

Supporting Information

Ruthenium-Catalyzed C-H Activation of Salicylaldehyde and Decarboxylative Coupling of Alkynoic Acids for the Selective synthesis of Homoisoflavonoids and Flavones

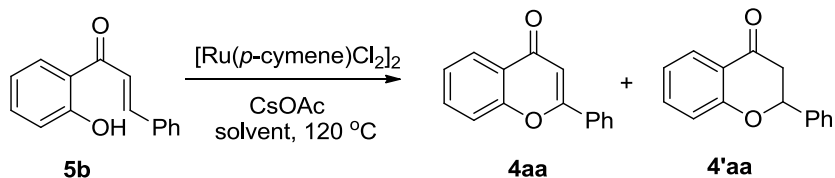
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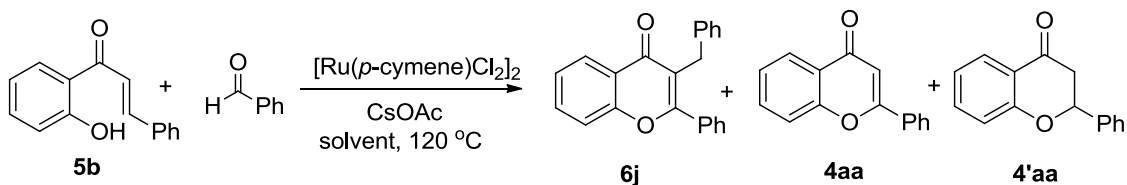
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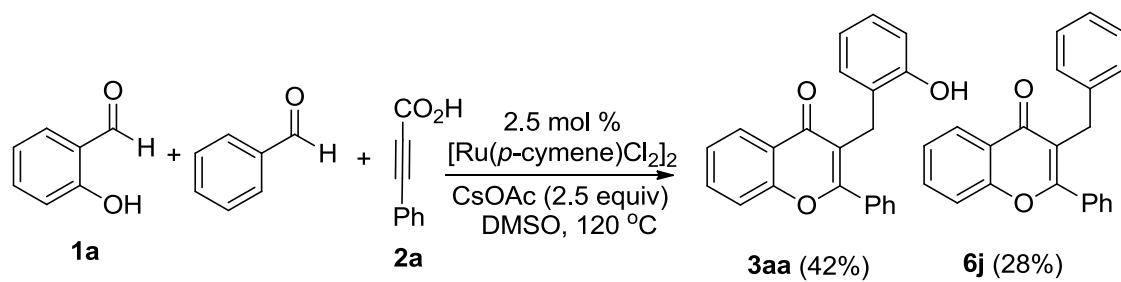
Table S1. The role of ruthenium and base in the reaction with **5b**

Entry	Solvent	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (mol %)	CsOAc (equiv)	Conv. 5b (%)	Yield (%)	
					4aa	4'aa
1	<i>t</i> -AmOH	2.5	2.0	95	58	23
2	<i>t</i> -AmOH	-	2.0	70	-	62
3	<i>t</i> -AmOH	2.5	-	30	-	21
4	<i>t</i> -AmOH	-	-	35	-	26
5	DMSO	2.5	2.0	91	72	9
6	DMSO	-	2.0	52	5	34
7	DMSO	2.5	-	5	-	-
8	DMSO	-	-	5	-	-

Table S2. The role of ruthenium and base in the reaction with **5b** and benzaldehyde.

Entry	Solvent	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (mol %)	CsOAc (equiv)	Conv. 5b (%)	Yield (%)		
					6j	4aa	4'aa
1	<i>t</i> -AmOH	2.5	2.0	74	-	54	6
2	<i>t</i> -AmOH	-	2.0	53	-	4	28
3	<i>t</i> -AmOH	2.5	-	16	-	5	4
4	<i>t</i> -AmOH	-	-	4	-	-	-
5	DMSO	2.5	2.0	92	80	-	-
6	DMSO	-	2.0	22	-	-	11
7	DMSO	2.5	-	4	-	-	-
8	DMSO	-	-	5	-	-	-

Scheme S1. Competitive experiment



S1. General information

All chemicals used were of reagent/analytical grade or of the highest purity available. All chemicals were purchased and used as such without further purification. Analytical thin layer chromatography (TLC) was performed on Merck pre-coated silica gel 60 F₂₅₄ plates. Visualization on TLC was achieved by the use of UV light (254 nm). ¹H NMR (500 and 600 MHz) and ¹³C NMR (125 and 150 MHz) was recorded in CDCl₃ on VARIAN VnmrJ. In ¹H NMR chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br (broad), s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), td (triplet of doublet), ddd (doublet of doublet of doublet), m (multiplet). Coupling constants *J*, were reported in hertz unit (Hz). ¹³C NMR was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center of a triplet at 77.0 ppm of chloroform-*d*. High resolution mass spectra (HRMS) were obtained using EI or ESI method. Flash column chromatography was performed with 300–400 mesh silica gel using ethyl acetate/*n*-hexane as an eluent to isolate the products.

S2. X-Ray Crystallography data

X-Ray Crystallography. Reflection data were collected on a Bruker APEX-II CCD-based diffractometer with graphite-monochromatized MoK α radiation (λ = 0.71073 Å). The hemisphere of reflection data were collected as ω scan frames at a rate of 0.5°/frame and an

exposure time of 10 s/frame. Cell parameters were determined and refined by the APEX2 program.¹ Data reduction was also performed by using the APEX2 program. The obtained data were corrected for Lorentz and polarization effects. An empirical absorption correction was applied by using the SADABS program. The structures of the compounds were solved by direct methods and refined by the full matrix least-squares methods using the SHELXTL program package with anisotropic thermal parameters for all non-hydrogen atoms.² CCDC 1576196, contain the supplementary crystallographic data for this paper. Selected bond lengths and angles in complexes are summarized in Table 1. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

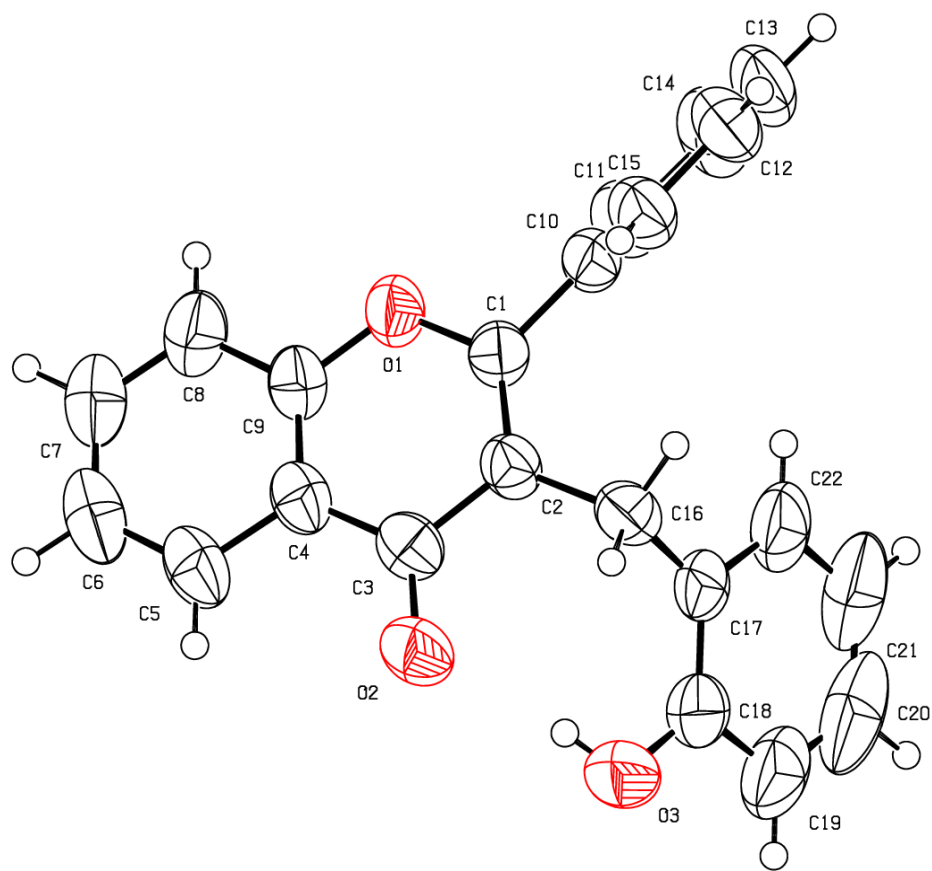


Table S3 . Crystallographic data and parameters for compound **3aa**.

	Compound 3aa
formula	C ₂₂ H ₁₅ O ₃
formula weight	327.34
crystal system	Monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	7.0355(16)
<i>b</i> (Å)	16.901(3)
<i>c</i> (Å)	14.017(3)
α (°)	90
β (°)	90.230(13)
γ (°)	90
<i>V</i> (Å ³)	1666.8(6)
<i>Z</i>	4
ρ_{calc} (g cm ⁻³)	1.304
μ (mm ⁻¹)	0.086
<i>F</i> (000)	684
<i>T</i> (K)	296(2)
scan mode	ω and ϕ
<i>hkl</i> range	-9 ≤ <i>h</i> ≤ 9, -21 ≤ <i>k</i> ≤ 21, -17 ≤ <i>l</i> ≤ 17
measd reflns	21936
unique reflns	3755
refined parameters	2074
<i>R</i> ₁ ^{<i>a</i>} (<i>I</i> > 2σ(<i>I</i>))	0.0861
<i>wR</i> ₂ ^{<i>b</i>} (<i>I</i> > 2σ(<i>I</i>))	0.2253
GOF on <i>F</i> ²	0.961
ρ_{fin} (max/min) (e Å ⁻³)	0.283/ -0.445

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR_2 = \{ [\sum w(F_o^2 - F_c^2)^2] / [\sum w(F_o^2)^2] \}^{1/2}.$$

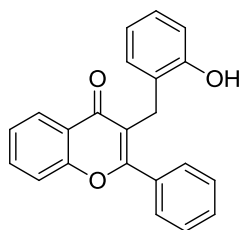
(1) Bruker-AXS (2014). APEX2. Version 2014.11-0. Madison, Wisconsin, USA.

(2) Sheldrick, G. *Acta Cryst. C* **2015**, *71*, 3-8.

S3. Synthesis of Homoisoflavonoids from aryl alkynoic acids

General Procedure for the synthesis of homoisoflavonoid from salicylaldehyde derivatives and aryl alkynoic acids: To a reaction flask, 2-hydroxy aryl aldehyde (1.0 mmol), aryl alkynoic acid (1.5 mmol), [Ru(*p*-cymene)Cl₂]₂ (15 mg, 0.025 mmol, 2.5 mol%), cesium acetate (479 mg, 2.5 mmol) and DMSO (10 mL) were added. The solution was stirred at 120 °C for 15 h. The resulting mixture was cooled and then diluted with water. The pH of the reaction mixture was adjusted to pH ~1 using HCl (aq). The crude product was extracted using ethyl acetate (2 × 25 mL). The organic layer was washed with water (2 × 25 mL) and followed by brine solution. The organic layer was dried over sodium sulfate. The solvent was removed under reduced pressure, and the resulting crude product was purified by column chromatography (eluent: 10% ethyl acetate /hexane) to obtain the pure product.

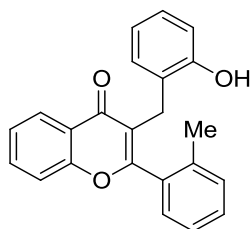
3-(2-Hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (3aa):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**3aa**) (134 mg, 0.410 mmol, 82% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.69 (s, 1H), 8.28 (ddd, *J* = 8.1, 1.7, 0.5 Hz, 1H), 7.70 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.66 – 7.62 (m, 5H), 7.49 – 7.40 (m, 2H), 7.08 – 7.00 (m, 1H), 6.90 (dd, *J* = 8.1, 1.3 Hz, 1H), 6.58 (td, *J* = 7.5, 1.3 Hz, 1H), 6.27 (dd, *J* = 7.6, 1.7 Hz, 1H), 3.94 (s, 2H); ¹³C

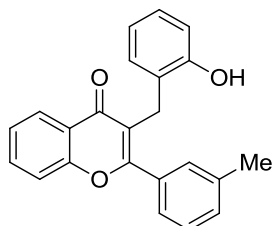
NMR (125 MHz, CDCl₃) δ 180.5, 164.5, 156.2, 155.2, 134.4, 133.0, 130.8, 130.4, 129.1, 128.9, 128.3, 126.1, 125.8, 125.4, 122.2, 121.6, 119.9, 118.2, 117.9, 25.8; HRMS (EI-MSES double focusing) m/z calcd. for C₂₂H₁₆O₃ [M]⁺: 328.1099; found: 328.1102.

3-(2-Hydroxybenzyl)-2-(*o*-tolyl)-4*H*-chromen-4-one (3ab):



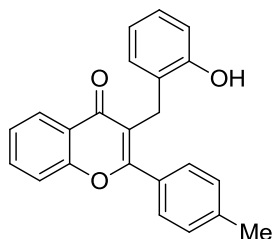
3-(*o*-Tolyl)propionic acid (240 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(*o*-tolyl)-4*H*-chromen-4-one (**3ab**) (121 mg, 0.355 mmol, 71% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.70 (s, 1H), 8.31 (dd, J = 7.9, 1.6 Hz, 1H), 7.74 – 7.68 (m, 1H), 7.58 – 7.51 (m, 1H), 7.47 – 7.44 (m, 5H), 7.08 – 7.00 (m, 1H), 6.92 – 6.86 (m, 1H), 6.57 (td, J = 7.5, 1.1 Hz, 1H), 6.19 (dd, J = 7.6, 1.4 Hz, 1H), 3.74 (s, 2H), 2.18 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 180.5, 165.0, 156.3, 155.3, 137.1, 134.4, 132.3, 130.9, 130.8, 130.6, 129.4, 128.3, 126.2, 126.2, 125.5, 125.1, 122.3, 122.2, 119.7, 117.9 (2C), 26.2, 19.4; HRMS (EI-MSES double focusing) m/z calcd. for C₂₃H₁₈O₃ [M]⁺: 342.1256; found: 342.1257.

3-(2-Hydroxybenzyl)-2-(*m*-tolyl)-4*H*-chromen-4-one (3ac):



3-(*m*-Tolyl)propionic acid (240 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(*m*-tolyl)-4*H*-chromen-4-one (**3ac**) (123 mg, 0.360 mmol, 72% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.70 (s, 1H), 8.28 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.70 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.52 (t, *J* = 7.9 Hz, 1H), 7.46 – 7.42 (m, 5H), 7.09 – 6.98 (m, 1H), 6.90 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.58 (td, *J* = 7.6, 1.3 Hz, 1H), 6.30 (dd, *J* = 7.7, 1.6 Hz, 1H), 3.92 (s, 2H), 2.50 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 180.5, 164.8, 156.2, 155.2, 138.8, 134.4, 132.9, 131.5, 130.5, 129.7, 128.9, 128.3, 126.2, 126.1, 125.8, 125.4, 122.2, 121.5, 119.8, 118.1, 117.9, 25.9, 21.5; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₃H₁₈O₃ [M]⁺: 342.1256; found: 342.1253.

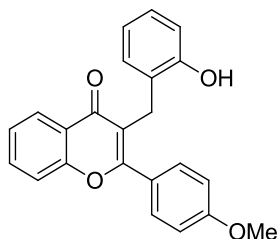
3-(2-Hydroxybenzyl)-2-(*p*-tolyl)-4*H*-chromen-4-one (3ad):



3-(*p*-Tolyl)propionic acid (240 mg, 1.0 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(*p*-tolyl)-4*H*-chromen-4-one (**3ad**) (120 mg, 0.350 mmol, 70 % yield); ¹H NMR (500 MHz, CDCl₃): δ 9.72 (s, 1H), 8.28 (ddd, *J* = 8.1, 1.7, 0.5 Hz, 1H), 7.69 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.46 – 7.43 (m, 2H), 7.43 – 7.40 (m, 2H), 7.10 – 6.99 (m, 1H), 6.90 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.59 (td, *J* = 7.5, 1.3 Hz, 1H), 6.33 (dd, *J* = 7.7, 1.6 Hz, 1H), 3.95 (s, 2H), 2.53 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 180.4, 164.7, 156.1, 155.1, 141.1, 134.3, 130.4, 130.2, 129.6, 129.0, 128.3, 126.1, 125.9, 125.3, 122.1, 121.5, 119.8, 118.2, 117.9,

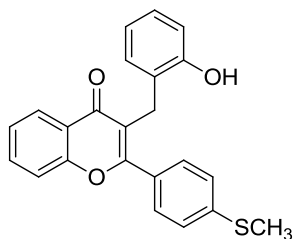
25.8, 21.6; HRMS (EI-MSES double focusing) m/z calcd. for $C_{23}H_{18}O_3$ $[M]^+$: 342.1256; found: 342.1253.

3-(2-Hydroxybenzyl)-2-(4-methoxyphenyl)-4*H*-chromen-4-one (3ae):



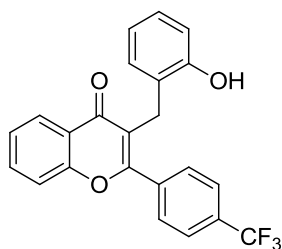
3-(4-Methoxyphenyl)propionic acid (264 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(4-methoxyphenyl)-4*H*-chromen-4-one (**3ae**) (134 mg, 0.375 mmol, 75% yield); 1H NMR (500 MHz, $CDCl_3$): δ 9.71 (s, 1H), 8.27 (dd, J = 8.1, 1.5 Hz, 1H), 7.68 (ddd, J = 8.7, 7.1, 1.7 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.45 (d, J = 8.4 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.16 – 7.10 (m, 2H), 7.07 – 7.01 (m, 1H), 6.90 (dd, J = 8.1, 1.0 Hz, 1H), 6.59 (td, J = 7.5, 1.2 Hz, 1H), 6.35 (dd, J = 7.7, 1.6 Hz, 1H), 3.97 (s, 2H), 3.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.5, 164.5, 161.4, 156.1, 155.1, 134.3, 130.8, 130.4, 128.3, 126.1, 126.0, 125.3, 125.3, 122.1, 121.4, 119.9, 118.2, 117.9, 114.3, 55.5, 25.9; HRMS (EI-MSES double focusing) m/z calcd. for $C_{23}H_{18}O_4$ $[M]^+$: 358.1205; found: 358.1203.

3-(2-Hydroxybenzyl)-2-(4-(methylthio)phenyl)-4*H*-chromen-4-one (3af):



3-(4-(Methylthio)phenyl)propionic acid (288 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(4-(methylthio)phenyl)-4*H*-chromen-4-one (**3af**) (129 mg, 0.345 mmol, 69% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.67 (s, 1H), 8.28 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.71 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 7.59 – 7.56 (m, 2H), 7.49 – 7.41 (m, 4H), 7.06 (td, *J* = 8.1, 1.7 Hz, 1H), 6.91 (dd, *J* = 8.1, 1.1 Hz, 1H), 6.61 (td, *J* = 7.5, 1.2 Hz, 1H), 6.38 (dd, *J* = 7.6, 1.6 Hz, 1H), 3.97 (s, 2H), 2.62 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 180.4, 164.0, 156.2, 155.1, 142.8, 134.4, 130.4, 129.5, 129.2, 128.3, 126.2, 125.9, 125.8, 125.4, 122.1, 121.6, 119.9, 118.2, 117.9, 25.8, 15.1; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₃H₁₈O₃S [M]⁺: 374.0977; found: 374.0976.

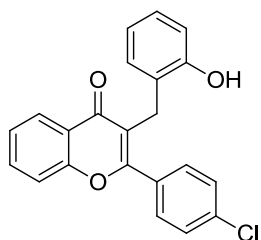
3-(2-Hydroxybenzyl)-2-(4-(trifluoromethyl)phenyl)-4*H*-chromen-4-one (3ag):



3-(4-(Trifluoromethyl)phenyl)propionic acid (321 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(4-(trifluoromethyl)phenyl)-4*H*-chromen-4-one (**3ag**) (139 mg, 0.350 mmol, 70% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.49 (s, 1H), 8.31 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.92 (d, *J* = 8.1 Hz, 2H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.74 (ddd, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.11 – 7.01 (m, 1H), 6.92 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.61 (td, *J* = 7.5, 1.3 Hz, 1H), 6.27 (dd, *J* = 7.7, 1.6 Hz, 1H), 3.91 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 180.2, 162.6, 156.1, 155.1, 136.4, 134.7, 132.7 (q, *J* = 32.8 Hz), 130.1, 129.8, 128.6, 126.2, 126.0 (q, *J*

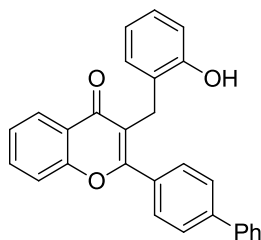
= 3.7 Hz), 125.7, 125.3, 123.6 (q, $J = 271.2$ Hz), 122.1, 122.0, 120.0, 118.3, 117.9, 25.8; HRMS (EI-MSES double focusing) m/z calcd. for $C_{23}H_{15}F_3O_3$ $[M]^+$: 396.0973; found: 396.0971.

2-(4-Chlorophenyl)-3-(2-hydroxybenzyl)-4*H*-chromen-4-one (3ah):



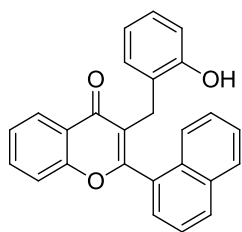
3-(4-Chlorophenyl)propionic acid (271 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 2-(4-chlorophenyl)-3-(2-hydroxybenzyl)-4*H*-chromen-4-one (**3ah**) (132 mg, 0.365 mmol, 73% yield); 1H NMR (500 MHz, $CDCl_3$): δ 9.56 (s, 1H), 8.28 (dd, $J = 8.3, 1.4$ Hz, 1H), 7.76 – 7.67 (m, 1H), 7.66 – 7.54 (m, 4H), 7.45 (d, $J = 7.9$ Hz, 2H), 7.05 (td, $J = 8.2, 1.6$ Hz, 1H), 6.90 (dd, $J = 8.1, 1.0$ Hz, 1H), 6.61 (td, $J = 7.5, 1.2$ Hz, 1H), 6.31 (dd, $J = 7.6, 1.6$ Hz, 1H), 3.91 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 180.3, 163.1, 156.1, 155.1, 137.1, 134.5, 131.4, 130.6, 130.2, 129.3, 128.5, 126.2, 125.5, 125.5, 122.1, 121.8, 119.9, 118.3, 117.9, 25.9; HRMS (EI-MSES double focusing) m/z calcd. for $C_{22}H_{15}ClO_3$ $[M]^+$: 362.0710; found: 362.0707.

2-([1,1'-Biphenyl]-4-yl)-3-(2-hydroxybenzyl)-4*H*-chromen-4-one (3ai):



3-([1,1'-Biphenyl]-4-yl)propionic acid (333 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 2-([1,1'-biphenyl]-4-yl)-3-(2-hydroxybenzyl)-4*H*-chromen-4-one (**3ai**) (131 mg, 0.325 mmol, 65% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.68 (s, 1H), 8.30 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.77 – 7.66 (m, 5H), 7.57 – 7.50 (m, 2H), 7.50 – 7.42 (m, 3H), 7.09 – 7.01 (m, 1H), 6.91 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.59 (td, *J* = 7.5, 1.3 Hz, 1H), 6.38 (dd, *J* = 7.7, 1.6 Hz, 1H), 4.00 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 180.4, 164.2, 156.2, 155.1, 143.6, 139.8, 134.4, 131.8, 130.4, 129.6, 129.0, 128.3, 128.2, 127.5, 127.2, 126.1, 125.8, 125.4, 122.2, 121.7, 119.9, 118.2, 117.9, 25.8; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₈H₂₀O₃ [M]⁺: 404.1412; found: 404.1410.

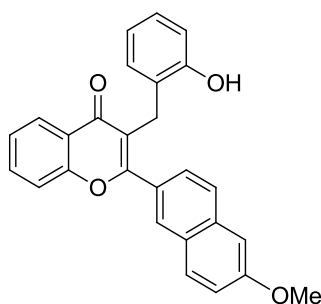
3-(2-Hydroxybenzyl)-2-(naphthalen-1-yl)-4*H*-chromen-4-one (3aj):



3-(Naphthalen-1-yl)propionic acid (294 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(naphthalen-1-yl)-4*H*-chromen-4-one (**3aj**) (134 mg, 0.355 mmol, 71% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.76 (s, 1H), 8.37 (ddd, *J* = 8.1, 1.7, 0.4 Hz, 1H), 8.16 (dd, *J* = 7.6, 1.5 Hz, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.76 – 7.68 (m, 3H), 7.67 – 7.60 (m, 2H), 7.53 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.50 (ddd, *J* = 8.2, 7.2, 1.1 Hz, 1H), 7.45 (ddd, *J* = 8.5, 0.9, 0.5 Hz, 1H), 7.05 – 6.96 (m, 1H), 6.89 (dd, *J* = 8.1, 1.3 Hz, 1H), 6.41 (td, *J* = 7.5, 1.3 Hz, 1H), 5.97 (dd, *J* = 7.7, 1.7 Hz, 1H), 3.88 (d, *J* = 14.4 Hz, 1H), 3.57 (d, *J* = 14.4 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 180.3, 163.8, 156.5, 155.3, 134.5, 133.6, 131.2, 130.8, 130.7, 130.0,

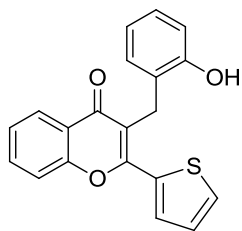
128.8, 128.2, 128.2, 127.6, 126.9, 126.2, 125.6, 125.2, 125.1, 124.7, 123.5, 122.4, 119.6, 118.1, 117.9, 26.5; HRMS (EI-MSES double focusing) m/z calcd. for $C_{26}H_{18}O_3$ $[M]^+$: 378.1256; found: 378.1257.

3-(2-Hydroxybenzyl)-2-(6-methoxynaphthalen-2-yl)-4H-chromen-4-one (3ak):



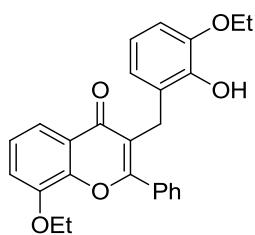
3-(6-Methoxynaphthalen-2-yl)propionic acid (339 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(6-methoxynaphthalen-2-yl)-4H-chromen-4-one (**3ak**) (139 mg, 0.340 mmol, 68% yield); 1H NMR (500 MHz, $CDCl_3$): δ 9.72 (s, 1H), 8.31 (dd, J = 8.1, 1.4 Hz, 1H), 8.07 (d, J = 1.1 Hz, 1H), 7.97 (d, J = 8.5 Hz, 1H), 7.87 (d, J = 8.9 Hz, 1H), 7.71 (ddd, J = 8.7, 7.1, 1.7 Hz, 1H), 7.67 (dd, J = 8.5, 1.8 Hz, 1H), 7.50 – 7.47 (m, 1H), 7.45 (ddd, J = 8.2, 7.2, 1.1 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.02 (td, J = 8.1, 1.7 Hz, 1H), 6.89 (dd, J = 8.1, 1.1 Hz, 1H), 6.51 (td, J = 7.5, 1.3 Hz, 1H), 6.26 (dd, J = 7.6, 1.6 Hz, 1H), 4.02 (s, 2H), 4.0 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 180.5, 164.8, 159.3, 156.2, 155.2, 135.5, 134.3, 130.5, 130.2, 129.3, 128.3, 128.1, 127.9, 127.6, 126.2, 126.1, 125.9, 125.4, 122.2, 121.7, 120.2, 119.8, 118.1, 117.9, 105.9, 55.5, 26.1; HRMS (EI-MSES double focusing) m/z calcd. for $C_{27}H_{20}O_4$ $[M]^+$: 408.1362; found: 408.1359.

3-(2-Hydroxybenzyl)-2-(thiophen-2-yl)-4H-chromen-4-one (3al):



3-(Thiophen-2-yl)propionic acid (228 mg, 1.5 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 3-(2-hydroxybenzyl)-2-(thiophen-2-yl)-4*H*-chromen-4-one (**3al**) (120 mg, 0.360 mmol, 72% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.43 (s, 1H), 8.45 – 8.11 (m, 1H), 7.72 (ddd, J = 6.2, 3.8, 1.2 Hz, 2H), 7.71 – 7.68 (m, 1H), 7.48 (dd, J = 8.5, 0.5 Hz, 1H), 7.42 (ddd, J = 8.1, 7.1, 1.0 Hz, 1H), 7.29 (dd, J = 5.1, 3.8 Hz, 1H), 7.11 – 7.04 (m, 1H), 6.93 (dd, J = 8.1, 1.2 Hz, 1H), 6.71 (dd, J = 7.7, 1.8 Hz, 1H), 6.66 (td, J = 7.3, 1.3 Hz, 1H), 4.19 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 180.1, 157.4, 155.9, 155.1, 134.5, 133.9, 131.2, 130.08, 130.07, 128.4, 127.8, 126.1, 125.8, 125.4, 121.9, 121.5, 120.2, 118.3, 117.8, 25.7; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{20}\text{H}_{14}\text{O}_3\text{S}$ $[\text{M}]^+$: 334.0664; found: 334.0660.

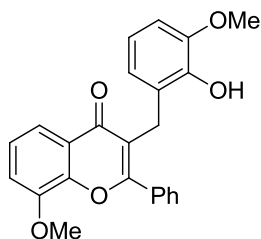
8-Ethoxy-3-(3-ethoxy-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (3ba):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 3-ethoxy-2-hydroxybenzaldehyde (166 mg, 1.0 mmol) afforded 8-ethoxy-3-(3-ethoxy-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**3ba**) (168 mg, 0.405 mmol, 81 % yield); ^1H NMR (500 MHz, CDCl_3): δ 7.80 (dd, J = 8.1, 1.4 Hz, 1H), 7.70 (s, 1H), 7.67 – 7.62 (m, 2H), 7.58 – 7.47 (m, 3H), 7.29 (t, J = 8.1 Hz, 1H), 7.16 (dd, J = 8.0, 1.4 Hz, 1H), 6.68 (dd, J = 8.1, 1.4 Hz, 1H), 6.59 (t, J = 8.0 Hz, 1H), 6.27 (dd, J = 7.8, 1.3

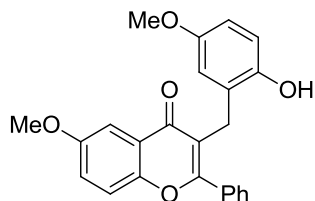
Hz, 1H), 4.18 (q, $J = 7.0$ Hz, 2H), 4.06 (q, $J = 7.0$ Hz, 2H), 3.98 (s, 2H), 1.46 (t, $J = 7$ Hz, 3H), 1.44 (t, $J = 7$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.3, 163.3, 148.1, 147.0, 144.2, 133.2, 130.4, 129.1, 128.64, 128.61, 126.1, 124.7, 123.6, 121.3, 120.4, 119.3, 116.9, 115.6, 110.6, 65.0, 64.4, 25.7, 14.9, 14.7; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{26}\text{H}_{24}\text{O}_5$ $[\text{M}]^+$: 416.1624; found: 416.1621.

3-(2-Hydroxy-3-methoxybenzyl)-8-methoxy-2-phenyl-4H-chromen-4-one (3ca):



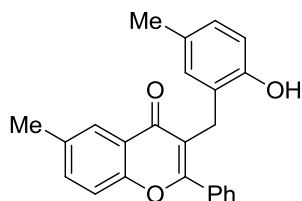
3-Phenylpropionic acid (219 mg, 1.5 mmol) and 2-hydroxy-3-methoxybenzaldehyde (152 mg, 1.0 mmol) afforded 3-(2-hydroxy-3-methoxybenzyl)-8-methoxy-2-phenyl-4H-chromen-4-one (**3ca**) (146 mg, 0.375 mmol, 75 % yield); ^1H NMR (500 MHz, CDCl_3): δ 8.22 (s, 1H), 7.82 (d, $J = 8.0$ Hz, 1H), 7.65 (d, $J = 6.6$ Hz, 2H), 7.58 – 7.52 (m, 3H), 7.33 (t, $J = 8.0$ Hz, 1H), 7.18 (d, $J = 7.9$ Hz, 1H), 6.69 (d, $J = 8.0$ Hz, 1H), 6.61 (t, $J = 7.7$ Hz, 1H), 6.20 (d, $J = 7.8$ Hz, 1H), 3.98 (s, 2H), 3.96 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.5, 163.6, 148.7, 148.2, 146.7, 144.1, 133.1, 130.5, 129.1, 128.7, 126.2, 124.8, 123.5, 121.5, 120.8, 119.4, 116.9, 114.3, 109.6, 56.3, 55.9, 25.6; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_5$ $[\text{M}]^+$: 388.1311; found: 388.1314.

3-(2-Hydroxy-5-methoxybenzyl)-6-methoxy-2-phenyl-4H-chromen-4-one (3da):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 2-hydroxy-5-methoxybenzaldehyde (152 mg, 1.0 mmol) afforded 3-(2-hydroxy-5-methoxybenzyl)-6-methoxy-2-phenyl-4H-chromen-4-one (**3da**) (144 mg, 0.370 mmol, 74% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.36 (s, 1H), 7.68 – 7.62 (m, 5H), 7.61 (d, J = 3.1 Hz, 1H), 7.39 (d, J = 9.1 Hz, 1H), 7.29 (dd, J = 9.2, 3.1 Hz, 1H), 6.82 (d, J = 8.8 Hz, 1H), 6.60 (dd, J = 8.8, 3.1 Hz, 1H), 5.83 (d, J = 3.1 Hz, 1H), 3.92 (s, 2H), 3.90 (s, 3H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.9, 164.0, 157.1, 152.9, 151.2, 148.8, 133.2, 130.7, 129.2, 128.9, 126.5, 124.9, 122.7, 120.9, 119.4, 118.8, 114.7, 114.1, 104.6, 55.9, 55.4, 25.9; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_5$ $[\text{M}]^+$: 388.1311; found: 388.1313.

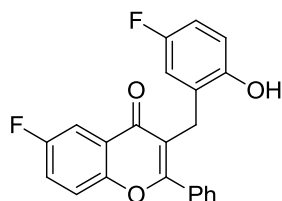
3-(2-Hydroxy-5-methylbenzyl)-6-methyl-2-phenyl-4H-chromen-4-one (3ea):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 2-hydroxy-5-methylbenzaldehyde (136 mg, 1.0 mmol) afforded 3-(2-hydroxy-5-methylbenzyl)-6-methyl-2-phenyl-4H-chromen-4-one (**3ea**) (142 mg, 0.400 mmol, 80% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.43 (s, 1H), 8.06 (d, J = 0.6 Hz, 1H), 7.70 – 7.60 (m, 5H), 7.50 (dd, J = 8.5, 1.9 Hz, 1H), 7.35 (d, J = 8.6 Hz, 1H), 6.82 (dd, J

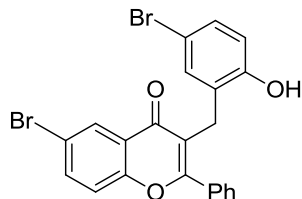
= 8.1, 1.6 Hz, 1H), 6.78 (d, J = 8.2 Hz, 1H), 5.97 (d, J = 1.5 Hz, 1H), 3.88 (s, 2H), 2.46 (s, 3H), 2.00 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 180.4, 164.3, 154.5, 152.7, 135.7, 135.4, 133.2, 130.9, 130.6, 129.2, 128.8, 128.7 (2C), 125.5, 125.3, 121.9, 121.5, 117.8, 117.7, 25.7, 21.0, 20.3; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{24}\text{H}_{20}\text{O}_3$ $[\text{M}]^+$: 356.1412; found: 356.1410.

6-Fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (3fa):



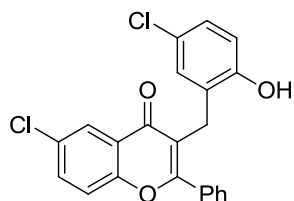
3-Phenylpropionic acid (219 mg, 1.5 mmol) and 5-fluoro-2-hydroxybenzaldehyde (140 mg, 1.5 mmol) afforded 6-fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (**3fa**) (137 mg, 0.375 mmol, 75% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.30 (s, 1H), 7.90 (dd, J = 8.2, 3.1 Hz, 1H), 7.72 – 7.55 (m, 5H), 7.49 (dd, J = 9.2, 4.3 Hz, 1H), 7.44 (ddd, J = 9.2, 7.5, 3.0 Hz, 1H), 6.82 (dd, J = 8.9, 5.1 Hz, 1H), 6.77 – 6.68 (m, 1H), 5.93 (dd, J = 9.3, 3.1 Hz, 1H), 3.88 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3): δ 179.7 (d, J = 2.5 Hz), 159.6 (d, J = 246.4 Hz), 156.3 (d, J = 239.5 Hz), 152.5 (d, J = 1.4 Hz), 151.0 (d, J = 2.0 Hz), 132.5, 131.1, 129.1 (d, J = 22.7 Hz), 126.6 (d, J = 7.2 Hz), 123.2 (d, J = 7.8 Hz), 122.9 (d, J = 25.5 Hz), 120.7, 120.2 (d, J = 8.2 Hz), 119.0 (d, J = 8.1 Hz), 116.1 (d, J = 22.8 Hz), 114.7 (d, J = 22.5 Hz), 110.8 (d, J = 23.7 Hz), 25.8; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{22}\text{H}_{14}\text{F}_2\text{O}_3$ $[\text{M}]^+$: 364.0911; found: 364.0908.

6-Bromo-3-(5-bromo-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (3ga):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 5-bromo-2-hydroxybenzaldehyde (201 mg, 1.0 mmol) afforded 6-Bromo-3-(5-bromo-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (**3ga**) (175 mg, 0.360 mmol, 72 % yield); ^1H NMR (500 MHz, CDCl_3): δ 9.40 (s, 1H), 8.41 (d, J = 2.5 Hz, 1H), 7.80 (dd, J = 8.9, 2.5 Hz, 1H), 7.70 – 7.64 (m, 3H), 7.62 – 7.57 (m, 2H), 7.38 (d, J = 8.9 Hz, 1H), 7.11 (dd, J = 8.6, 2.5 Hz, 1H), 6.76 (d, J = 8.7 Hz, 1H), 6.25 (d, J = 2.5 Hz, 1H), 3.84 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 179.2, 165.2, 154.9, 154.3, 137.6, 132.9, 132.3, 131.2, 131.1, 129.2, 128.9, 128.7, 127.4, 123.4, 121.3, 120.0, 119.9, 118.9, 111.5, 25.7; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{22}\text{H}_{14}\text{Br}_2\text{O}_3$ $[\text{M}]^+$: 483.9310; found: 483.9307.

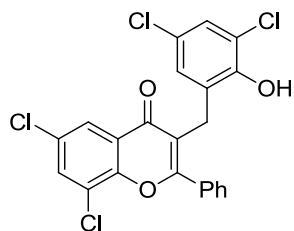
6-Chloro-3-(5-chloro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (3ha):



3-Phenylpropionic acid (220 mg, 1.5 mmol) and 5-chloro-2-hydroxybenzaldehyde (157 mg, 1.0 mmol) afforded 6-Chloro-3-(5-chloro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (**3ha**) (137 mg, 0.346 mmol, 69% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.40 (s, 1H), 8.25 (d, J = 2.6 Hz, 1H), 7.69 – 7.64 (m, 4H), 7.60 (dd, J = 8, 1.8 Hz, 2H), 7.44 (d, J = 9.0 Hz, 1H), 6.98 (dd, J = 8.7, 2.7 Hz, 1H), 6.81 (d, J = 8.7 Hz, 1H), 6.13 (d, J = 2.6 Hz, 1H), 3.85 (s, 2H); ^{13}C NMR (125

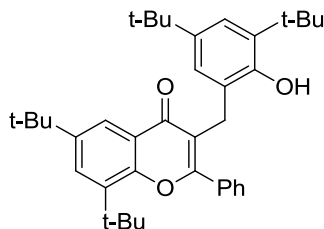
MHz, CDCl₃) δ 179.3, 165.1, 154.5, 153.8, 134.8, 132.3, 131.5, 131.2, 129.9, 129.2, 128.9, 128.2, 126.9, 125.4, 124.3, 123.0, 121.2, 119.7, 119.4, 25.7; HRMS (EI-MSES double focusing) m/z calcd. for C₂₂H₁₄Cl₂O₃ [M]⁺: 396.0320; found: 396.0321.

6,8-Dichloro-3-(3,5-dichloro-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (3ia):



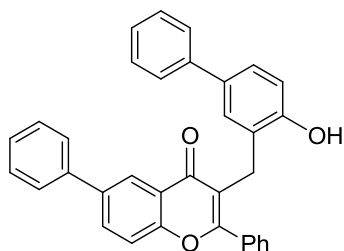
3-Phenylpropionic acid (219 mg, 1.5 mmol) and 3,5-dichloro-2-hydroxybenzaldehyde (191 mg, 1.0 mmol) afforded 6,8-dichloro-3-(3,5-dichloro-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**3ia**) (149 mg, 0.320 mmol, 64% yield); ¹H NMR (500 MHz, CDCl₃): δ 8.84 (s, 1H), 8.15 (d, J = 2.5 Hz, 1H), 7.77 (d, J = 2.5 Hz, 1H), 7.68 – 7.60 (m, 5H), 7.15 (d, J = 2.6 Hz, 1H), 6.22 (d, J = 2.6 Hz, 1H), 3.94 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 178.4, 164.9, 150.5, 149.5, 134.5, 131.7, 131.5, 131.2, 129.2, 128.9, 128.2, 128.1, 127.8, 124.44, 124.41, 124.2, 123.9, 122.9, 120.5, 26.3; HRMS (EI-MSES double focusing) m/z calcd. for C₂₂H₁₂Cl₄O₃ [M]⁺: 463.9541; found: 463.9543.

6,8-Di-*tert*-butyl-3-(3,5-di-*tert*-butyl-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (3ja) :



3-Phenylpropionic acid (220 mg, 1.5 mmol) and 3,5-di-tert-butyl-2-hydroxybenzaldehyde (235 mg, 1.0 mmol) afforded 6,8-di-tert-butyl-3-(3,5-di-tert-butyl-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**3ja**) (180 mg, 0.326 mmol, 65% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.86 (s, 1H), 8.14 (d, *J* = 2.5 Hz, 1H), 7.72 (d, *J* = 2.5 Hz, 1H), 7.70 – 7.67 (m, 2H), 7.67 – 7.63 (m, 3H), 7.09 (d, *J* = 2.5 Hz, 1H), 6.16 (d, *J* = 2.5 Hz, 1H), 3.96 (s, 2H), 1.41 (s, 9H), 1.41 (s, 9H), 1.38 (s, 9H), 1.1 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 181.0, 163.2, 153.2, 151.5, 147.7, 141.1, 138.2, 137.6, 133.7, 130.4, 129.2, 129.1, 129.1, 126.2, 124.8, 122.6, 122.4, 121.6, 119.9, 35.2, 35.1, 35.0, 33.9, 31.5, 31.4, 29.9, 29.8, 25.7; HRMS (EI-MSES double focusing) *m/z* calcd. for C₃₈H₄₈O₃ [M]⁺: 552.3603; found: 552.3605.

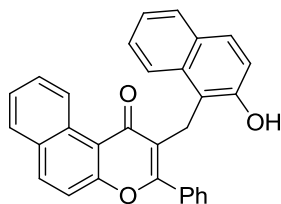
3-((4-Hydroxy-[1,1'-biphenyl]-3-yl)methyl)-2,6-diphenyl-4*H*-chromen-4-one (3ka) :



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 4-hydroxy-[1,1'-biphenyl]-3-carbaldehyde (198 mg, 1.0 mmol) afforded 3-((4-hydroxy-[1,1'-biphenyl]-3-yl)methyl)-2,6-diphenyl-4*H*-chromen-4-one (**3ka**) (178 mg, 0.370 mmol, 74 % yield); ¹H NMR (500 MHz, CDCl₃): δ 9.74 (s, 1H), 8.52 (d, *J* = 2.3 Hz, 1H), 7.96 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.74 – 7.63 (m, 7H), 7.55 (d, *J* = 8.7 Hz, 1H), 7.49 (t, *J* = 7.9 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.36 – 7.29 (m, 3H), 7.28 – 7.20 (m, 3H), 6.96 (d, *J* = 8.4 Hz, 1H), 6.49 (d, *J* = 2.3 Hz, 1H), 4.03 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 180.5, 164.7, 155.6, 154.8, 140.5, 139.1, 138.6, 133.4, 133.1, 132.5, 130.8, 129.1, 129.1, 129.0, 128.4,

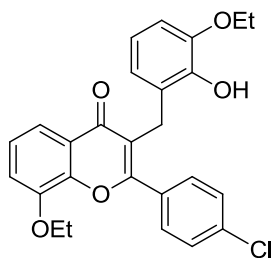
127.9, 127.2, 126.8, 126.3, 126.2, 125.9, 123.8, 122.3, 121.6, 118.5, 118.4, 25.8; HRMS (EI-MSES double focusing) m/z calcd. for $C_{34}H_{24}O_3$ $[M]^+$: 480.1725; found: 480.1724.

