Supplementary Materials

Anticancer Evaluation of Novel Benzofuran-Indole Hybrids as EGFR Inhibitors Against Non-Small Cell Lung Cancer Cells

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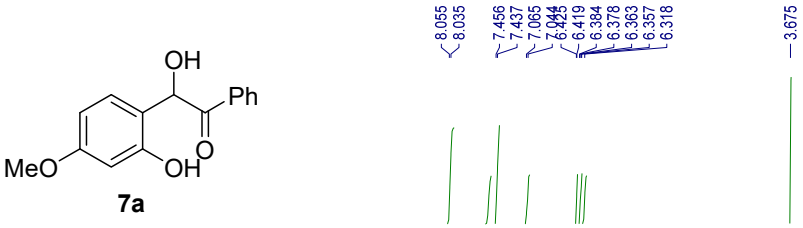
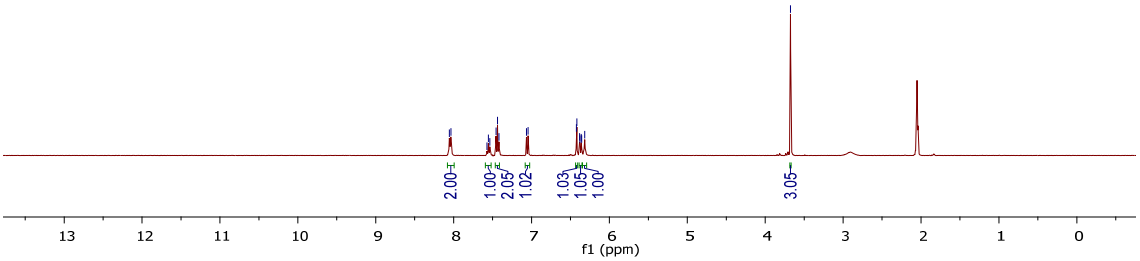
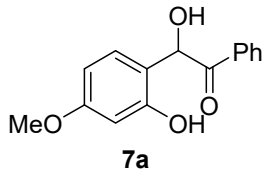


7a

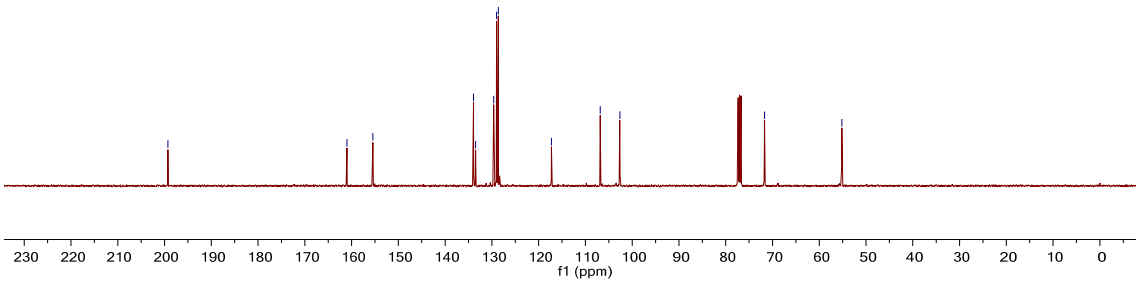
^{1}H NMR spectrum of 7a (400 MHz, $(CD_3)_2CO$)

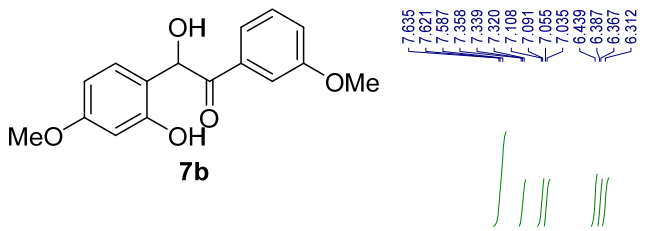




7a

^{13}C NMR spectrum of 7a (100 MHz, $CDCl_3$)





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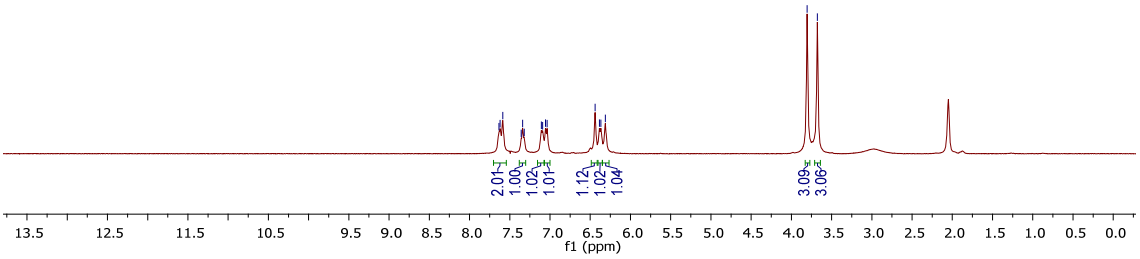
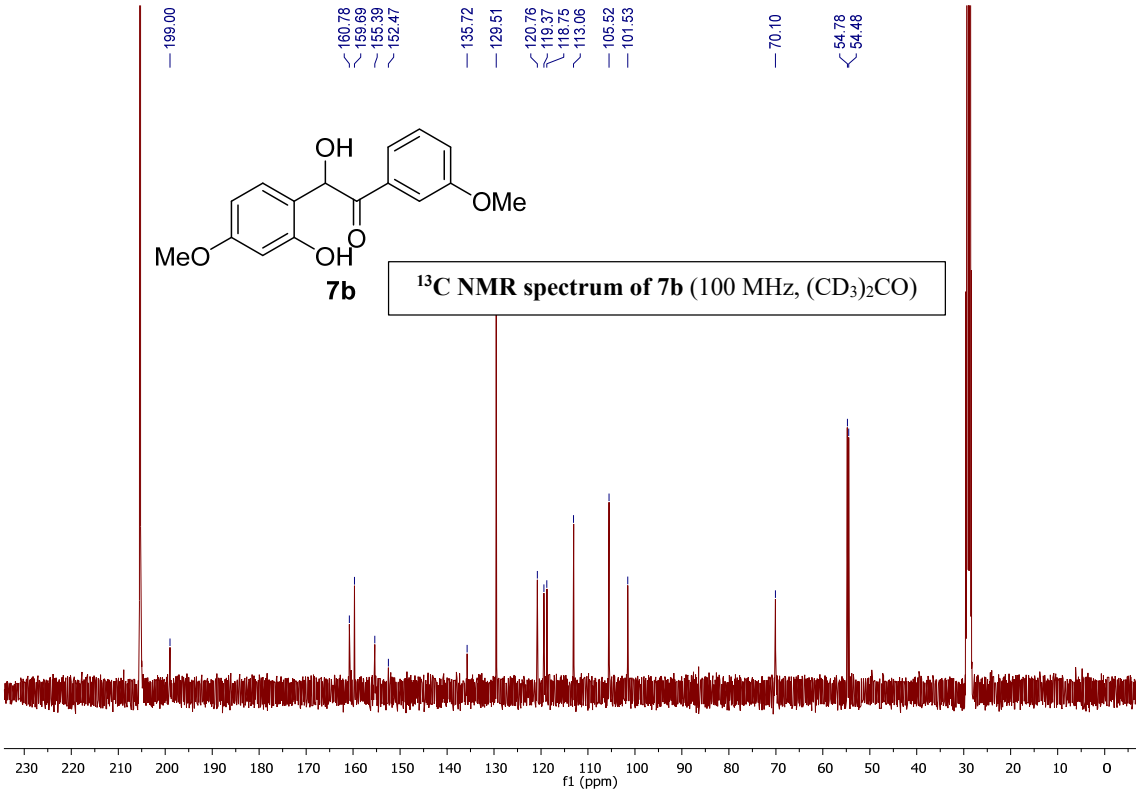
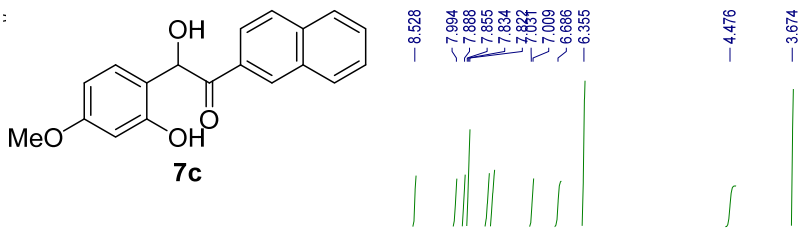
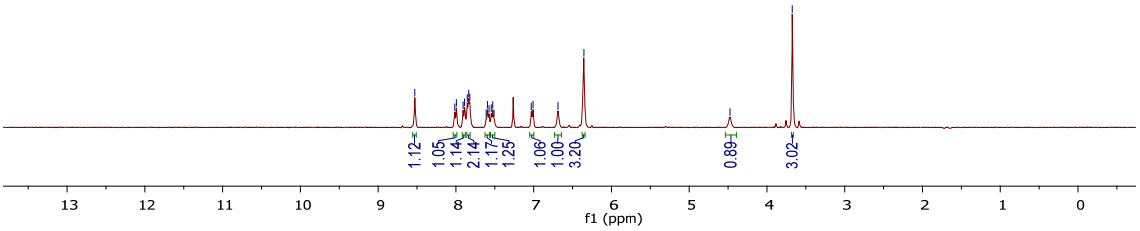


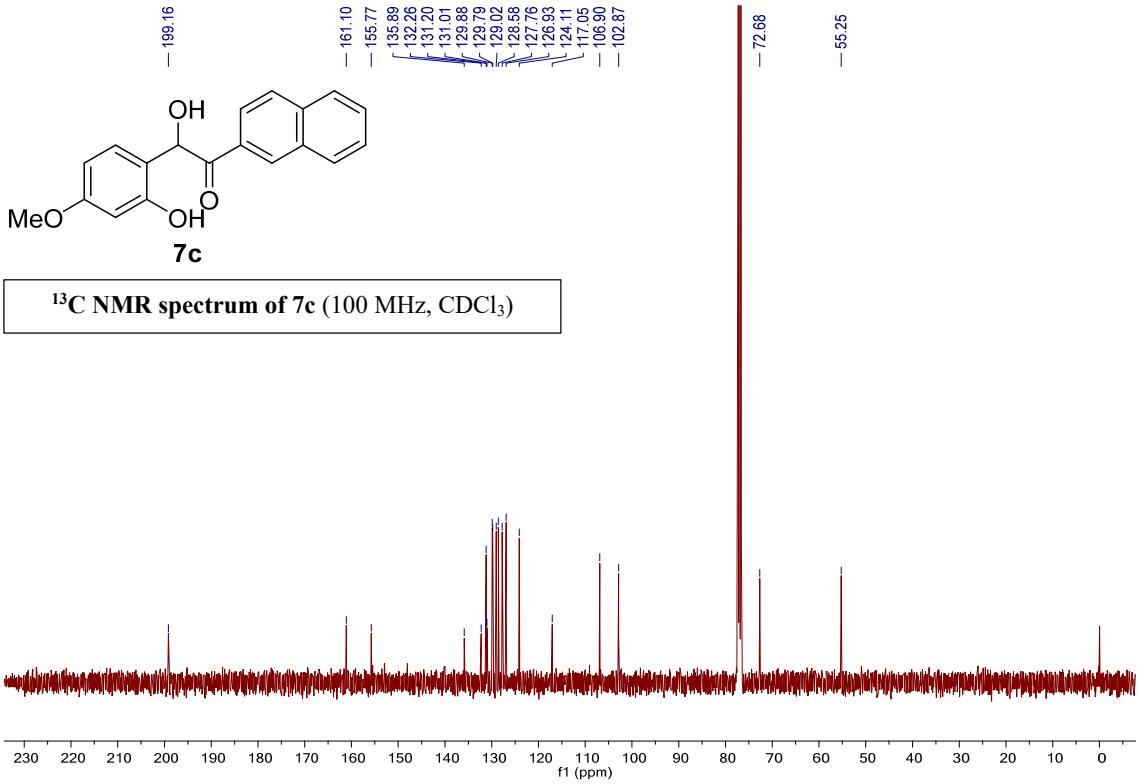


^{13}C NMR spectrum of 7b (100 MHz, $(CD_3)_2CO$)

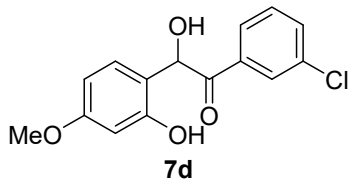


^{1}H NMR spectrum of 7c (400 MHz, $CDCl_3$)

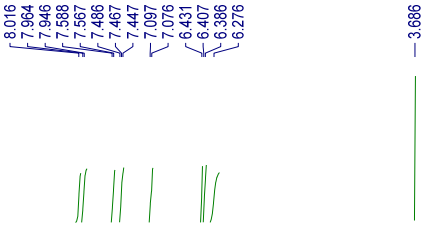




^{13}C NMR spectrum of 7c (100 MHz, $CDCl_3$)



7d



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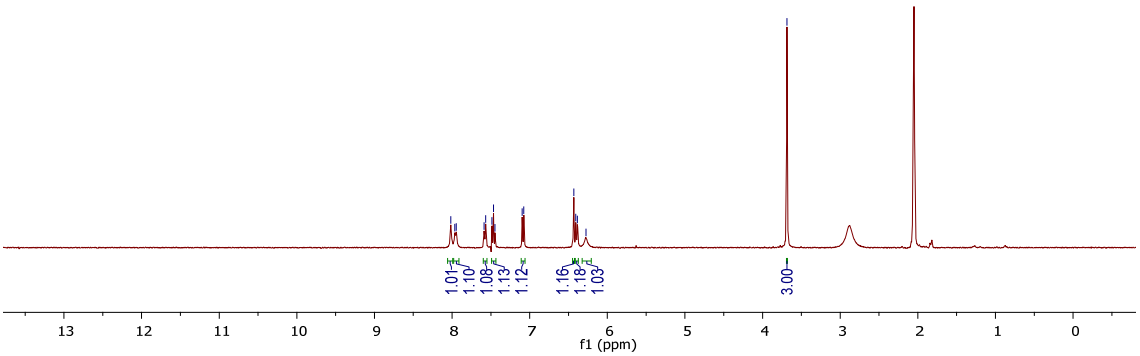
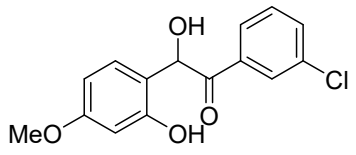
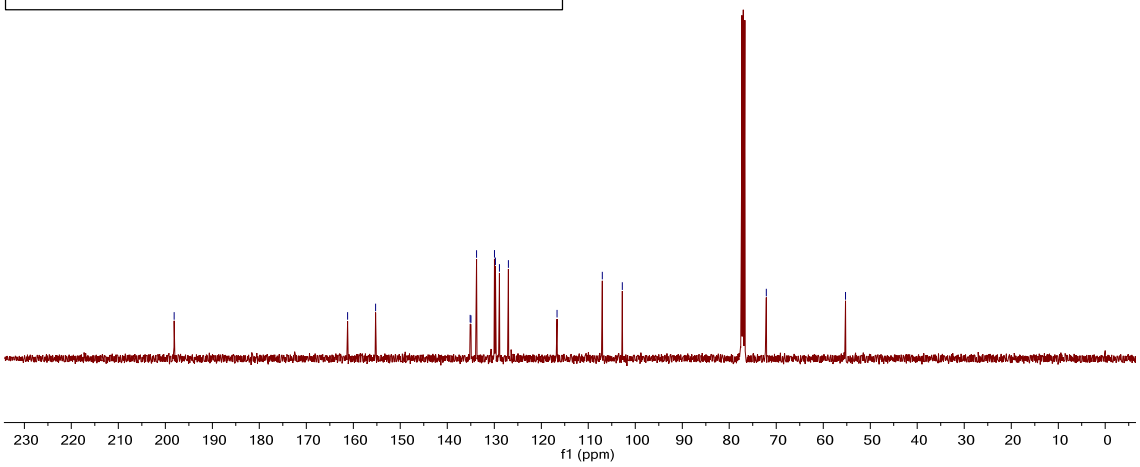
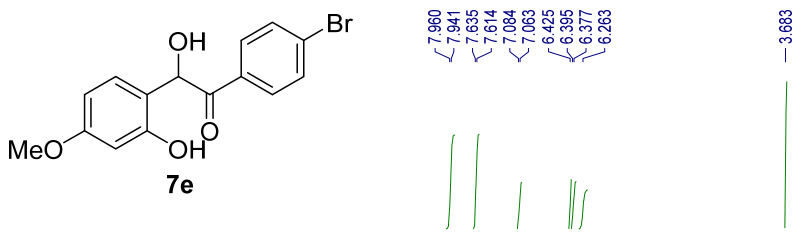




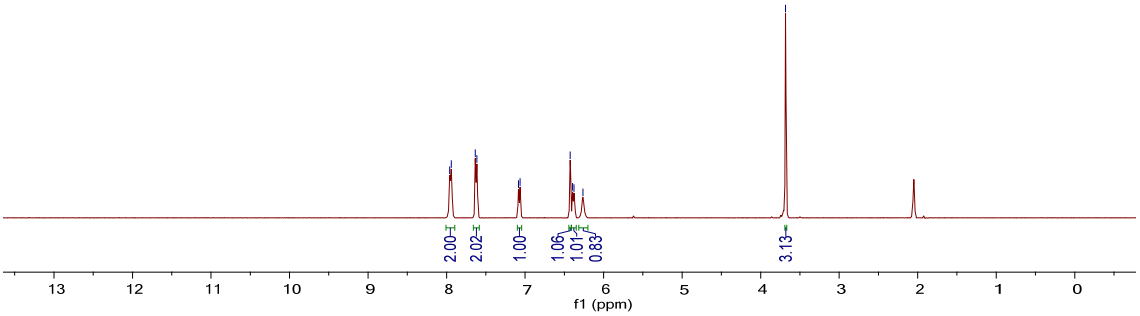
7d

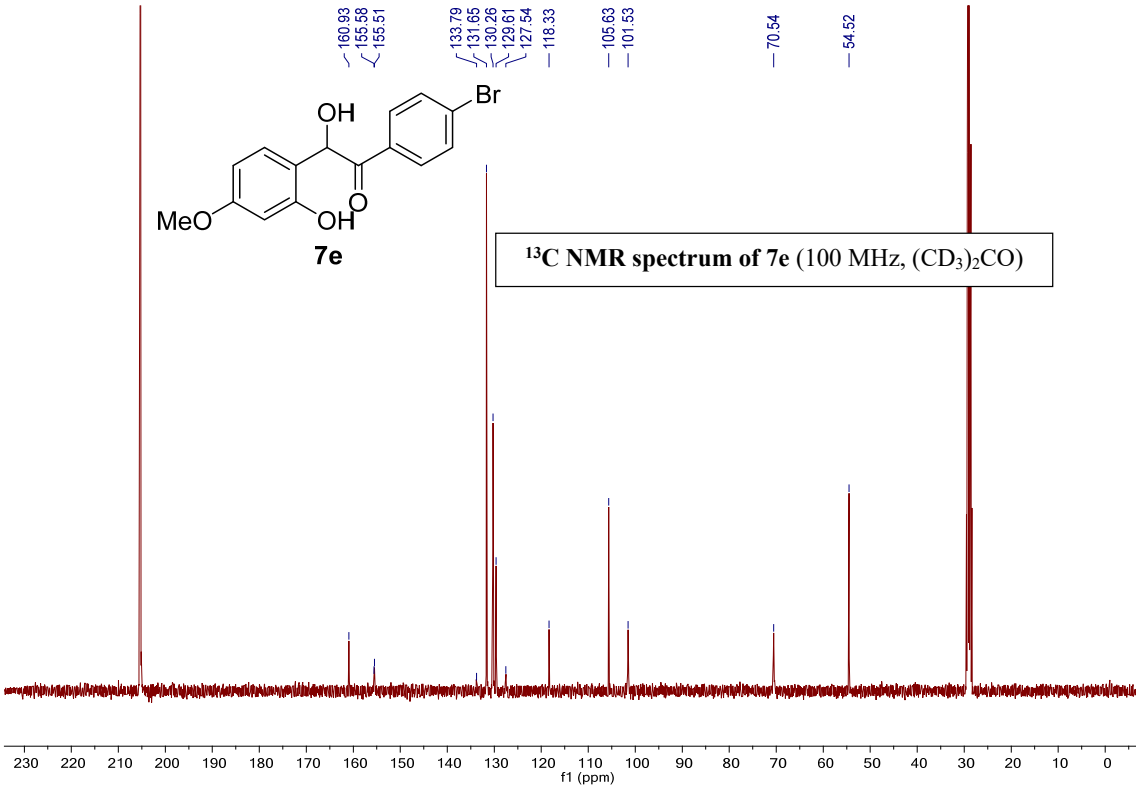
^{13}C NMR spectrum of 7d (100 MHz, $CDCl_3$)



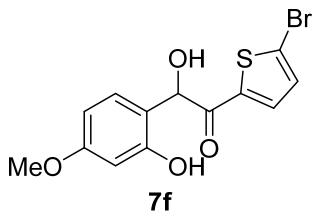


^{1}H NMR spectrum of 7e (400 MHz, $(CD_3)_2CO$)

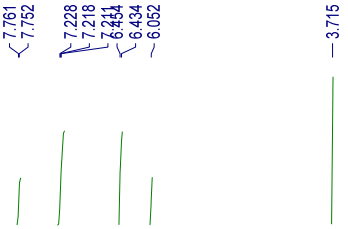




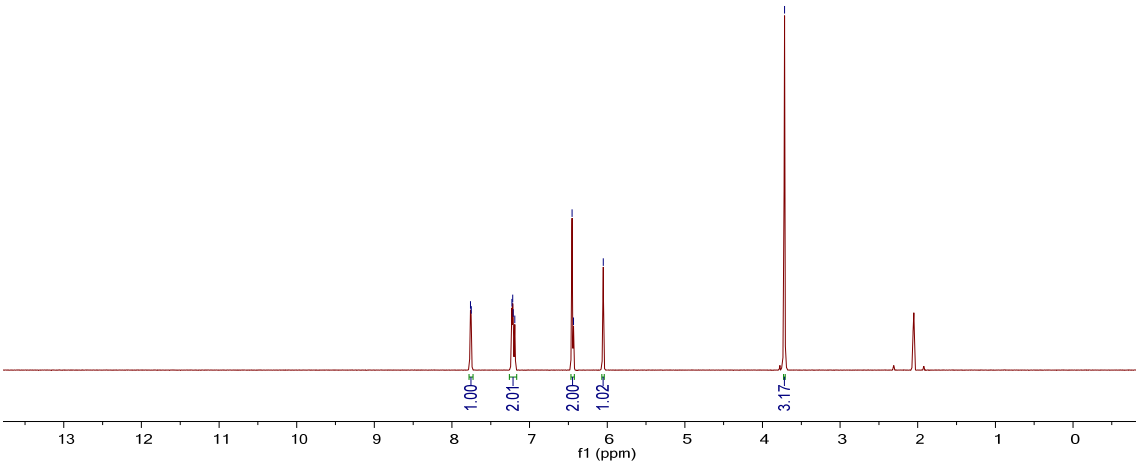
^{13}C NMR spectrum of 7e (100 MHz, $(CD_3)_2CO$)



7f



^{1}H NMR spectrum of 7f (400 MHz, $(CD_3)_2CO$)



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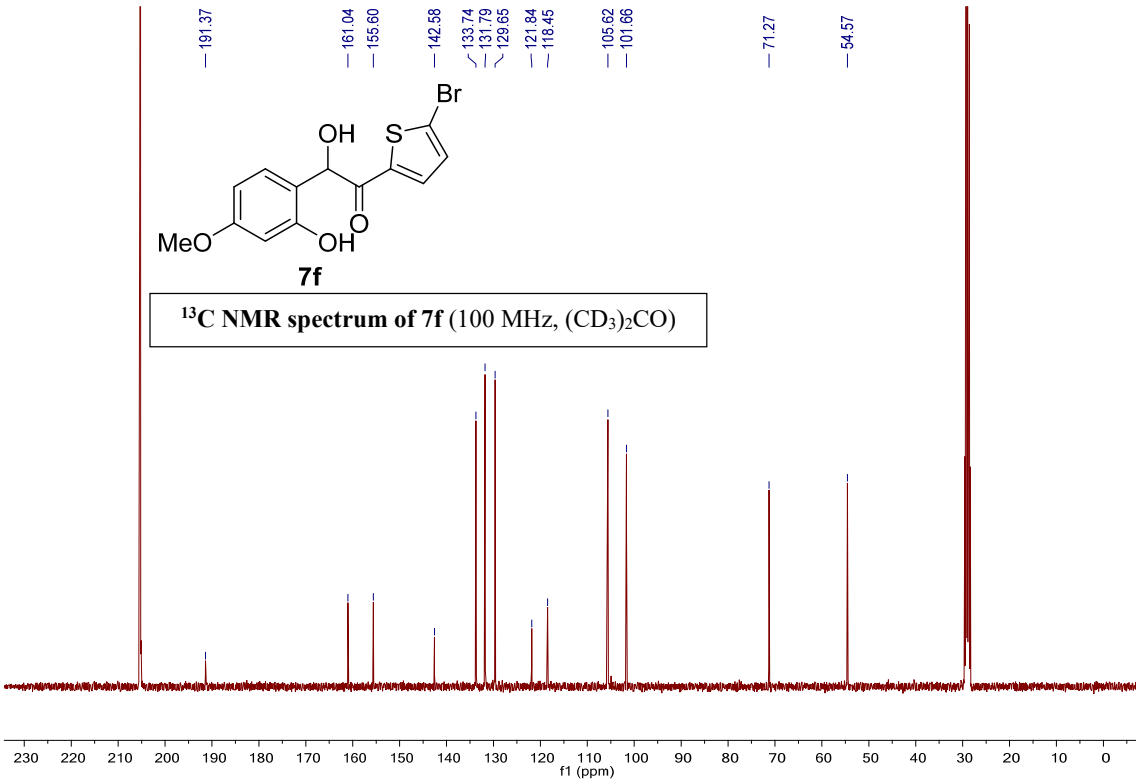
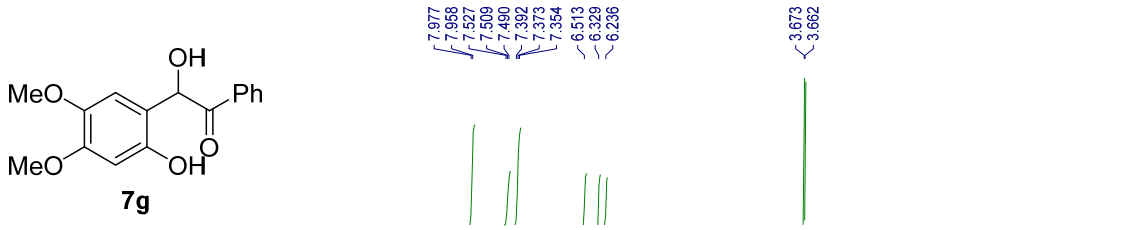


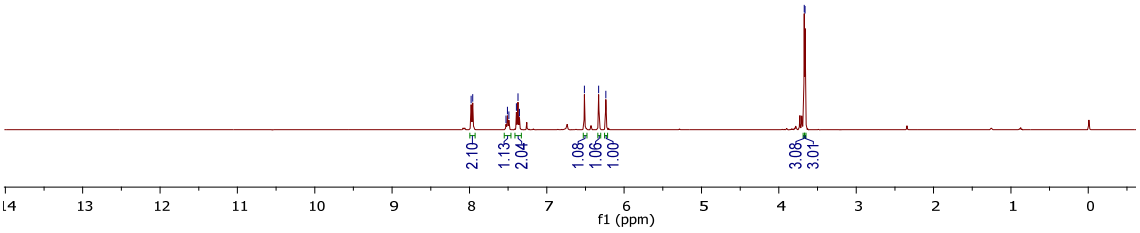
7f

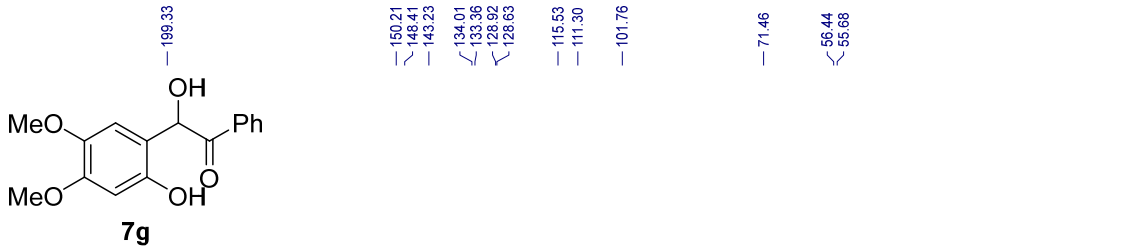
^{13}C NMR spectrum of 7f (100 MHz, $(CD_3)_2CO$)



7g

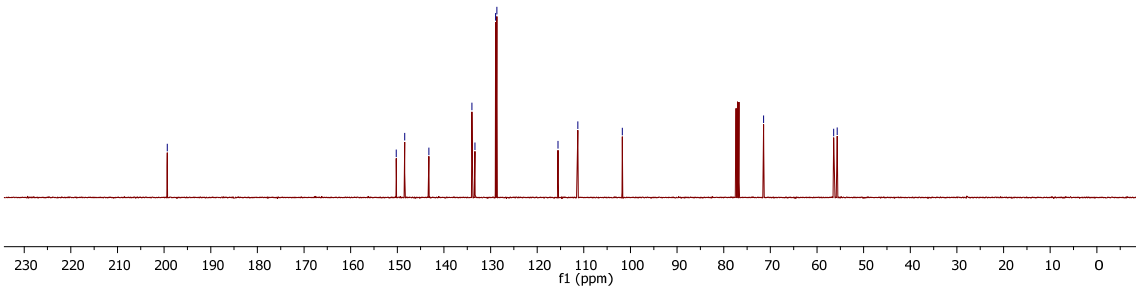
^{1}H NMR spectrum of 7g (400 MHz, $CDCl_3$)

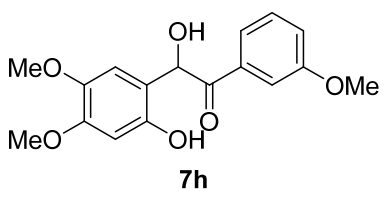




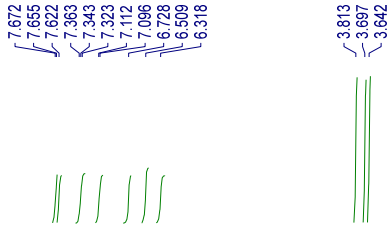
7g

^{13}C NMR spectrum of 7g (100 MHz, $CDCl_3$)

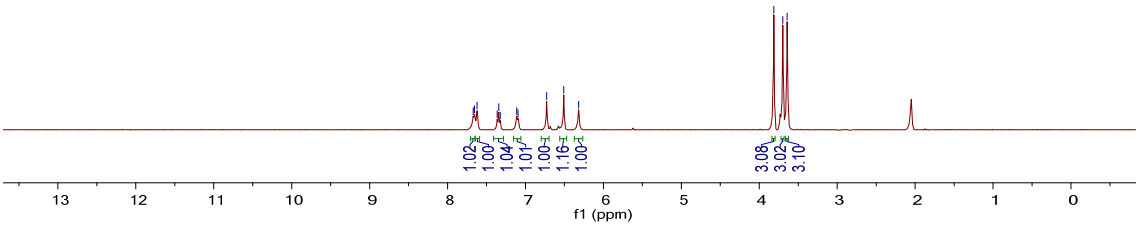


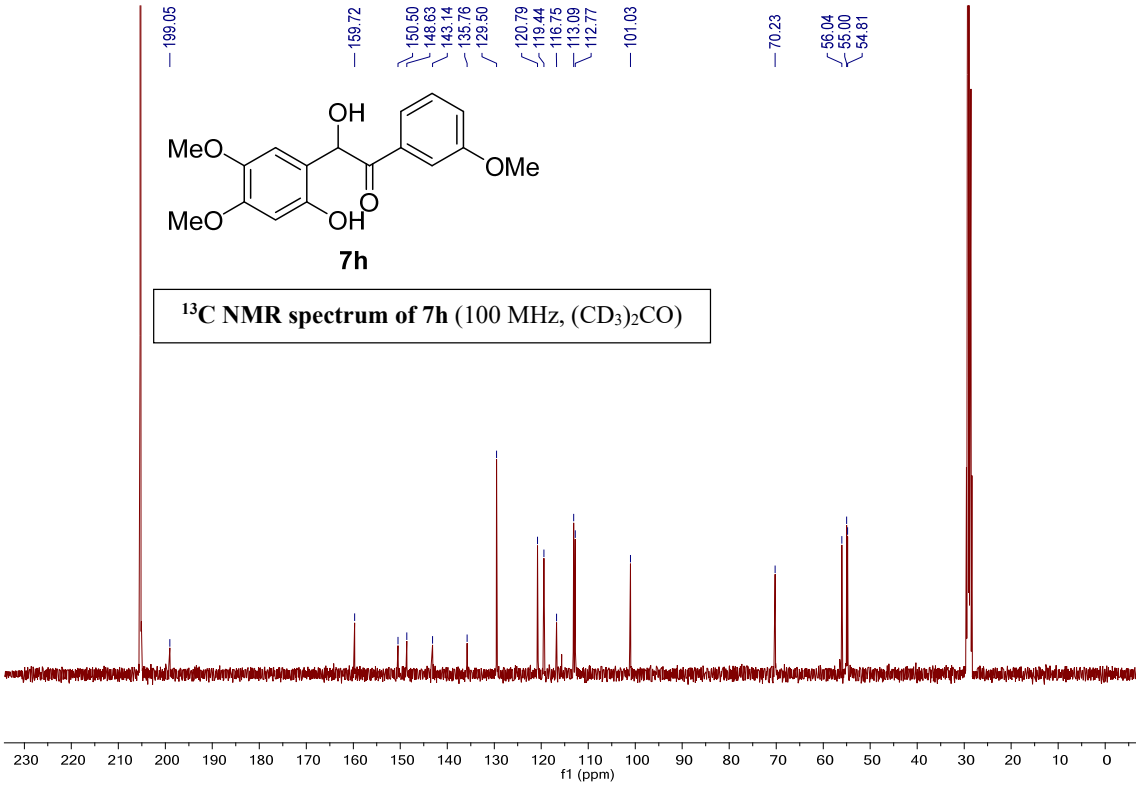


7h



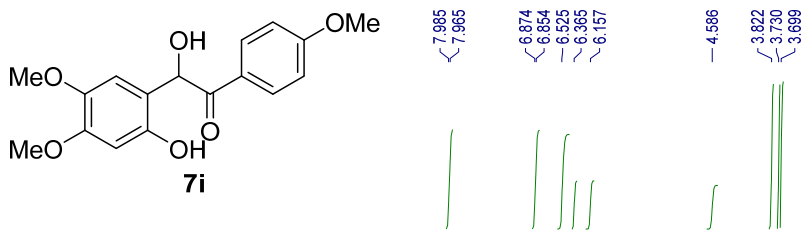
^{1}H NMR spectrum of 7h (400 MHz, $(CD_3)_2CO$)



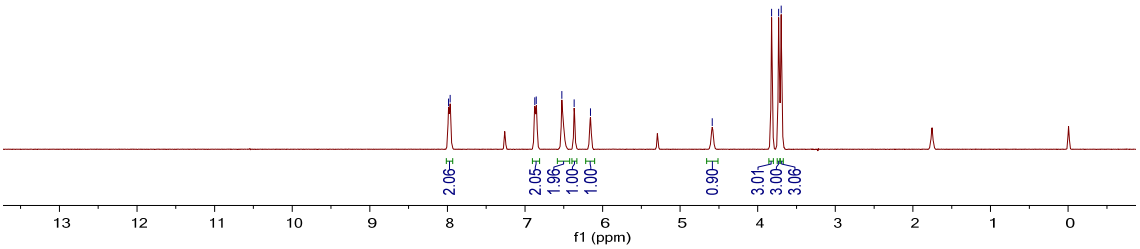


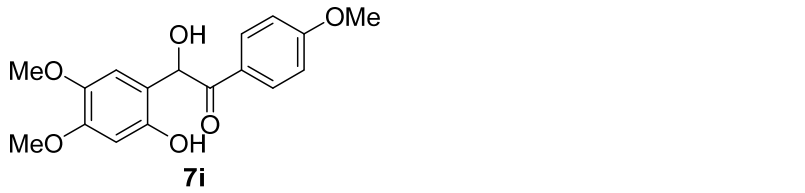
7h

^{13}C NMR spectrum of 7h (100 MHz, $(CD_3)_2CO$)

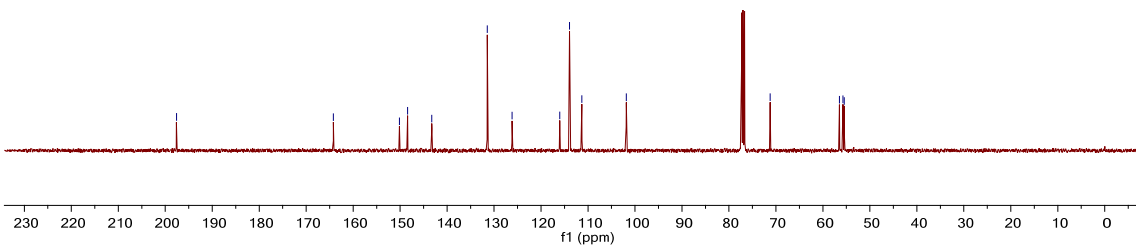


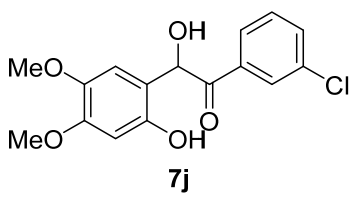
^{1}H NMR spectrum of 7i (400 MHz, $CDCl_3$)



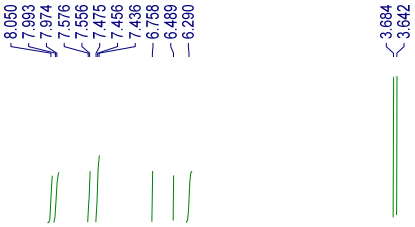


^{13}C NMR spectrum of 7i (100 MHz, $CDCl_3$)

