Supporting Information

A versatile approach to flavones *via* one-pot Pd(II)-catalyzed dehydrogenation/oxidative boron-Heck coupling sequence of chromanones

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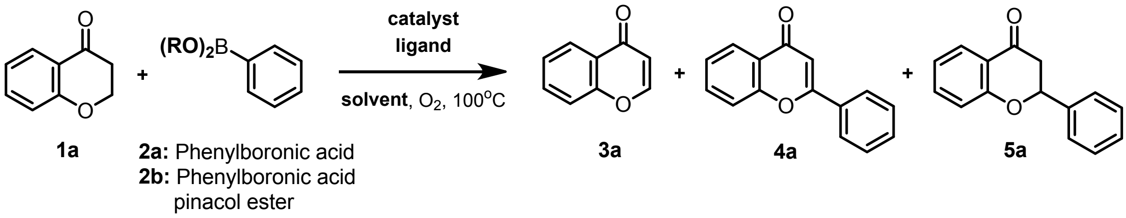
Detailed Optimization

Table S1. Additional Optimization for Pd (II)-Catalyzed Dehydrogenation/Oxidative Heck Coupling Sequence of chromanone **1a**[a]



entry	2a or 2b (equiv)	catalyst (equiv)	ligand (equiv)	solvent	Isolated Yield(%)		
					3a	4a	5a
1	2a (3)	$Pd(TFA)_2$(0.15)		AcOH	0	0	0
2	2a (3)	$Pd(TFA)_2$(0.15)	DMSO (0.3)	AcOH	34	13	9
3	2a (3)	$Pd(TFA)_2$(0.15)		DMSO	43	0	0
4	2a (3)	$Pd(TFA)_2$(0.15)	pyridine (0.3)	DMSO	76	2	0
5	2a (3)	$Pd(TFA)_2$(0.15)	DMAP (0.3)	DMSO	70	2	0
6	2a (3)	$Pd(TFA)_2$(0.15)	bipyridine (0.3)	DMSO	35	11	11
7	2a (3)	$Pd(TFA)_2$(0.15)	phenanthroline (0.3)	DMSO	24	19	9
8	2a (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMSO	1	42	25
9	2a (3)	$Pd(TFA)_2$(0.15)	DMSO (0.3)	DMF	0	0	0
10	2a (3)	$Pd(TFA)_2$(0.15)	DMAP (0.3)	DMF	0	0	0
11	2a (3)	$Pd(TFA)_2$(0.15)	Bipyridine (0.3)	DMF	0	21	3
12	2a (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	0	13	4
13	2a (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	0	35	0
14	2b (3)	$Pd(TFA)_2$(0.05)	5-NO_2-phenanthroline (0.1)	DMSO	36	52	3
15	2b (3)	$Pd(TFA)_2$(0.1)	5-NO_2-phenanthroline (0.2)	DMSO	13	72	1
16	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMSO	0	93	1
17	2b (3)	$Pd(TFA)_2$(0.2)	5-NO_2-phenanthroline (0.4)	DMSO	0	96	0
18	2b (1.5)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMSO	0	72	0
19	2b (3)	$Pd(TFA)_2$(0.05)	5-NO_2-phenanthroline (0.1)	DMF	24	48	5
20	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	0	70	0
21	2b (3)	$Pd(TFA)_2$(0.2)	5-NO_2-phenanthroline (0.4)	DMF	0	78	0
22	2b (1.5)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	26	39	0
23	2b (3)	$Pd(OAc)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMSO	0	70	1
24	2b (3)	$Pd(OAc)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	34	40	0

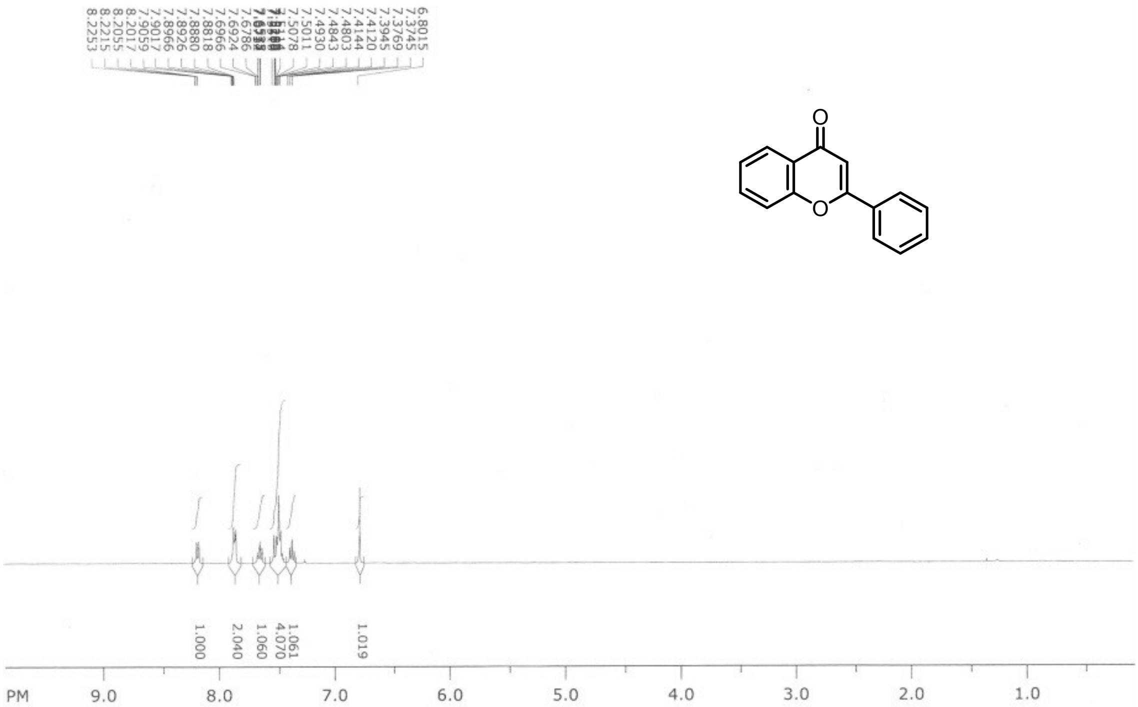
25	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	toluene	57	2	3
26	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	CH_3CN[b]	52	4	13
27	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	Dioxane	51	1	1
28	2b (3)	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	THF[b]	72	3	3
29	2a (1.5)[c]	$Pd(TFA)_2$(0.15)	DMSO(0.3)	AcOH	0	0	0
30	2a (1.5)[c]	$Pd(TFA)_2$(0.1)	phenanthroline(0.2)	DMF	26	13	22
31	2a (1.5)[c]	$Pd(TFA)_2$(0.15)	phenanthroline(0.3)	DMF	5	43	20
32	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	DMF	3	49	1
33	2a (3)[c]	$Pd(TFA)_2$(0.15)	phenanthroline(0.3)	DMF	14	33	25
34	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	2,9-dimethyl-1,10-phenanthroline(0.4)	DMF	12	0	0
35	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	4,7-dihydroxy-1,10-phenanthroline(0.4)	DMF	0	0	0
36	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	bipyridine(0.4)	DMF	0	44	6
37	2a (1.5)[c]	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	10	45	5
38	2a (3)[c]	$Pd(TFA)_2$(0.15)	5-NO_2-phenanthroline (0.3)	DMF	4	55	4
39	2a (3)[c]	$Pd(TFA)_2$(0.2)	5-NO_2-phenanthroline (0.4)	DMF	0	66	13
40	2a (1.5)[c]	$Pd(OAc)_2$(0.15)	phenanthroline(0.3)	DMF	13	15	5
41	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	DMSO	63	21	3
42	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	Dioxane	16	3	20
43	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	AcOH	0	0	0
44	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	toluene	3	5	32
45	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	CH_3CN[b]	41	0	23
46	2a (1.5)[c]	$Pd(TFA)_2$(0.2)	phenanthroline(0.4)	HMPA	0	12	0
47	2b (3)[c]	$Pd(TFA)_2$(0.15)	Phenanthroline(0.3)	DMF	0	79	0

[a]Reaction conditions: To a solution of Pd catalyst, and ligand in anhydrous solvent (1mL) were added chromanone (**1a**) and phenyl boronic acid (**2a**) or its pinacol ester (**2b**) under O_2 atmosphere. The reaction mixture was stirred at 100°C until complete consumption of the starting material on TLC. Then, the reaction mixture was diluted with EtOAc and filtered through a pad of celite. The filtrate was concentrated *in vacuo* and purified by column chromatography on silica gel (EtOAc/Hexanes). [b]Reflux condition. [c]Reagent **2** was added to reaction mixture after 24h.