2-((2-Hydroxynaphthalen-1-yl)methyl)-3-phenyl-1H-benzo[f]chromen-1-one (3la) :



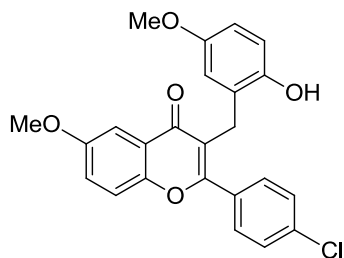
3-Phenylpropionic acid (219 mg, 1.5 mmol) and 2-hydroxy-1-naphthaldehyde (172 mg, 1.0 mmol) afforded 2-((2-hydroxynaphthalen-1-yl)methyl)-3-phenyl-1H-benzo[f]chromen-1-one (**3la**) (154 mg, 0.360 mmol, 72% yield); 1H NMR (500 MHz, $CDCl_3$): δ 10.89 (s, 1H), 9.96 (d, J = 8.7 Hz, 1H), 8.07 (d, J = 9.1 Hz, 1H), 7.93 – 7.89 (m, 2H), 7.87 (d, J = 7.9 Hz, 1H), 7.78 – 7.71 (m, 4H), 7.66 – 7.58 (m, 3H), 7.50 (d, J = 9.1 Hz, 1H), 7.28 (d, J = 8.8 Hz, 1H), 7.12 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H), 6.94 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 6.86 (d, J = 8.6 Hz, 1H), 4.49 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 182.2, 161.3, 157.5, 153.9, 136.4, 133.6, 133.3, 131.2, 130.6, 130.1, 129.9, 129.5, 129.3, 129.1, 128.8, 128.5, 128.4, 127.3, 126.8, 125.5, 122.93, 122.90, 122.3, 121.1, 117.9, 117.1, 115.4, 23.0; HRMS (EI-MSES double focusing) m/z calcd. for $C_{30}H_{20}O_3$ $[M]^+$: 428.1412; found: 428.1414.

2-(4-Chlorophenyl)-8-ethoxy-3-(3-ethoxy-2-hydroxybenzyl)-4H-chromen-4-one (3bh):



3-(4-Chlorophenyl)propionic acid (271 mg, 1.5 mmol) and 3-ethoxy-2-hydroxybenzaldehyde (166 mg, 1.0 mmol) afforded 2-(4-chlorophenyl)-8-ethoxy-3-(3-ethoxy-2-hydroxybenzyl)-4*H*-chromen-4-one (**3bh**) (162 mg, 0.360 mmol, 72% yield); ¹H NMR (500 MHz, CDCl₃): δ 7.79 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.61 – 7.54 (m, 2H), 7.50 – 7.45 (m, 2H), 7.30 (t, *J* = 8.1 Hz, 1H), 7.19 (s, 1H), 7.17 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.70 (dd, *J* = 8.1, 1.4 Hz, 1H), 6.63 (t, *J* = 8.0 Hz, 1H), 6.36 (dd, *J* = 7.8, 1.2 Hz, 1H), 4.18 (t, *J* = 7.0 Hz, 2H), 4.08 (q, *J* = 7.0 Hz, 2H), 3.96 (s, 2H), 1.47 (t, *J* = 7.0 Hz, 3H), 1.44 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.9, 161.8, 148.1, 146.9, 146.7, 143.9, 136.6, 131.7, 130.4, 128.9, 125.7, 124.7, 123.6, 121.0, 120.5, 119.4, 116.9, 115.6, 110.4, 65.0, 64.4, 25.6, 14.9, 14.7; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₆H₂₃ClO₃ [M]⁺: 450.1234; found: 450.1233.

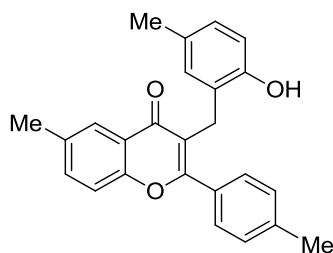
2-(4-Chlorophenyl)-3-(2-hydroxy-5-methoxybenzyl)-6-methoxy-4*H*-chromen-4-one (3dh):



3-(4-Chlorophenyl)propionic acid (271 mg, 1.5 mmol) and 2-hydroxy-5-methoxybenzaldehyde (152 mg, 1.5 mmol) afforded 2-(4-chlorophenyl)-3-(2-hydroxy-5-methoxybenzyl)-6-methoxy-4*H*-chromen-4-one (**3dh**) (156 mg, 0.370 mmol, 74% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.23 (s, 1H), 7.61 (s, 4H), 7.59 (d, *J* = 3 Hz, 1H), 7.39 (d, *J* = 9.2 Hz, 1H), 7.30 (dd, *J* = 9.2, 3.1 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 1H), 6.61 (dd, *J* = 8.8, 3.1 Hz, 1H), 5.86 (d, *J* = 3.1 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 2H), 3.53 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 179.8, 162.6, 157.2, 152.9, 151.2, 148.8, 137.0, 131.6, 130.6, 129.3, 126.3, 125.1, 122.7, 121.1, 119.4, 118.9, 114.9, 113.9,

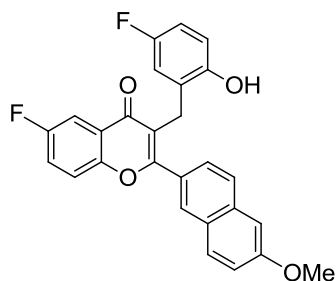
104.6, 55.9, 55.4, 25.9; HRMS (EI-MSES double focusing) m/z calcd. for $C_{24}H_{19}ClO_5$ $[M]^+$: 422.0921; found: 422.0922.

3-(2-Hydroxy-5-methylbenzyl)-6-methyl-2-(*p*-tolyl)-4*H*-chromen-4-one (3ed):



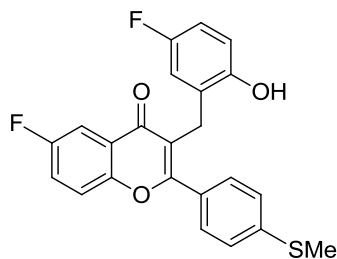
3-(*p*-Tolyl)propionic acid (240 mg, 1.5 mmol) and 2-hydroxy-5-methylbenzaldehyde (136 mg, 1.0 mmol) afforded **3-(2-hydroxy-5-methylbenzyl)-6-methyl-2-(*p*-tolyl)-4*H*-chromen-4-one (3ed)** (142 mg, 0.385 mmol, 77% yield); 1H NMR (500 MHz, $CDCl_3$): δ 9.48 (s, 1H), 8.05 (d, J = 0.9 Hz, 1H), 7.52 (d, J = 8.1 Hz, 2H), 7.48 (dd, J = 8.6, 1.9 Hz, 1H), 7.43 (d, J = 7.9 Hz, 2H), 7.34 (d, J = 8.6 Hz, 1H), 6.83 (dd, J = 8.2, 1.8 Hz, 1H), 6.79 (d, J = 8.2 Hz, 1H), 6.04 (d, J = 1.7 Hz, 1H), 3.89 (s, 2H), 2.53 (s, 3H), 2.46 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 180.4, 164.5, 154.5, 152.7, 140.9, 135.6, 135.3, 130.9, 130.4, 129.5, 129.1, 128.7, 128.67, 125.7, 125.3, 121.9, 121.4, 117.8, 117.6, 25.7, 21.6, 21.0, 20.4; HRMS (EI-MSES double focusing) m/z calcd. for $C_{25}H_{22}O_3$ $[M]^+$: 370.1569; found: 370.1570.

6-Fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-(6-methoxynaphthalen-2-yl)-4*H*-chromen-4-one (3fk):



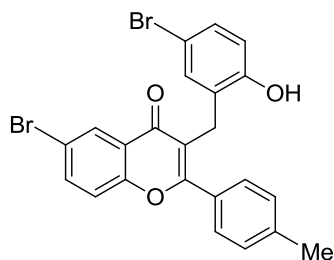
3-(6-Methoxynaphthalen-2-yl)propionic acid (339 mg, 1.5 mmol) and 5-fluoro-2-hydroxybenzaldehyde (140 mg, 1.0 mmol) afforded 6-fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-(6-methoxynaphthalen-2-yl)-4*H*-chromen-4-one (**3fk**) (164 mg, 0.385 mmol, 77 % yield); ^1H NMR (500 MHz, CDCl_3): δ 9.37 (s, 1H), 8.06 (d, J = 1.4 Hz, 1H), 7.99 (d, J = 8.6 Hz, 1H), 7.92 (dd, J = 8.2, 3.0 Hz, 1H), 7.88 (d, J = 9.0 Hz, 1H), 7.65 (dd, J = 8.4, 1.6 Hz, 1H), 7.51 (dd, J = 9.2, 4.2 Hz, 1H), 7.45 (ddd, J = 9.2, 7.6, 3.1 Hz, 1H), 7.32 – 7.27 (m, 2H), 6.83 (dd, J = 8.9, 5.1 Hz, 1H), 6.77 – 6.68 (m, 1H), 5.97 (dd, J = 9.3, 3.1 Hz, 1H), 4.01 (s, 3H), 3.96 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3): δ 179.7 (d, J = 2.6 Hz), 165.2, 159.6 (d, J = 246.3 Hz), 159.4, 156.3 (d, J = 236.1 Hz), 152.5 (d, J = 1.2 Hz), 151.0 (d, J = 2.0 Hz), 135.6, 130.2, 129.3, 128.1, 127.8, 127.4, 126.9 (d, J = 7.1 Hz), 125.8, 123.2 (d, J = 7.8 Hz), 122.9 (d, J = 25.5 Hz), 120.7, 120.5, 120.2 (d, J = 8.1 Hz), 119.0 (d, J = 8.1 Hz), 116.2 (d, J = 22.6 Hz), 114.7 (d, J = 22.5 Hz), 110.8 (d, J = 23.7 Hz), 105.9, 55.5, 26.1; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{27}\text{H}_{18}\text{F}_2\text{O}_4$ $[\text{M}]^+$: 444.1173; found: 444.1177.

6-Fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-(4-(methylthio)phenyl)-4H-chromen-4-one (3ff) :



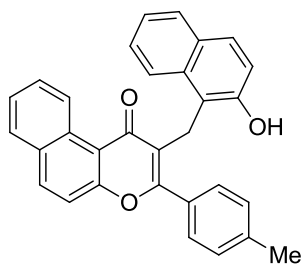
3-(4-(Methylthio)phenyl)propionic acid (288 mg, 1.5 mmol) and 5-fluoro-2-hydroxybenzaldehyde (140 mg, 1.0 mmol) afforded 6-fluoro-3-(5-fluoro-2-hydroxybenzyl)-2-(4-(methylthio)phenyl)-4H-chromen-4-one (**3ff**) (151 mg, 0.385 mmol, 77% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.28 (s, 1H), 8.12 – 7.74 (m, 1H), 7.60 – 7.52 (m, 2H), 7.52 – 7.39 (m, 4H), 6.83 (dd, $J = 8.9, 5.1$ Hz, 1H), 6.73 (ddd, $J = 8.9, 8.2, 3.2$ Hz, 1H), 6.05 (dd, $J = 9.2, 3.1$ Hz, 1H), 3.90 (s, 2H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 179.6 (d, $J = 2.5$ Hz), 164.4, 159.6 (d, $J = 246.3$ Hz), 156.4 (d, $J = 236.0$ Hz), 152.4 (d, $J = 1.3$ Hz), 150.9 (d, $J = 2.0$ Hz), 143.4, 129.3, 128.5, 126.8 (d, $J = 7.2$ Hz), 125.9, 123.2 (d, $J = 7.8$ Hz), 122.9 (d, $J = 25.5$ Hz), 120.6, 120.2 (d, $J = 8.1$ Hz), 119.1 (d, $J = 8.1$ Hz), 116.1 (d, $J = 22.7$ Hz), 114.8 (d, $J = 22.5$ Hz), 110.8 (d, $J = 23.7$ Hz), 25.8, 15.1; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{23}\text{H}_{16}\text{F}_2\text{O}_3\text{S}$ $[\text{M}]^+$: 410.0788; found: 410.0786.

6-Bromo-3-(5-bromo-2-hydroxybenzyl)-2-(p-tolyl)-4H-chromen-4-one (3gd):



3-(*p*-Tolyl)propionic acid (240 mg, 1.5 mmol) and 5-bromo-2-hydroxybenzaldehyde (201 mg, 1.0 mmol) afforded 6-bromo-3-(5-bromo-2-hydroxybenzyl)-2-(*p*-tolyl)-4*H*-chromen-4-one (**3gd**) (180 mg, 0.360 mmol, 72 % yield); ¹H NMR (500 MHz, CDCl₃): δ 9.41 (s, 1H), 8.40 (d, *J* = 2.4 Hz, 1H), 7.78 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.55 – 7.42 (m, 4H), 7.37 (d, *J* = 8.9 Hz, 1H), 7.11 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.75 (d, *J* = 8.7 Hz, 1H), 6.28 (d, *J* = 2.5 Hz, 1H), 3.85 (s, 2H), 2.54 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 179.2, 165.5, 154.9, 154.3, 141.7, 137.5, 132.9, 131.1, 129.8, 129.4, 128.8, 128.6, 127.5, 123.4, 121.2, 119.97, 119.89, 118.9, 111.5, 25.7, 21.6; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₃H₁₆Br₂O₃ [M]⁺: 497.9466; found: 497.9463.

2-((2-Hydroxynaphthalen-1-yl)methyl)-3-(*p*-tolyl)-1*H*-benzo[*f*]chromen-1-one (3kd):



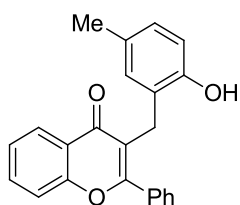
3-(*p*-Tolyl)propionic acid (240 mg, 1.5 mmol) and 2-hydroxy-1-naphthaldehyde (172 mg, 1.0 mmol) afforded 2-((2-hydroxynaphthalen-1-yl)methyl)-3-(*p*-tolyl)-1*H*-benzo[*f*]chromen-1-one (**3kd**) (168 mg, 0.380 mmol, 76% yield); ¹H NMR (500 MHz, CDCl₃): δ 10.90 (s, 1H), 10.07 – 9.85 (m, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.89 – 7.84 (m, 1H), 7.82 – 7.77 (m, 2H), 7.74 (ddd, *J* = 8.6, 7.0, 1.4 Hz, 1H), 7.65 – 7.62 (m, 1H), 7.61 – 7.57 (m, 2H), 7.52 (dd, *J* = 8.4, 0.6 Hz, 2H), 7.49 (d, *J* = 9.1 Hz, 1H), 7.28 (d, *J* = 8.8 Hz, 1H), 7.13 (ddd, *J* = 8.0, 6.7, 1.3 Hz, 1H), 6.96 (ddd, *J* = 8.1, 6.7, 1.4 Hz, 1H), 6.91 (dd, *J* = 8.1, 0.5 Hz, 1H), 4.49 (s, 2H), 2.57 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 182.2, 161.5, 157.5, 153.8, 141.7, 136.2, 133.6, 130.6, 130.4, 130.1, 129.8, 129.7, 129.5, 129.3, 128.7, 128.5, 128.3, 127.3, 126.7, 125.4, 123.1, 122.7, 122.3, 121.1, 118.1,

117.1, 115.4, 23.1, 21.7; HRMS (EI-MSES double focusing) m/z calcd. for $C_{31}H_{22}O_3$ $[M]^+$: 442.1569; found: 442.1570.

S4. Synthesis of homoisoflavonoid from 2'-hydroxychalcone

General Procedure for the synthesis of homoisoflavonoid from 2'-hydroxychalcone and aldehydes: To a reaction flask, 2'-hydroxy chalcone (1.0 mmol), 2-hydroxy aryl aldehyde or aryl aldehyde (1.0 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (15 mg, 0.025 mmol, 2.5 mol%), cesium acetate (385 mg, 2.0 mmol) and DMSO (10 mL) were added. The solution was stirred at 120 °C for 12 h. The resulting mixture was cooled and then diluted with water. The pH of the mass was adjusted to pH ~1 using con. HCl. The crude product was extracted using ethyl acetate (2 x 25). The organic layer was washed with water (2 x 25) and followed by brine solution. The organic layer was dried over sodium sulfate. The solvent was removed under reduced pressure, and the resulting crude product was purified by simple column chromatography (eluent = 10% ethyl acetate/ hexane) to obtain the pure product.

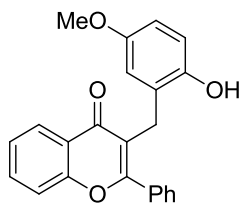
3-(2-Hydroxy-5-methylbenzyl)-2-phenyl-4H-chromen-4-one (6a):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and 2-hydroxy-5-methylbenzaldehyde (137 mg, 1.0 mmol) afforded 3-(2-hydroxy-5-methylbenzyl)-2-phenyl-4H-chromen-4-one (**6a**) (251 mg, 0.732

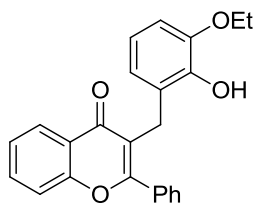
mmol, 73% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.37 (s, 1H), 8.28 (dd, J = 8.1, 1.4 Hz, 1H), 7.68 – 7.71 (m, 1H), 7.67 – 7.62 (m, 5H), 7.46 – 7.41 (m, 2H), 6.83 (dd, J = 8.2, 2.0 Hz, 1H), 6.79 (d, J = 8.2 Hz, 1H), 5.99 (d, J = 2.0 Hz, 1H), 3.89 (s, 2H), 2.01 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) : δ 180.3, 164.4, 156.1, 152.7, 134.3, 133.1, 130.9, 130.7, 129.1, 128.8, 128.76, 128.74, 126.1, 125.3, 122.2, 121.7, 117.9, 117.8, 25.7, 20.3; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{23}\text{H}_{18}\text{O}_3$ $[\text{M}]^+$: 342.1256; found: 342.1259.

3-(2-Hydroxy-5-methoxybenzyl)-2-phenyl-4*H*-chromen-4-one (6b):



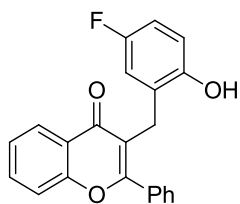
2'-Hydroxychalcone (225 mg, 1.0 mmol) and 2-hydroxy-5-methoxybenzaldehyde (153 mg, 1.0 mmol) afforded 3-(2-hydroxy-5-methoxybenzyl)-2-phenyl-4*H*-chromen-4-one (**6b**) (291 mg, 0.813 mmol, 81 % yield); ^1H NMR (500 MHz, CDCl_3): δ 9.25 (s, 1H), 8.27 (dd, J = 8.1, 1.6 Hz, 1H), 7.73 – 7.65 (m, 3H), 7.65 – 7.62 (m, 3H), 7.48 – 7.38 (m, 2H), 6.82 (d, J = 8.8 Hz, 1H), 6.60 (dd, J = 8.8, 3.1 Hz, 1H), 5.83 (d, J = 3.1 Hz, 1H), 3.91 (s, 2H), 3.49 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) : δ 180.3, 164.3, 156.2, 152.9, 148.8, 134.4, 133.1, 130.7, 129.2, 129.0, 126.4, 126.1, 125.4, 122.2, 121.6, 118.9, 117.9, 114.7, 114.2, 55.4, 25.8; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{23}\text{H}_{18}\text{O}_4$ $[\text{M}]^+$: 358.1205; found: 358.1204.

3-(3-Ethoxy-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (6c):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and 3-ethoxy-2-hydroxybenzaldehyde (167 mg, 1.0 mmol) afforded 3-(3-ethoxy-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**6c**) (262 mg, 0.702 mmol, 70 % yield); ¹H NMR (500 MHz, CDCl₃): δ 8.26 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.71 – 7.66 (m, 2H), 7.63 – 7.59 (m, 2H), 7.56 – 7.50 (m, 3H), 7.49 – 7.46 (m, 1H), 7.42 – 7.39 (m, 1H), 6.69 (dd, *J* = 8.1, 1.3 Hz, 1H), 6.60 (t, *J* = 8.0 Hz, 1H), 6.28 (dd, *J* = 7.8, 1.3 Hz, 1H), 4.07 (q, *J* = 7.0 Hz, 2H), 3.96 (s, 2H), 1.44 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) : δ 179.3, 163.6, 156.2, 147.0, 144.2, 133.8, 133.2, 130.4, 128.8, 128.6, 126.2, 126.1, 125.0, 122.5, 121.3, 120.6, 119.3, 117.9, 110.6, 64.4, 25.7, 14.9; HRMS (ESI) *m/z* calcd. for C₂₄H₂₀O₄ [M+Na]⁺: 395.1259; found C₂₄H₂₀O₄ [M+Na]⁺: 395.1257.

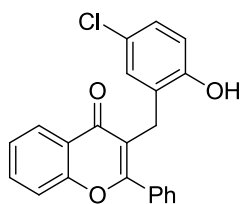
3-(5-Fluoro-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (6d):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and 5-fluoro-2-hydroxybenzaldehyde (141 mg, 1.0 mmol) afforded 3-(5-fluoro-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**6d**) (285 mg, 0.823 mmol, 82% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.51 (s, 1H), 8.28 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.71 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.68 – 7.61 (m, 5H), 7.51 – 7.41 (m, 2H), 6.83 (dd, *J* = 8.9, 5.1 Hz, 1H), 6.77 – 6.68 (m, 1H), 5.95 (dd, *J* = 9.4, 3.1 Hz, 1H), 3.89 (s, 2H); ¹³C NMR (125

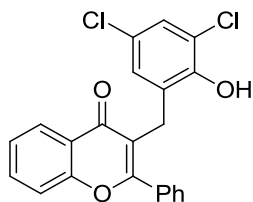
MHz, CDCl₃) : δ 180.3, 164.6, 156.2 (d, J = 235.9 Hz), 156.1, 151.1 (d, J = 1.9 Hz), 134.5, 132.7, 130.9, 129.0 (d, J = 12.7 Hz), 126.8 (d, J = 7.2 Hz), 126.1, 125.5, 122.1, 121.1, 118.9 (d, J = 8.1 Hz), 117.9, 116.1 (d, J = 22.8 Hz), 114.6 (d, J = 22.5 Hz), 25.8 (d, J = 1.0 Hz); HRMS (EI-MSES double focusing) m/z calcd. for C₂₂H₁₅FO₃ [M]⁺: 346.1005; found: 346.1002.

3-(5-Chloro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (6e):



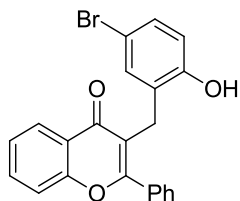
2'-Hydroxychalcone (225 mg, 1.0 mmol) and 5-chloro-2-hydroxybenzaldehyde (157 mg, 1.0 mmol) afforded 3-(5-chloro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (**6e**) (269 mg, 0.742 mmol, 74% yield); ¹H NMR (500 MHz, CDCl₃): δ 9.69 (s, 1H), 8.28 (dd, J = 8.1, 1.4 Hz, 1H), 7.73-7.70 (m, 1H), 7.69 – 7.64 (m, 3H), 7.63 – 7.59 (m, 2H), 7.52 – 7.38 (m, 2H), 6.97 (dd, J = 8.6, 2.7 Hz, 1H), 6.80 (d, J = 8.6 Hz, 1H), 6.14 (d, J = 2.6 Hz, 1H), 3.86 (s, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 180.4, 164.9, 156.2, 153.9, 134.6, 132.7, 130.9, 130.0, 129.1, 128.9, 128.1, 127.2, 126.1, 125.5, 124.1, 122.1, 121.0, 119.4, 118.0, 25.7; HRMS (ESI) m/z calcd. for C₂₂H₁₅Cl₂O₃ [M+Na]⁺: 385.0607; found C₂₂H₁₅Cl₂O₃ [M+Na]⁺: 385.0606.

3-(3,5-Dichloro-2-hydroxybenzyl)-2-phenyl-4H-chromen-4-one (6f):



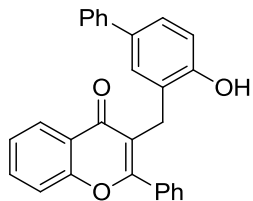
2'-hydroxychalcone (225 mg, 1.0 mmol) and 3,5-dichloro-2-hydroxybenzaldehyde (192 mg, 1.0 mmol) afforded 3-(3,5-dichloro-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**6f**) (311 mg, 0.783 mmol, 78 % yield); ¹H NMR (500 MHz, CDCl₃): δ 10.00 (s, 1H), 8.29 (ddd, *J* = 8.1, 1.7, 0.5 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.69 – 7.62 (m, 3H), 7.61 – 7.57 (m, 2H), 7.52 – 7.40 (m, 2H), 7.13 (d, *J* = 2.6 Hz, 1H), 6.10 (d, *J* = 2.6 Hz, 1H), 3.89 (s, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 180.2, 165.1, 156.2, 150.1, 134.7, 132.5, 131.1, 129.1, 128.9, 128.5, 128.2, 128.1, 126.2, 125.7, 123.9, 123.2, 122.0, 120.4, 118.0, 26.3; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₂H₁₄Cl₂O₃ [M]⁺: 396.0320; found: 396.0316.

3-(5-Bromo-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (6g):



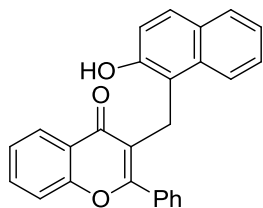
2'-Hydroxychalcone (225 mg, 1.0 mmol) and 5-bromo-2-hydroxybenzaldehyde (202 mg, 1.0 mmol) afforded 3-(5-bromo-2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one (**6g**) (315 mg, 0.773 mmol, 77 % yield); ¹H NMR (500 MHz, CDCl₃): δ 9.70 (s, 1H), 8.50 – 8.16 (m, 1H), 7.77 – 7.70 (m, 1H), 7.69 – 7.63 (m, 3H), 7.63 – 7.58 (m, 2H), 7.51 – 7.42 (m, 2H), 7.10 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.76 (d, *J* = 8.6 Hz, 1H), 6.26 (d, *J* = 2.5 Hz, 1H), 3.85 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) : δ 180.4, 164.9, 156.2, 154.4, 134.6, 132.9, 132.6, 130.9, 129.1, 128.9, 127.7, 126.1, 125.6, 122.1, 121.0, 119.8, 118.0, 111.4, 25.7; HRMS (ESI) *m/z* calcd. for C₂₂H₁₅BrO₃ [M+Na]⁺: 429.0102; found C₂₂H₁₅BrO₃ [M+Na]⁺: 429.0101.

3-((4-Hydroxy-[1,1'-biphenyl]-3-yl)methyl)-2-phenyl-4*H*-chromen-4-one (6h):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and 4-hydroxy-[1,1'-biphenyl]-3-carbaldehyde (199 mg, 1.0 mmol) afforded 3-((4-hydroxy-[1,1'-biphenyl]-3-yl)methyl)-2-phenyl-4*H*-chromen-4-one (**6h**) (304 mg, 0.752 mmol, 75% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.75 (s, 1H), 8.31 (dd, J = 8.1, 1.3 Hz, 1H), 7.75 – 7.67 (m, 3H), 7.66 – 7.61 (m, 3H), 7.49 – 7.43 (m, 2H), 7.35 – 7.28 (m, 3H), 7.27 (d, J = 1.4 Hz, 1H), 7.25 – 7.21 (m, 2H), 6.95 (d, J = 8.4 Hz, 1H), 6.48 (d, J = 2.4 Hz, 1H), 4.00 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) : δ 180.5, 164.6, 156.2, 154.8, 140.5, 134.5, 133.1, 132.5, 130.8, 129.1, 129.05, 129.03, 128.4, 126.8, 126.3, 126.25, 126.16, 125.9, 125.5, 122.2, 121.6, 118.4, 117.9, 25.8; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{28}\text{H}_{20}\text{O}_3$ $[\text{M}]^+$: 404.1412; found: 404.1414.

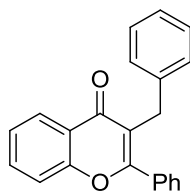
3-((2-Hydroxynaphthalen-1-yl)methyl)-2-phenyl-4*H*-chromen-4-one (6i):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and 2-hydroxy-1-naphthaldehyde (173 mg, 1.0 mmol) afforded 3-((2-Hydroxynaphthalen-1-yl)methyl)-2-phenyl-4*H*-chromen-4-one (**6i**) (266 mg, 0.702 mmol, 70 % yield); ^1H NMR (500 MHz, CDCl_3): δ 10.59 (s, 1H), 8.21 (dd, J = 8.1, 1.6 Hz, 1H), 7.90 – 7.83 (m, 2H), 7.74 – 7.70 (m, 3H), 7.69 – 7.63 (m, 2H), 7.60 (d, J = 8.8 Hz, 1H), 7.45 (d, J = 8.1 Hz, 1H), 7.38 (ddd, J = 8.1, 7.2, 1.1 Hz, 1H), 7.26 (d, J = 8.8 Hz, 1H), 7.13 (ddd,

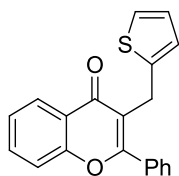
$J = 8.0, 6.9, 1.1$ Hz, 1H), 6.94 (ddd, $J = 8.3, 6.8, 1.4$ Hz, 1H), 6.79 (d, $J = 8.2$ Hz, 1H), 4.41 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) : δ 180.9, 163.8, 156.1, 153.7, 134.4, 133.5, 133.4, 131.4, 129.8, 129.3, 129.0, 128.8, 128.5, 126.1, 125.5, 125.3, 122.9, 122.4, 121.9, 121.2, 120.6, 117.9, 117.7, 22.9; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{26}\text{H}_{18}\text{O}_3$ $[\text{M}]^+$: 378.1256; found: 378.1259.

3-Benzyl-2-phenyl-4*H*-chromen-4-one (6j):



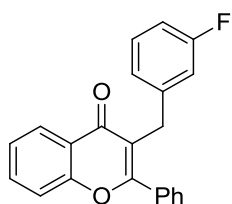
2'-Hydroxychalcone (225 mg, 1.0 mmol) and benzaldehyde (106 mg, 1.0 mmol) afforded 3-benzyl-2-phenyl-4*H*-chromen-4-one (**6j**) (204 mg, 0.652 mmol, 65 % yield); ^1H NMR (500 MHz, CDCl_3): δ 8.27 (ddd, $J = 8.0, 1.7, 0.5$ Hz, 1H), 7.70 – 7.65 (m, 1H), 7.59 – 7.55 (m, 2H), 7.54 – 7.50 (m, 1H), 7.49 – 7.45 (m, 3H), 7.41 (ddd, $J = 8.1, 7.1, 1.05$ Hz, 1H), 7.24 – 7.20 (m, 2H), 7.17 – 7.12 (m, 3H), 3.98 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) : δ 178.2, 162.9, 156.2, 140.1, 133.5, 133.2, 130.4, 128.6, 128.5, 128.3, 128.1, 126.1, 125.9, 124.9, 123.0, 120.6, 117.9, 31.2; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{22}\text{H}_{16}\text{O}_2$ $[\text{M}]^+$: 312.1150; found: 312.1147.

2-Phenyl-3-(thiophen-2-ylmethyl)-4*H*-chromen-4-one (6k):



2'-Hydroxychalcone (225 mg, 1.0 mmol) and thiophene-2-carbaldehyde (113 mg, 1.0 mmol) afforded 2-phenyl-3-(thiophen-2-ylmethyl)-4*H*-chromen-4-one (**6k**) (224 mg, 0.702 mmol, 70 % yield); ¹H NMR (500 MHz, CDCl₃): δ 8.30 – 8.27 (m, 1H), 7.71 – 7.63 (m, 3H), 7.56 – 7.49 (m, 3H), 7.49 – 7.45 (m, 1H), 7.42 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 7.09 (dd, *J* = 5.2, 1.2 Hz, 1H), 6.87 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.77 – 6.76 (m, 1H), 4.09 (s, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 177.9, 162.8, 156.2, 142.8, 133.6, 132.9, 130.6, 128.7, 128.6, 126.6, 126.1, 124.9, 124.9, 123.6, 123.0, 120.5, 117.9, 26.3; HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₀H₁₄O₂S [M]⁺: 318.0715; found: 318.0714.

3-(3-Fluorobenzyl)-2-phenyl-4*H*-chromen-4-one (**6l**) :

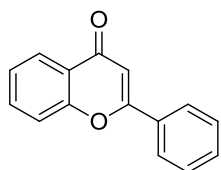


2'-Hydroxychalcone (225 mg, 1.0 mmol) and 3-fluorobenzaldehyde (125 mg, 1.0 mmol) afforded 3-(3-fluorobenzyl)-2-phenyl-4*H*-chromen-4-one (**6l**) (239 mg, 0.722 mmol, 72 % yield); ¹H NMR (500 MHz, CDCl₃): δ 8.37 – 8.16 (dd, , *J* = 8.0, 0.3 Hz 1H), 7.69 (ddd, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.57 – 7.51 (m, 2H), 7.51 – 7.46 (m, 3H), 7.42 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 7.25 – 7.11 (m, 2H), 6.92 – 6.80 (m, 1H), 6.83 (m, 2H), 3.96 (s, 2H); ¹³C NMR (125 MHz, CDCl₃) : δ 178.1, 163.2, 162.9 (d, *J* = 243.8 Hz), 156.2, 142.7 (d, *J* = 7.2 Hz), 133.7, 133.0, 130.5, 129.7 (d, *J* = 8.3 Hz), 128.6, 128.5, 128.2 (d, *J* = 33.6 Hz), 126.1, 125.0, 123.7 (d, *J* = 2.8

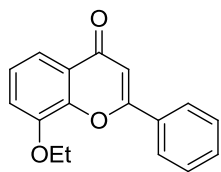
Hz), 119.9, 117.9, 114.9 (d, $J = 21.5$ Hz), 112.9 (d, $J = 21.0$ Hz), 31.0 (d, $J = 1.6$ Hz); HRMS (EI-MSES double focusing) m/z calcd. for $C_{22}H_{15}FO_2$ $[M]^+$: 330.1056; found: 330.1052.

S5. Experimental Procedure for Flavones

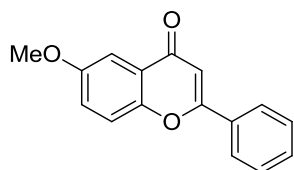
General Procedure for the Synthesis of flavone from salicylaldehyde and arylpropionic acids: To a reaction flask, salicylaldehyde (1.0 mmol), Phenyl propiolic acid (1.0 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (15 mg, 2.5 mol%), cesium acetate (384 mg, 2.0 mmol) and *tert*-Amyl alcohol (5 mL) were added. The solution was stirred at 100 °C for 12 h. The reaction mass was concentrated to dryness. Water was added and the crude product was extracted using ethyl acetate (2 x 25). The organic layer was washed with brine (1 x 25) and dried over sodium sulfate. The solvent was removed under reduced pressure, and the resulting crude product was purified by column chromatography (eluent = 10% ethyl acetate/hexane) to obtain the pure product.



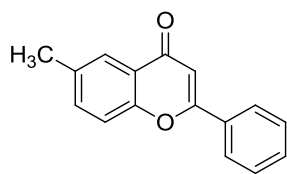
2-Phenyl-4H-chromen-4-one (4aa)¹: 3-Phenylpropionic acid (146 mg, 1.0 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 2-phenyl-4H-chromen-4-one (**4aa**) (133 mg, 0.599 mmol, 60% yield); 1H NMR (500 MHz, $CDCl_3$): δ 8.24 (ddd, $J = 8.0, 1.7, 0.4$ Hz 1H), 7.93 (dd, $J = 8.1, 1.6$ Hz 2H), 7.71 (dd, $J = 7.1, 1.7$ Hz 1H), 7.61 – 7.50 (m, 4H), 7.43 (ddd, $J = 8.1, 7.1, 1.1$ Hz, 1H), 6.84 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 178.5, 163.4, 156.3, 133.8, 131.8, 131.6, 129.0, 126.3, 125.7, 125.2, 123.9, 118.1, 107.6; MS (EI) m/z : 222 $[M]^+$.



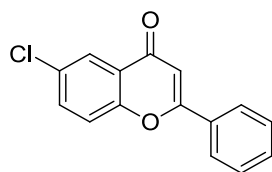
8-Ethoxy-2-phenyl-4H-chromen-4-one (4ba)²: 3-Phenylpropionic acid (146 mg, 1.0 mmol) and 3-ethoxy-2-hydroxybenzaldehyde (166 mg, 1.0 mmol) afforded 8-ethoxy-2-phenyl-4H-chromen-4-one (**4ba**) (144 mg, 0.539 mmol, 54% yield); ¹H NMR (500 MHz, CDCl₃): δ 7.98 (dd, *J* = 7.7, 4.3 Hz, 2H), 7.77 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.58 – 7.50 (m, 3H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.19 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.85 (s, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 1.57 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 178.6, 162.9, 148.5, 146.8, 131.9, 131.5, 129.0, 126.3, 125.0, 124.8, 116.4, 115.7, 107.2, 65.0, 14.8; MS (EI) *m/z*: 266 [M]⁺.



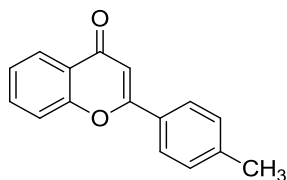
6-Methoxy-2-phenyl-4H-chromen-4-one (4da)³: 3-Phenylpropionic acid (146 mg, 1.0 mmol) and 2-hydroxy-5-methoxybenzaldehyde (152 mg, 1.0 mmol) afforded 6-methoxy-2-phenyl-4H-chromen-4-one (**4da**) (194 mg, 0.769 mmol, 77% yield); ¹H NMR (500 MHz, CDCl₃): 7.92 (dd, *J* = 8.0, 1.8 Hz, 2H), 7.60 (d, *J* = 3.1 Hz, 1H), 7.55 – 7.49 (m, 4H), 7.29 (dd, *J* = 9.1, 3.1 Hz, 1H), 6.82 (s, 1H), 3.92 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 178.3, 163.2, 156.9, 151.1, 131.9, 131.5, 129.0, 126.2, 124.6, 123.8, 119.5, 106.9, 104.8, 55.9; MS (EI) *m/z*: 252 [M]⁺.



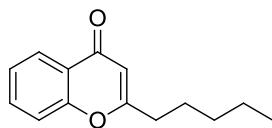
6-Methyl-2-phenyl-4H-chromen-4-one (4ea)⁴: 3-Phenylpropionic acid (146 mg, 1.0 mmol) and 2-hydroxy-5-methylbenzaldehyde (136 mg, 1.0 mmol) afforded 6-methyl-2-phenyl-4H-chromen-4-one (**4ea**) (161 mg, 0.679 mmol, 68% yield); ¹H NMR (500 MHz, CDCl₃): 8.02 (d, *J* = 0.7 Hz, 1H), 7.96 – 7.90 (m, 2H), 7.57 – 7.49 (m, 4H), 7.47 (d, *J* = 8.6 Hz, 1H), 6.81 (s, 1H), 2.47 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 178.6, 163.2, 154.6, 135.2, 134.9, 131.9, 131.5, 128.9, 126.2, 125.0, 123.6, 117.8, 107.4, 20.9; MS (EI) *m/z*: 236 [M]⁺.



6-Chloro-2-phenyl-4H-chromen-4-one (4ha)¹: 3-Phenylpropionic acid (146 mg, 1.0 mmol) and 5-chloro-2-hydroxybenzaldehyde (156 mg, 1.0 mmol) afforded 6-chloro-2-phenyl-4H-chromen-4-one (**4ha**) (154 mg, 0.599 mmol, 60% yield); ¹H NMR (500 MHz, CDCl₃): δ 8.20 (d, *J* = 2.6 Hz, 1H), 7.92 (dd, *J* = 8.3, 1.8 Hz, 2H), 7.65 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.59 – 7.50 (m, 4H), 6.83 (s, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 177.2, 163.7, 154.6, 133.9, 131.8, 131.4, 131.2, 129.1, 126.3, 125.2, 124.9, 119.8, 107.5; MS (EI) *m/z*: 256 [M]⁺.



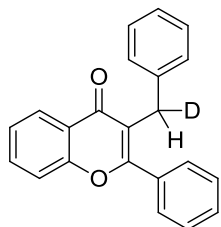
2-(*p*-Tolyl)-4*H*-chromen-4-one (4ad)¹: 3-(*p*-Tolyl)propionic acid (150 mg, 1.0 mmol) and salicylaldehyde (111 mg, 1.0 mmol) afforded 2-(*p*-tolyl)-4*H*-chromen-4-one (**4ad**) (170 mg, 0.719 mmol, 72% yield); ¹H NMR (500 MHz, CDCl₃): δ 8.23 (ddd, *J* = 7.9, 1.7, 0.4 Hz, 1H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.69 (ddd, *J* = 8.8, 7.2, 1.8 Hz, 1H), 7.57 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.42 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 7.33 (dd, *J* = 8.6, 0.7 Hz, 2H), 6.80 (s, 1H), 2.44 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 178.5, 163.6, 156.2, 142.2, 133.6, 129.8, 128.9, 126.2, 125.7, 125.1, 123.9, 118.0, 106.9, 21.5; MS (EI) *m/z*: 236 [M]⁺.



2-Pentyl-4*H*-chromen-4-one (4am)¹: 2-octynoic acid (140 mg, 1.0 mmol) and salicylaldehyde (122 mg, 1.0 mmol) afforded 2-pentyl-4*H*-chromen-4-one (**4am**) (119 mg, 0.549 mmol, 55% yield); ¹H NMR (500 MHz, CDCl₃): δ 8.18 (ddd, *J* = 7.9, 1.7, 0.5 Hz, 1H), 7.63 (ddd, *J* = 8.5, 7.2, 1.8 Hz, 1H), 7.42 (ddd, *J* = 8.5, 1.1, 0.5 Hz, 1H), 7.37 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 6.18 (s, 1H), 2.61 (t, *J* = 7.7 Hz, 2H), 1.81 – 1.65 (m, 2H), 1.44 – 1.31 (m, 4H), 0.95 – 0.89 (m, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 178.4, 169.8, 156.5, 133.4, 125.6, 124.9, 123.7, 117.8, 109.8, 34.3, 31.1, 26.5, 22.3, 13.9; MS (EI) *m/z*: 216 [M]⁺.

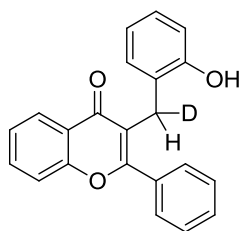
S6. Control experiments

3-Benzyl-2-phenyl-4*H*-chromen-4-one-*d* (**6j-D**):



2'-Hydroxychalcone (191 mg, 1.0 mmol) and benzaldehyde-*d* (107 mg, 1.0 mmol) afforded 3-benzyl-2-phenyl-4*H*-chromen-4-one-*d* (**6j-D**) (194 mg, 0.62 mmol, 62% yield); ¹H NMR (500 MHz, CDCl₃): δ 8.26 (ddd, *J* = 8.0, 1.7, 0.5 Hz, 1H), 7.68 (ddd, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.59 – 7.55 (m, 2H), 7.54 – 7.50 (m, 1H), 7.50 – 7.45 (m, 3H), 7.41 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.17 – 7.11 (m, 3H), 3.98 (s, 0.75H), 3.97 (s, 0.55H); ¹³C NMR (125 MHz, CDCl₃): δ 178.3, 162.9, 156.2, 140.1, 133.6, 133.2, 130.4, 128.6, 128.6, 128.4, 128.1, 126.1, 125.9, 124.9, 123.0, 120.6, 117.9, 31.2, 30.9 (t, *J*=20.3 Hz); HRMS (EI-MSES double focusing) *m/z* calcd. for C₂₂H₁₅DO₂ [M]⁺: 313.1213; found: 313.1209.

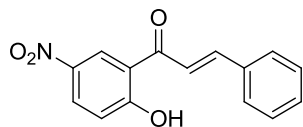
3-(2-Hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one-*d* (**3aa-D**):



3-Phenylpropionic acid (178 mg, 1.218 mmol) and salicylaldehyde-*d* (100 mg, 0.812 mmol) afforded 3-(2-hydroxybenzyl)-2-phenyl-4*H*-chromen-4-one-*d* (**3aa-D**) (103 mg, 0.385 mmol,

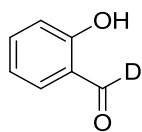
77% yield); ^1H NMR (500 MHz, CDCl_3): δ 9.67 (s, 1H), 8.29 (dd, J = 8.1, 1.6 Hz, 1H), 7.70 (ddd, J = 8.7, 7.1, 1.7 Hz, 1H), 7.64 (s, 5H), 7.52 – 7.40 (m, 2H), 7.08 – 7.00 (m, 1H), 6.90 (dd, J = 8.1, 1.1 Hz, 1H), 6.57 (td, J = 7.5, 1.2 Hz, 1H), 6.26 (dd, J = 7.7, 1.7 Hz, 1H), 3.94 (s, 0.06H), 3.93 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 180.4, 164.5, 156.2, 155.2, 134.4, 133.0, 130.7, 130.3, 129.1, 128.9, 128.3, 126.1, 125.7, 125.4, 122.2, 121.6, 119.8, 118.2, 117.9, 25.5 (t, J = 19.2); HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{22}\text{H}_{15}\text{DO}_3$ $[\text{M}]^+$: 329.1162; found: 329.1173.