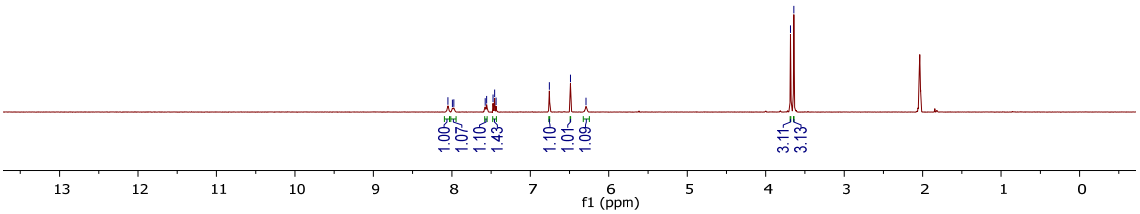


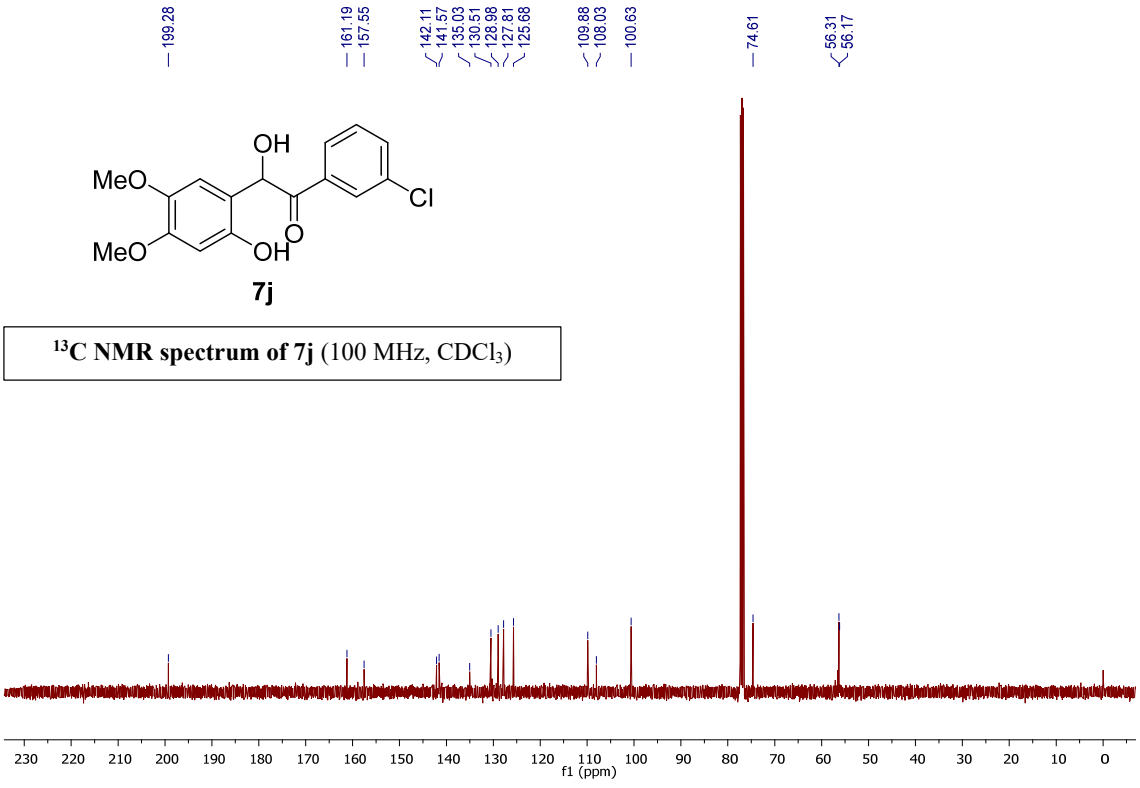


7j



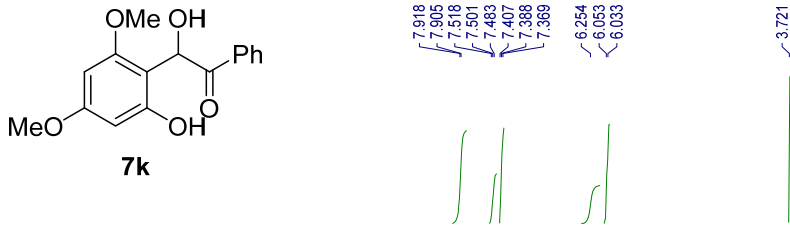
^{1}H NMR spectrum of 7j (400 MHz, $(CD_3)_2CO$)



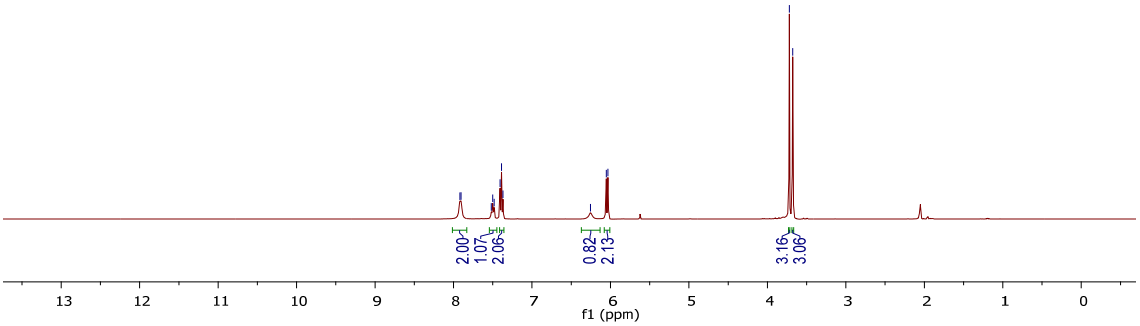


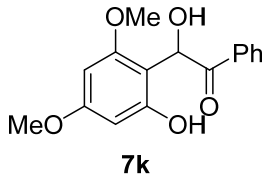
7j

^{13}C NMR spectrum of 7j (100 MHz, $CDCl_3$)

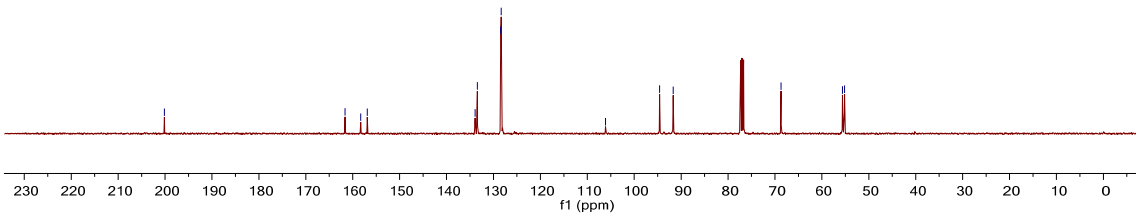


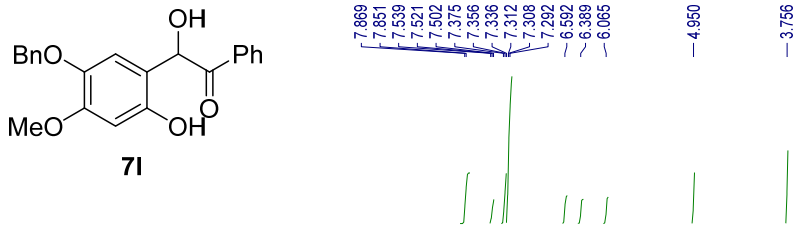
^{1}H NMR spectrum of 7k (400 MHz, $(CD_3)_2CO$)





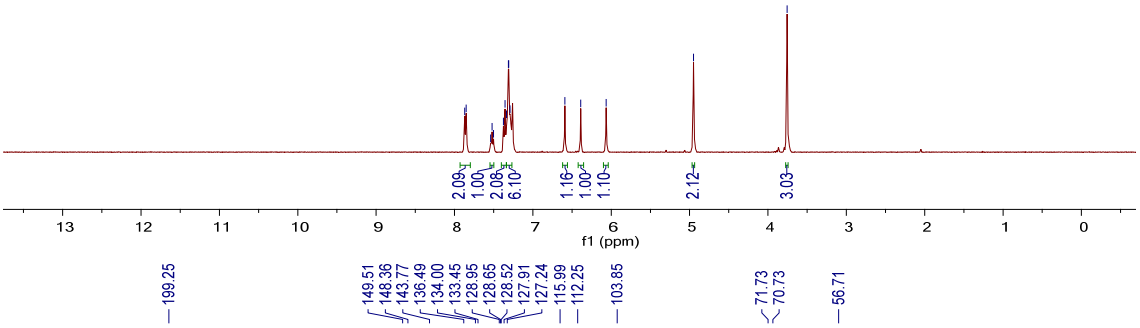
^{13}C NMR spectrum of 7k (100 MHz, $CDCl_3$)





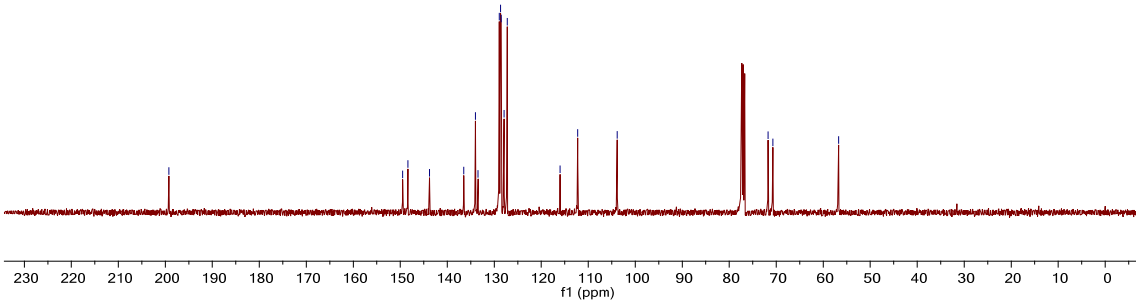
7l

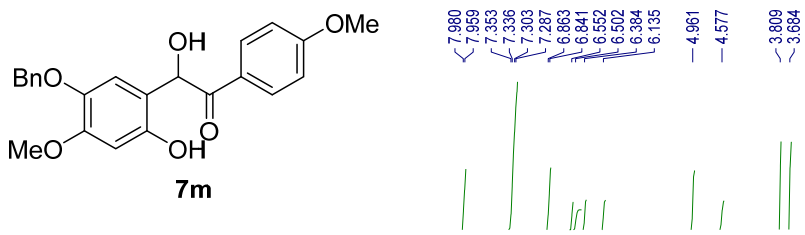
^{1}H NMR spectrum of 7l (400 MHz, $CDCl_3$)



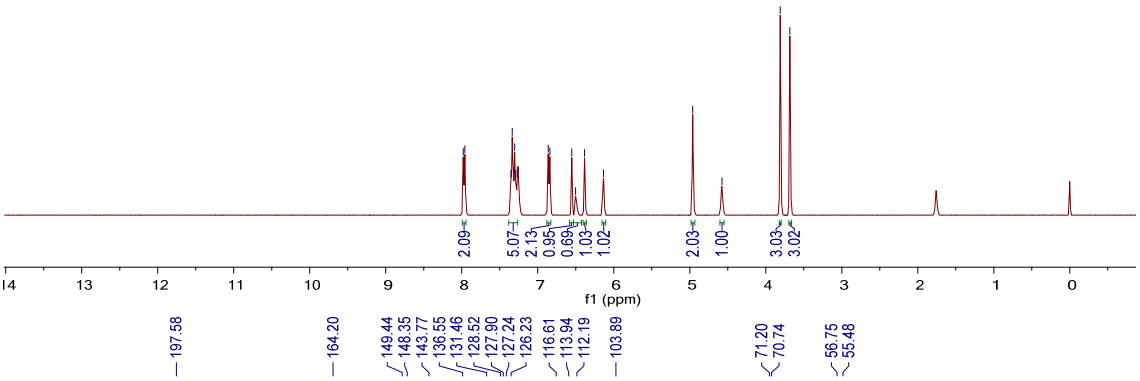
7l

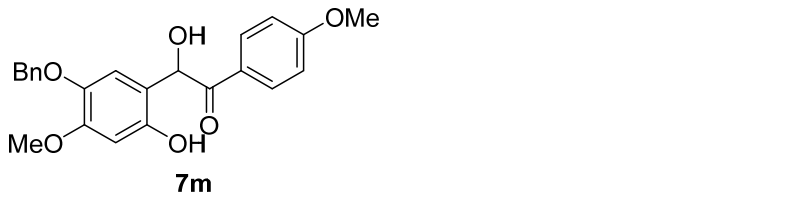
^{13}C NMR spectrum of 7l (100 MHz, $CDCl_3$)



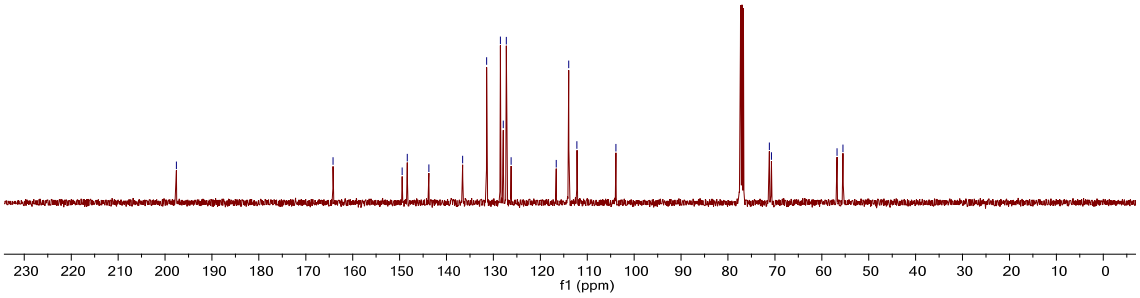


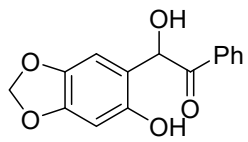
^{1}H NMR spectrum of 7m (400 MHz, $CDCl_3$)



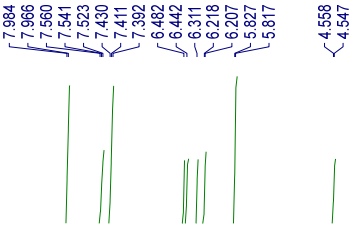


^{13}C NMR spectrum of 7m (100 MHz, $CDCl_3$)

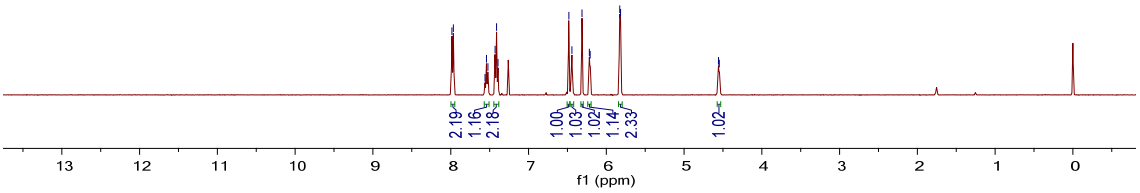


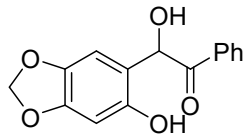


7n



^{1}H NMR spectrum of 7n (400 MHz, $CDCl_3$)





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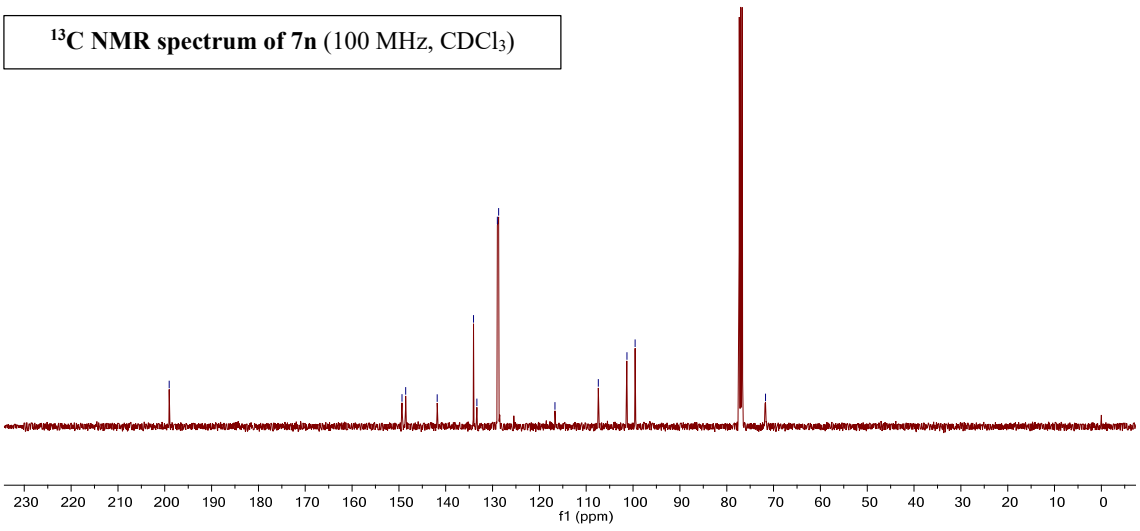
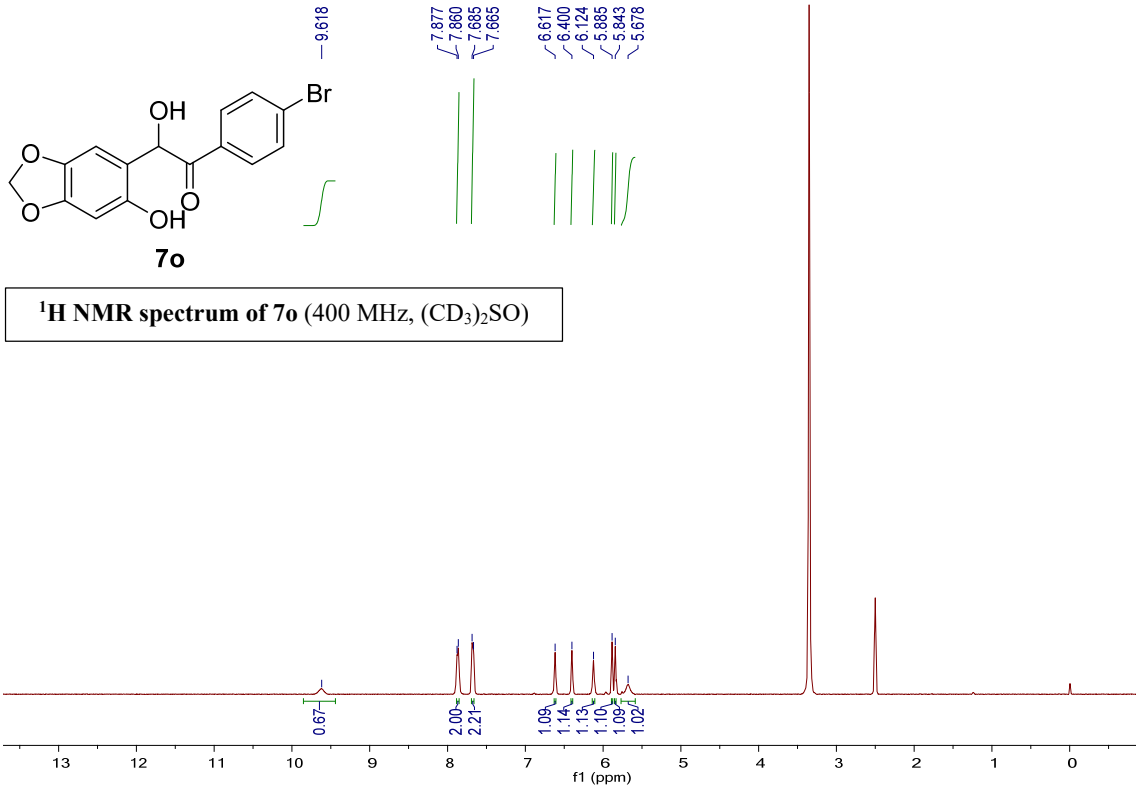
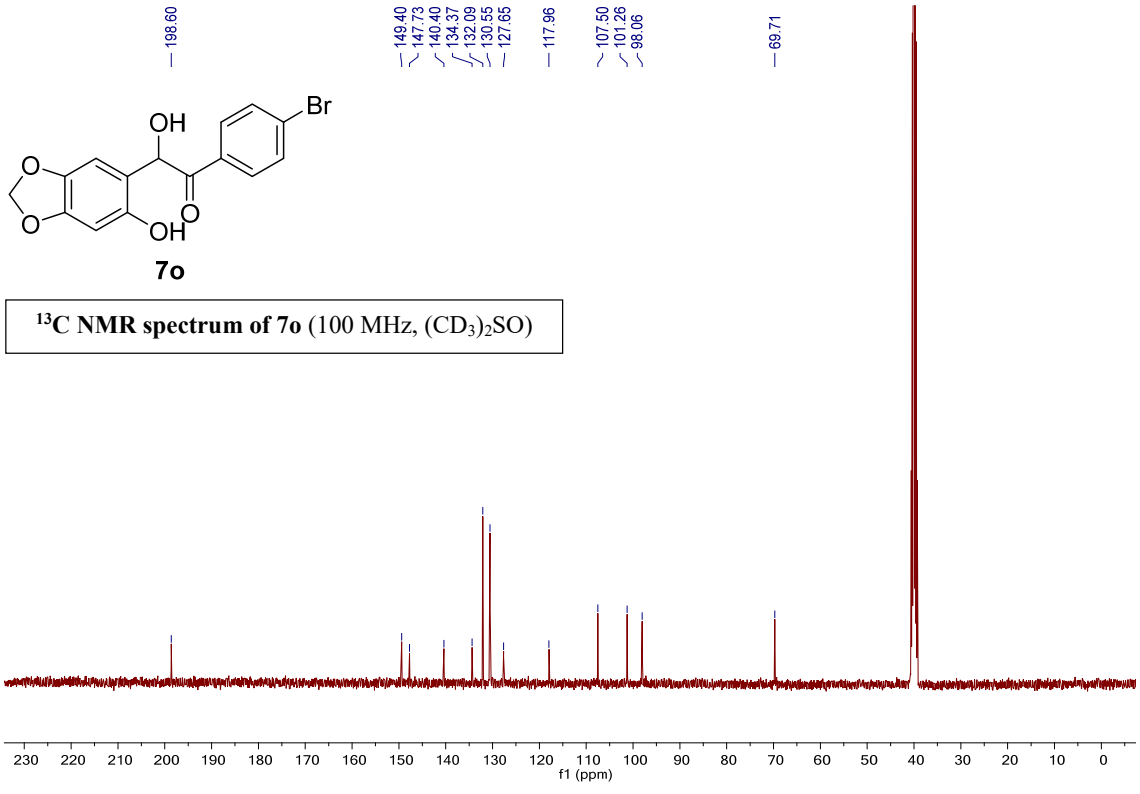


^{13}C NMR spectrum of 7n (100 MHz, $CDCl_3$)



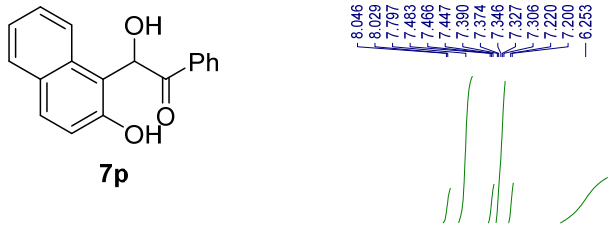
7o

^{1}H NMR spectrum of 7o (400 MHz, $(CD_3)_2SO$)

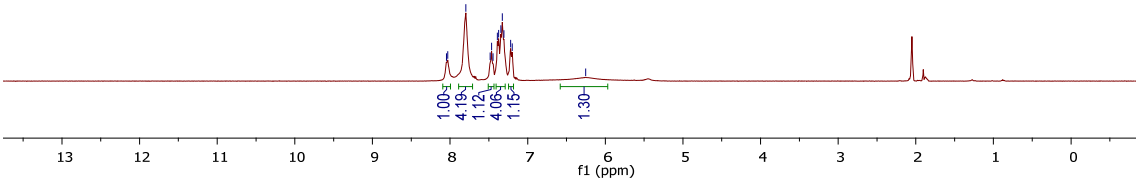


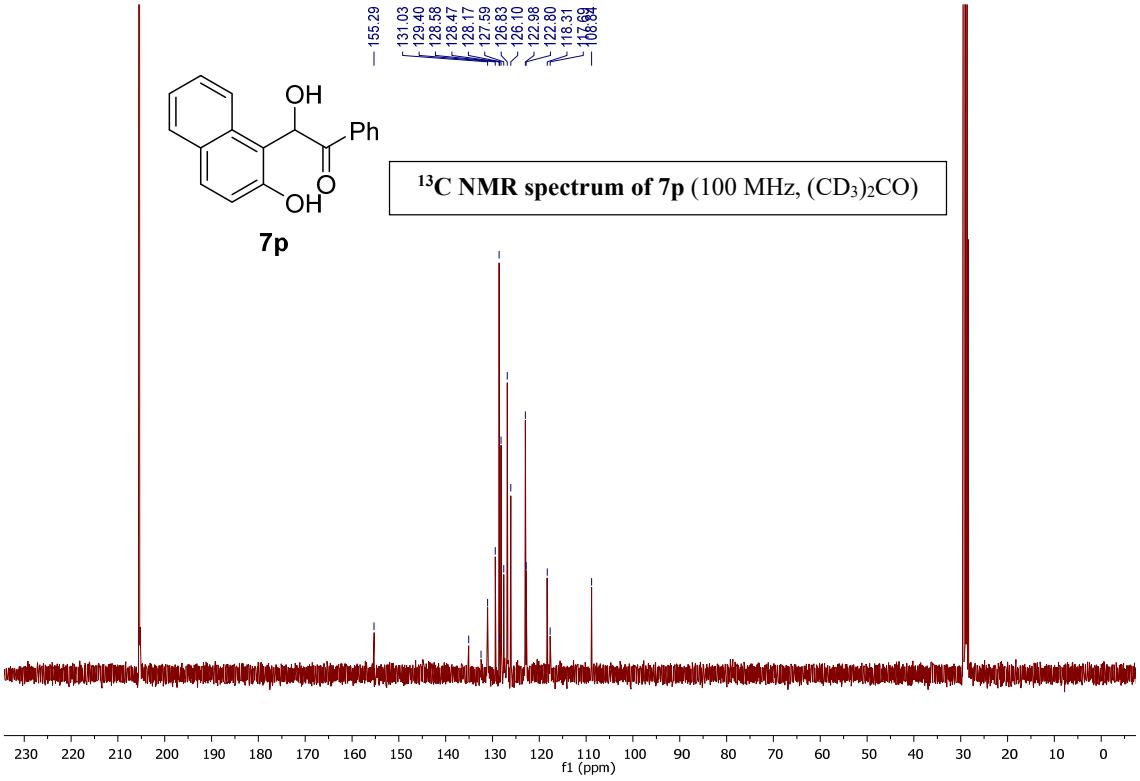
7o

^{13}C NMR spectrum of 7o (100 MHz, $(CD_3)_2SO$)

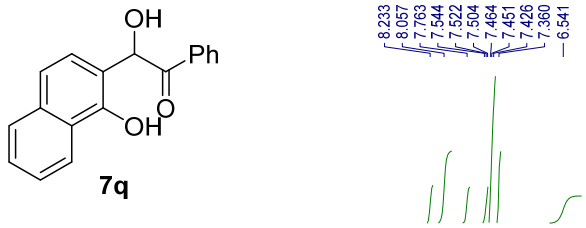


^{1}H NMR spectrum of 7p (400 MHz, $(CD_3)_2CO$)

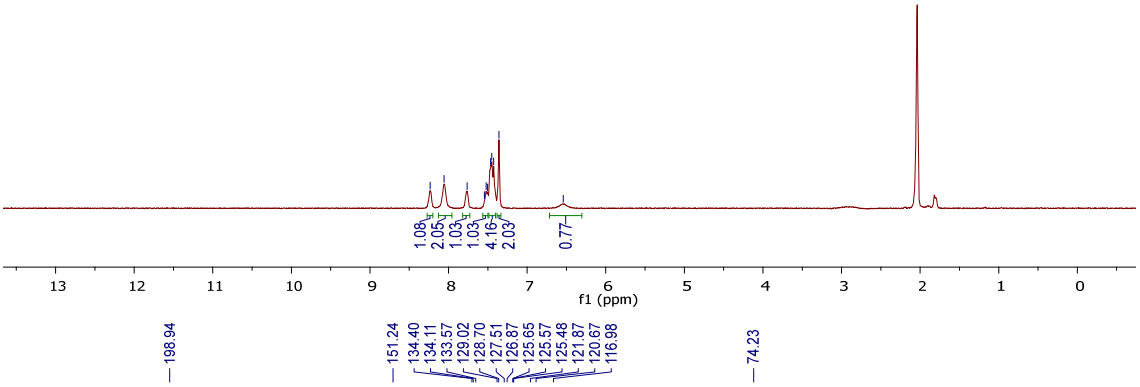


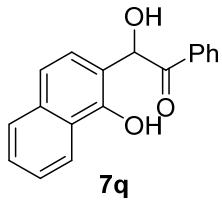


^{13}C NMR spectrum of 7p (100 MHz, $(CD_3)_2CO$)

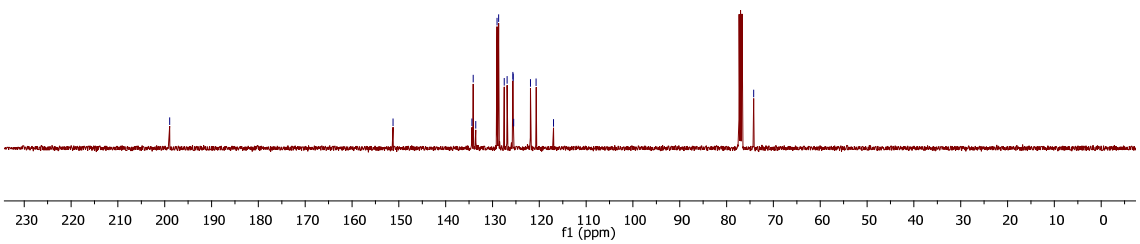


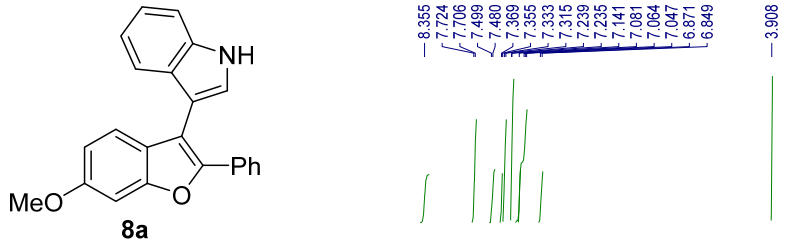
^{1}H NMR spectrum of 7q (400 MHz, $(CD_3)_2CO$)





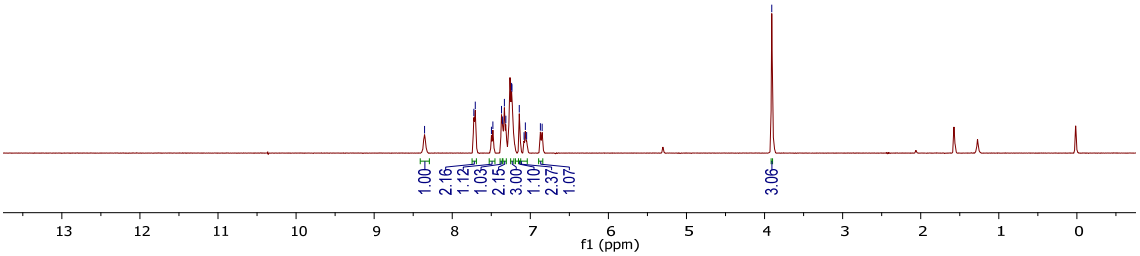
^{13}C NMR spectrum of 7q (100 MHz, $CDCl_3$)





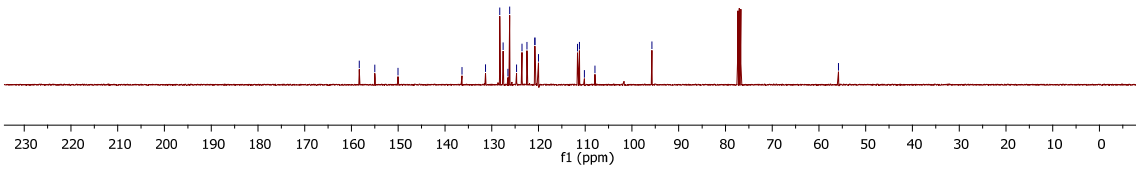
8a

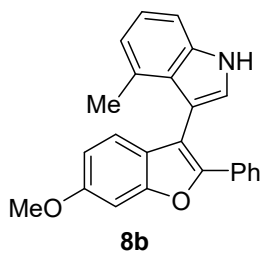
^{1}H NMR spectrum of 8a (400 MHz, $CDCl_3$)



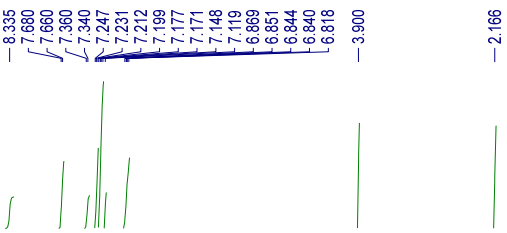
8a

^{13}C NMR spectrum of 8a (100 MHz, $CDCl_3$)

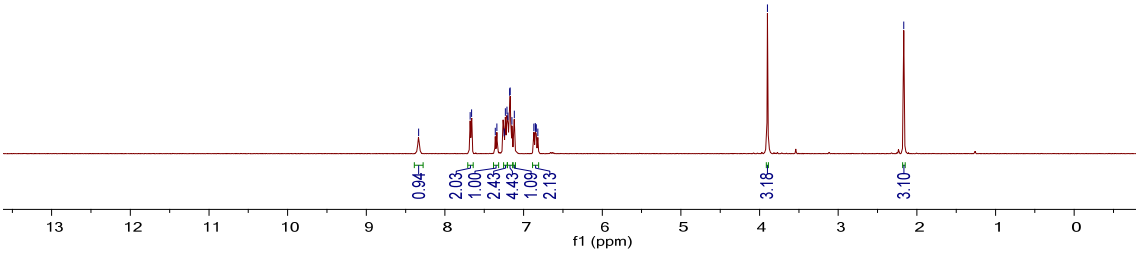


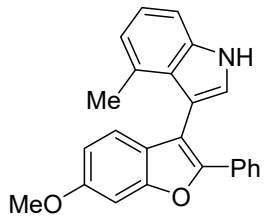


8b



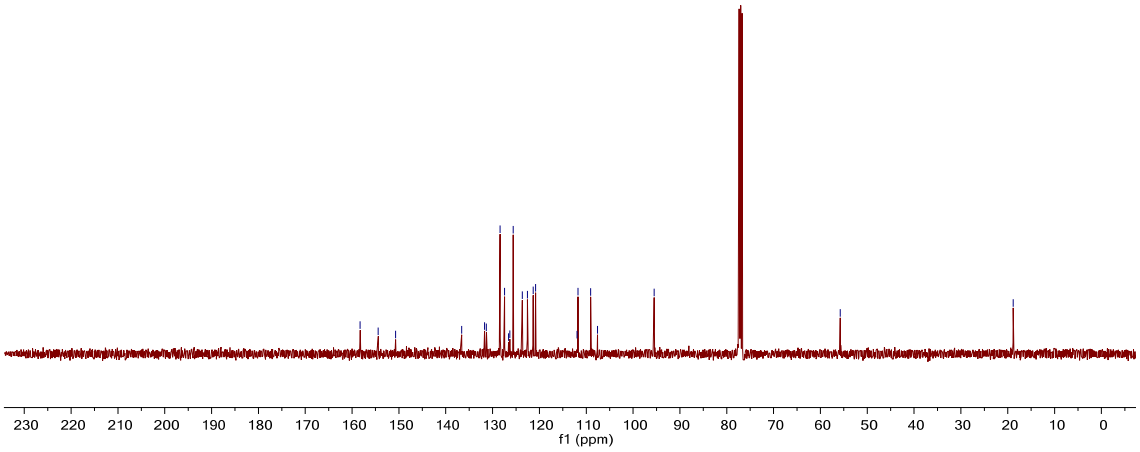
^{1}H NMR spectrum of 8b (400 MHz, $CDCl_3$)

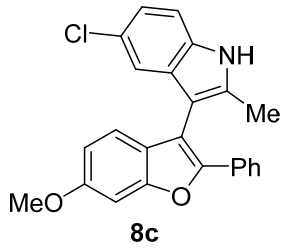




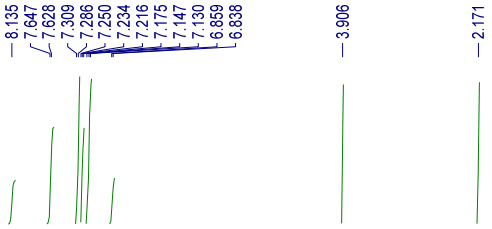
8b

^{13}C NMR spectrum of 8b (100 MHz, $CDCl_3$)

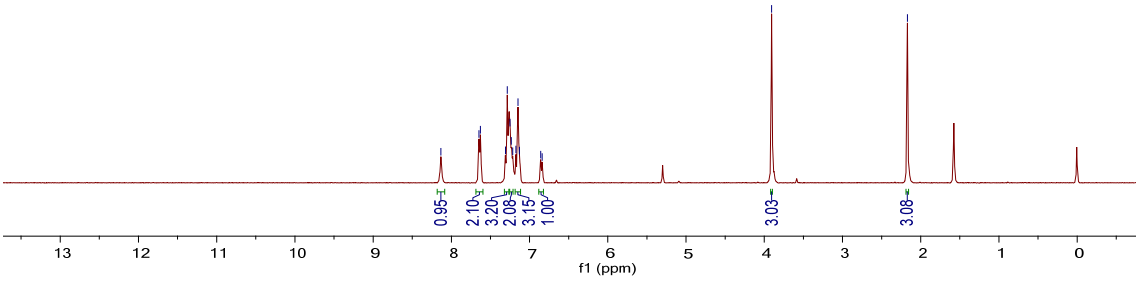


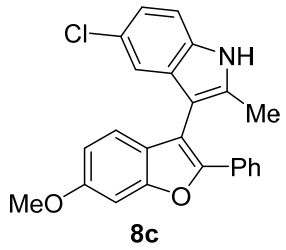


8c



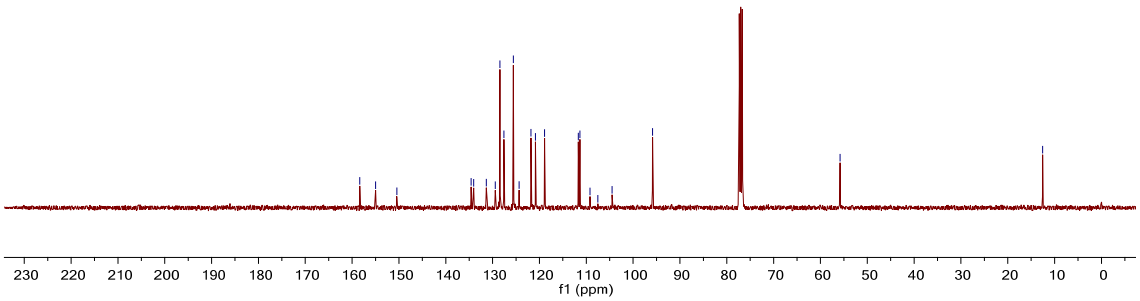
^{1}H NMR spectrum of 8c (400 MHz, $CDCl_3$)

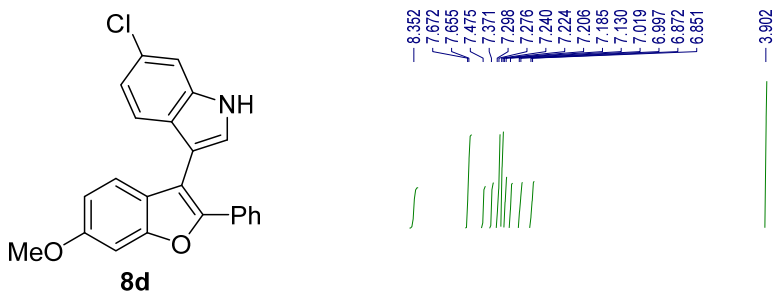




8c

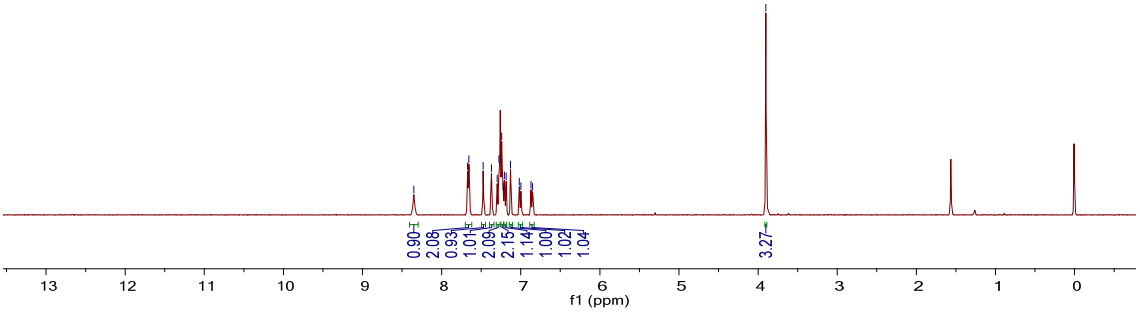
^{13}C NMR spectrum of 8c (100 MHz, $CDCl_3$)

