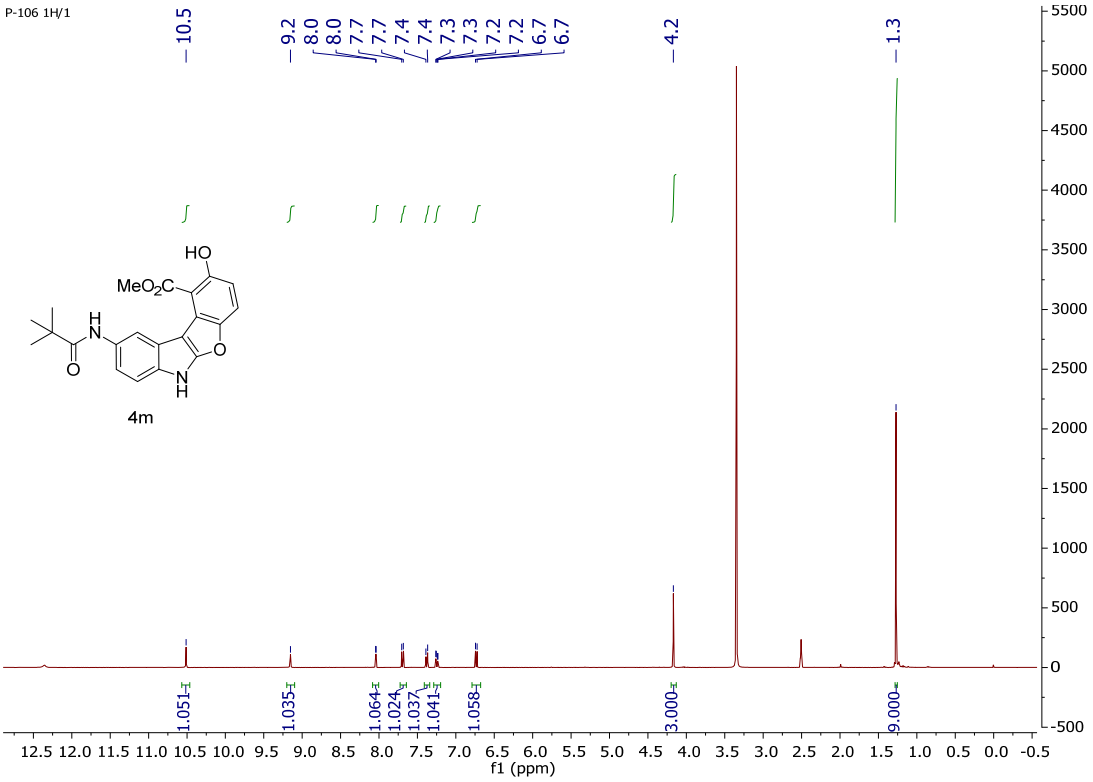

P-87/2
169.4
167.1
158.7
156.4
149.4
140.0
124.0
122.6
122.3
121.6
120.4
117.5
112.3
109.9
105.7
98.4
52.8
51.8
HO
MeO2C
MeO2C
O
N
H
4j
f1 (ppm)

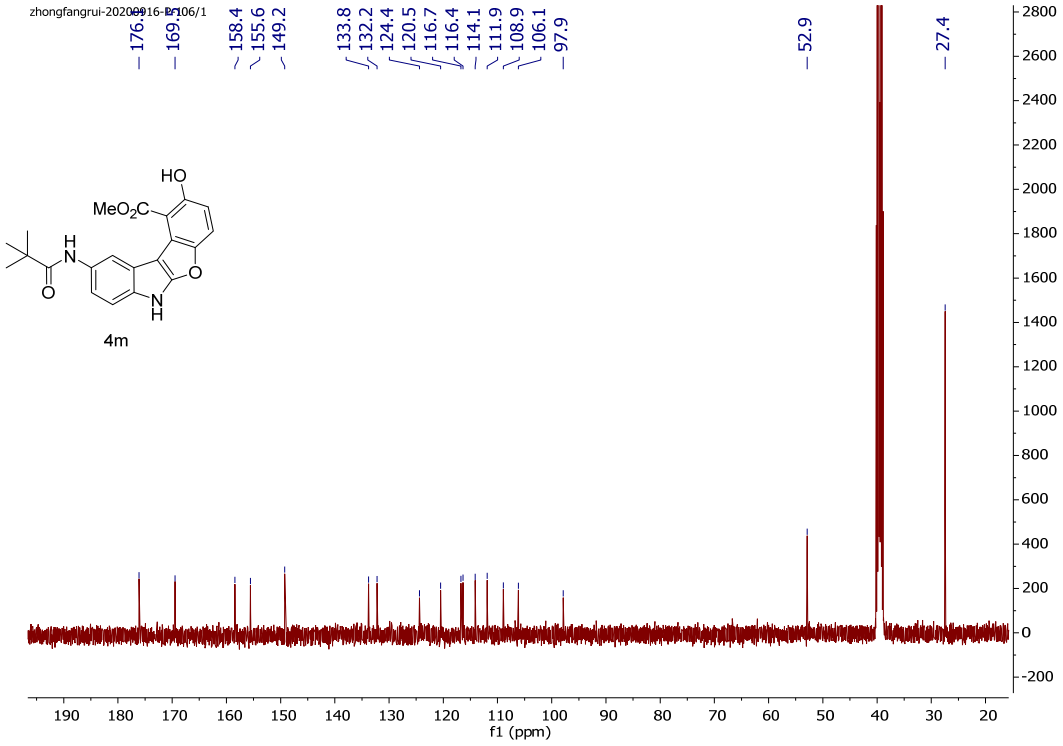

P-105 1H 13C/1
12.4
10.4
9.9
7.7
7.7
7.6
7.6
7.6
7.6
7.5
7.5
7.3
7.3
7.3
6.9
6.9
6.9
6.7
6.7
4.0
2.3
HO
MeO2C
TsHN
O
N
H
4k
1.022
1.000
0.995
1.060
2.056
1.056
3.153
1.033
1.018
3.045
3.081
f1 (ppm)