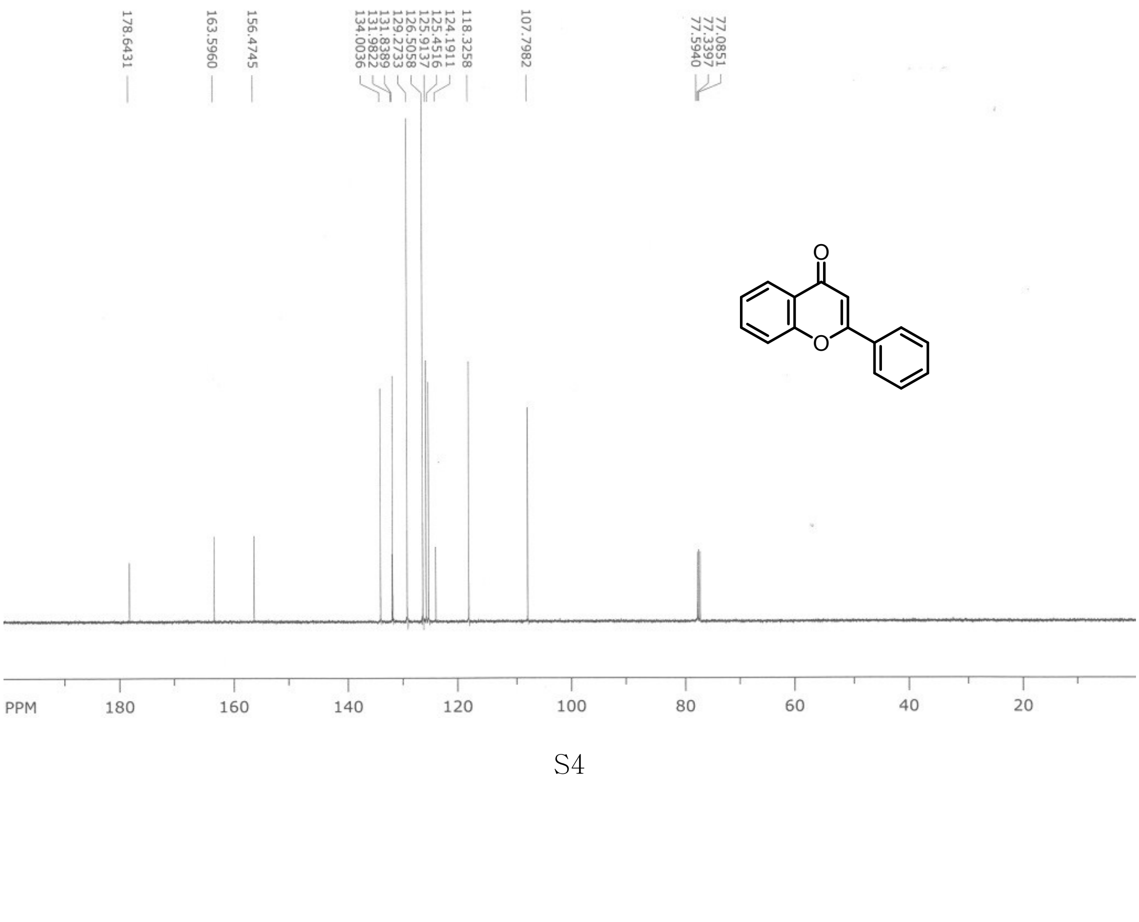
^{1}H NMR and ^{13}C NMR spectra

Compound 4a

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

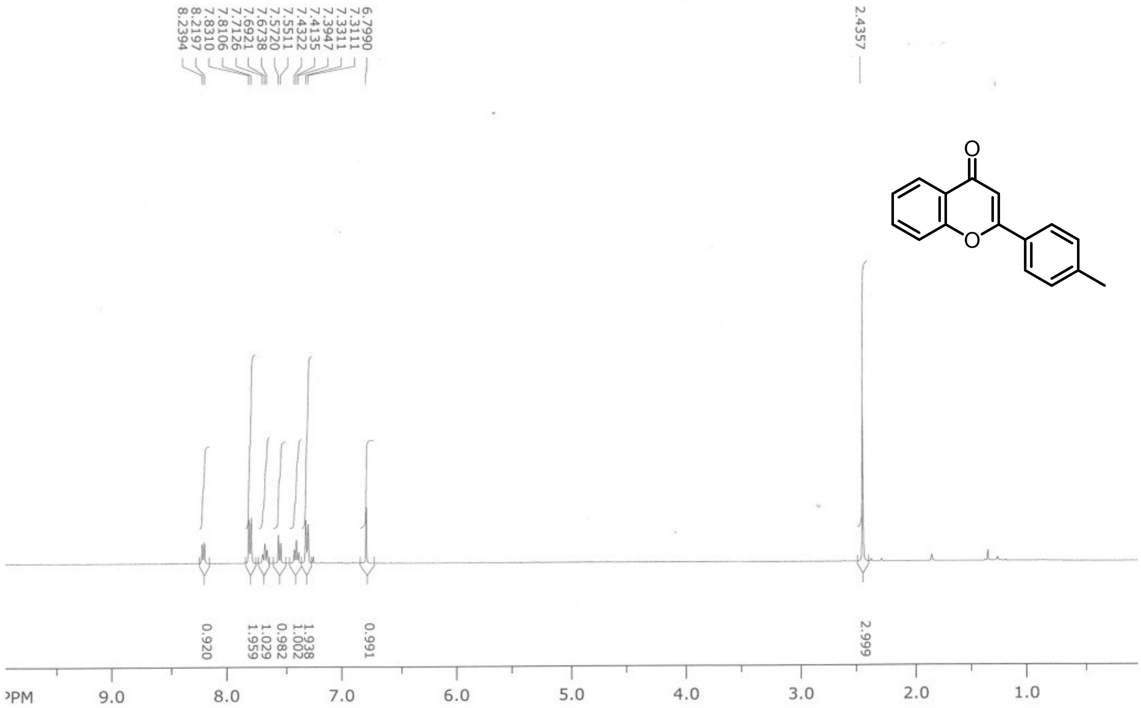


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

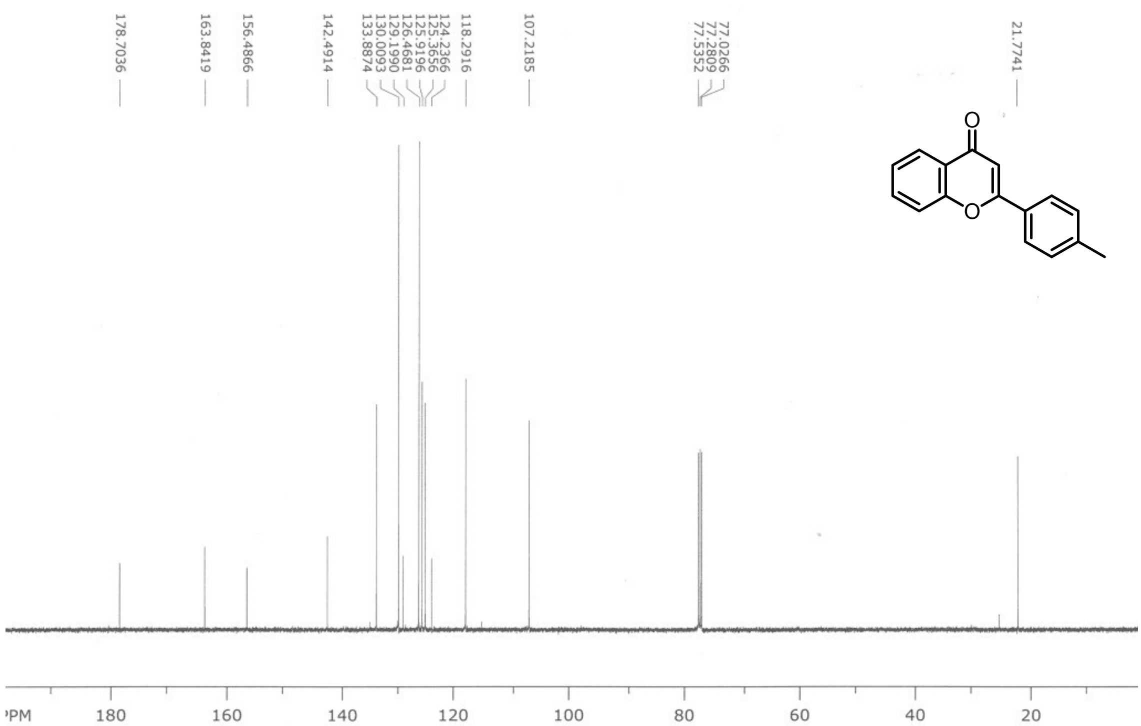


Compound 4b

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

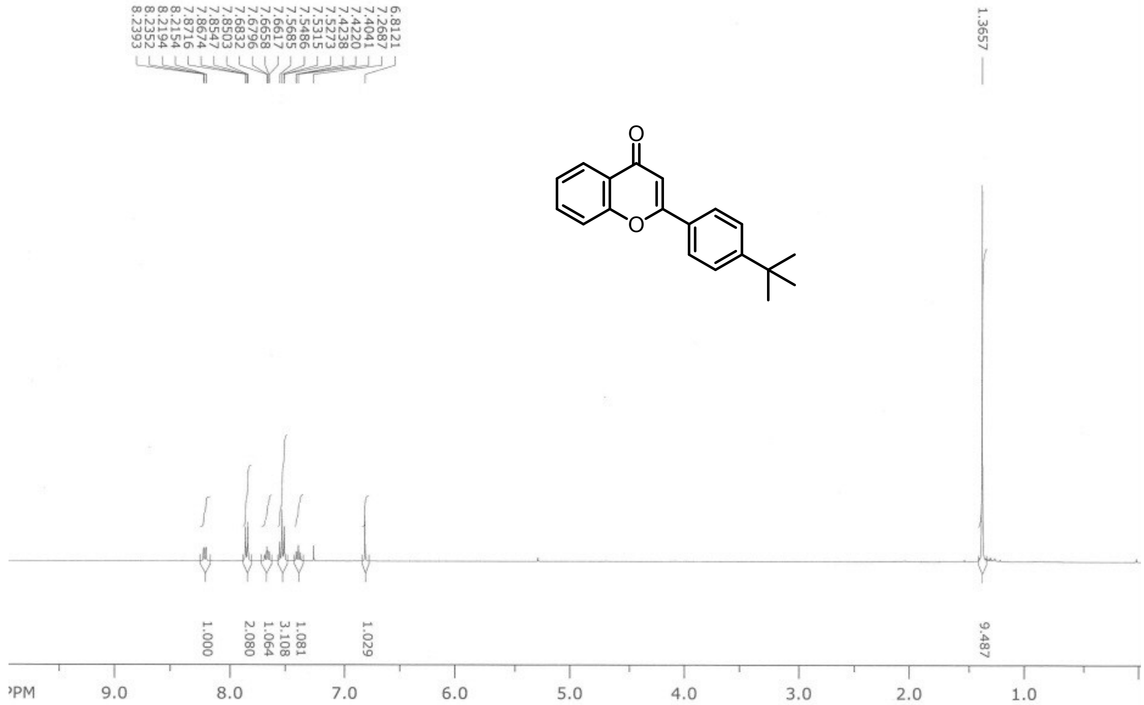


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Compound 4c

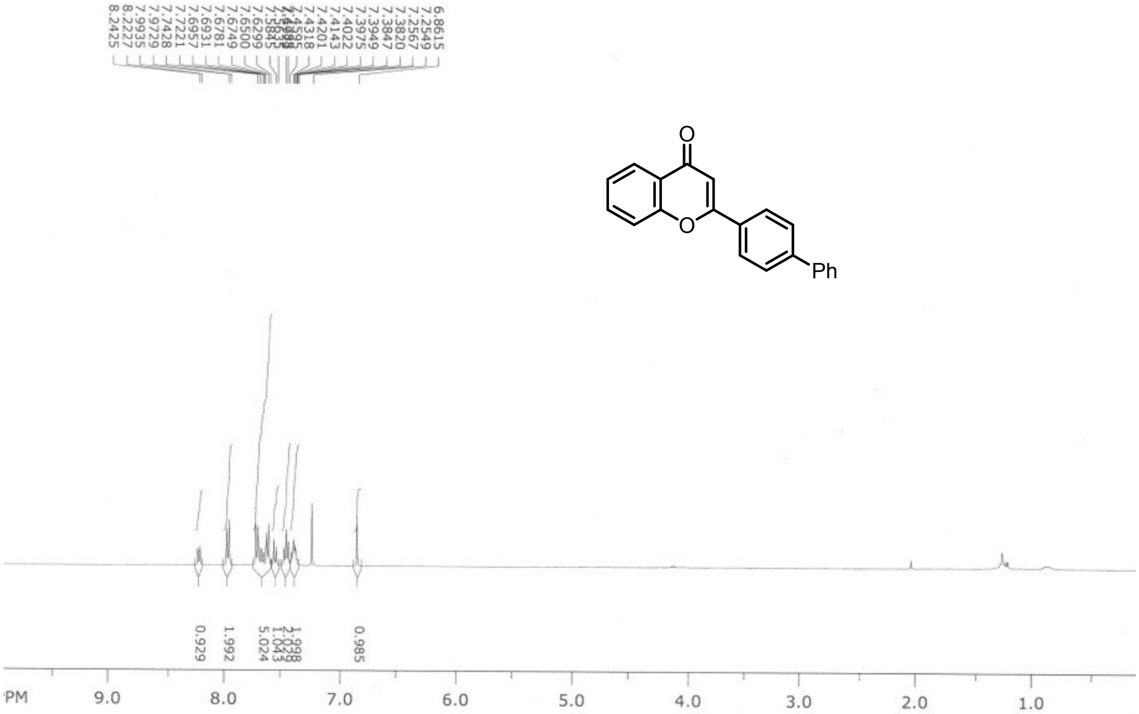
▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



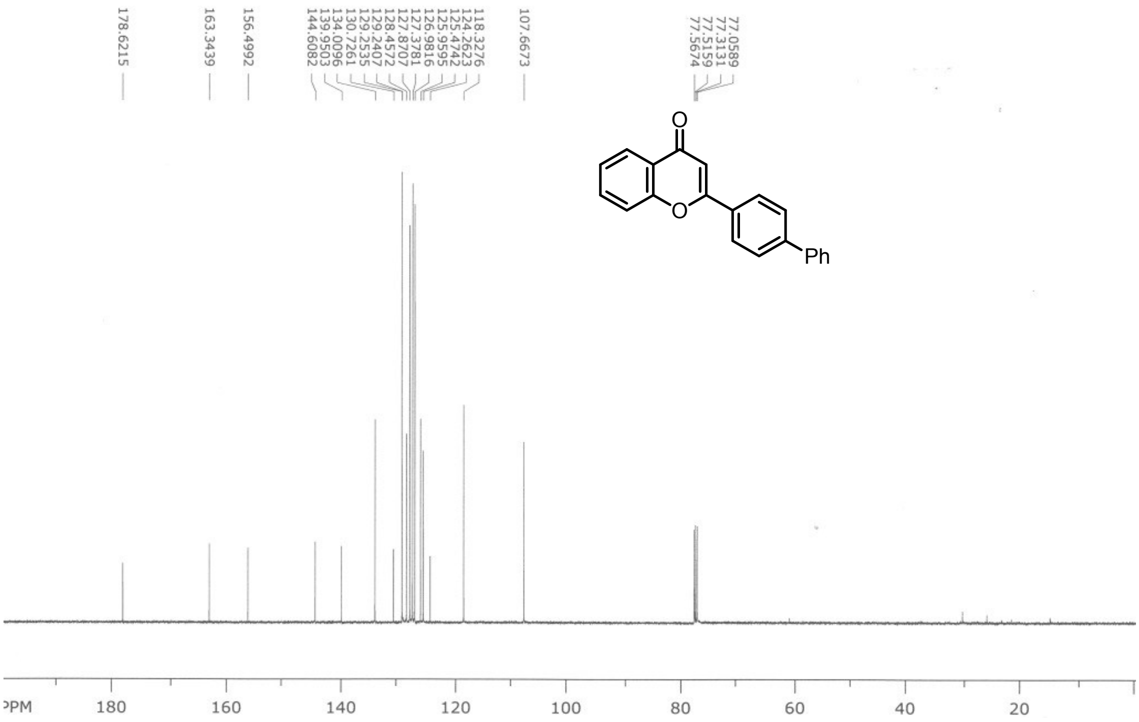
▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