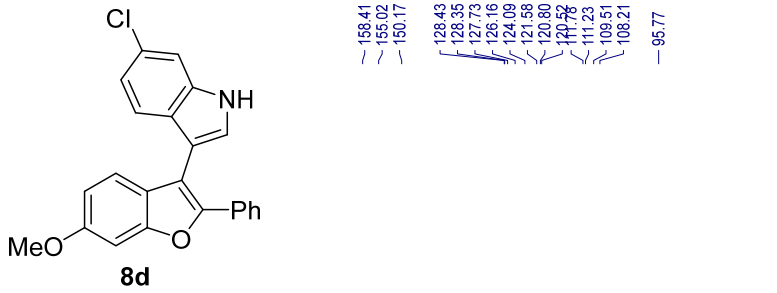




8d

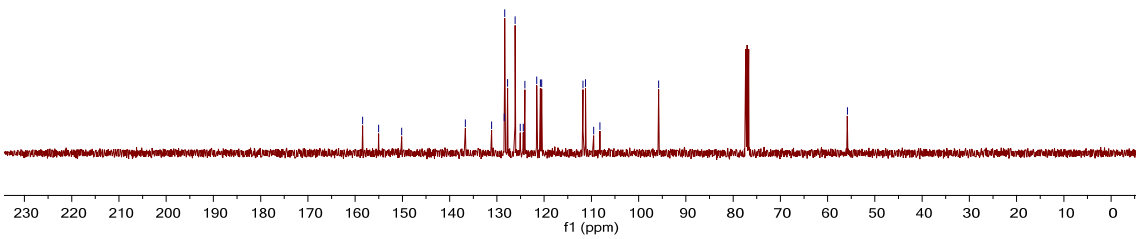
^{1}H NMR spectrum of 8d (400 MHz, $CDCl_3$)

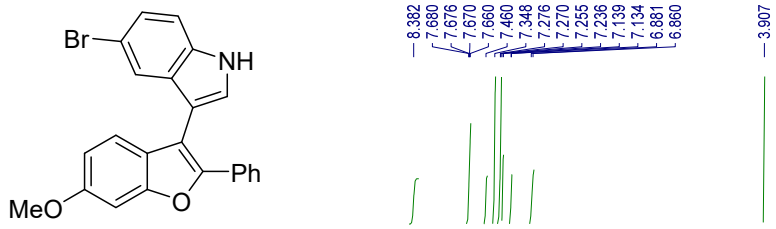




8d

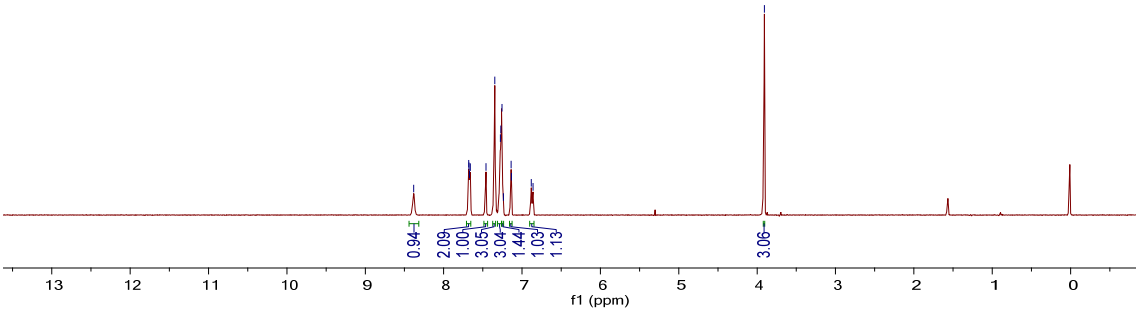
^{13}C NMR spectrum of 8d (100 MHz, $CDCl_3$)





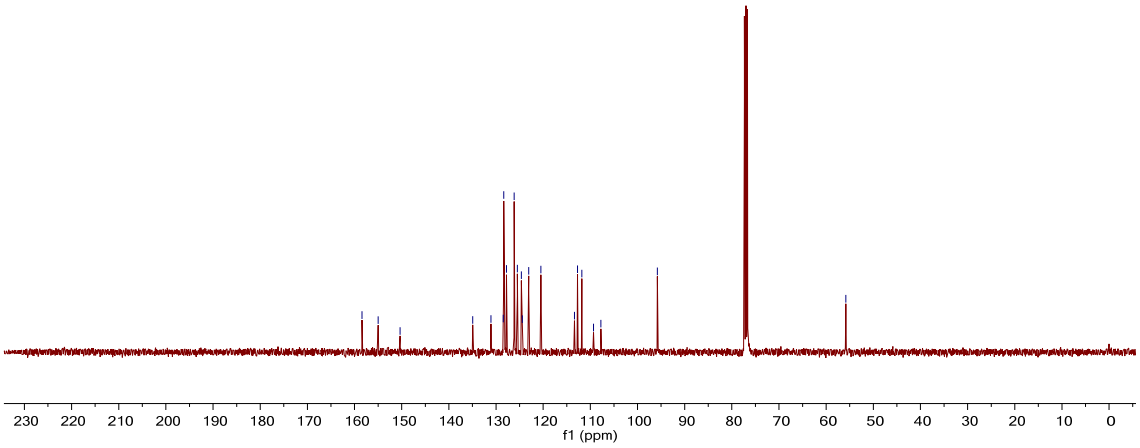
8e

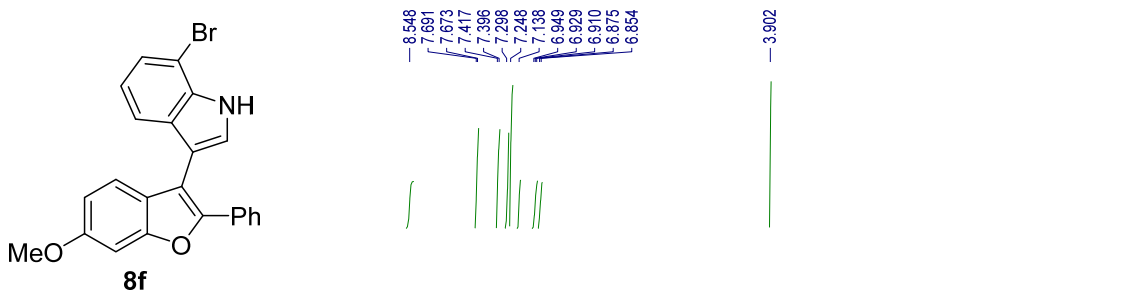
^{1}H NMR spectrum of 8e (400 MHz, $CDCl_3$)



8e

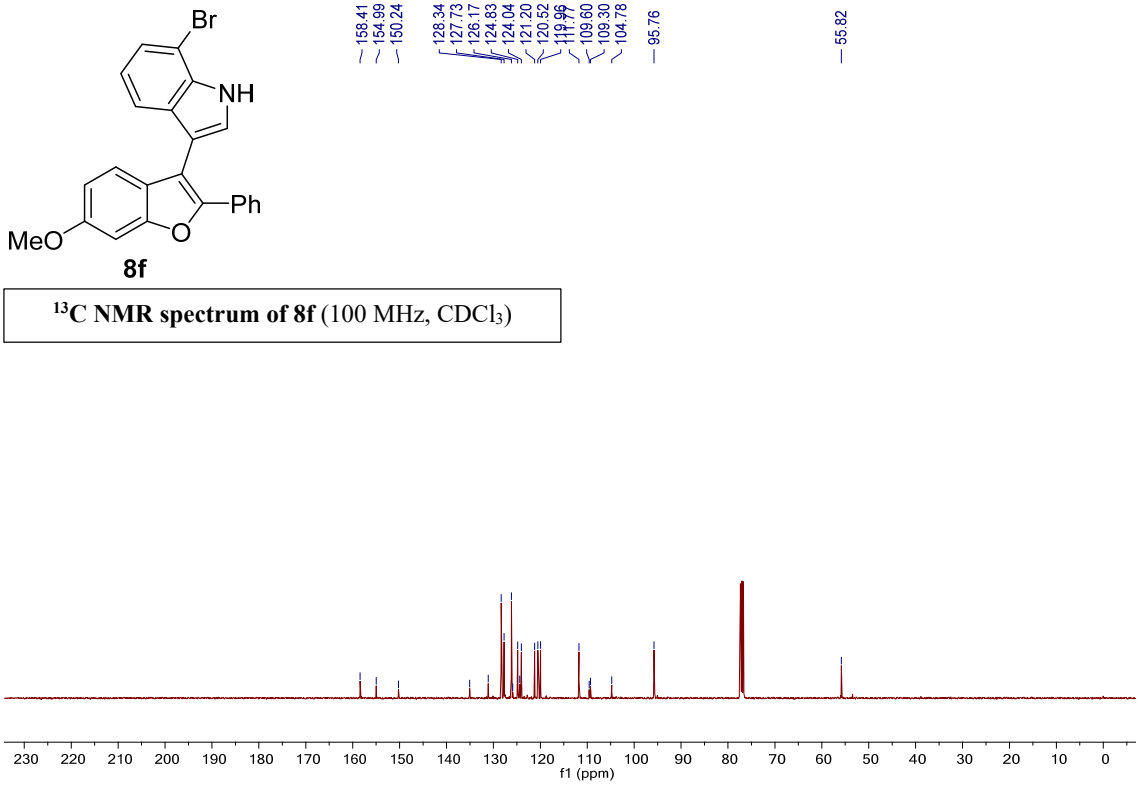
^{13}C NMR spectrum of 8e (100 MHz, $CDCl_3$)





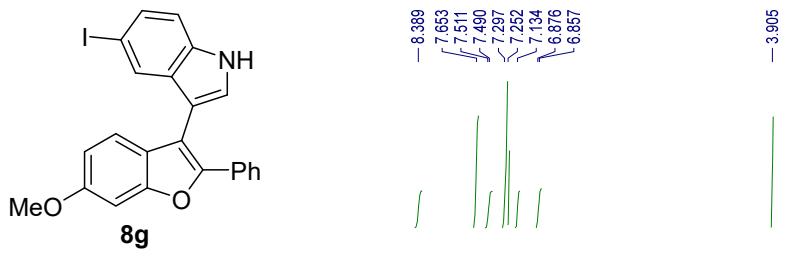
8f

^{1}H NMR spectrum of 8f (400 MHz, $CDCl_3$)

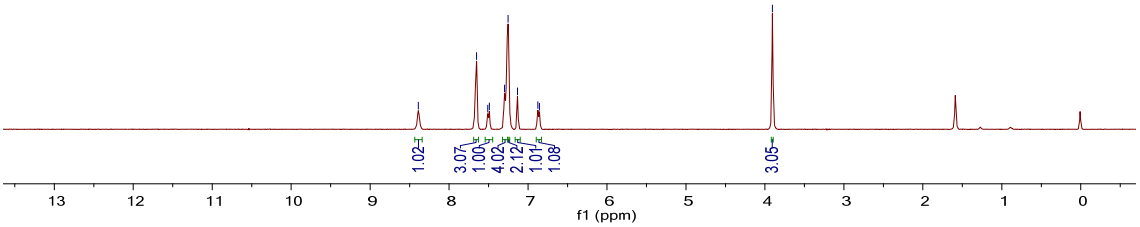


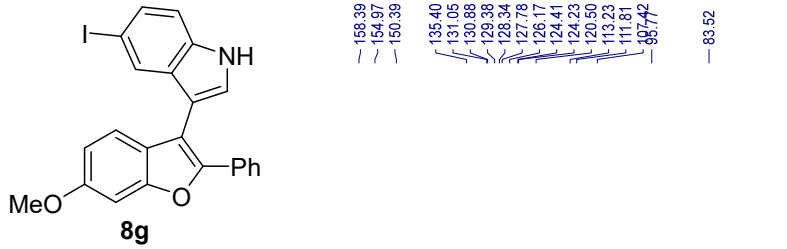
8f

^{13}C NMR spectrum of 8f (100 MHz, $CDCl_3$)

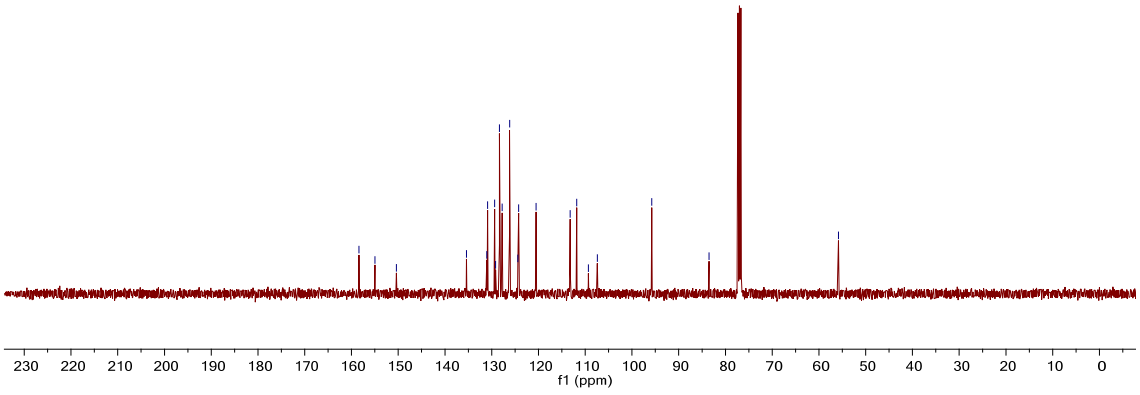


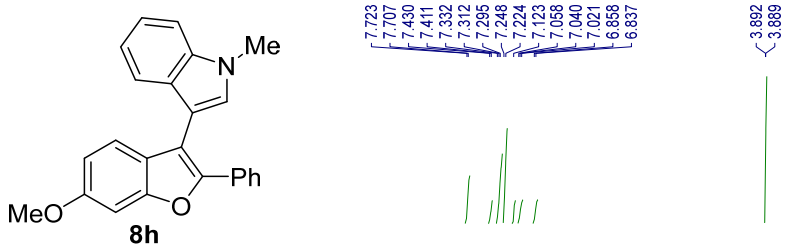
^{1}H NMR spectrum of 8g (400 MHz, $CDCl_3$)



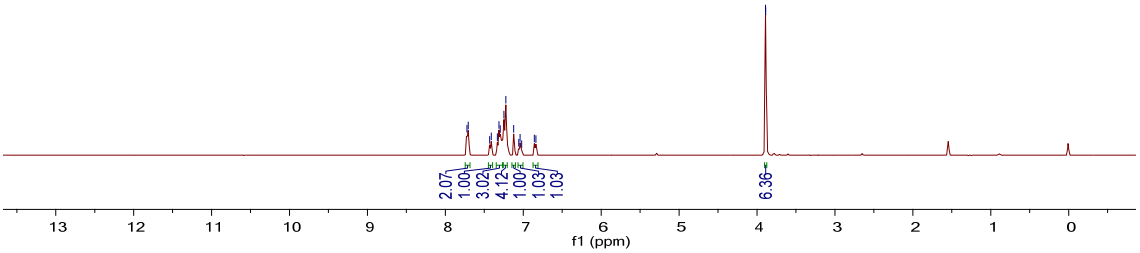


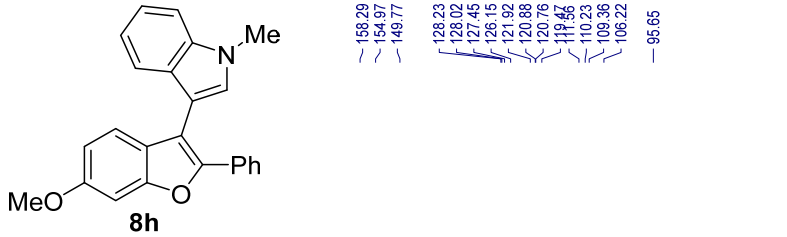
^{13}C NMR spectrum of 8g (100 MHz, $CDCl_3$)



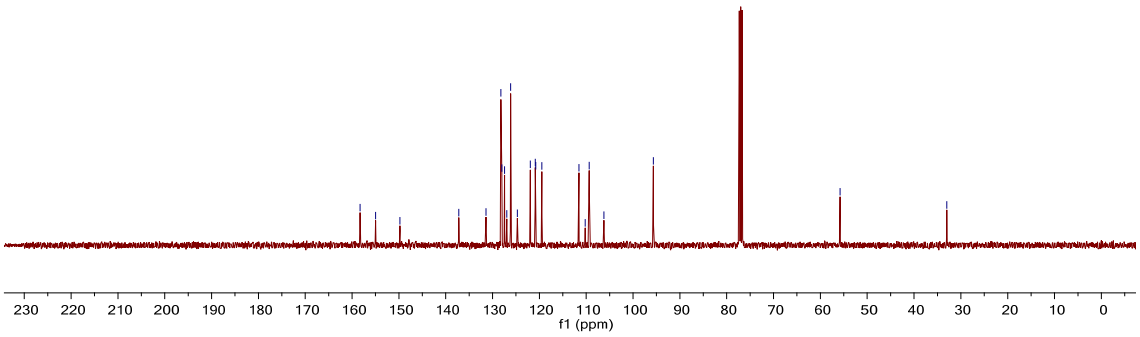


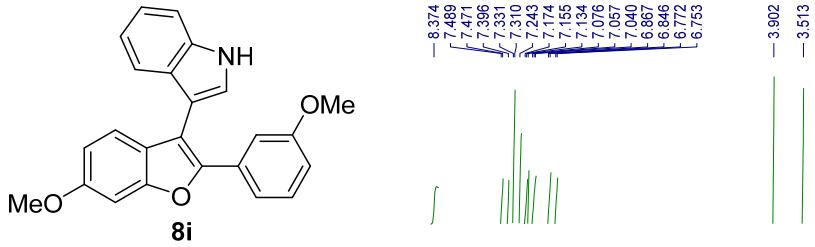
^{1}H NMR spectrum of 8h (400 MHz, $CDCl_3$)





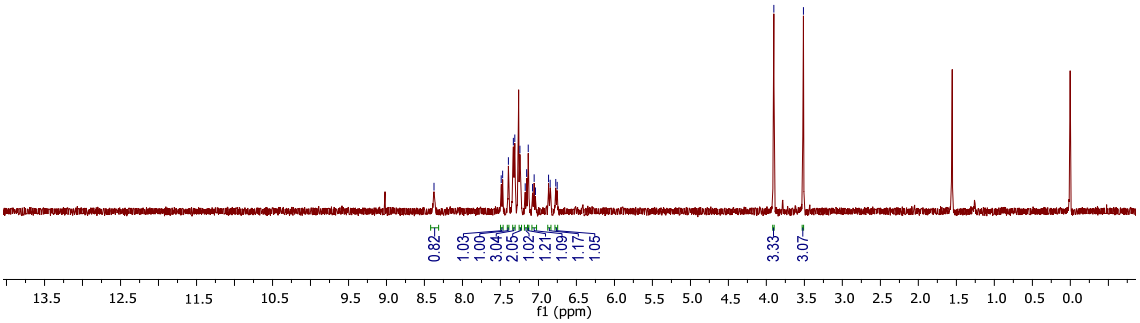
^{13}C NMR spectrum of 8h (100 MHz, $CDCl_3$)

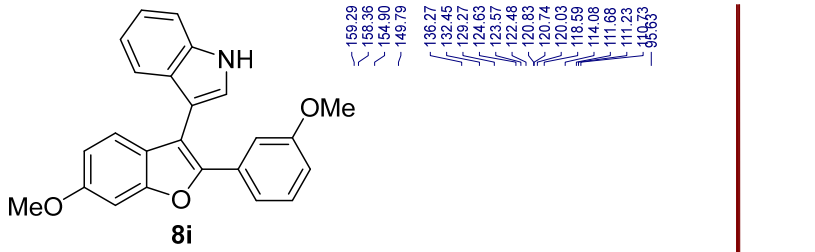




8i

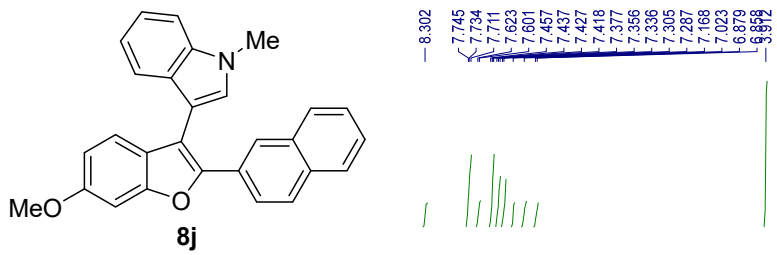
^{1}H NMR spectrum of 8i (400 MHz, $CDCl_3$)





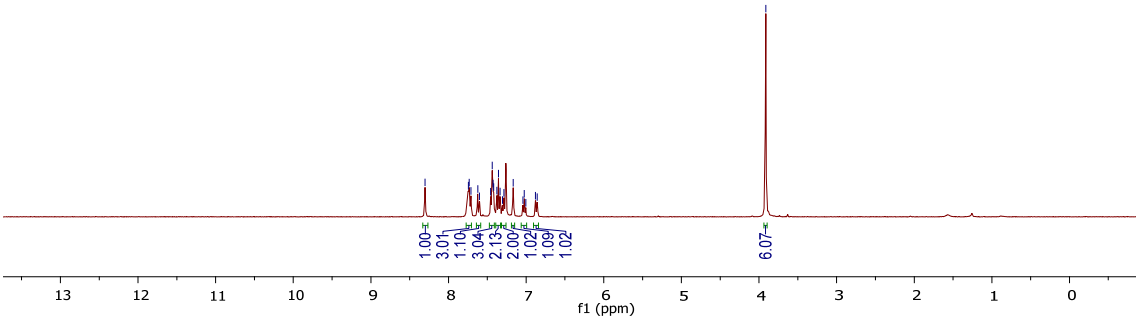
8i

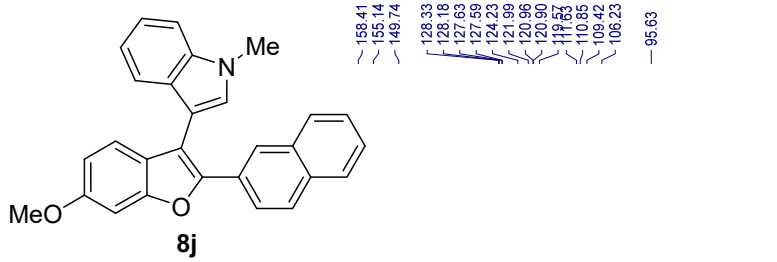
^{13}C NMR spectrum of 8i (100 MHz, $CDCl_3$)



8j

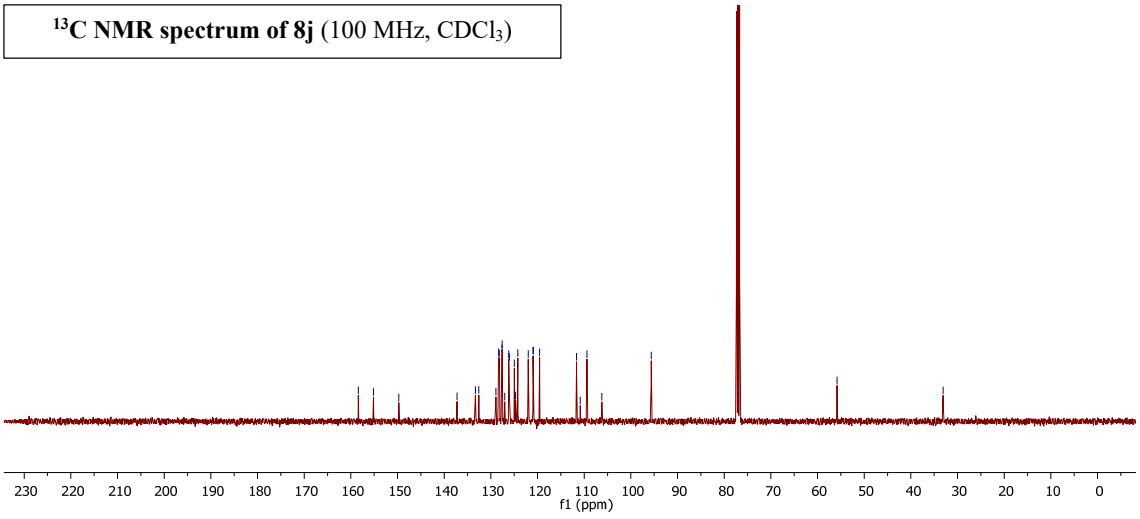
^{1}H NMR spectrum of 8j (400 MHz, $CDCl_3$)

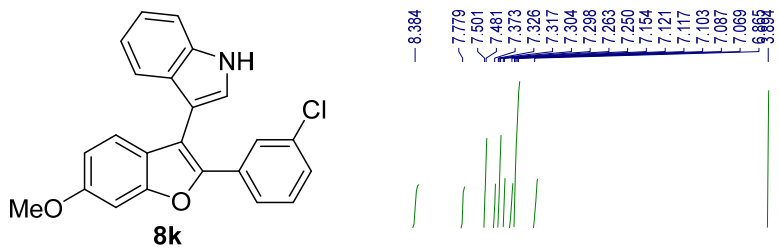




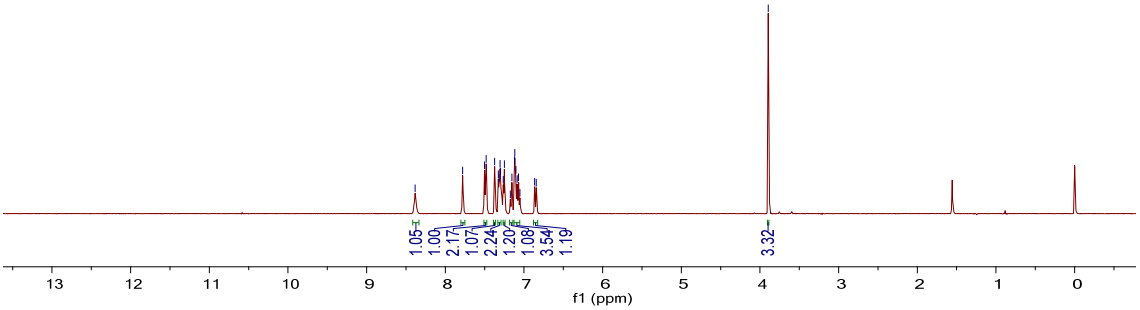
8j

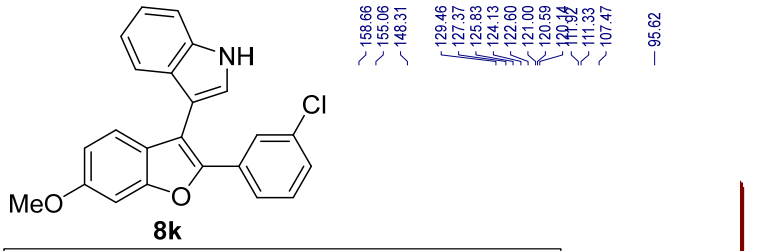
^{13}C NMR spectrum of 8j (100 MHz, $CDCl_3$)



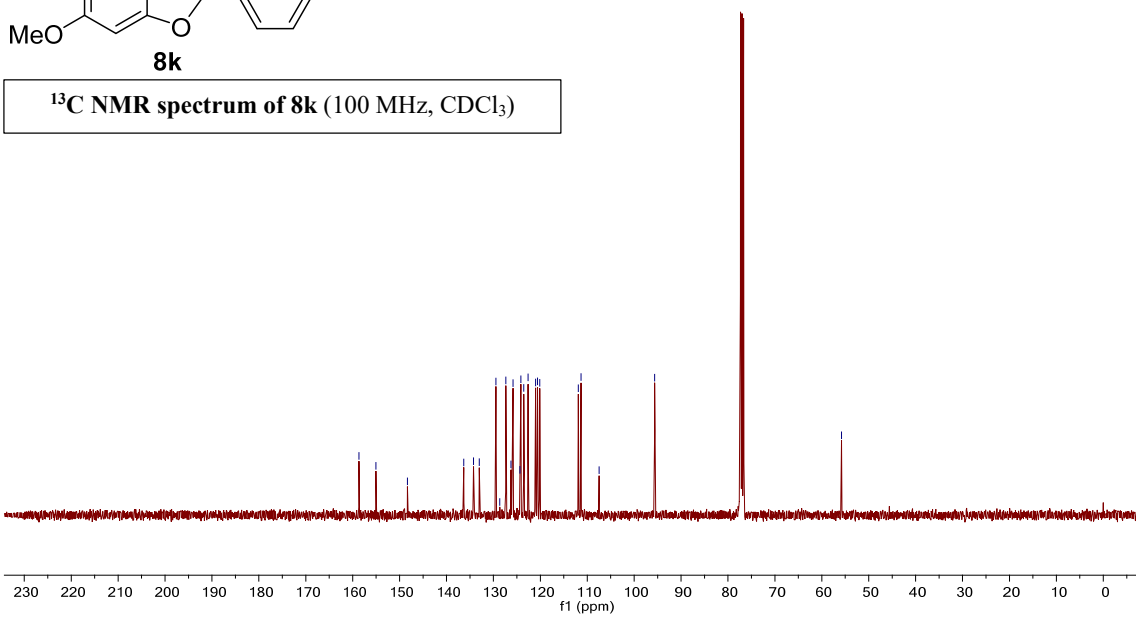


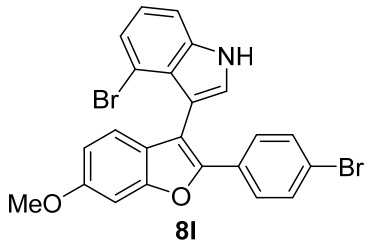
^{1}H NMR spectrum of 8k (400 MHz, $CDCl_3$)



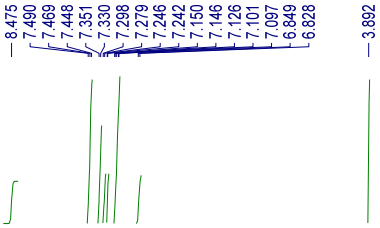


^{13}C NMR spectrum of 8k (100 MHz, $CDCl_3$)

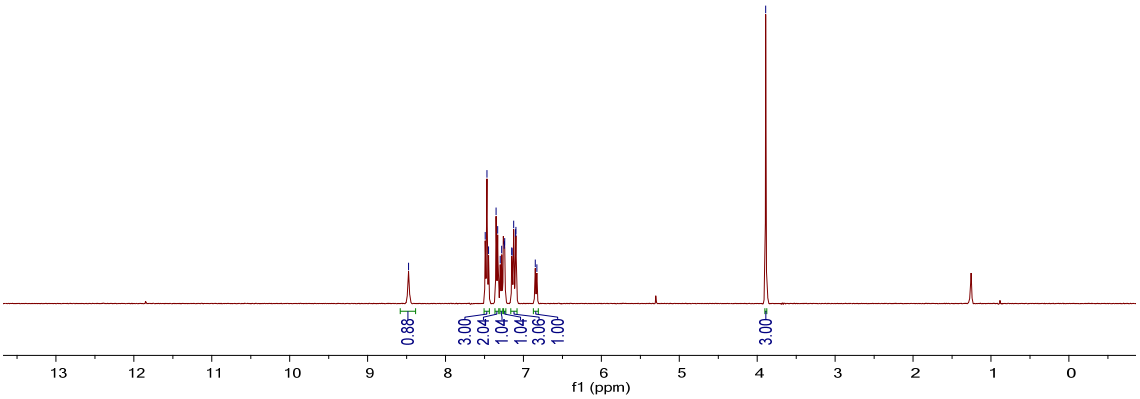


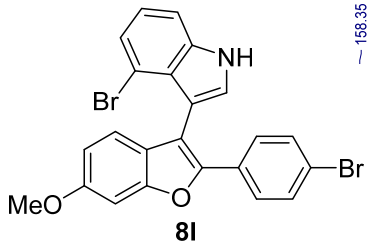


8l



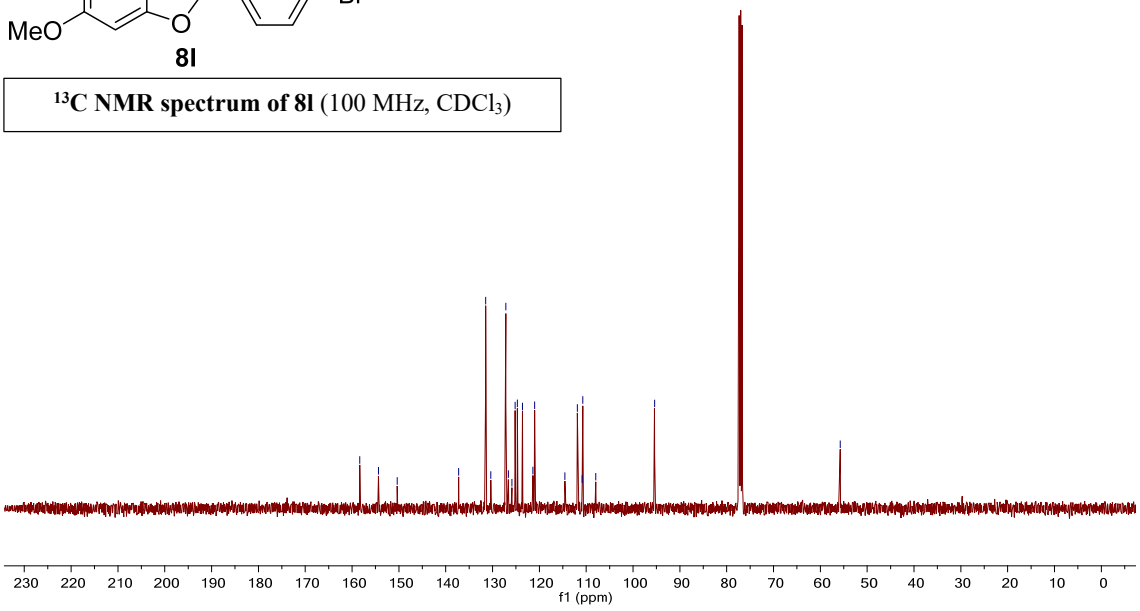
^{1}H NMR spectrum of 8l (400 MHz, $CDCl_3$)

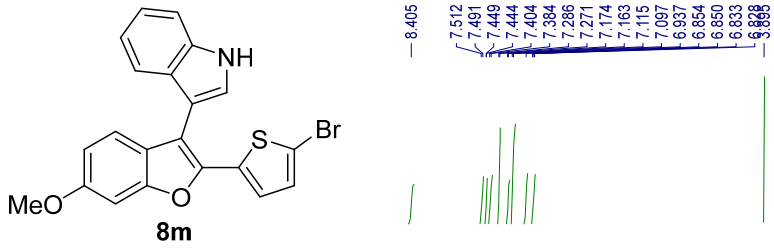




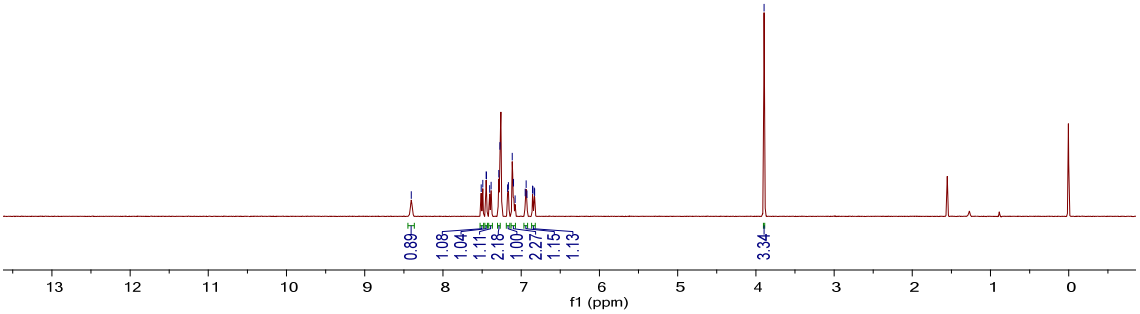
8l

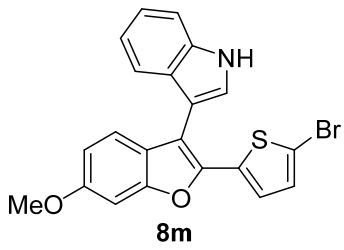
^{13}C NMR spectrum of 8l (100 MHz, $CDCl_3$)

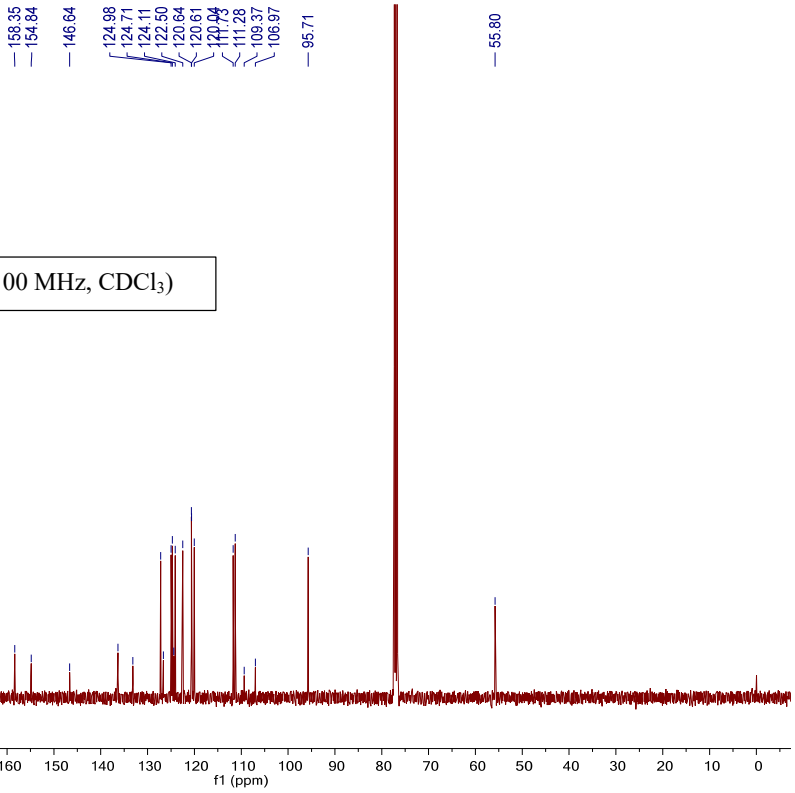




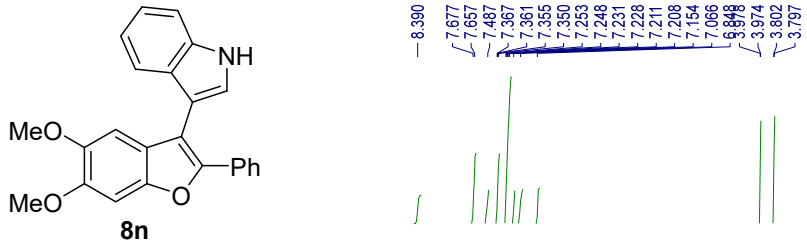
^{1}H NMR spectrum of 8m (400 MHz, $CDCl_3$)





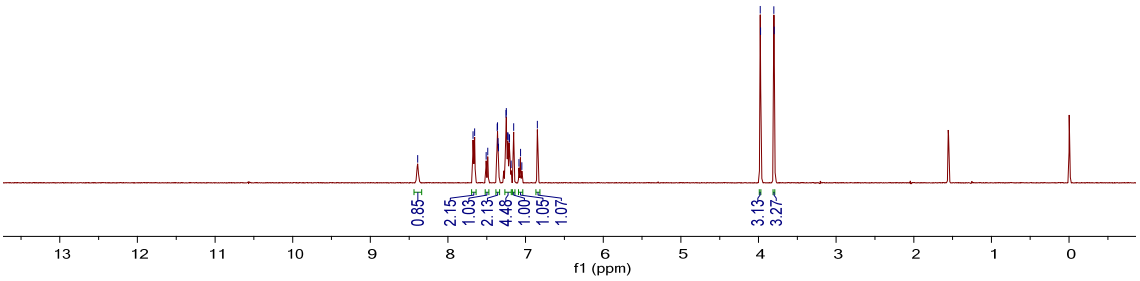


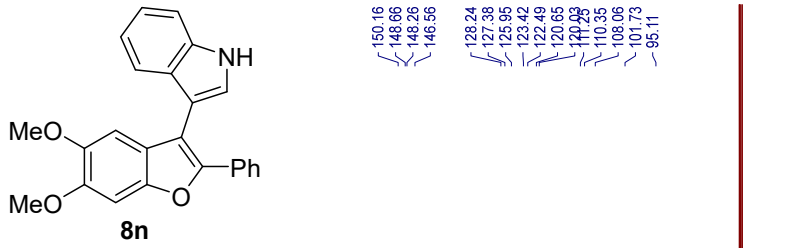
^{13}C NMR spectrum of 8m (100 MHz, $CDCl_3$)