(*E*)-1-(2-Hydroxy-5-nitrophenyl)-3-phenylprop-2-en-1-one (6ma):



3-Phenylpropionic acid (219 mg, 1.5 mmol) and 2-hydroxy-5-nitrobenzaldehyde (167 mg, 1.0 mmol) afforded (*E*)-1-(2-hydroxy-5-nitrophenyl)-3-phenylprop-2-en-1-one (**6ma**) (108 mg, 0.400 mmol, 40% yield); Refer the manuscript more information; ^1H NMR (500 MHz, CDCl_3): δ 13.59 (s, 1H), 8.91 (d, J = 2.7 Hz, 1H), 8.39 (dd, J = 9.2, 2.7 Hz, 1H), 8.05 (d, J = 15.4 Hz, 1H), 7.75 – 7.73 (m, 2H), 7.69 (d, J = 15.4 Hz, 1H), 7.51 – 7.49 (m, 3H), 7.14 (d, J = 9.2 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 192.8, 168.5, 148.1, 139.5, 133.9, 131.8, 130.9, 129.2, 129.2, 126.1, 119.7, 118.8, 118.4; HRMS (EI-MSES double focusing) m/z calcd. for $\text{C}_{15}\text{H}_{11}\text{NO}_4$ $[\text{M}]^+$: 269.0688; found: 269.0686.

Synthesis of Salicylaldehyde-*d*:



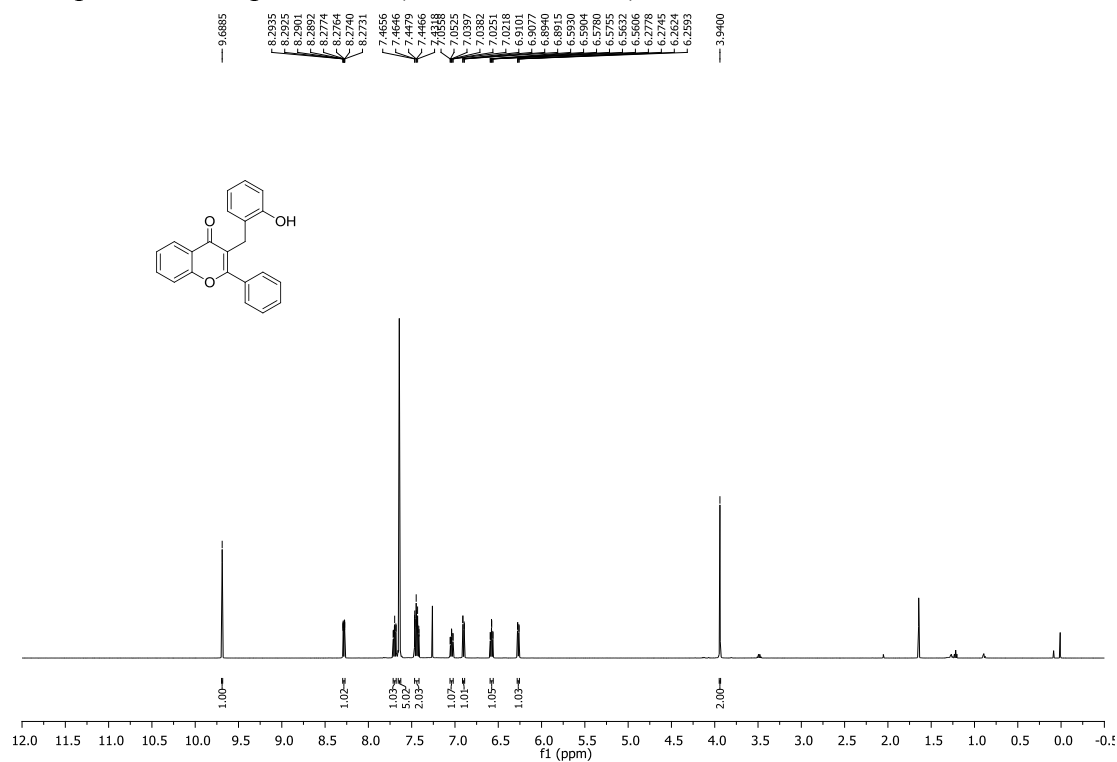
Synthesis of salicylaldehyde-*d* was performed using the known literature procedure¹; ¹H NMR (500 MHz, CDCl₃): δ 11.04 (s, 1H), 7.65 – 7.44 (m, 2H), 7.09 – 6.90 (m, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 196.3 (t, *J* = 26.9 Hz), 161.7, 136.9, 133.7, 120.6 (t, *J* = 2.9 Hz), 119.8, 117.6.

S7. References

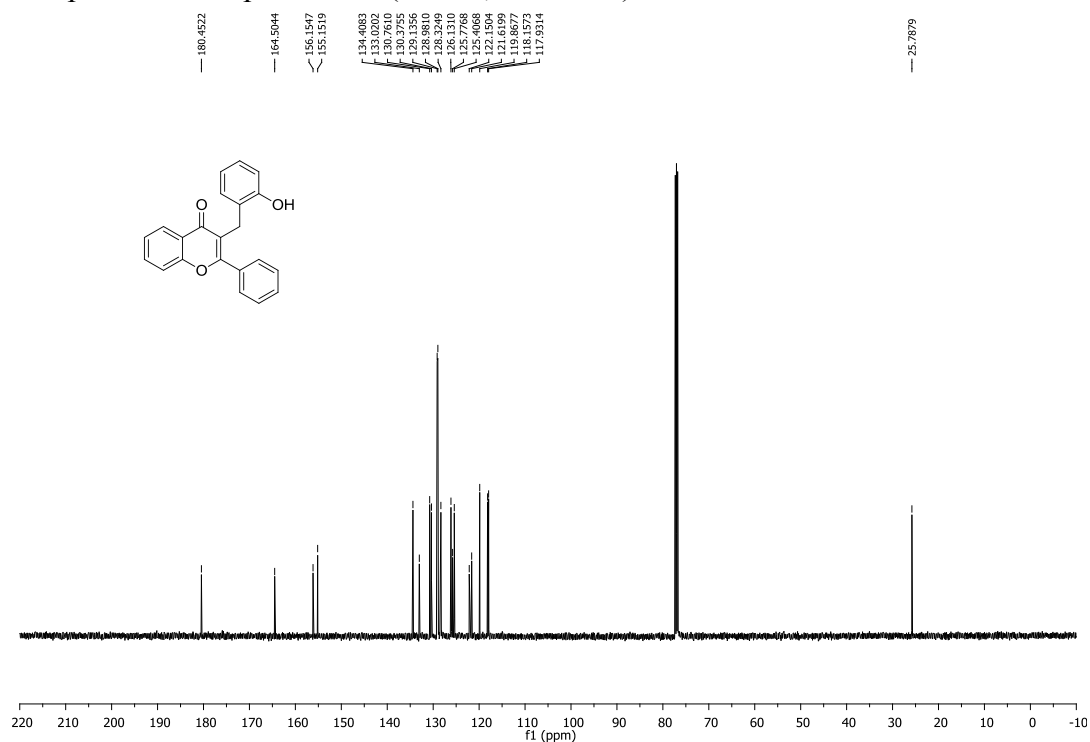
1. Baruah, S.; Kaishap, P. P.; Gogoi, S. *Chem. Commun.* **2016**, 52, 13004.
2. Liu, J.; Song, W.; Yue, Y.; Liu, R.; Yi, H.; Zhuo, K.; Lei, A. *Chem. Commun.* **2015**, 51, 17576.
3. Yoshida, M.; Fujino, Y.; Doi, T. *Org. Lett.* **2011**, 13, 4526.
4. Zhu, X.; Chen, Y.; Chen, Y.; Wang, J.; Su, W. *Lett. Org. Chem.* **2014**, 11, 621.

S8. Spectral Copies of ^1H and ^{13}C NMR of the Compounds

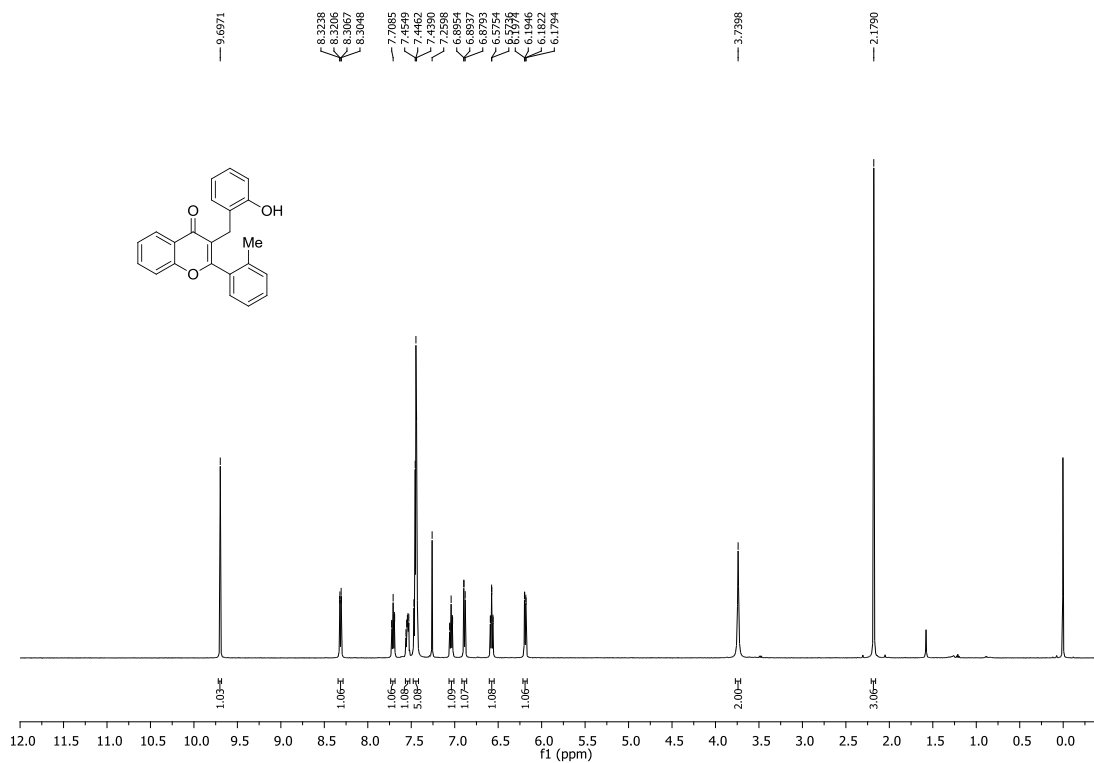
^1H NMR spectra of compound **3aa** (CDCl_3 , 500 MHz)



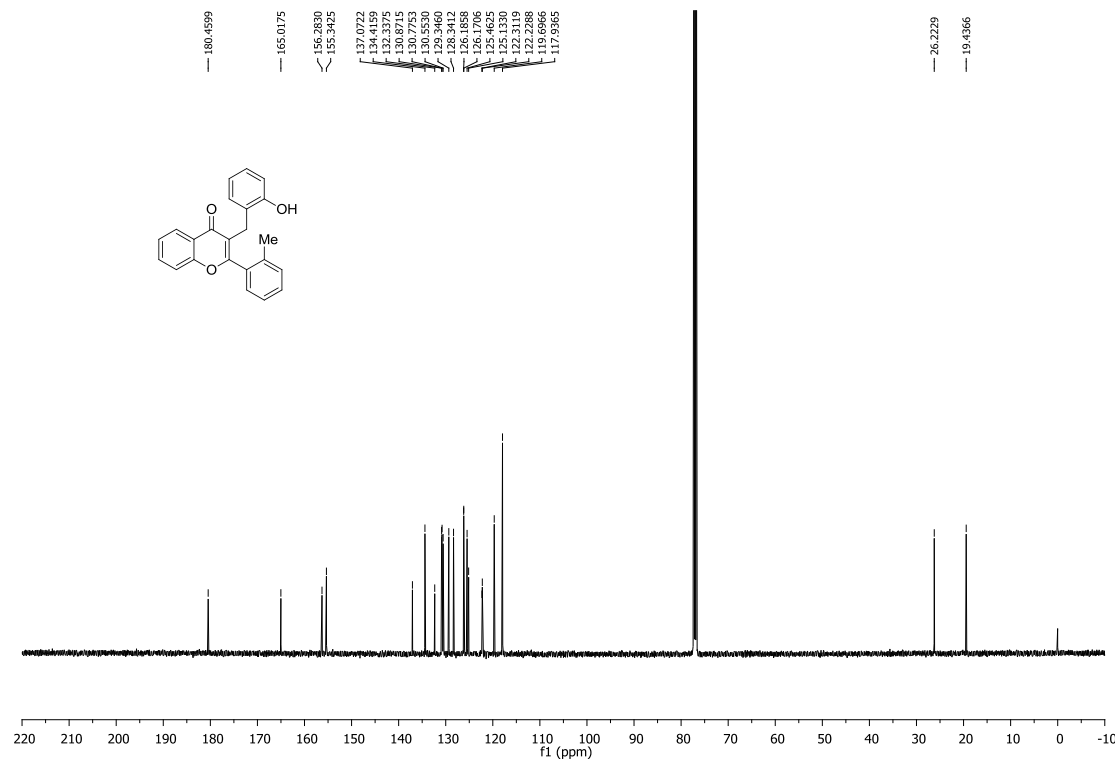
^{13}C NMR spectra of compound **3aa** (CDCl_3 , 125 MHz)



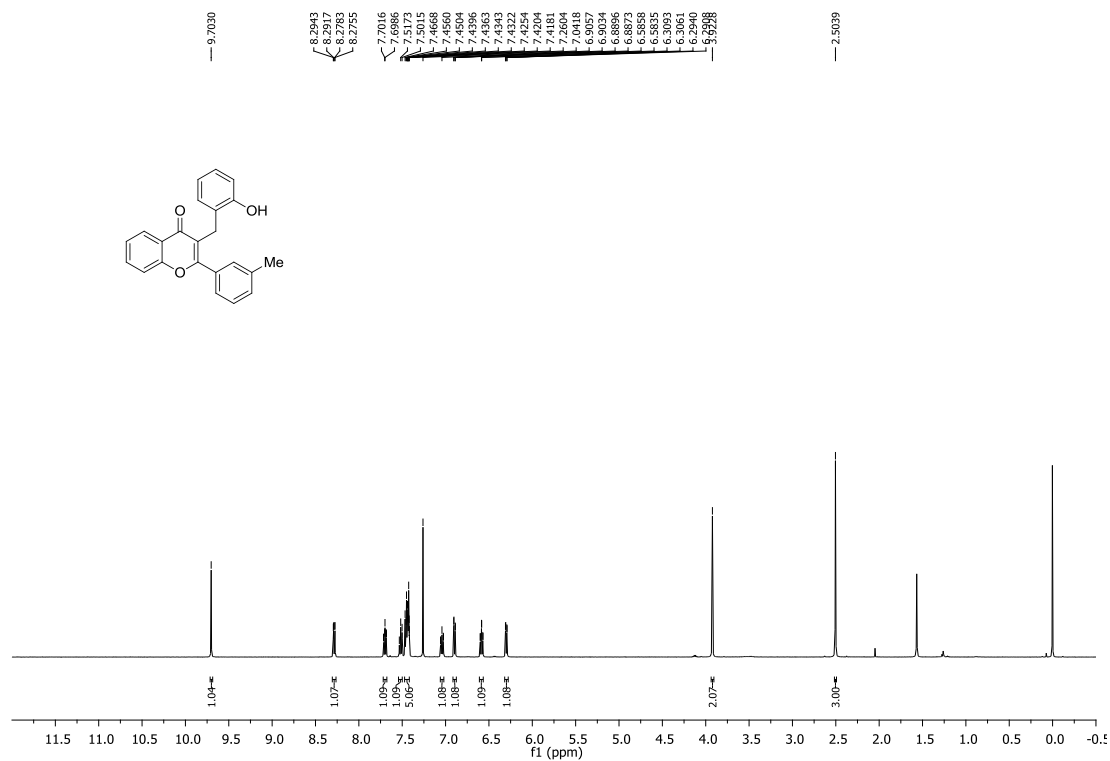
^1H NMR spectra of compound **3ab** (CDCl_3 , 500 MHz)



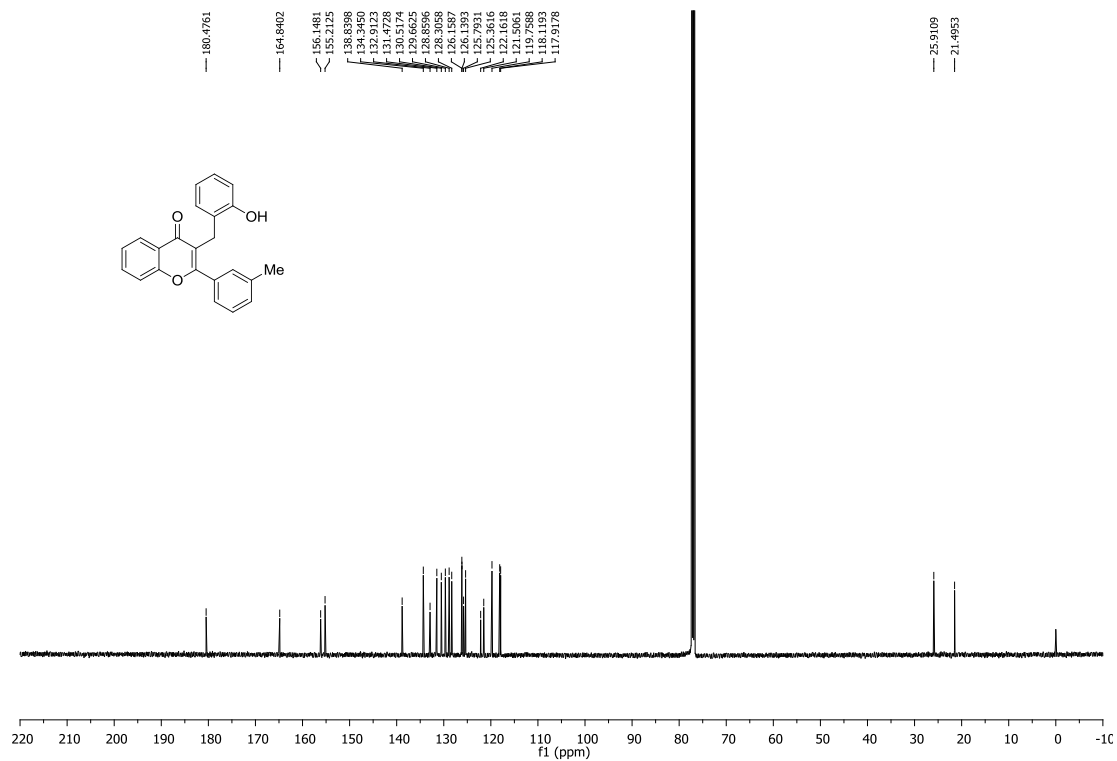
^{13}C NMR spectra of compound **3ab** (CDCl_3 , 125 MHz)



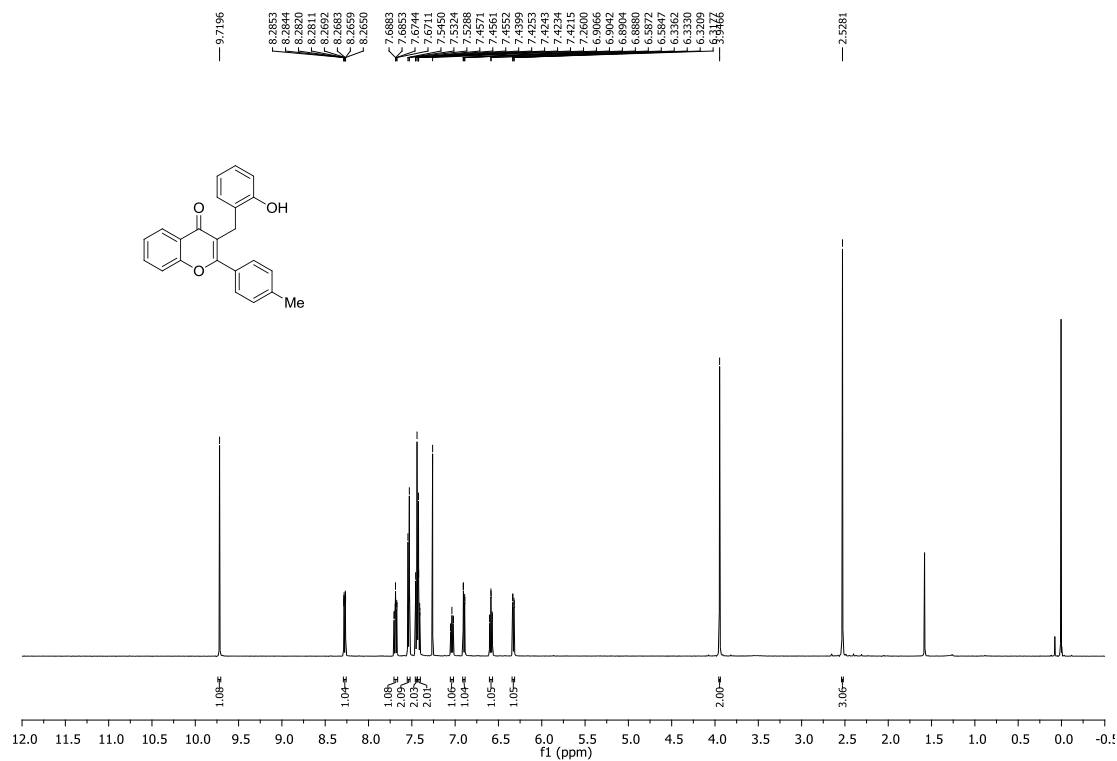
^1H NMR spectra of compound **3ac** (CDCl_3 , 500 MHz)



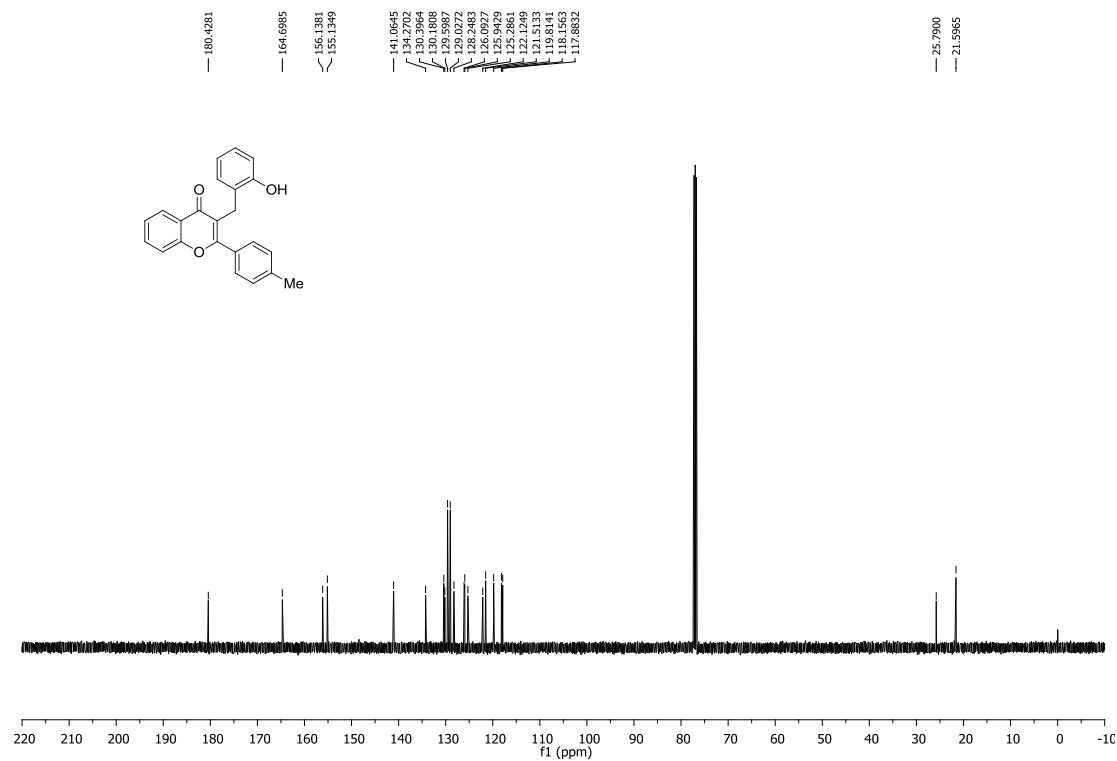
^{13}C NMR spectra of compound **3ac** (CDCl_3 , 125 MHz)



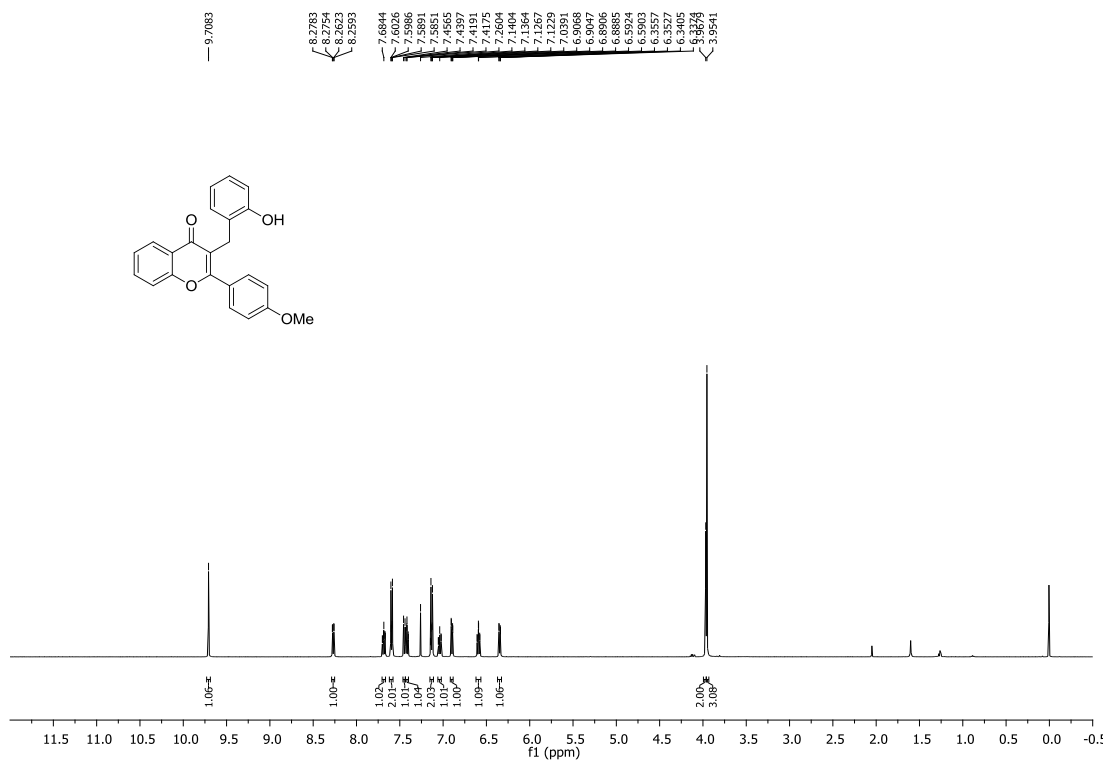
¹H NMR spectra of compound **3ad** (CDCl₃, 500 MHz)



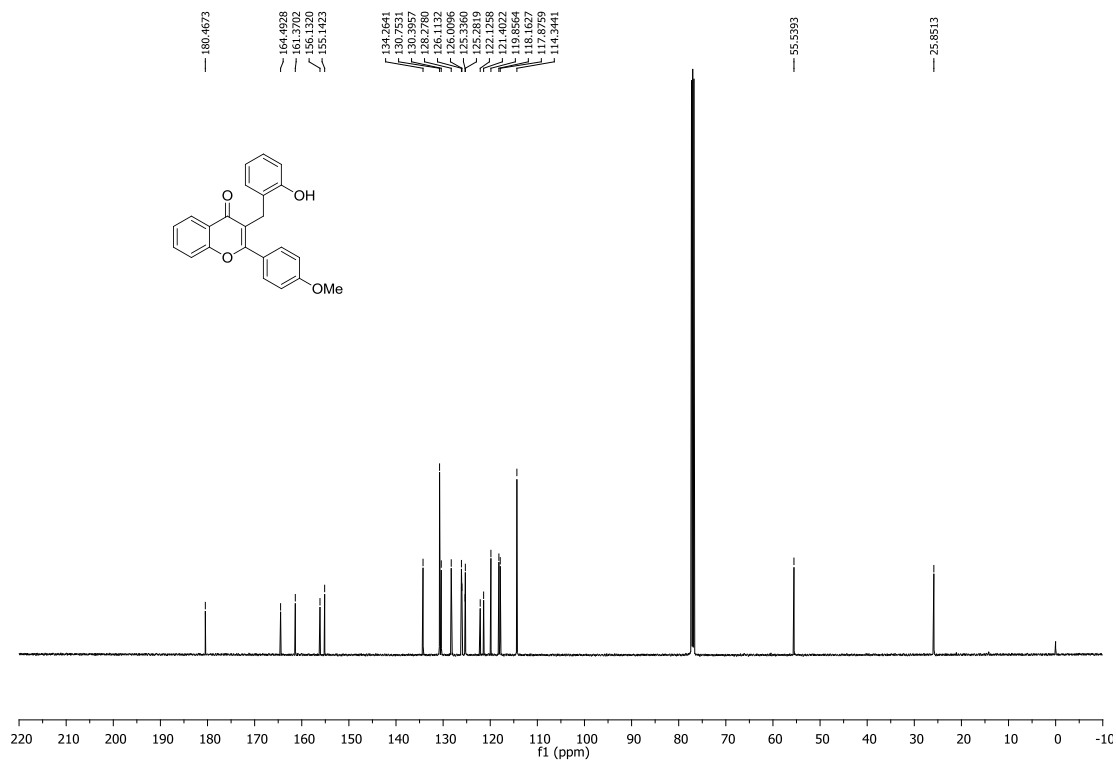
¹³C NMR spectra of compound **3ad** (CDCl₃, 125 MHz)



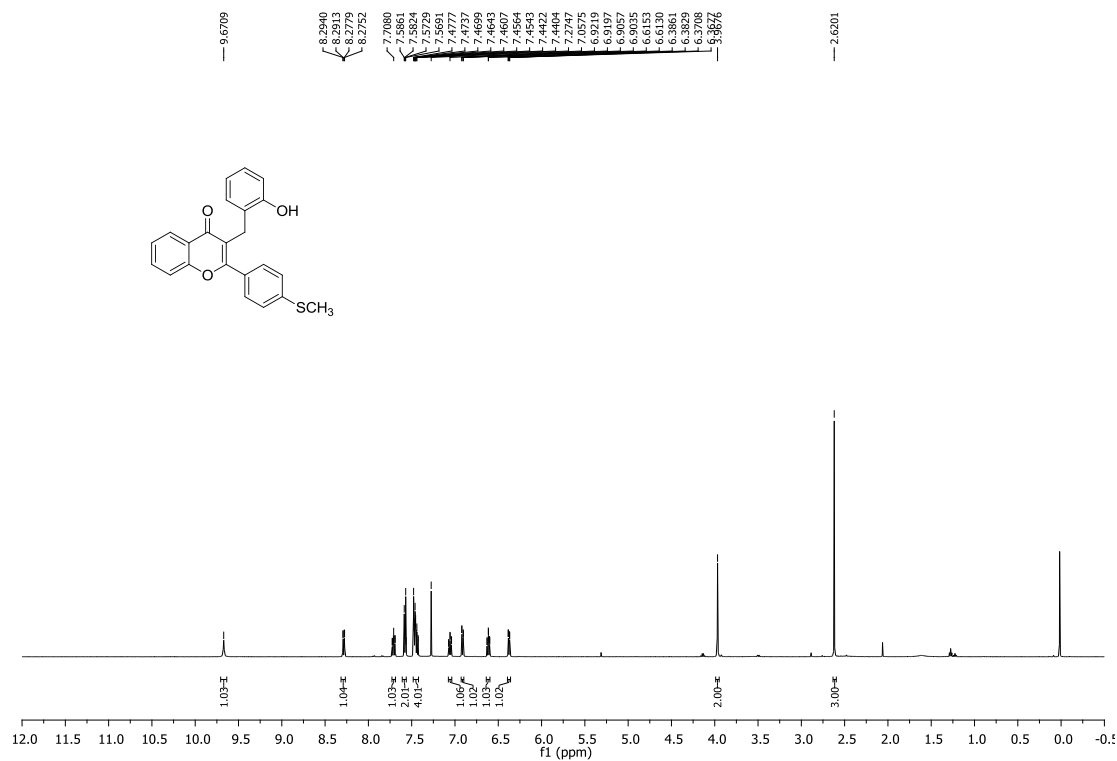
^1H NMR spectra of compound **3ae** (CDCl_3 , 500 MHz)



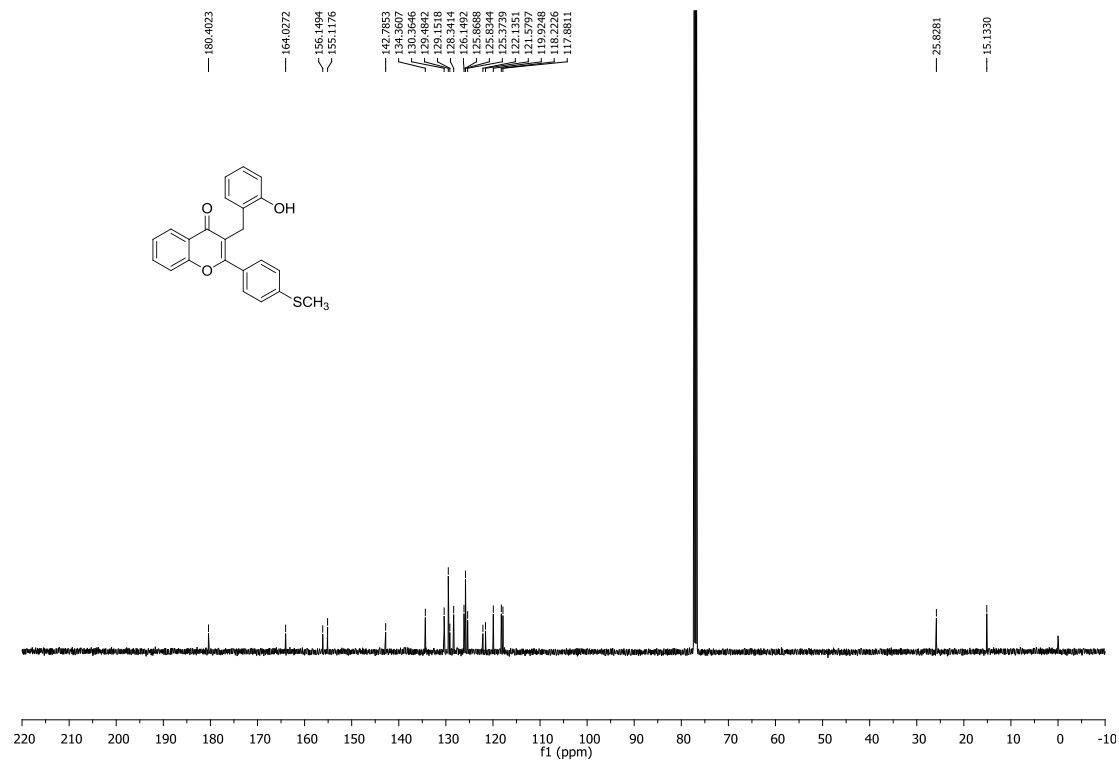
^{13}C NMR spectra of compound **3ae** (CDCl_3 , 125 MHz)



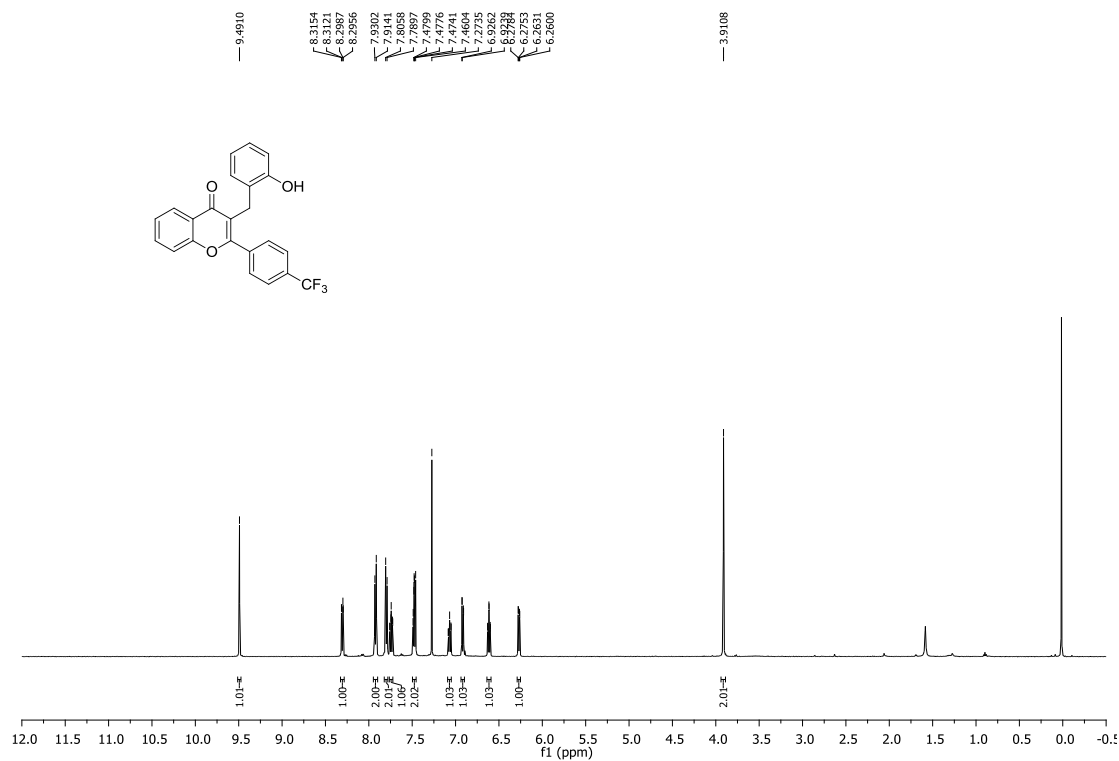
^1H NMR spectra of compound **3af** (CDCl_3 , 500 MHz)



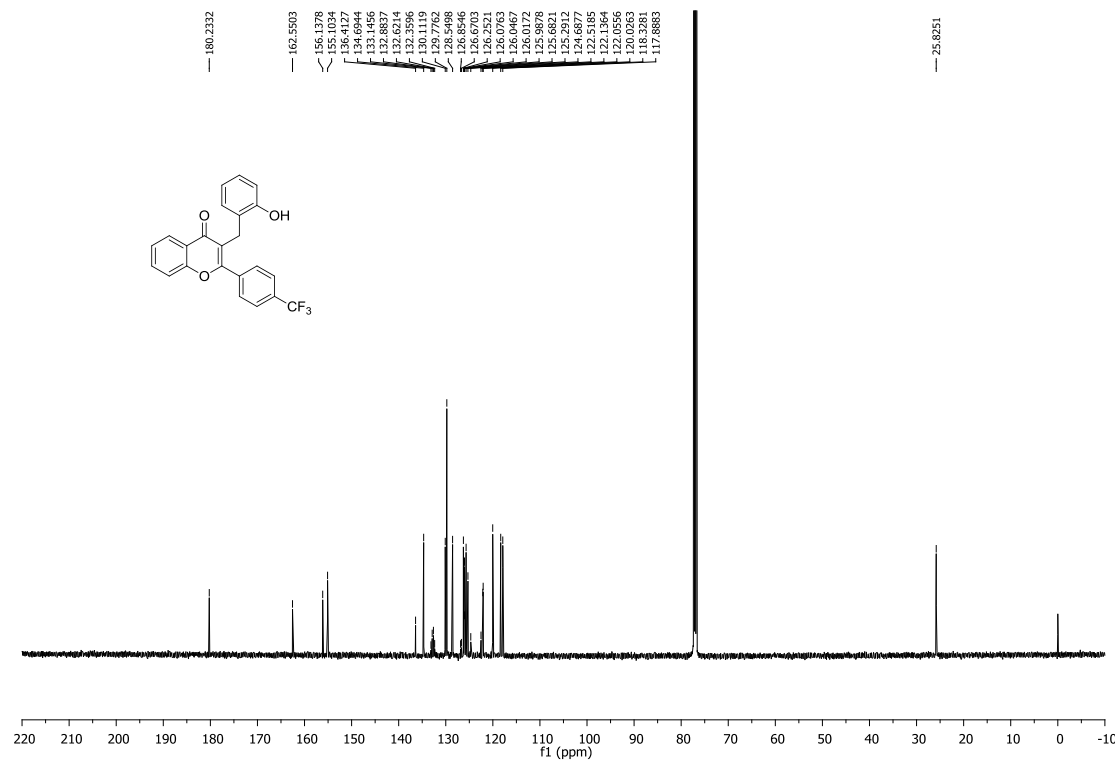
^{13}C NMR spectra of compound **3af** (CDCl_3 , 125 MHz)



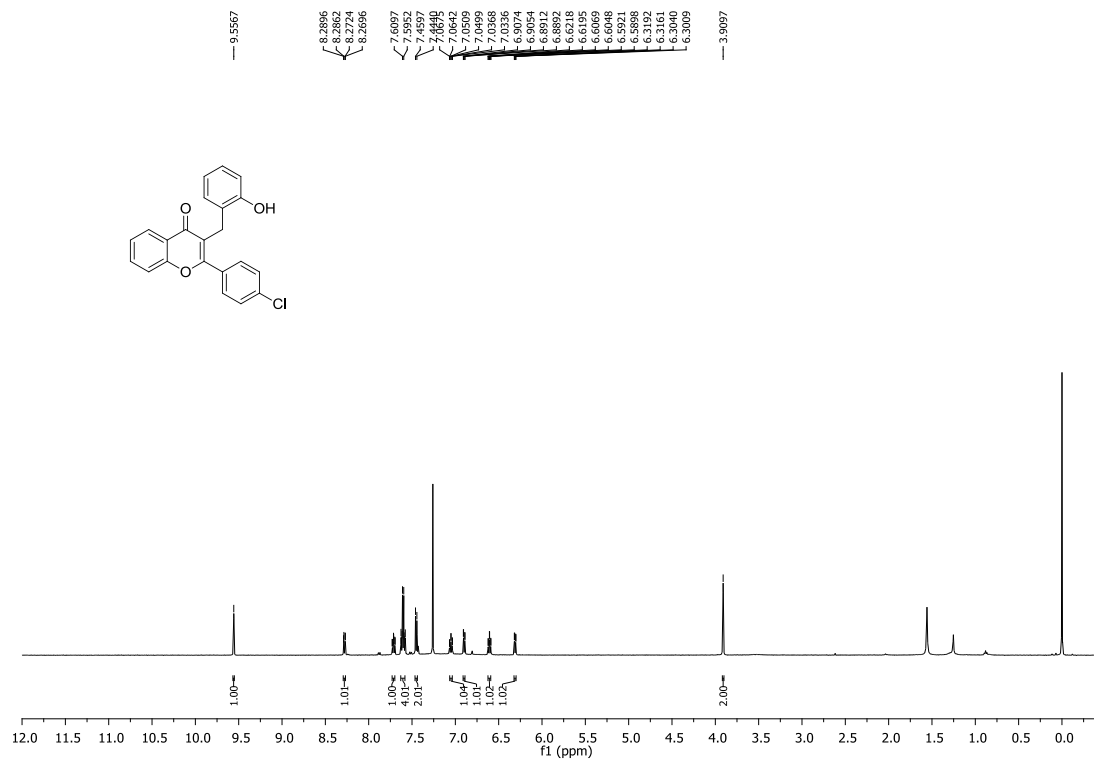
¹H NMR spectra of compound **3ag** (CDCl₃, 500 MHz)