Compound 4d

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

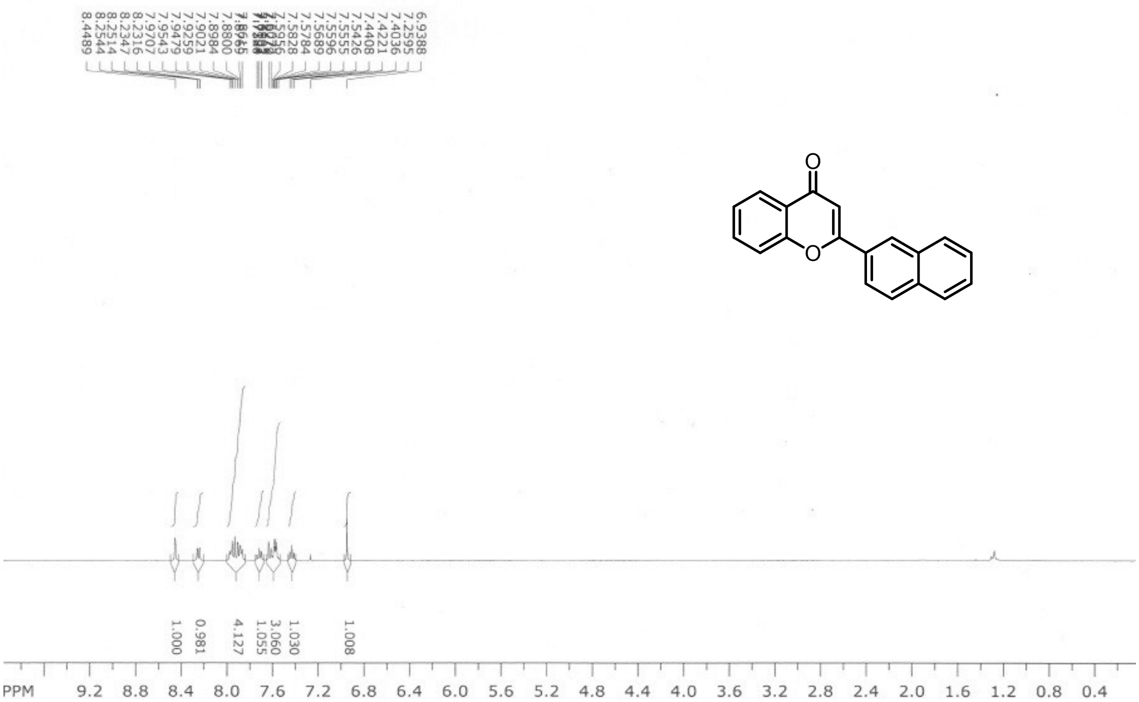


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

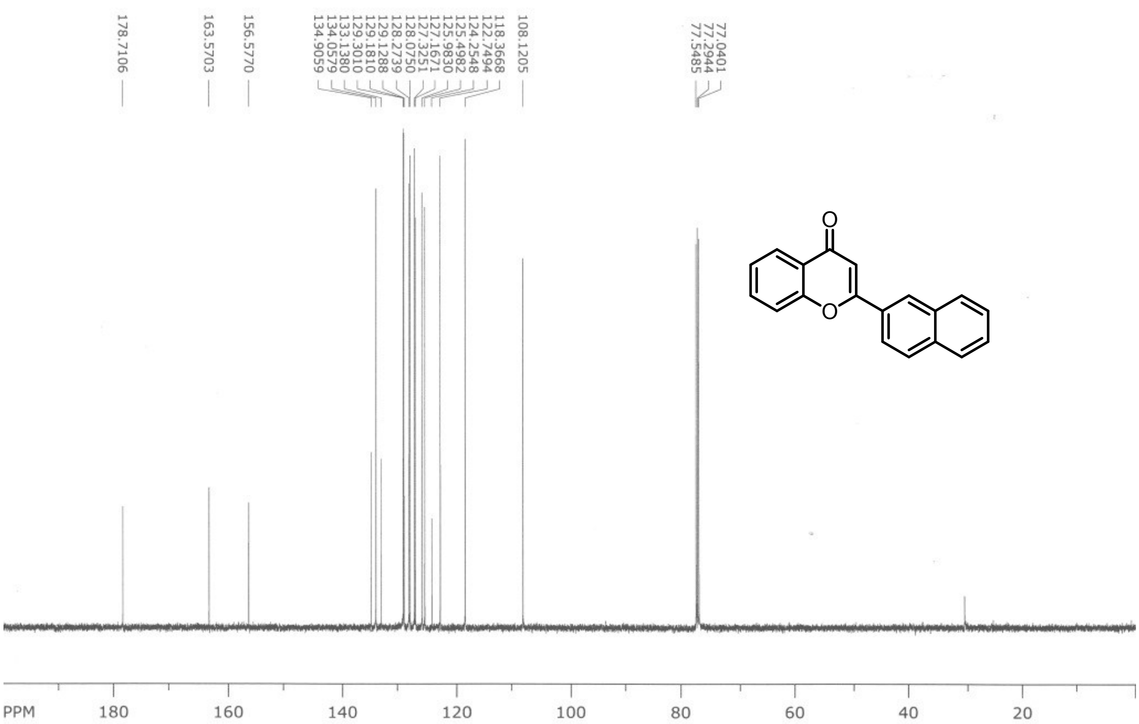


Compound 4e

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

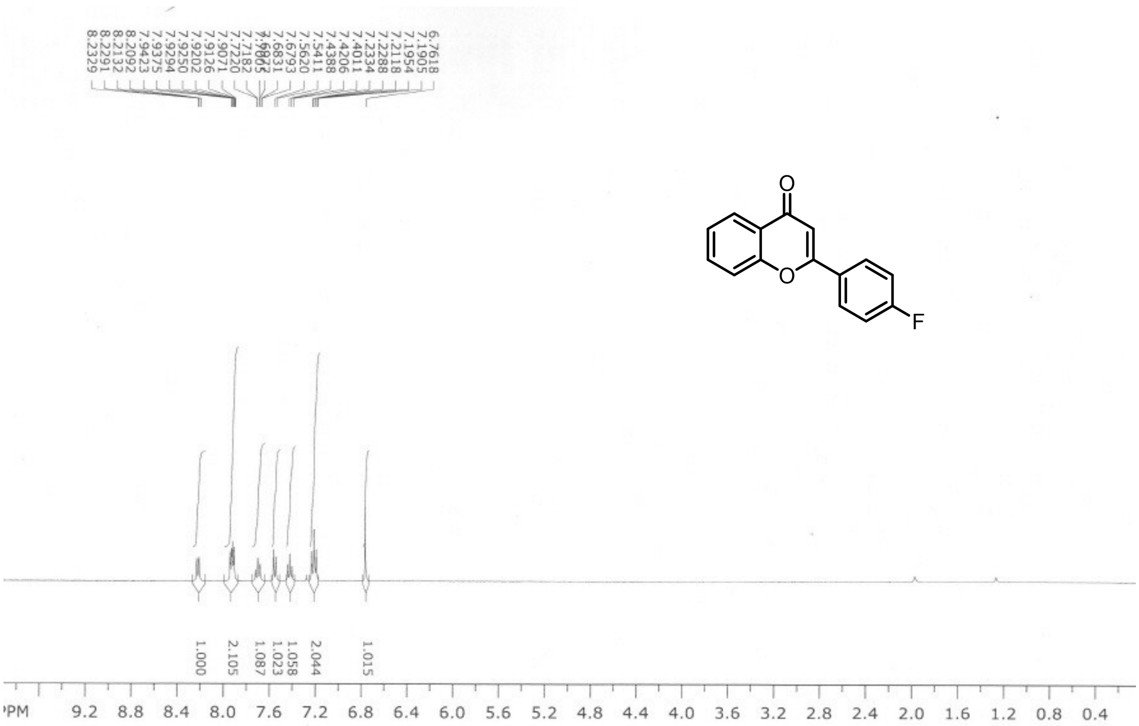


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

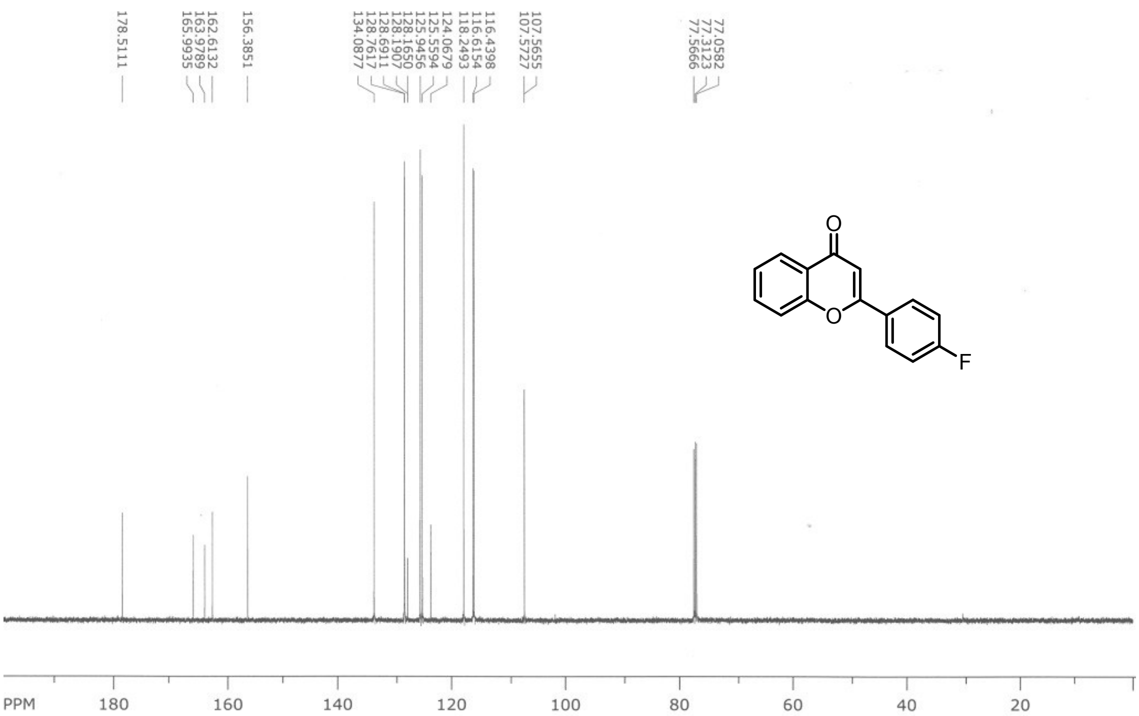


Compound 4f

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

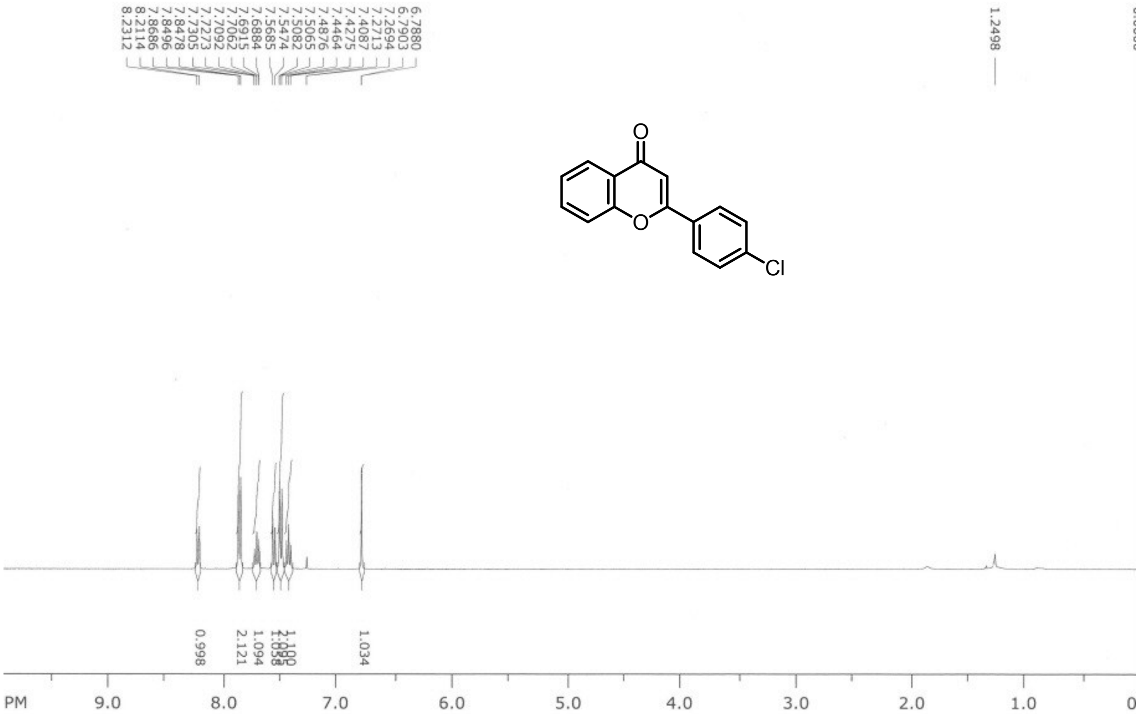


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

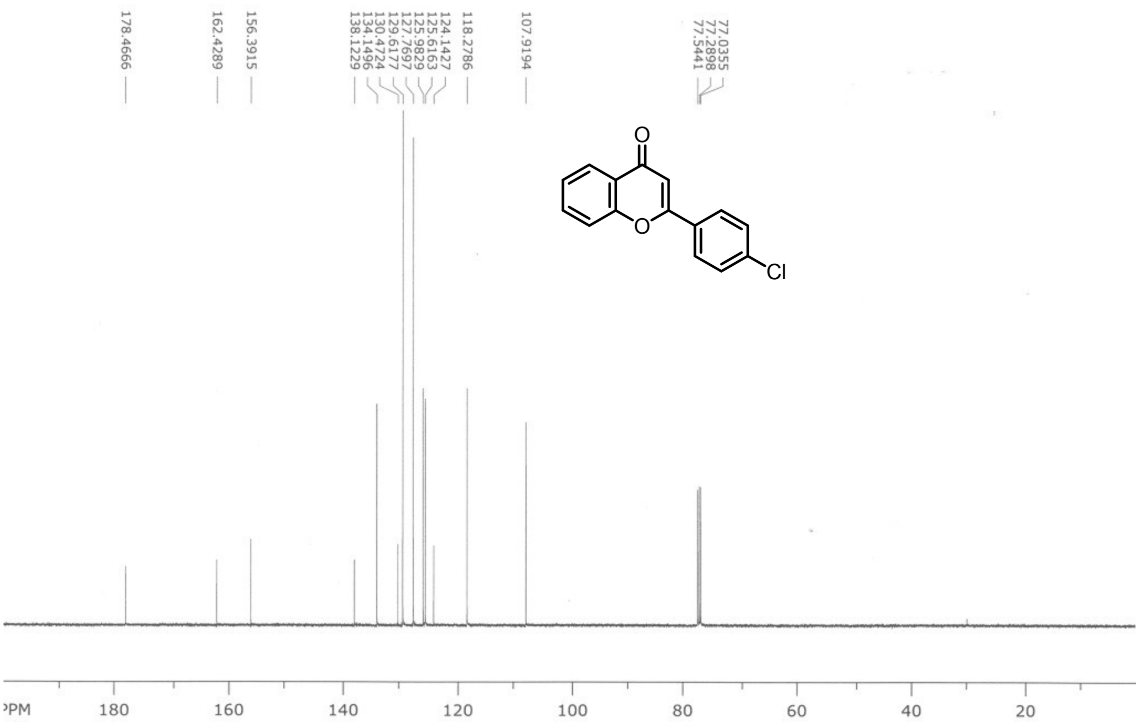


Compound 4g

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

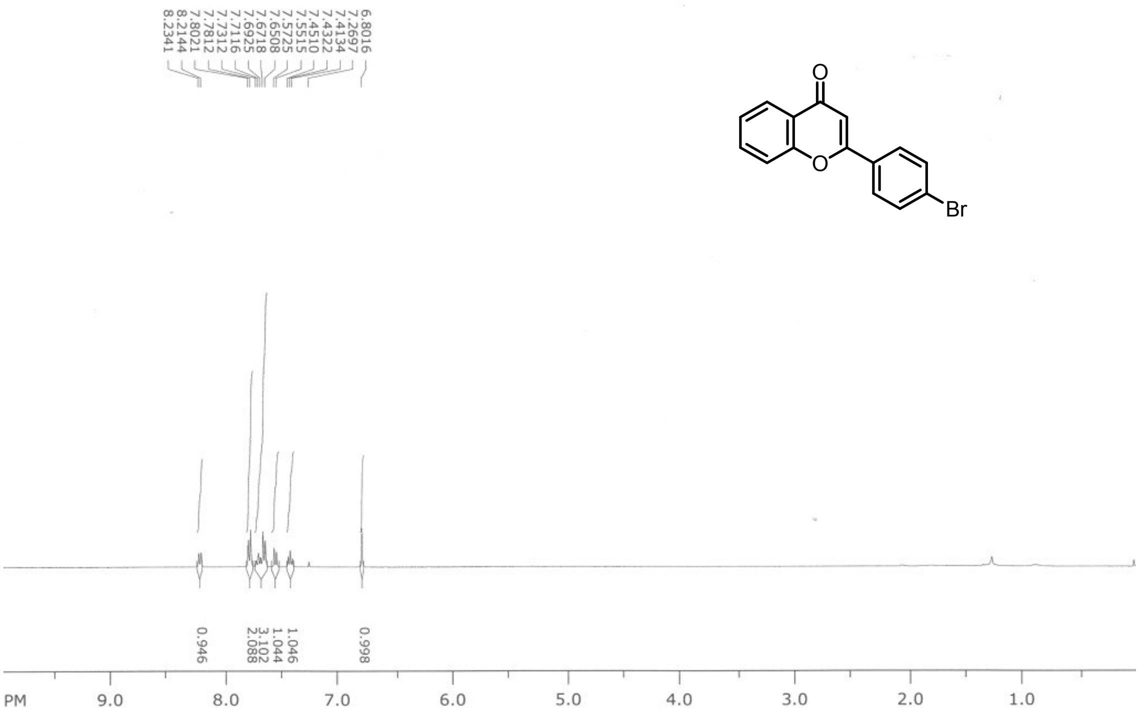


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

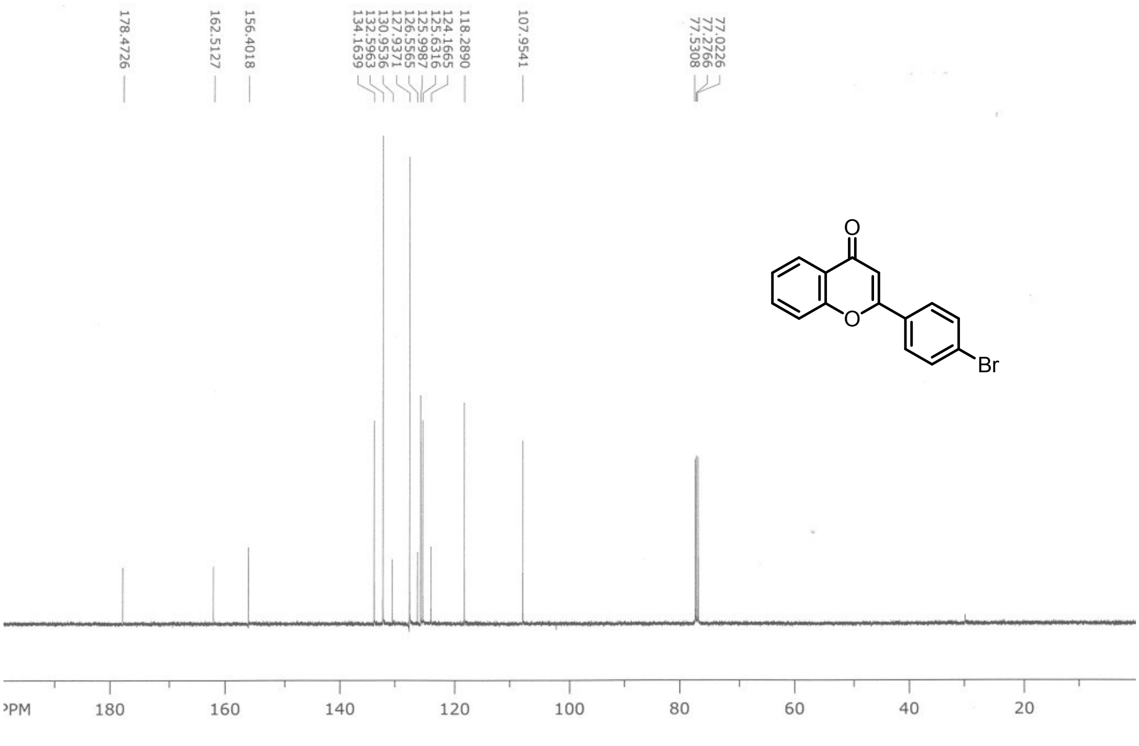


Compound 4h

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

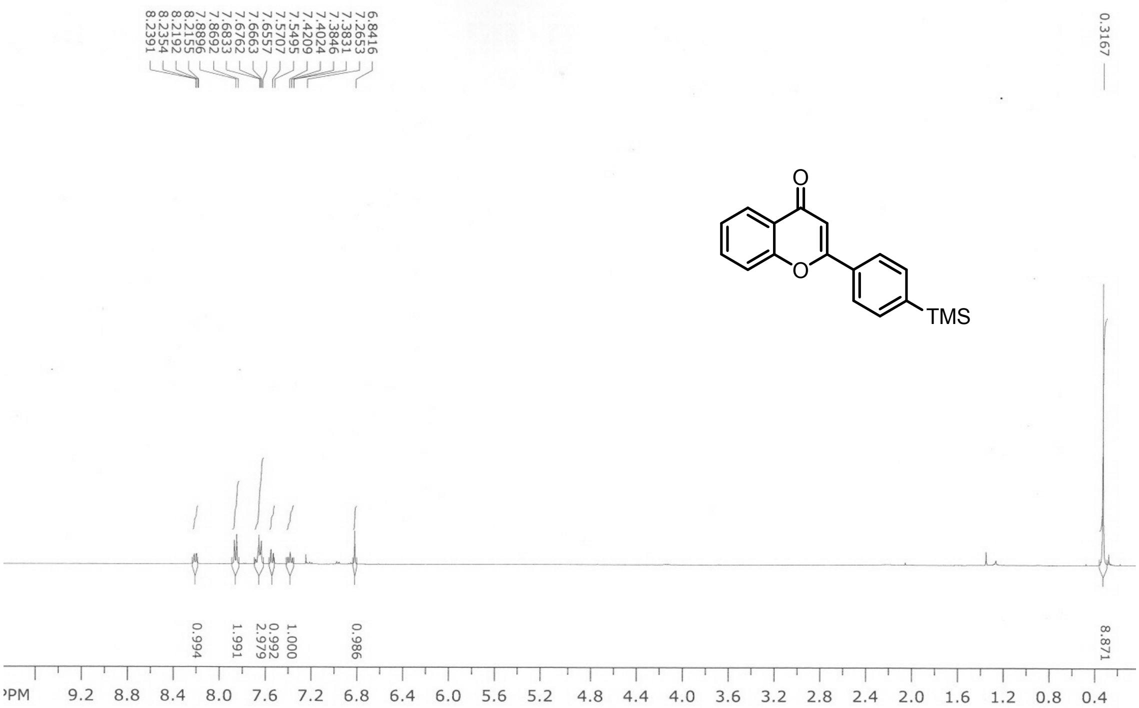


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Compound 4i

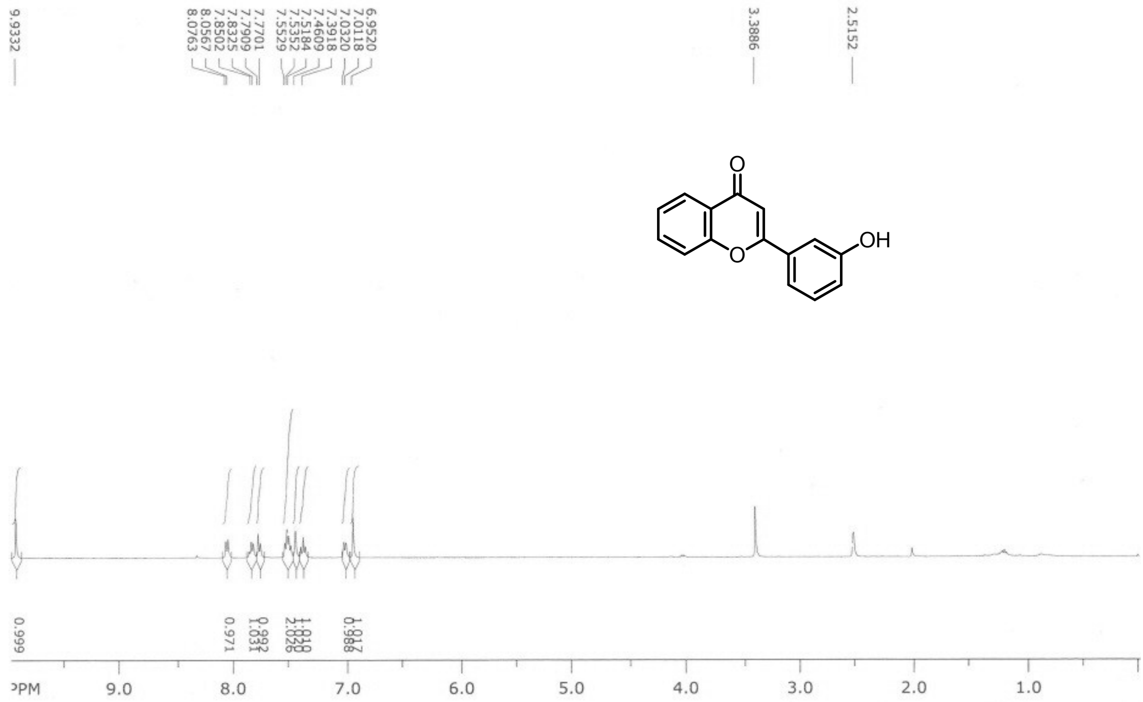
▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