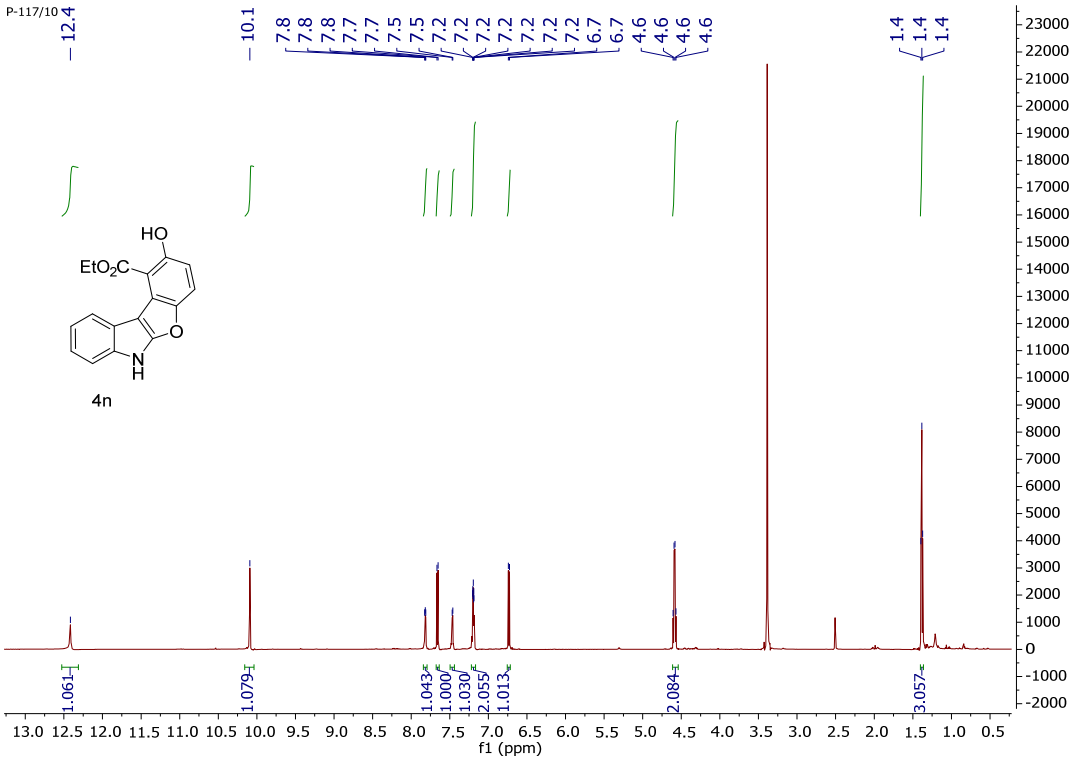

P-105 1H 13C/2
169.1
158.2
155.3
149.2
142.8
136.8
134.7
130.3
129.4
126.8
124.2
120.8
117.1
116.7
115.1
112.6
109.2
106.4
97.7
52.7
20.9
HO
MeO2C
TsHN
O
N
H
4k
f1 (ppm)

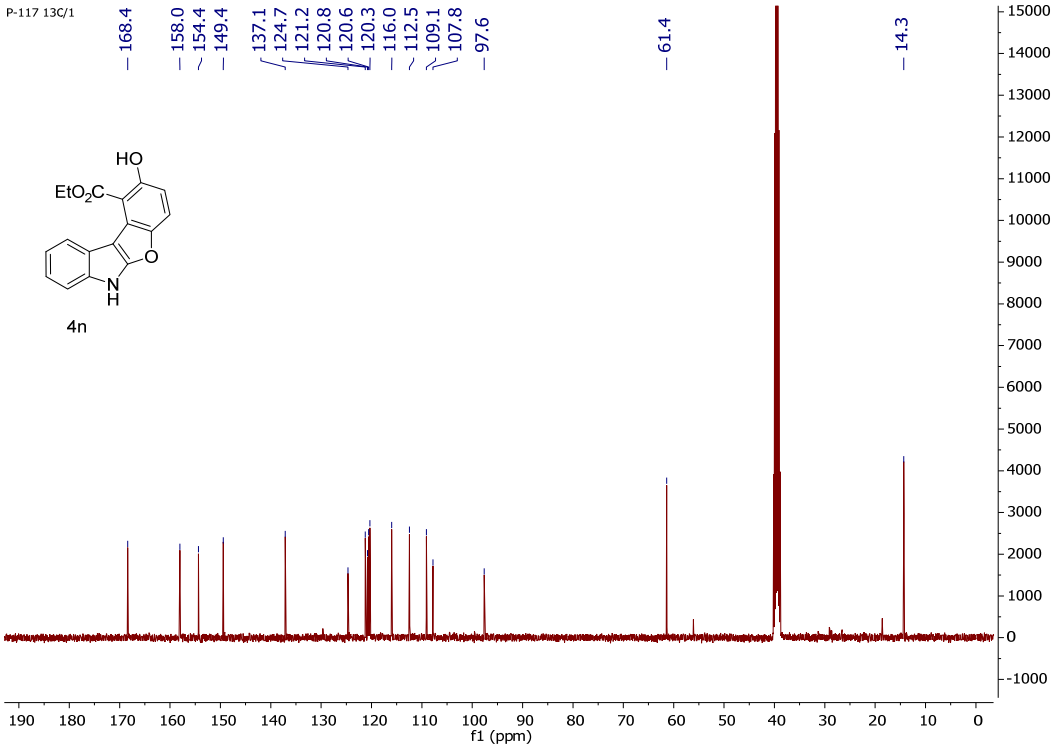

P-108 1H/1
8.0
7.5
7.5
7.5
7.5
7.3
7.3
7.3
7.3
7.1
7.1
7.1
7.1
6.7
6.7
6.7
6.7
4.3
4.3
4.3
1.6
HO
MeO2C
BocHN
O
N
H
4l
0.809
0.936
1.169
1.067
1.050
3.000
9.229
f1 (ppm)