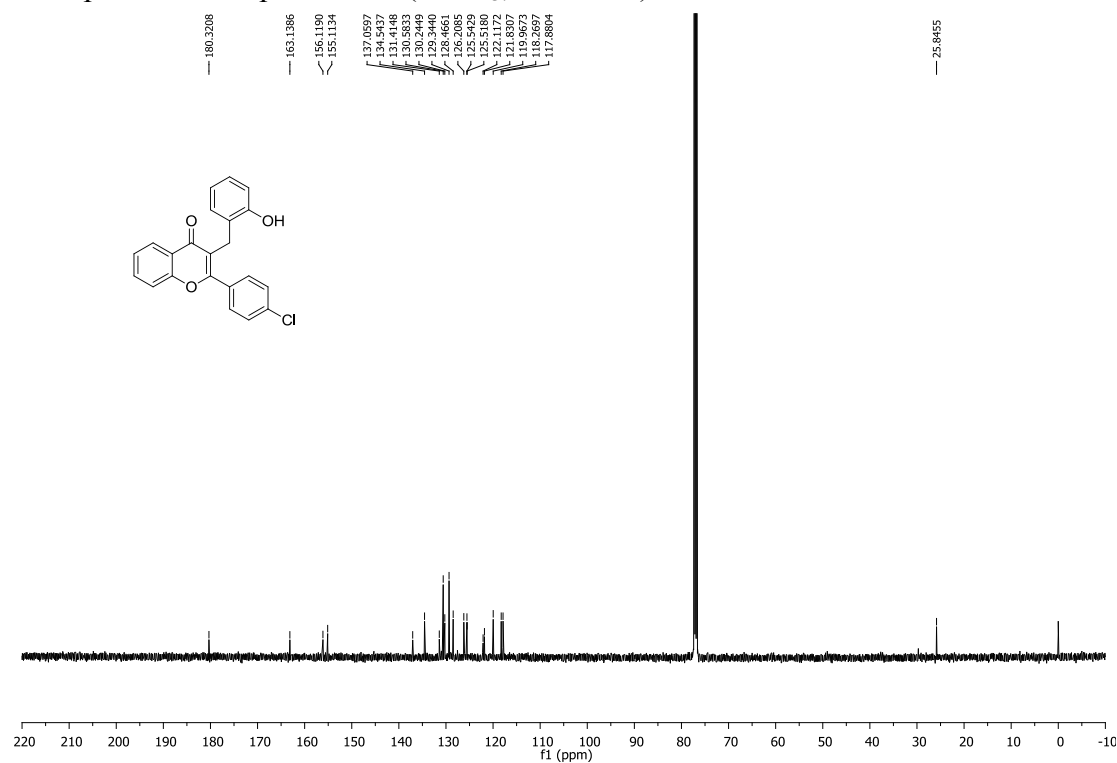
¹³C NMR spectra of compound **3ag** (CDCl₃, 125 MHz)



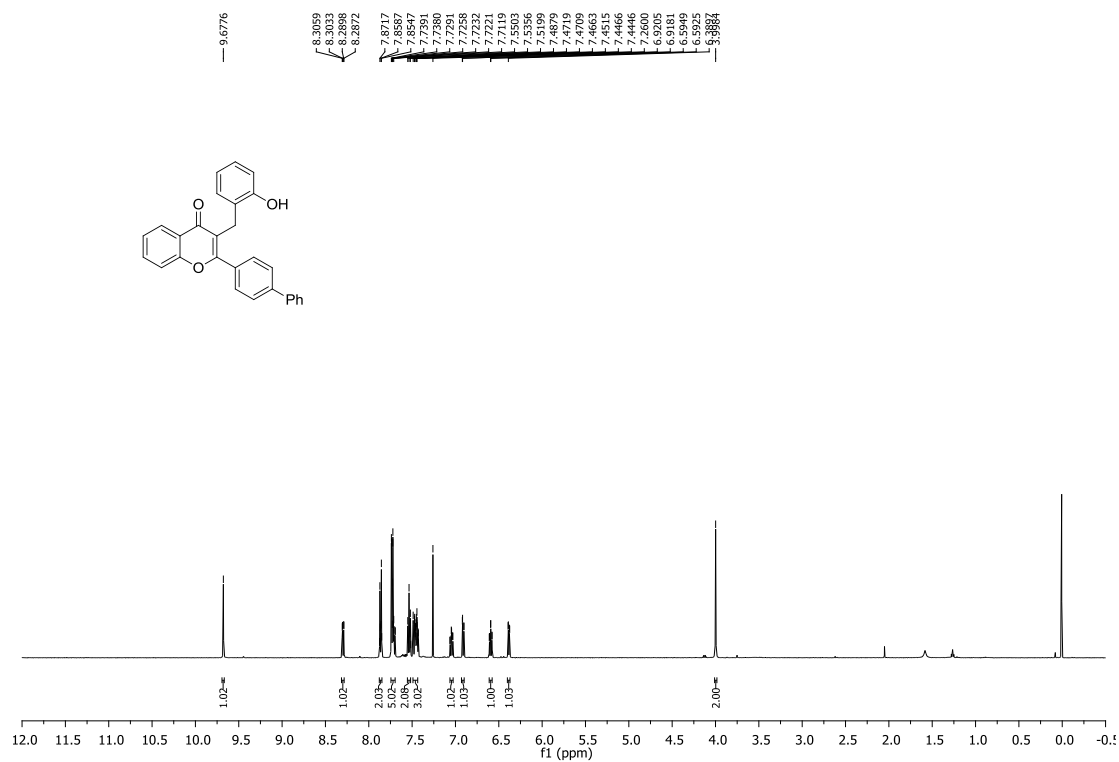
^1H NMR spectra of compound **3ah** (CDCl_3 , 500 MHz)



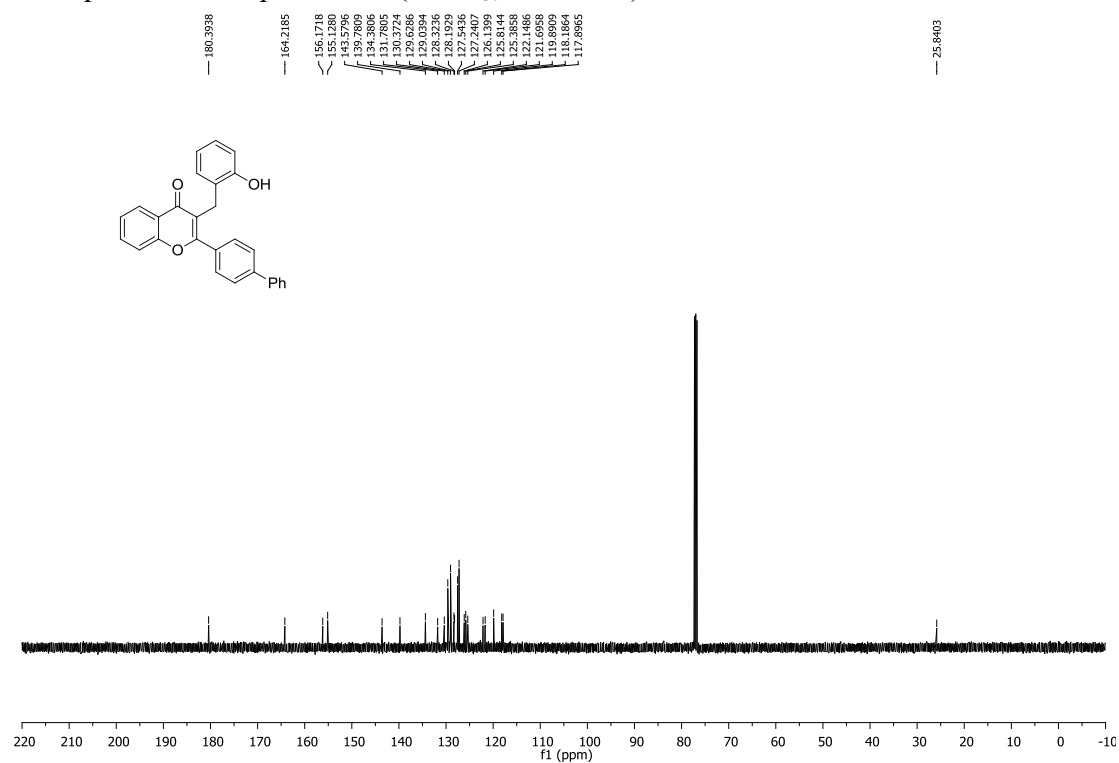
^{13}C NMR spectra of compound **3ah** (CDCl_3 , 125 MHz)



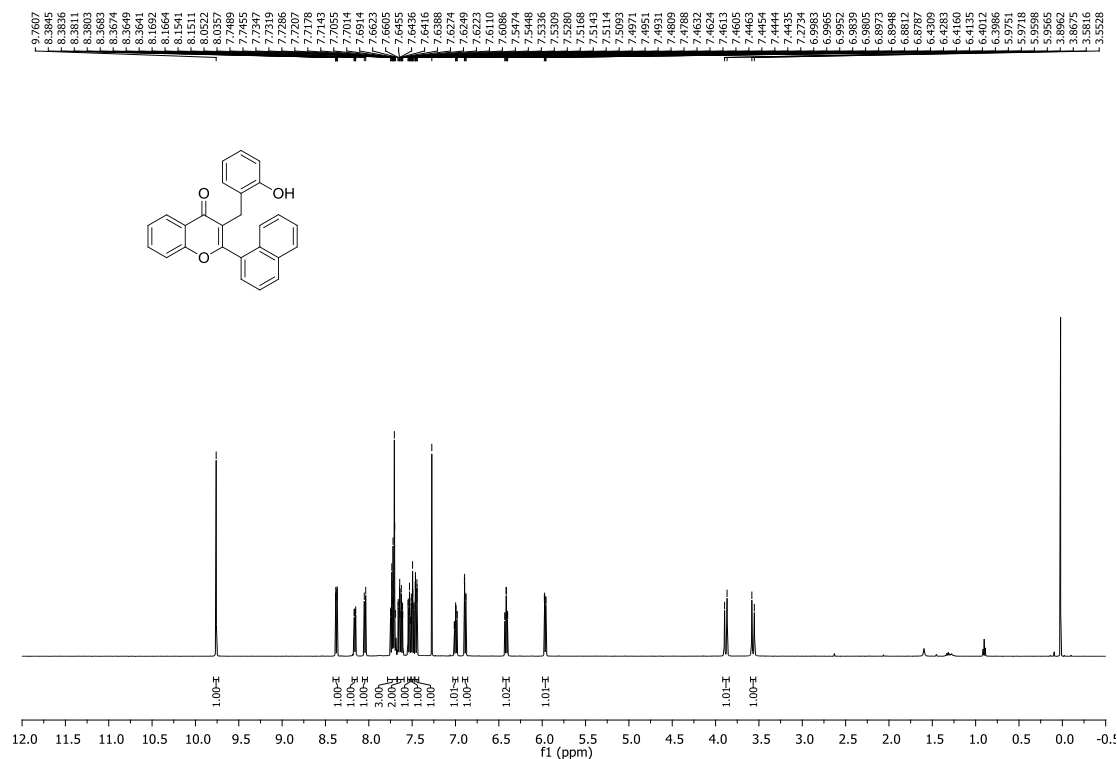
^1H NMR spectra of compound **3ai** (CDCl_3 , 500 MHz)



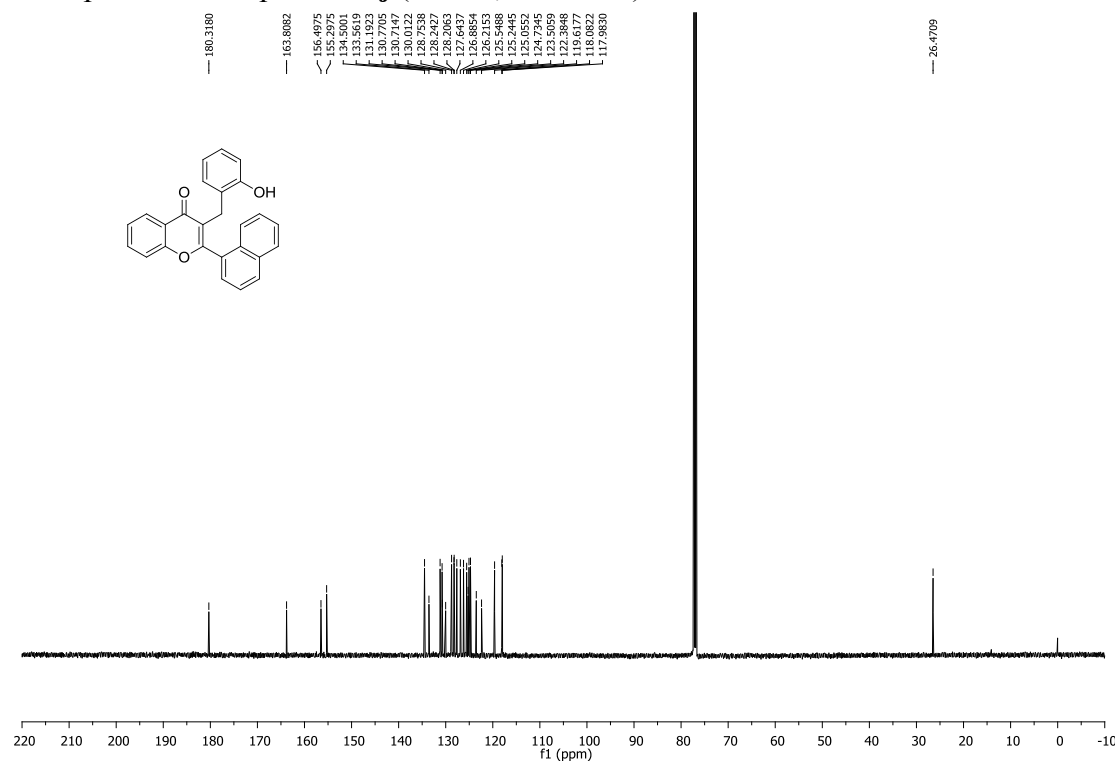
^{13}C NMR spectra of compound **3ai** (CDCl_3 , 125 MHz)



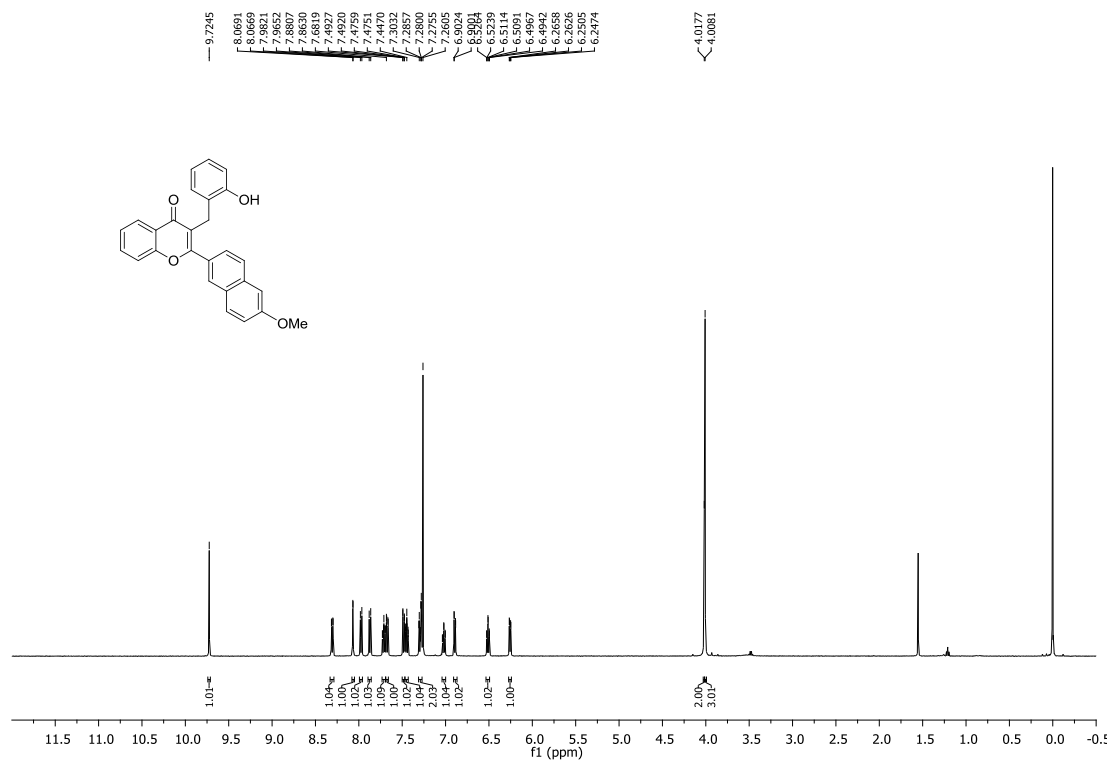
¹H NMR spectra of compound **3aj** (CDCl₃, 500 MHz)



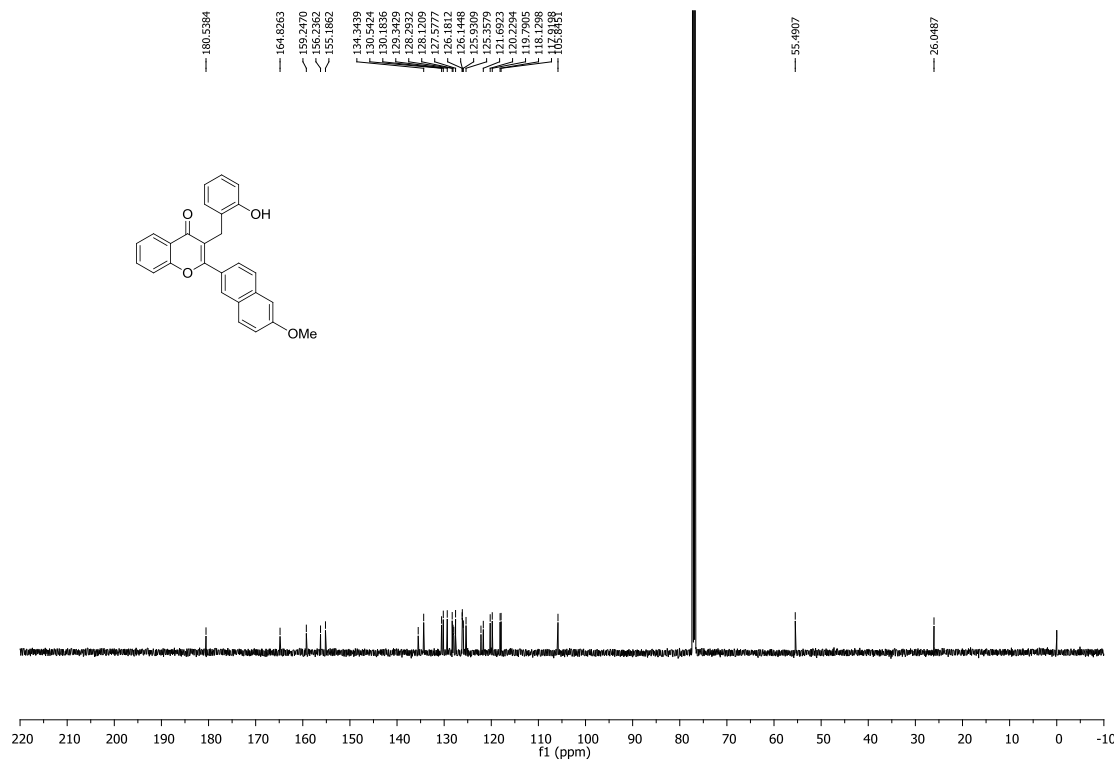
¹³C NMR spectra of compound **3aj** (CDCl₃, 125 MHz)



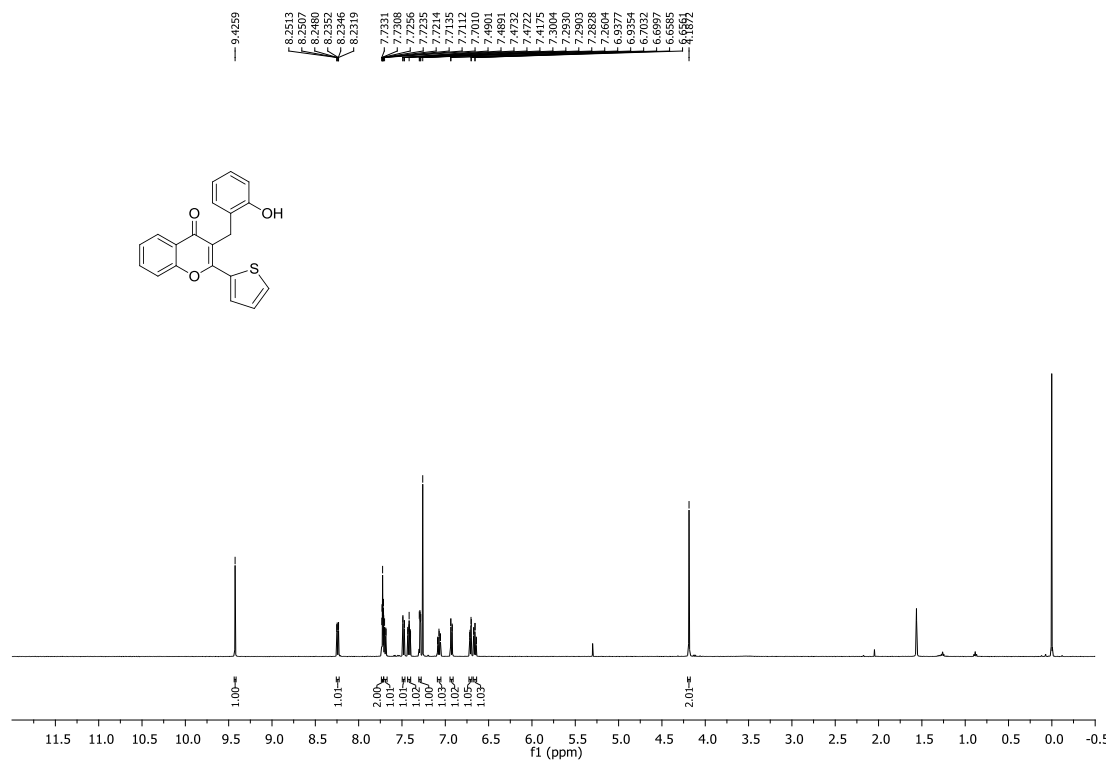
^1H NMR spectra of compound **3ak** (CDCl_3 , 500 MHz)



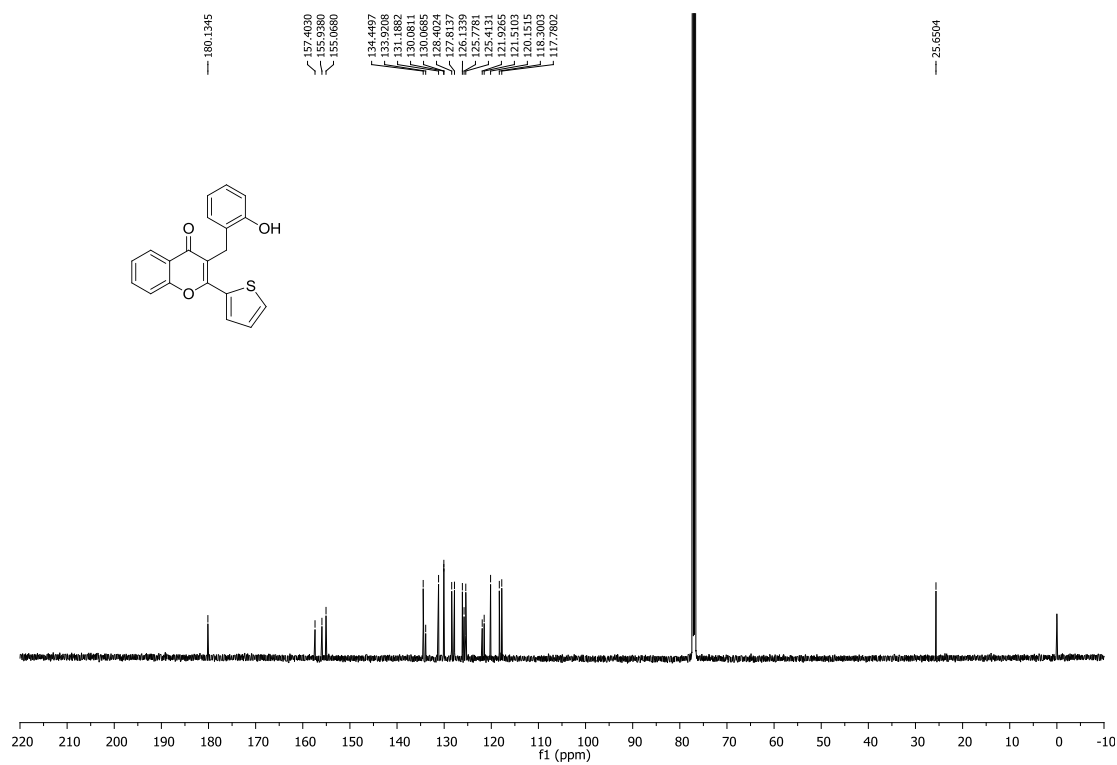
^{13}C NMR spectra of compound **3ak** (CDCl_3 , 125 MHz)



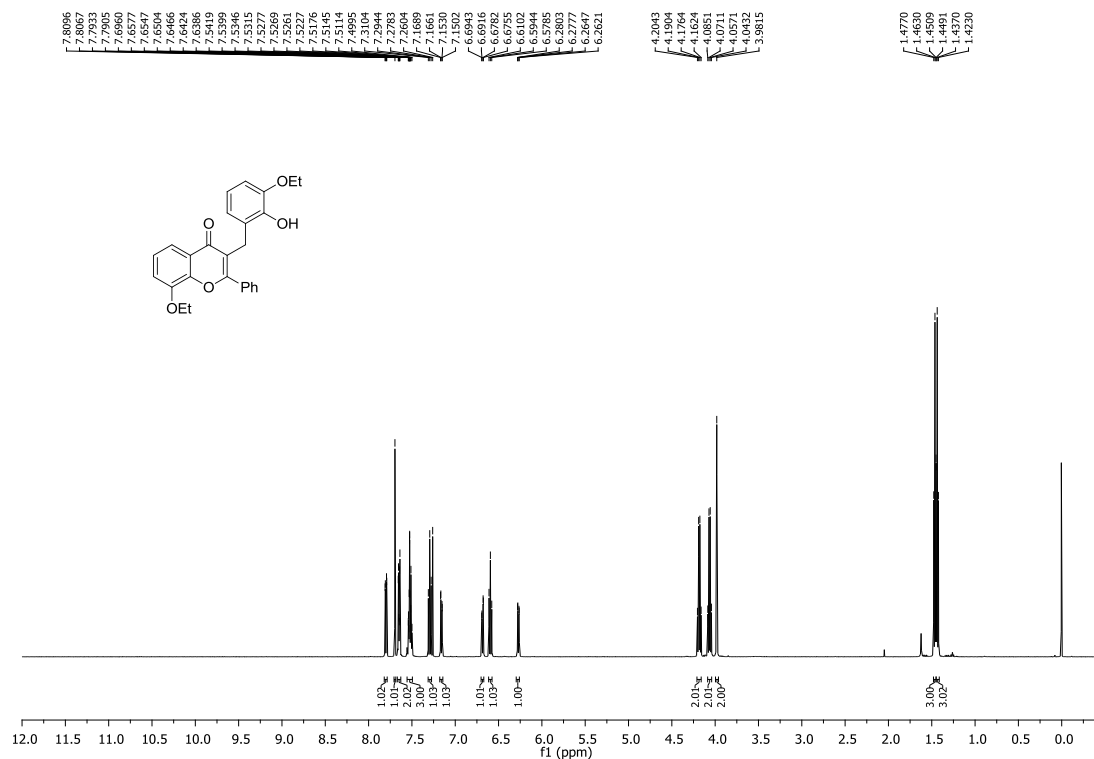
^1H NMR spectra of compound **3al** (CDCl_3 , 500 MHz)



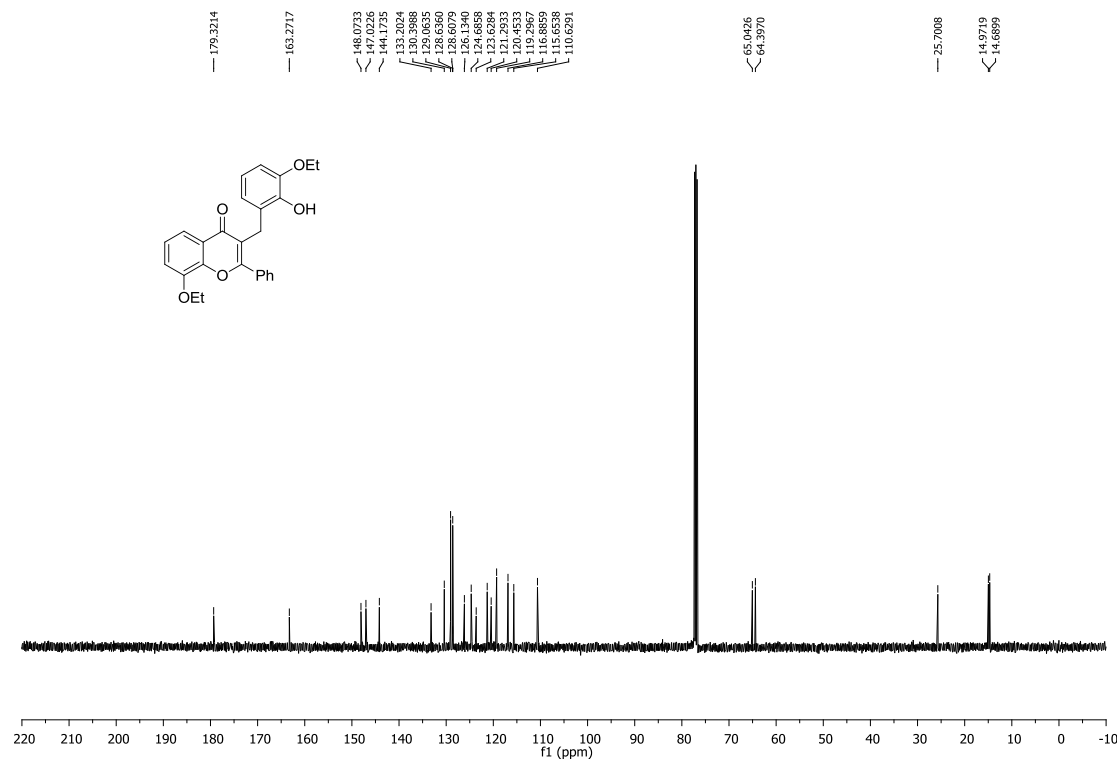
^{13}C NMR spectra of compound **3al** (CDCl_3 , 125 MHz)



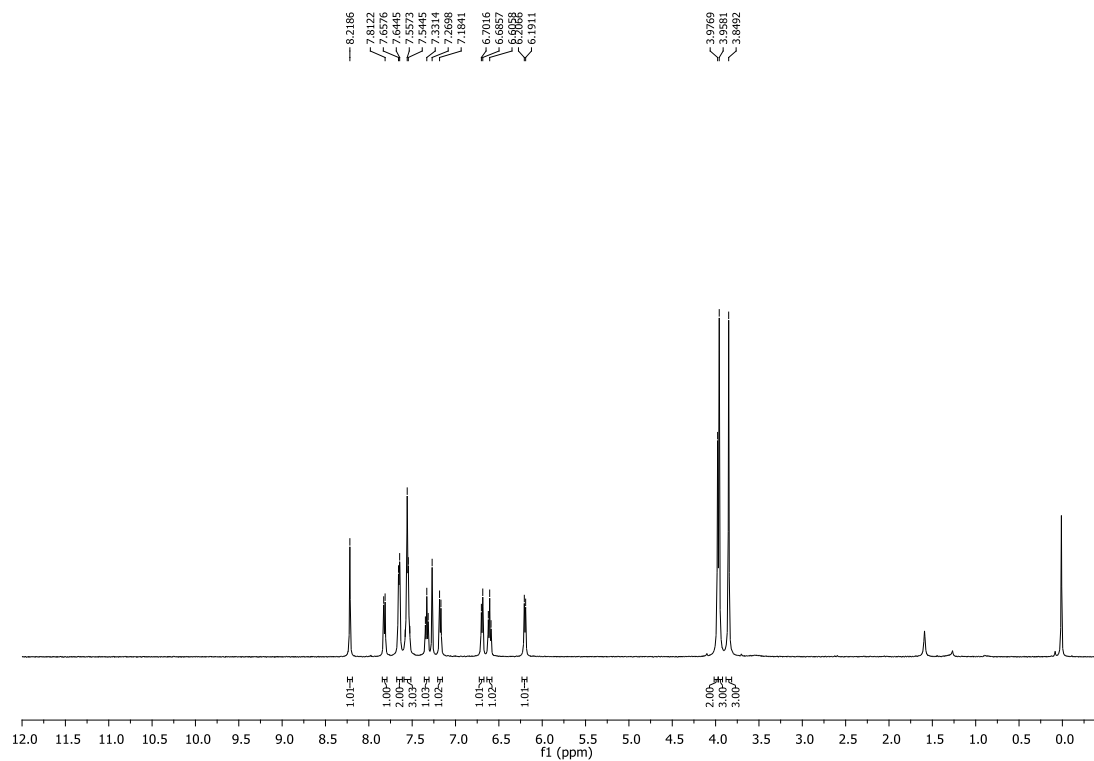
¹H NMR spectra of compound **3ba** (CDCl₃, 500 MHz)



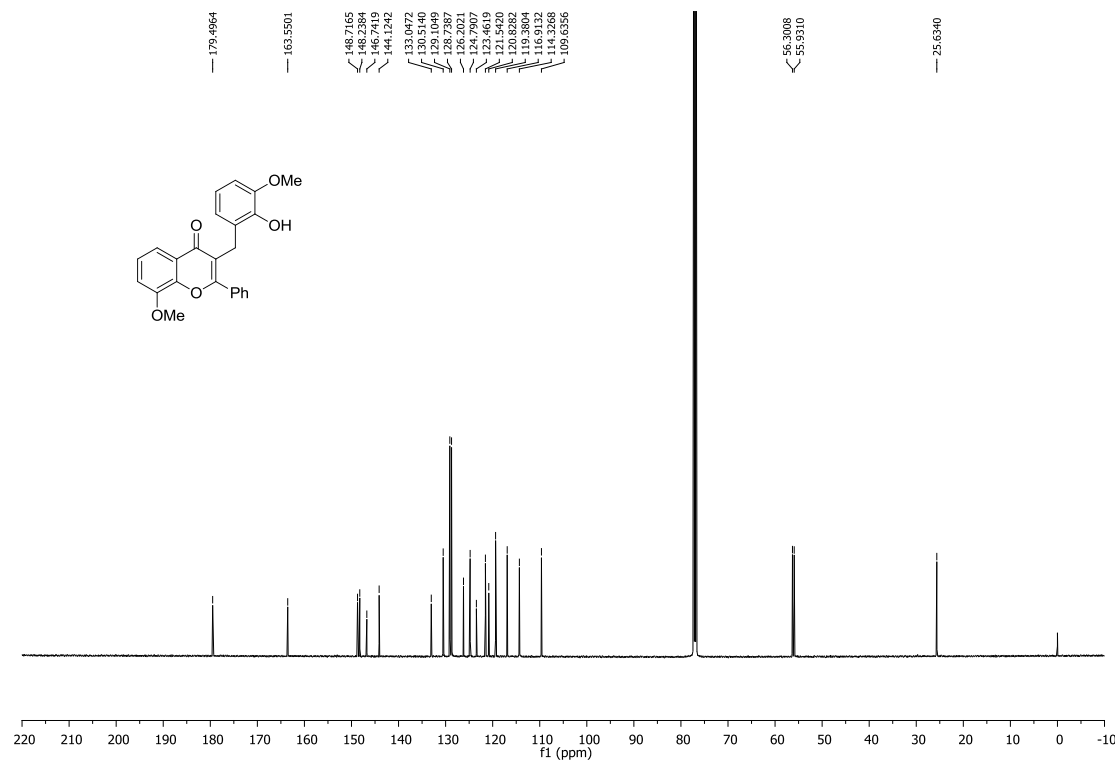
¹³C NMR spectra of compound **3ba** (CDCl₃, 125 MHz)



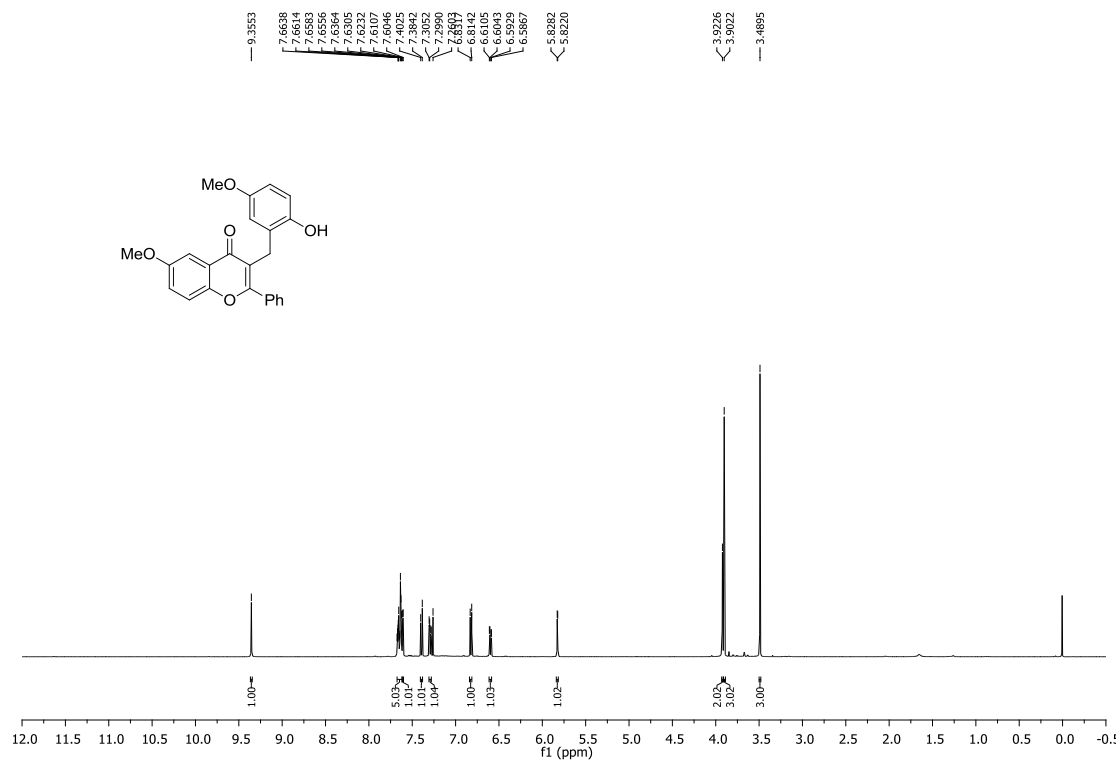
^1H NMR spectra of compound **3ca** (CDCl_3 , 500 MHz)



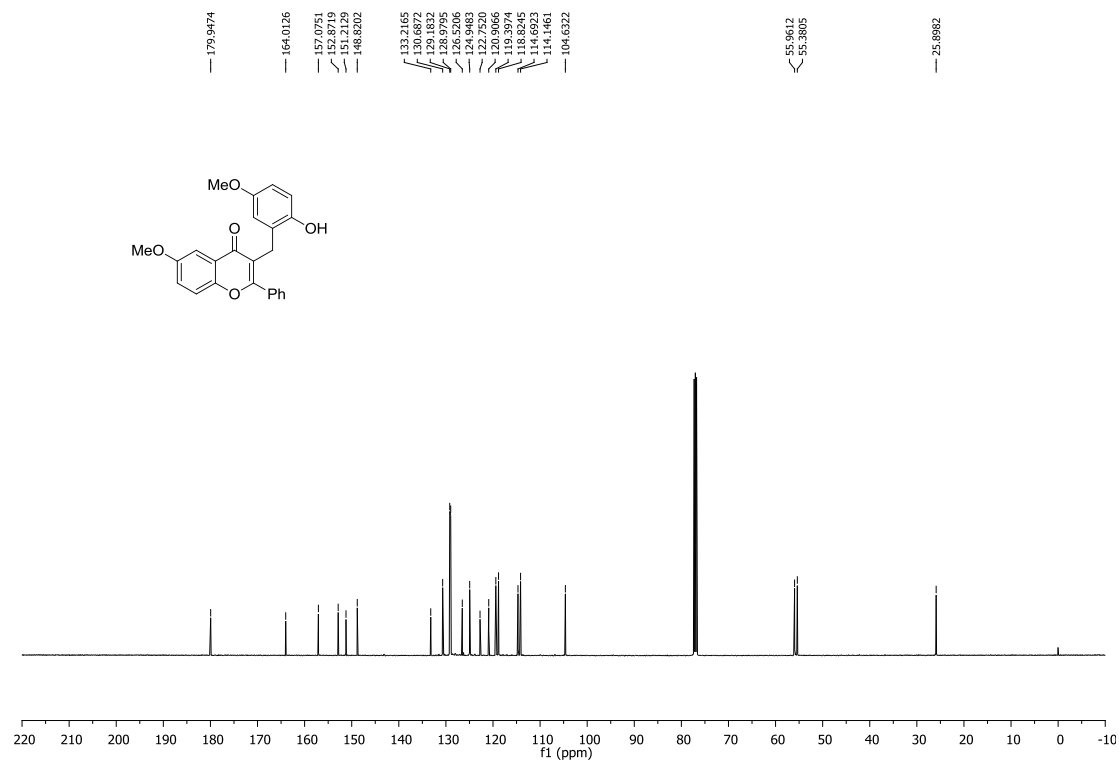
^{13}C NMR spectra of compound **3ca** (CDCl_3 , 125 MHz)



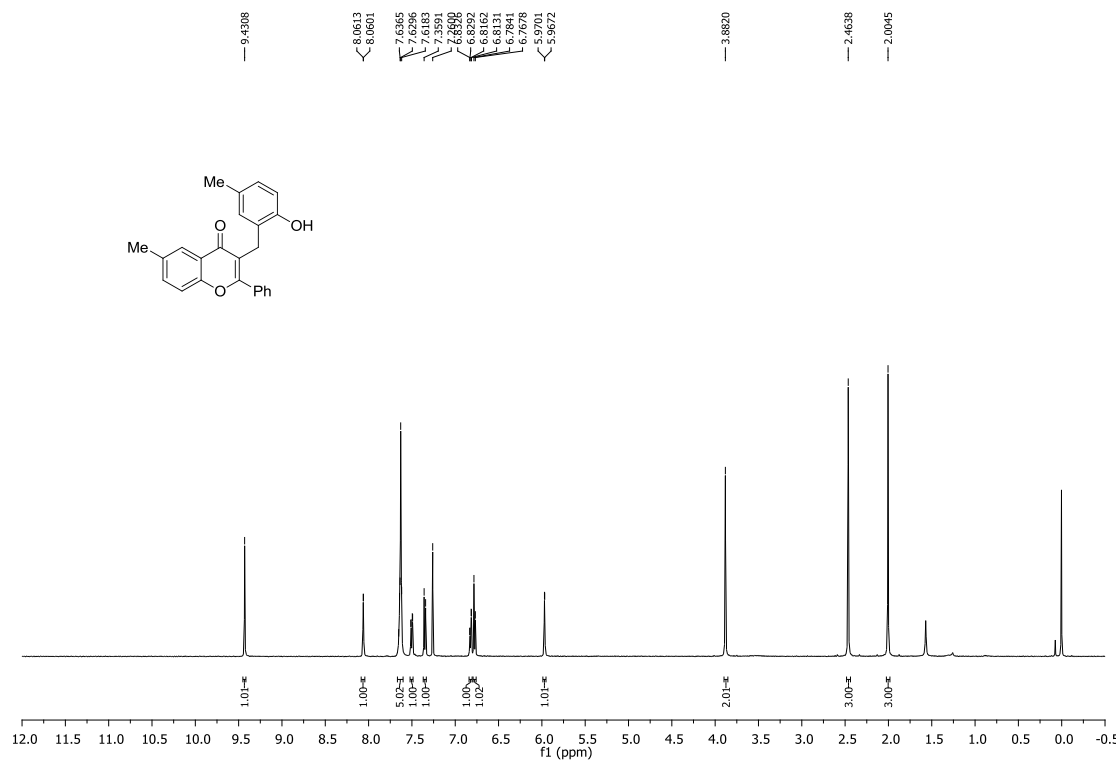
^1H NMR spectra of compound **3da** (CDCl_3 , 500 MHz)