8n

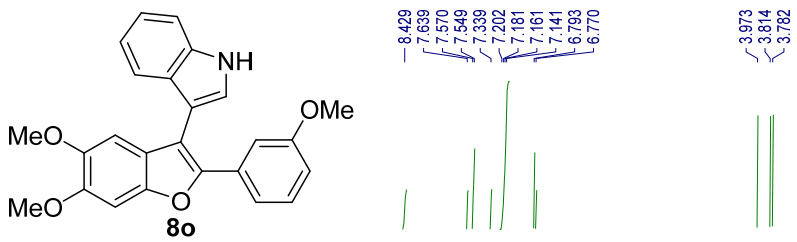
^{1}H NMR spectrum of 8n (400 MHz, $CDCl_3$)



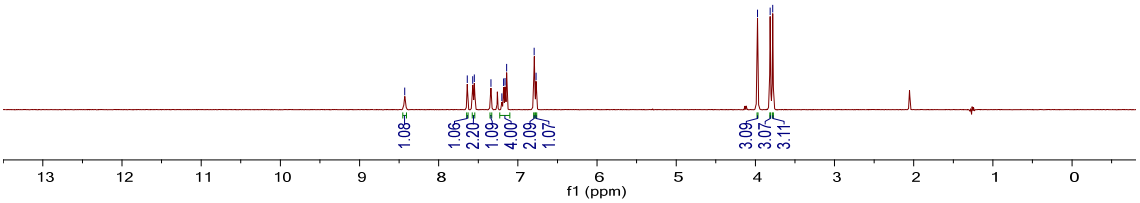


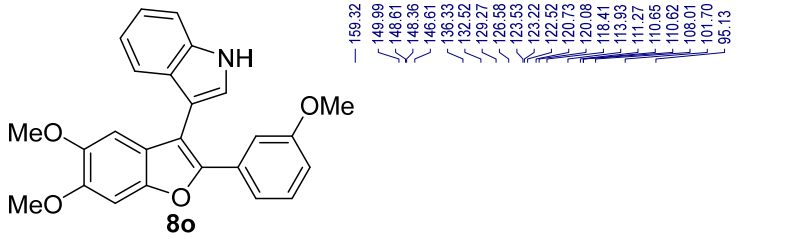
8n

^{13}C NMR spectrum of 8n (100 MHz, $CDCl_3$)

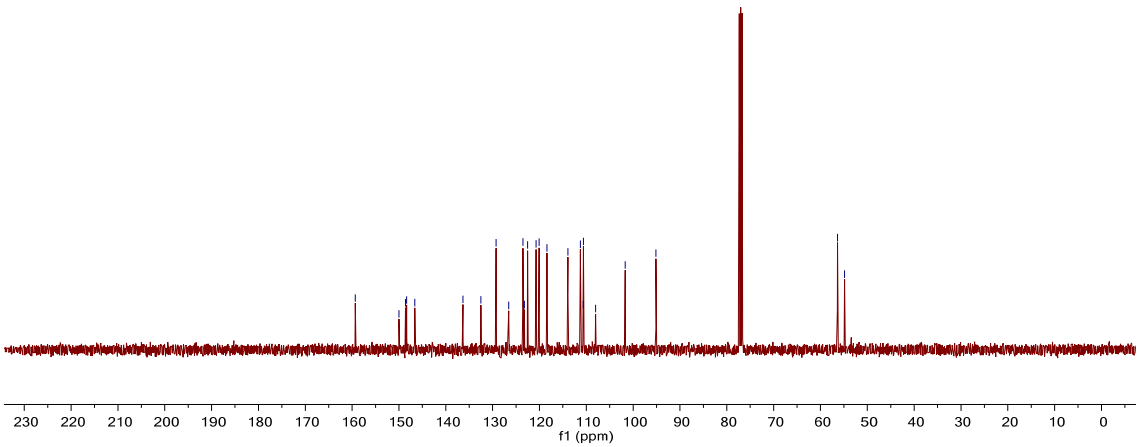


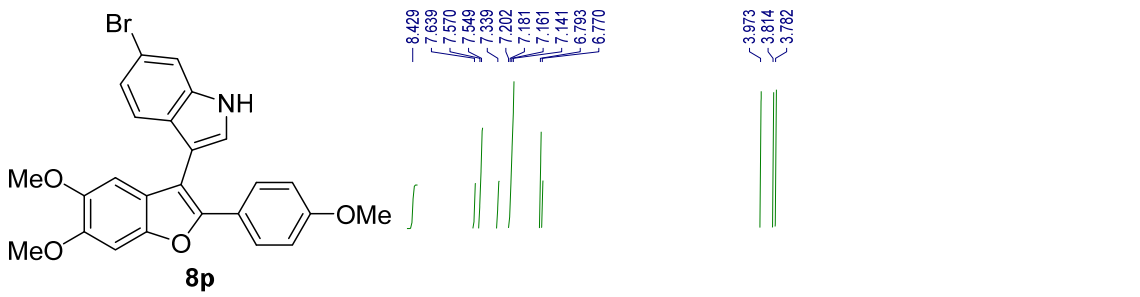
^{1}H NMR spectrum of 8o (400 MHz, $CDCl_3$)





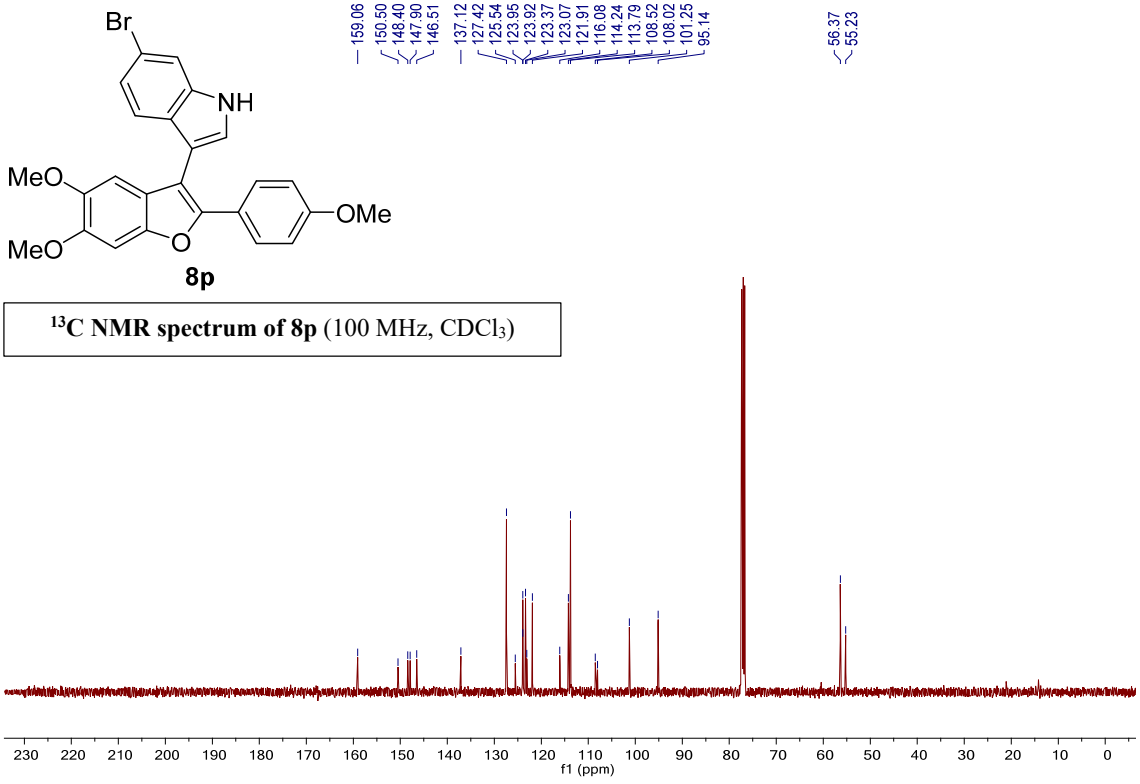
^{13}C NMR spectrum of 8o (100 MHz, $CDCl_3$)





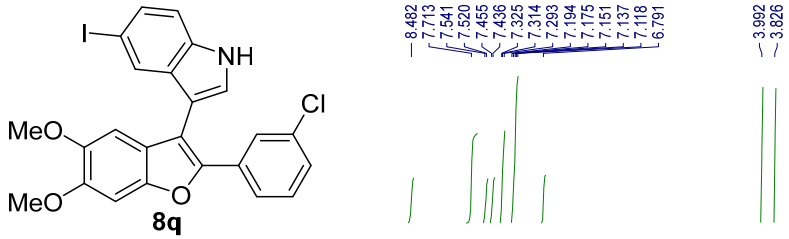
8p

^{1}H NMR spectrum of 8p (400 MHz, $CDCl_3$)

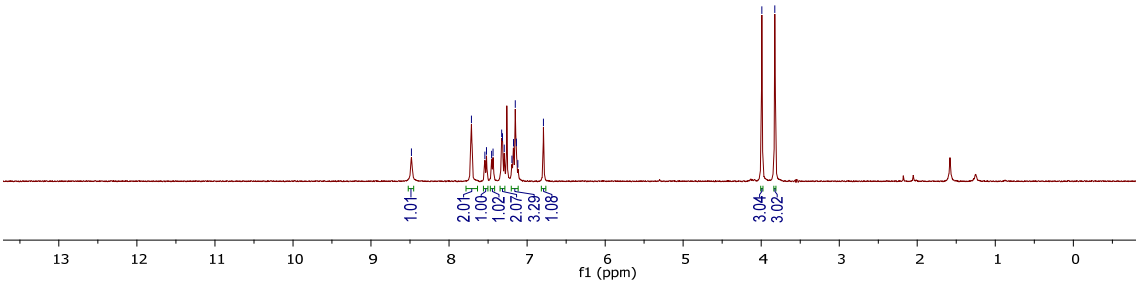


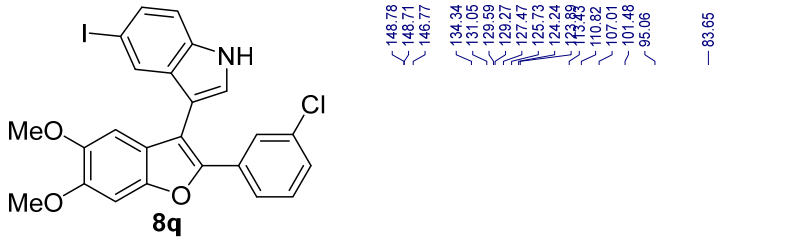
8p

^{13}C NMR spectrum of 8p (100 MHz, $CDCl_3$)

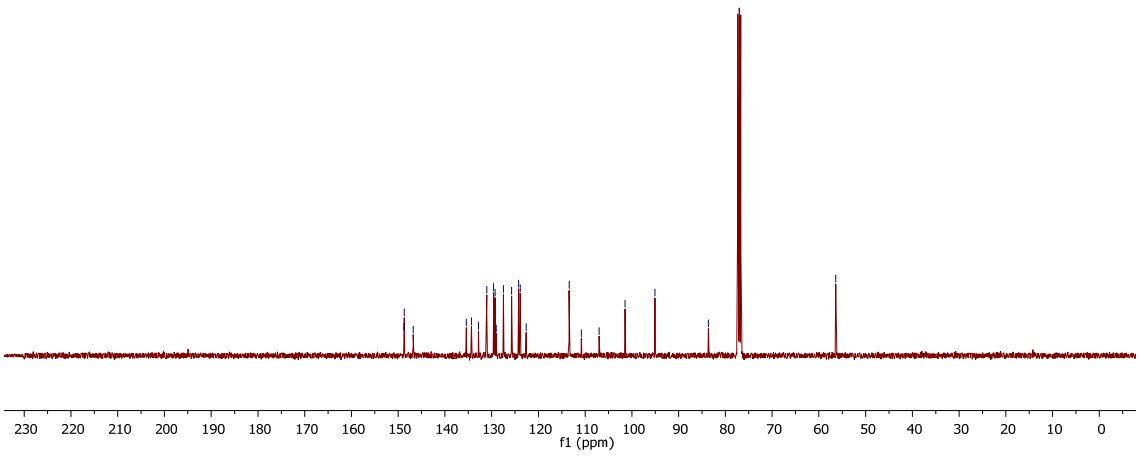


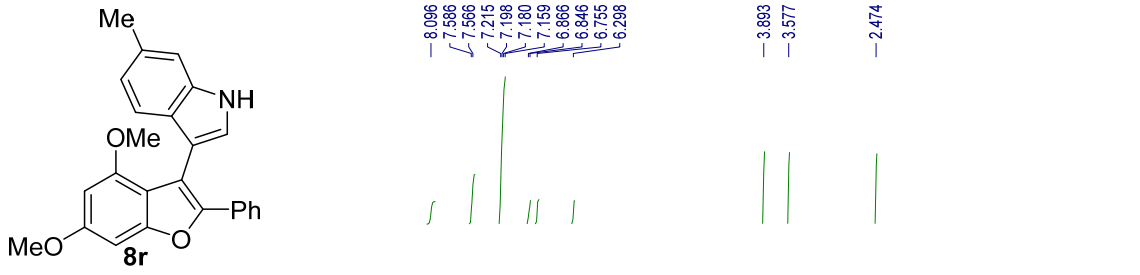
^{1}H NMR spectrum of 8q (400 MHz, $CDCl_3$)



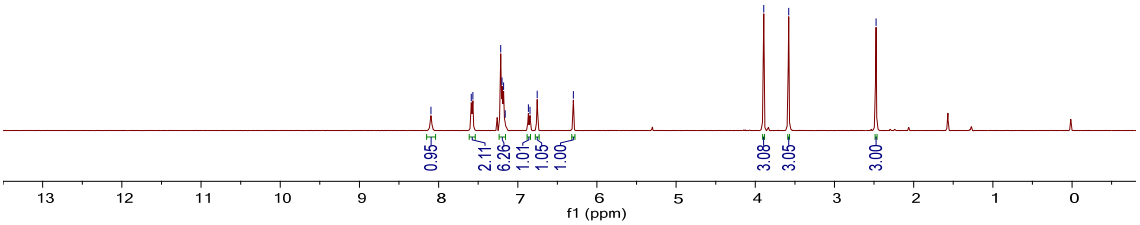


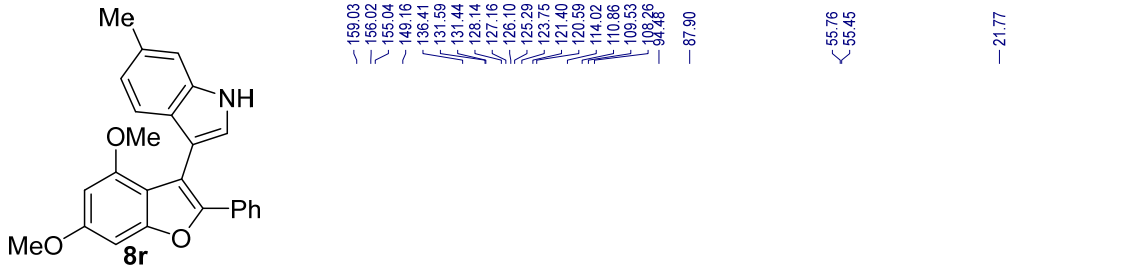
^{13}C NMR spectrum of 8q (100 MHz, $CDCl_3$)



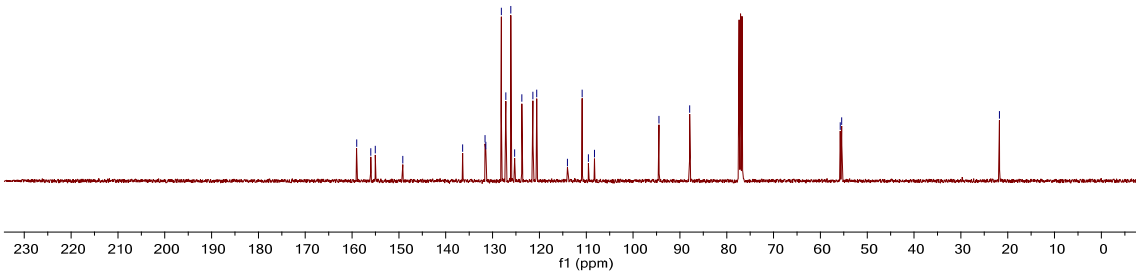


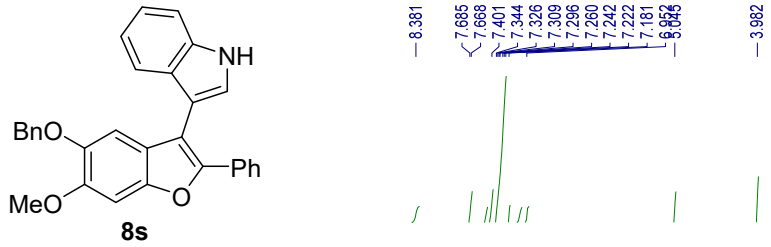
^{1}H NMR spectrum of 8r (400 MHz, $CDCl_3$)





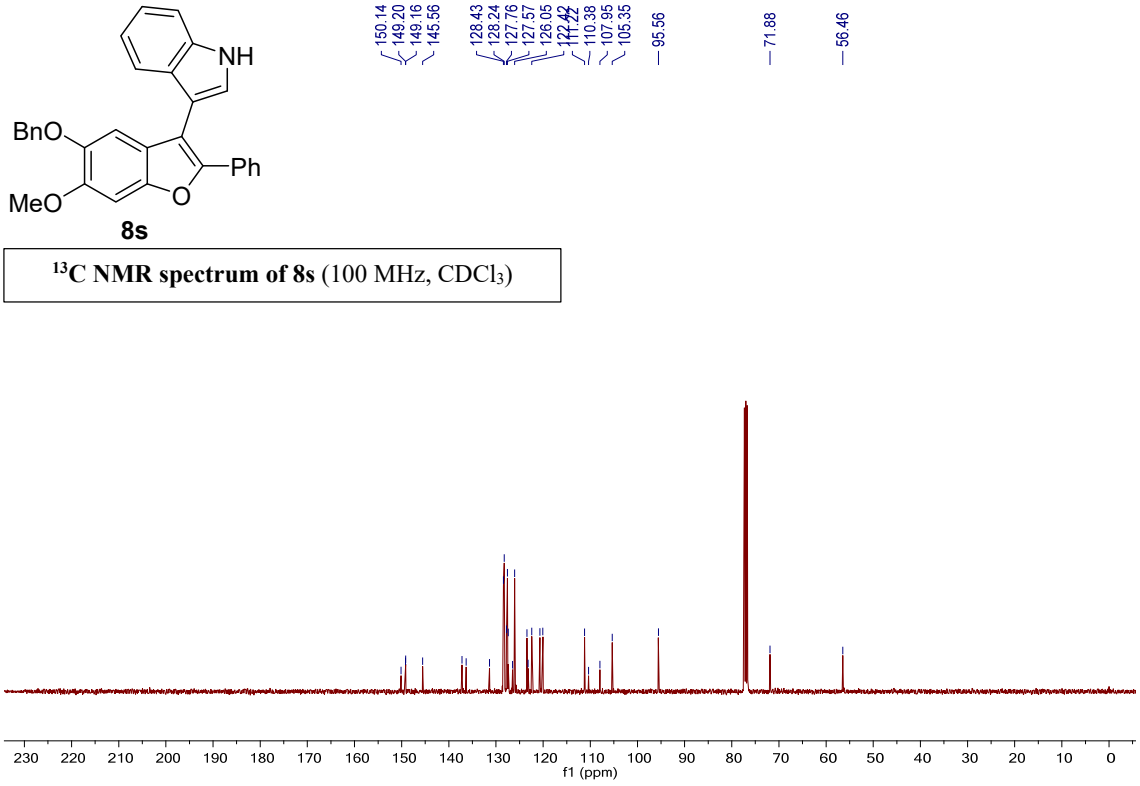
^{13}C NMR spectrum of 8r (100 MHz, $CDCl_3$)





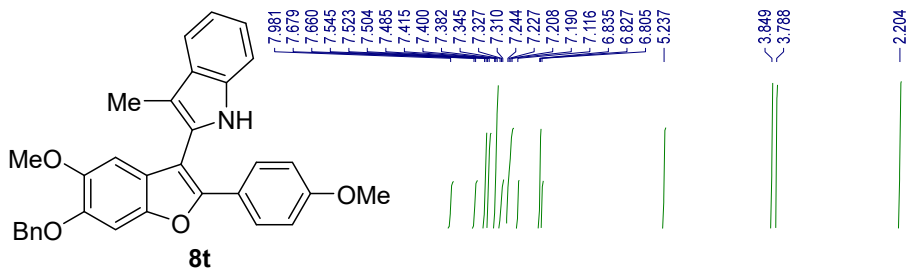
8s

^{1}H NMR spectrum of 8s (400 MHz, $CDCl_3$)



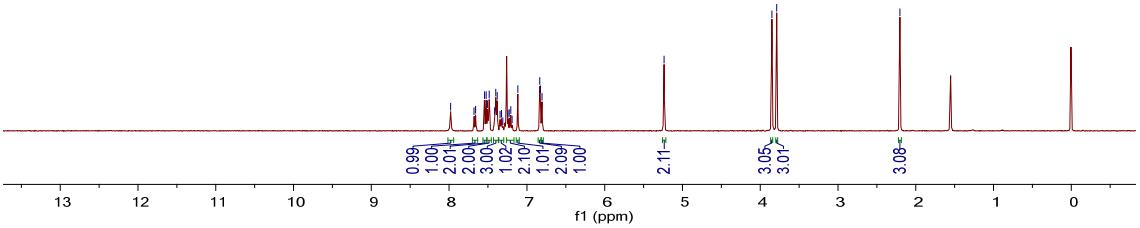
8s

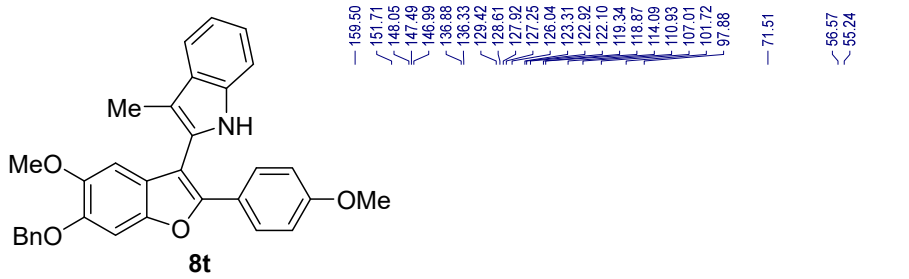
^{13}C NMR spectrum of 8s (100 MHz, $CDCl_3$)



8t

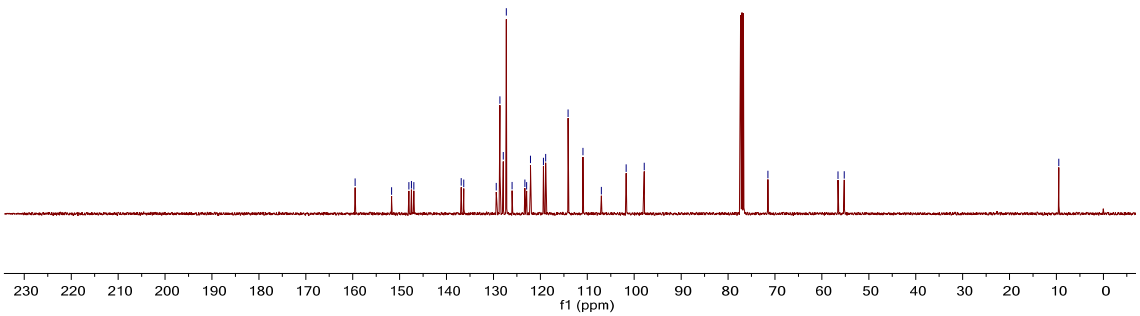
^{1}H NMR spectrum of 8t (400 MHz, $CDCl_3$)

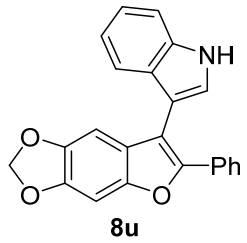




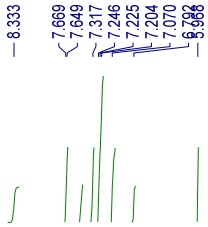
8t

^{13}C NMR spectrum of 8t (100 MHz, $CDCl_3$)

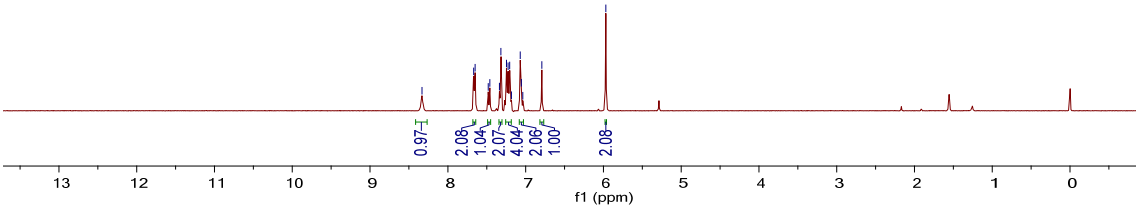


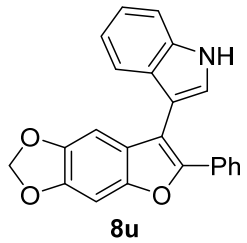


8u



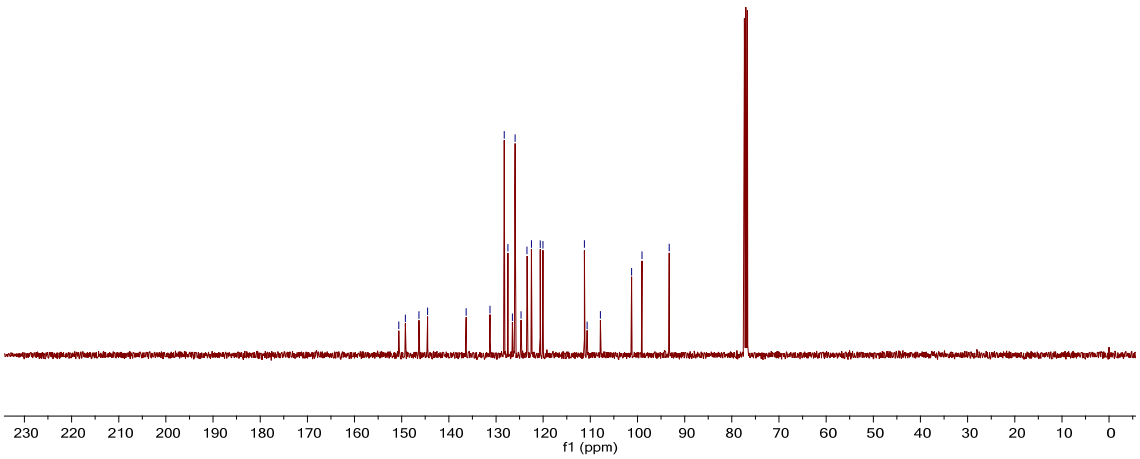
^{1}H NMR spectrum of 8u (400 MHz, $CDCl_3$)

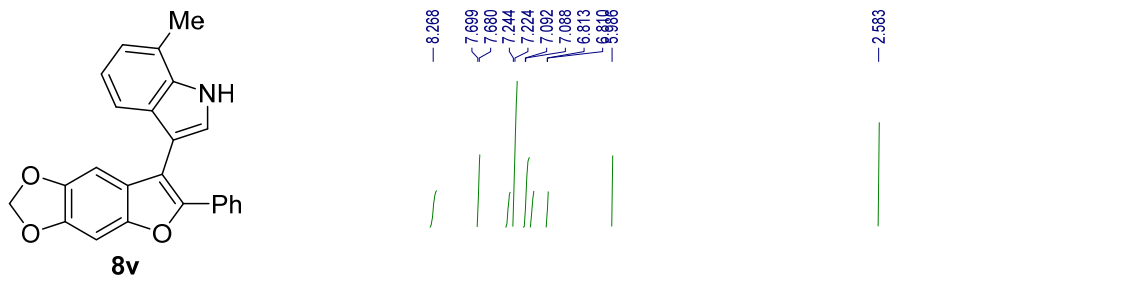




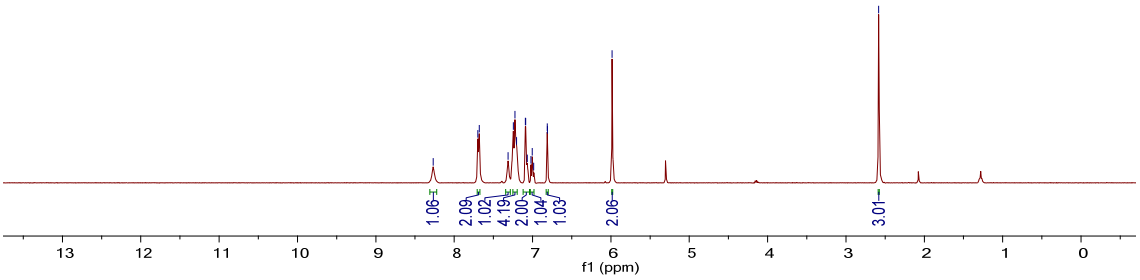
8u

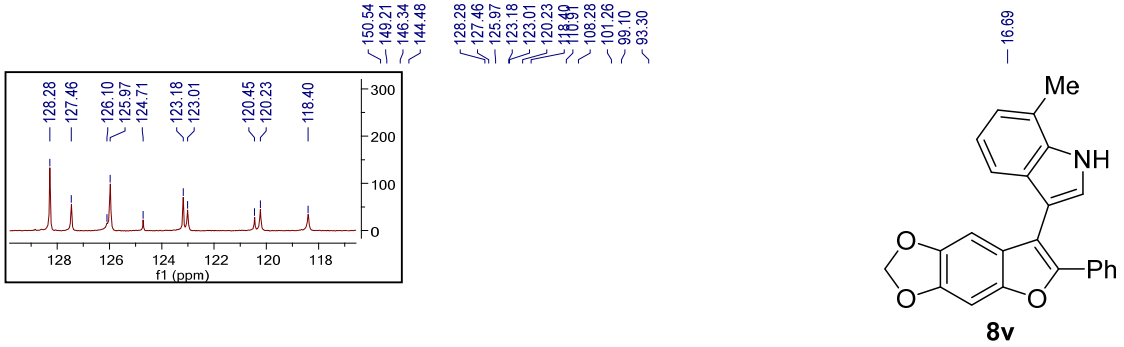
^{13}C NMR spectrum of 8u (100 MHz, $CDCl_3$)



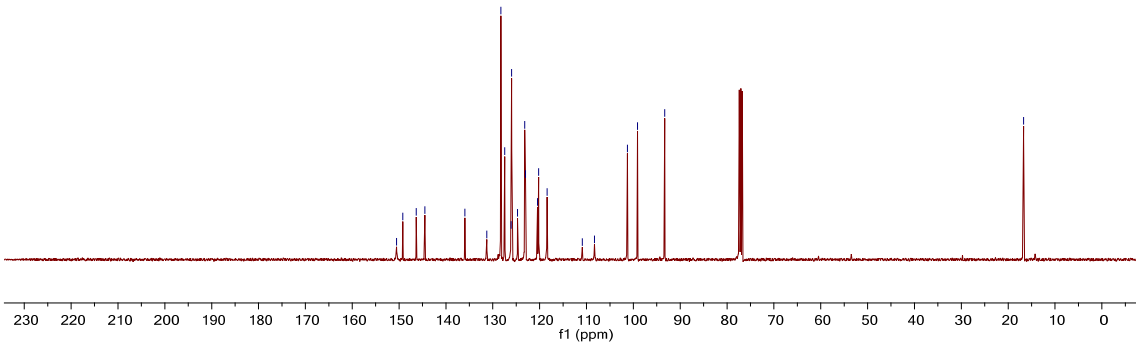


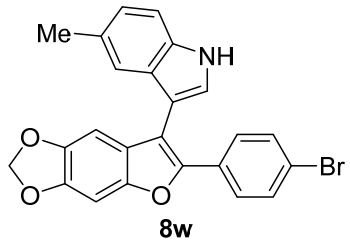
^{1}H NMR spectrum of 8v (400 MHz, $CDCl_3$)

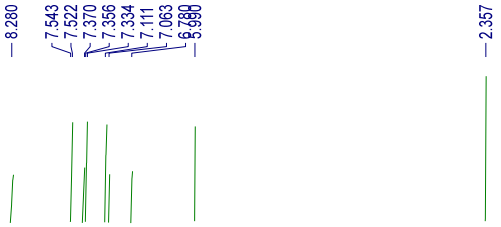




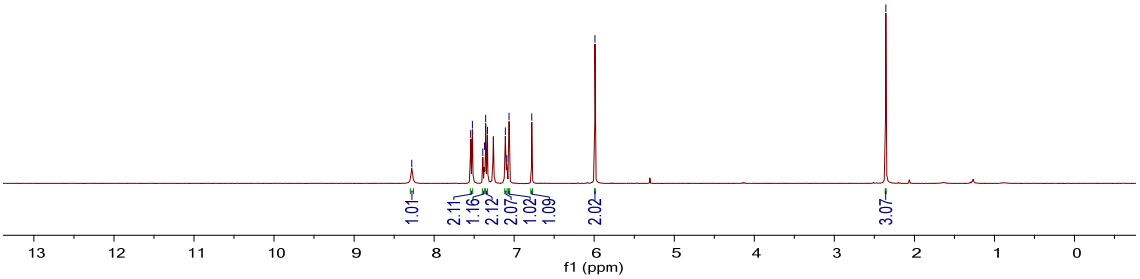
^{13}C NMR spectrum of 8v (100 MHz, $CDCl_3$)

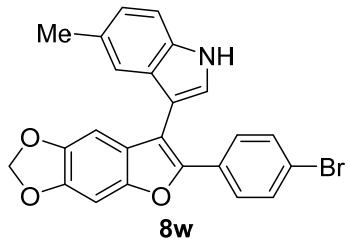


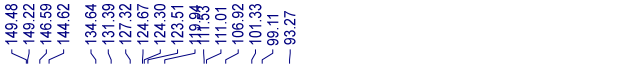




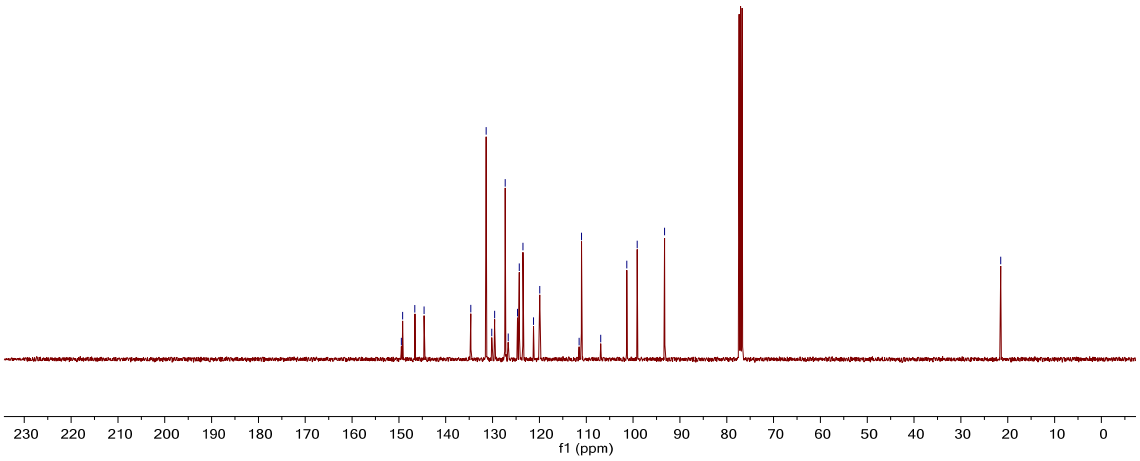
^{1}H NMR spectrum of 8w (400 MHz, $CDCl_3$)

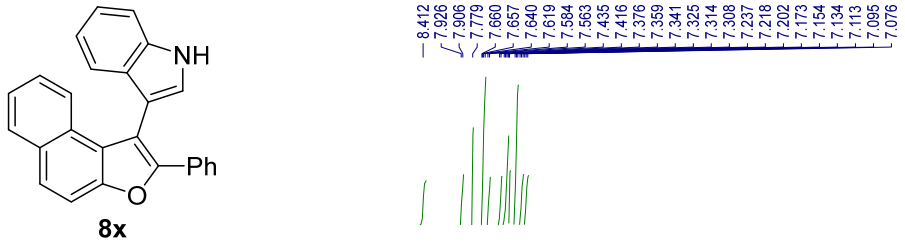




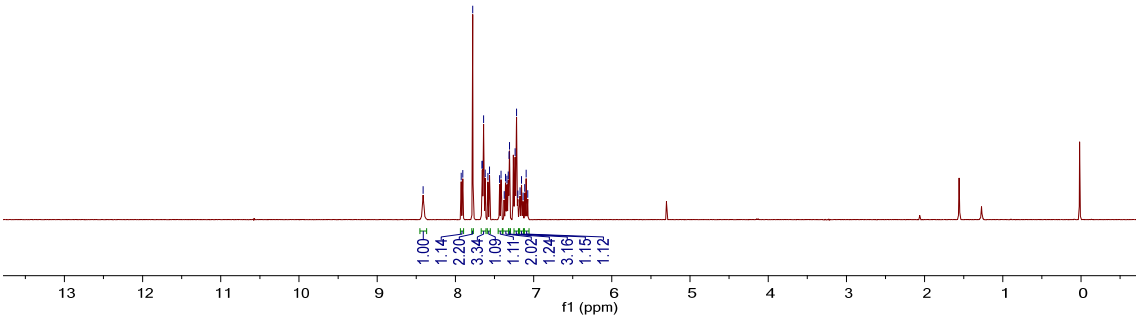


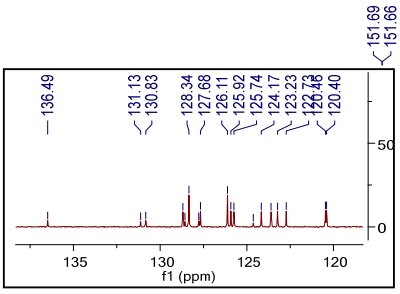
^{13}C NMR spectrum of 8w (100 MHz, $CDCl_3$)

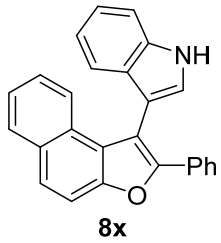




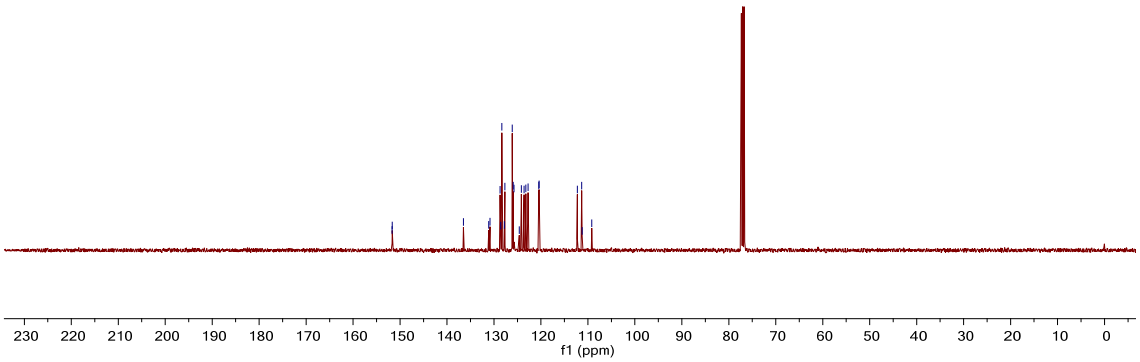
^{1}H NMR spectrum of 8x (400 MHz, $CDCl_3$)