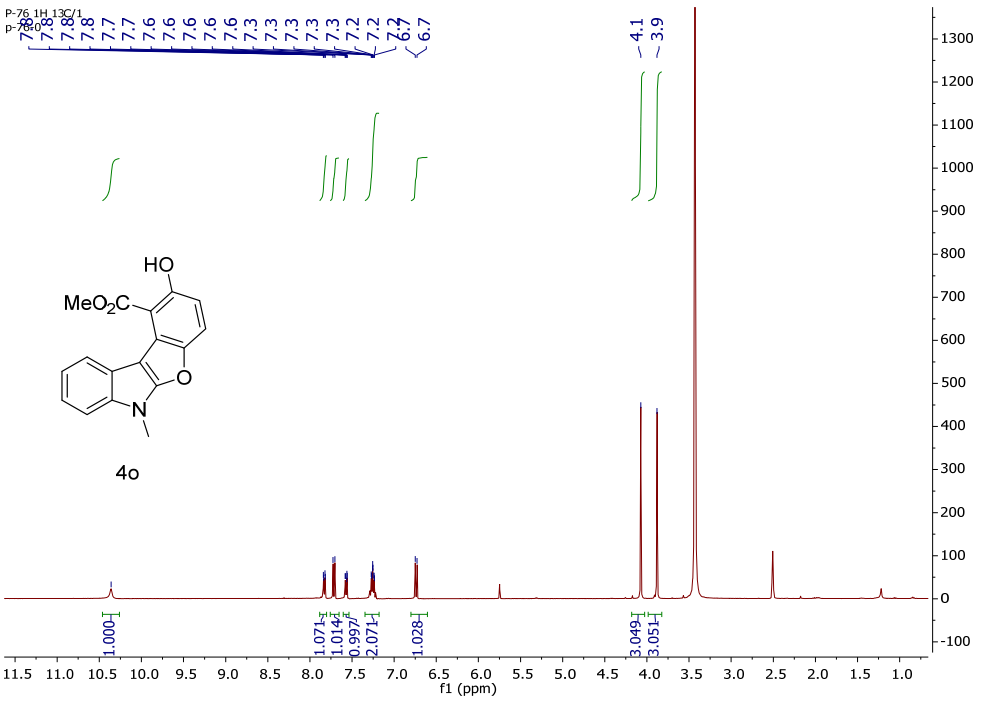

zhongfangrui-20200916-P-108/1
13C NMR (101 MHz, DMSO
116.48, 112.13, 108.81, 106.49, 97.
160.4
158.4
155.2
152.2
149.2
133.0
127.4
120.8
116.5
111.1
108.8
106.5
97.8
78.5
53.0
28.3
HO
MeO2C
BocHN
O
N
H
4l
f1 (ppm)

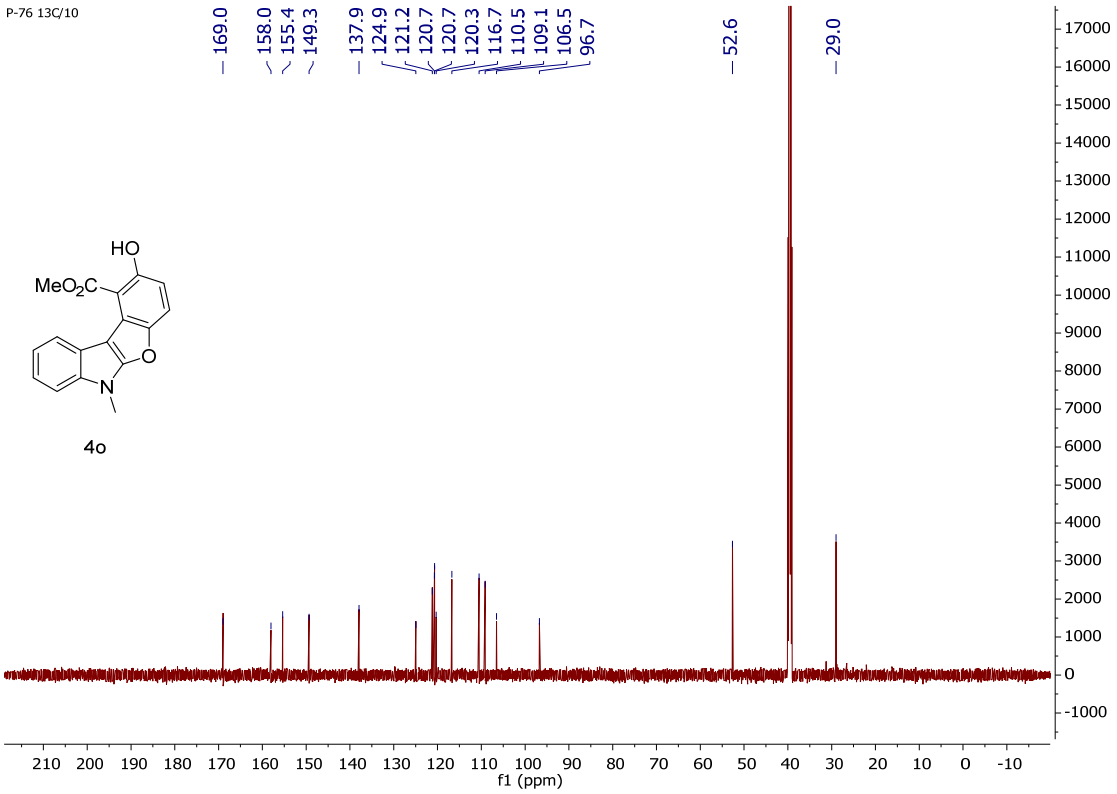

P-106 1H/1
10.5
9.2
8.0
8.0
7.7
7.7
7.4
7.4
7.3
7.3
7.2
7.2
6.7
6.7
4.2
1.3
HO
MeO2C
H
N
O
O
N
H
4m
1.051
1.035
1.064
1.024
1.037
1.041
1.058
3.000
9.000
f1 (ppm)