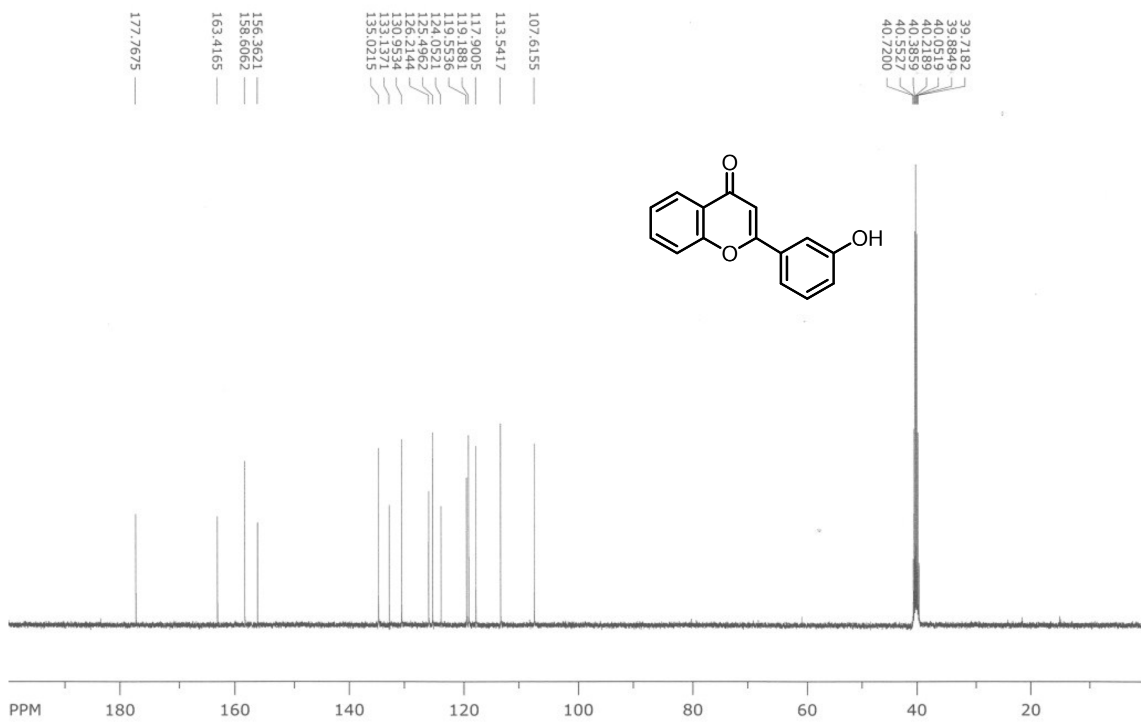
▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

Compound 4j

▼ ^{1}H-NMR (DMSO-d$_6$, 400 MHz)

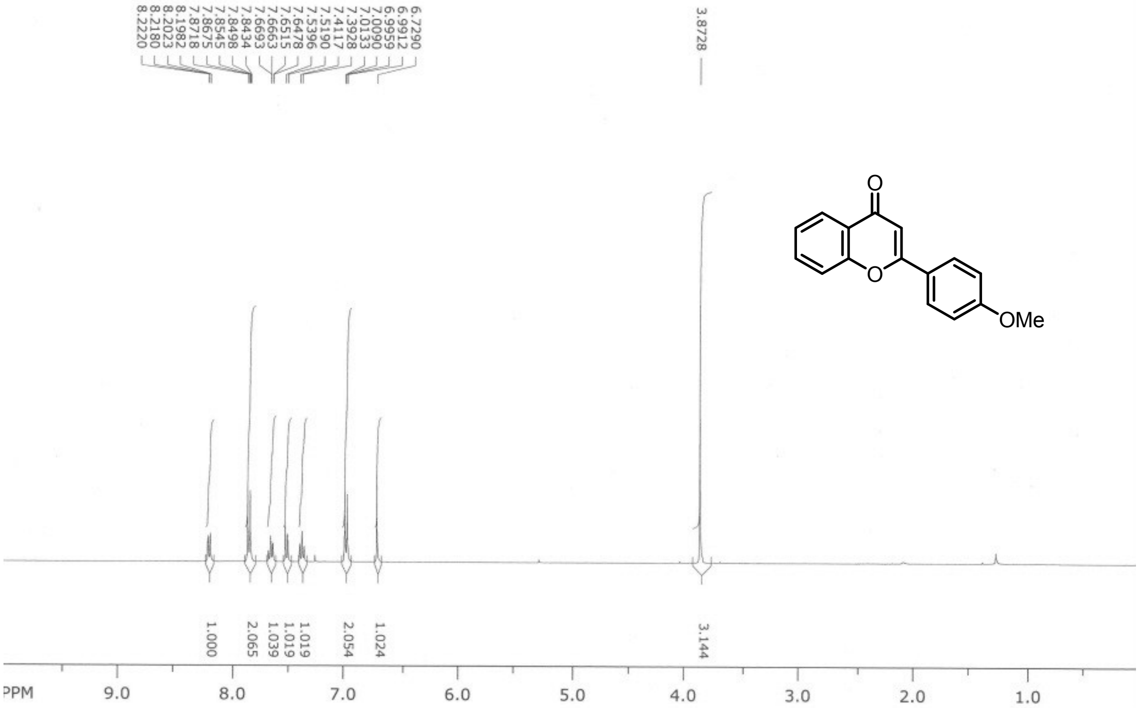


▼ ^{13}C-NMR (DMSO-d$_6$, 125 MHz)