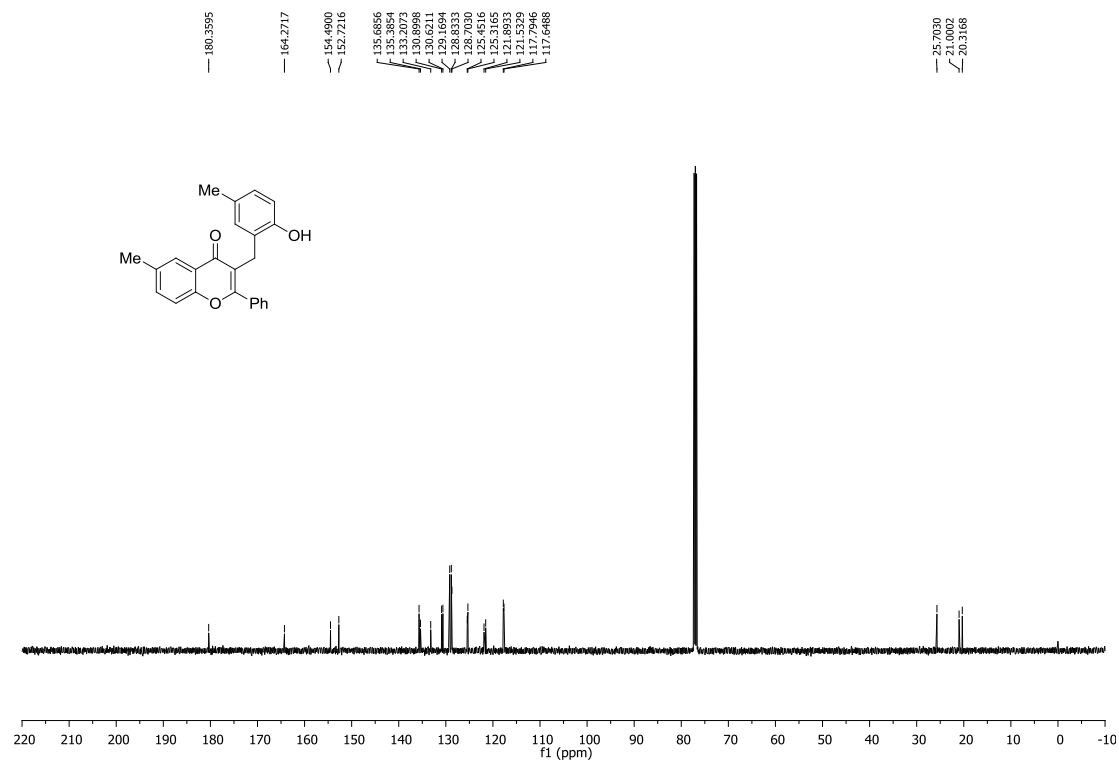
^{13}C NMR spectra of compound **3da** (CDCl_3 , 125 MHz)



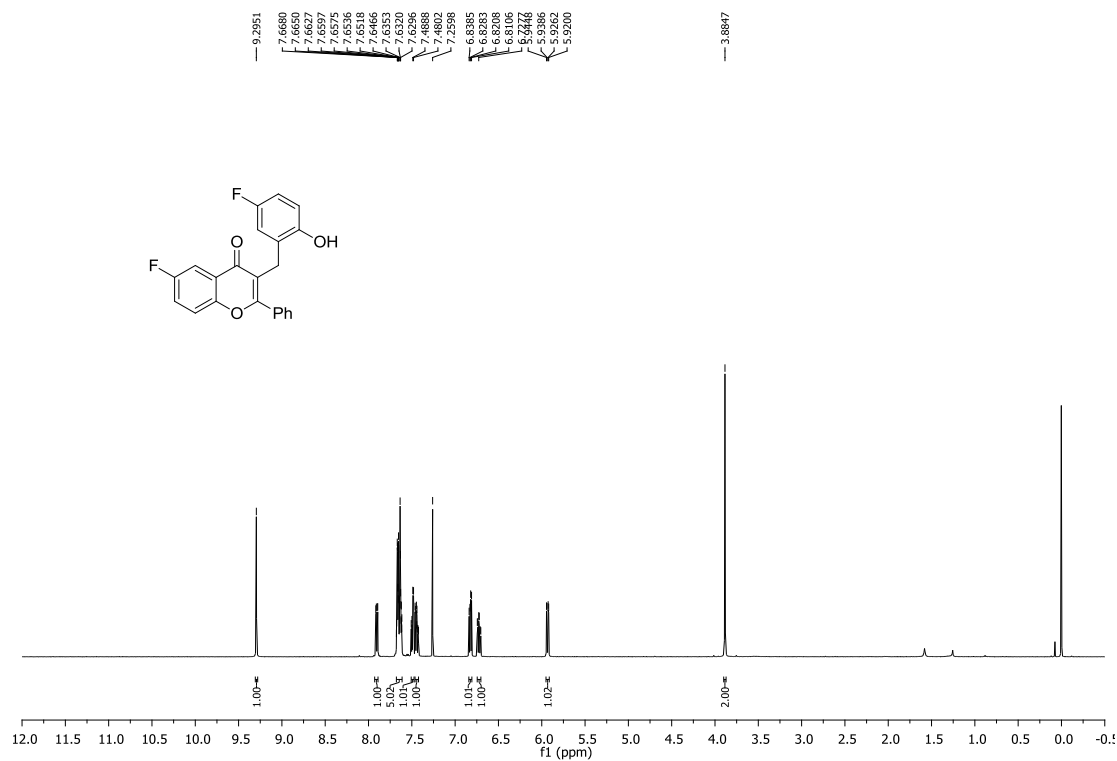
¹H NMR spectra of compound **3ea** (CDCl₃, 500 MHz)



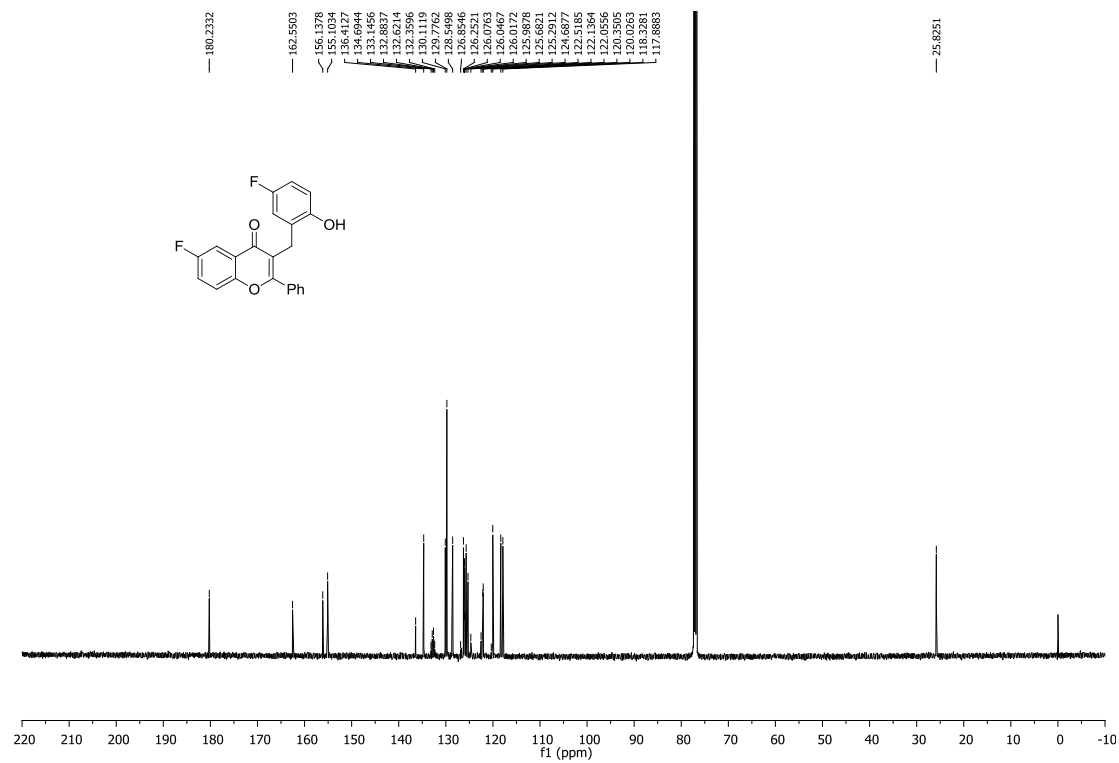
¹³C NMR spectra of compound **3ea** (CDCl₃, 125 MHz)



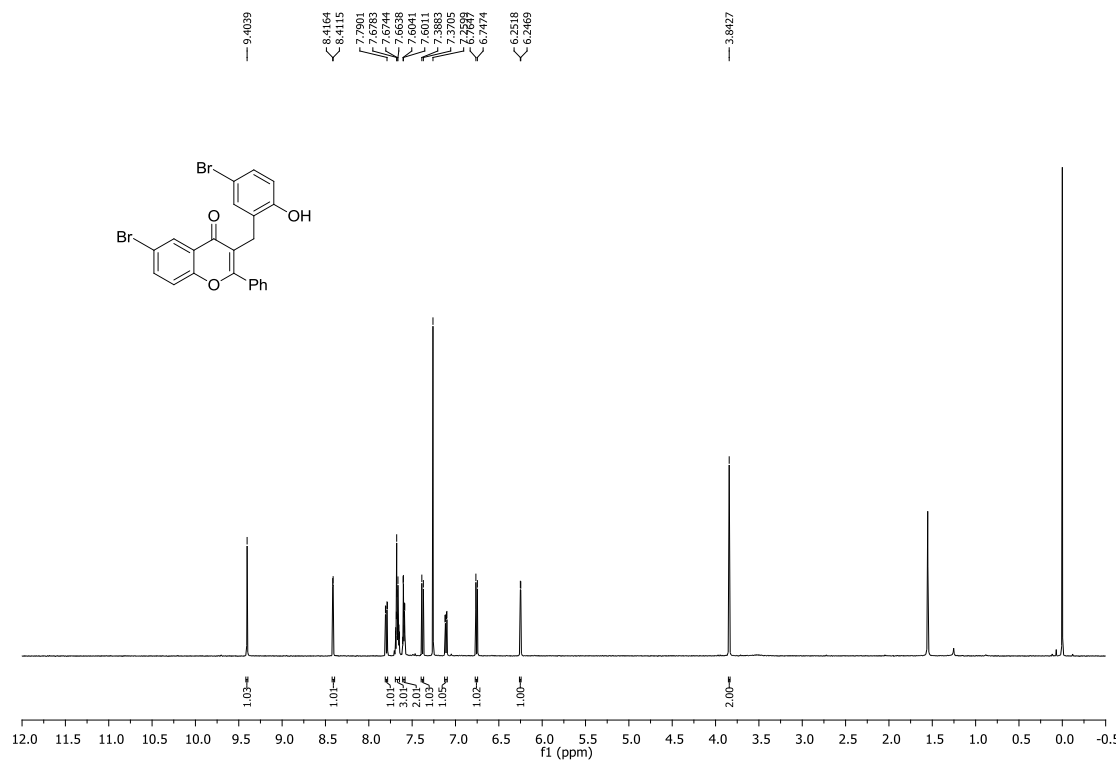
¹H NMR spectra of compound **3fa** (CDCl₃, 500 MHz)



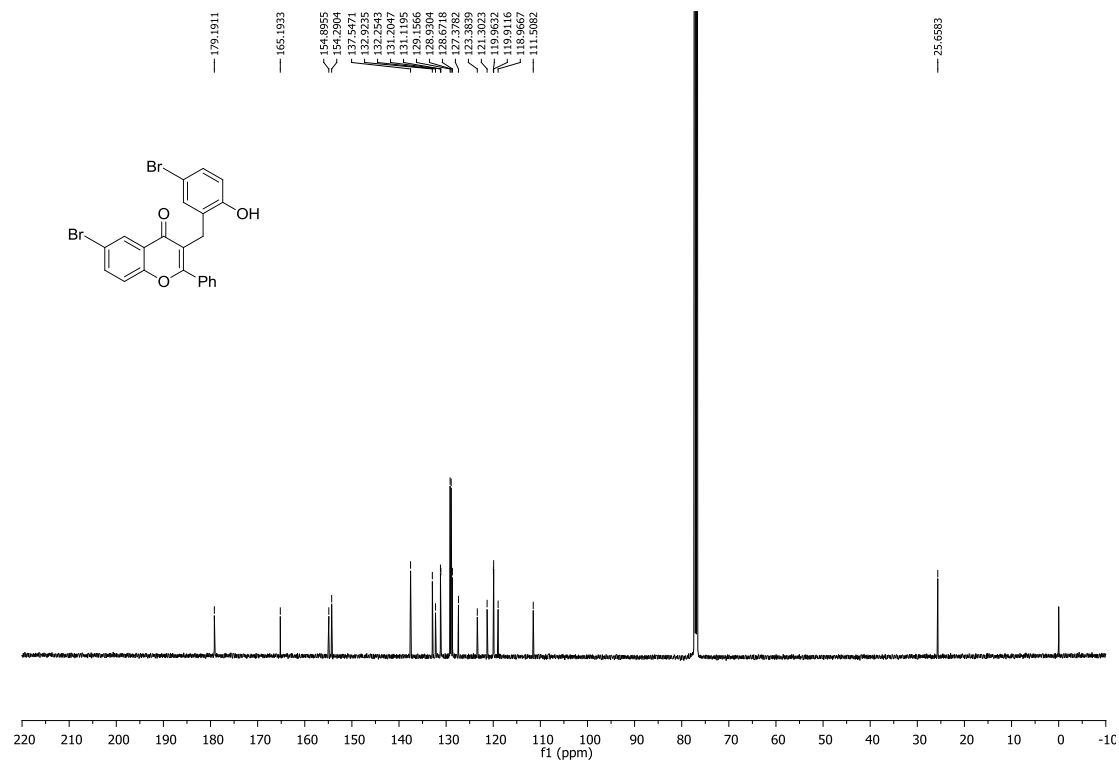
¹³C NMR spectra of compound **3fa** (CDCl₃, 125 MHz)



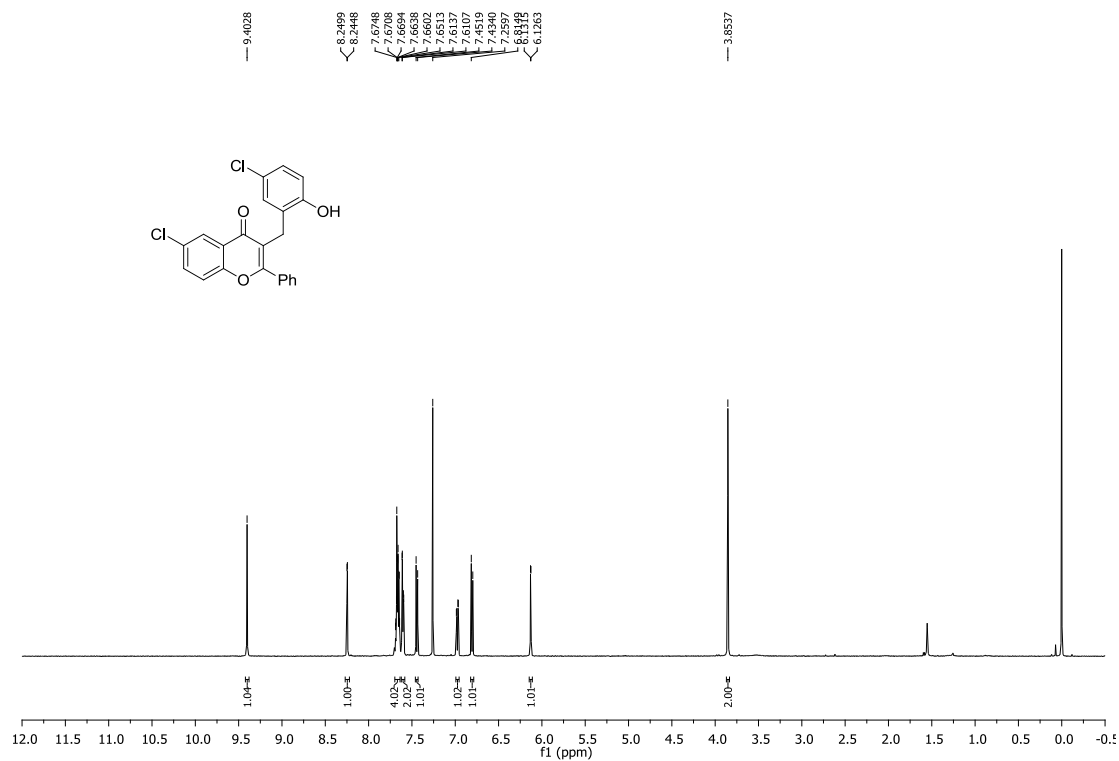
^1H NMR spectra of compound **3ga** (CDCl_3 , 500 MHz)



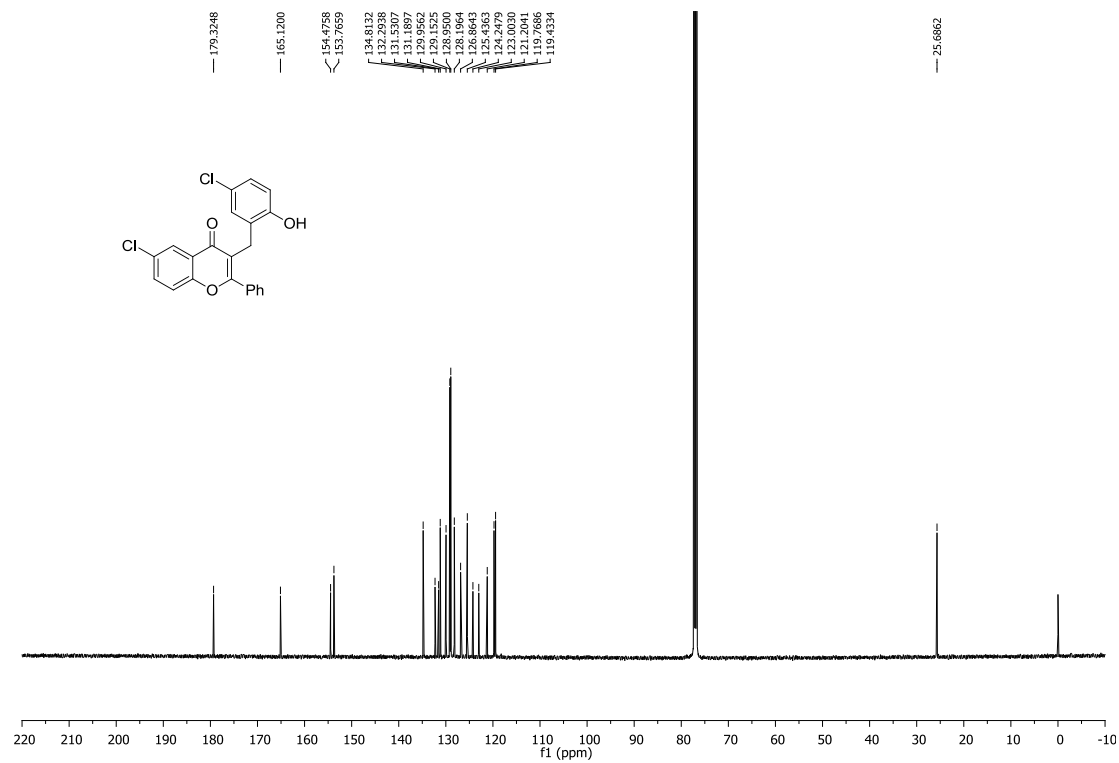
^{13}C NMR spectra of compound **3ga** (CDCl_3 , 125 MHz)



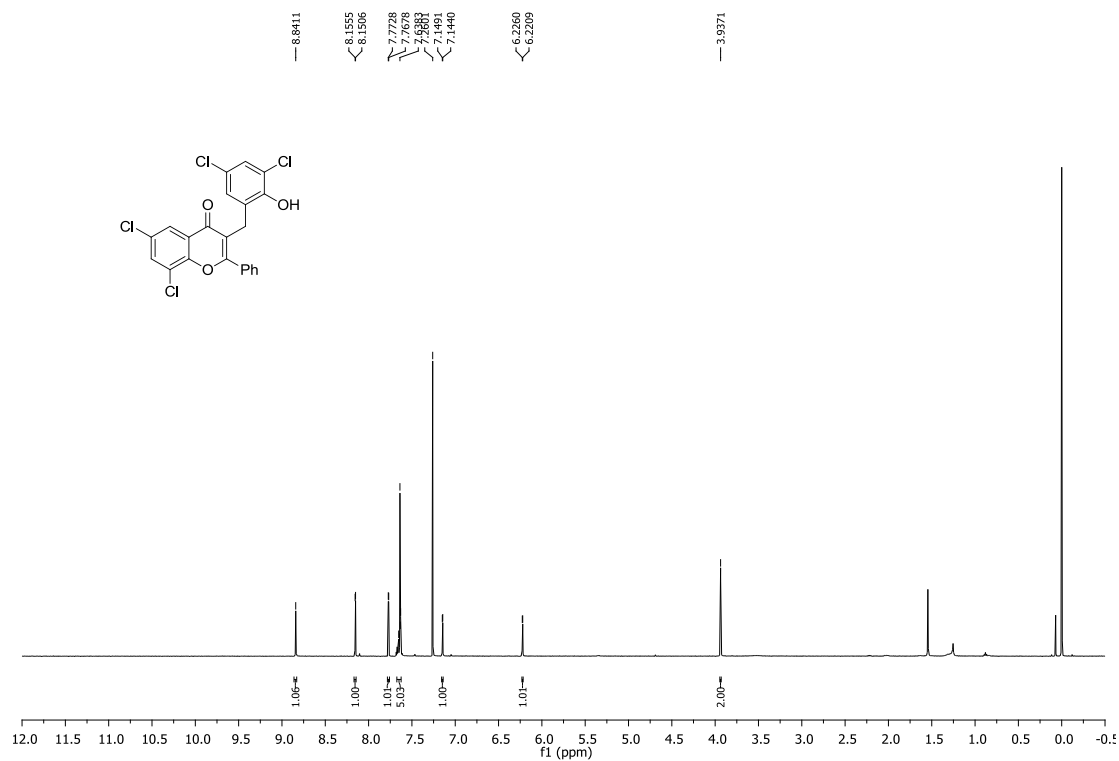
^1H NMR spectra of compound **3ha** (CDCl_3 , 500 MHz)



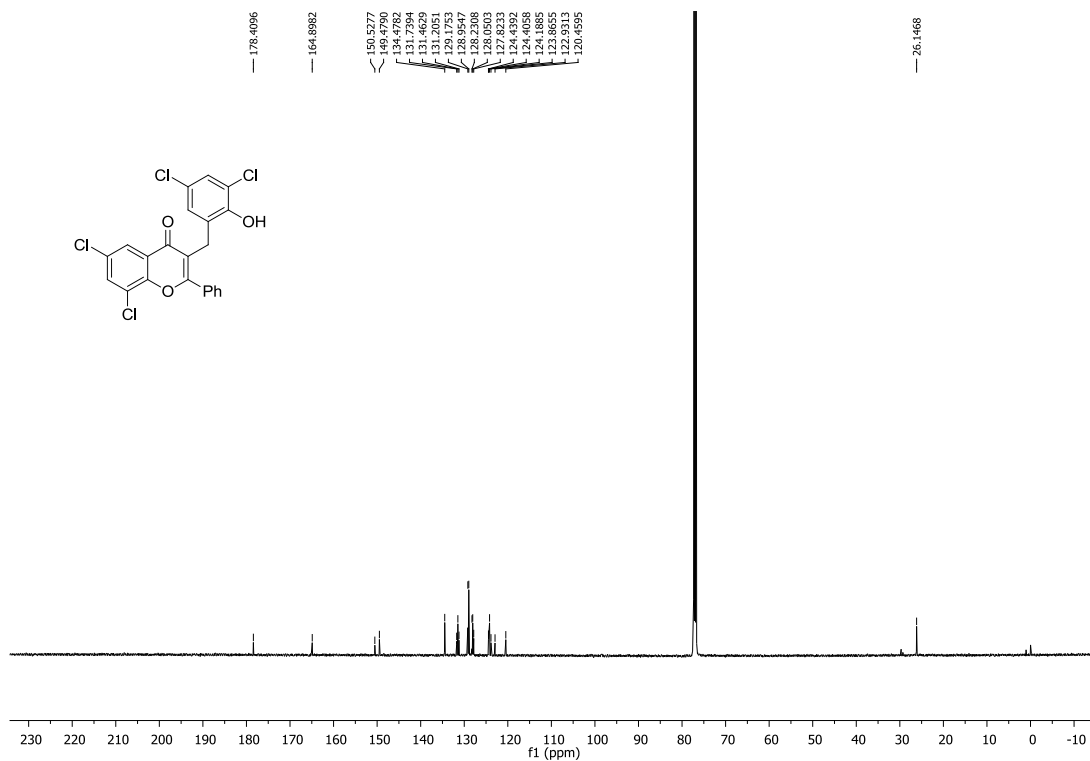
^{13}C NMR spectra of compound **3ha** (CDCl_3 , 125 MHz)



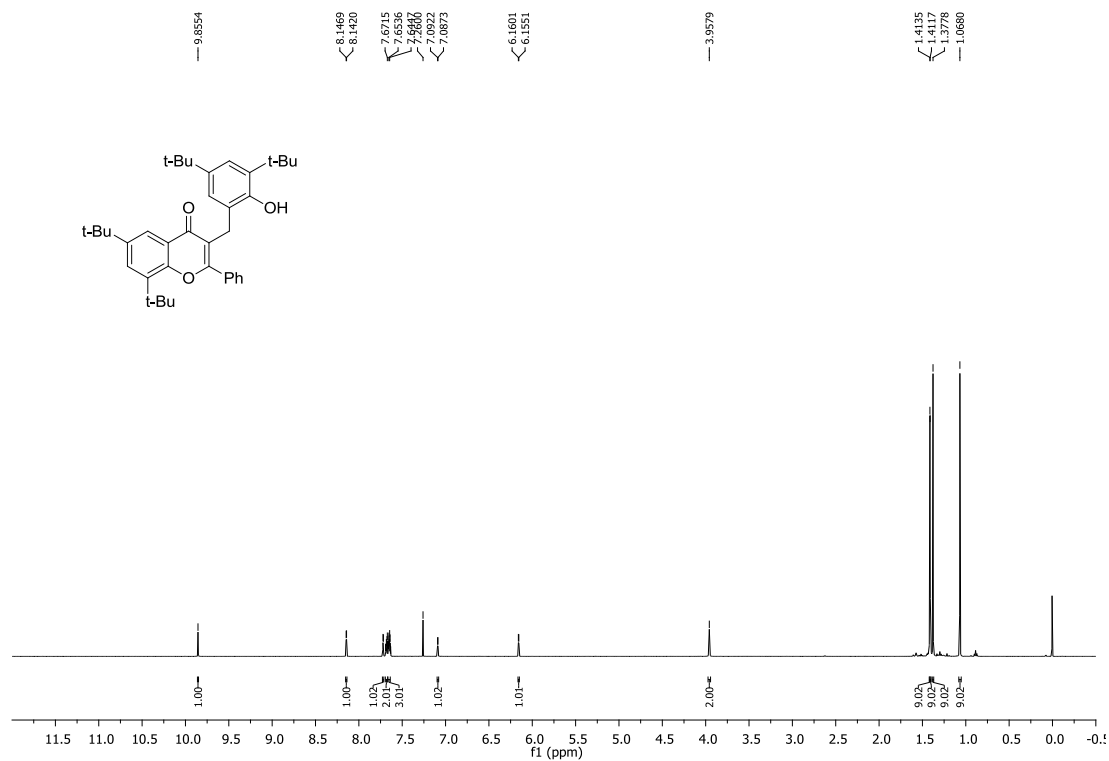
^1H NMR spectra of compound **3ia** (CDCl_3 , 500 MHz)



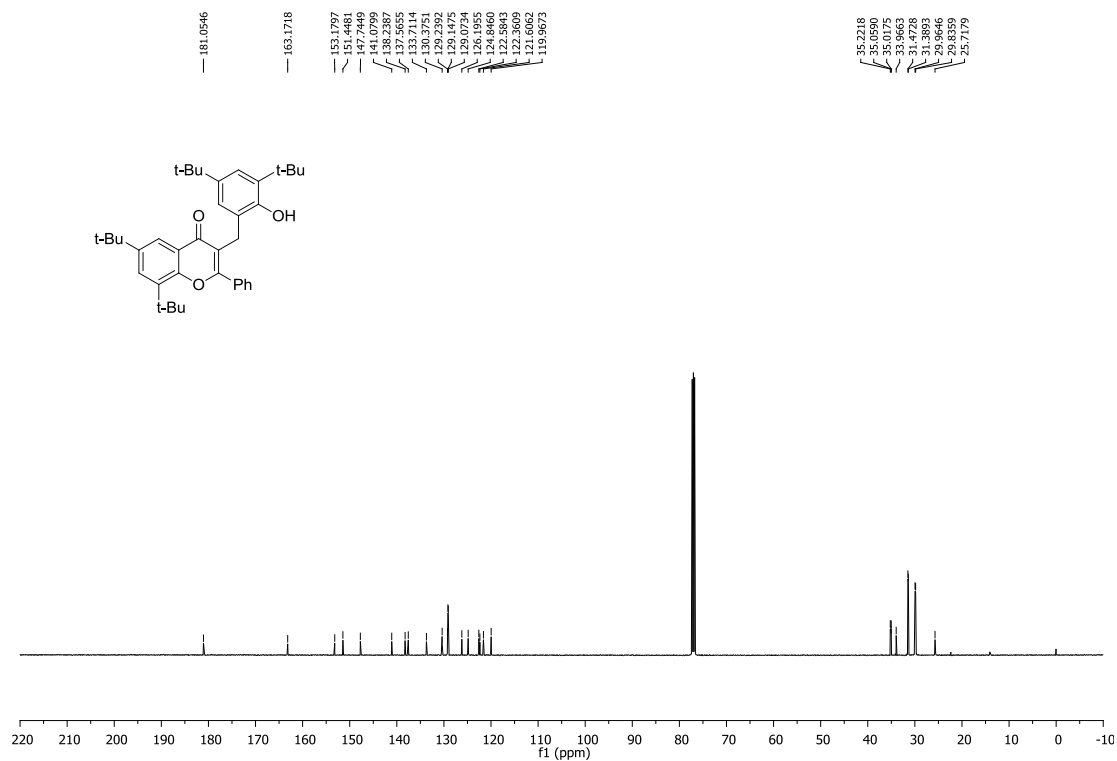
^{13}C NMR spectra of compound **3ia** (CDCl_3 , 125 MHz)



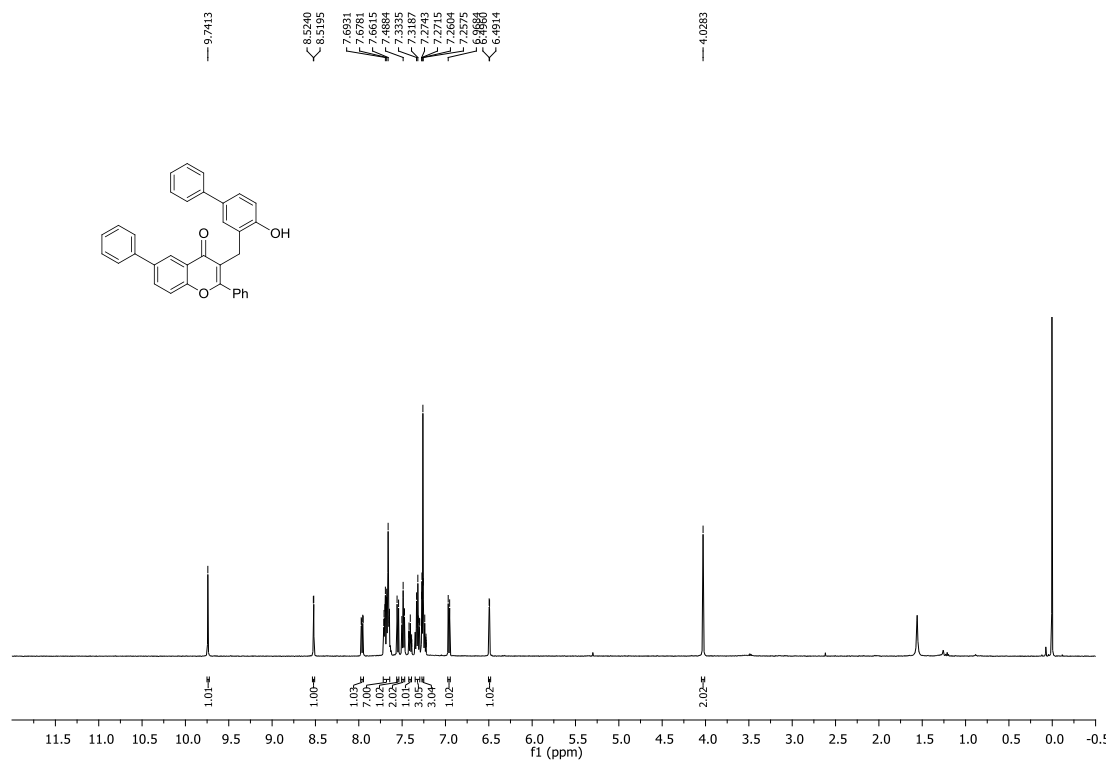
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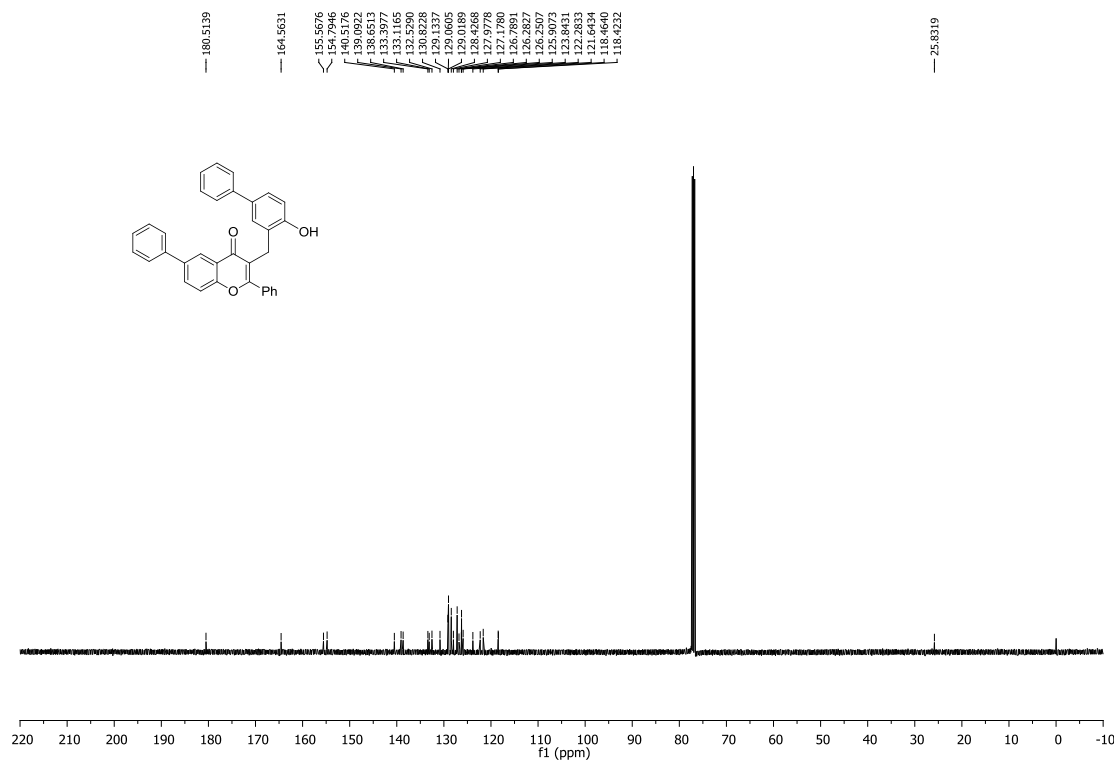
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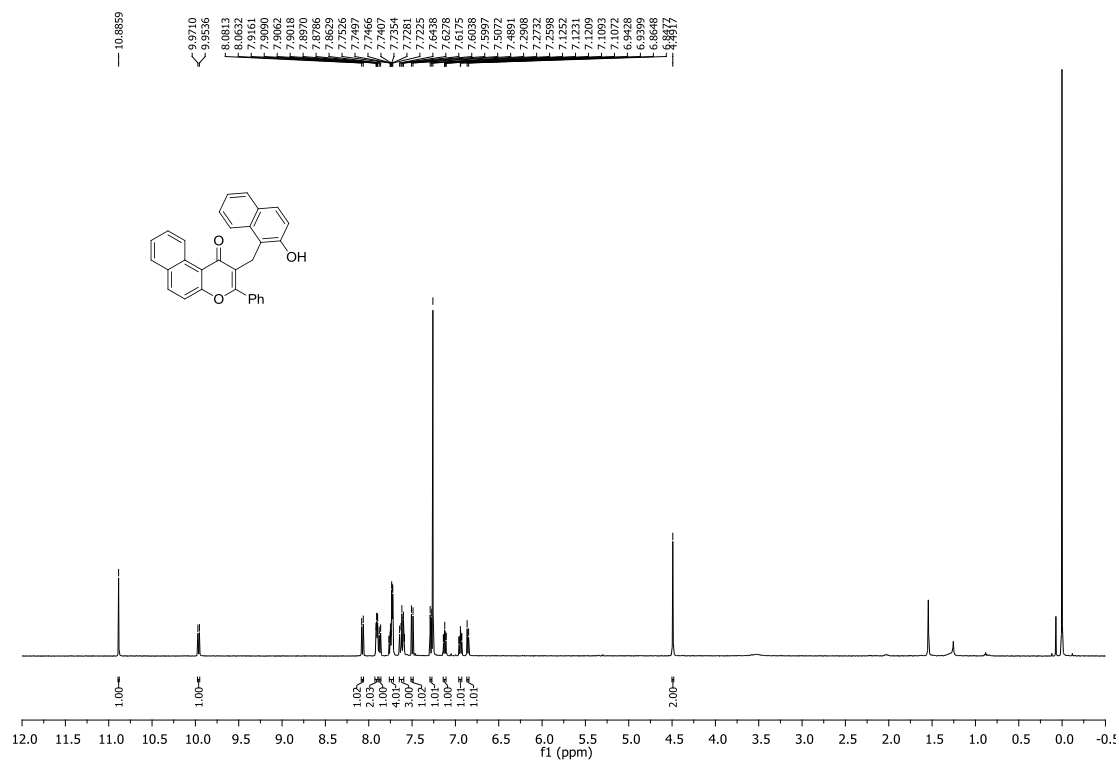
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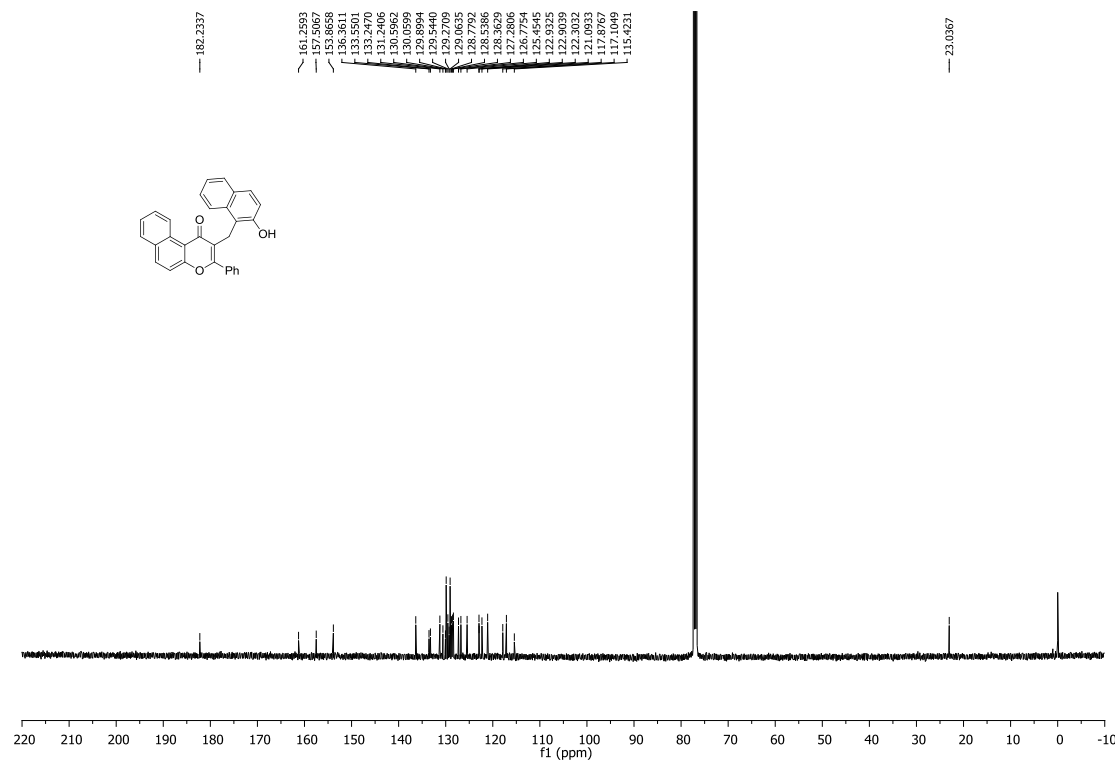
¹³C NMR spectra of compound **3ka** (CDCl₃, 125 MHz)



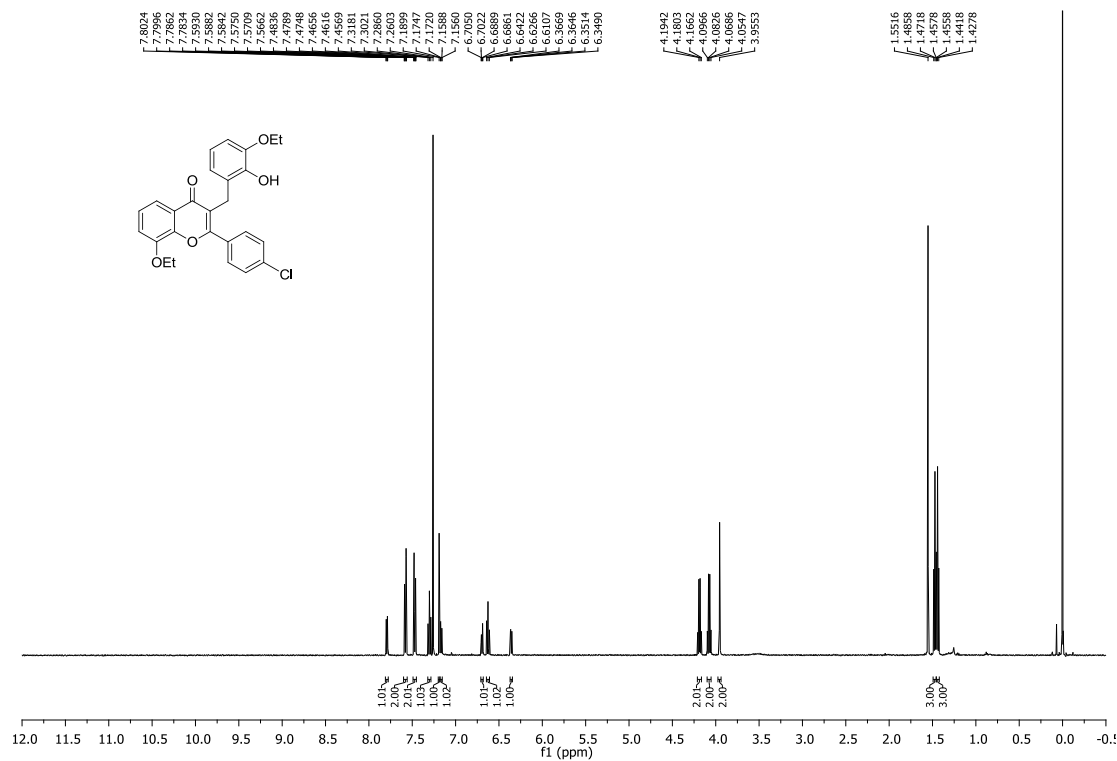
^1H NMR spectra of compound **3la** (CDCl_3 , 500 MHz)