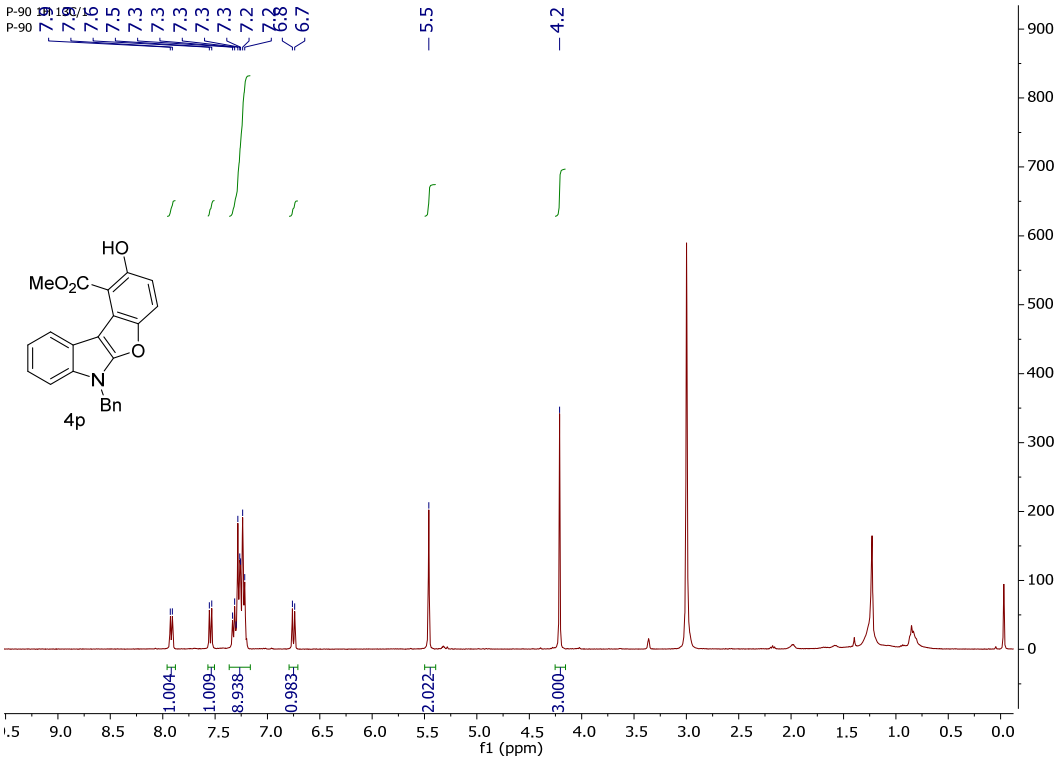

zhongfangrui-20200916-P106/1
176.
169.
158.4
155.6
149.2
133.8
132.2
124.4
120.5
116.7
116.4
114.1
111.9
108.9
106.1
97.9
52.9
27.4
HO
MeO2C
H
N
O
O
N
H
4m
f1 (ppm)

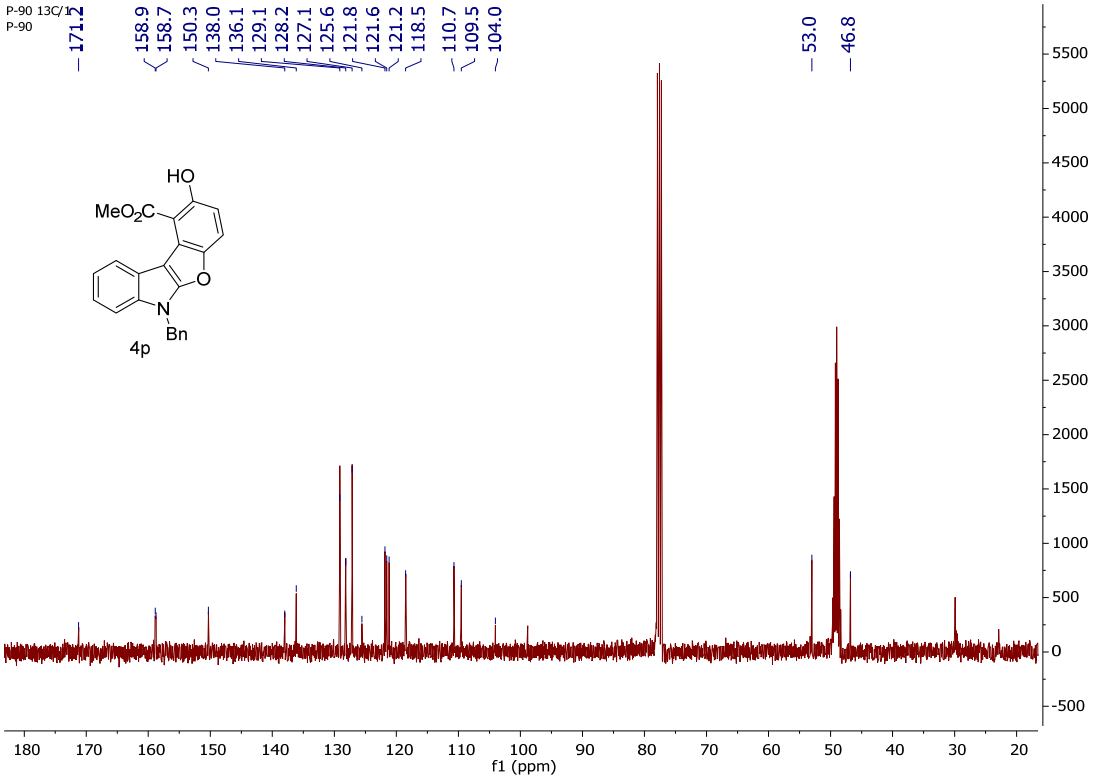

P-117/10
12.4
10.1
7.8
7.8
7.8
7.7
7.7
7.5
7.5
7.2
7.2
7.2
7.2
7.2
7.2
7.2
6.7
6.7
4.6
4.6
4.6
4.6
1.4
1.4
1.4
HO
EtO2C
O
N
H
4n
1.061
1.079
1.043
1.000
1.030
2.055
1.013
2.084
3.057
f1 (ppm)

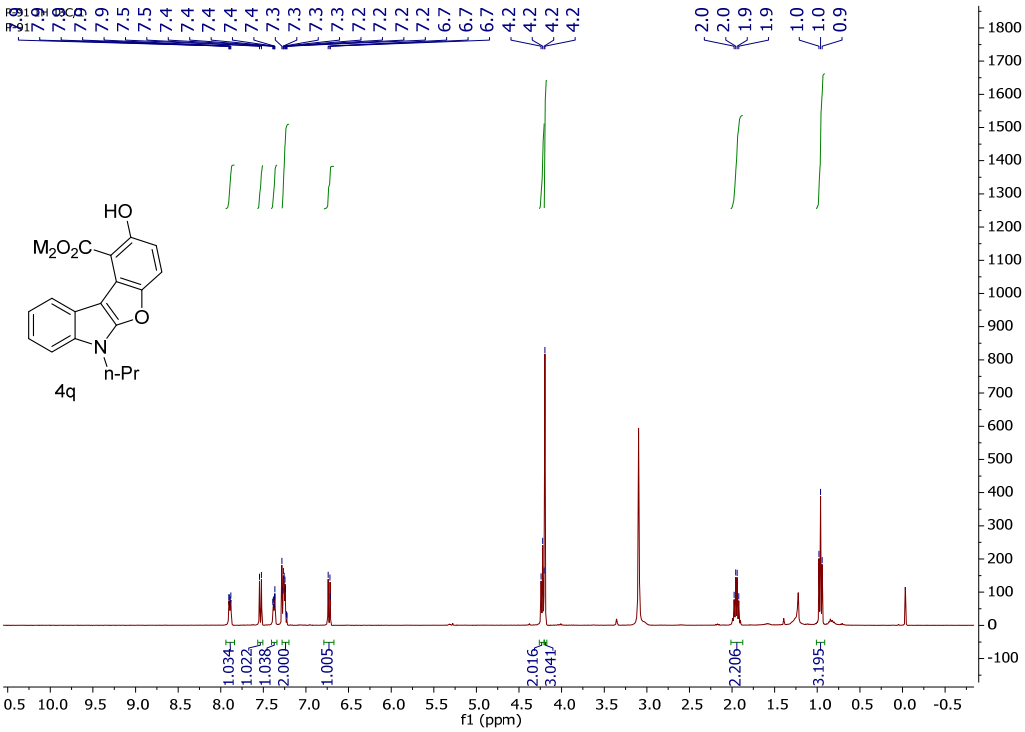

P-117 13C/1
168.4
158.0
154.4
149.4
137.1
124.7
121.2
120.8
120.6
120.3
116.0
112.5
109.1
107.8
97.6
61.4
14.3
HO
EtO2C
O
N
H
4n
f1 (ppm)