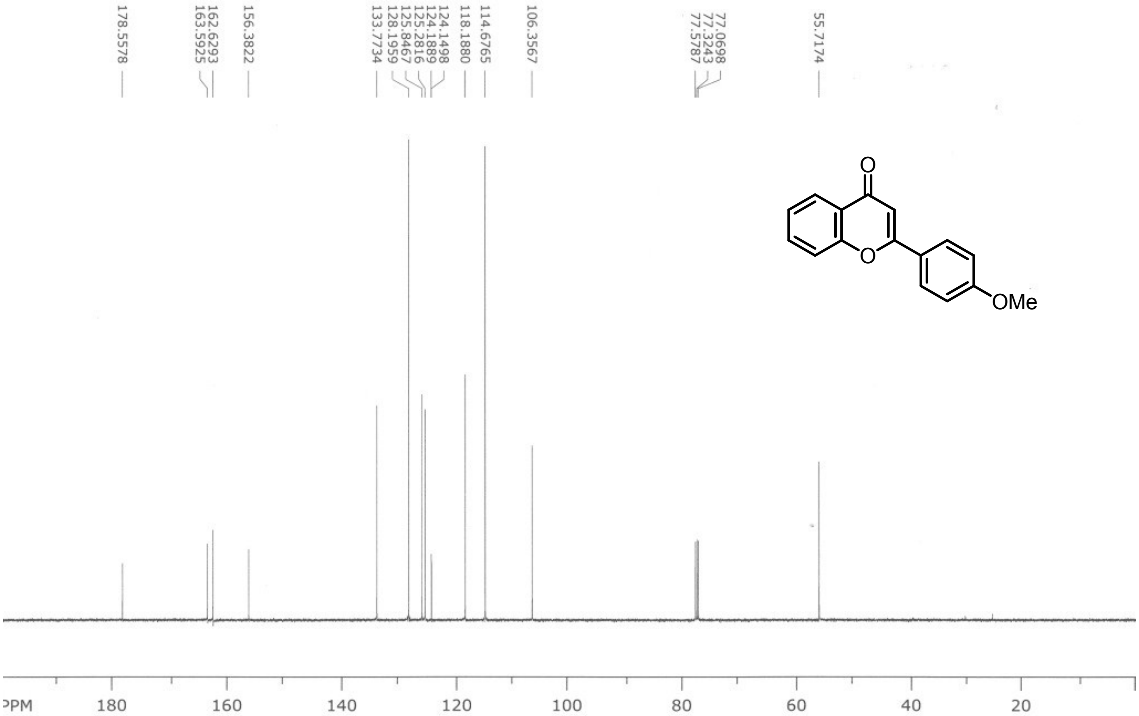


Compound 4k

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

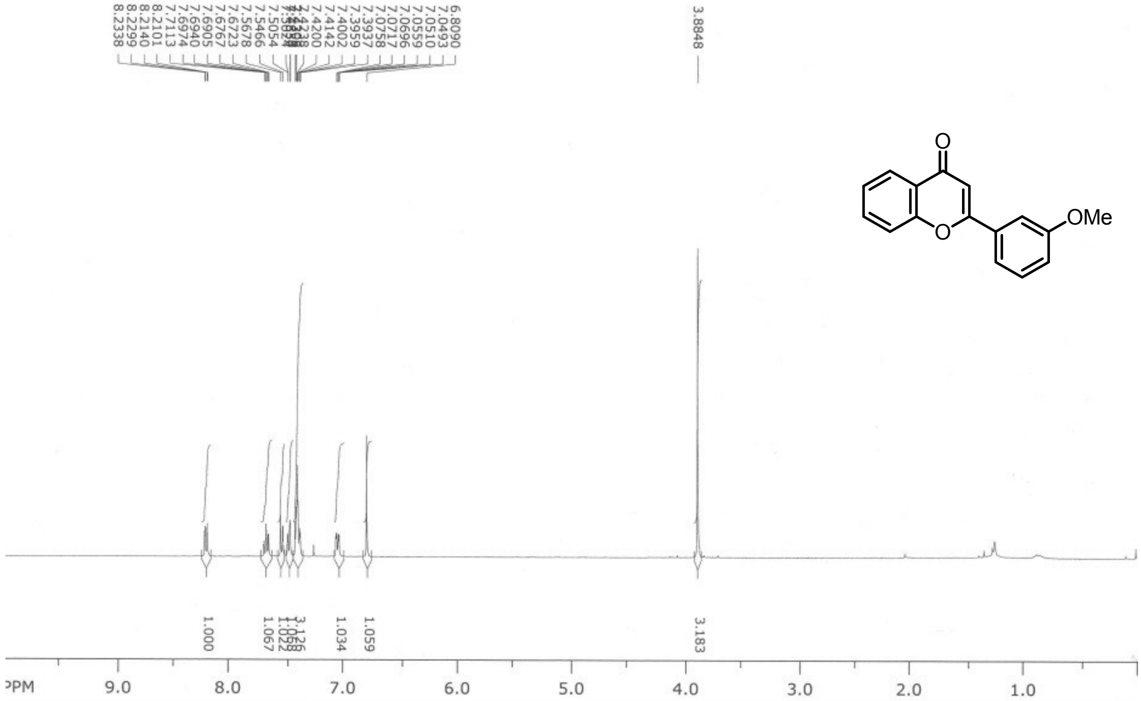


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

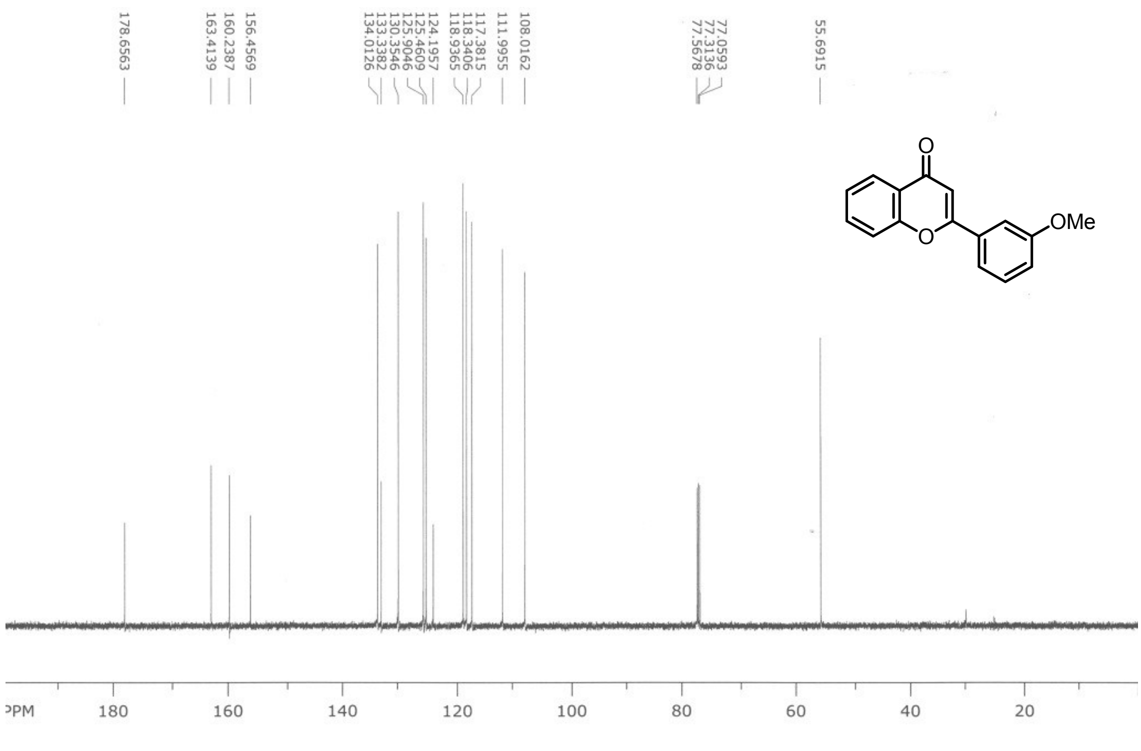


Compound 4l

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

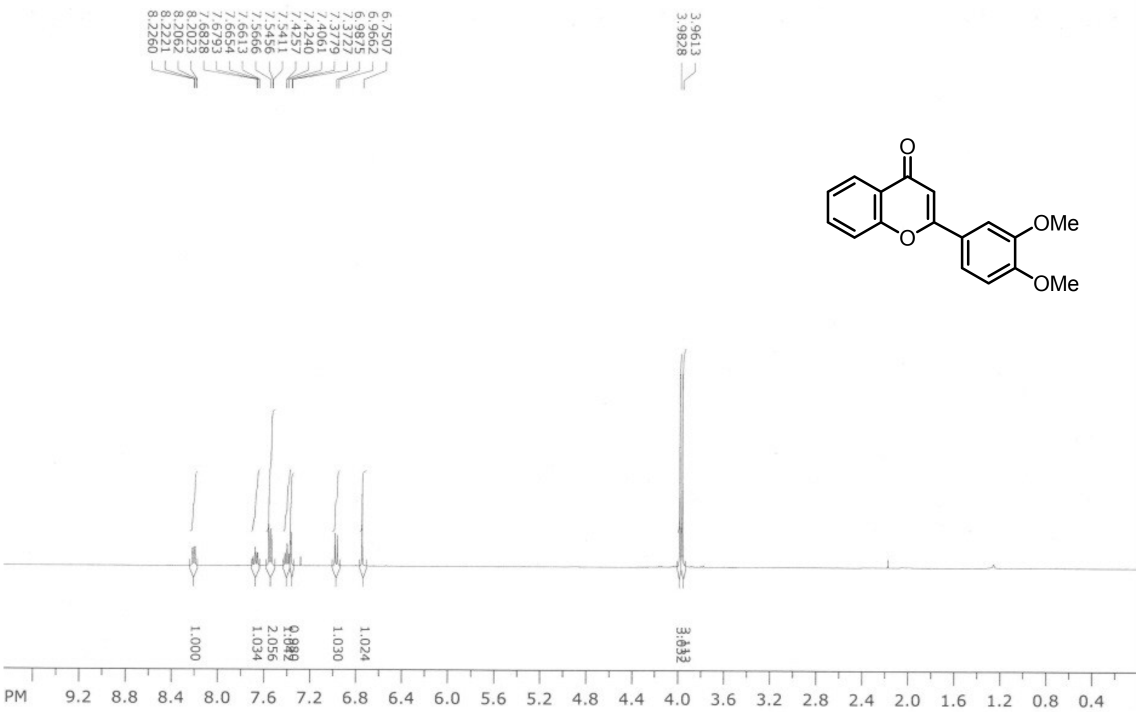


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Compound 4m

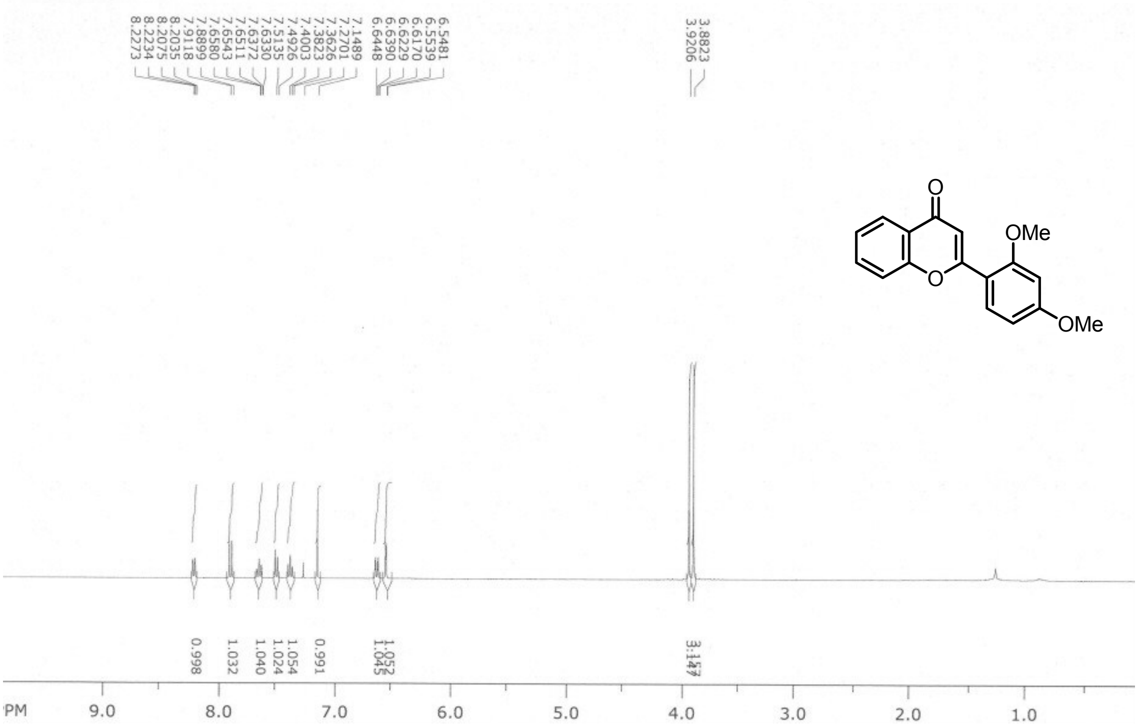
▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



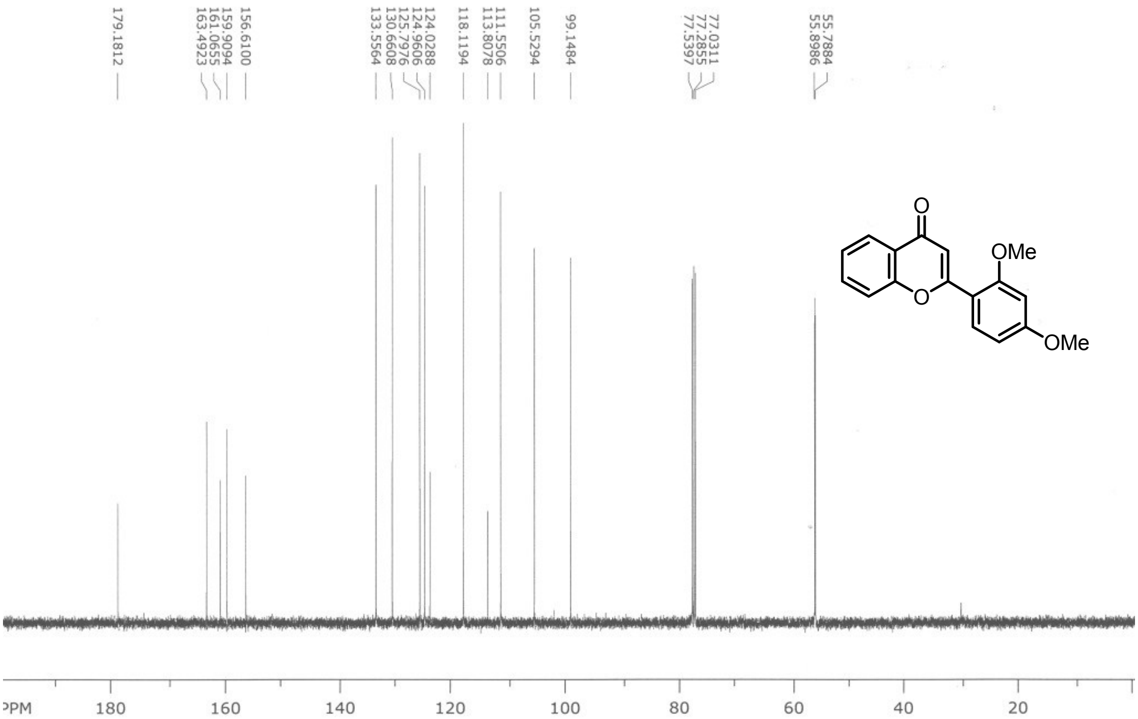
▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

Compound 4n

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



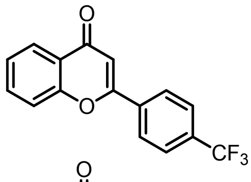
▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

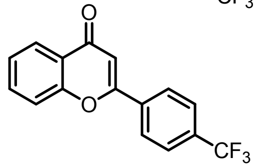


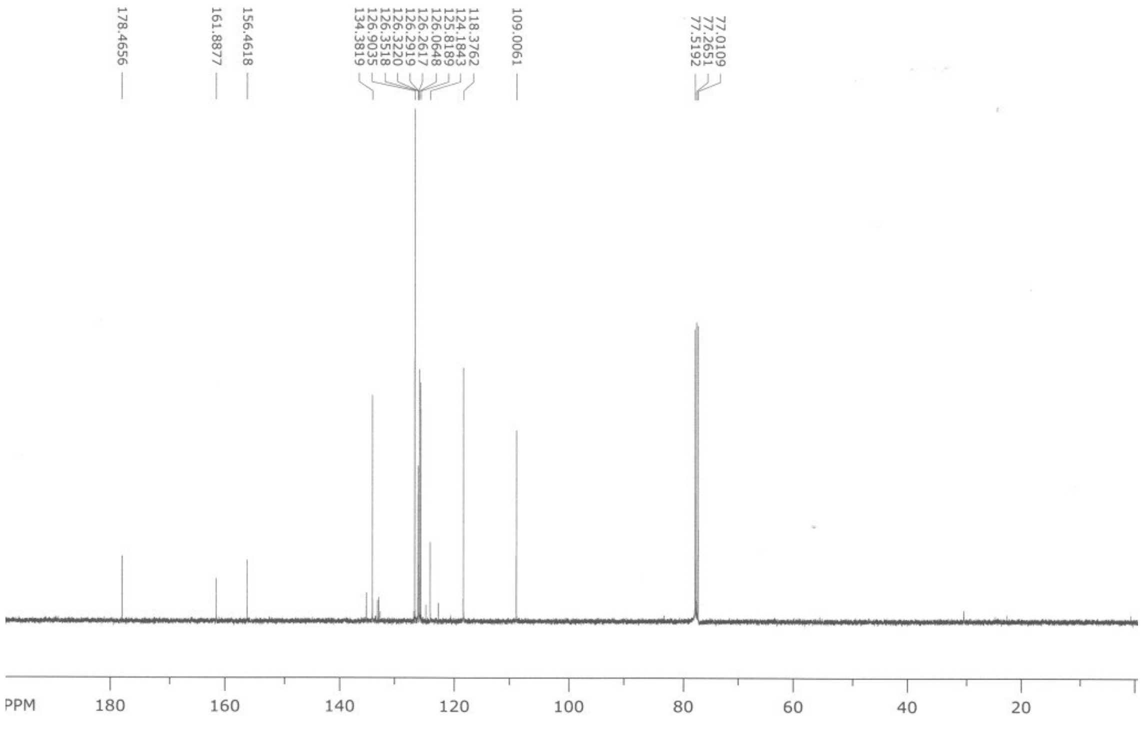
Compound 4o

▼ **^{1}H-NMR ($CDCl_3$, 400 MHz)**

▼ **^{13}C-NMR ($CDCl_3$,125 MHz)**

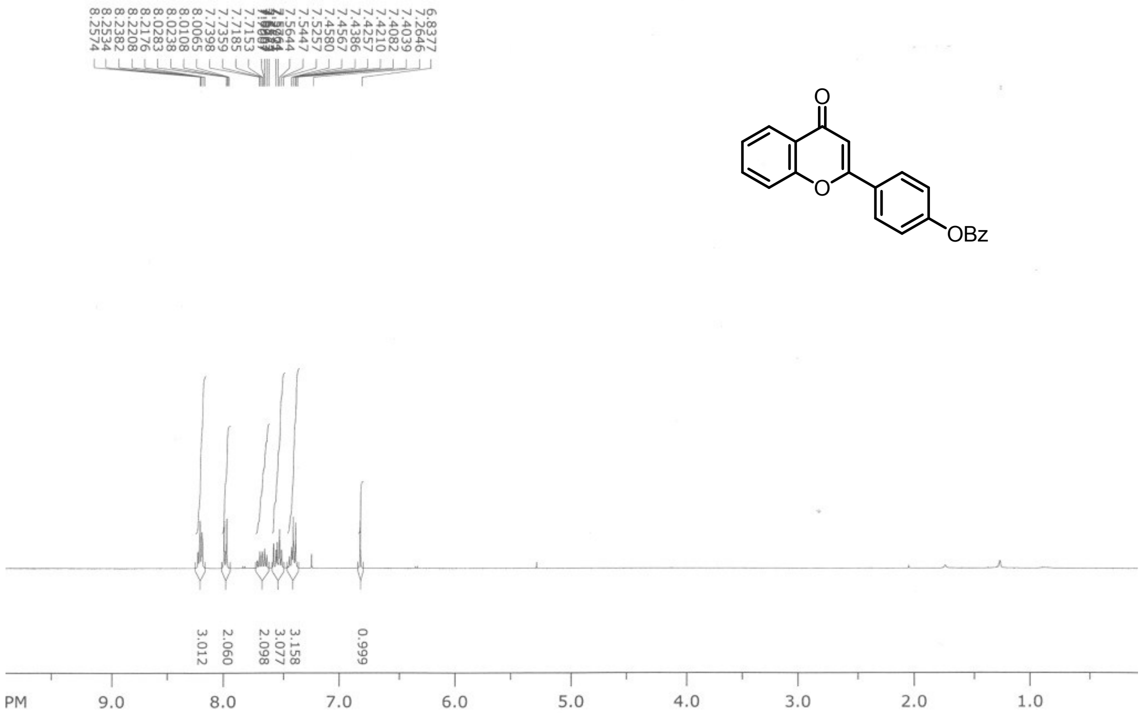




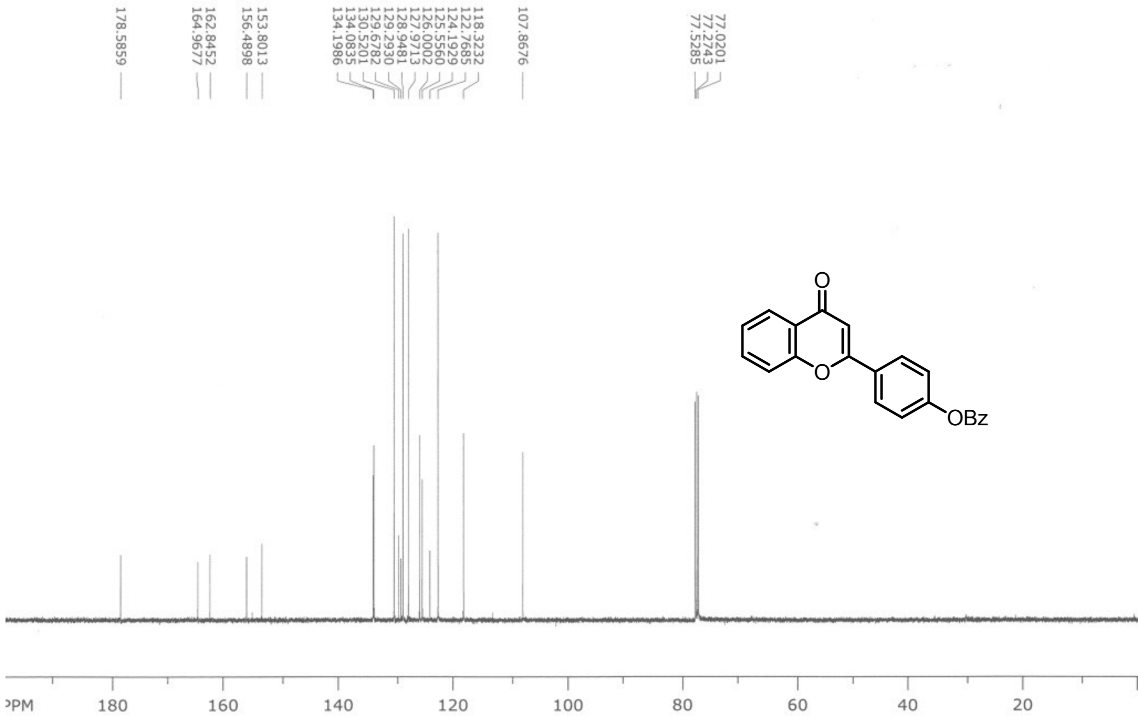


Compound 4p

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

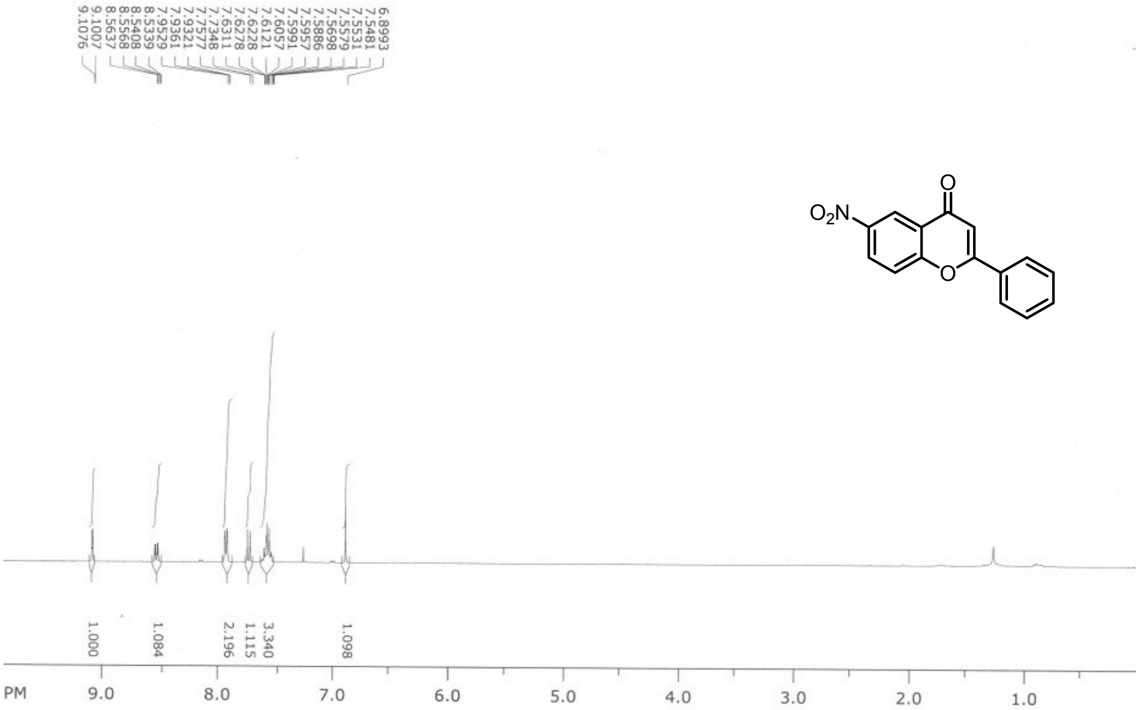


▼ ^{13}C-NMR ($CDCl_3$, 100 MHz)