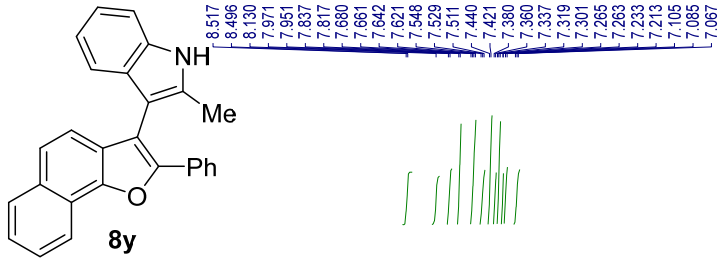




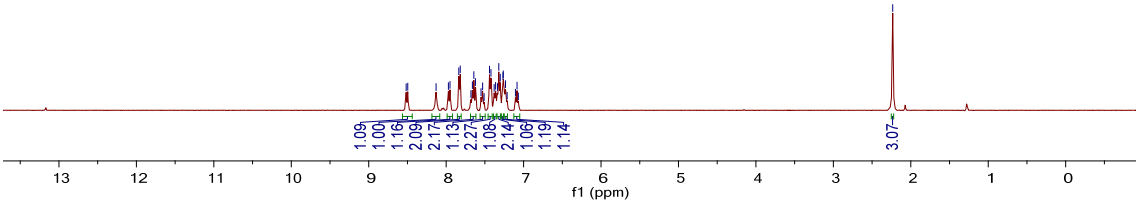


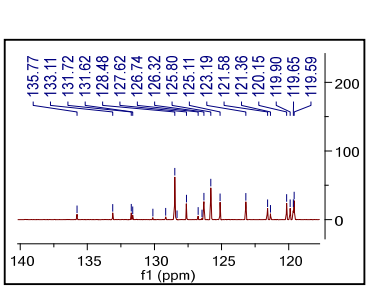
^{13}C NMR spectrum of 8x (100 MHz, $CDCl_3$)

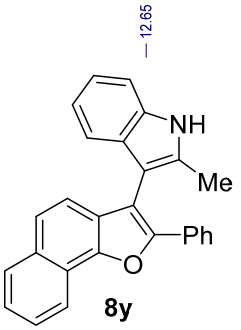




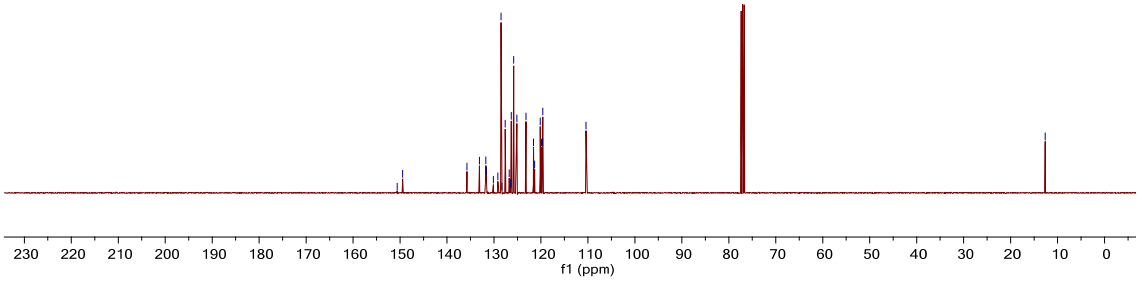
^{1}H NMR spectrum of 8y (400 MHz, $CDCl_3$)

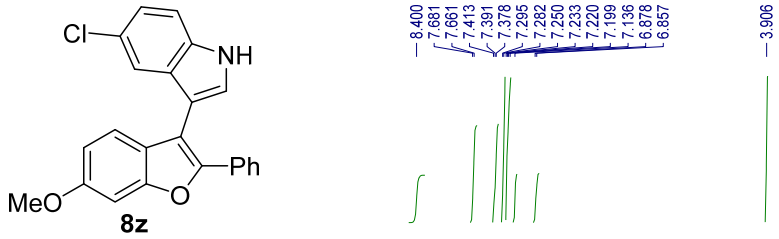




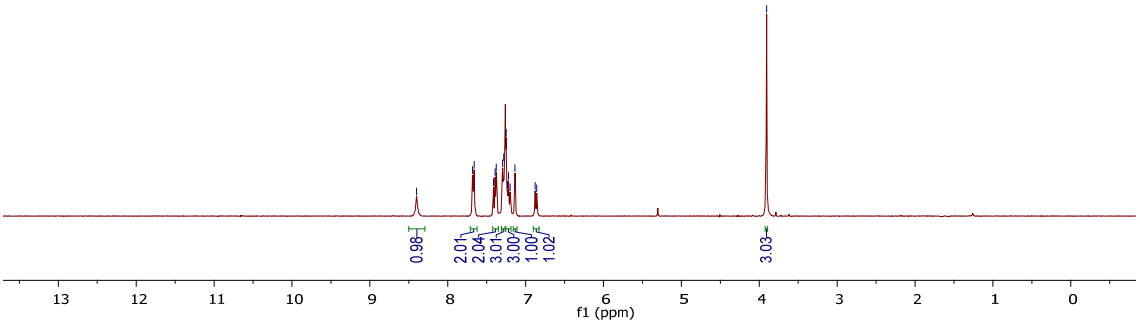


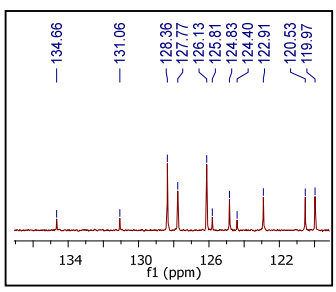
^{13}C NMR spectrum of 8y (100 MHz, $CDCl_3$)



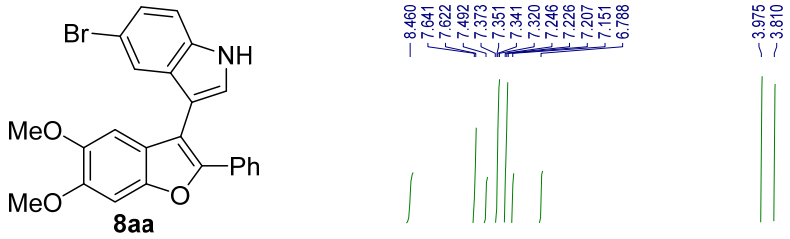


^{1}H NMR spectrum of 8z (400 MHz, $CDCl_3$)

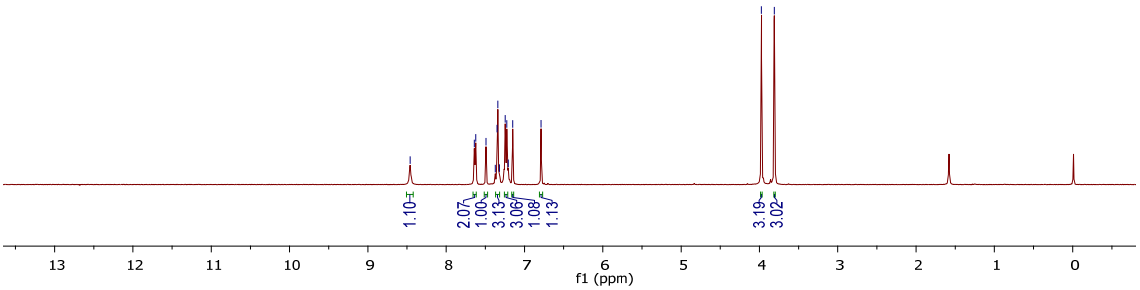


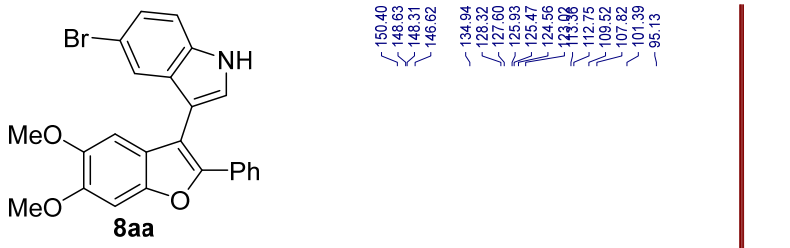


^{13}C NMR spectrum of 8z (100 MHz, $CDCl_3$)

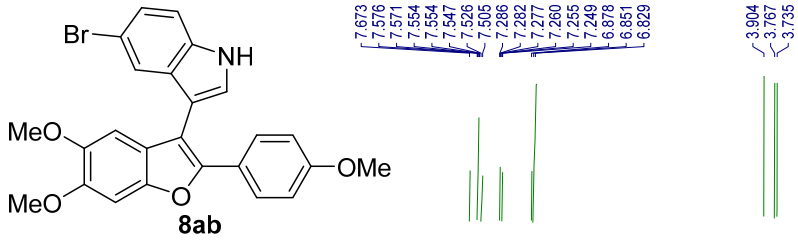


^{1}H NMR spectrum of 8aa (400 MHz, $CDCl_3$)

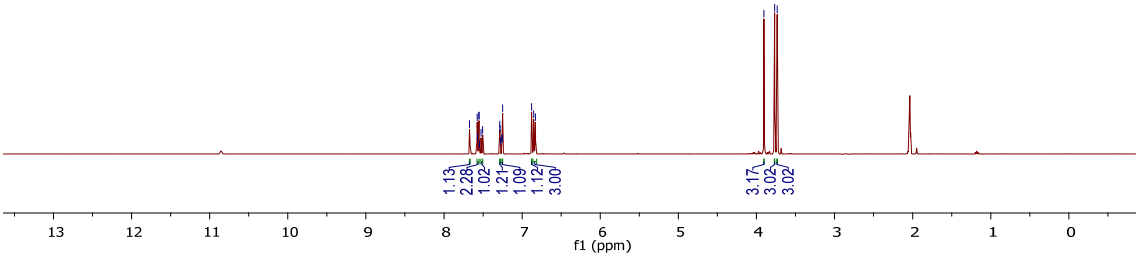


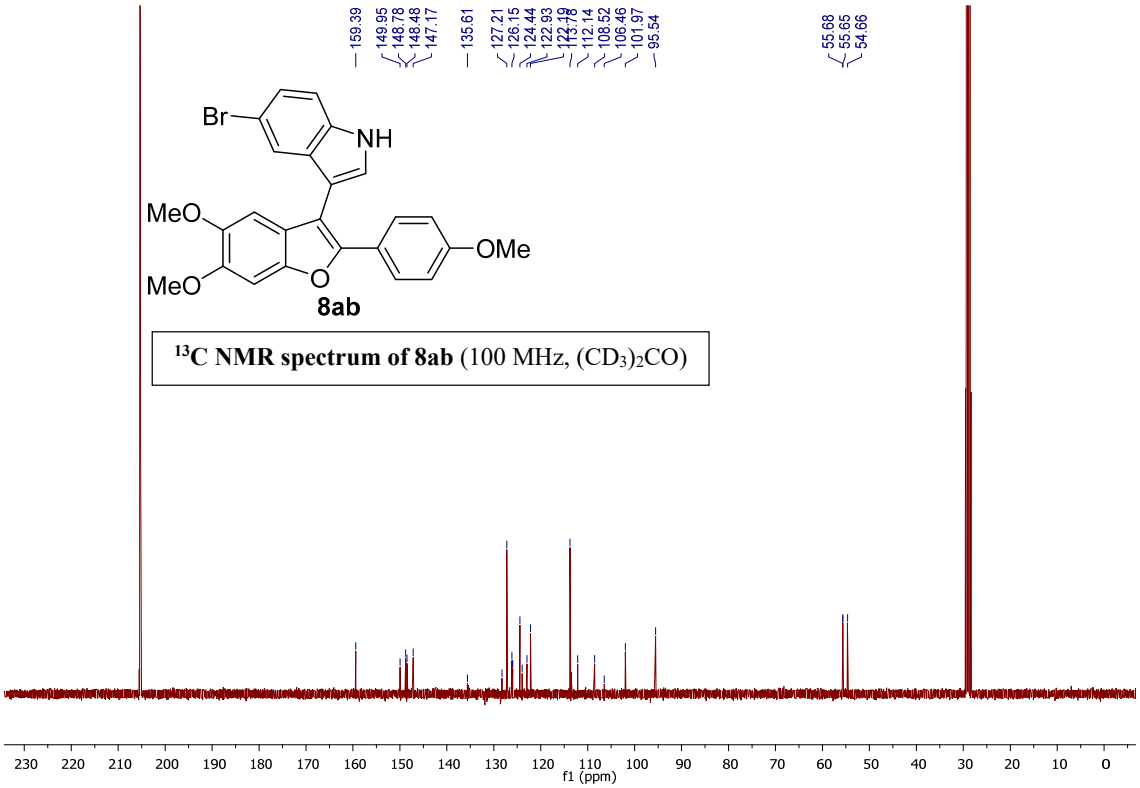


^{13}C NMR spectrum of 8aa (100 MHz, $CDCl_3$)

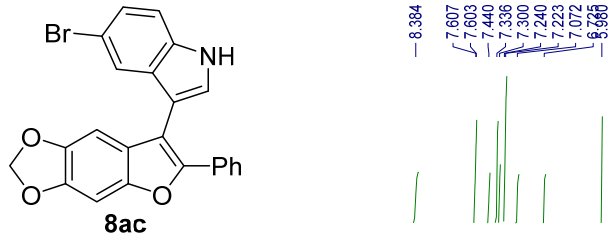


^{1}H NMR spectrum of 8ab (400 MHz, $(CD_3)_2CO$)

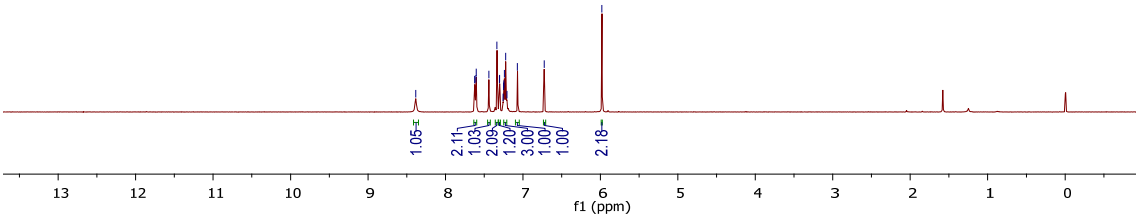


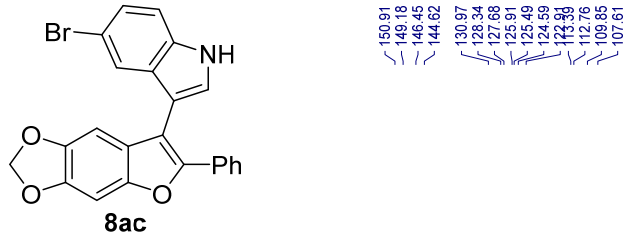


^{13}C NMR spectrum of 8ab (100 MHz, $(CD_3)_2CO$)

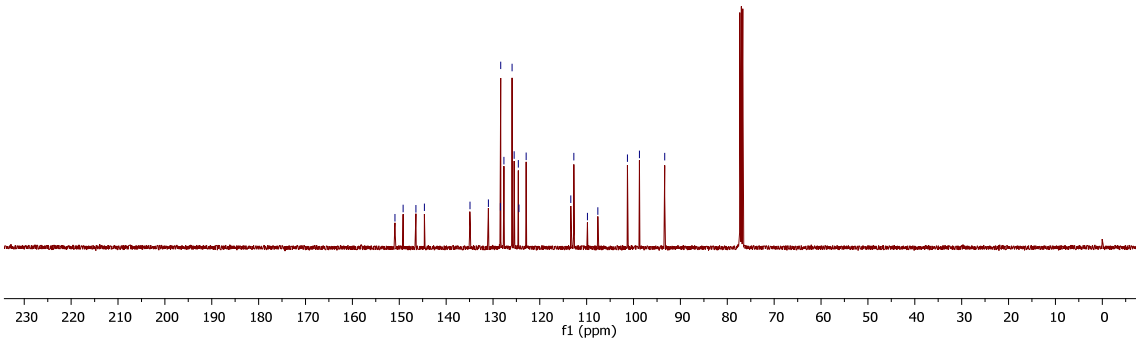


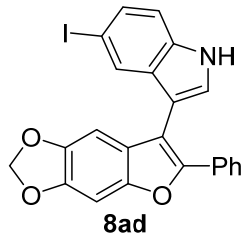
^{1}H NMR spectrum of 8ac (400 MHz, $CDCl_3$)

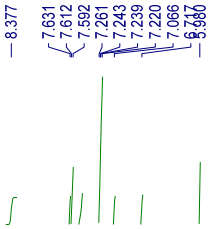




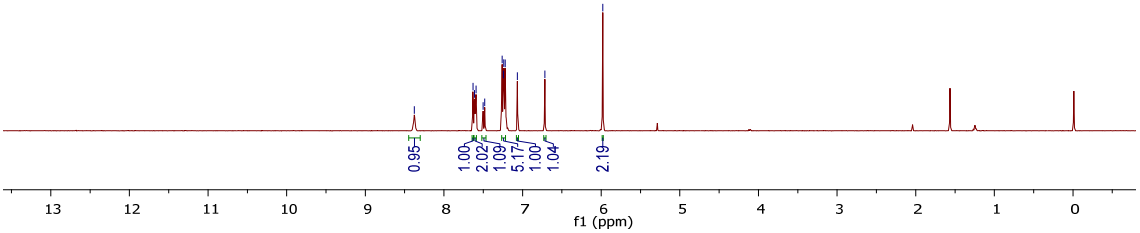
^{13}C NMR spectrum of 8ac (100 MHz, $CDCl_3$)

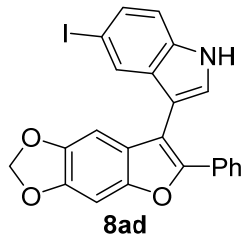




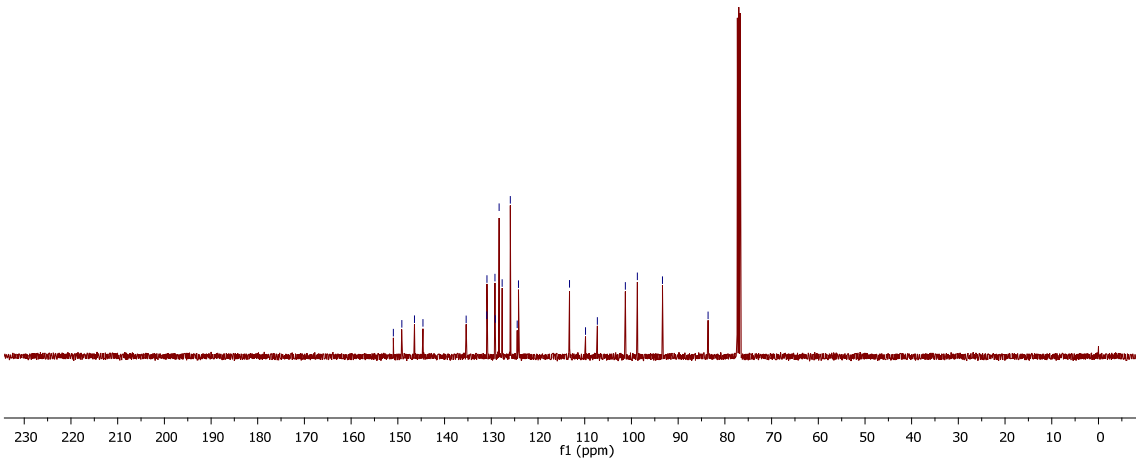


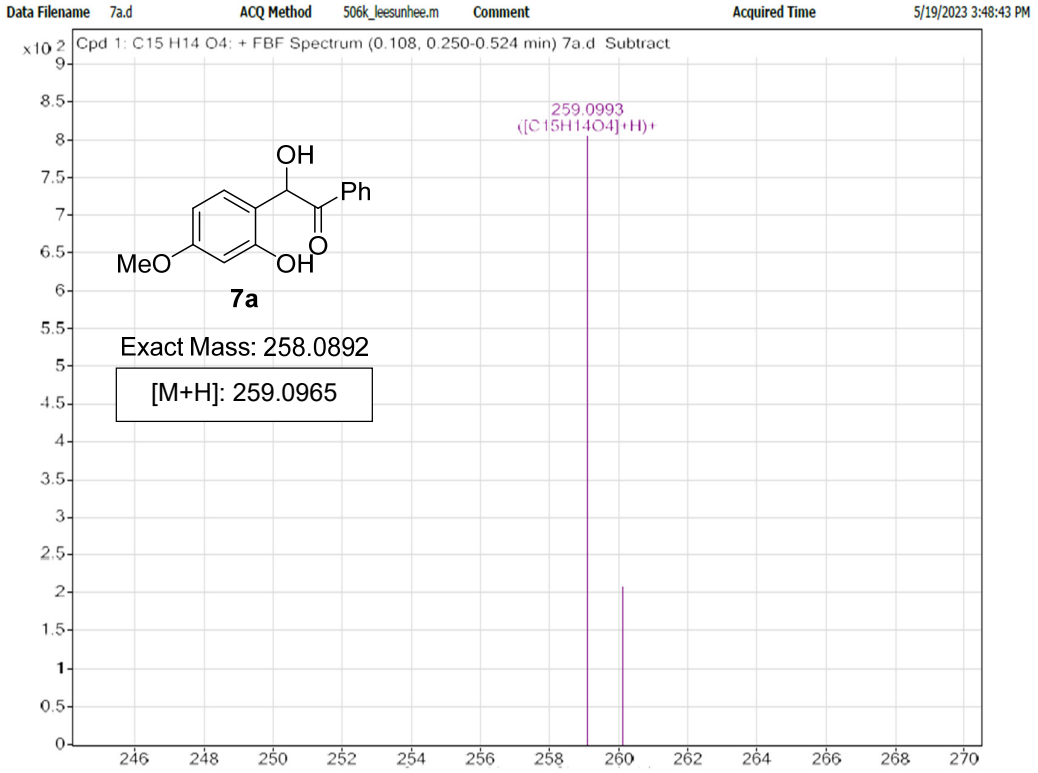
^{1}H NMR spectrum of 8ad (400 MHz, $CDCl_3$)

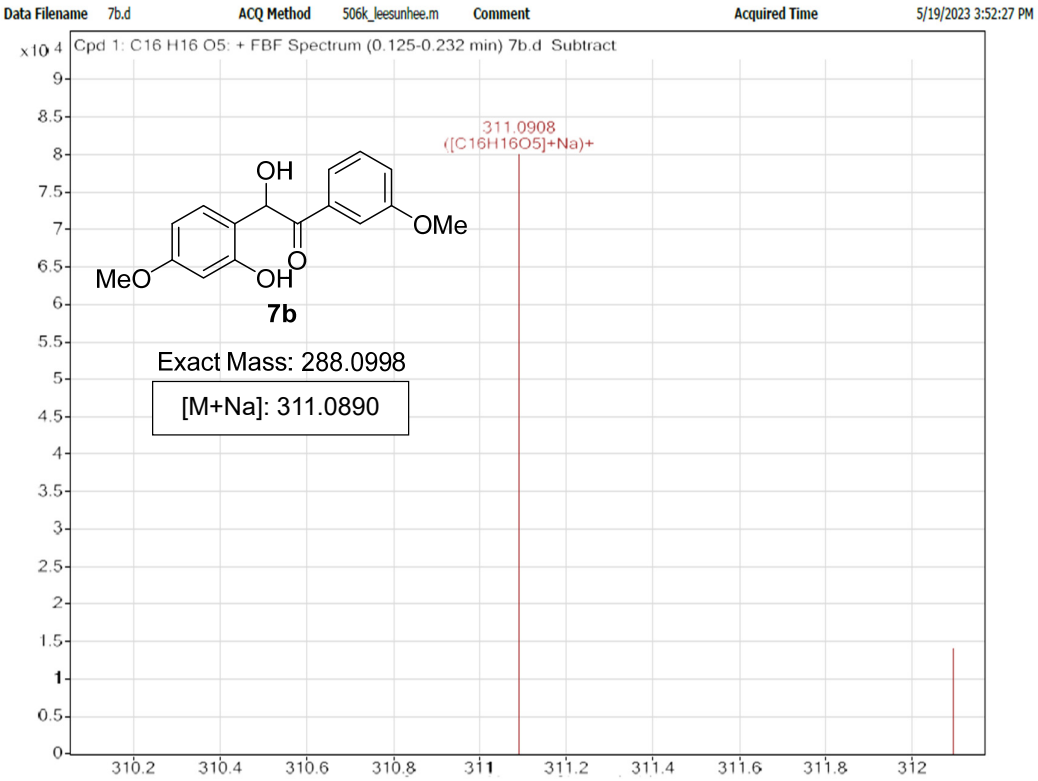


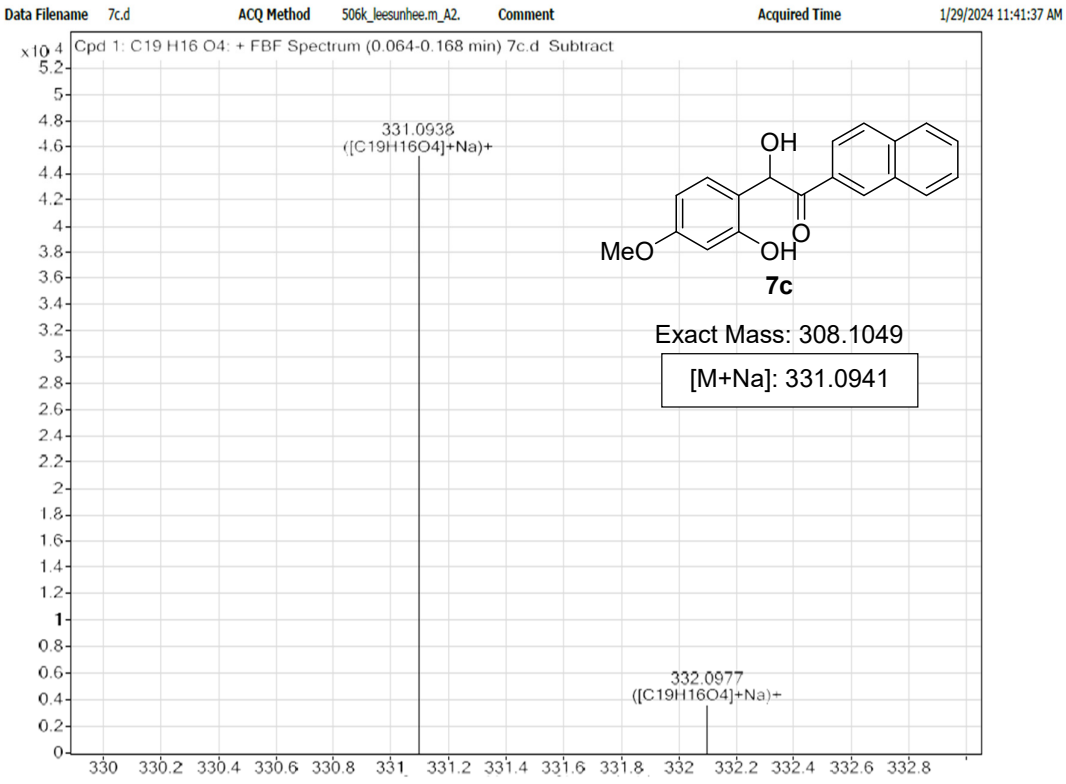


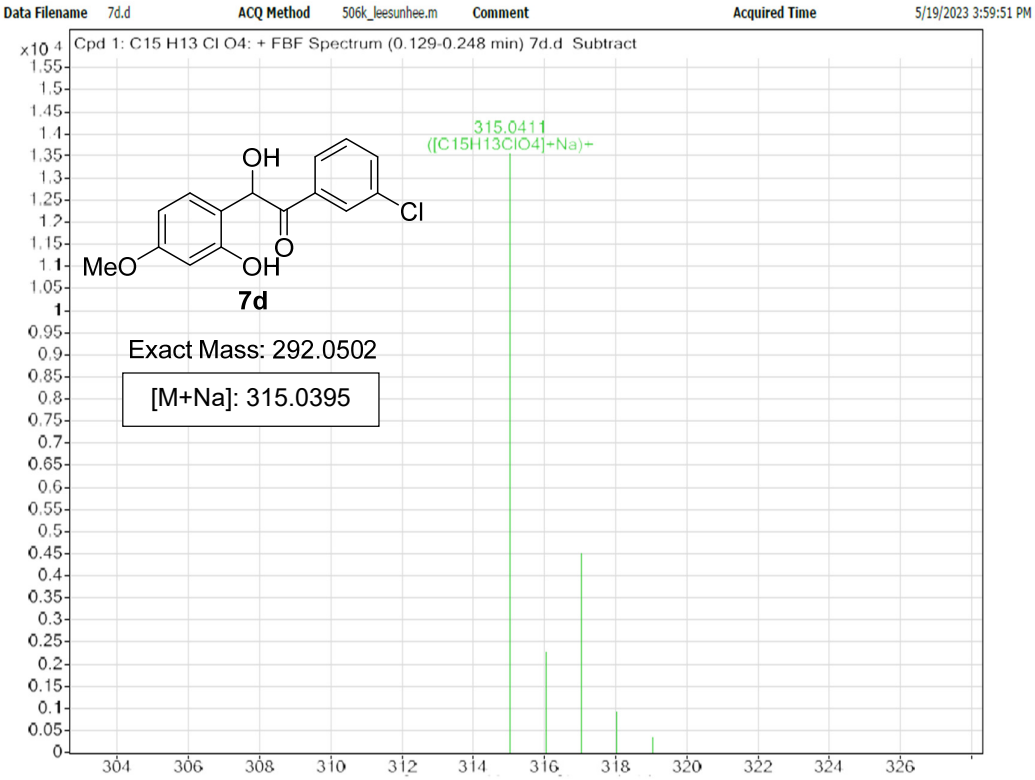
^{13}C NMR spectrum of 8ad (100 MHz, $CDCl_3$)

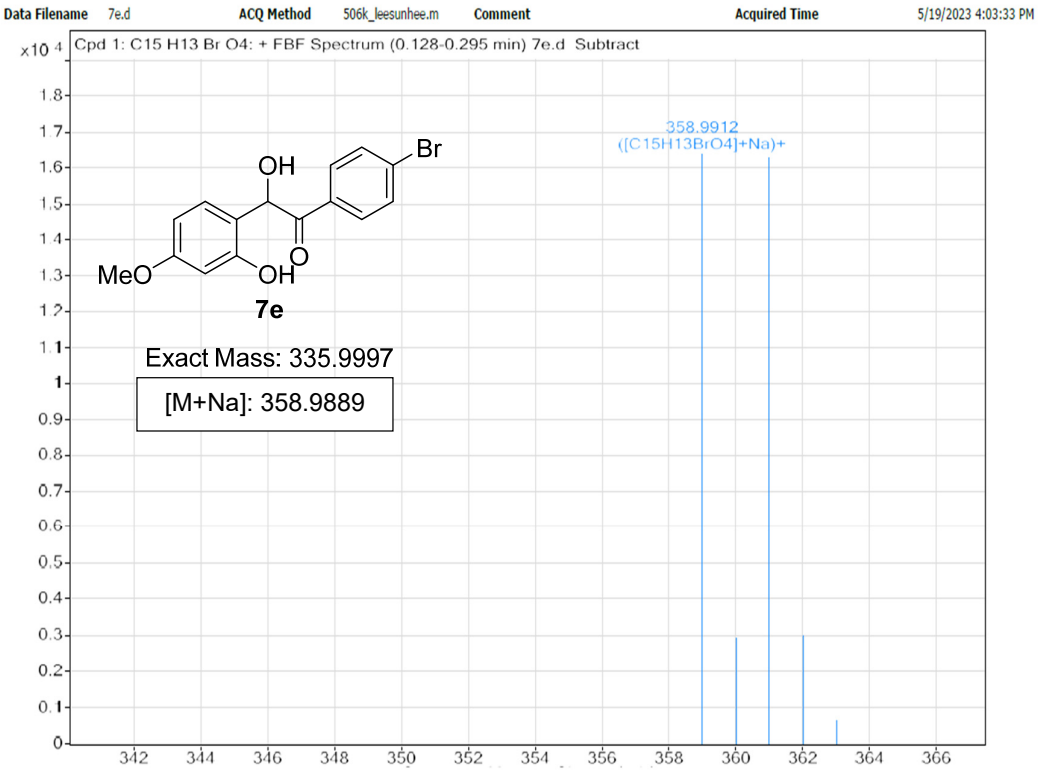


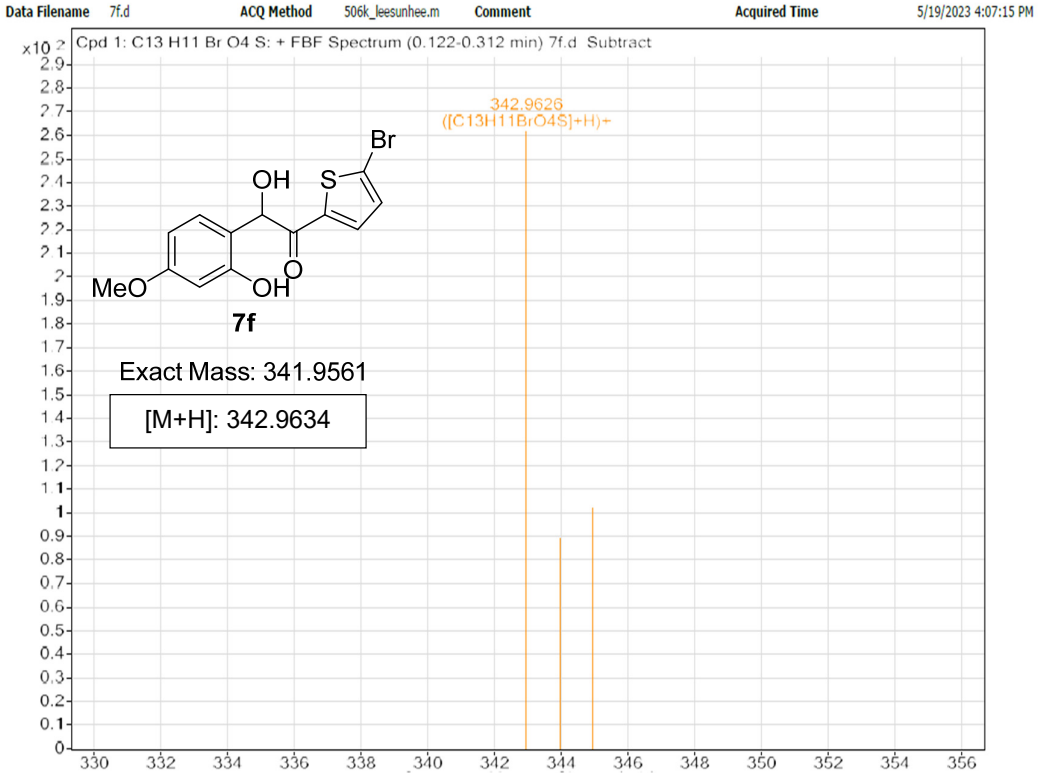

Data Filename 7a.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 3:48:43 PM
Cpd 1: C15 H14 O4: + FBF Spectrum (0.108, 0.250-0.524 min) 7a.d Subtract
x10 2
259.0993
([C15H14O4]+H)+
OH
Ph
O
MeO
OH
7a
Exact Mass: 258.0892
[M+H]: 259.0965

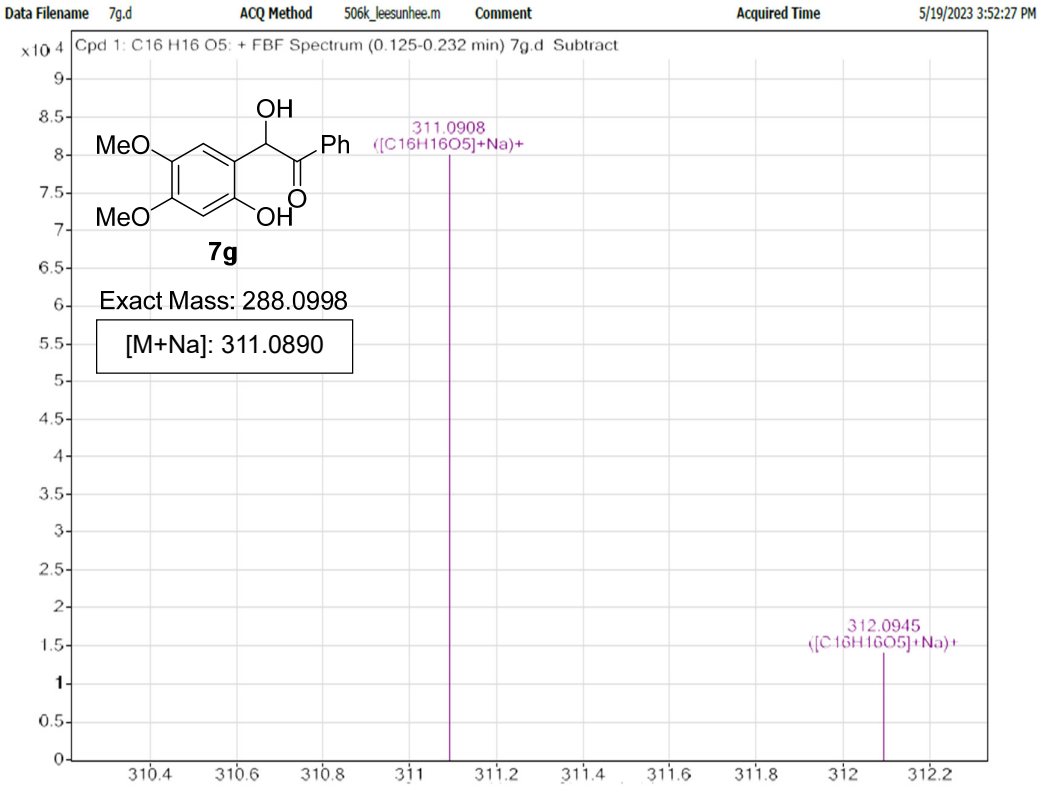

Data Filename 7b.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 3:52:27 PM
Cpd 1: C16 H16 O5: + FBF Spectrum (0.125-0.232 min) 7b.d Subtract
x10 4
311.0908
([C16H16O5]+Na)+
OH
OMe
O
MeO
OH
7b
Exact Mass: 288.0998
[M+Na]: 311.0890