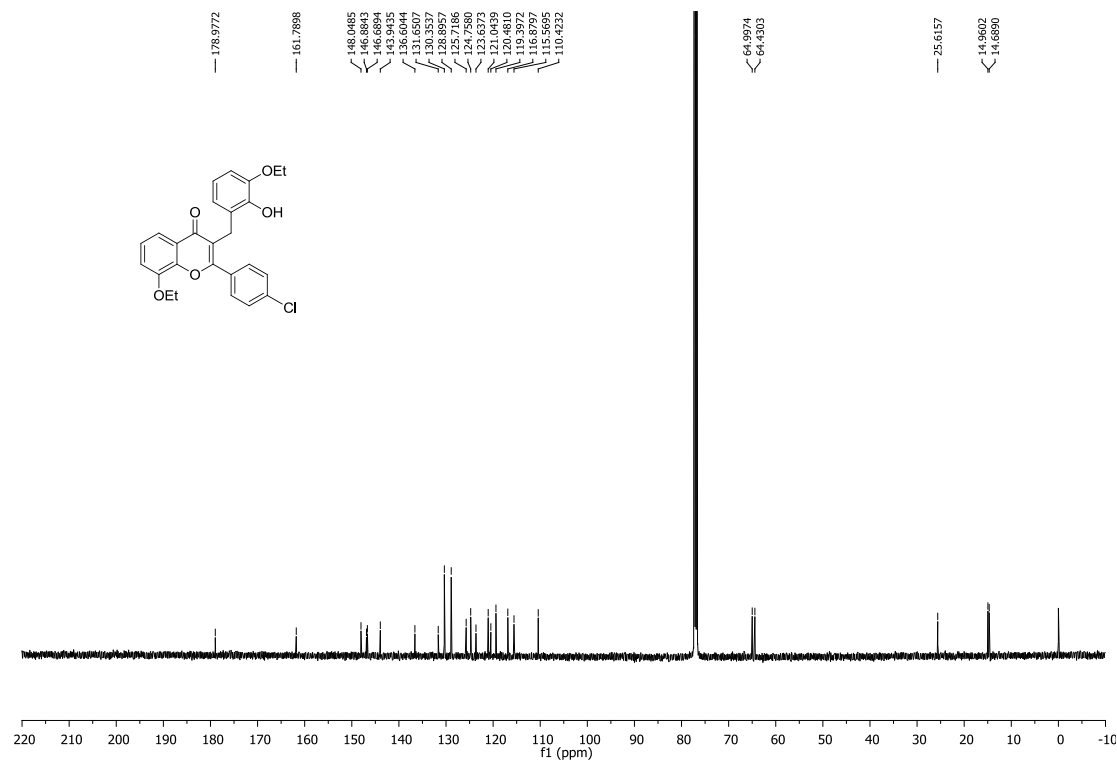
^{13}C NMR spectra of compound **3la** (CDCl_3 , 125 MHz)



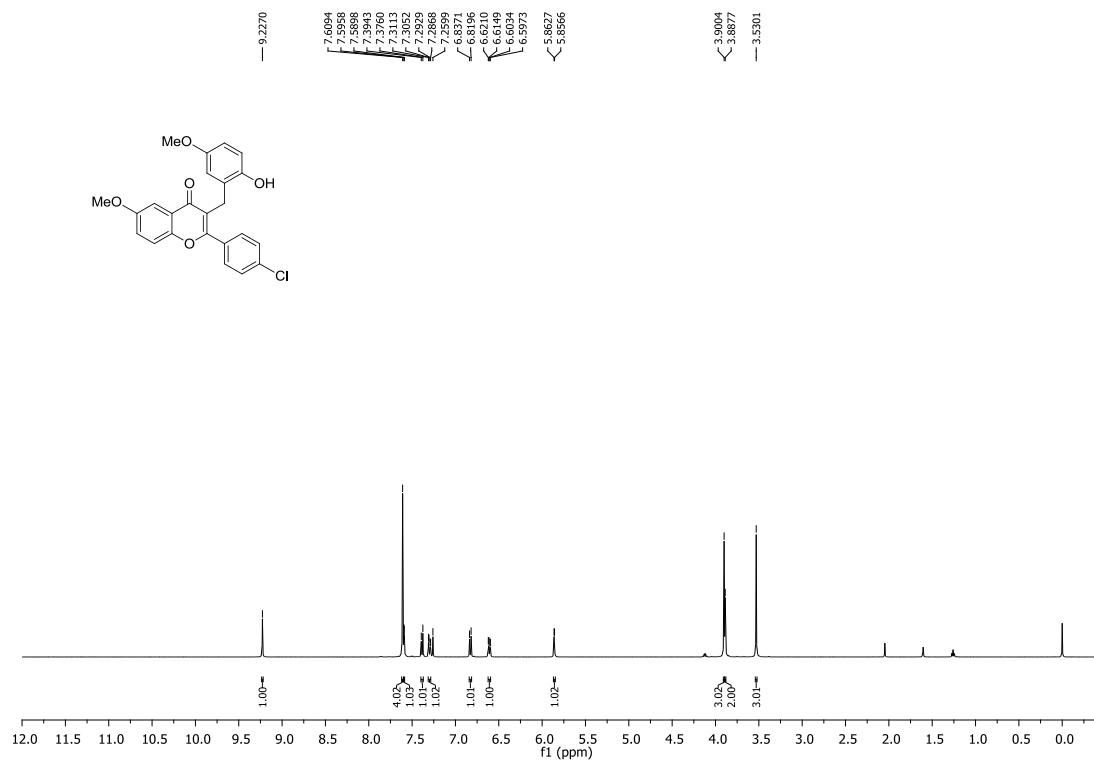
¹H NMR spectra of compound **3bh** (CDCl₃, 500 MHz)



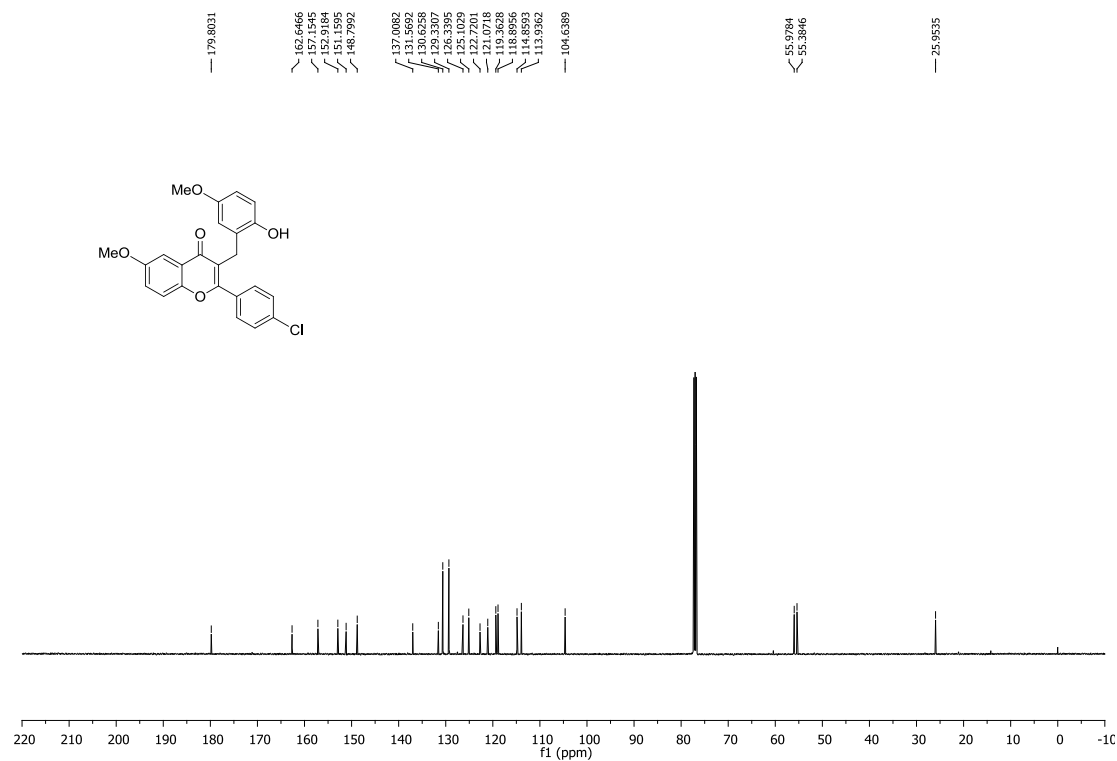
¹³C NMR spectra of compound **3bh** (CDCl₃, 125 MHz)



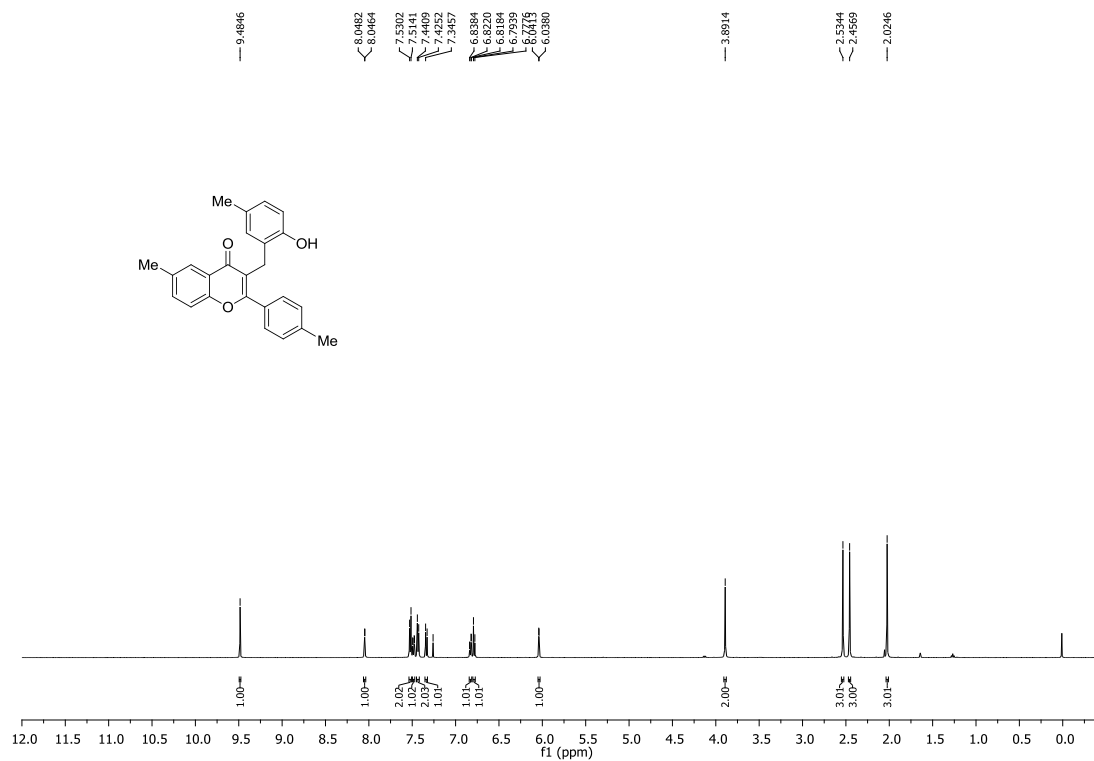
^1H NMR spectra of compound **3dh** (CDCl_3 , 500 MHz)



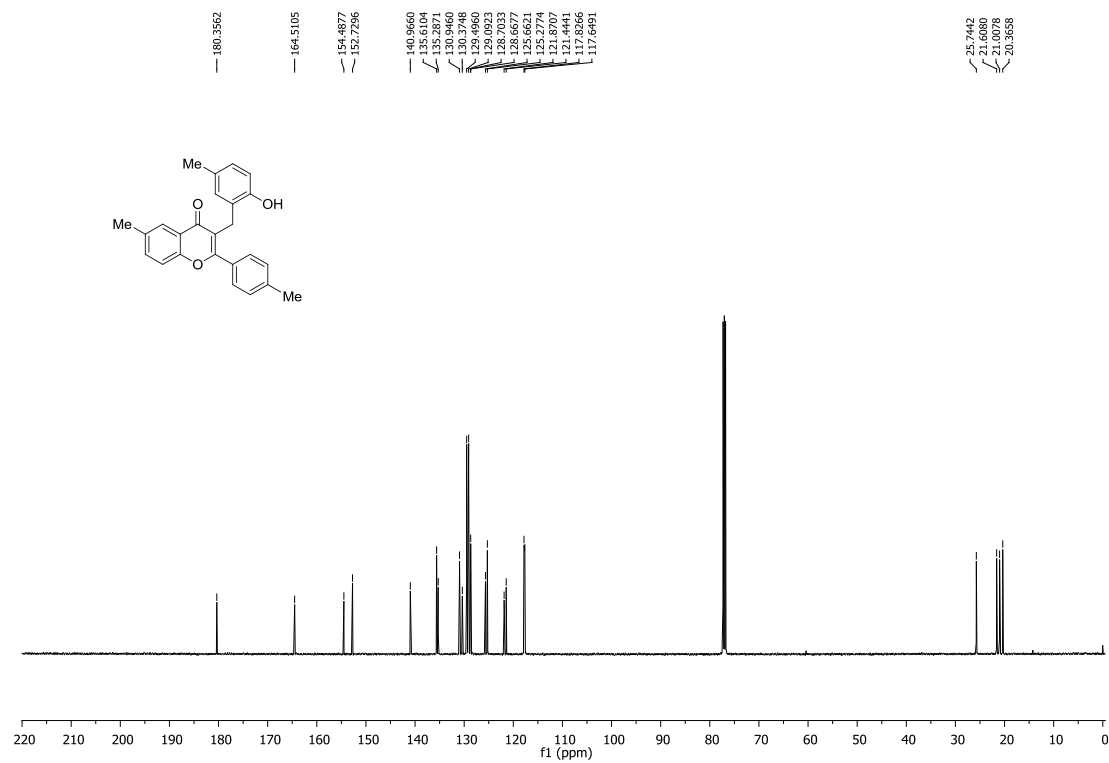
^{13}C NMR spectra of compound **3dh** (CDCl_3 , 125 MHz)



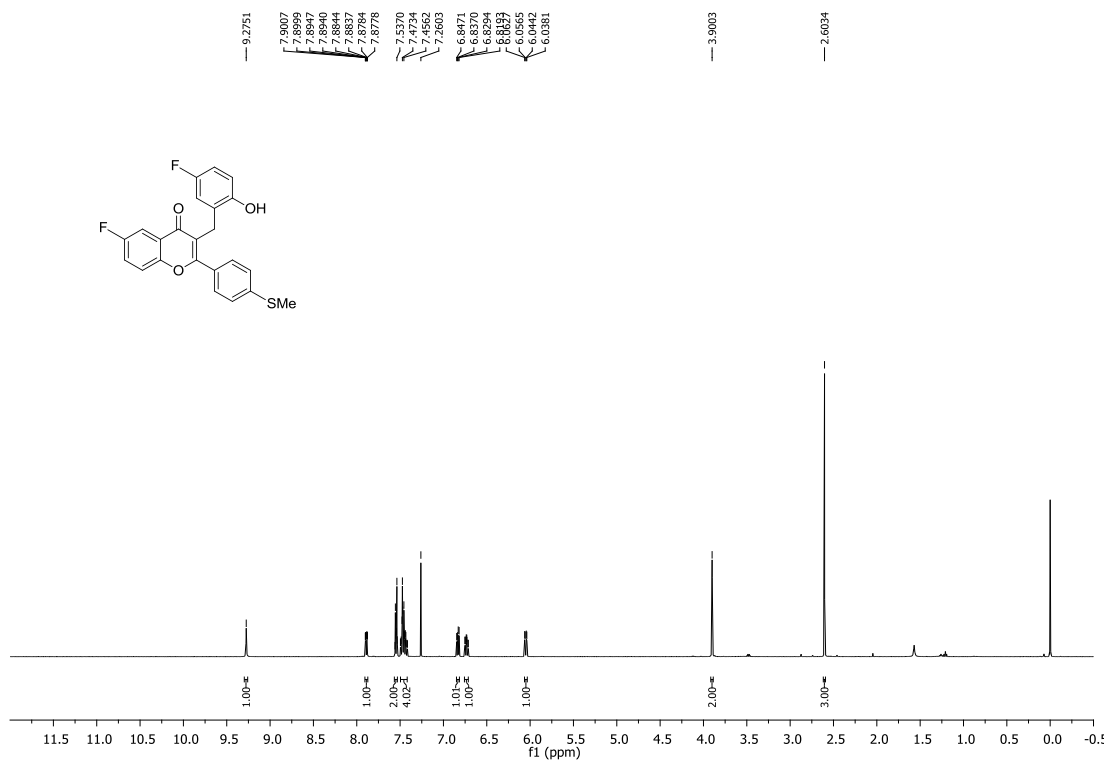
^1H NMR spectra of compound **3ed** (CDCl_3 , 500 MHz)



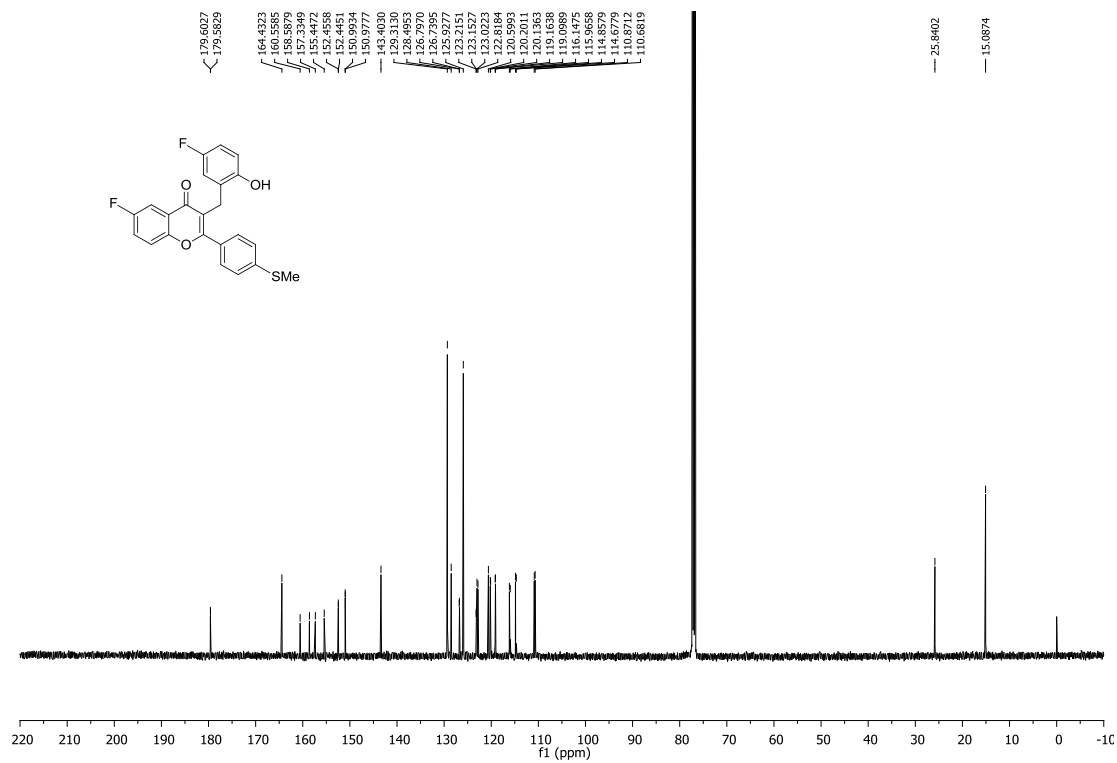
^{13}C NMR spectra of compound **3ed** (CDCl_3 , 125 MHz)



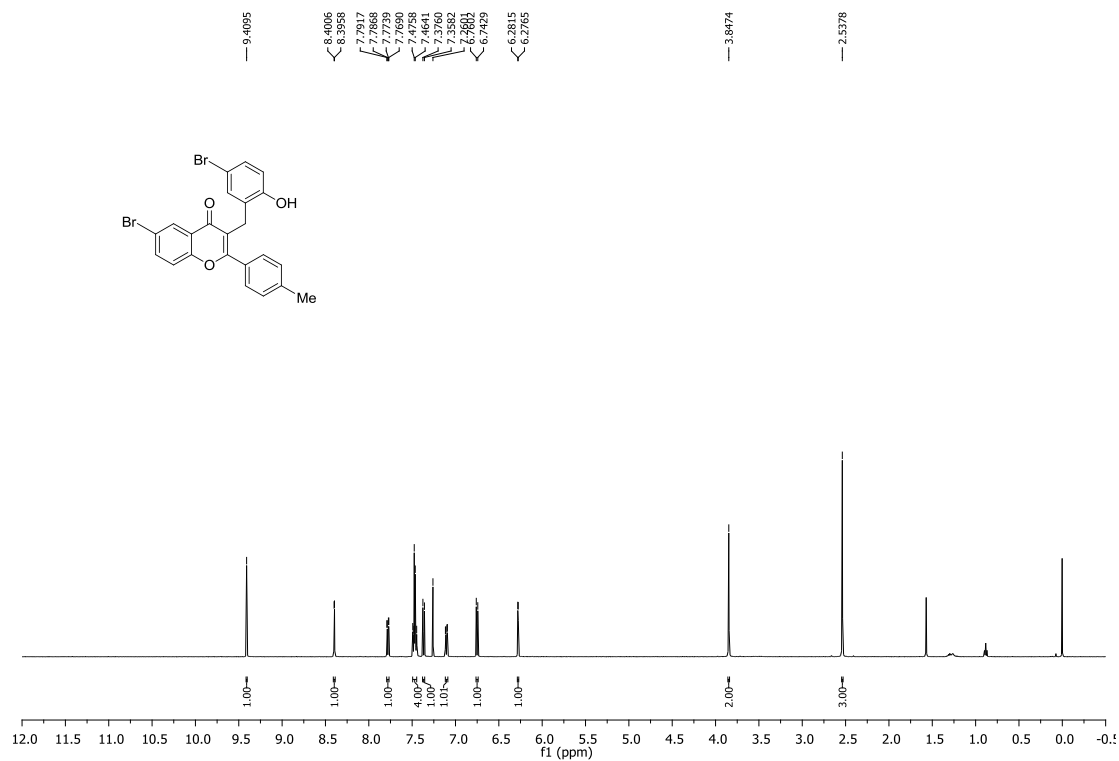
^1H NMR spectra of compound **3ff** (CDCl_3 , 500 MHz)



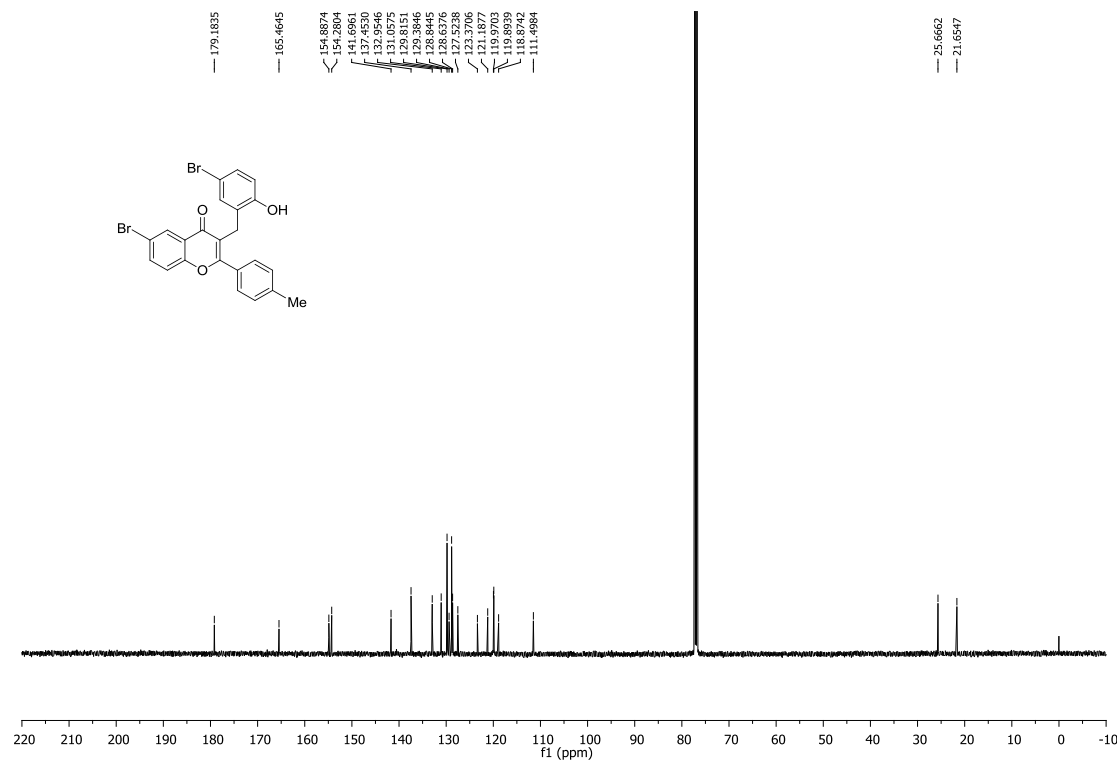
^{13}C NMR spectra of compound **3ff** (CDCl_3 , 125 MHz)



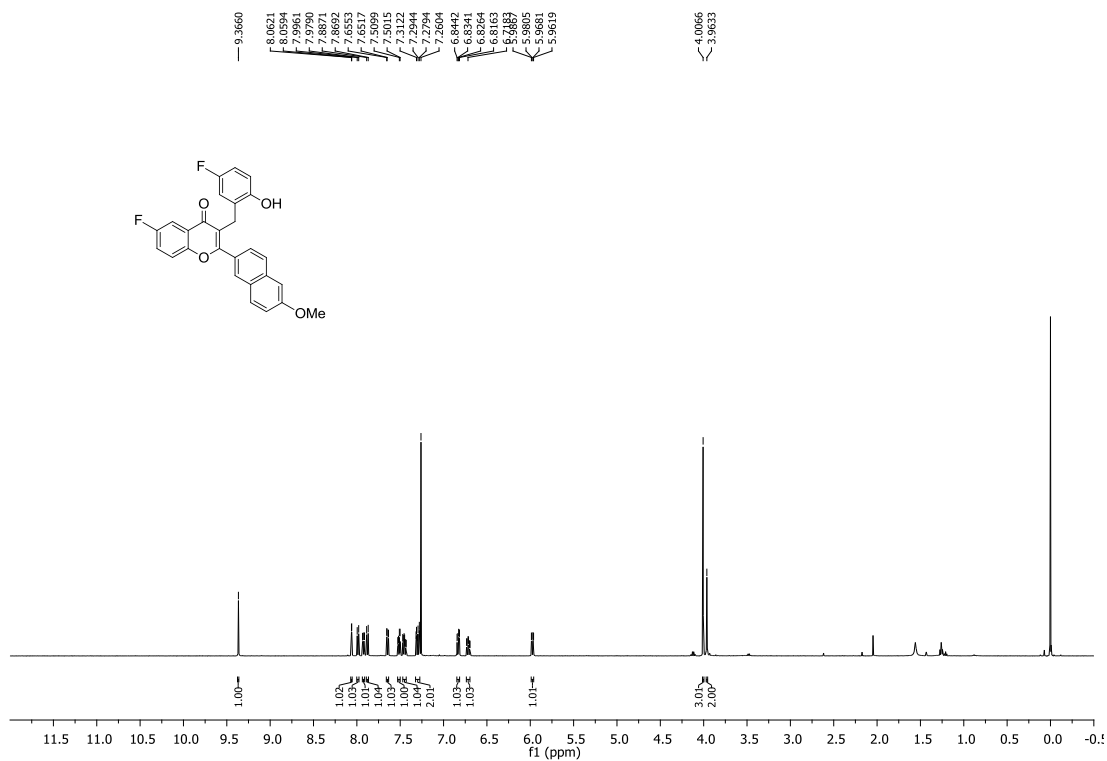
^1H NMR spectra of compound **3gd** (CDCl_3 , 500 MHz)



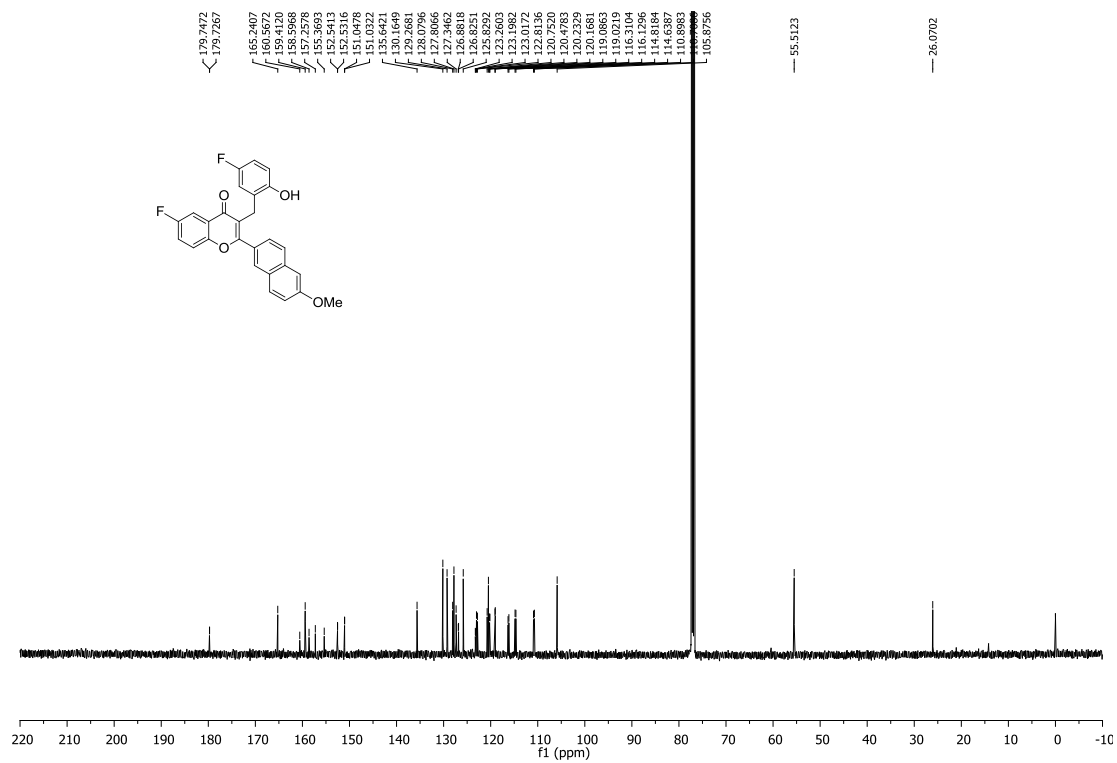
^{13}C NMR spectra of compound **3gd** (CDCl_3 , 125 MHz)



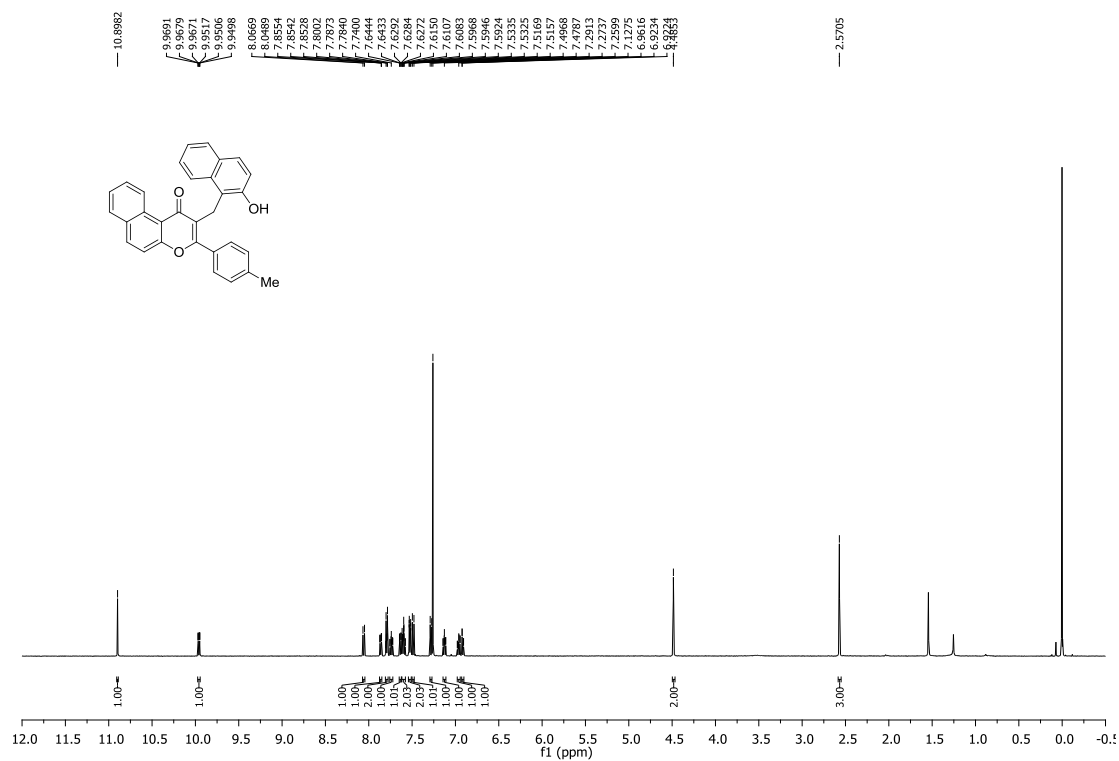
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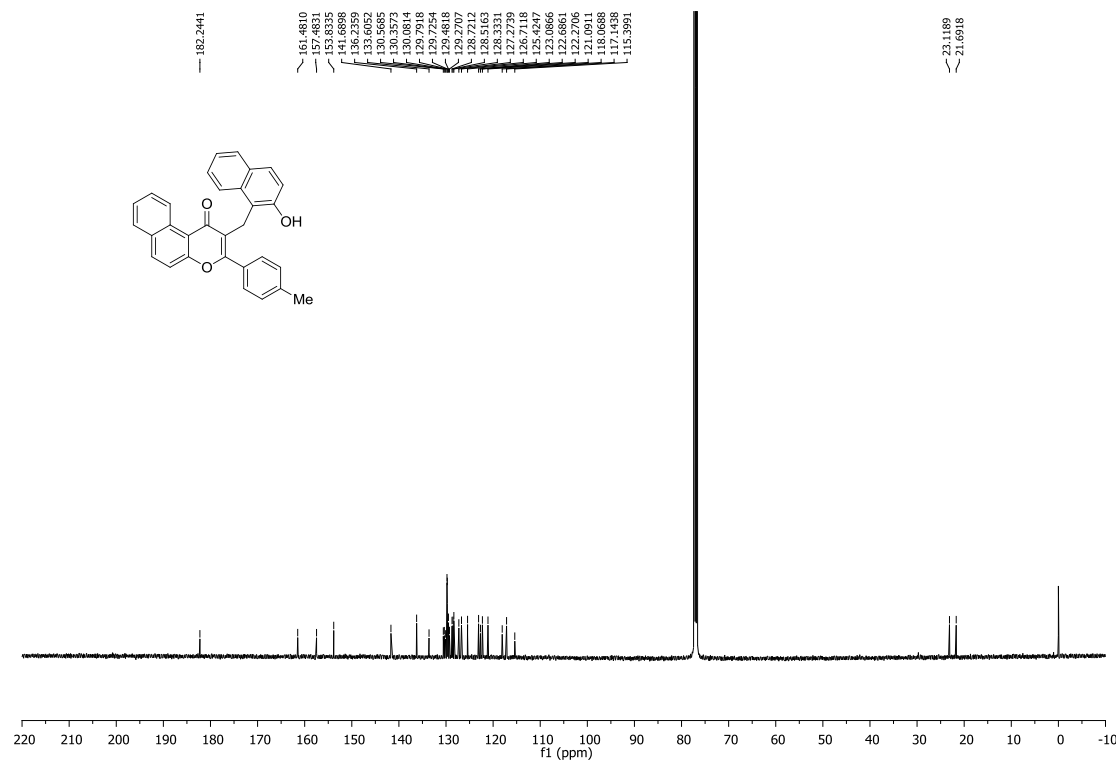
¹³C NMR spectra of compound **3fk** (CDCl₃, 125 MHz)



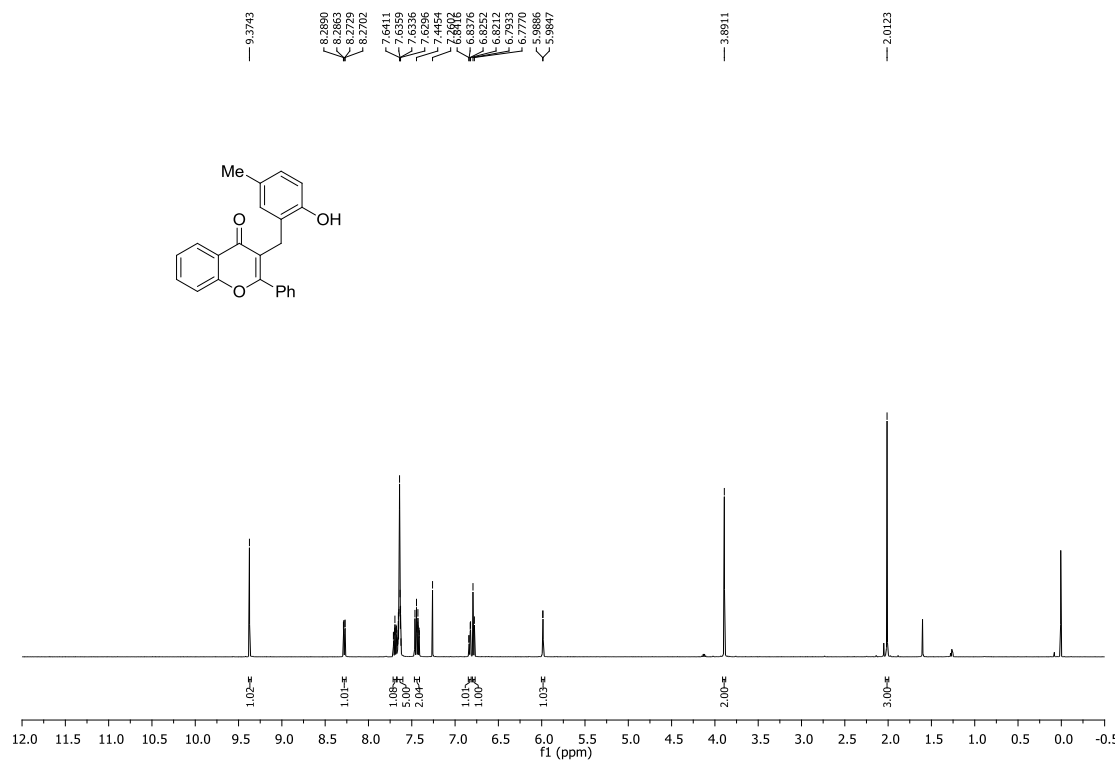
¹H NMR spectra of compound **3kd** (CDCl₃, 500 MHz)



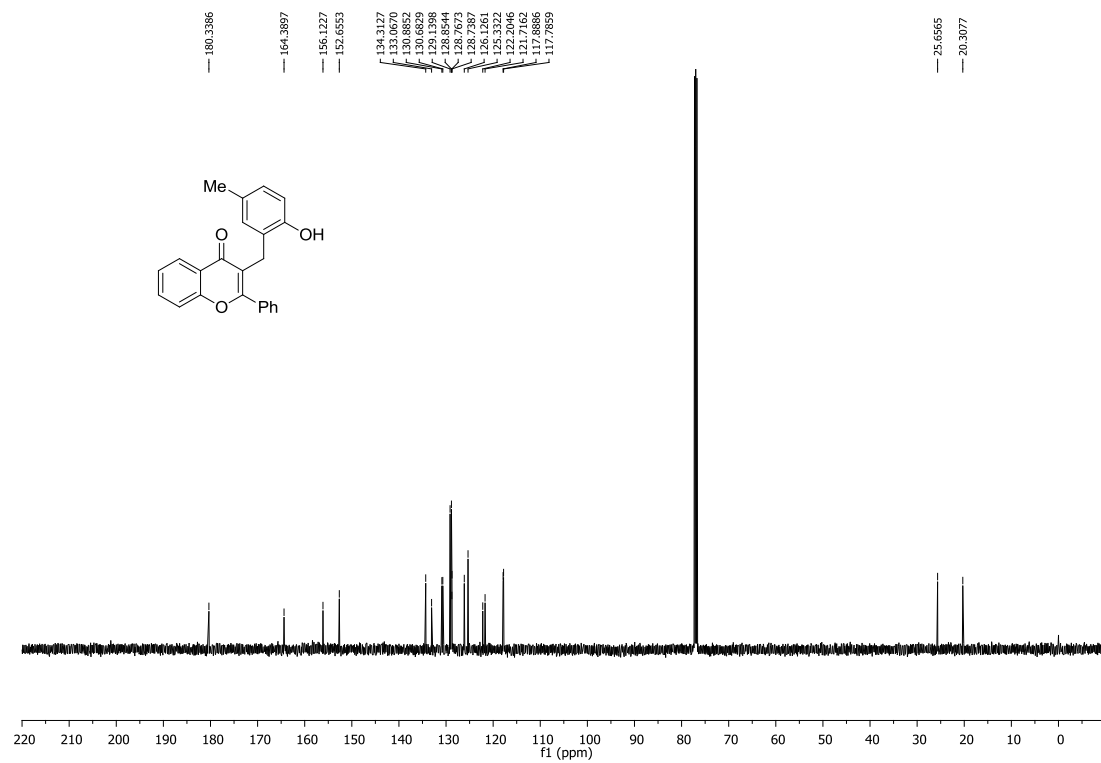
¹³C NMR spectra of compound **3kd** (CDCl₃, 125 MHz)



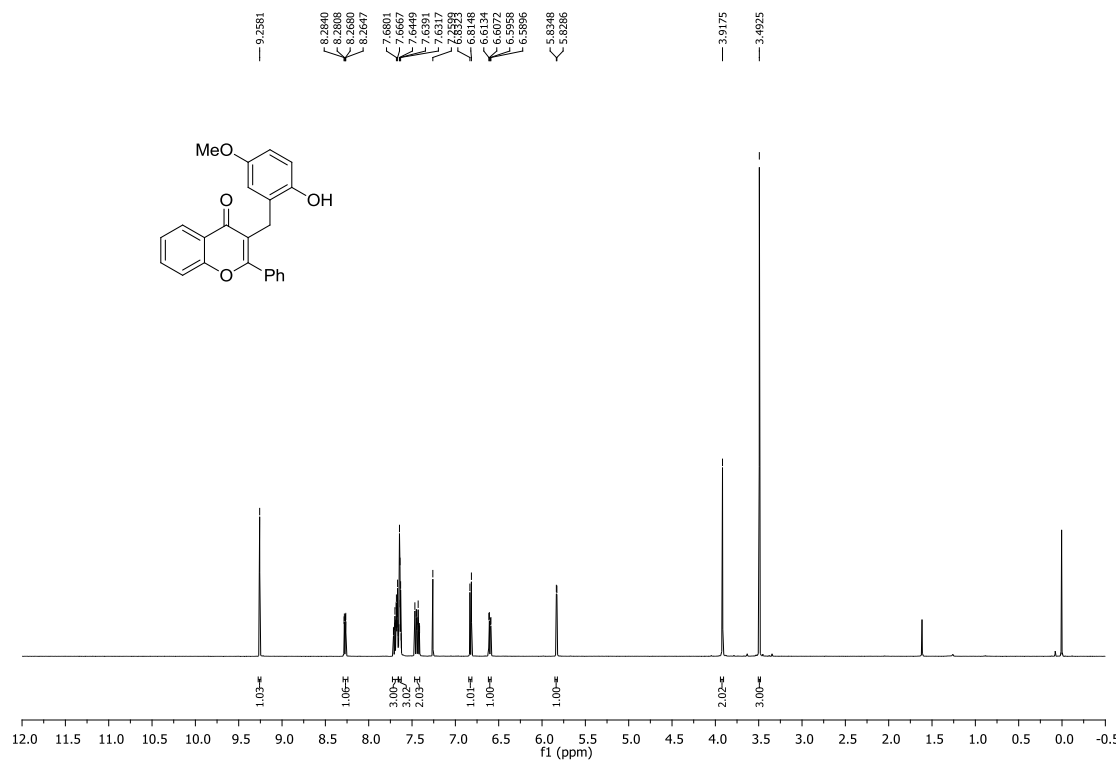
^1H NMR spectra of compound **6a** (CDCl_3 , 500 MHz)



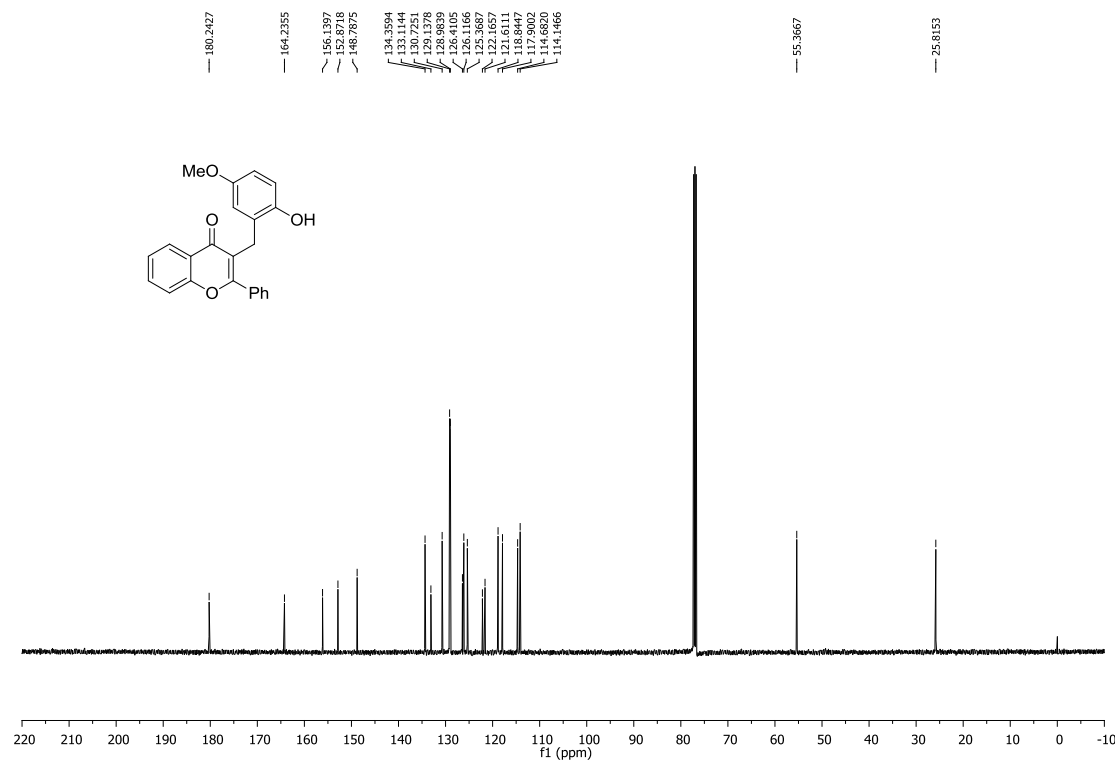
^{13}C NMR spectra of compound **6a** (CDCl_3 , 125 MHz)