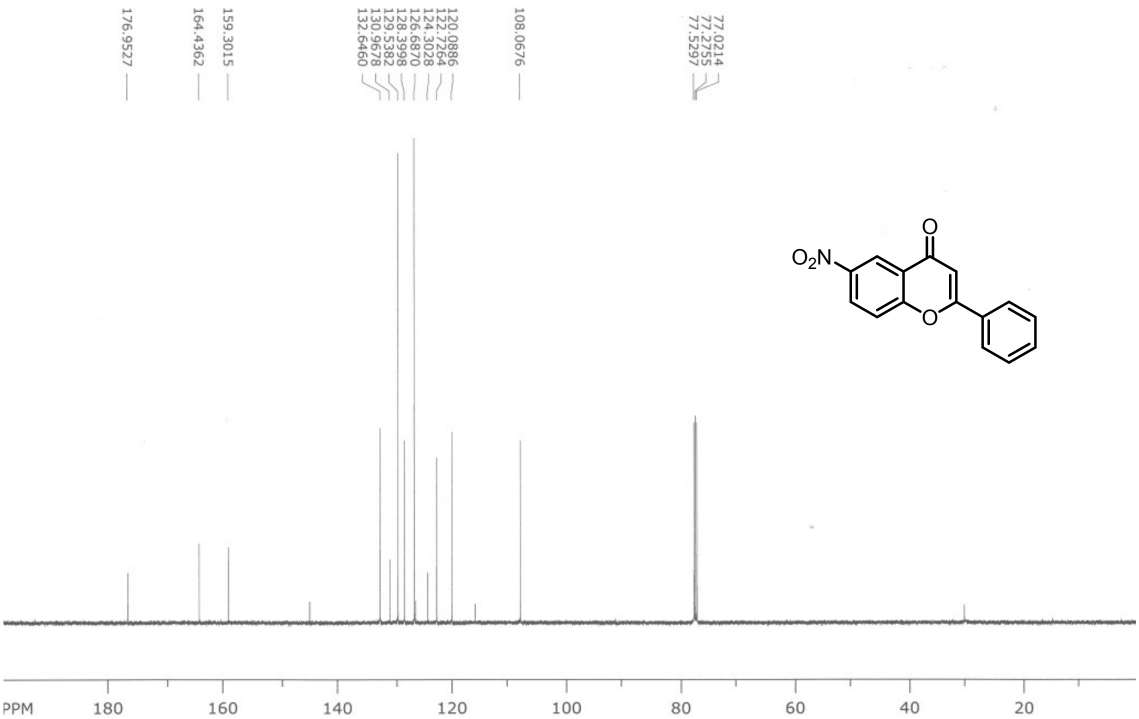


Compound 4q

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

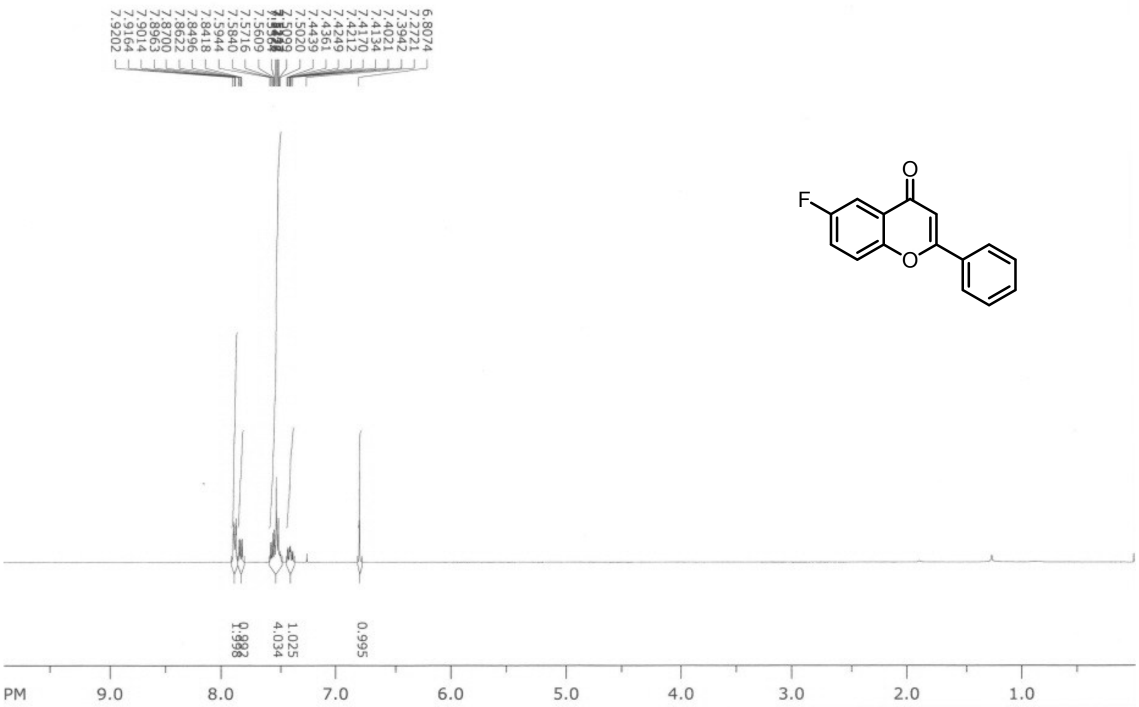


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

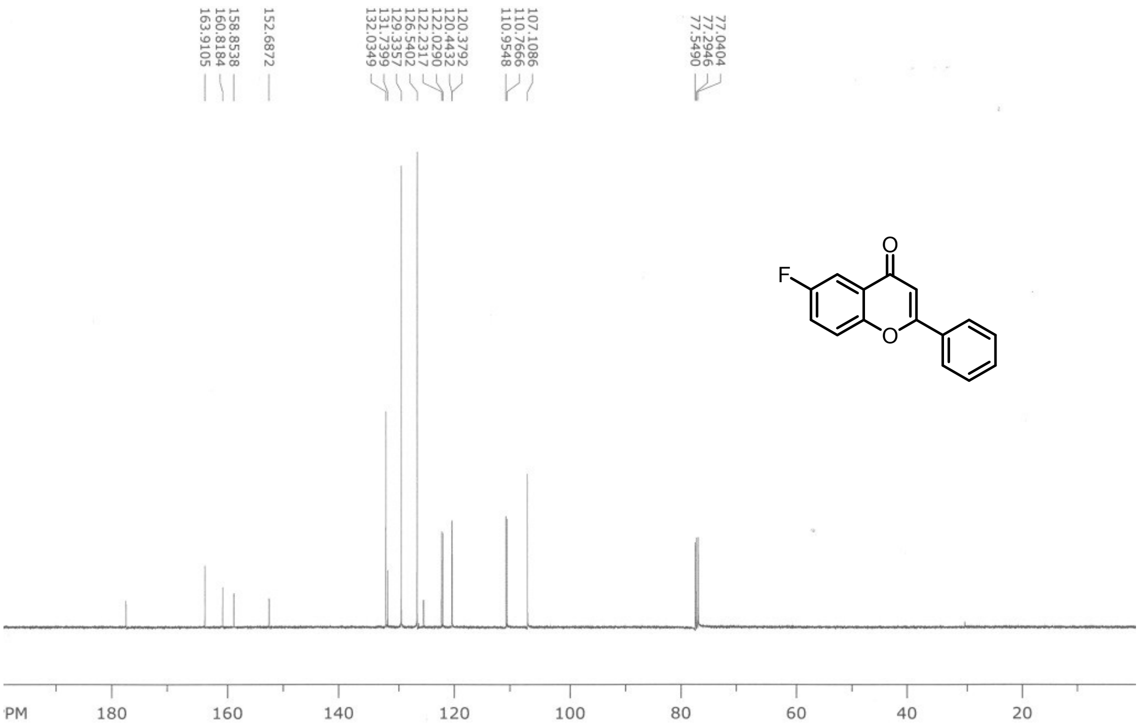


Compound 4r

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

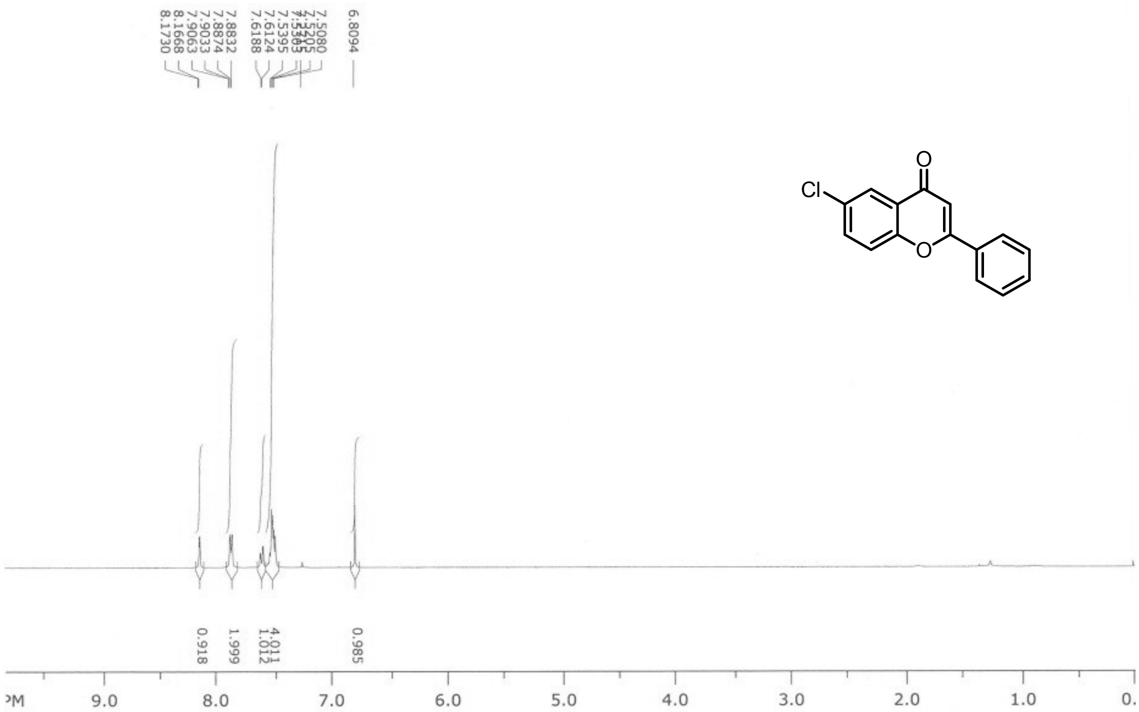


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

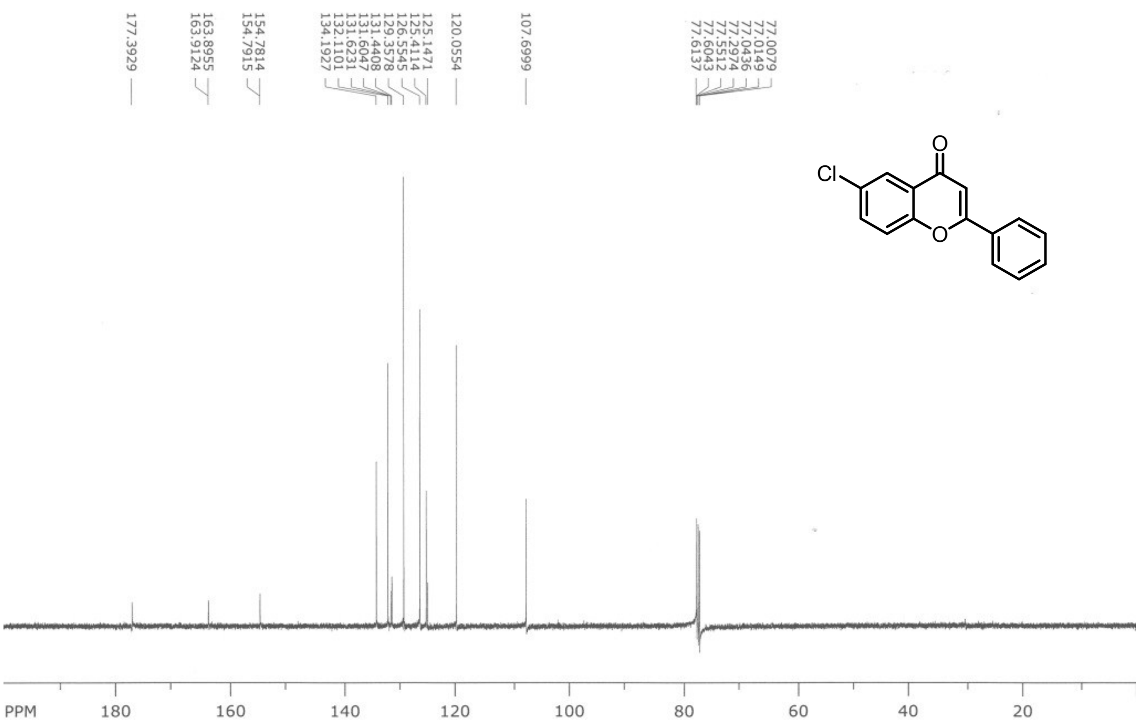


Compound 4s

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

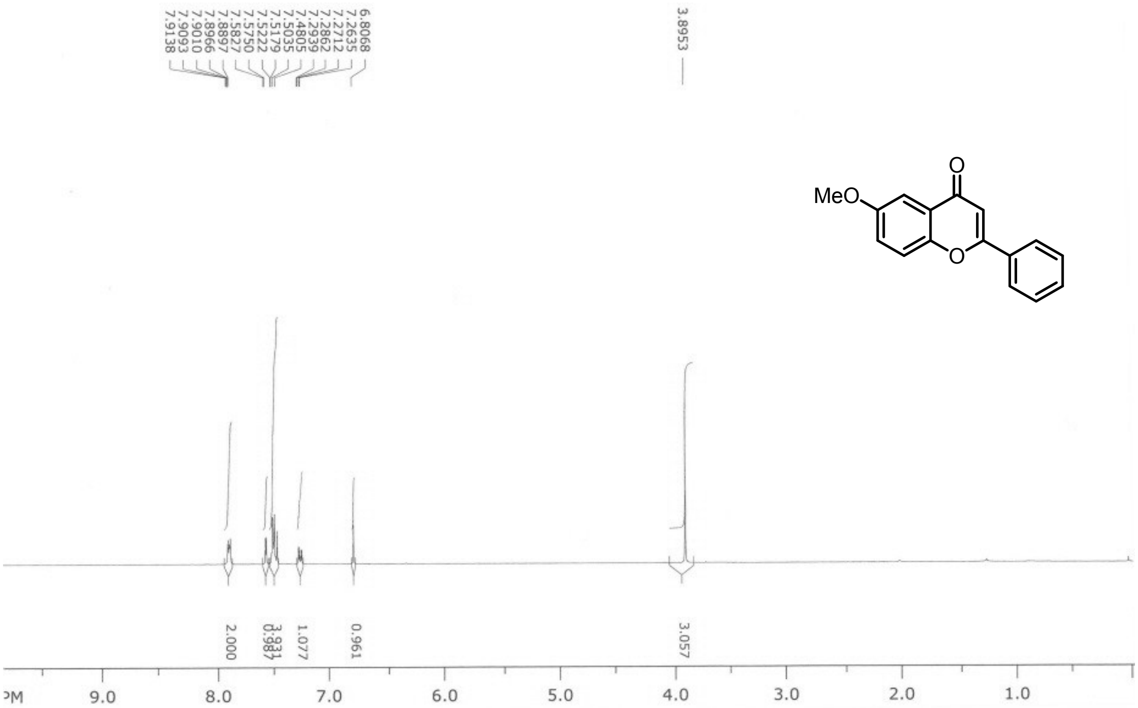


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

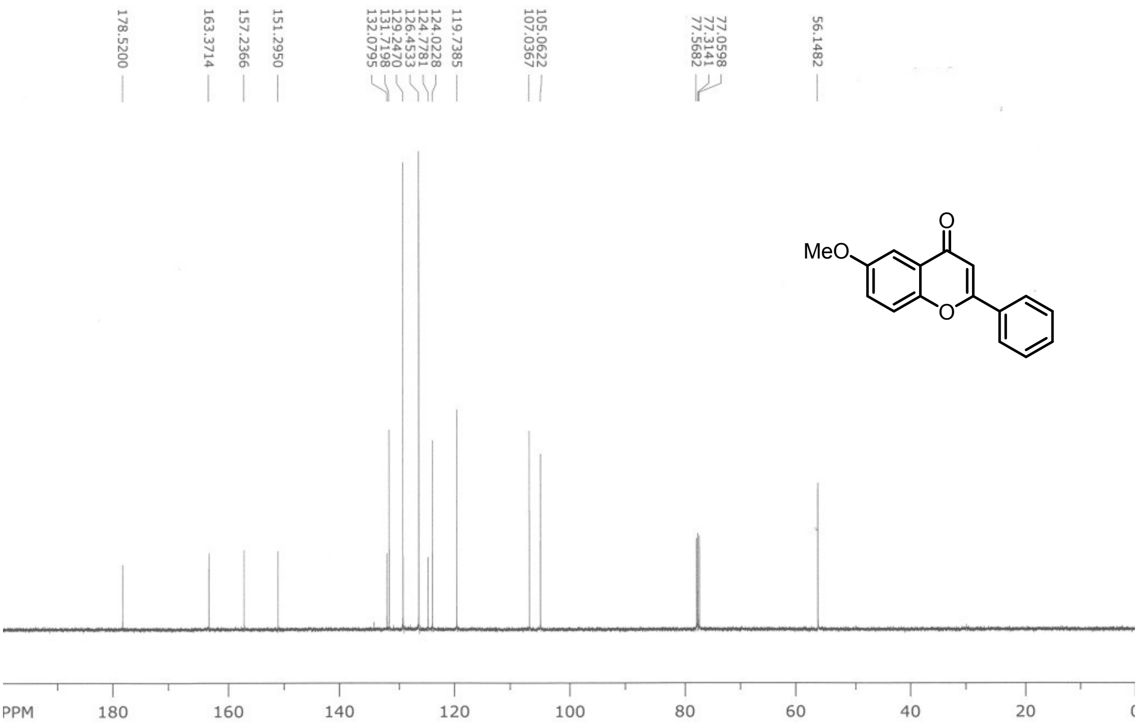