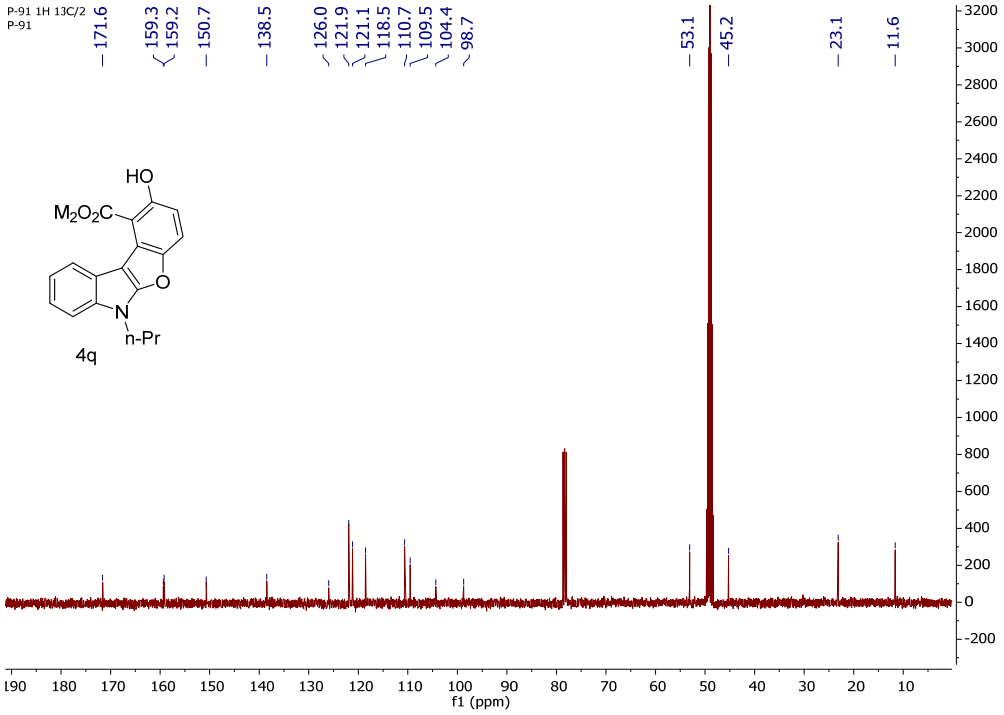

P-76 1H 13C/1
p-76.0
HO
MeO2C
O
N
4o
f1 (ppm)

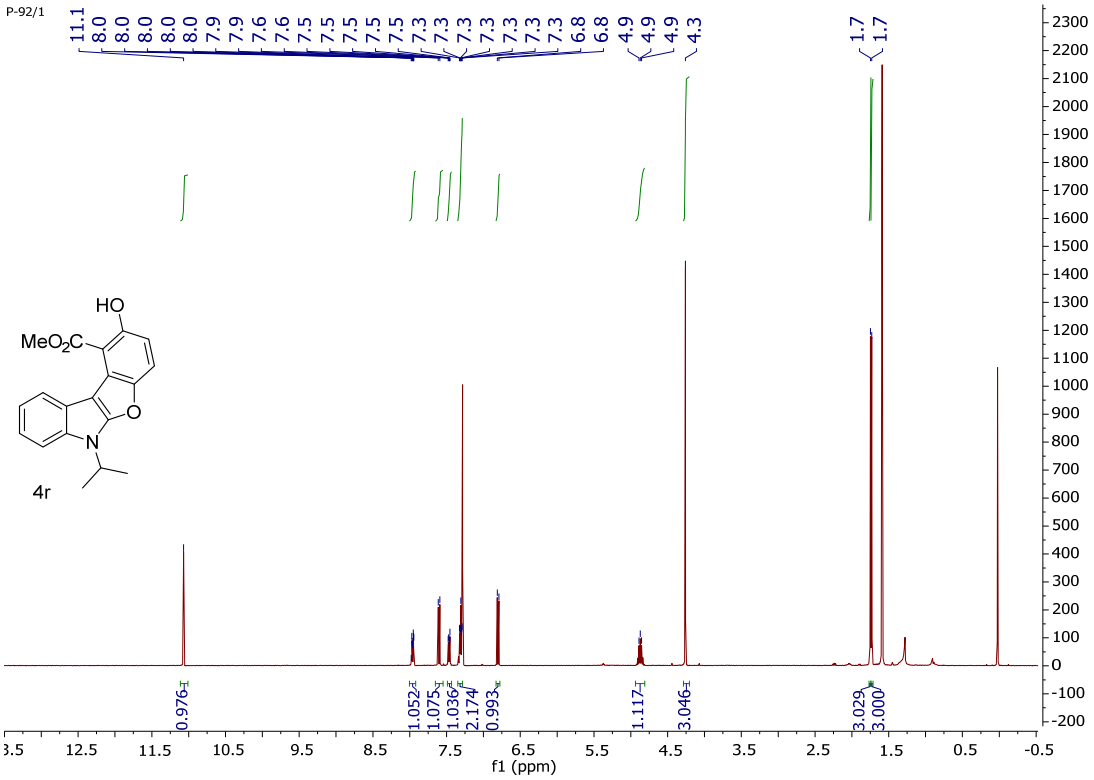

P-76 13C/10
HO
MeO2C
O
N
4o
f1 (ppm)