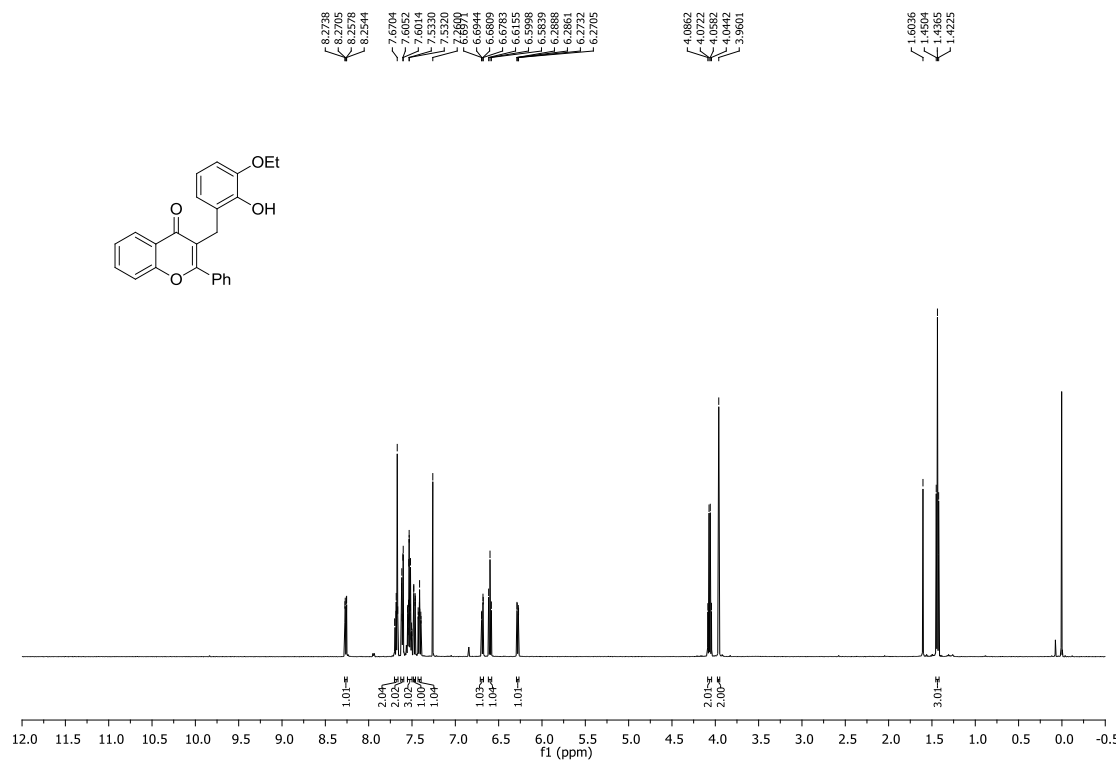
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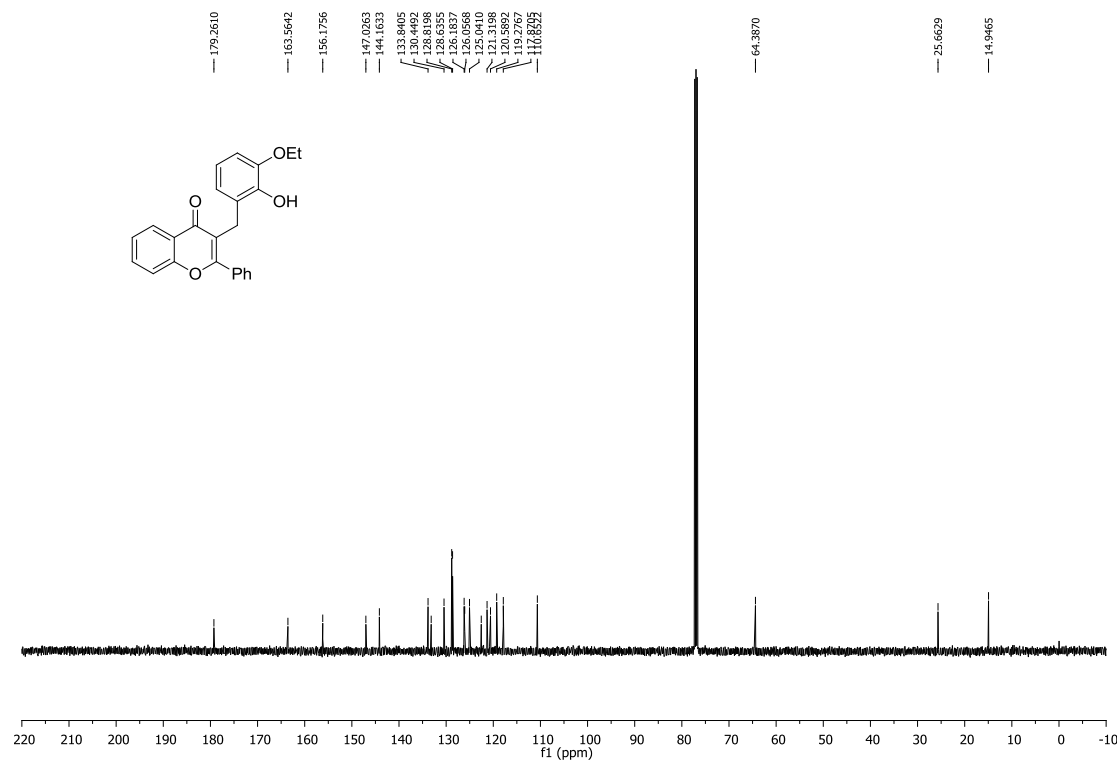
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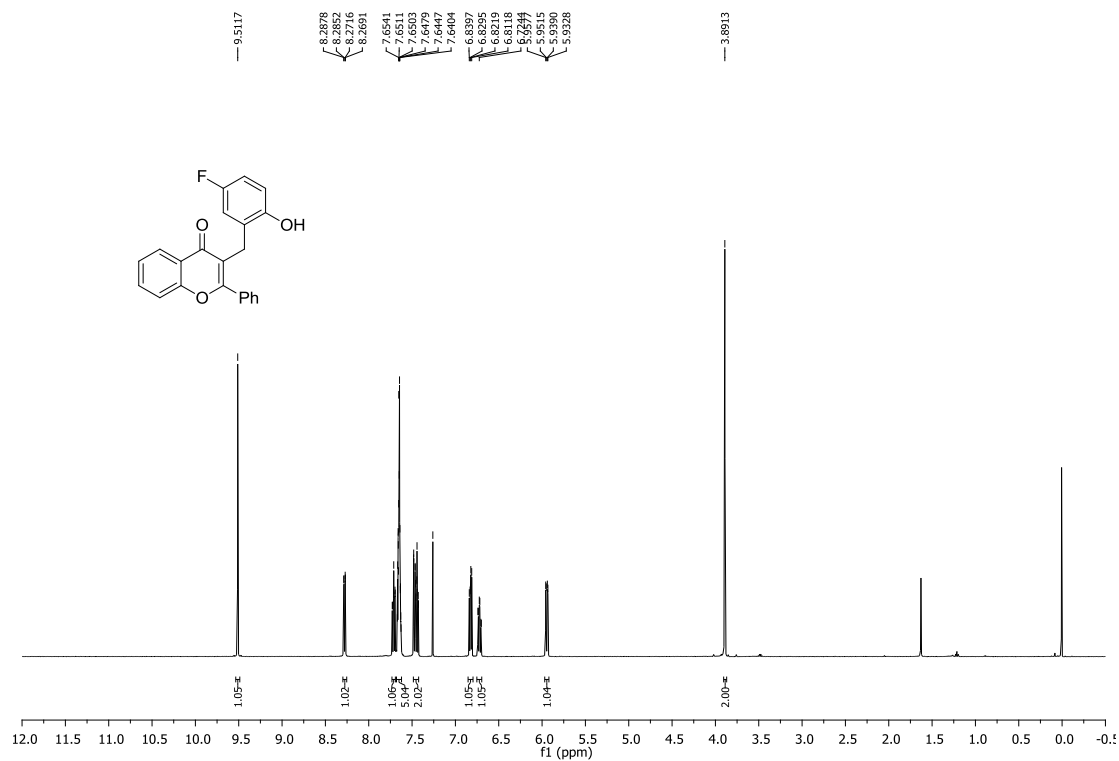
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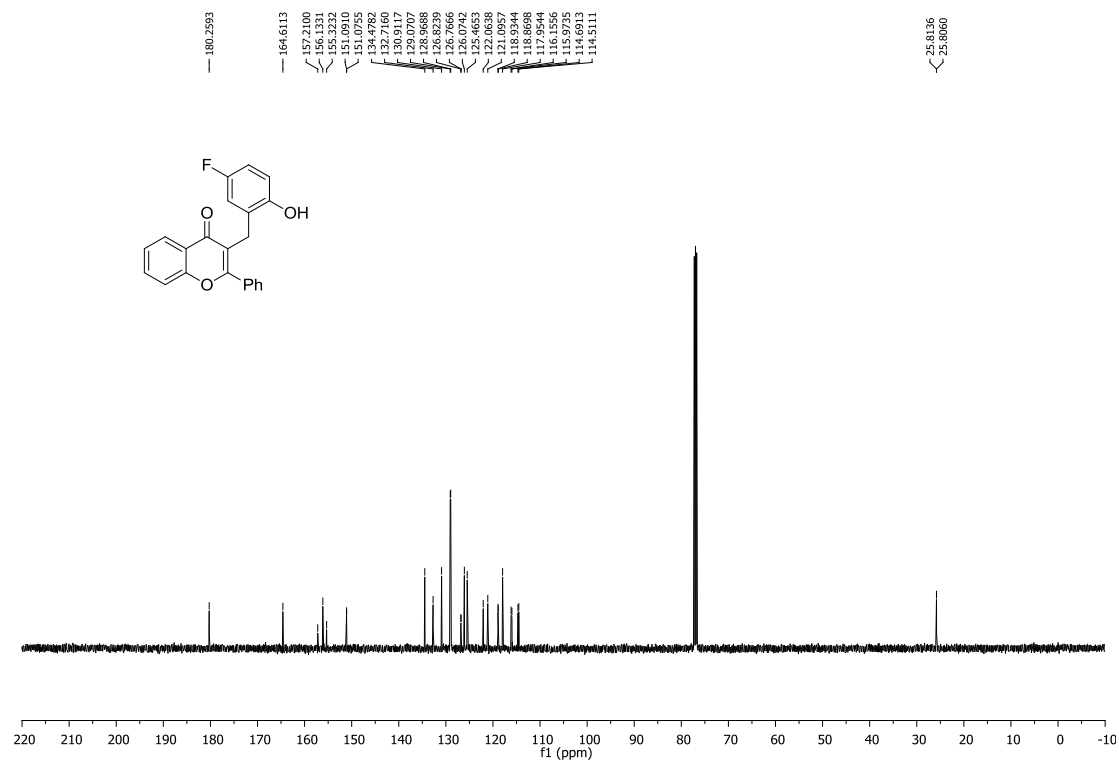
^{13}C NMR spectra of compound **6c** (CDCl_3 , 125 MHz)



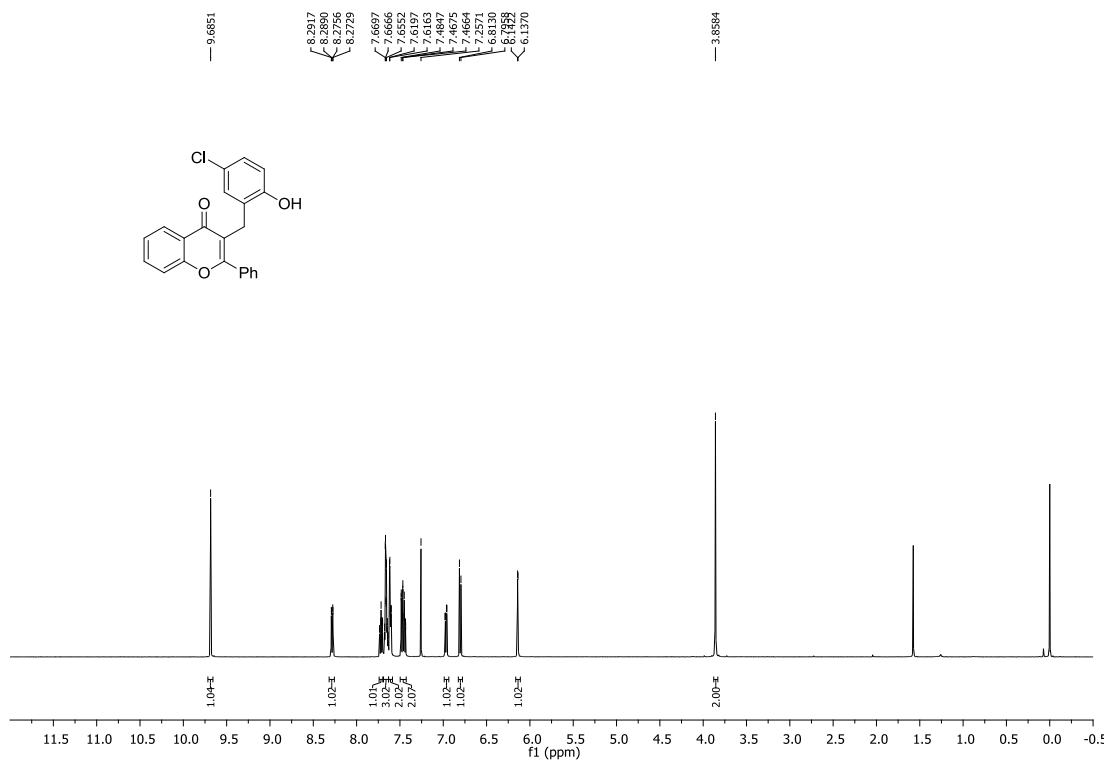
^1H NMR spectra of compound **6d** (CDCl_3 , 500 MHz)



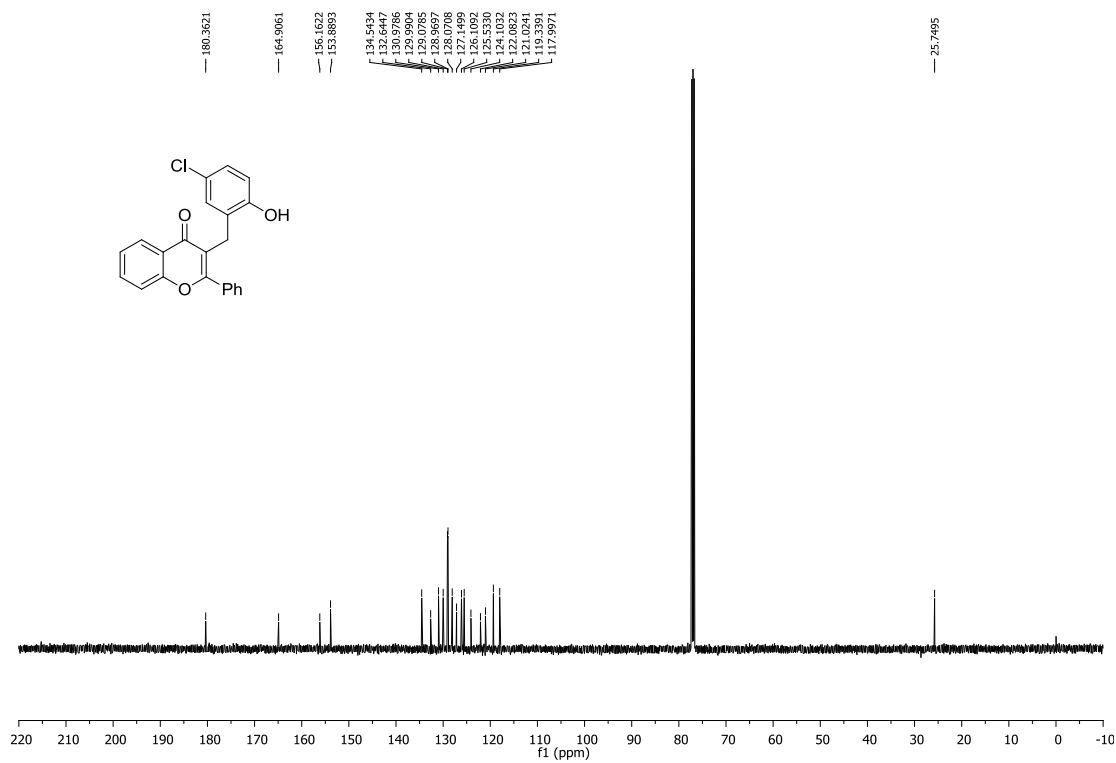
^{13}C NMR spectra of compound **6d** (CDCl_3 , 125 MHz)



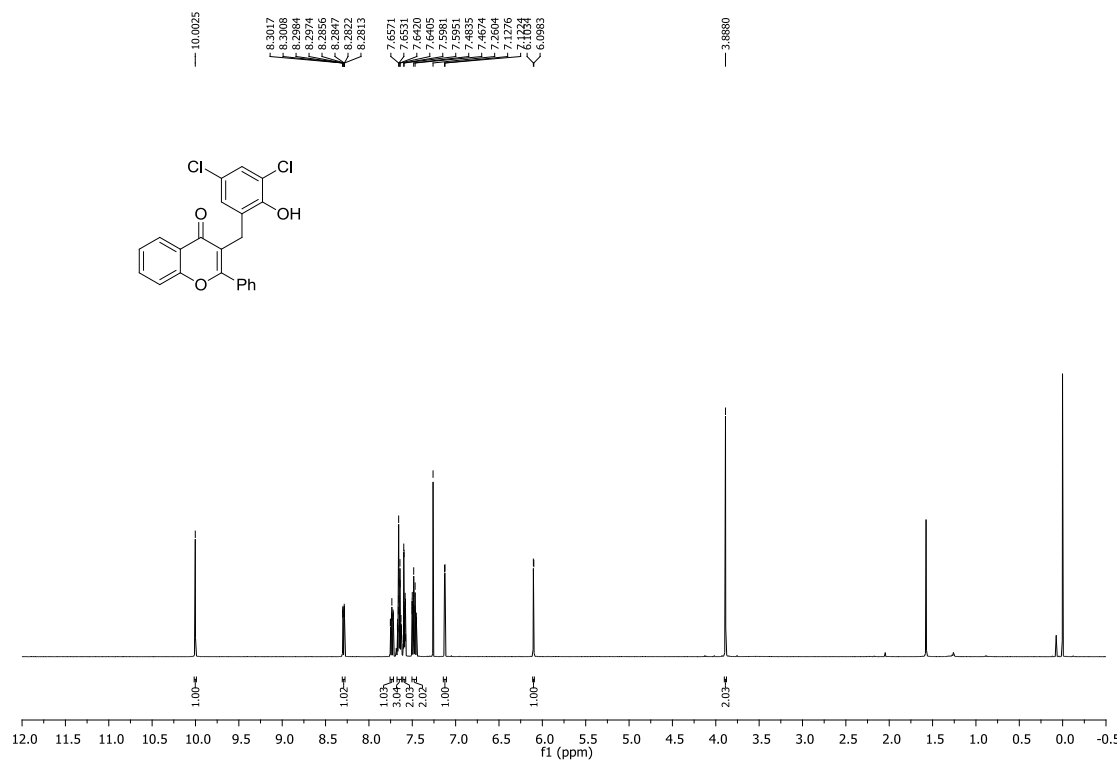
¹H NMR spectra of compound **6e** (CDCl₃, 500 MHz)



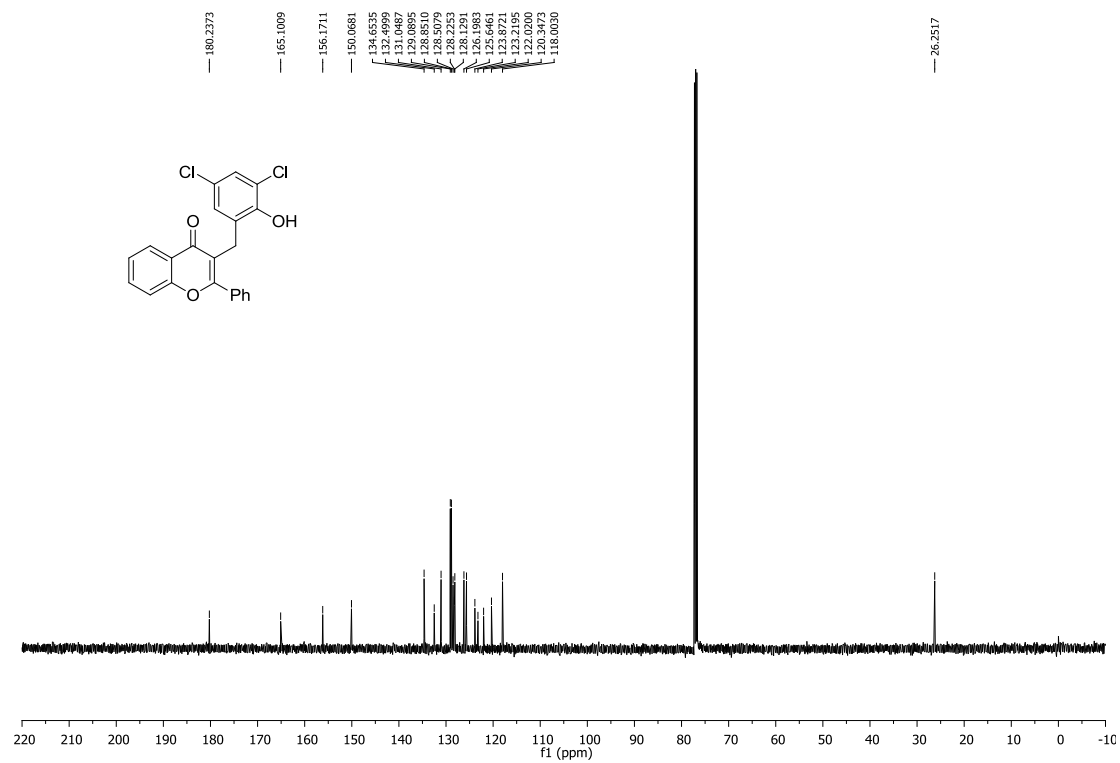
¹³C NMR spectra of compound **6e** (CDCl₃, 125 MHz)



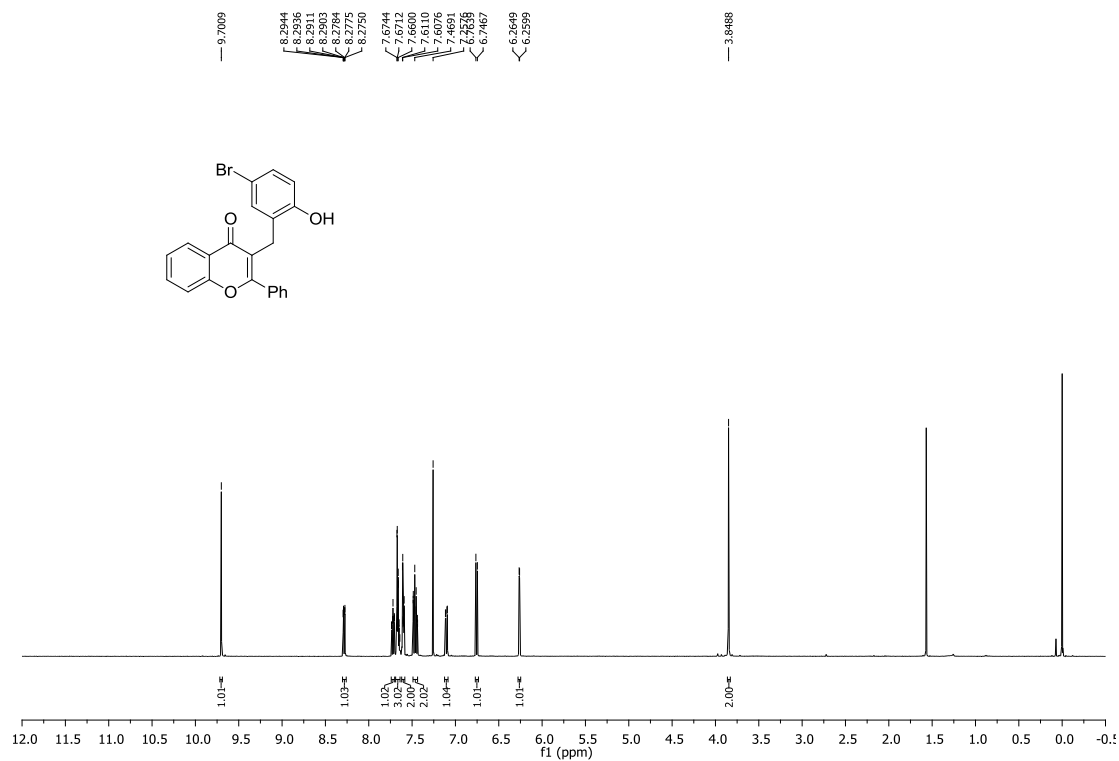
^1H NMR spectra of compound **6f** (CDCl_3 , 500 MHz)



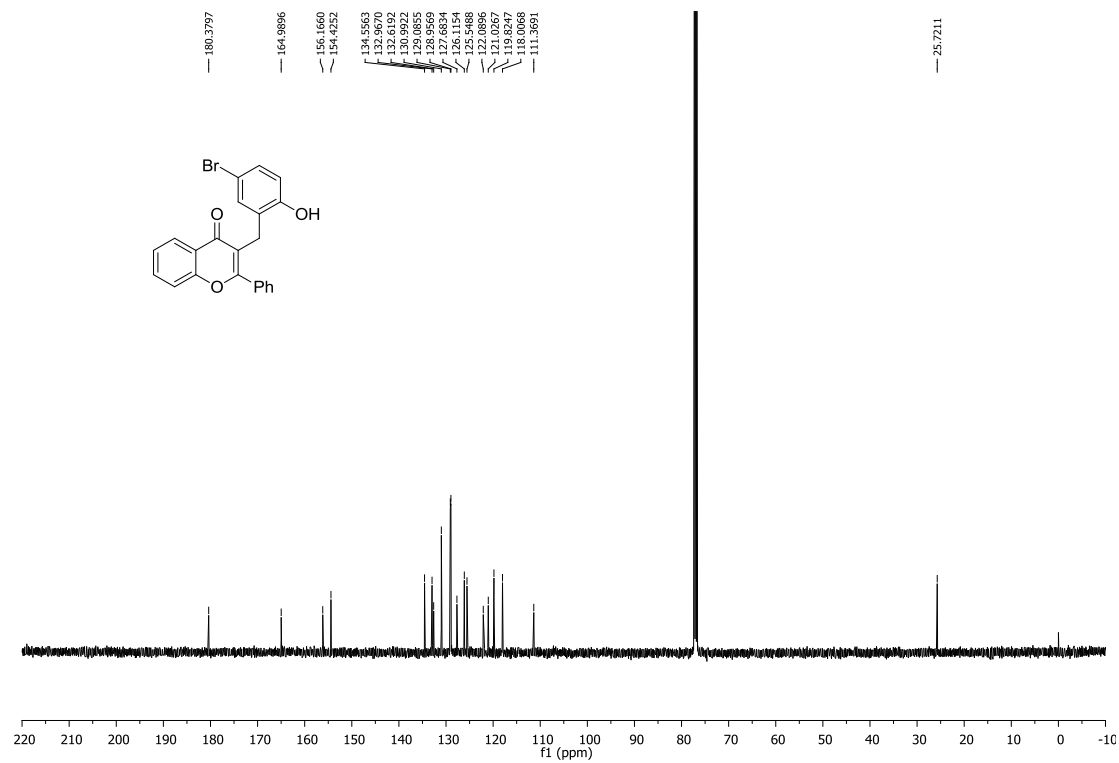
^{13}C NMR spectra of compound **6f** (CDCl_3 , 125 MHz)



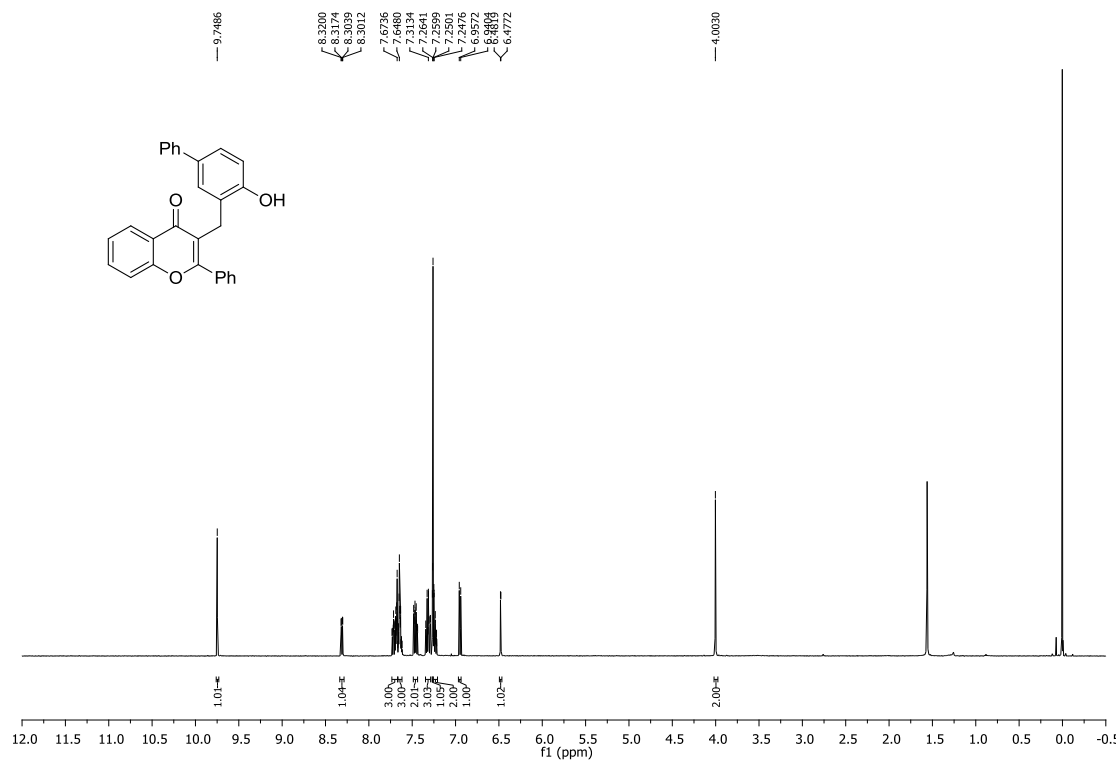
^1H NMR spectra of compound **6g** (CDCl_3 , 500 MHz)



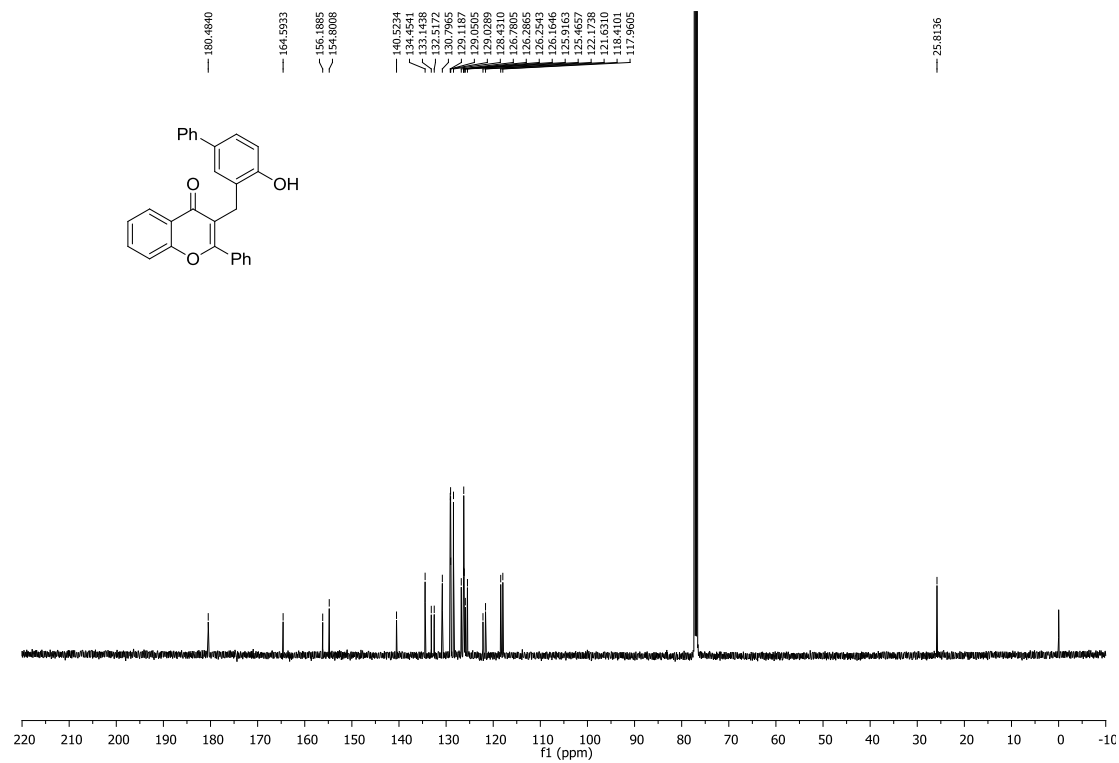
^{13}C NMR spectra of compound **6g** (CDCl_3 , 125 MHz)



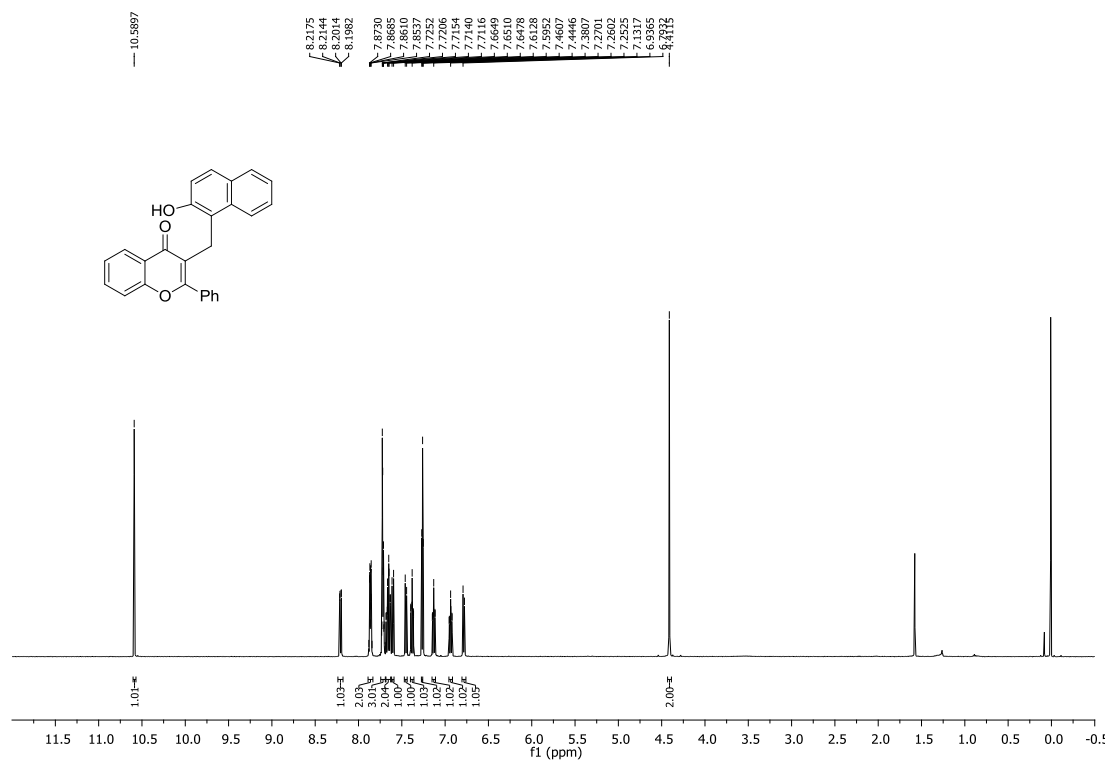
¹H NMR spectra of compound **6h** (CDCl₃, 500 MHz)



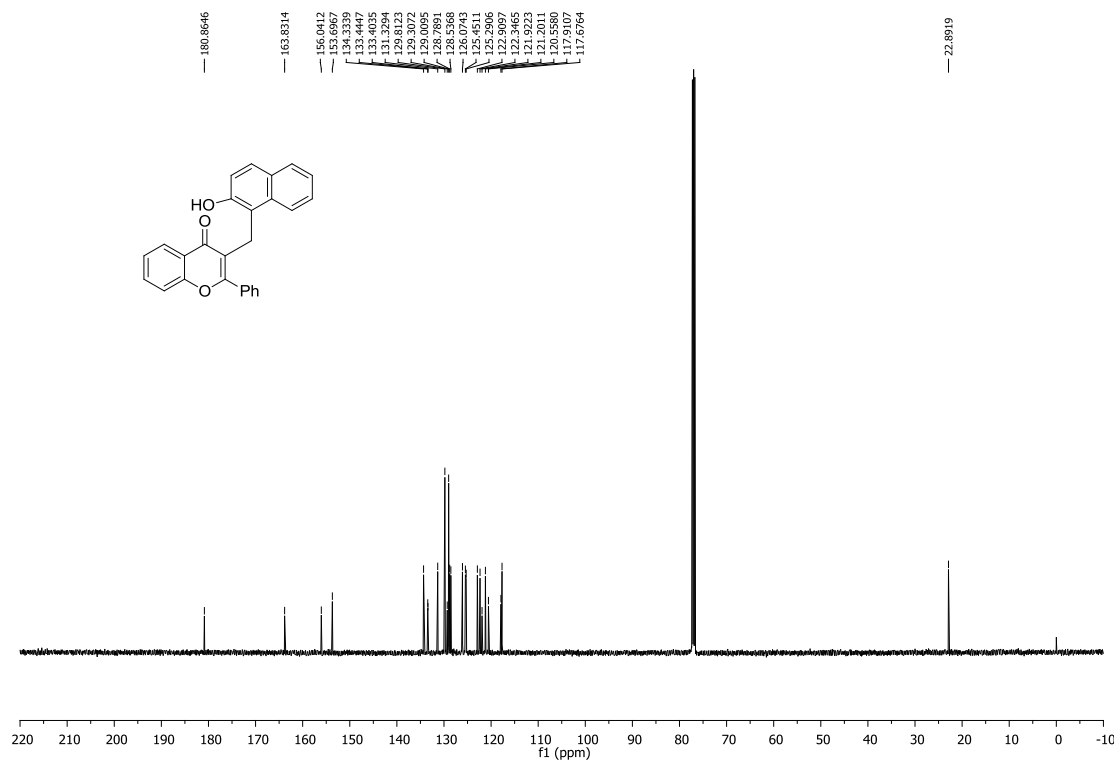
¹³C NMR spectra of compound **6h** (CDCl₃, 125 MHz)



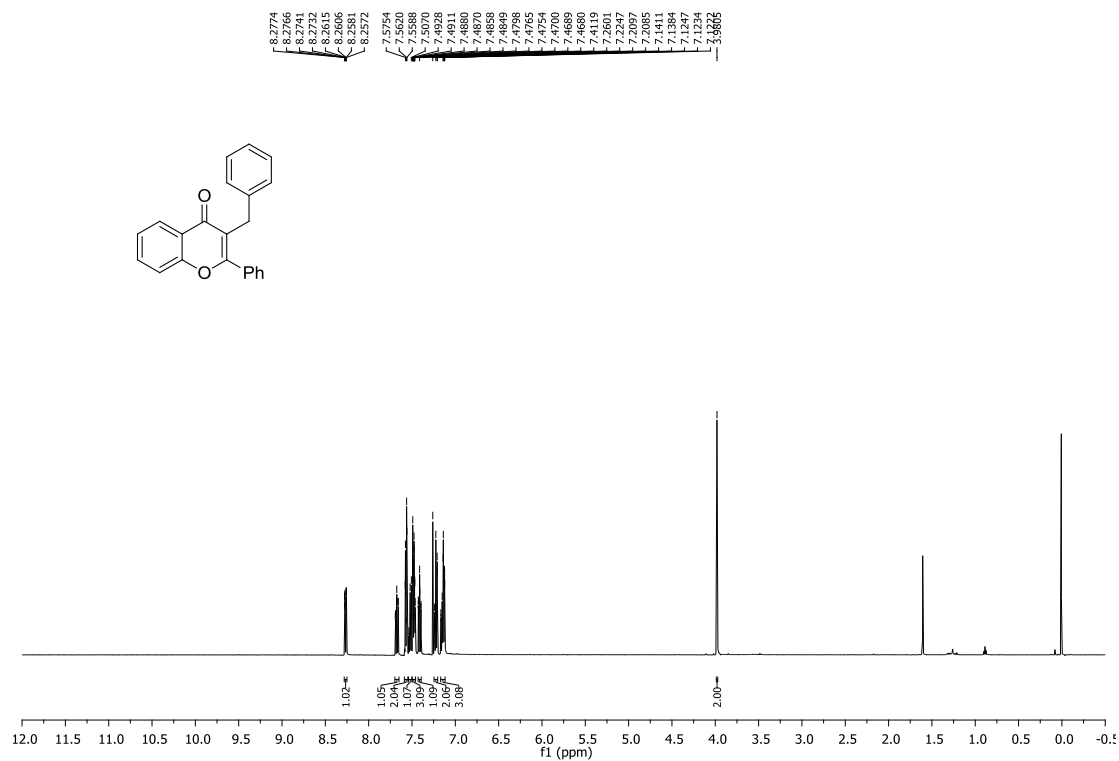
¹H NMR spectra of compound **6i** (CDCl₃, 500 MHz)



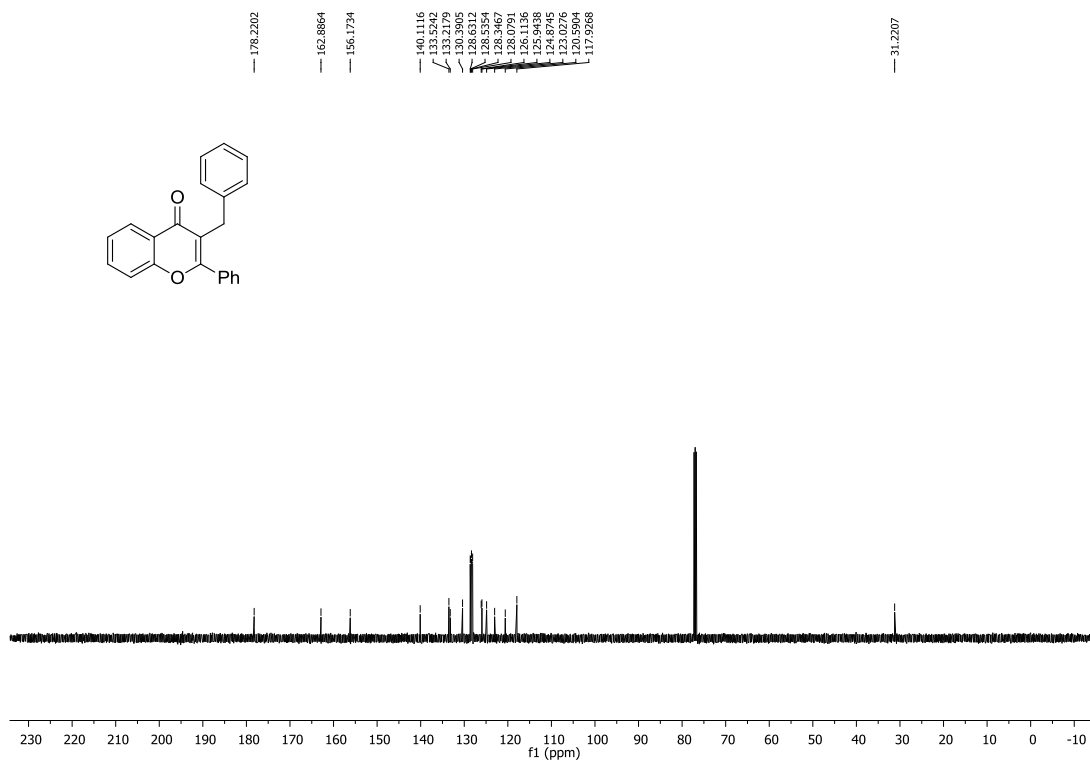
¹³C NMR spectra of compound **6i** (CDCl₃, 125 MHz)