Compound 4t

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

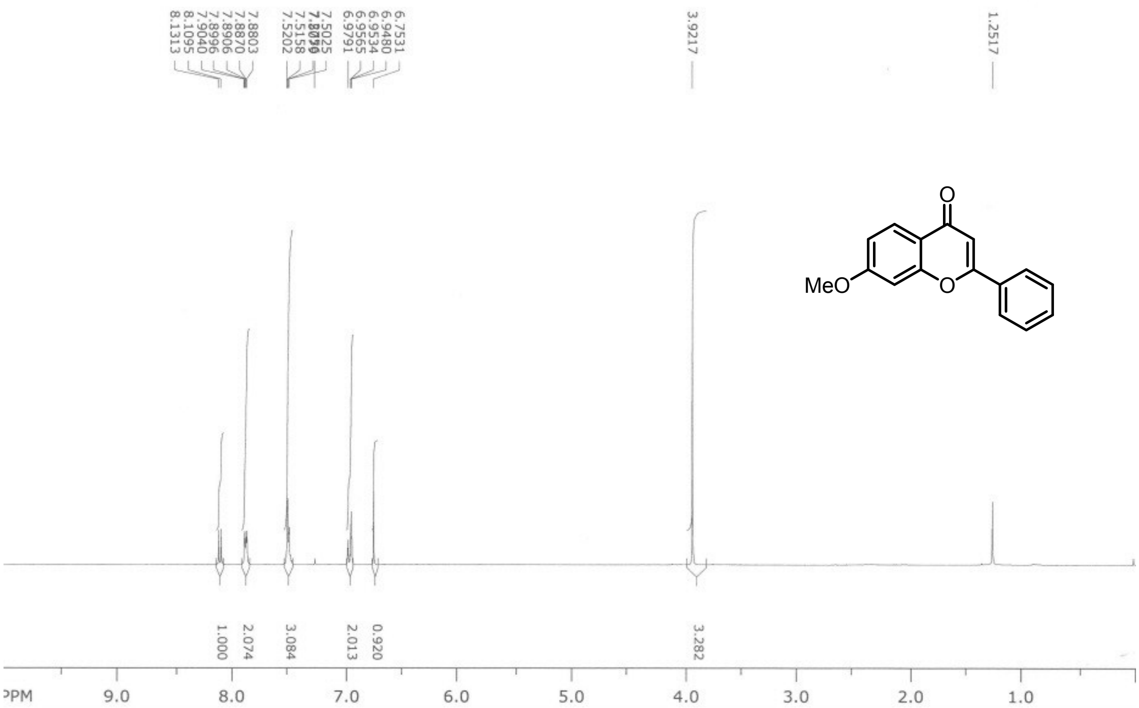


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

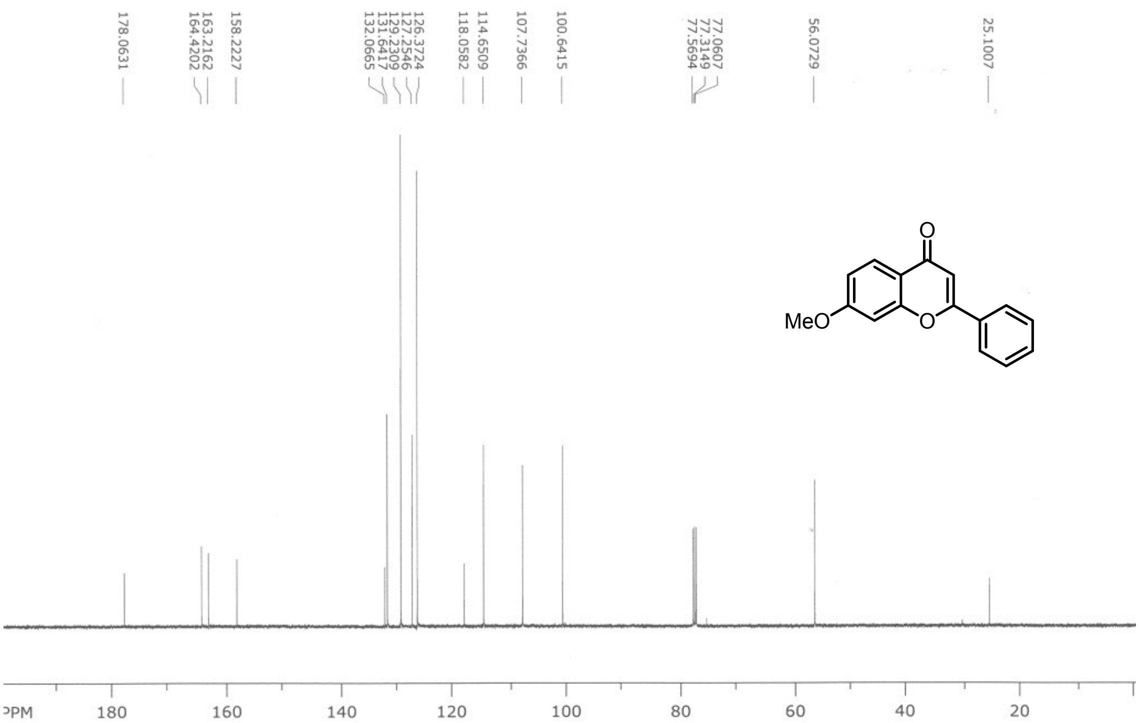


Compound 4u

▼ ^{1}H-NMR (CDCl$_3$, 400 MHz)



▼ ^{13}C-NMR (CDCl$_3$, 125 MHz)



Compound 4v

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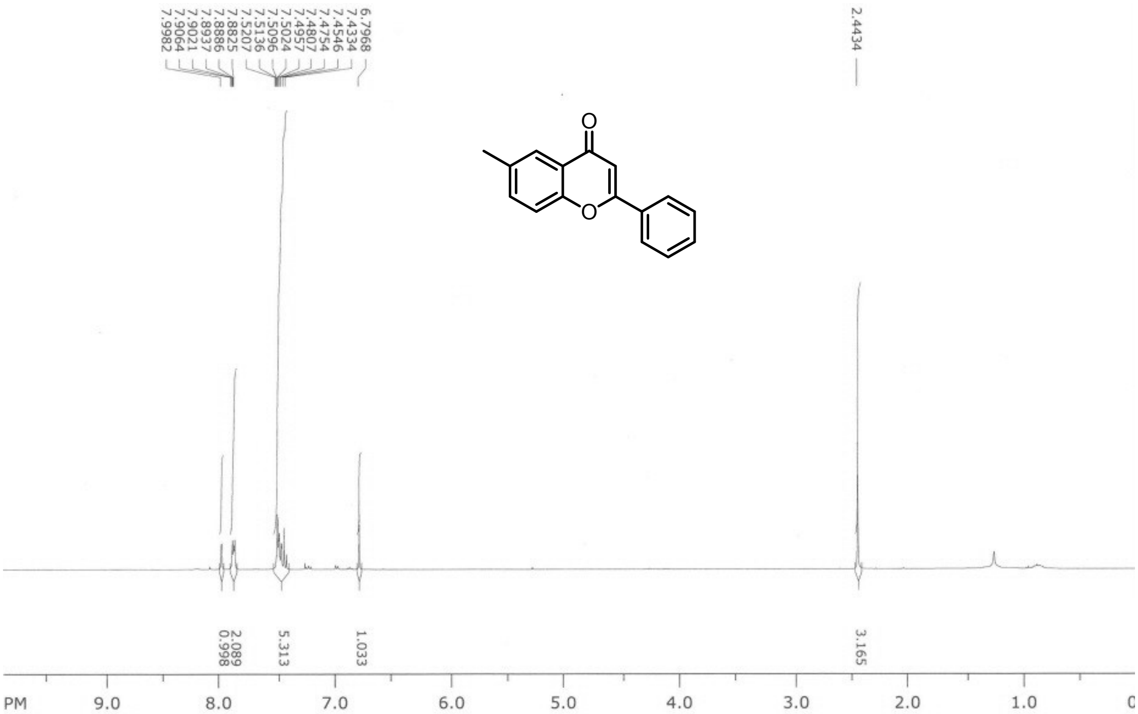
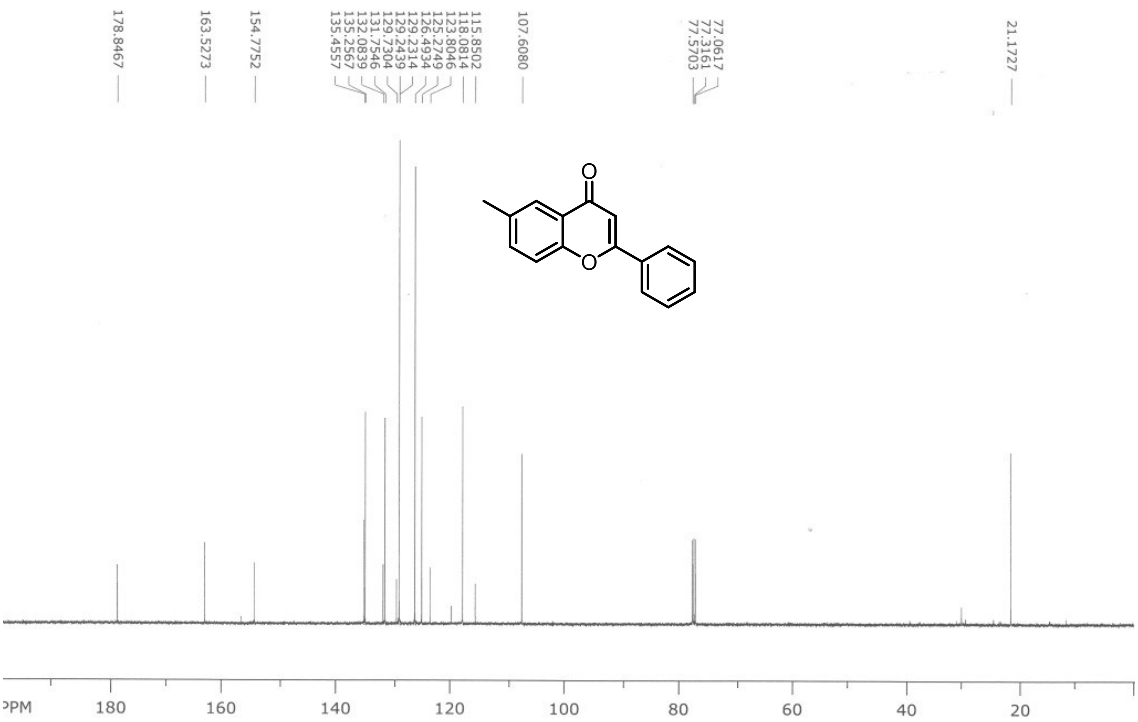


▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Compound 4w

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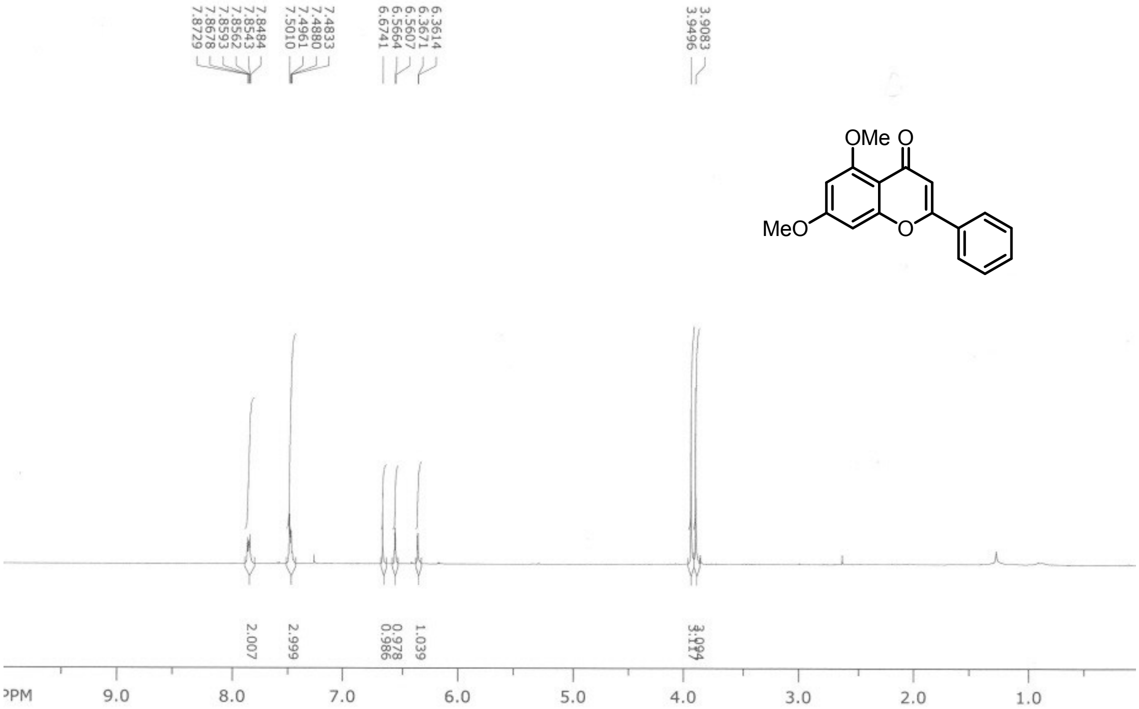
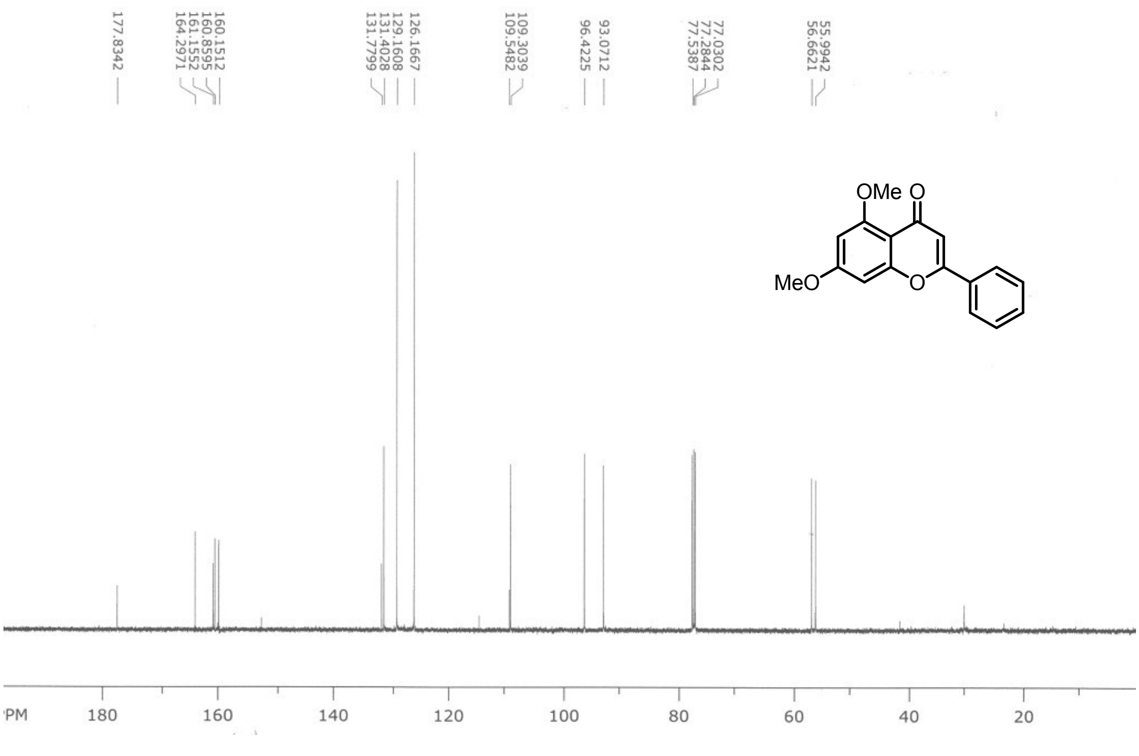