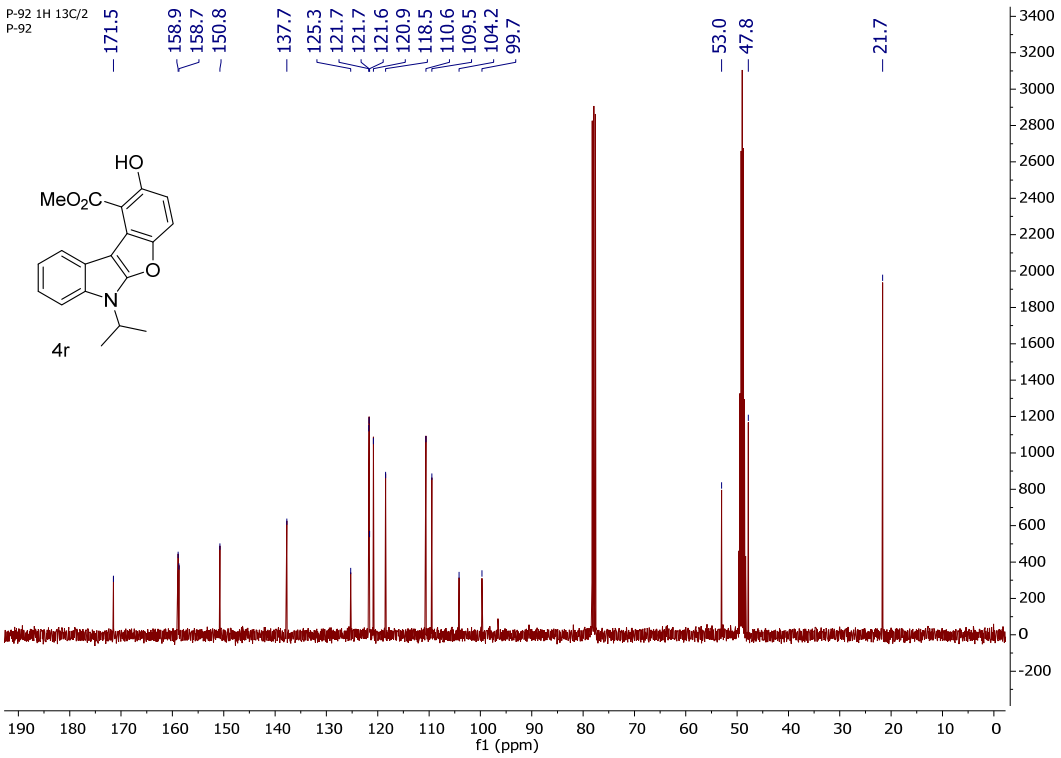

HO
MeO2C
O
N
Bn
4p
f1 (ppm)

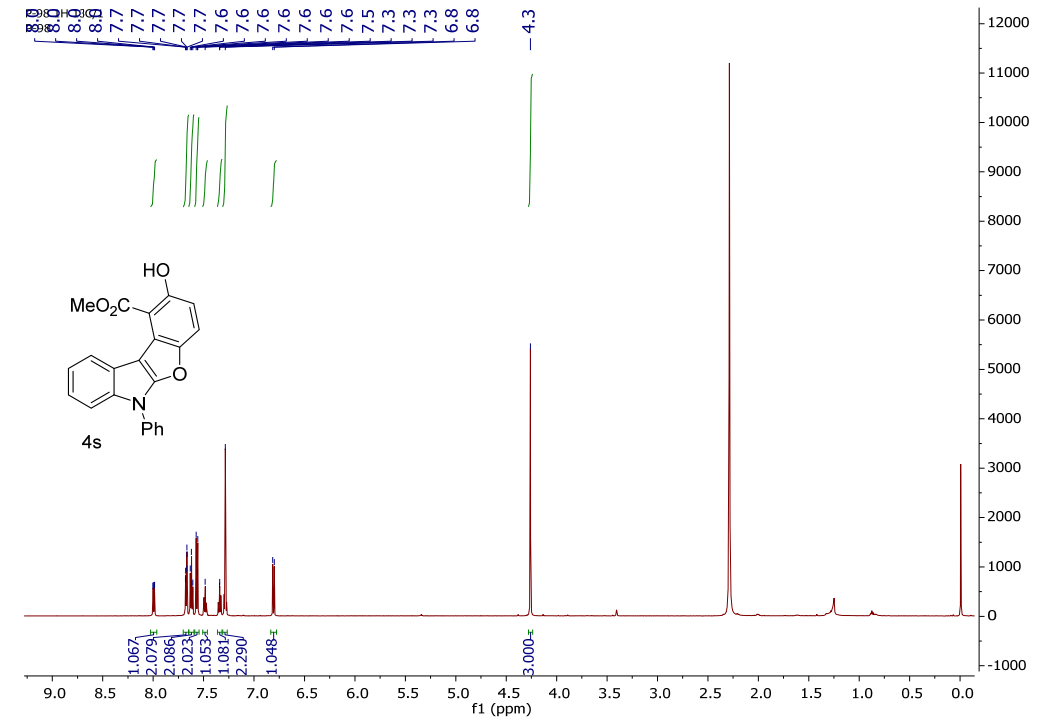

HO
MeO2C
O
N
Bn
4p
f1 (ppm)

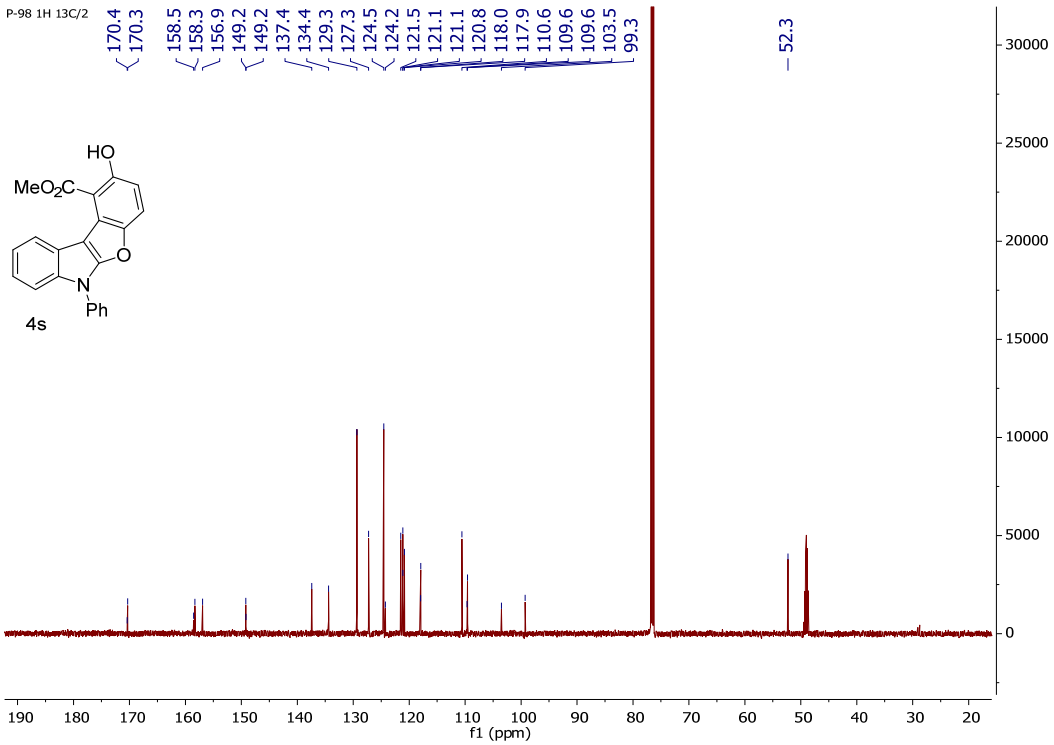

HO
M2O2C
O
N
n-Pr
4q
f1 (ppm)