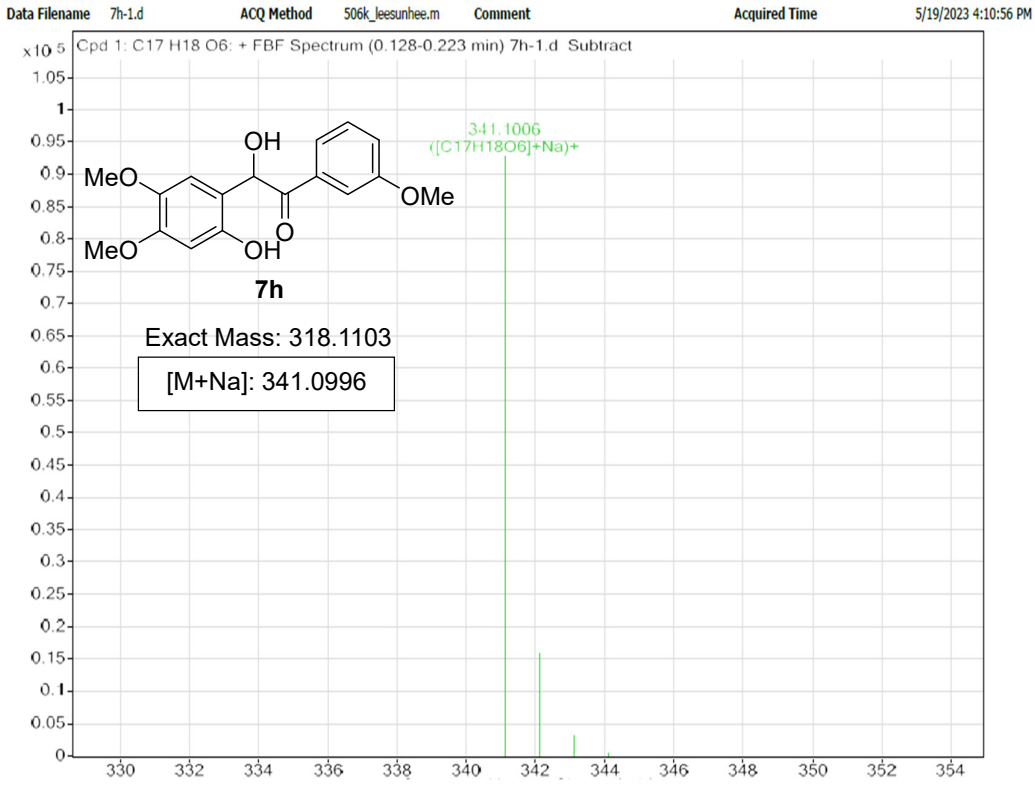

Data Filename 7c.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 11:41:37 AM
Cpd 1: C19 H16 O4: + FBF Spectrum (0.064-0.168 min) 7c.d Subtract
331.0938
([C19H16O4]+Na)+
332.0977
([C19H16O4]+Na)+
OH
MeO
OH
O
7c
Exact Mass: 308.1049
[M+Na]: 331.0941

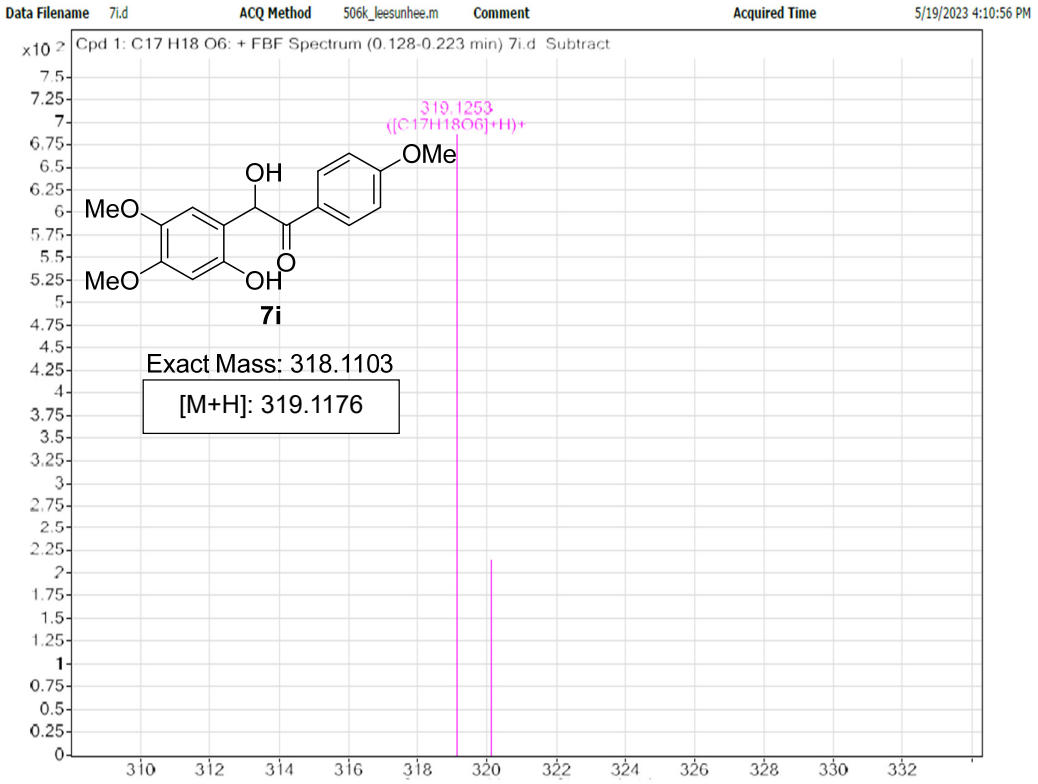

Data Filename 7d.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 3:59:51 PM
Cpd 1: C15 H13 Cl O4: + FBF Spectrum (0.129-0.248 min) 7d.d Subtract
315.0411
([C15H13ClO4]+Na)+
OH
Cl
O
MeO
OH
7d
Exact Mass: 292.0502
[M+Na]: 315.0395

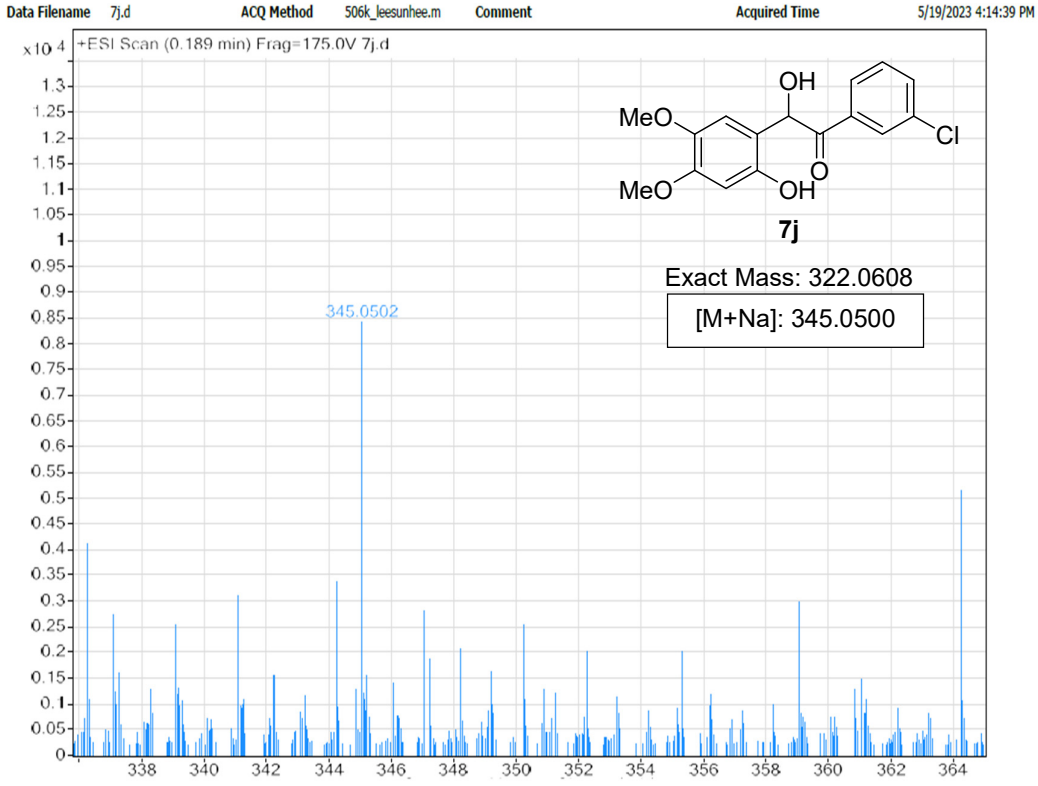

Data Filename 7e.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:03:33 PM
Cpd 1: C15 H13 Br O4: + FBF Spectrum (0.128-0.295 min) 7e.d Subtract
x10 4
358.9912
([C15H13BrO4]+Na)+
OH
Br
O
MeO
OH
7e
Exact Mass: 335.9997
[M+Na]: 358.9889

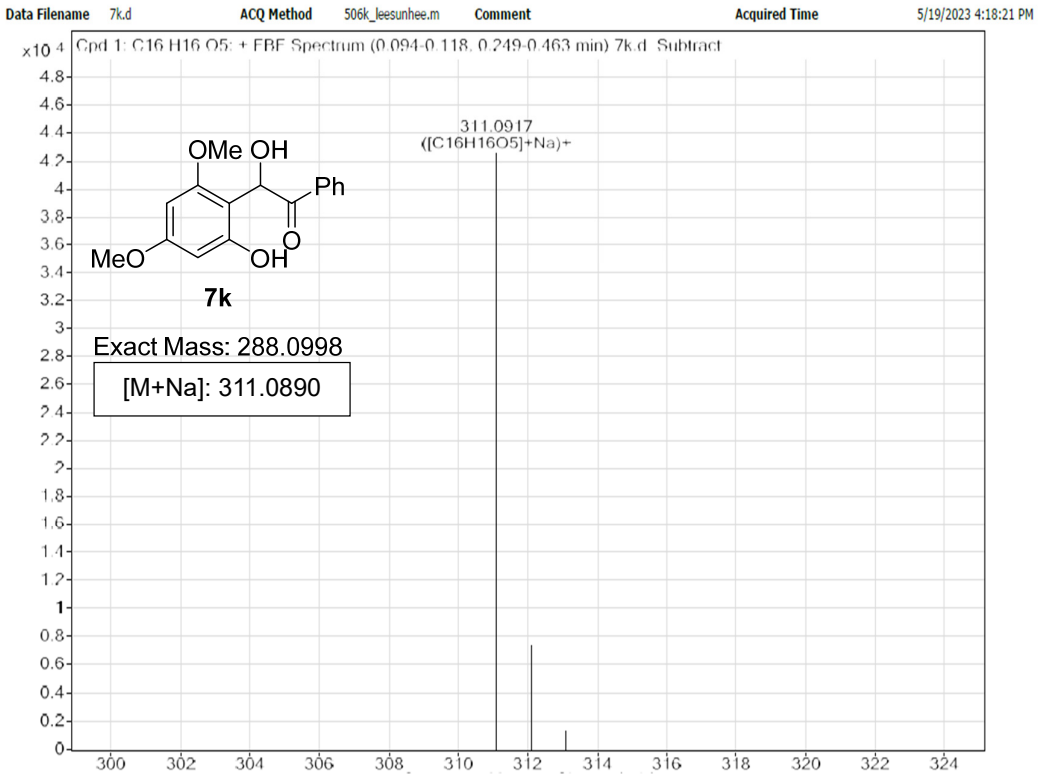

Data Filename 7f.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:07:15 PM
Cpd 1: C13 H11 Br O4 S: + FBF Spectrum (0.122-0.312 min) 7f.d Subtract
x10 2
342.9626
([C13H11BrO4S]+H)+
Br
OH
S
O
MeO
OH
7f
Exact Mass: 341.9561
[M+H]: 342.9634

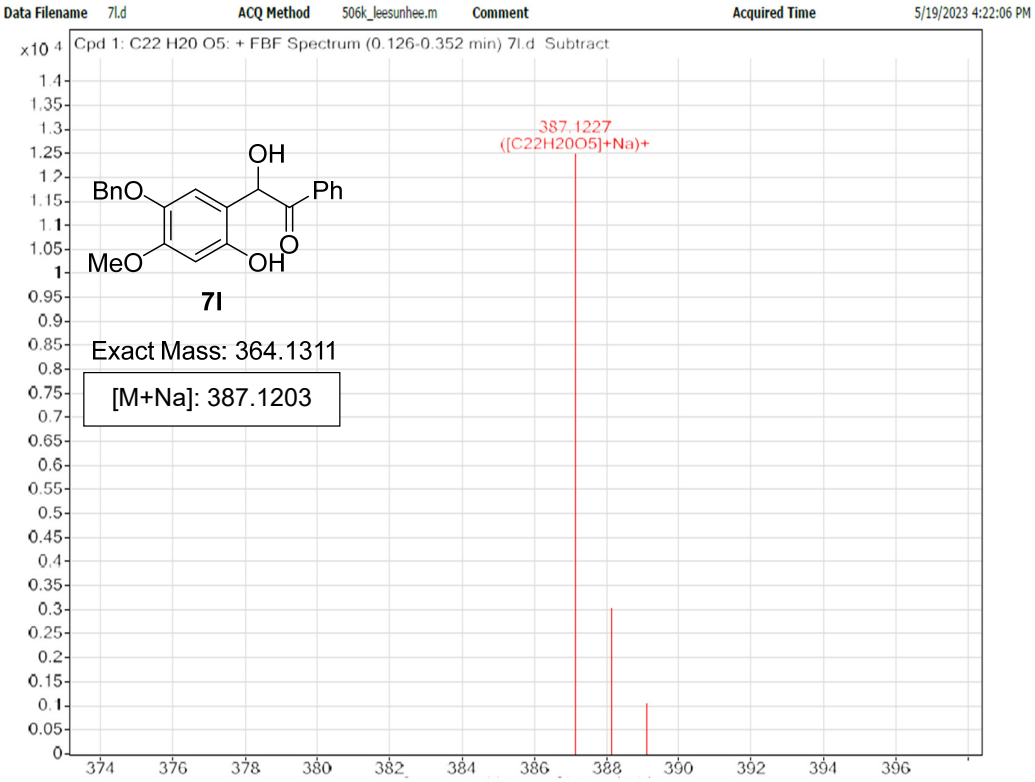

Data Filename 7g.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 3:52:27 PM
Cpd 1: C16 H16 O5: + FBF Spectrum (0.125-0.232 min) 7g.d Subtract
x10 4
311.0908
([C16H16O5]+Na)+
312.0945
([C16H16O5]+Na)+
OH
MeO
Ph
O
MeO
OH
7g
Exact Mass: 288.0998
[M+Na]: 311.0890

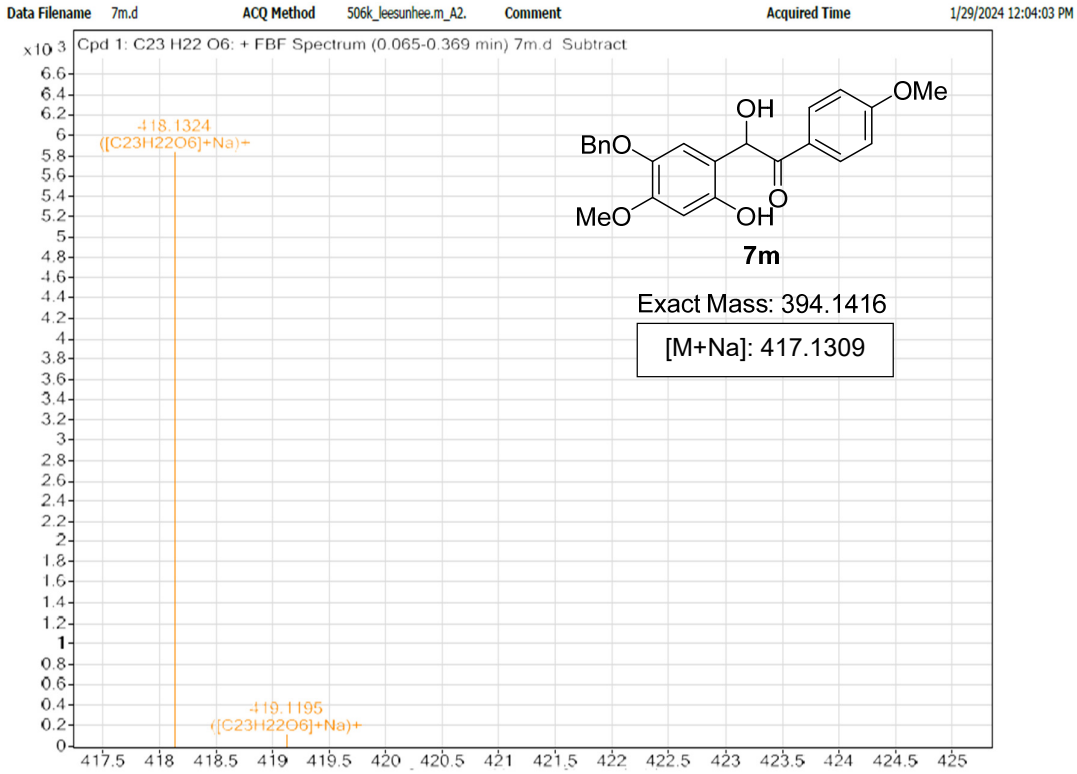

Data Filename 7h-1.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:10:56 PM
Cpd 1: C17 H18 O6: + FBF Spectrum (0.128-0.223 min) 7h-1.d Subtract
x10 5
341.1006
([C17H18O6]+Na)+
OH
MeO
OMe
O
MeO
OH
7h
Exact Mass: 318.1103
[M+Na]: 341.0996

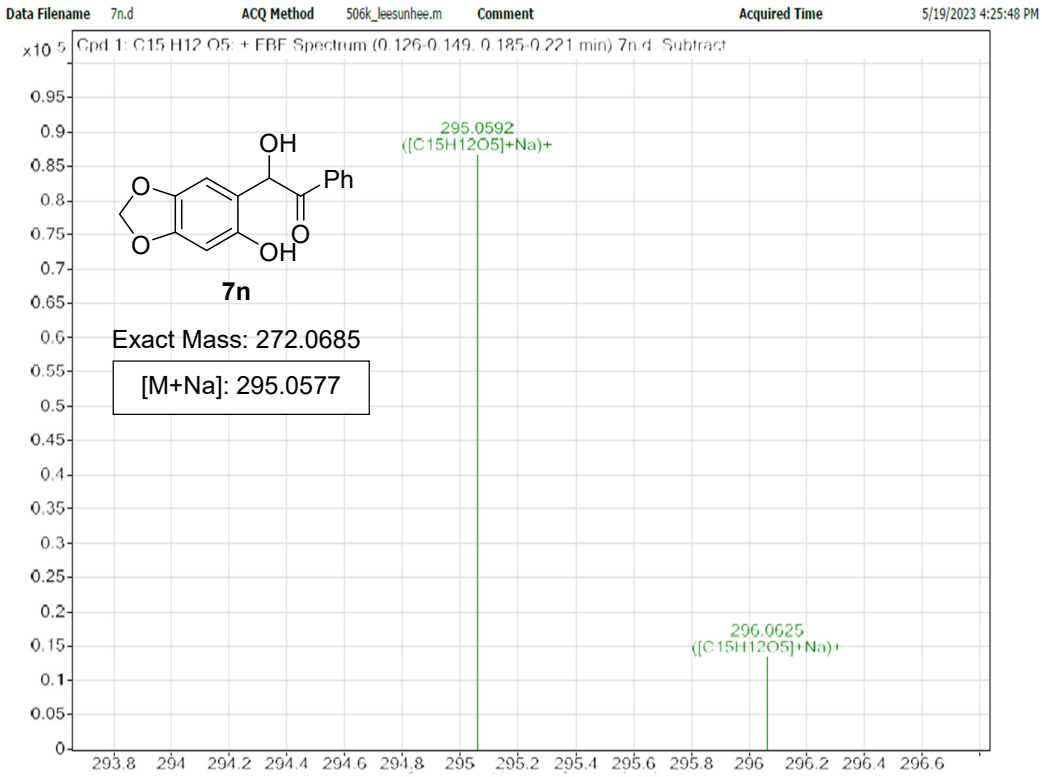

Data Filename 7i.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:10:56 PM
Cpd 1: C17 H18 O6: + FBF Spectrum (0.128-0.223 min) 7i.d Subtract
x10 2
319.1253
([C17H18O6]+H)+
OMe
OH
MeO
MeO
OH
O
7i
Exact Mass: 318.1103
[M+H]: 319.1176

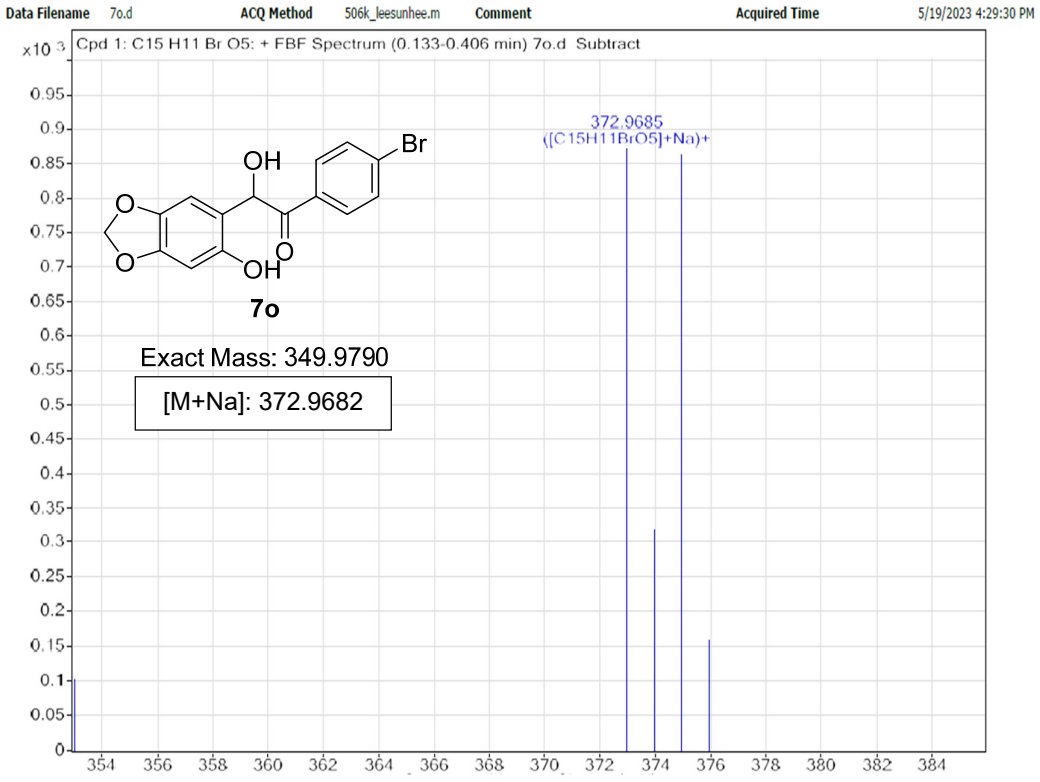

Data Filename 7j.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:14:39 PM
x10 4
+ESI Scan (0.189 min) Frag=175.0V 7j.d
345.0502
OH
MeO
MeO
OH
Cl
O
7j
Exact Mass: 322.0608
[M+Na]: 345.0500

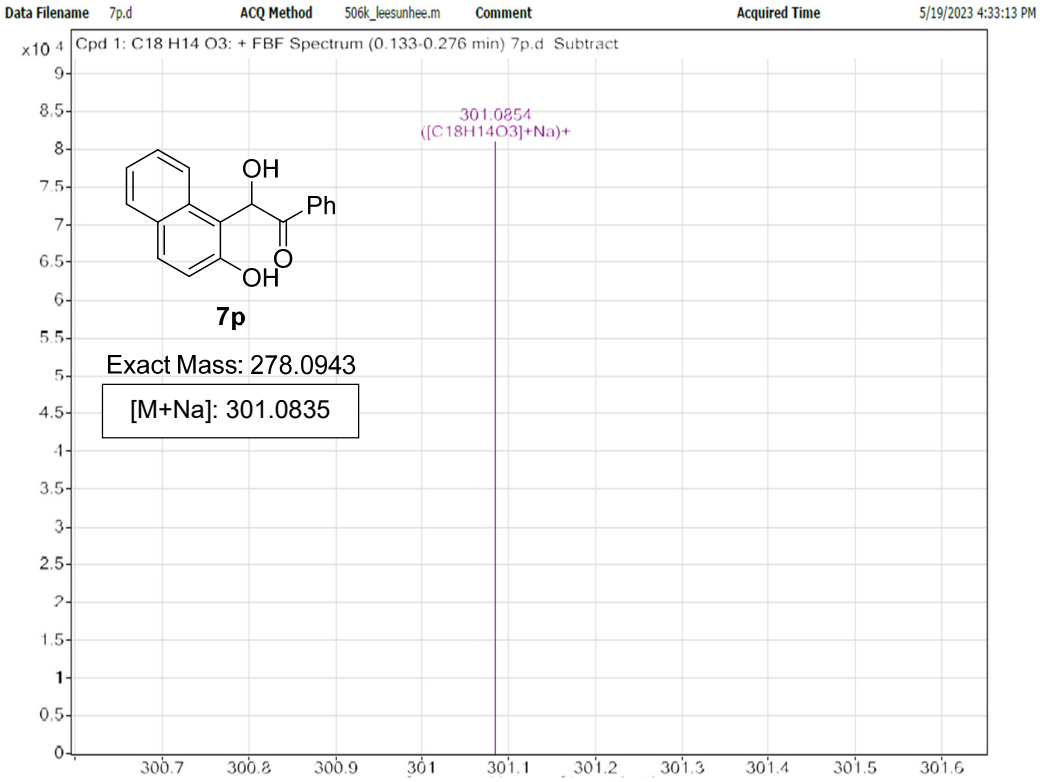

Data Filename 7k.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:18:21 PM
Cpd 1: C16 H16 O5: + FBF Spectrum (0.094-0.118, 0.249-0.463 min) 7k.d Subtract
x10 4
311.0917
([C16H16O5]+Na)+
OMe OH
Ph
MeO
OH
O
7k
Exact Mass: 288.0998
[M+Na]: 311.0890

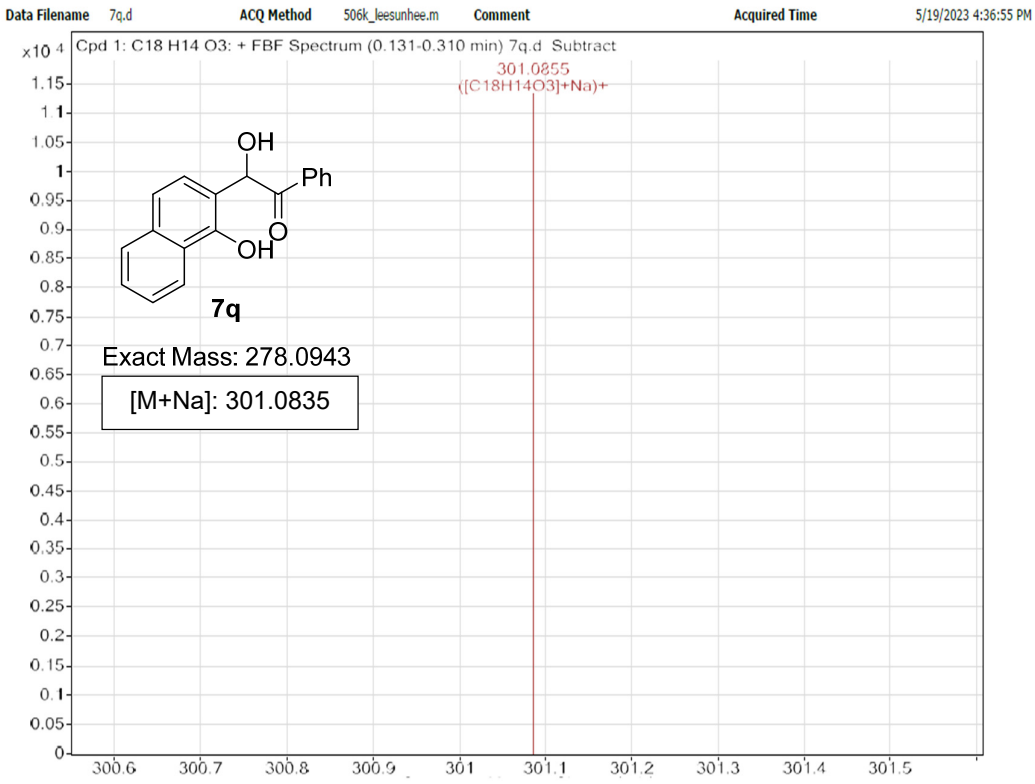

Data Filename 7l.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:22:06 PM
Cpd 1: C22 H20 O5: + FBF Spectrum (0.126-0.352 min) 7l.d Subtract
x10 4
387.1227
([C22H20O5]+Na)+
OH
BnO
Ph
MeO
OH
O
7l
Exact Mass: 364.1311
[M+Na]: 387.1203

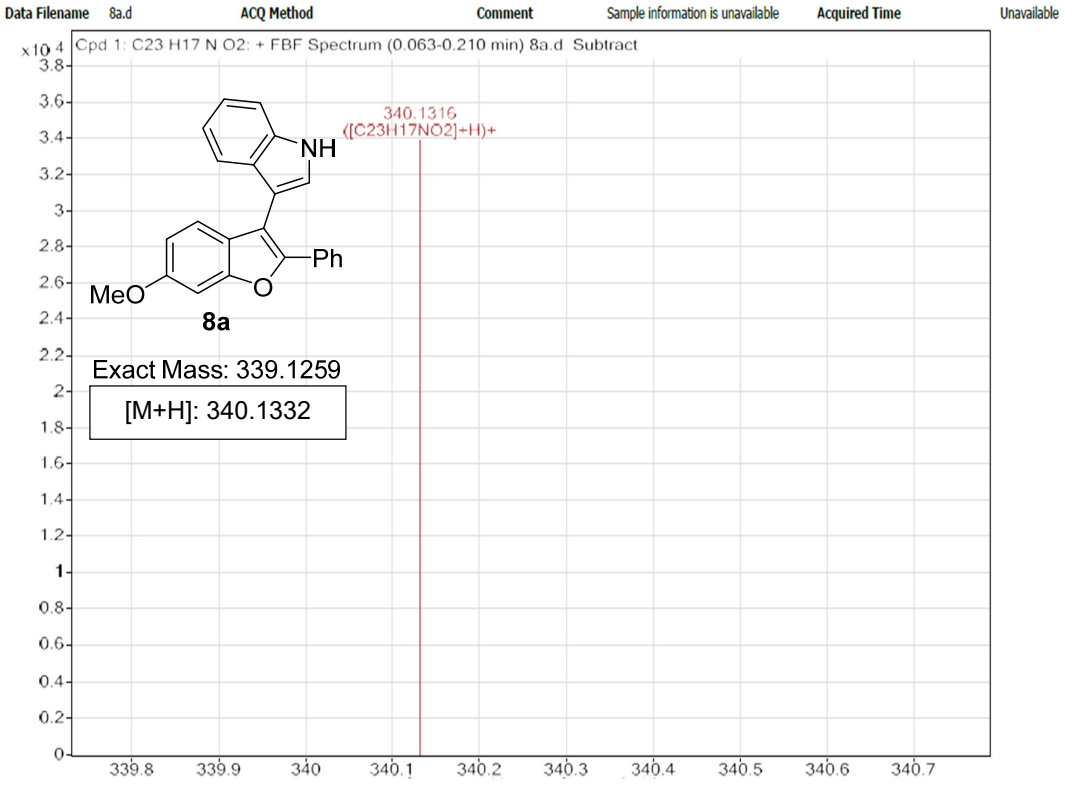

Data Filename 7m.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 12:04:03 PM
Cpd 1: C23 H22 O6: + FBF Spectrum (0.065-0.369 min) 7m.d Subtract
x10 3
418.1324
([C23H22O6]+Na)+
419.1195
([C23H22O6]+Na)+
OMe
OH
BnO
MeO
OH
O
7m
Exact Mass: 394.1416
[M+Na]: 417.1309

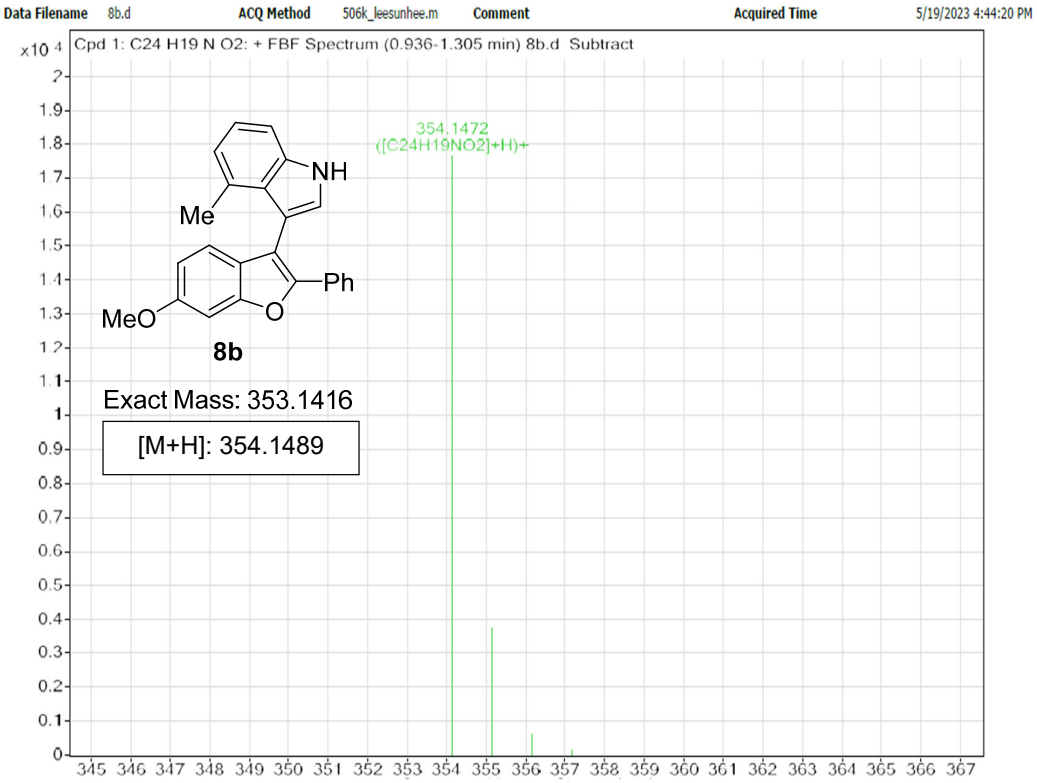

Data Filename 7n.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:25:48 PM
Cpd 1: C15 H12 O5: + FBF Spectrum (0.126-0.149, 0.185-0.221 min) 7n.d Subtract
x10 5
295.0592
([C15H12O5]+Na)+
296.0625
([C15H12O5]+Na)+
OH
Ph
O
O
O
OH
7n
Exact Mass: 272.0685
[M+Na]: 295.0577

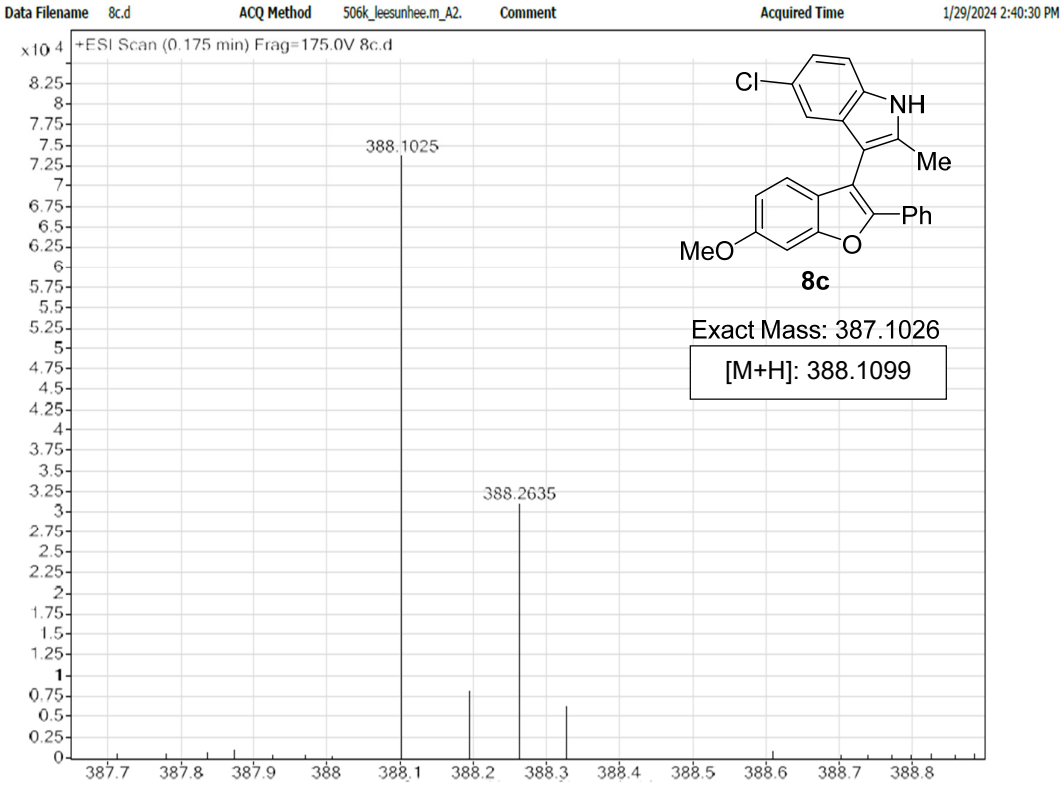

Data Filename 7o.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:29:30 PM
Cpd 1: C15 H11 Br O5: + FBF Spectrum (0.133-0.406 min) 7o.d Subtract
x10 3
372.9685
([C15H11BrO5]+Na)+
OH
Br
O
O
O
OH
7o
Exact Mass: 349.9790
[M+Na]: 372.9682

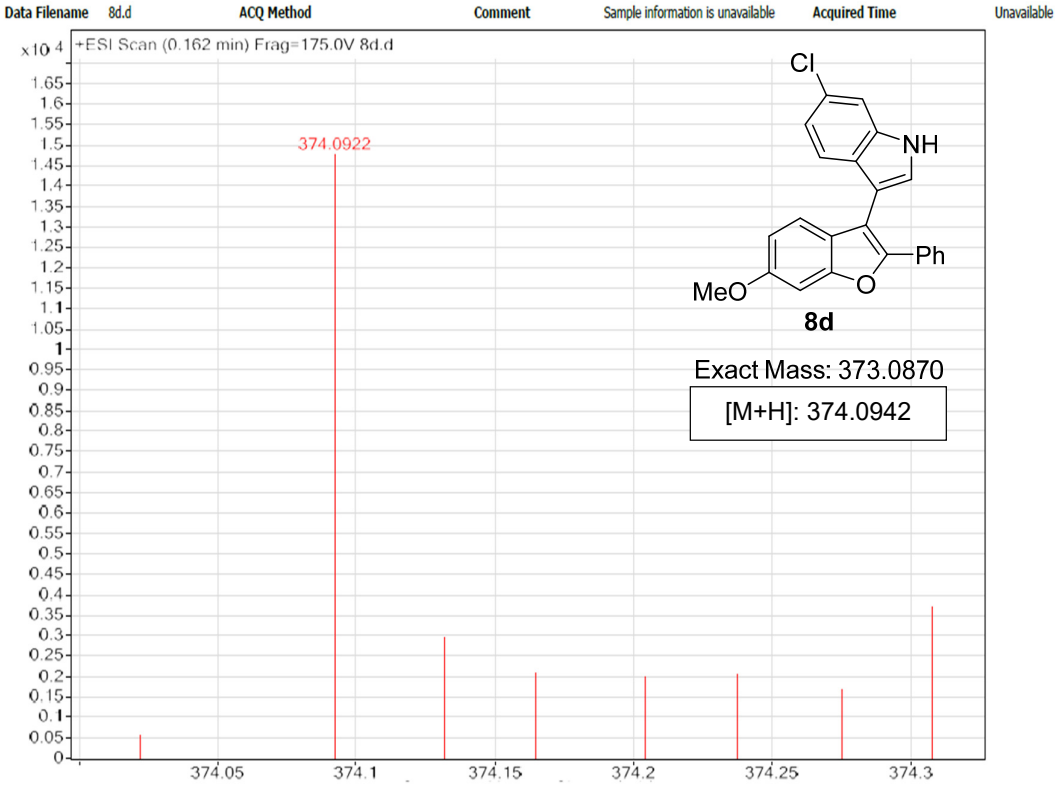

Data Filename 7p.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:33:13 PM
Cpd 1: C18 H14 O3: + FBF Spectrum (0.133-0.276 min) 7p.d Subtract
x10 4
301.0854
([C18H14O3]+Na)+
OH
Ph
O
OH
7p
Exact Mass: 278.0943
[M+Na]: 301.0835