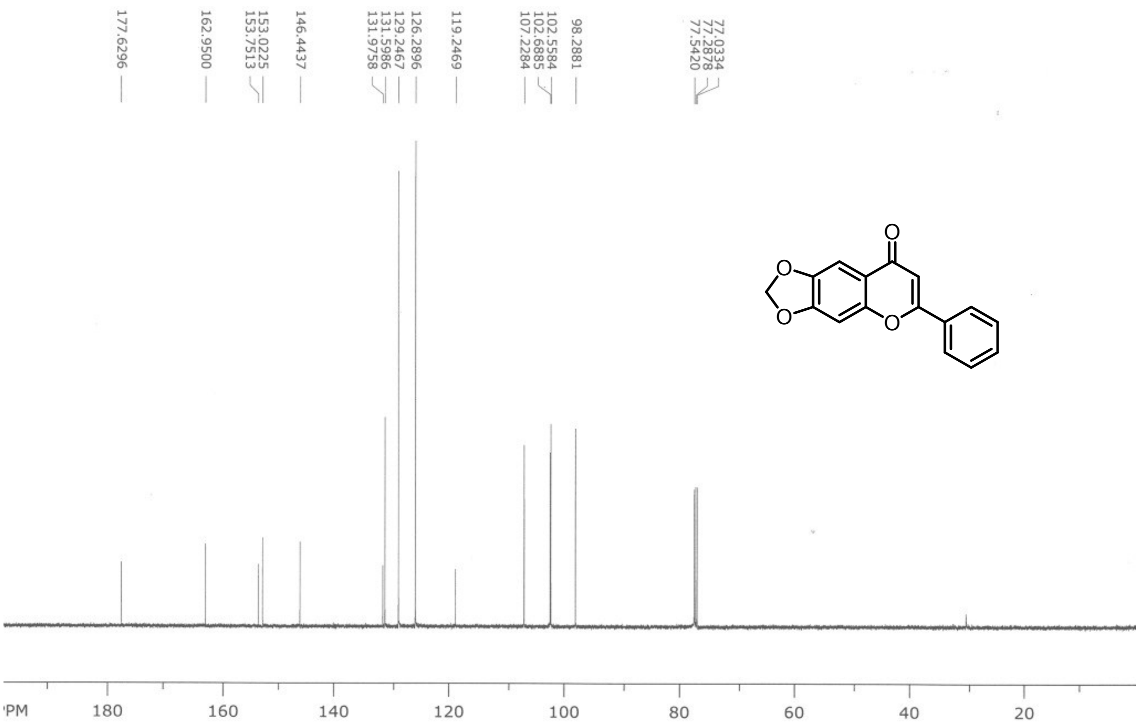
▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Compound 4x

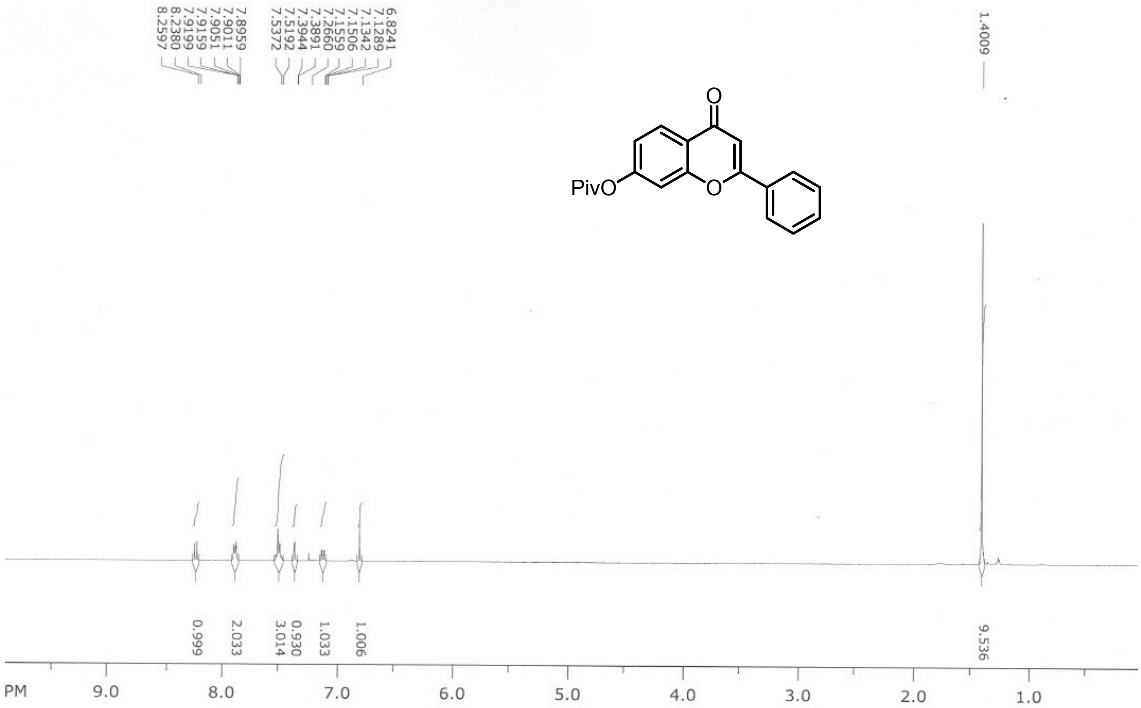
▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)

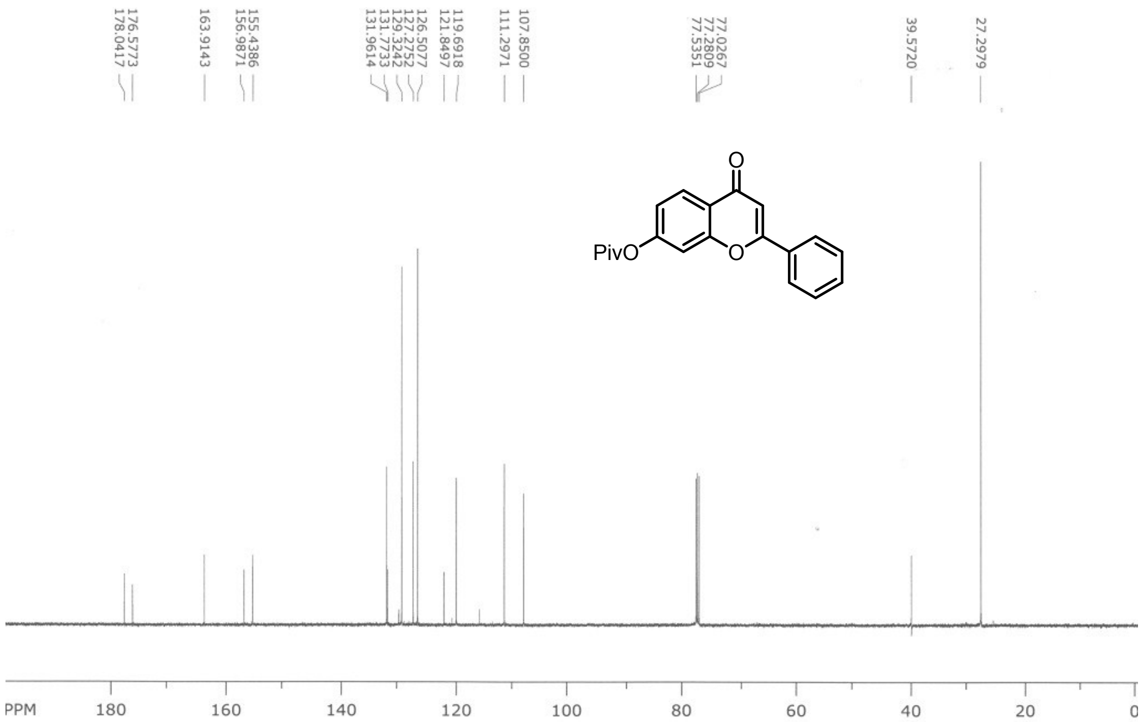


Compound 4y

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

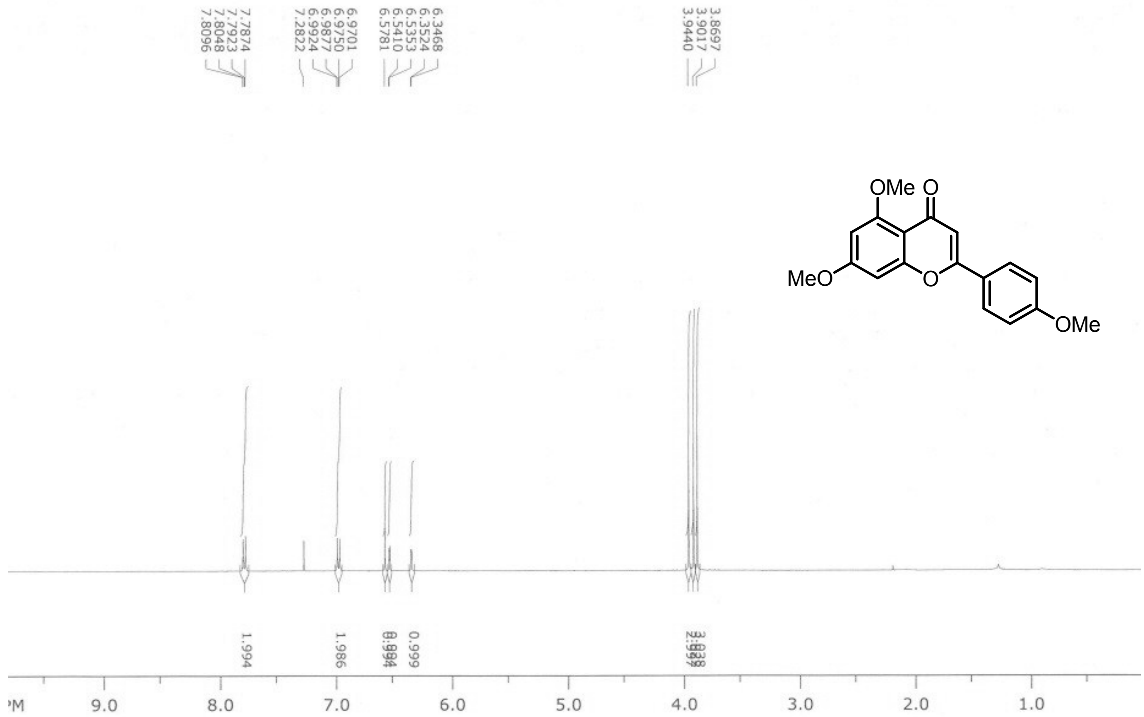


▼ ^{13}C-NMR ($CDCl_3$,125 MHz)

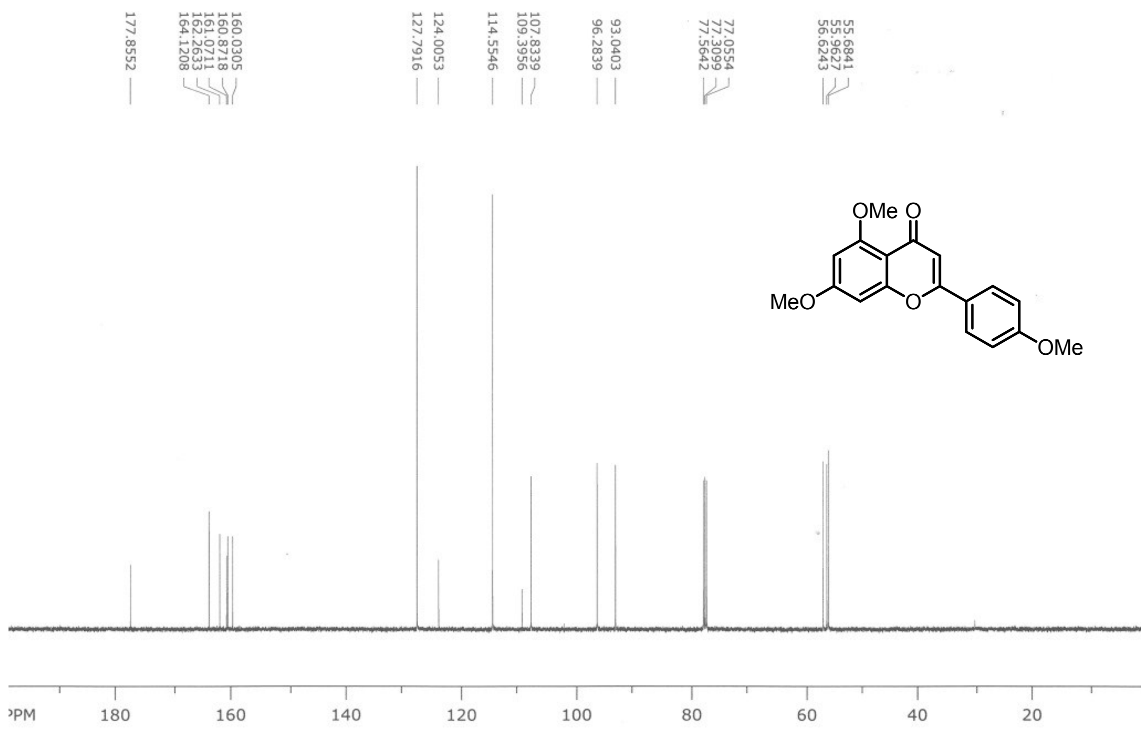


Compound 7

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)

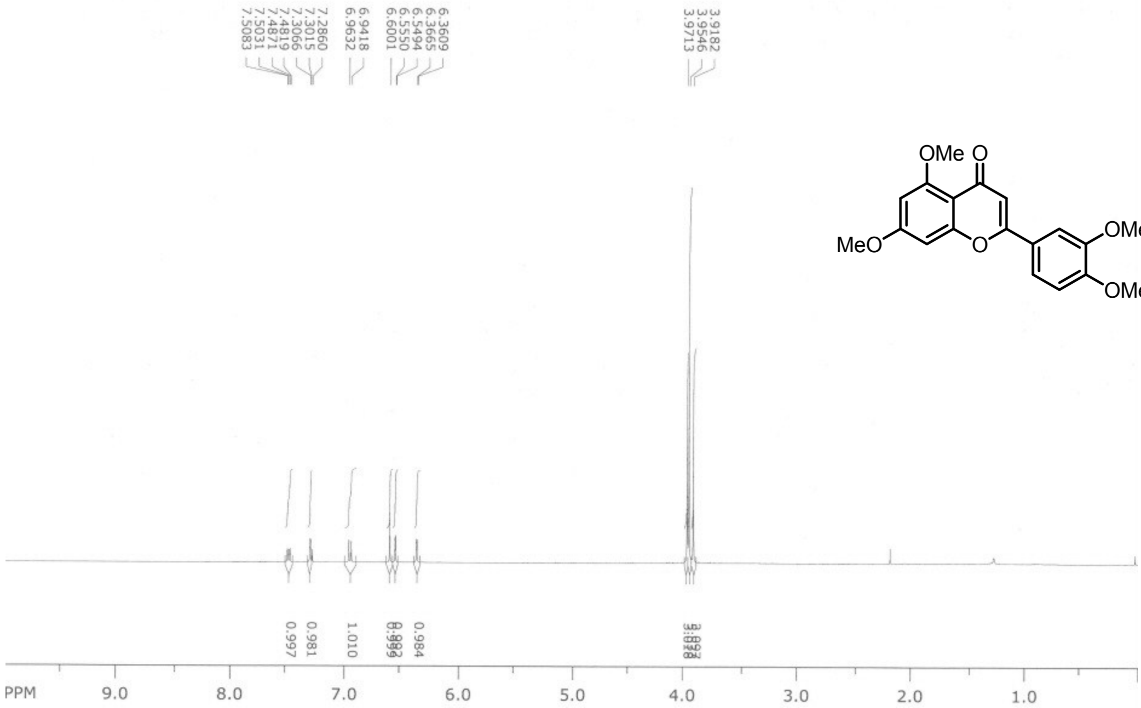


▼ ^{13}C-NMR ($CDCl_3$, 100 MHz)



Compound 9

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



▼ ^{13}C-NMR ($CDCl_3$, 100 MHz)