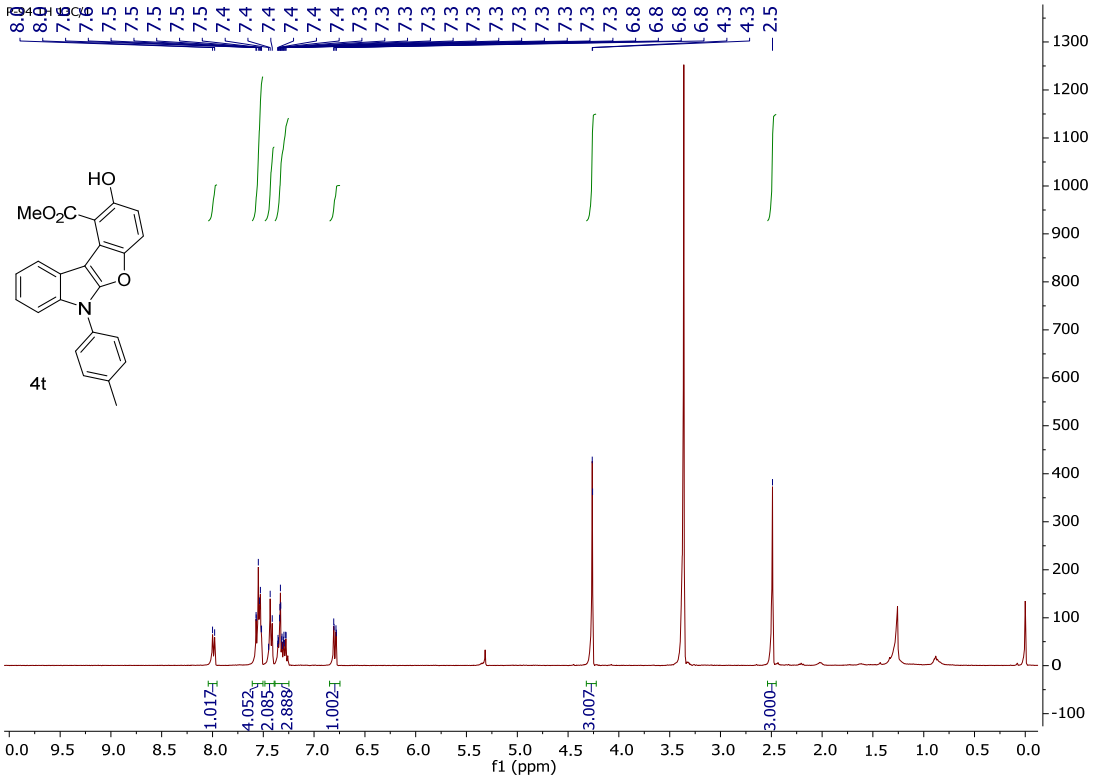

P-91 1H 13C/2
P-91
HO
M2O2C
O
N
n-Pr
4q
f1 (ppm)

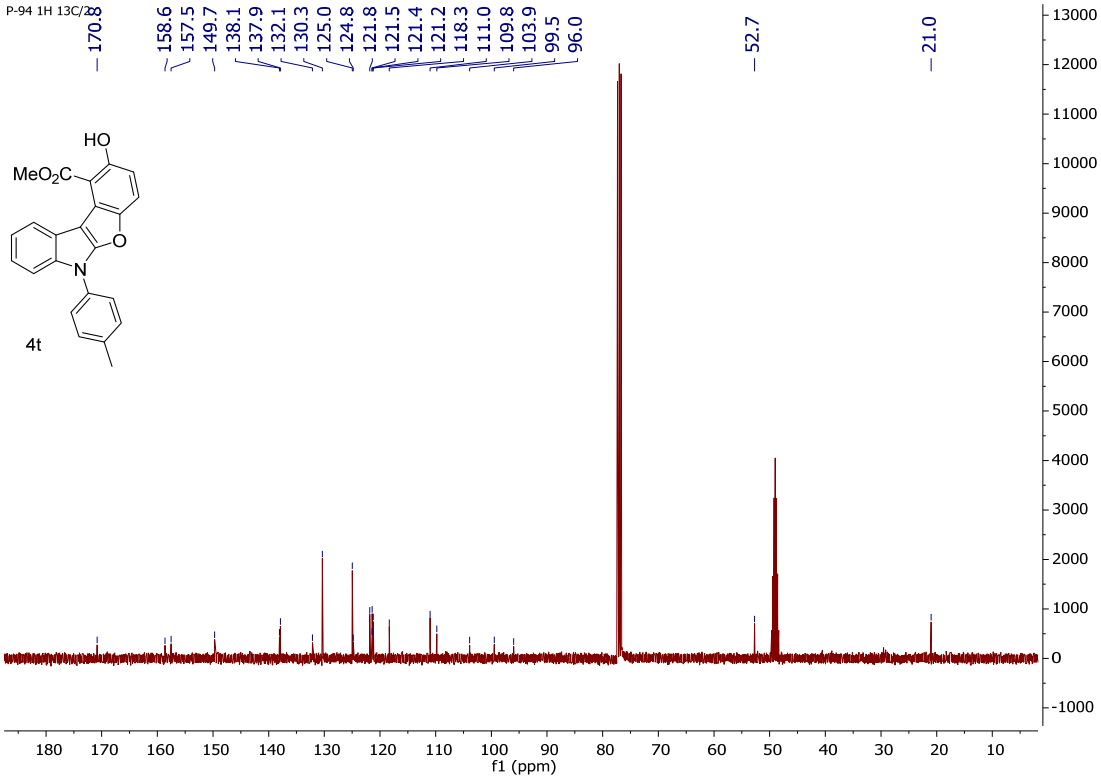

P-92/1
HO
MeO2C
O
N
4r
f1 (ppm)