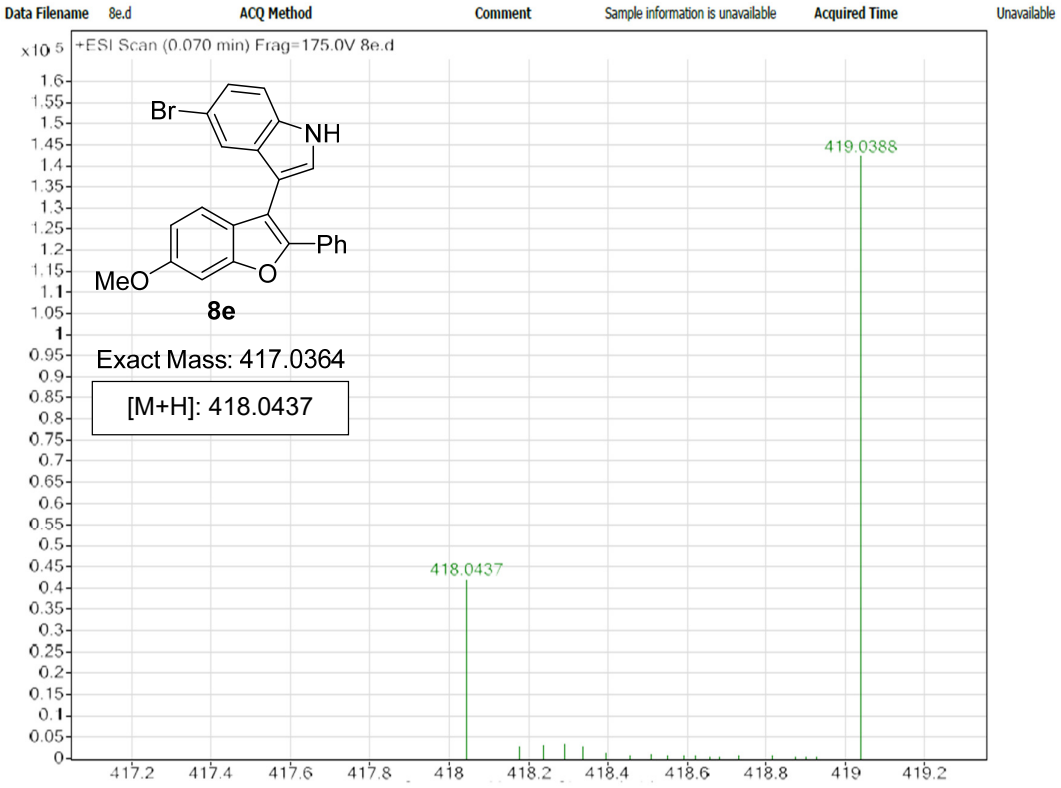

Data Filename 7q.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:36:55 PM
Cpd 1: C18 H14 O3: + FBF Spectrum (0.131-0.310 min) 7q.d Subtract
301.0855
([C18H14O3]+Na)+
OH
Ph
O
OH
7q
Exact Mass: 278.0943
[M+Na]: 301.0835

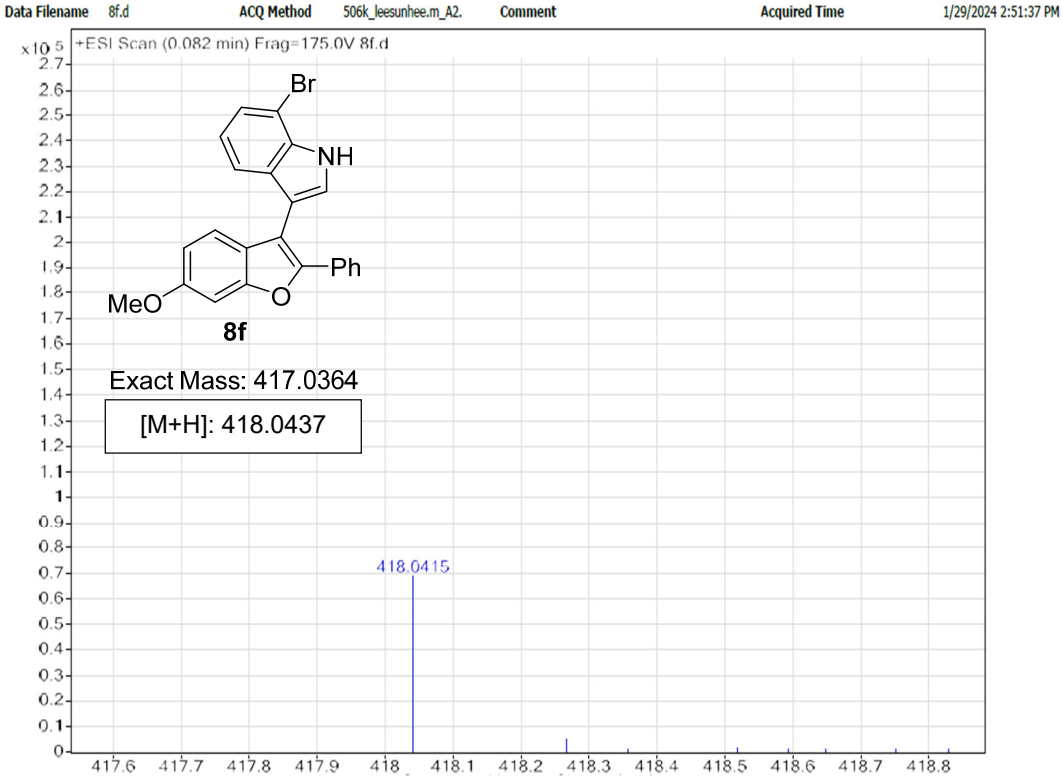

Data Filename 8a.d
ACQ Method
Comment Sample information is unavailable
Acquired Time Unavailable
Cpd 1: C23 H17 N O2: + FBF Spectrum (0.063-0.210 min) 8a.d Subtract
x10 4
340.1316
([C23H17NO2]+H)+
NH
Ph
MeO
O
8a
Exact Mass: 339.1259
[M+H]: 340.1332

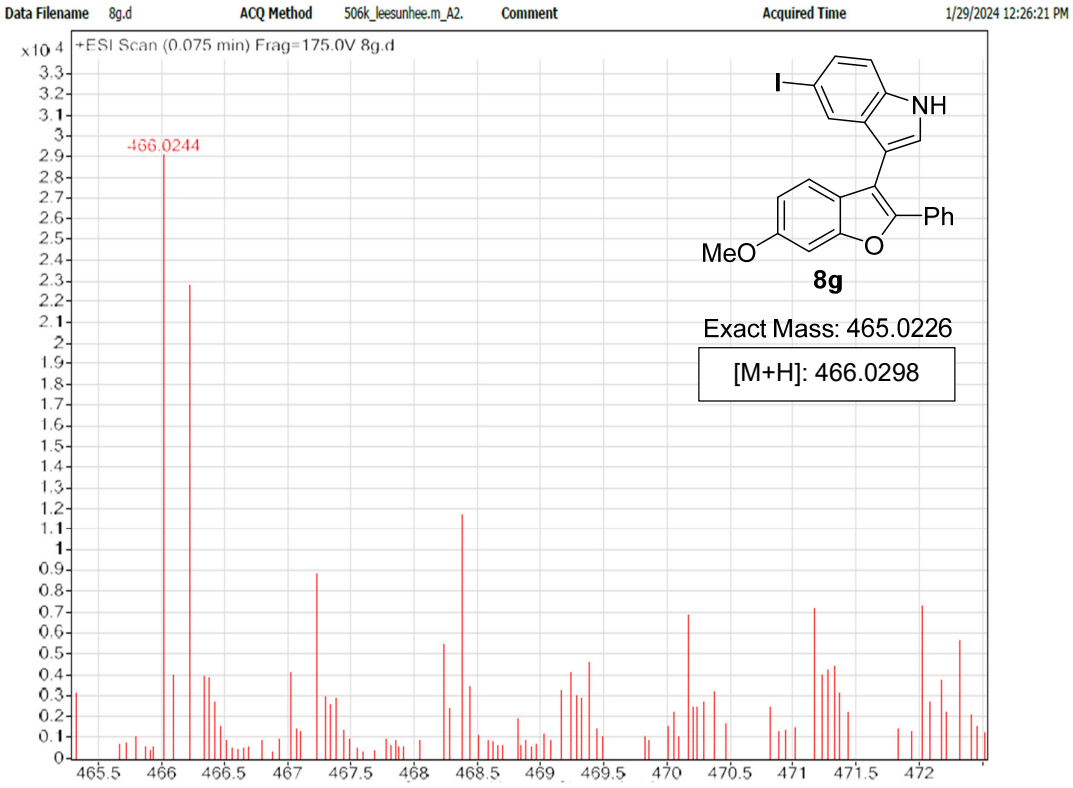

Data Filename 8b.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 4:44:20 PM
Cpd 1: C24 H19 N O2: + FBF Spectrum (0.936-1.305 min) 8b.d Subtract
x10 4
354.1472
([C24H19NO2]+H)+
NH
Me
Ph
MeO
O
8b
Exact Mass: 353.1416
[M+H]: 354.1489

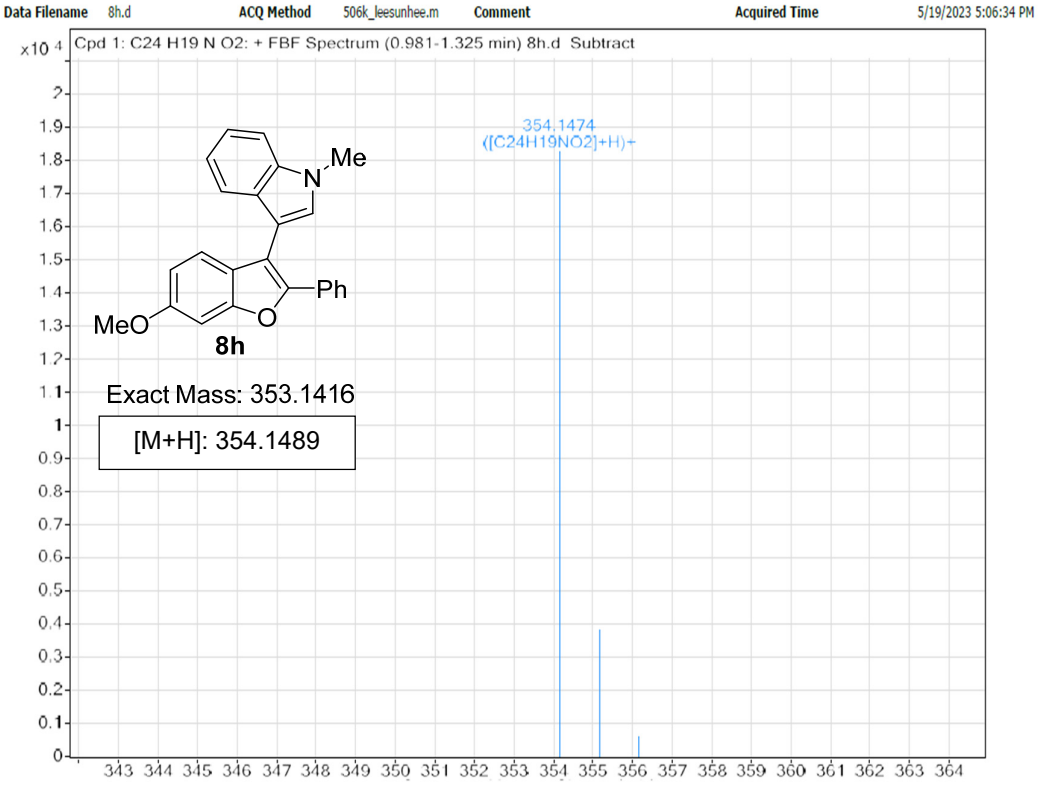

Data Filename 8c.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 2:40:30 PM
+ESI Scan (0.175 min) Frag=175.0V 8c.d
388.1025
388.2635
Cl
NH
Me
Ph
MeO
O
8c
Exact Mass: 387.1026
[M+H]: 388.1099

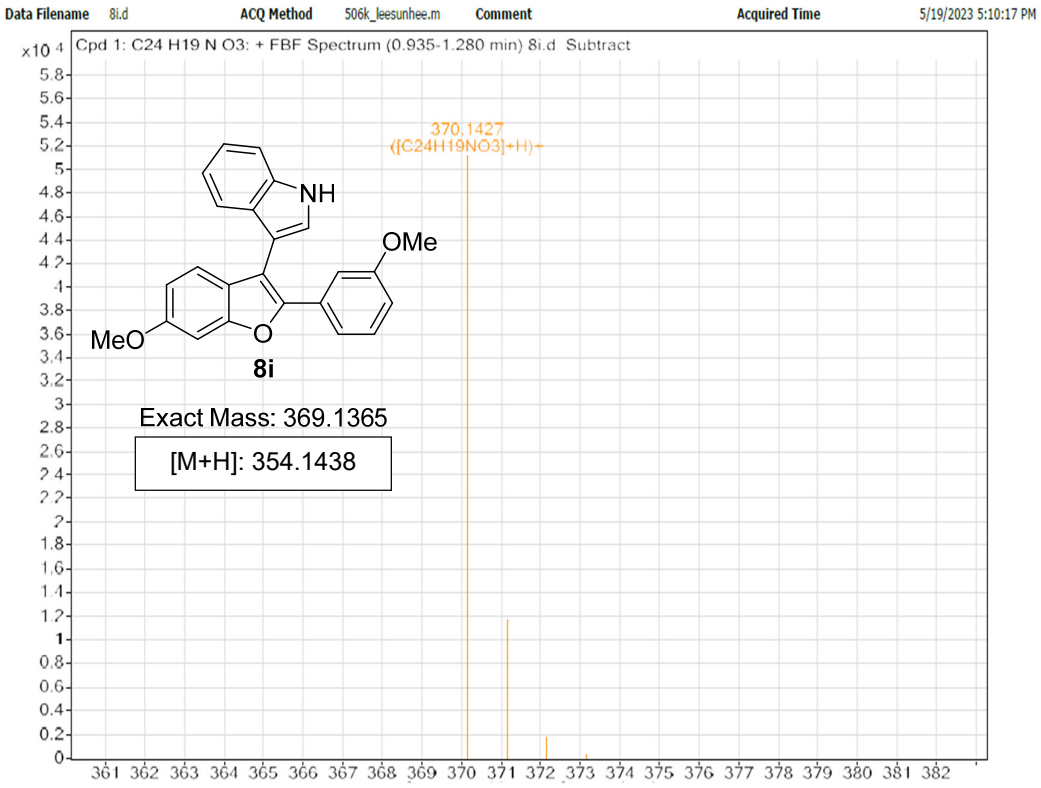

Data Filename 8d.d
ACQ Method
Comment
Sample information is unavailable
Acquired Time
Unavailable
+ESI Scan (0.162 min) Frag=175.0V 8d.d
374.0922
Cl
NH
Ph
MeO
O
8d
Exact Mass: 373.0870
[M+H]: 374.0942

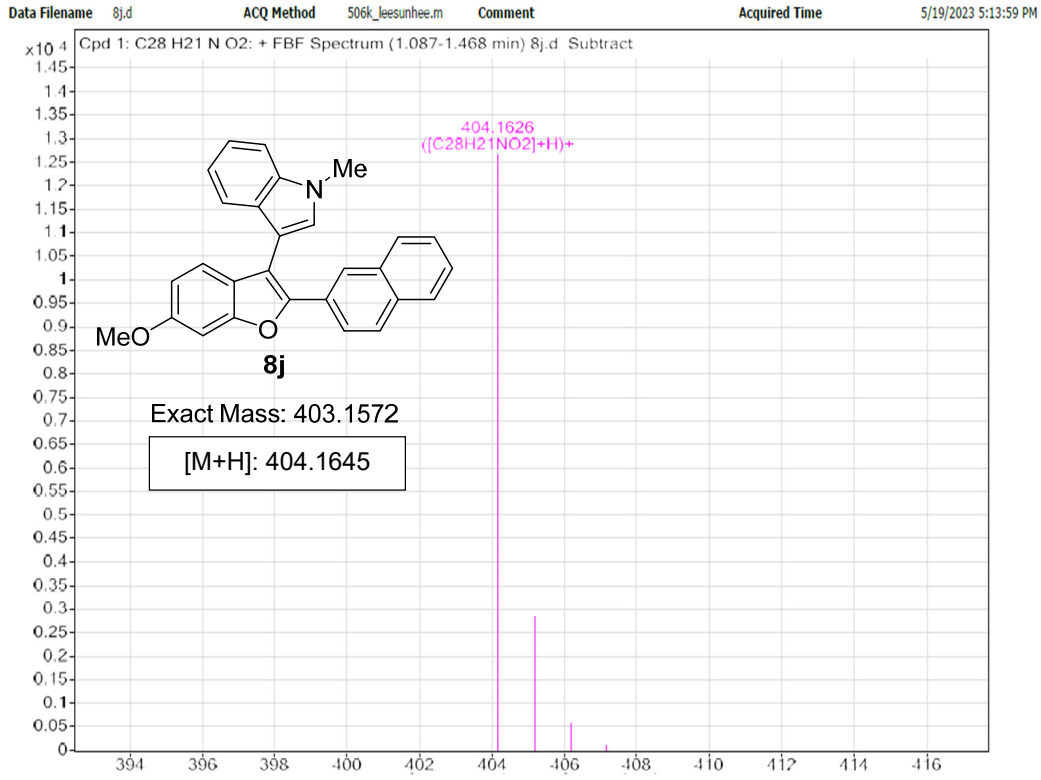

Data Filename 8e.d
ACQ Method
Comment
Sample information is unavailable
Acquired Time
Unavailable
+ESI Scan (0.070 min) Frag=175.0V 8e.d
x10 5
Br
NH
Ph
MeO
O
8e
Exact Mass: 417.0364
[M+H]: 418.0437
419.0388
418.0437
417.2
417.4
417.6
417.8
418
418.2
418.4
418.6
418.8
419
419.2

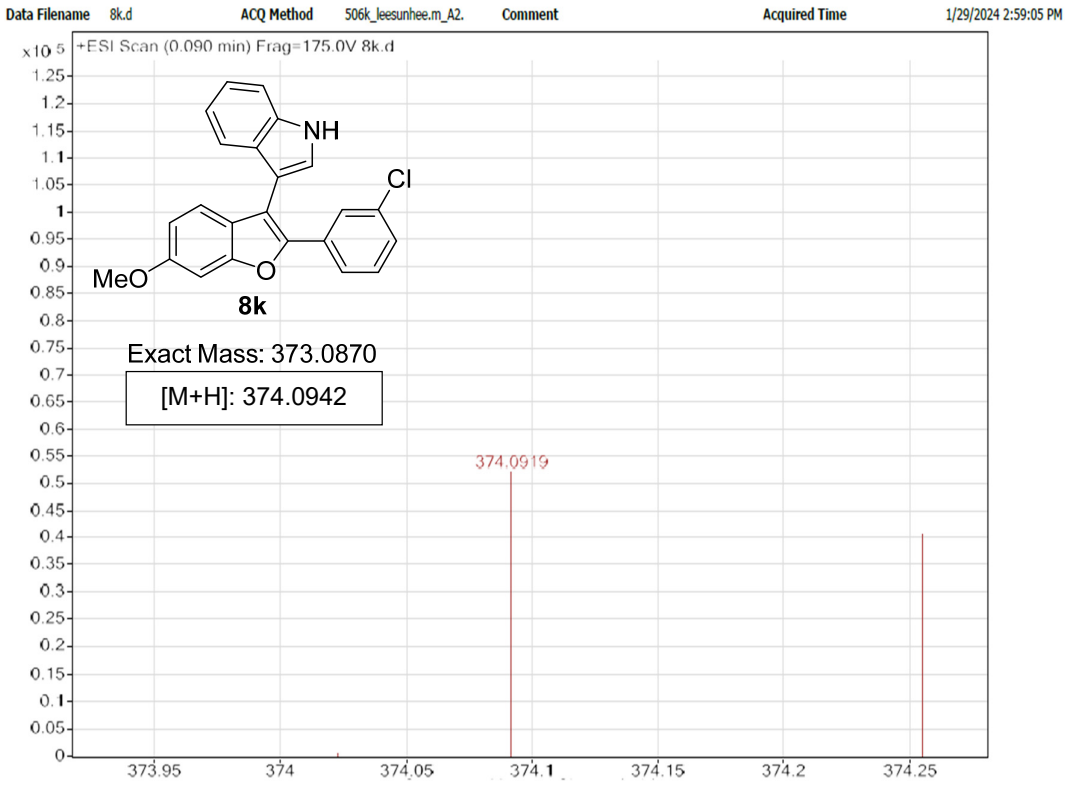

Data Filename 8f.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 2:51:37 PM
+ESI Scan (0.082 min) Frag=175.0V 8f.d
x10 5
Br
NH
Ph
MeO
O
8f
Exact Mass: 417.0364
[M+H]: 418.0437
418.0415
417.6
417.7
417.8
417.9
418
418.1
418.2
418.3
418.4
418.5
418.6
418.7
418.8

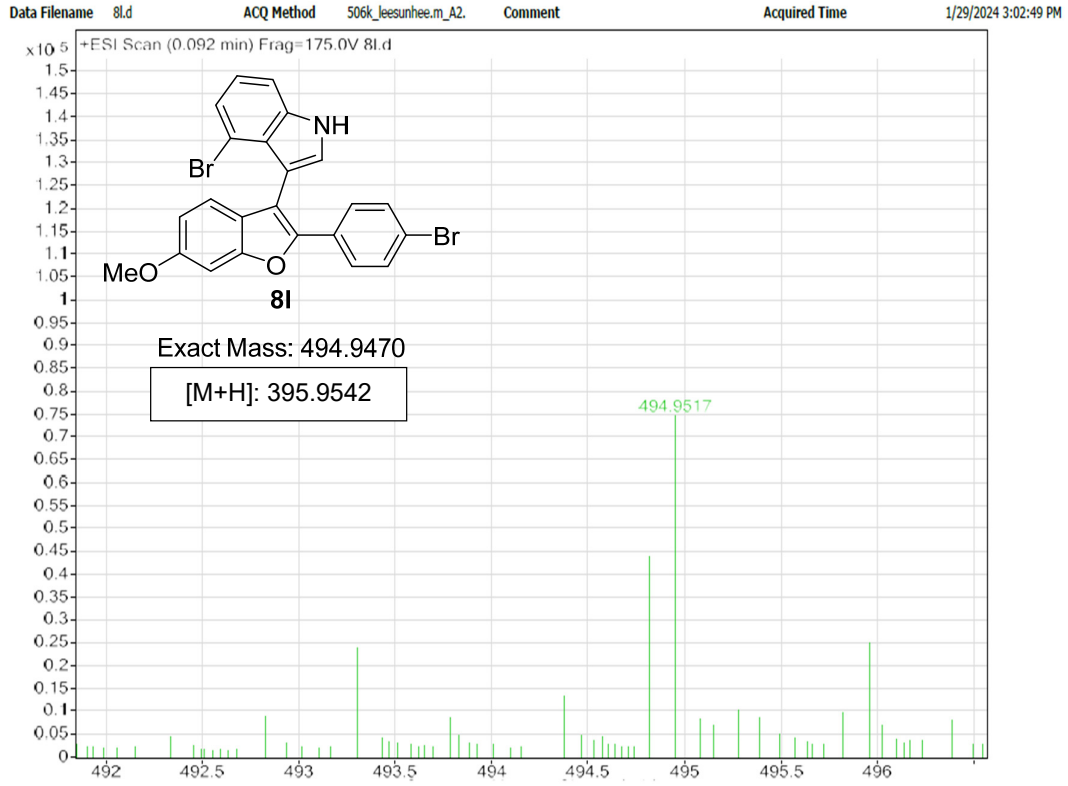

Data Filename 8g.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 12:26:21 PM
+ESI Scan (0.075 min) Frag=175.0V 8g.d
466.0244
I
NH
Ph
MeO
O
8g
Exact Mass: 465.0226
[M+H]: 466.0298

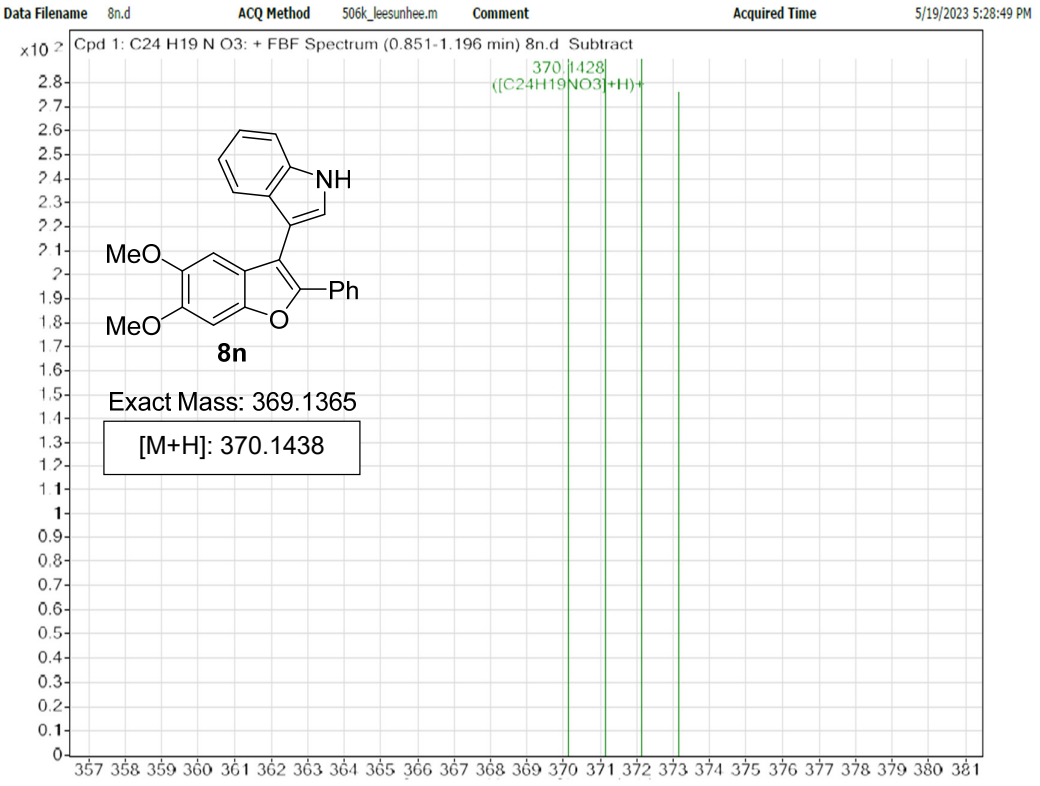

Data Filename 8h.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:06:34 PM
Cpd 1: C24 H19 N O2: + FBF Spectrum (0.981-1.325 min) 8h.d Subtract
354.1474
([C24H19NO2]+H)+
Me
N
Ph
MeO
O
8h
Exact Mass: 353.1416
[M+H]: 354.1489

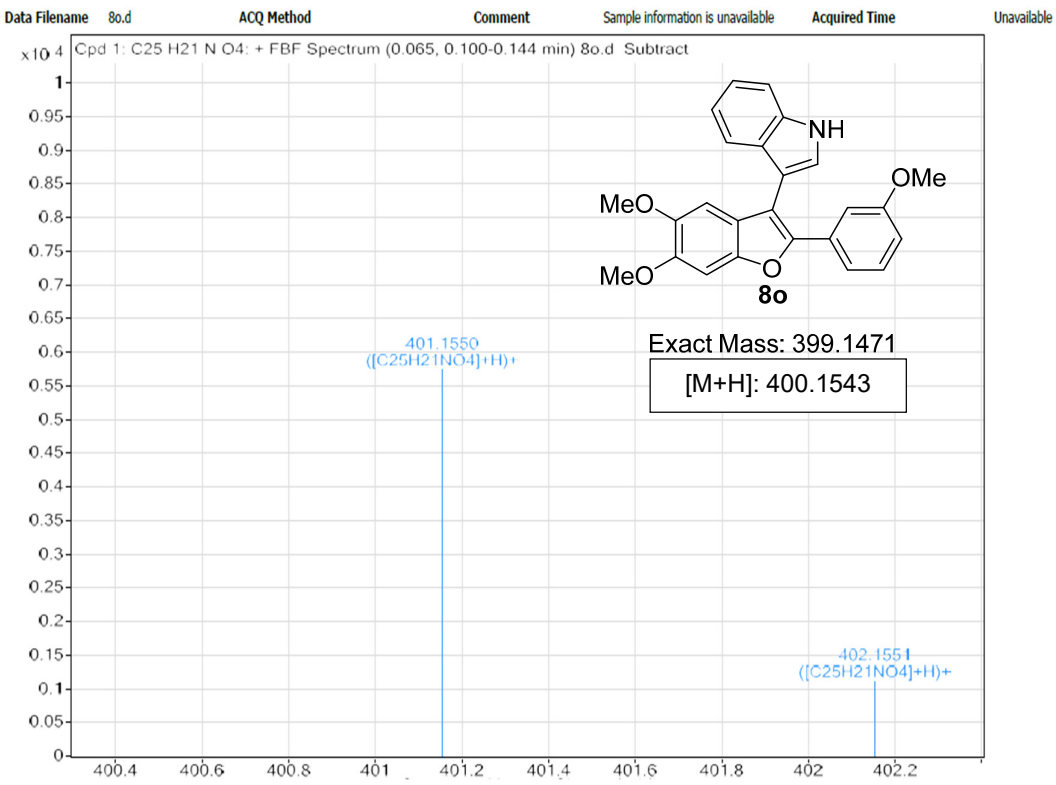

Data Filename 8i.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:10:17 PM
Cpd 1: C24 H19 N O3: + FBF Spectrum (0.935-1.280 min) 8i.d Subtract
370.1427
([C24H19NO3]+H)+
NH
OMe
MeO
O
8i
Exact Mass: 369.1365
[M+H]: 354.1438

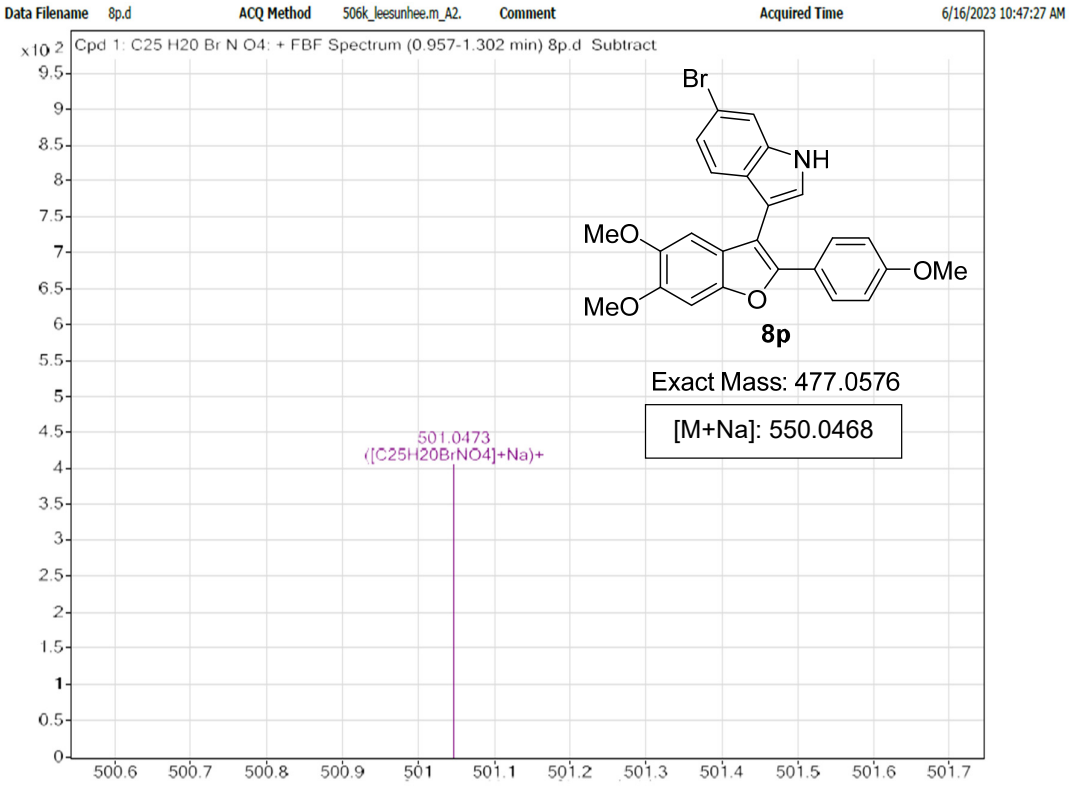

Data Filename 8j.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:13:59 PM
Cpd 1: C28 H21 N O2: + FBF Spectrum (1.087-1.468 min) 8j.d Subtract
404.1626
([C28H21NO2]+H)+
Me
N
MeO
O
8j
Exact Mass: 403.1572
[M+H]: 404.1645

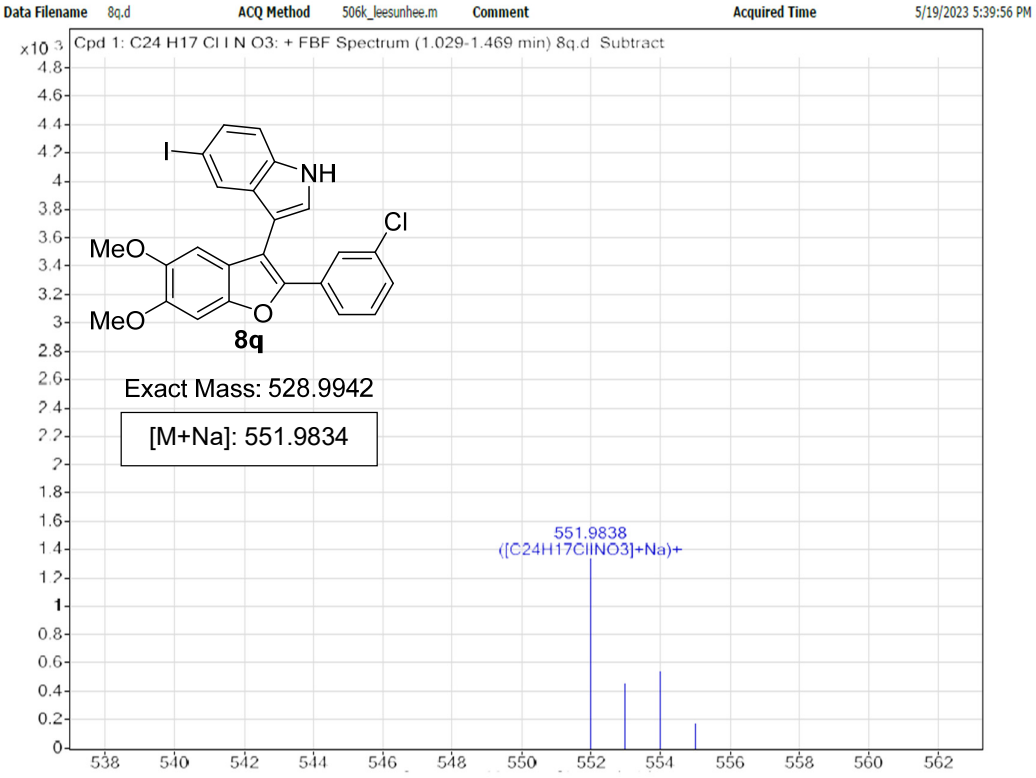

Data Filename 8k.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 2:59:05 PM
+ESI Scan (0.090 min) Frag=175.0V 8k.d
NH
Cl
MeO
O
8k
Exact Mass: 373.0870
[M+H]: 374.0942
374.0919

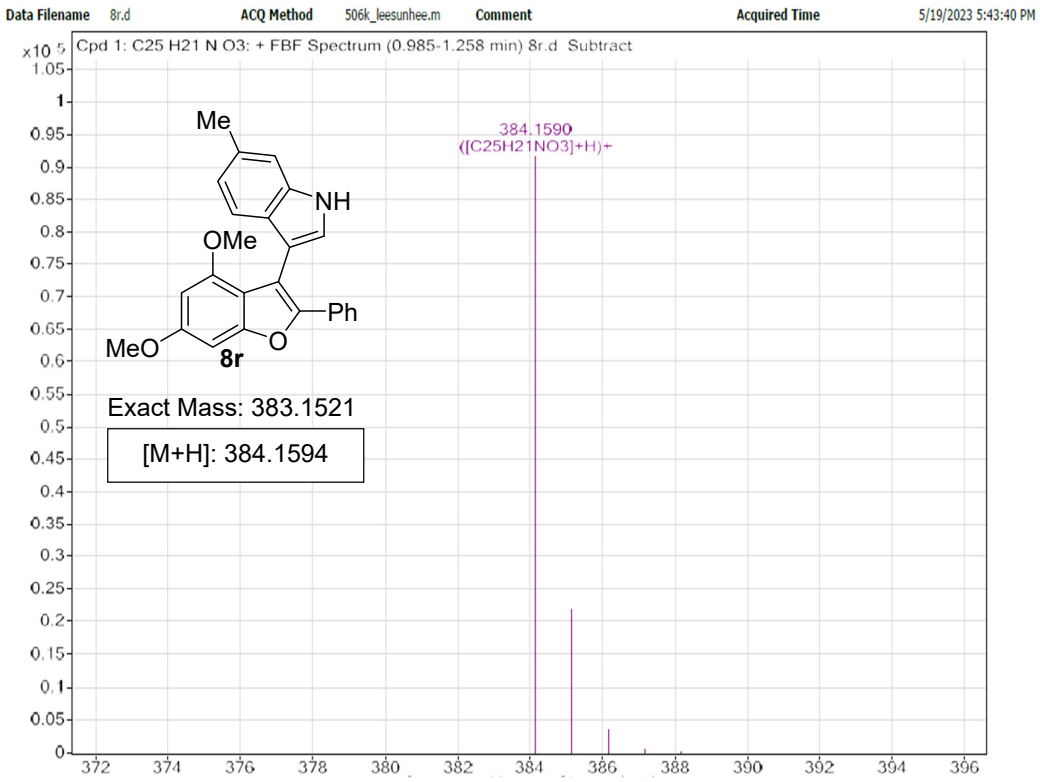

Data Filename 8l.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 3:02:49 PM
+ESI Scan (0.092 min) Frag=175.0V 8l.d
NH
Br
Br
MeO
O
8l
Exact Mass: 494.9470
[M+H]: 395.9542
494.9517

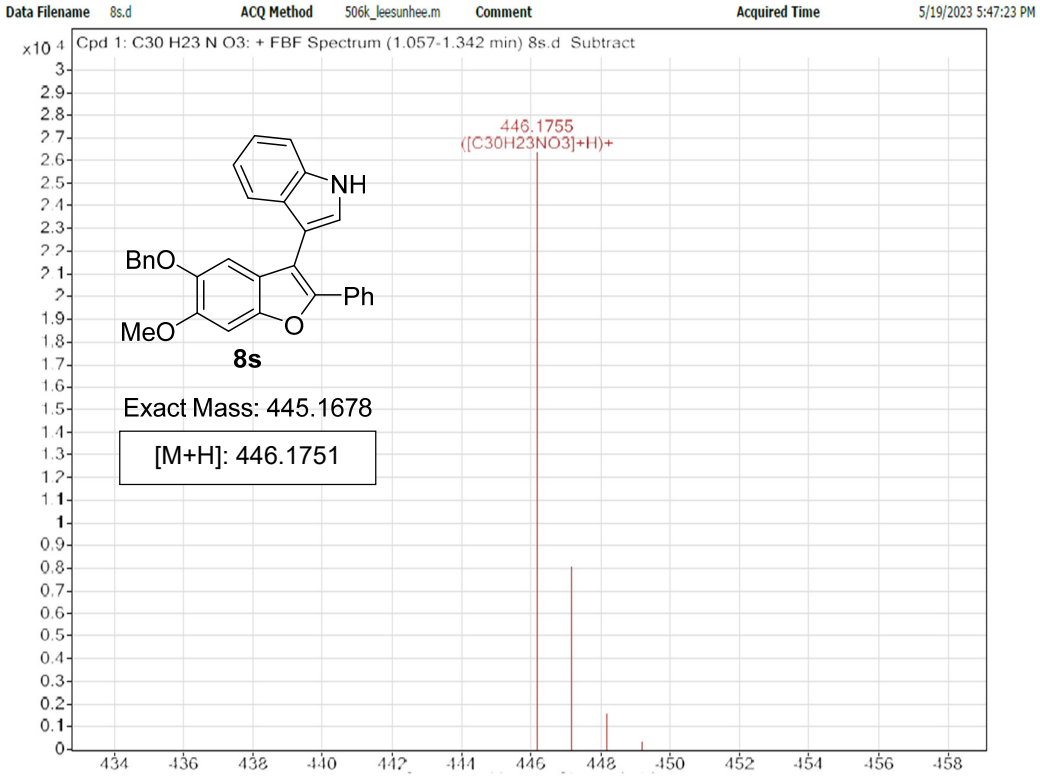

Data Filename 8n.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:28:49 PM
Cpd 1: C24 H19 N O3: + FBF Spectrum (0.851-1.196 min) 8n.d Subtract
x10 2
370.1428
([C24H19NO3]+H)+
NH
MeO
Ph
MeO
O
8n
Exact Mass: 369.1365
[M+H]: 370.1438

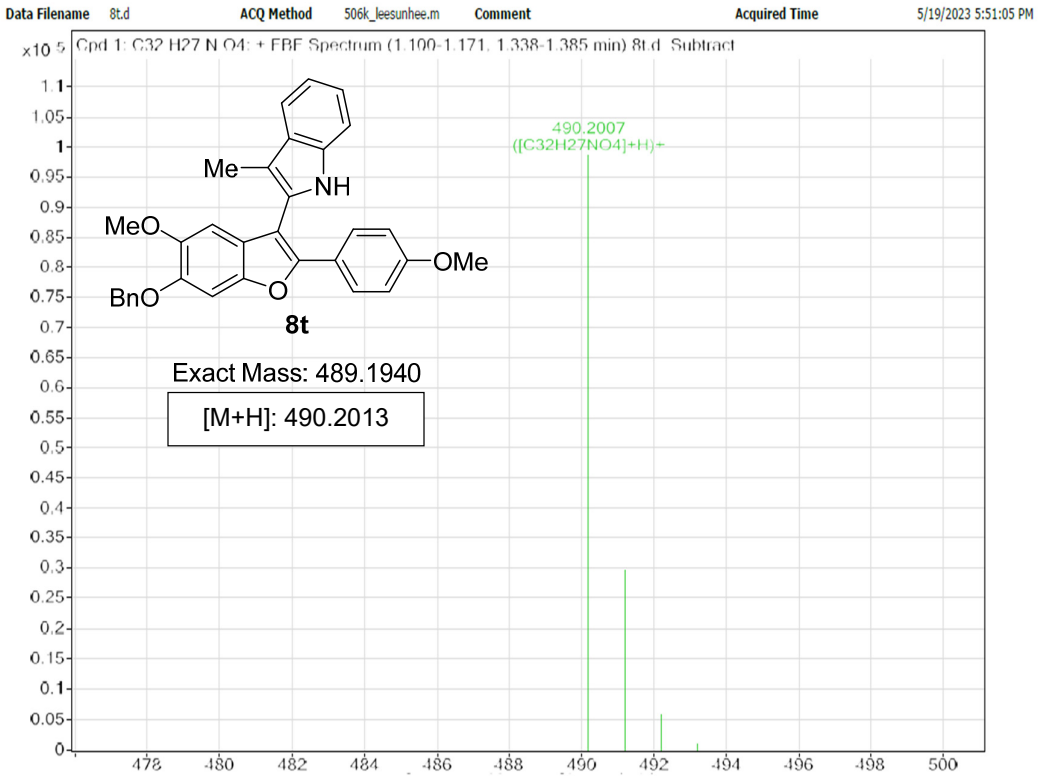

Data Filename 8o.d
ACQ Method
Comment Sample information is unavailable
Acquired Time Unavailable
Cpd 1: C25 H21 N O4: + FBF Spectrum (0.065, 0.100-0.144 min) 8o.d Subtract
x10 4
NH
OMe
MeO
MeO
O
8o
401.1550
([C25H21NO4]+H)+
Exact Mass: 399.1471
[M+H]: 400.1543
402.1551
([C25H21NO4]+H)+

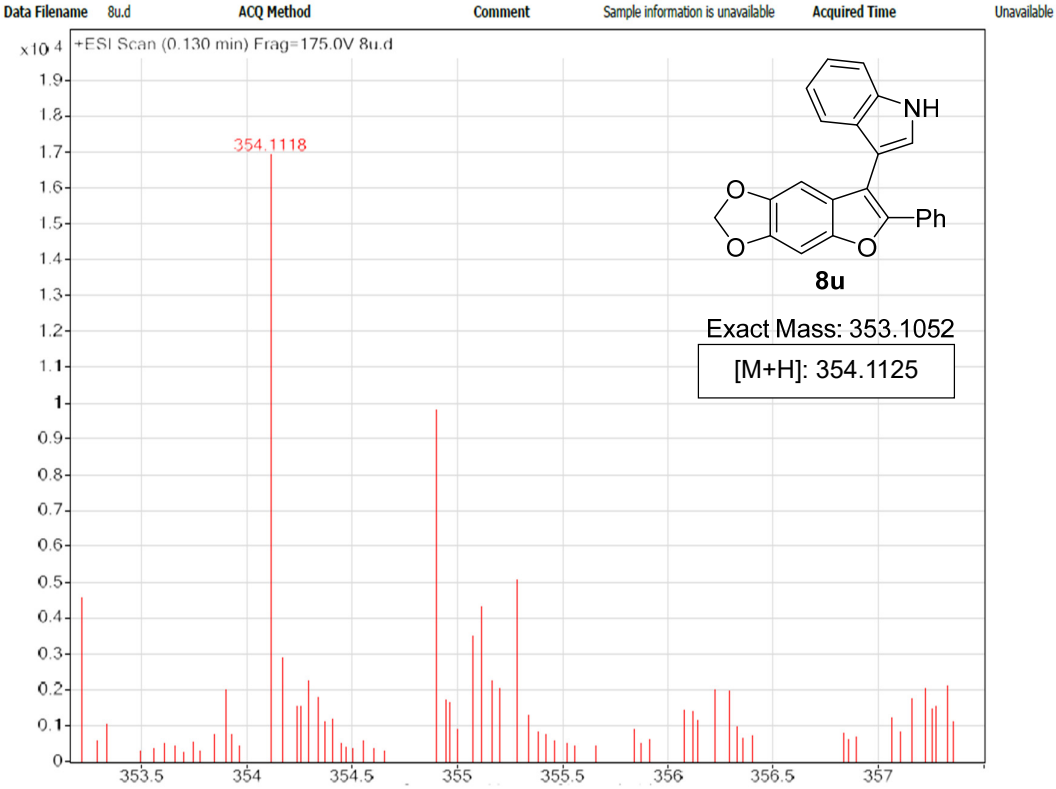

Data Filename 8p.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 6/16/2023 10:47:27 AM
Cpd 1: C25 H20 Br N O4: + FBF Spectrum (0.957-1.302 min) 8p.d Subtract
x10 2
Br
NH
MeO
MeO
OMe
O
8p
Exact Mass: 477.0576
[M+Na]: 550.0468
501.0473
([C25H20BrNO4]+Na)+

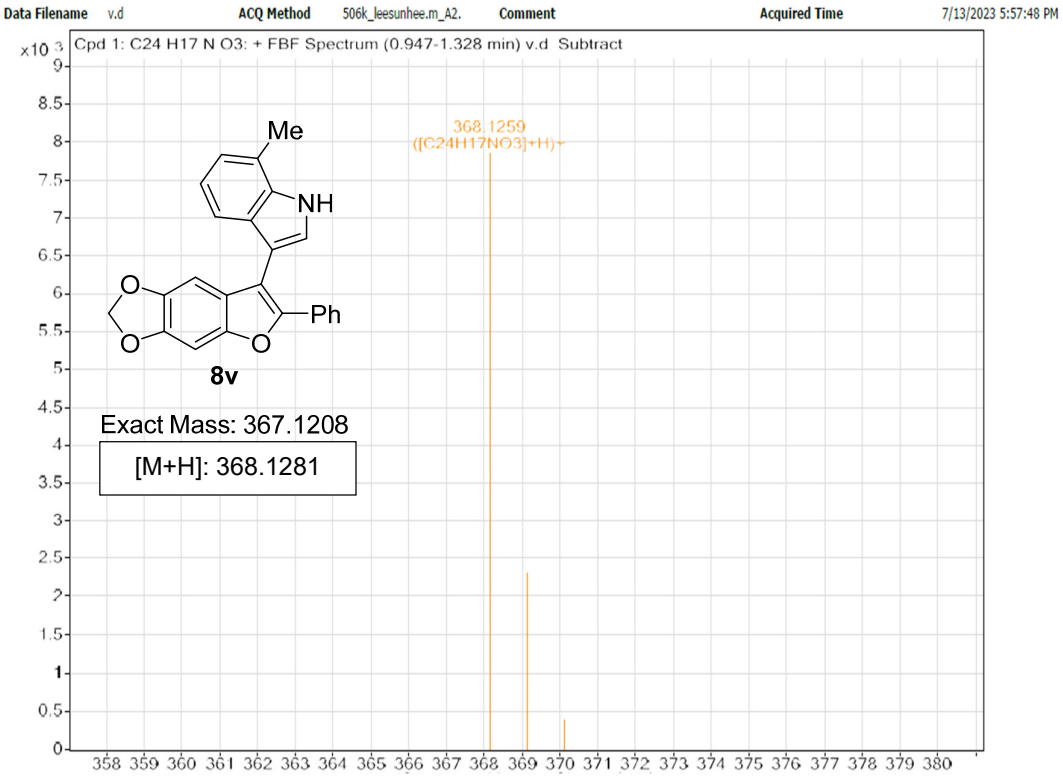

Data Filename 8q.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:39:56 PM
Cpd 1: C24 H17 Cl I N O3: + FBF Spectrum (1.029-1.469 min) 8q.d Subtract
x10 3
I
NH
Cl
MeO
MeO
O
8q
Exact Mass: 528.9942
[M+Na]: 551.9834
551.9838
([C24H17ClINO3]+Na)+

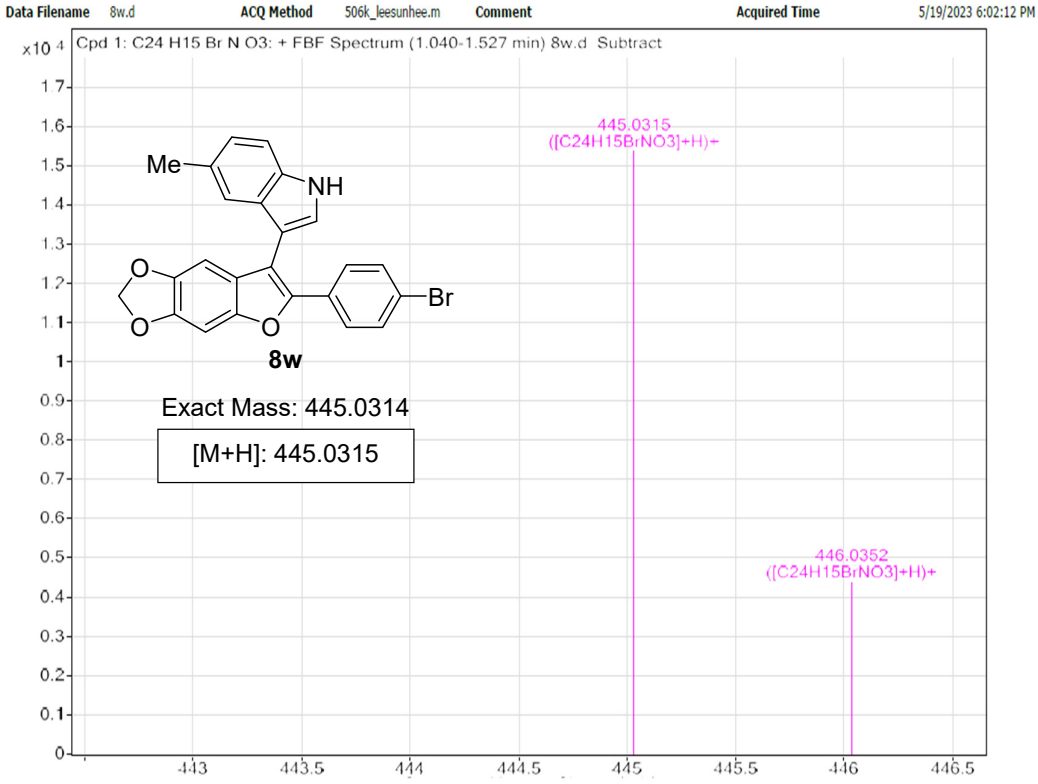

Data Filename 8r.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:43:40 PM
Cpd 1: C25 H21 N O3: + FBF Spectrum (0.985-1.258 min) 8r.d Subtract
x10 5
384.1590
([C25H21NO3]+H)+
Me
NH
OMe
Ph
MeO
O
8r
Exact Mass: 383.1521
[M+H]: 384.1594

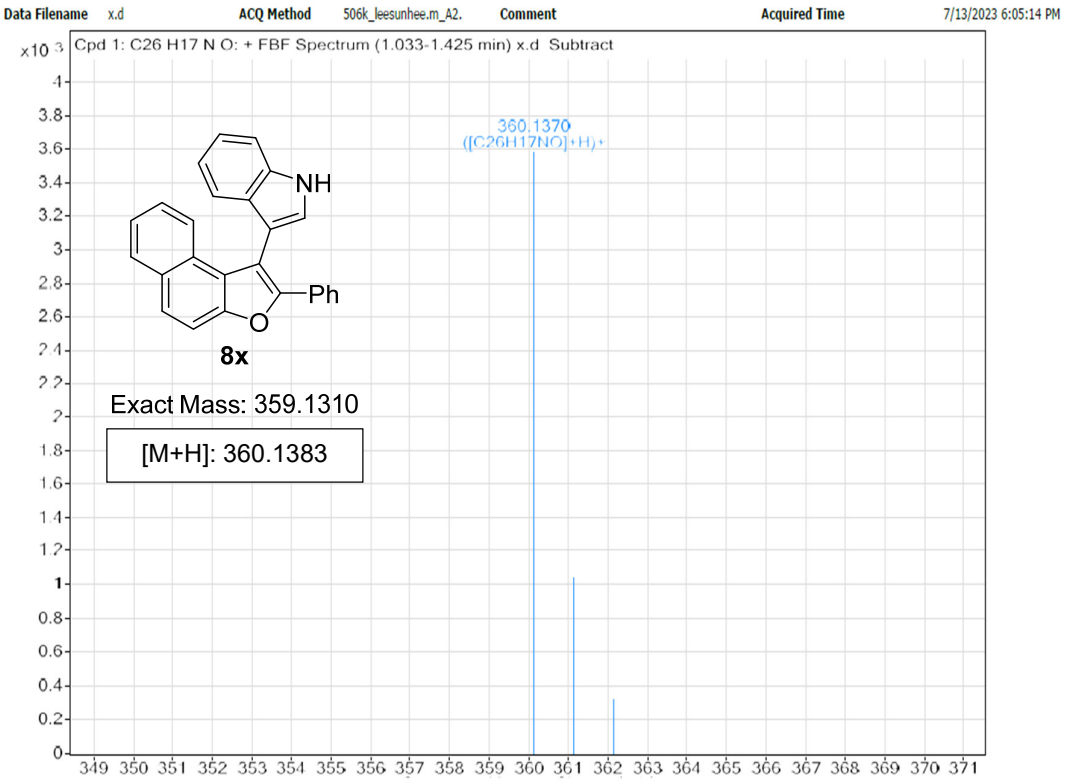

Data Filename 8s.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:47:23 PM
Cpd 1: C30 H23 N O3: + FBF Spectrum (1.057-1.342 min) 8s.d Subtract
x10 4
446.1755
([C30H23NO3]+H)+
NH
BnO
Ph
MeO
O
8s
Exact Mass: 445.1678
[M+H]: 446.1751

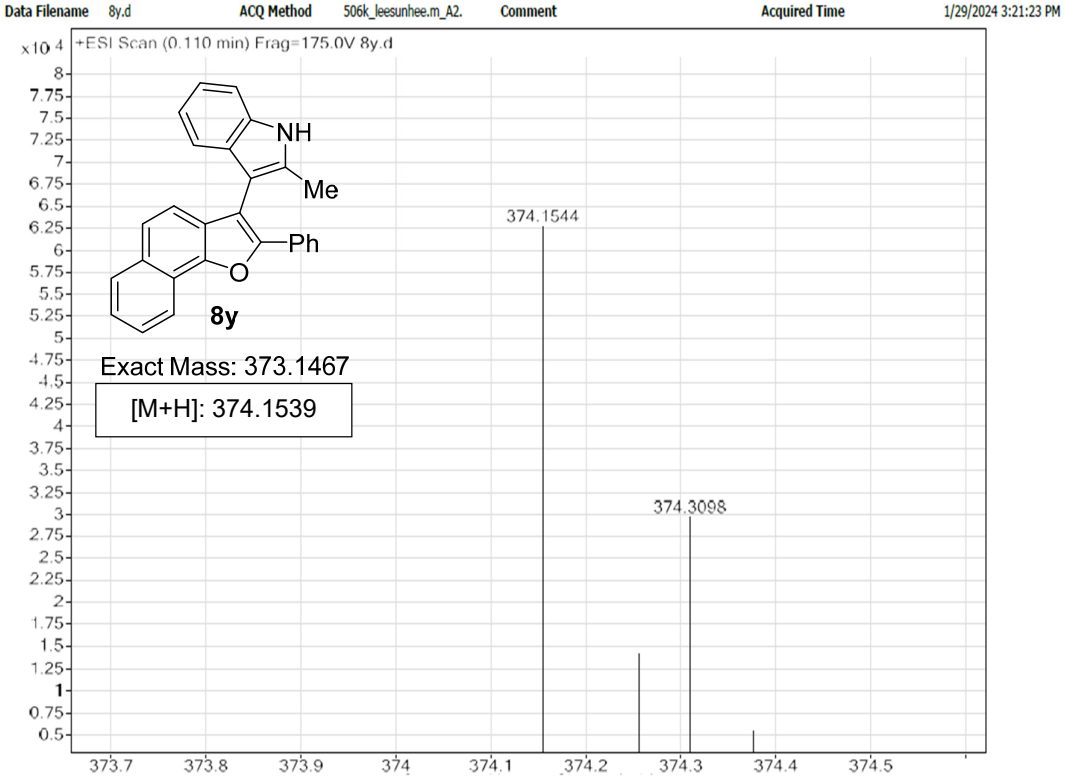

Data Filename 8t.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 5:51:05 PM
Cpd 1: C32 H27 N O4: + EBF Spectrum (1.100-1.171, 1.338-1.385 min) 8t.d, Subtract
490.2007
([C32H27NO4]+H)+
Me
NH
MeO
OMe
BnO
O
8t
Exact Mass: 489.1940
[M+H]: 490.2013

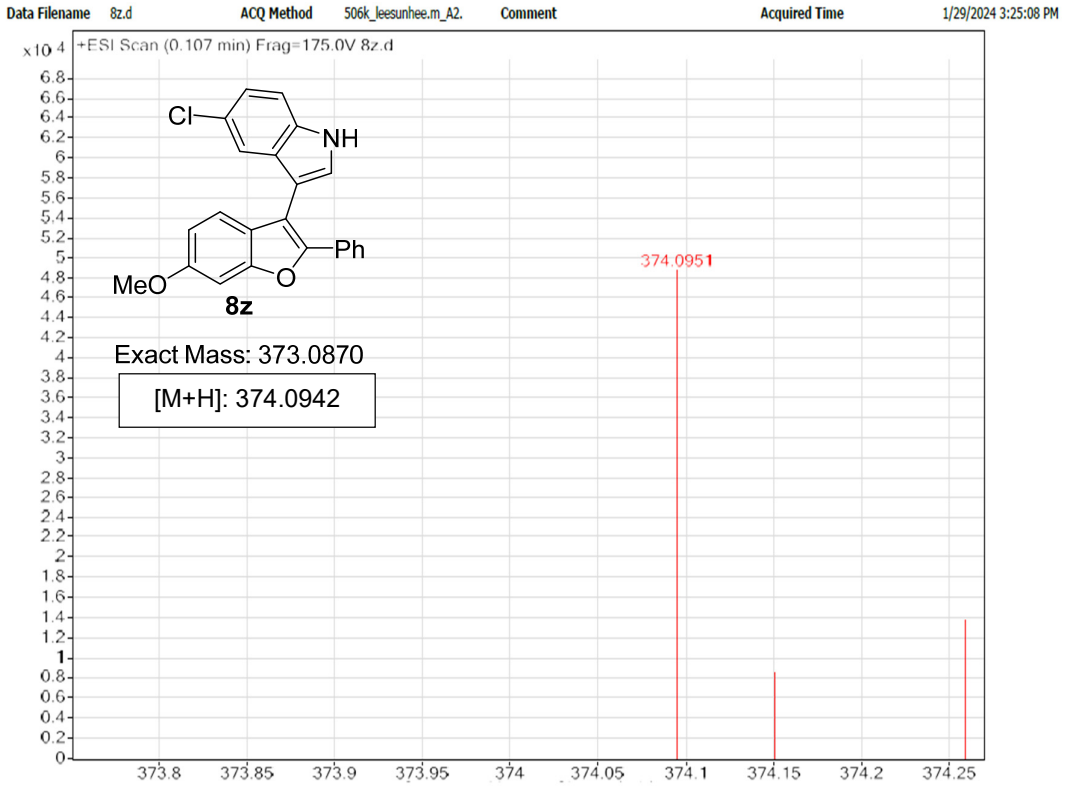

Data Filename 8u.d
ACQ Method
Comment
Sample information is unavailable
Acquired Time
Unavailable
+ESI Scan (0.130 min) Frag=175.0V 8u.d
354.1118
NH
O
O
O
Ph
8u
Exact Mass: 353.1052
[M+H]: 354.1125

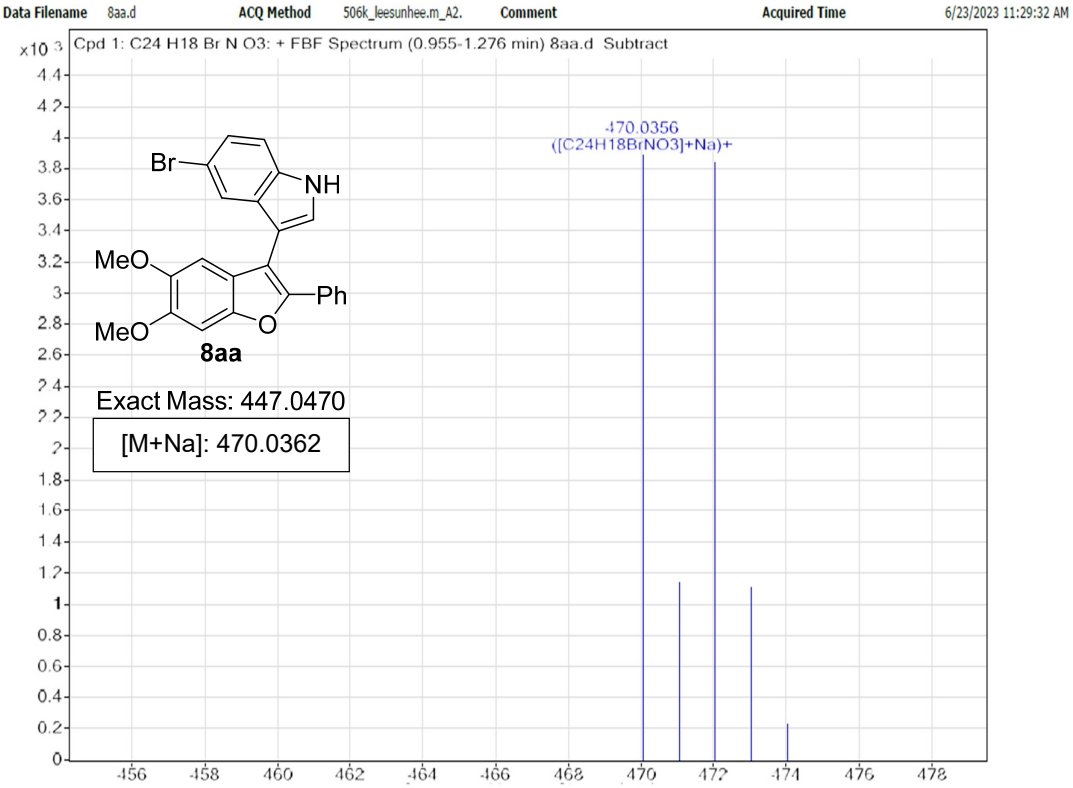

Data Filename v.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 7/13/2023 5:57:48 PM
Cpd 1: C24 H17 N O3: + FBF Spectrum (0.947-1.328 min) v.d Subtract
x10 3
368.1259
([C24H17NO3]+H)+
Me
NH
O
O
O
Ph
8v
Exact Mass: 367.1208
[M+H]: 368.1281

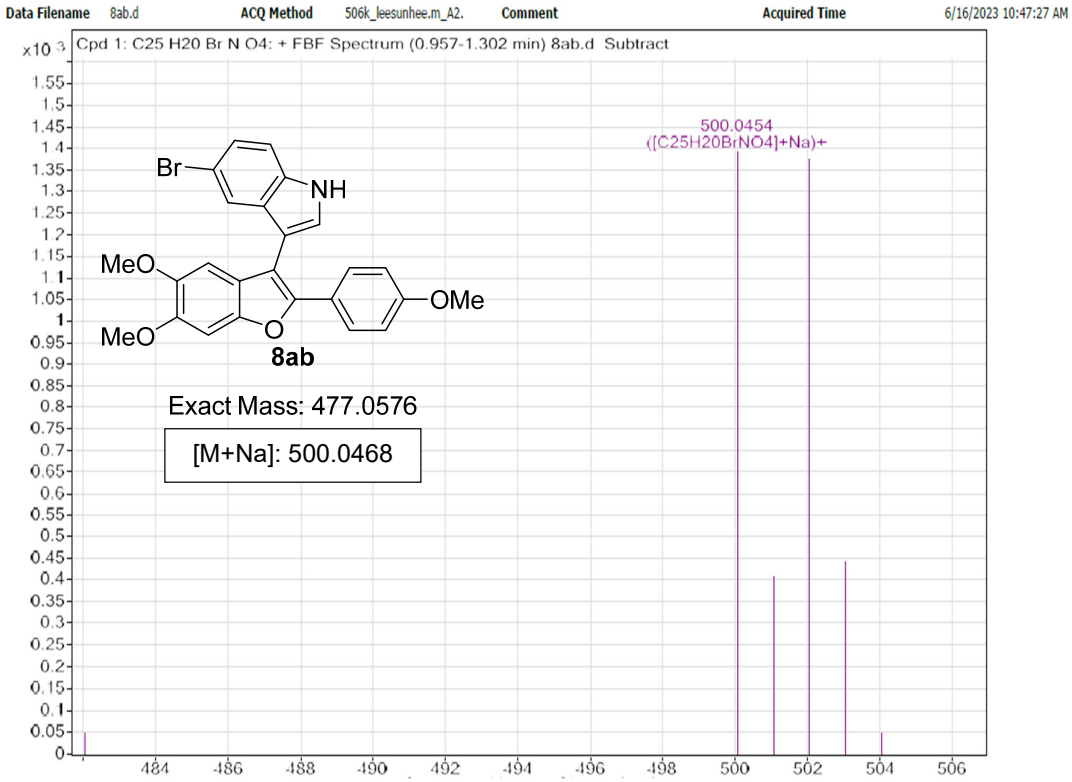

Data Filename 8w.d
ACQ Method 506k_leesunhee.m
Comment
Acquired Time 5/19/2023 6:02:12 PM
Cpd 1: C24 H15 Br N O3: + FBF Spectrum (1.040-1.527 min) 8w.d Subtract
x10 4
445.0315
([C24H15BrNO3]+H)+
Me
NH
O
O
O
Br
8w
Exact Mass: 445.0314
[M+H]: 445.0315
446.0352
([C24H15BrNO3]+H)+

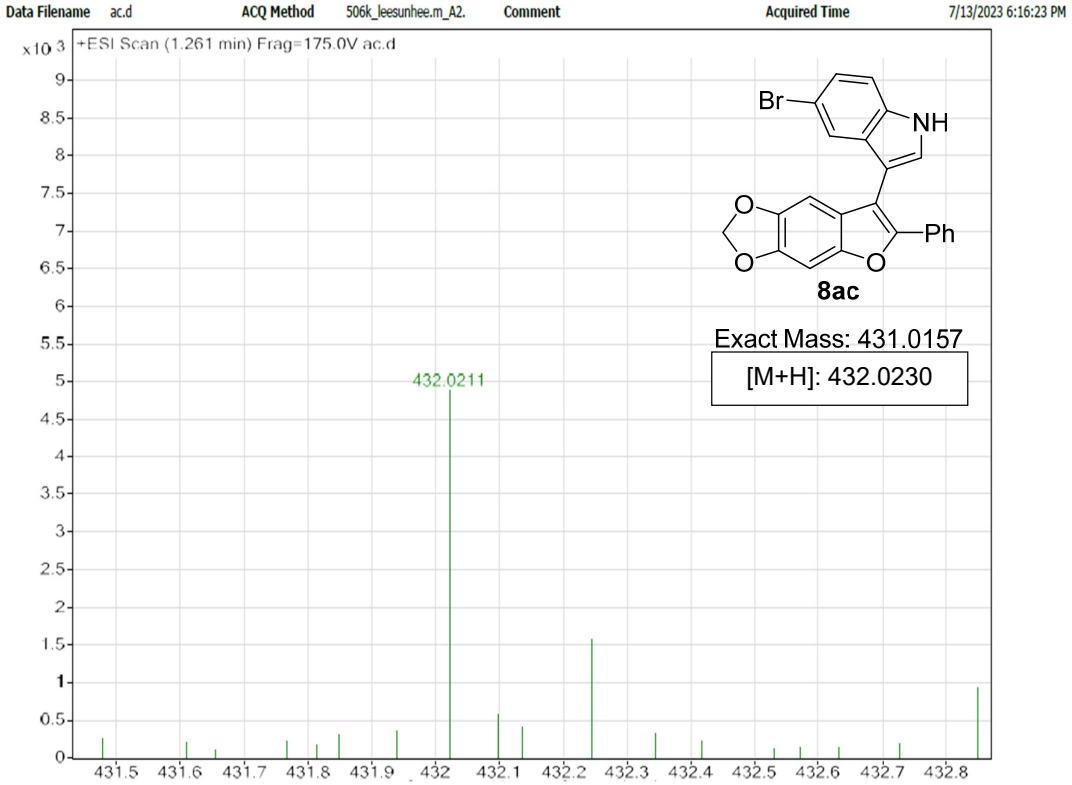

Data Filename x.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 7/13/2023 6:05:14 PM
Cpd 1: C26 H17 N O: + FBF Spectrum (1.033-1.425 min) x.d Subtract
x10 3
360.1370
([C26H17NO]+H)+
NH
Ph
O
8x
Exact Mass: 359.1310
[M+H]: 360.1383

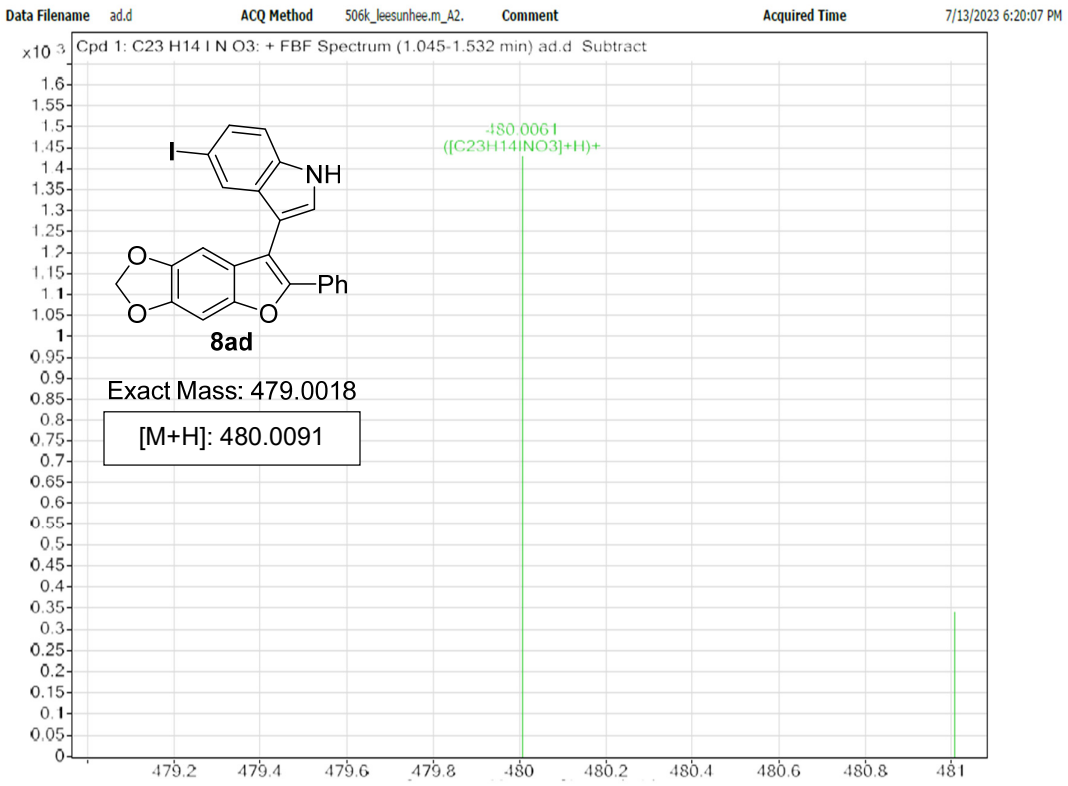

Data Filename 8y.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 3:21:23 PM
+ESI Scan (0.110 min) Frag=175.0V 8y.d
x10 4
NH
Me
Ph
O
8y
Exact Mass: 373.1467
[M+H]: 374.1539
374.1544
374.3098


Data Filename 8z.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 1/29/2024 3:25:08 PM
+ESI Scan (0.107 min) Frag=175.0V 8z.d
Cl
NH
Ph
MeO
O
8z
374.0951
Exact Mass: 373.0870
[M+H]: 374.0942

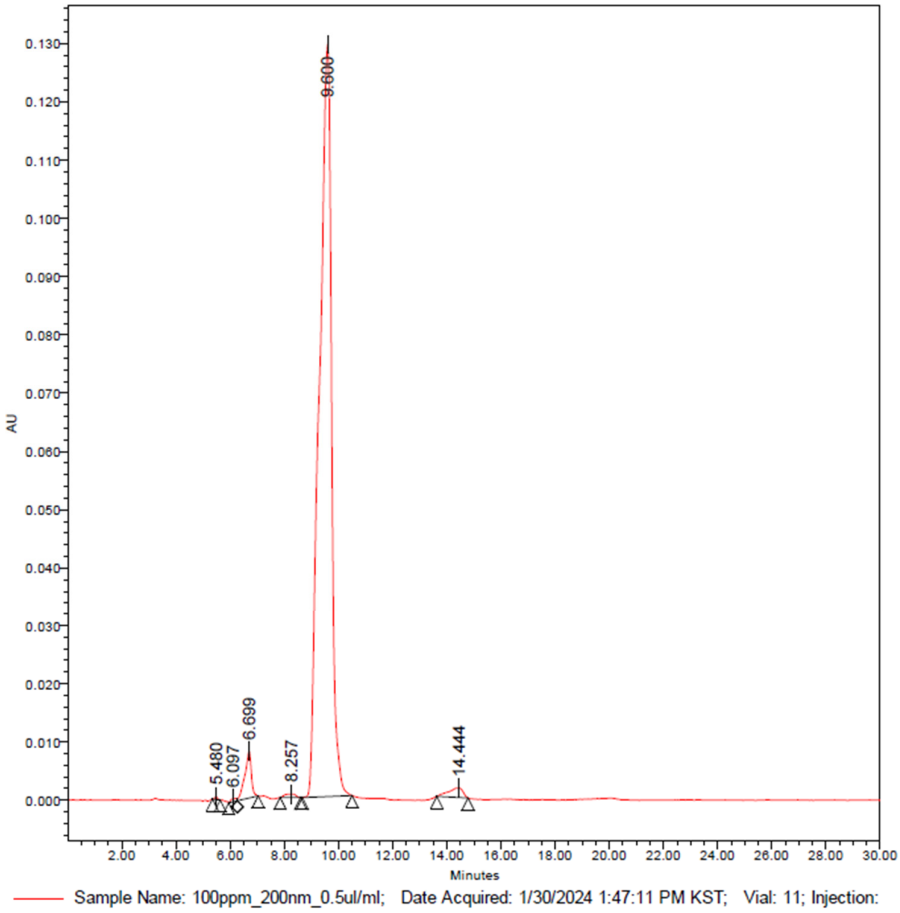

Data Filename 8aa.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 6/23/2023 11:29:32 AM
Cpd 1: C24 H18 Br N O3: + FBF Spectrum (0.955-1.276 min) 8aa.d Subtract
Br
NH
MeO
Ph
MeO
O
8aa
470.0356
([C24H18BrNO3]+Na)+
Exact Mass: 447.0470
[M+Na]: 470.0362


Data Filename 8ab.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 6/16/2023 10:47:27 AM
Cpd 1: C25 H20 Br N O4: + FBF Spectrum (0.957-1.302 min) 8ab.d Subtract
500.0454
([C25H20BrNO4]+Na)+
Br
NH
MeO
MeO
OMe
O
8ab
Exact Mass: 477.0576
[M+Na]: 500.0468


Data Filename ac.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 7/13/2023 6:16:23 PM
+ESI Scan (1.261 min) Frag=175.0V ac.d
Br
NH
O
O
O
Ph
8ac
Exact Mass: 431.0157
[M+H]: 432.0230
432.0211


Data Filename ad.d
ACQ Method 506k_leesunhee.m_A2.
Comment
Acquired Time 7/13/2023 6:20:07 PM
Cpd 1: C23 H14 I N O3: + FBF Spectrum (1.045-1.532 min) ad.d Subtract
x10 3
480.0061
([C23H14INO3]+H)+
I
NH
O
O
O
Ph
8ad
Exact Mass: 479.0018
[M+H]: 480.0091
1.6
1.55
1.5
1.45
1.4
1.35
1.3
1.25
1.2
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
479.2
479.4
479.6
479.8
480
480.2
480.4
480.6
480.8
481

Purity of 8aa measured by HPLC



Peak Summary with Statistics
Name:

	Sample Name	Vial	Inj	Retention Time (min)	Area	% Area	Height
1	100ppm_200nm_0.5ul/ml	11	1	5.480	3532	0.08	510
2	100ppm_200nm_0.5ul/ml	11	1	6.097	7370	0.17	497
3	100ppm_200nm_0.5ul/ml	11	1	14.444	60905	1.44	1617
4	100ppm_200nm_0.5ul/ml	11	1	8.257	16691	0.39	601
5	100ppm_200nm_0.5ul/ml	11	1	9.600	4013420	94.75	129276
6	100ppm_200nm_0.5ul/ml	11	1	6.699	134010	3.16	8022
Mean				8.429			
Std. Dev.				3.308			
% RSD				39.24			

8aa HPLC conditions	
Column	CHIRALPAK® C18 UG 5 μm, 4.6 mm i.d. × 250 mm
Mobile phase	Acetonitrile : Water = 8 : 2
Flow rate	0.5 mL/min
Injection volume	10 μL
Detection	254 nm
Column Temperature	25 °C
Auto-sampler temperature	25 °C
Retention time	9.6 minutes