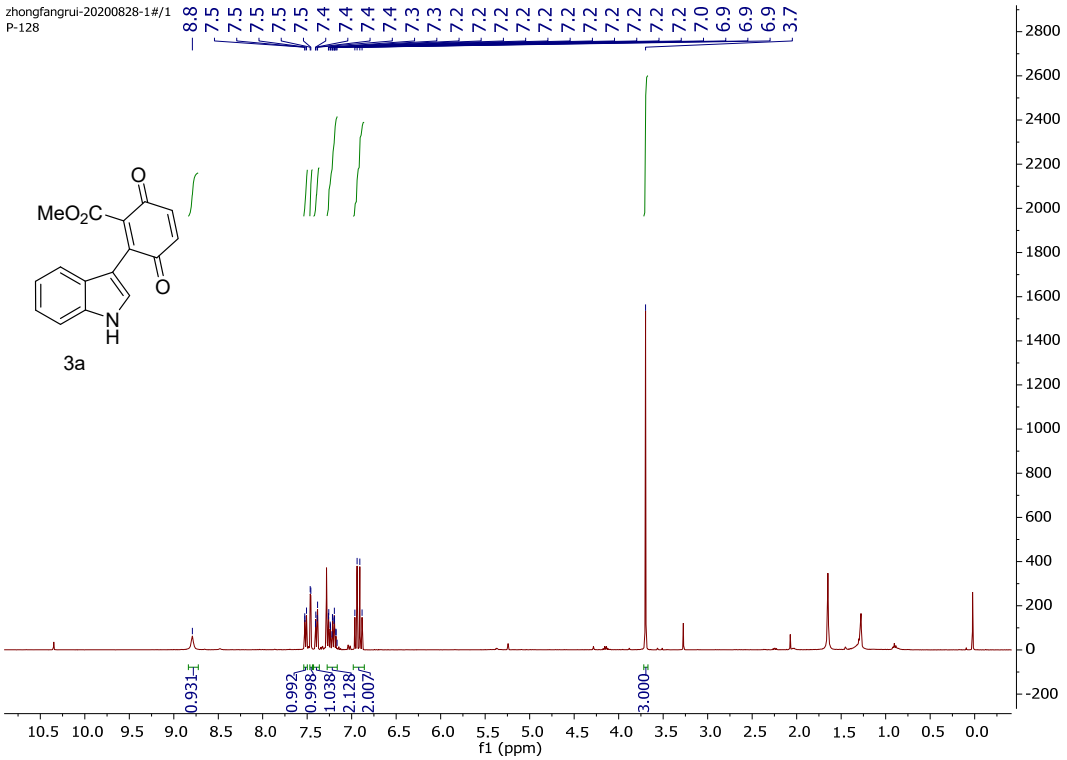

P-92 1H 13C/2
P-92
HO
MeO2C
O
N
4r
f1 (ppm)

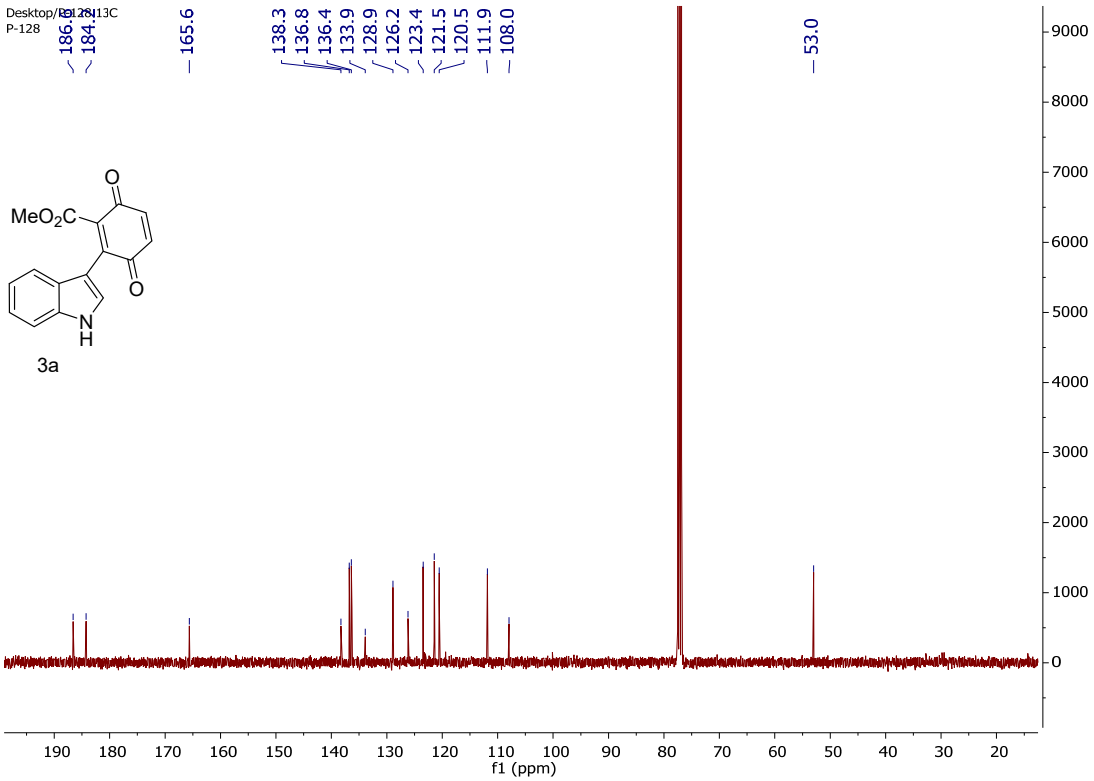

8.1
8.0
7.7
7.7
7.7
7.7
7.7
7.6
7.6
7.6
7.6
7.6
7.6
7.5
7.3
7.3
7.3
6.8
6.8
4.3
HO
MeO2C
O
N
Ph
4s
1.067
2.079
2.086
2.023
1.053
1.081
2.290
1.048
3.000
f1 (ppm)


P-98 1H 13C/2
170.4
170.3
158.5
158.3
156.9
149.2
149.2
137.4
134.4
129.3
127.3
124.5
124.2
121.5
121.1
121.1
120.8
118.0
117.9
110.6
109.6
109.6
103.5
99.3
52.3
HO
MeO2C
O
N
Ph
4s
f1 (ppm)


HO
MeO2C
O
N
4t
f1 (ppm)


HO
MeO2C
O
N
4t
f1 (ppm)


zhongfangrui-20200828-1#/1
P-128
8.8
7.5
7.5
7.5
7.5
7.5
7.4
7.4
7.4
7.4
7.3
7.3
7.2
7.2
7.2
7.2
7.2
7.2
7.2
7.2
7.2
7.2
7.0
6.9
6.9
6.9
3.7
MeO2C
O
O
N
H
3a
0.931
0.992
0.998
1.038
2.128
2.007
3.000
f1 (ppm)


Desktop/zhongfangrui-20200828-1#/1
P-128
186.1
184.1
165.6
138.3
136.8
136.4
133.9
128.9
126.2
123.4
121.5
120.5
111.9
108.0
53.0
MeO2C
O
O
N
H
3a
f1 (ppm)