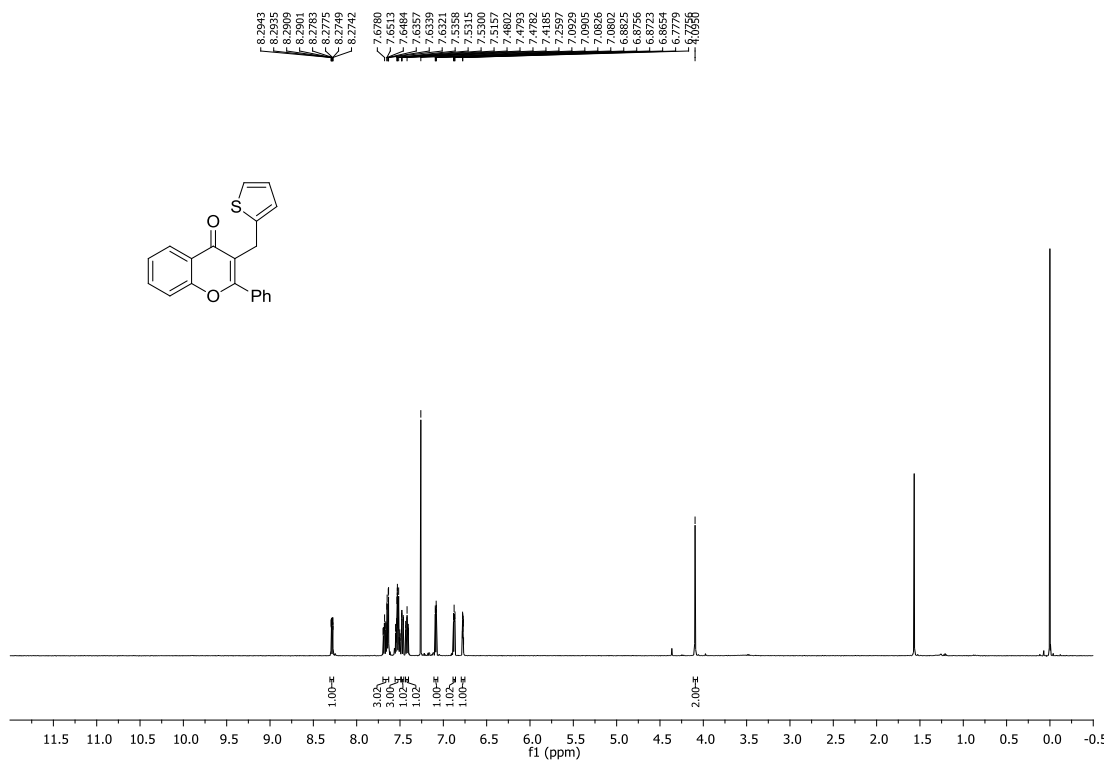
¹H NMR spectra of compound **6j** (CDCl₃, 500 MHz)



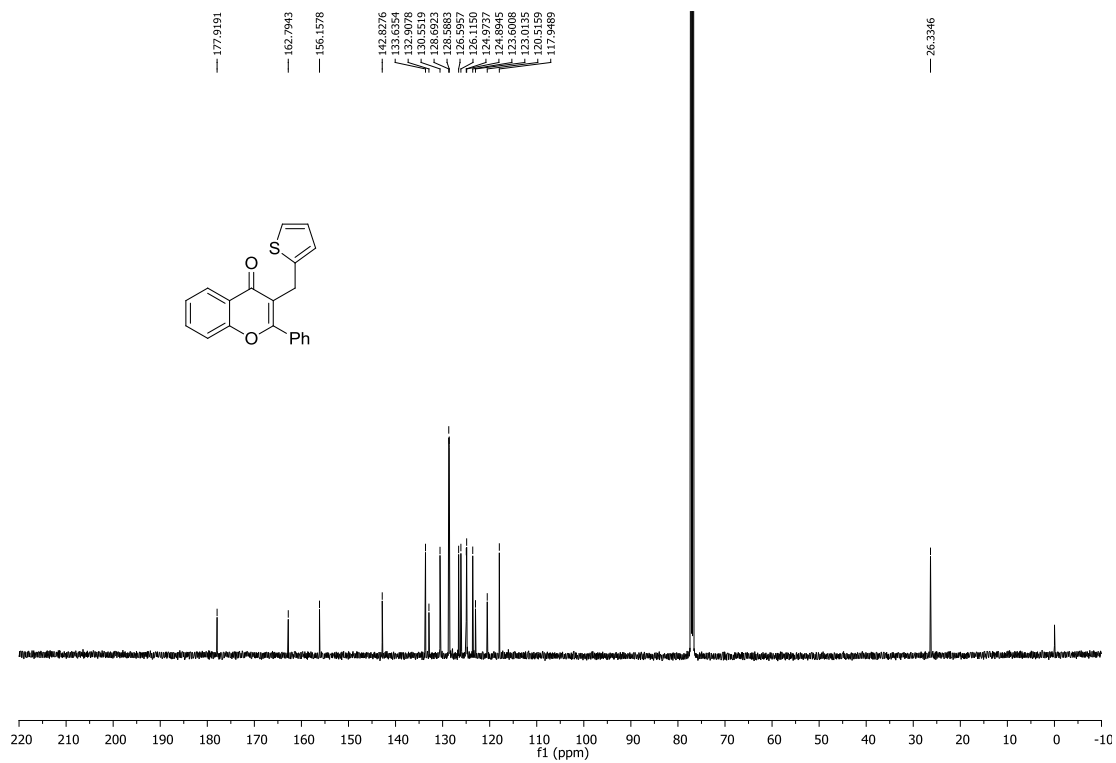
¹³C NMR spectra of compound **6j** (CDCl₃, 125 MHz)



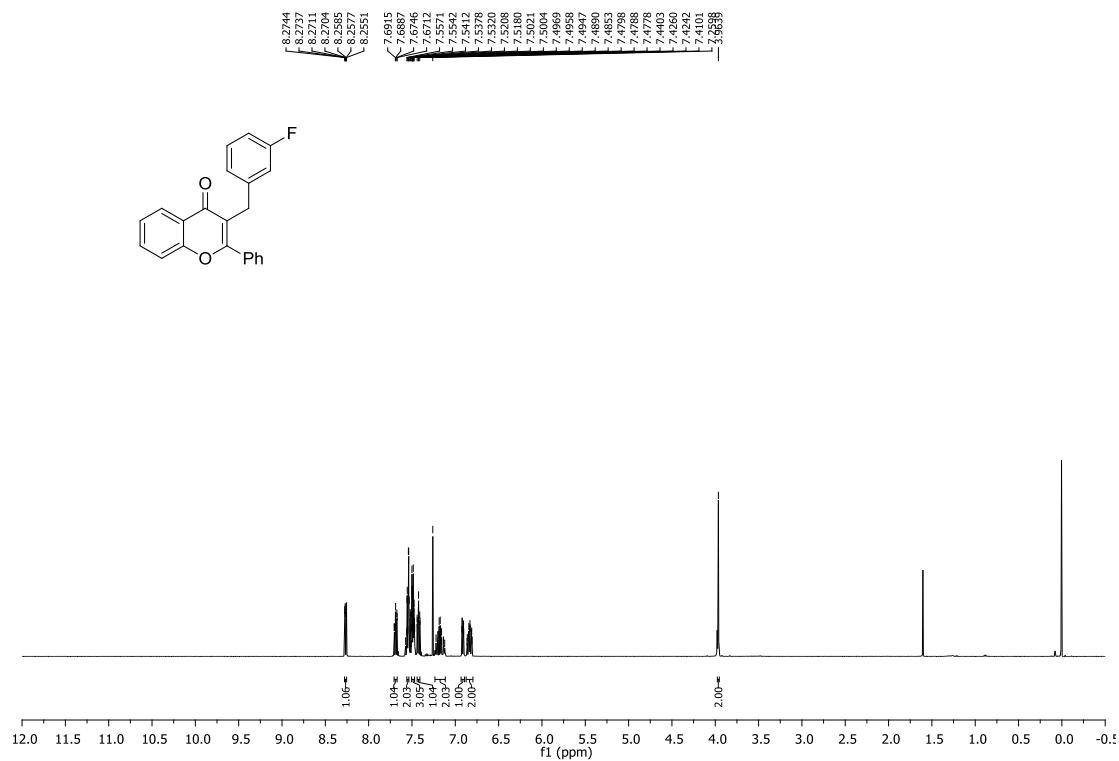
^1H NMR spectra of compound **6k** (CDCl_3 , 500 MHz)



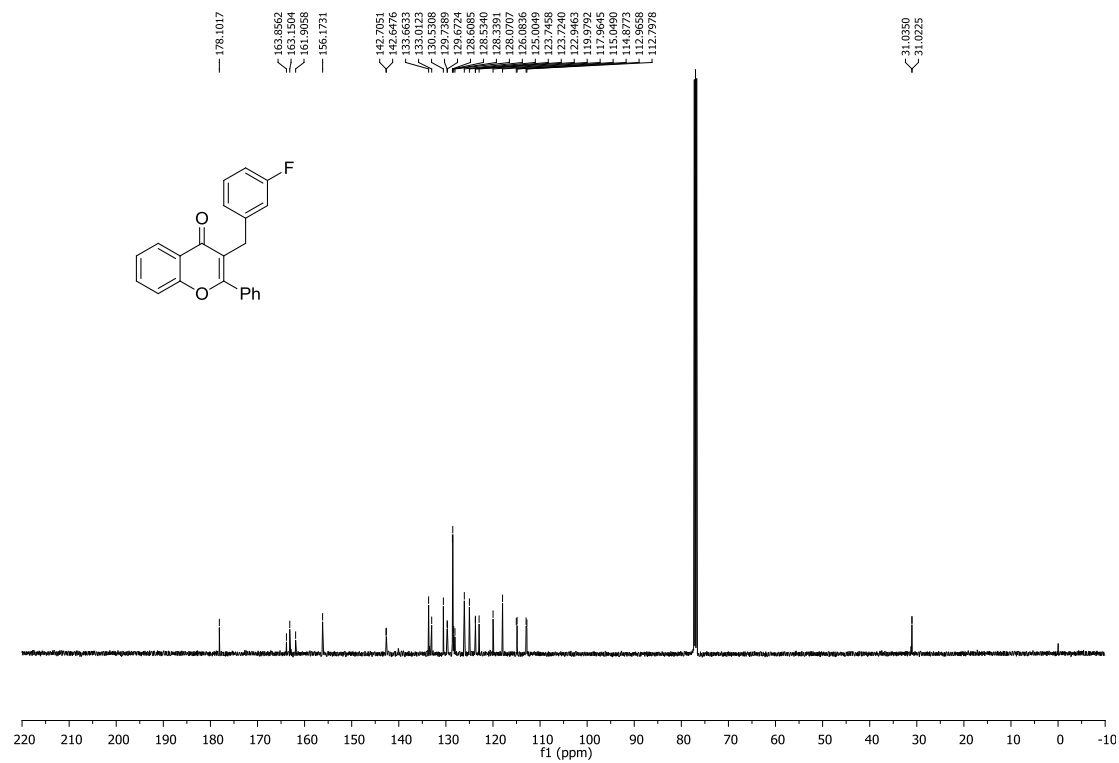
^{13}C NMR spectra of compound **6k** (CDCl_3 , 125 MHz)



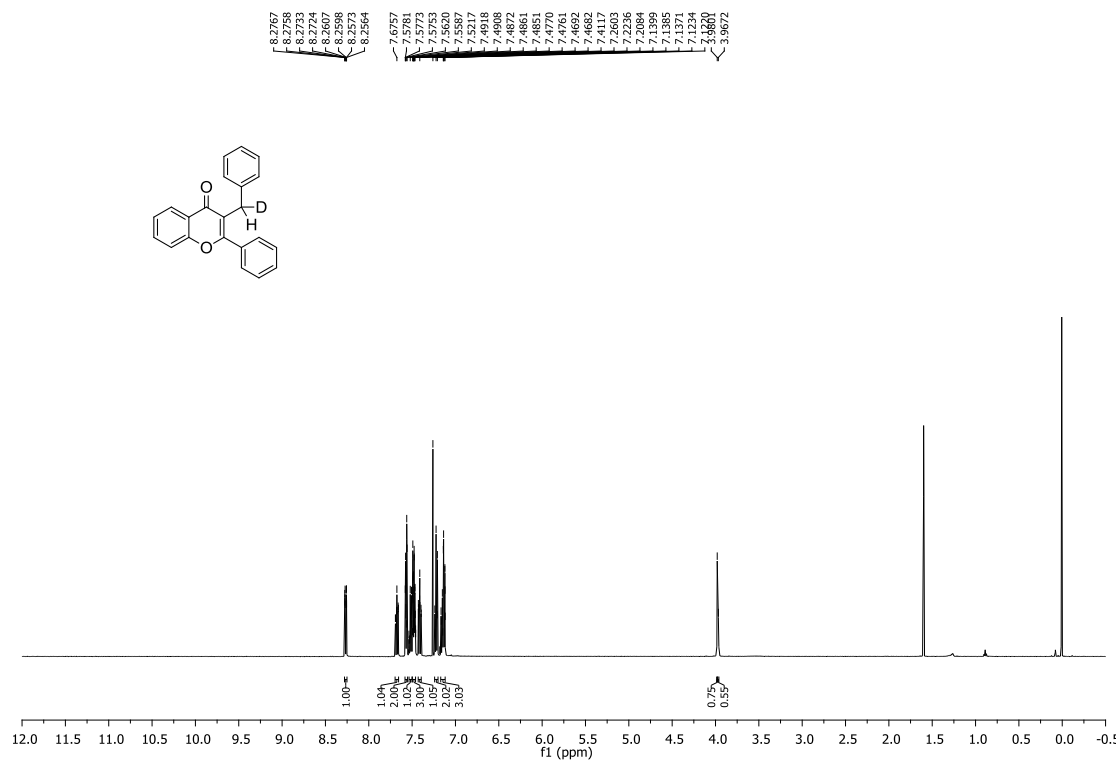
¹H NMR spectra of compound **6l** (CDCl₃, 500 MHz)



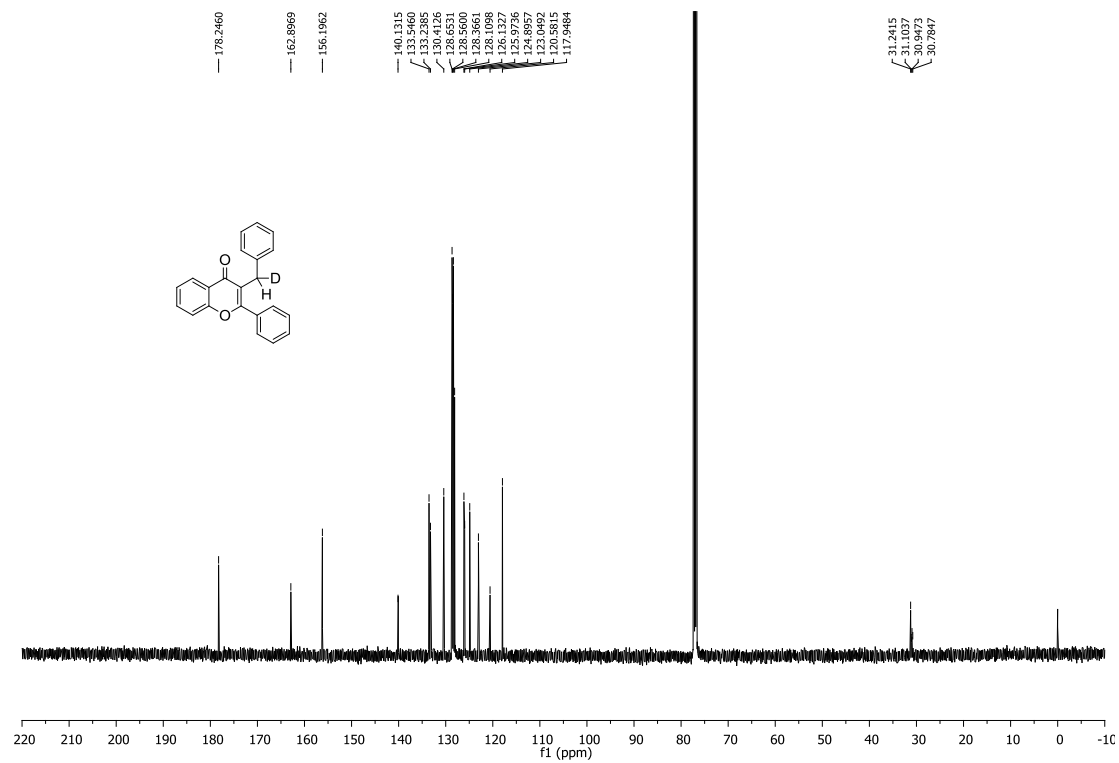
¹³C NMR spectra of compound **6l** (CDCl₃, 125 MHz)



^1H NMR spectra of compound **3j-D** (CDCl_3 , 500 MHz)



^{13}C NMR spectra of compound **3j-D** (CDCl_3 , 125 MHz)

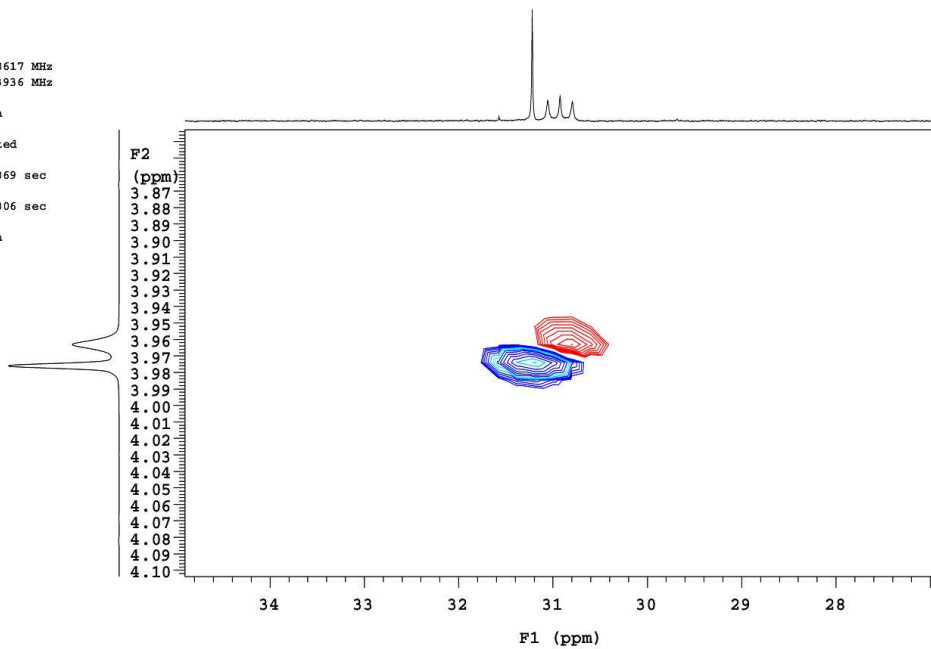


2D NMR spectra of compound **3j-D** (CDCl₃, 600 MHz)

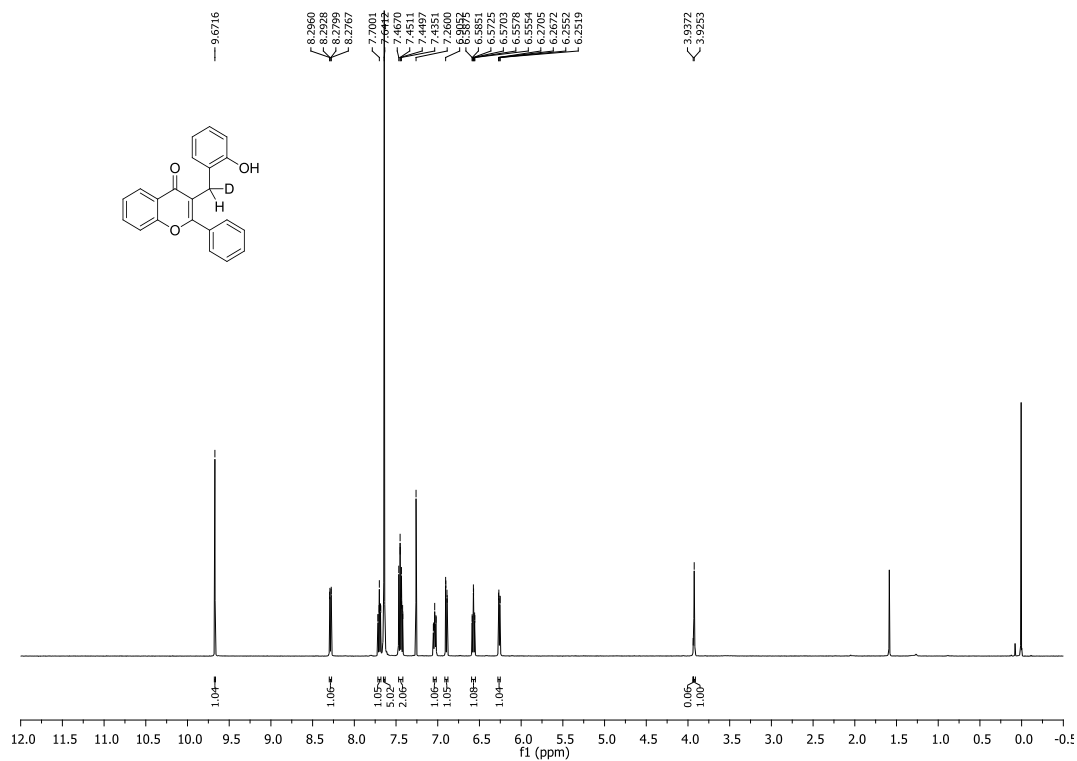
CER1530
 temp=25degC
 gHSQCAD

 Temp. 25.0 C / 298.1 K
 Operator: vnmr1

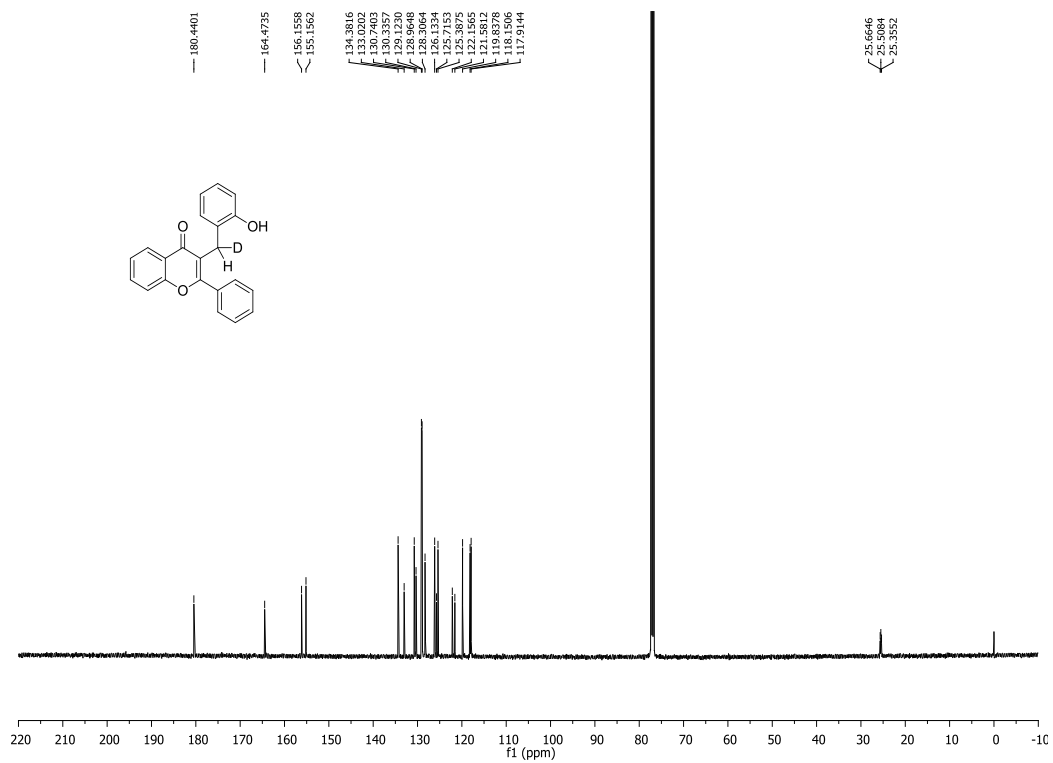
 Relax. delay 1.000 sec
 Acq. time 0.150 sec
 Width 6648.9 Hz
 2D Width 30177.3 Hz
 8 repetitions
 2 x 200 increments
 OBSERVE H1, 599.9868617 MHz
 DECOUPLE C13, 150.8803936 MHz
 Power 43 dB
 on during acquisition
 off during delay
 W40_cold_tube modulated
 DATA PROCESSING
 Gauss apodization 0.069 sec
 F1 DATA PROCESSING
 Gauss apodization 0.006 sec
 FT size 2048 x 2048
 Total time 1 hr, 4 min



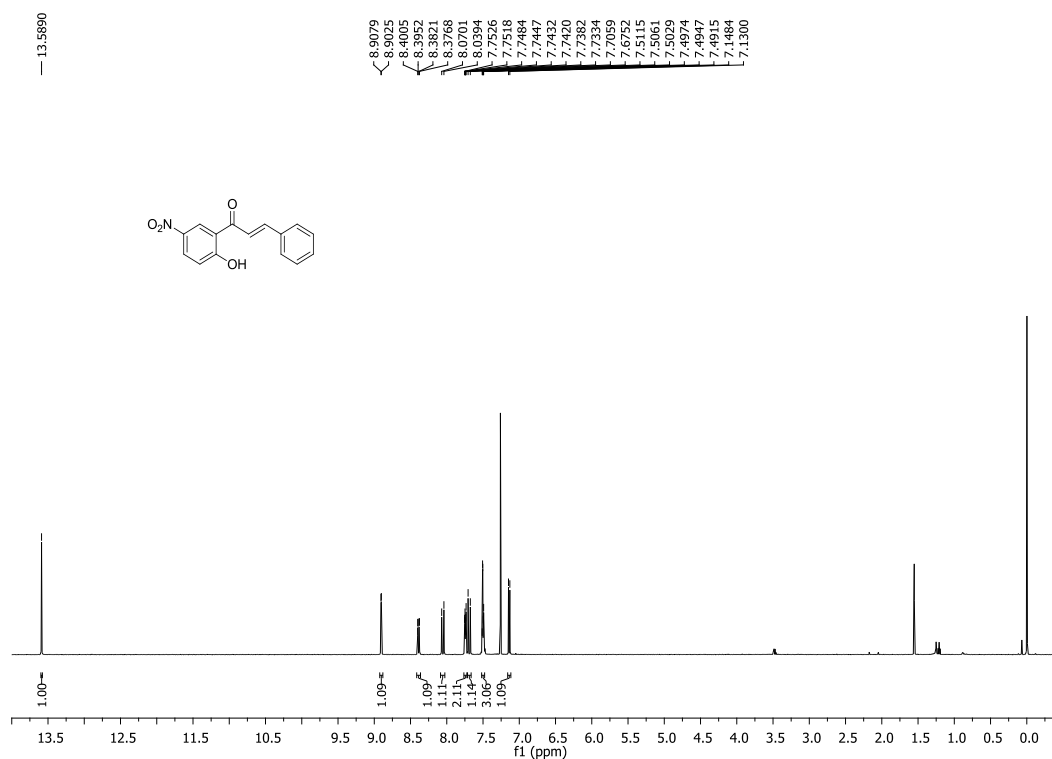
^1H NMR spectra of compound **3aa-D** (CDCl_3 , 500 MHz)



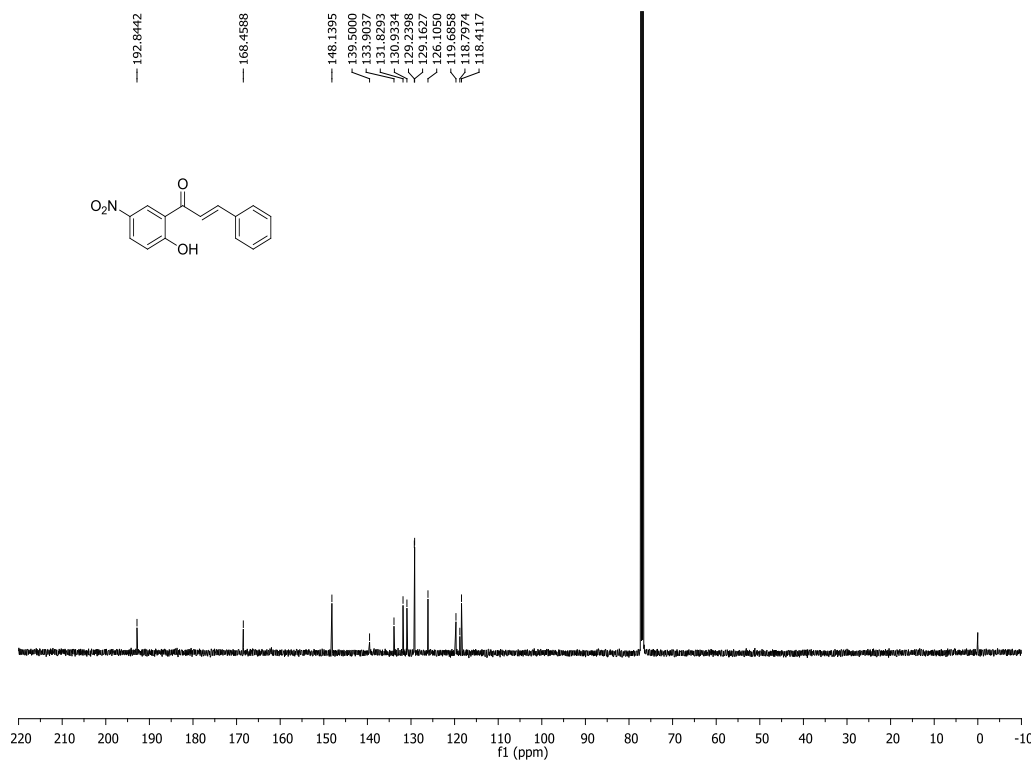
^{13}C NMR spectra of compound **3aa-D** (CDCl_3 , 125 MHz)



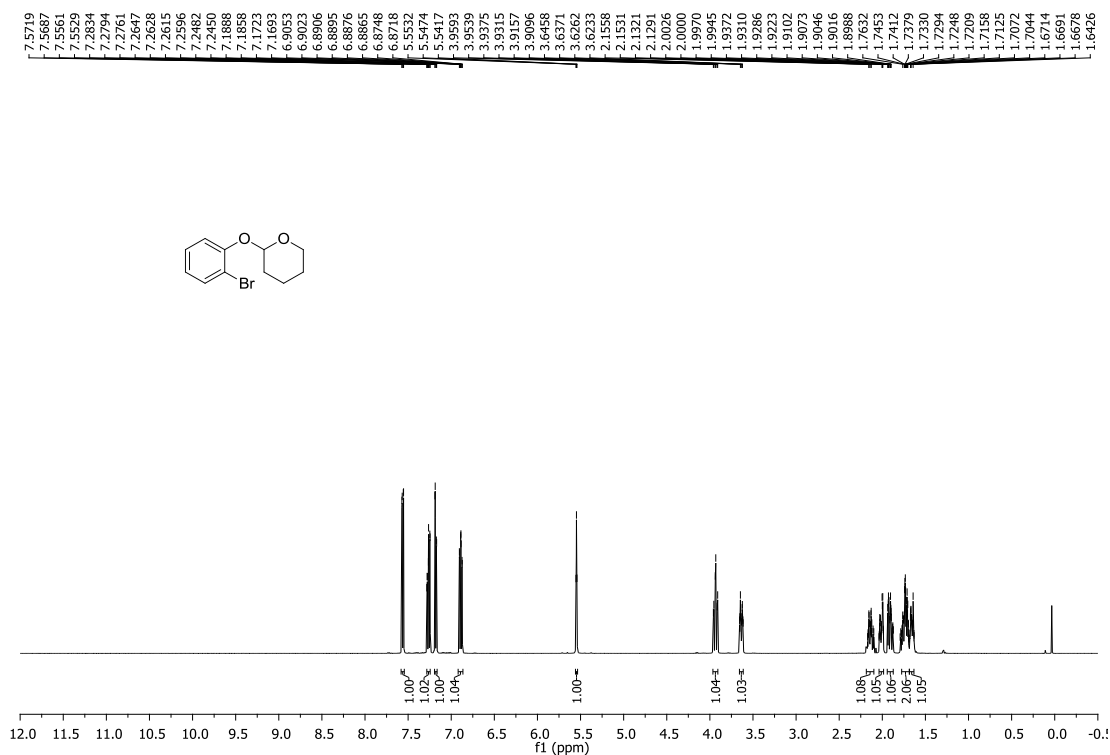
^1H NMR spectra of compound **5ma** (CDCl_3 , 500 MHz)



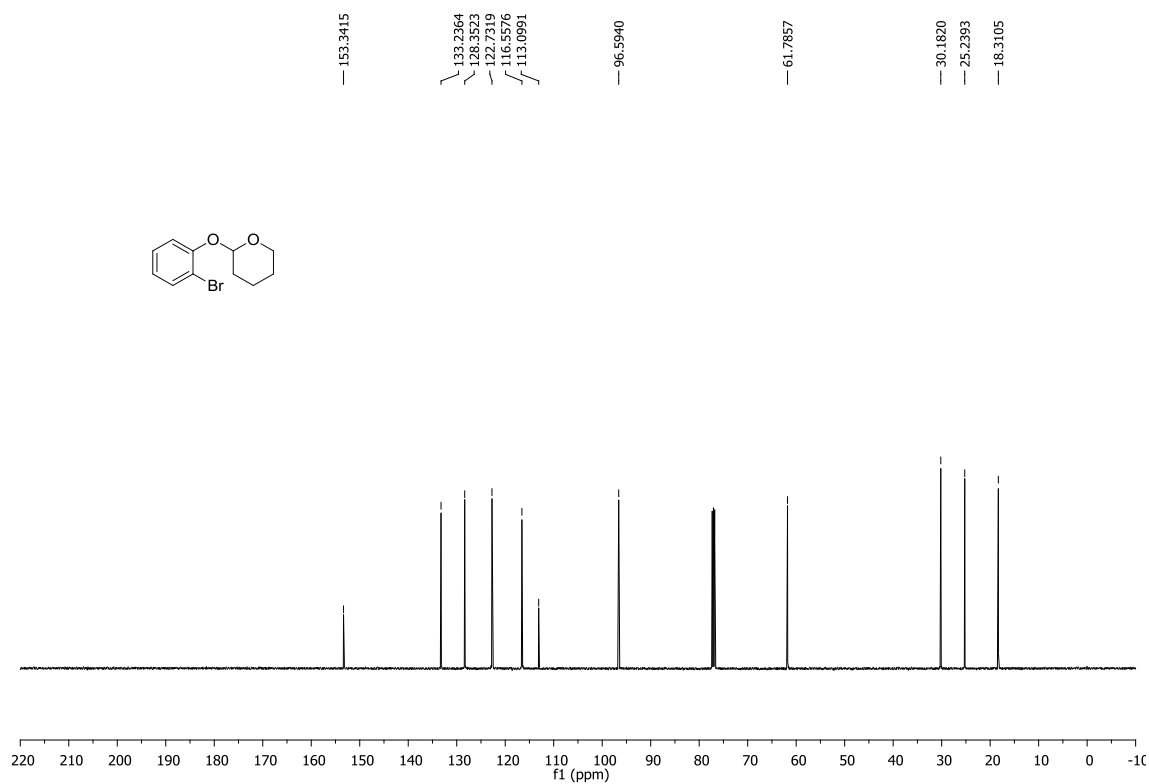
^{13}C NMR spectra of compound **5ma** (CDCl_3 , 125 MHz)



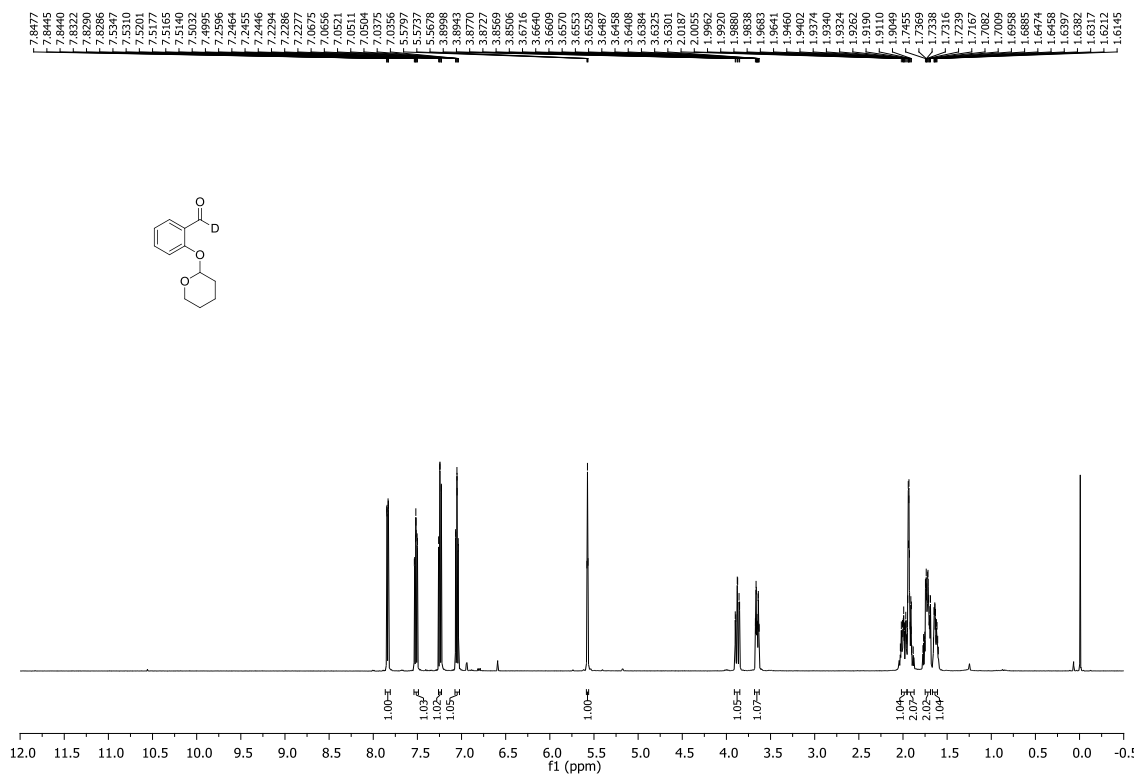
¹H NMR spectra of compound A (CDCl₃, 500 MHz)



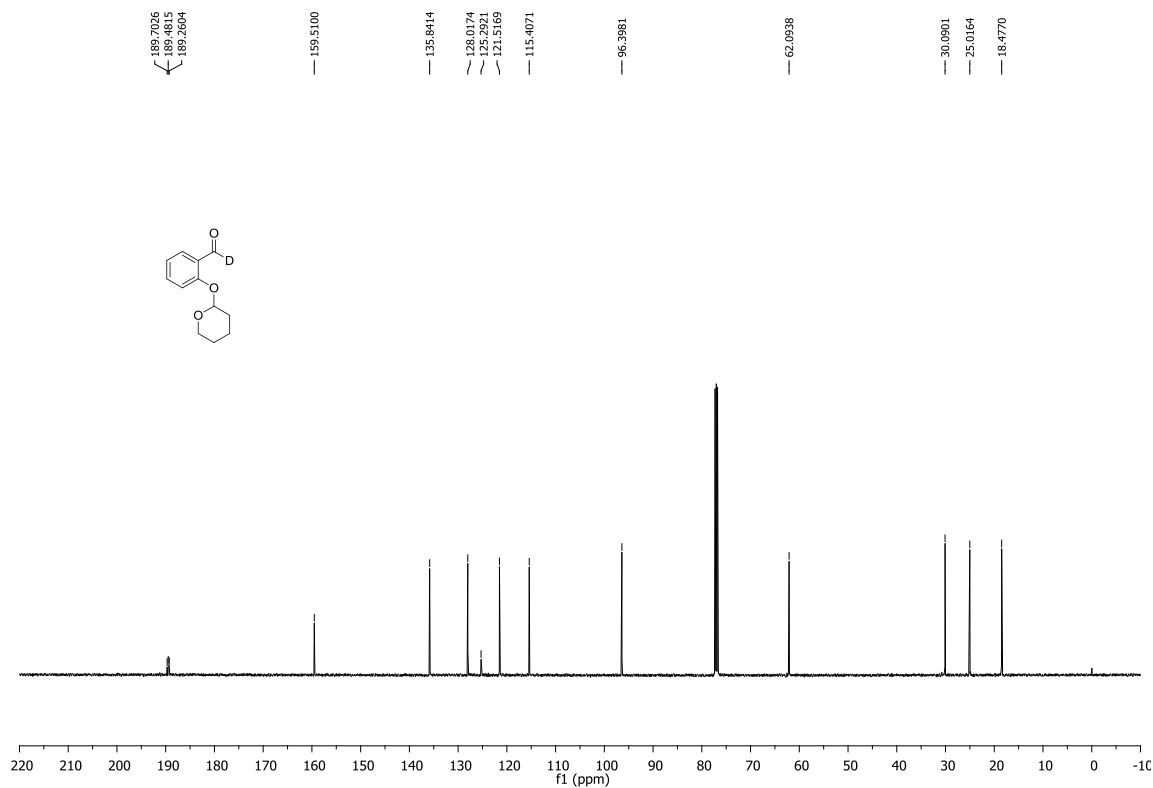
¹³C NMR spectra of compound A (CDCl₃, 125 MHz)



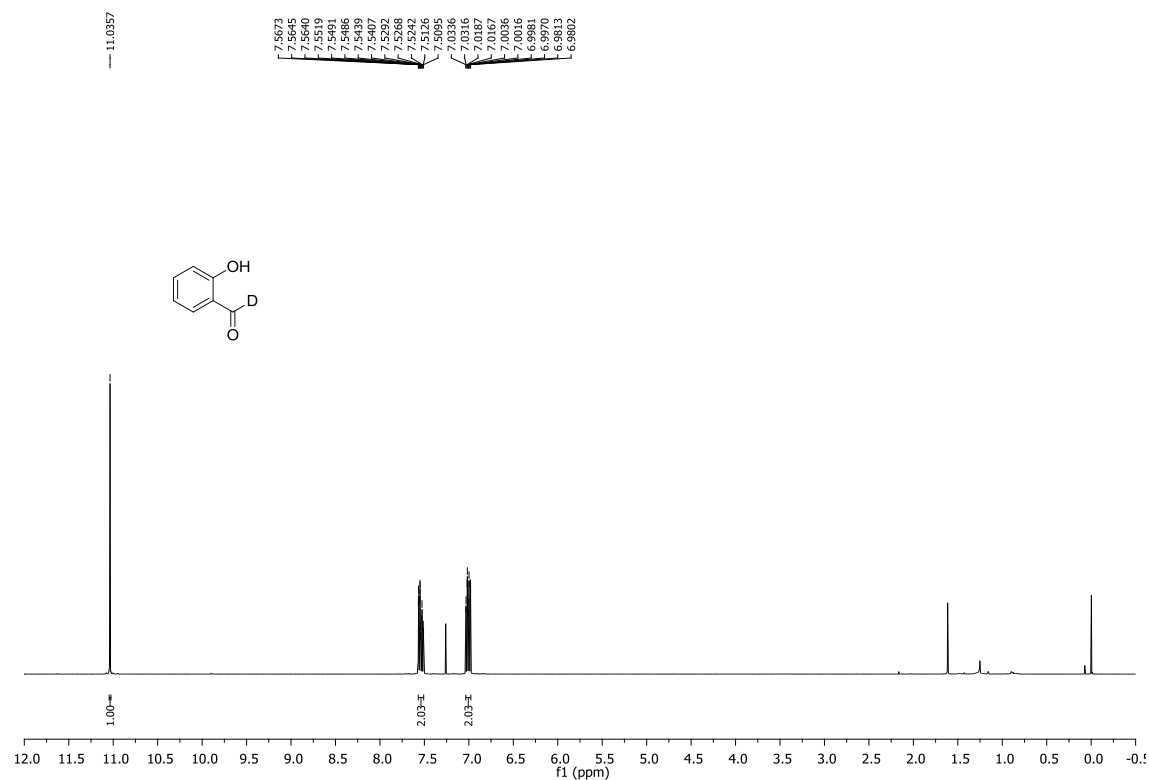
¹H NMR spectra of compound **B** (CDCl₃, 125 MHz)



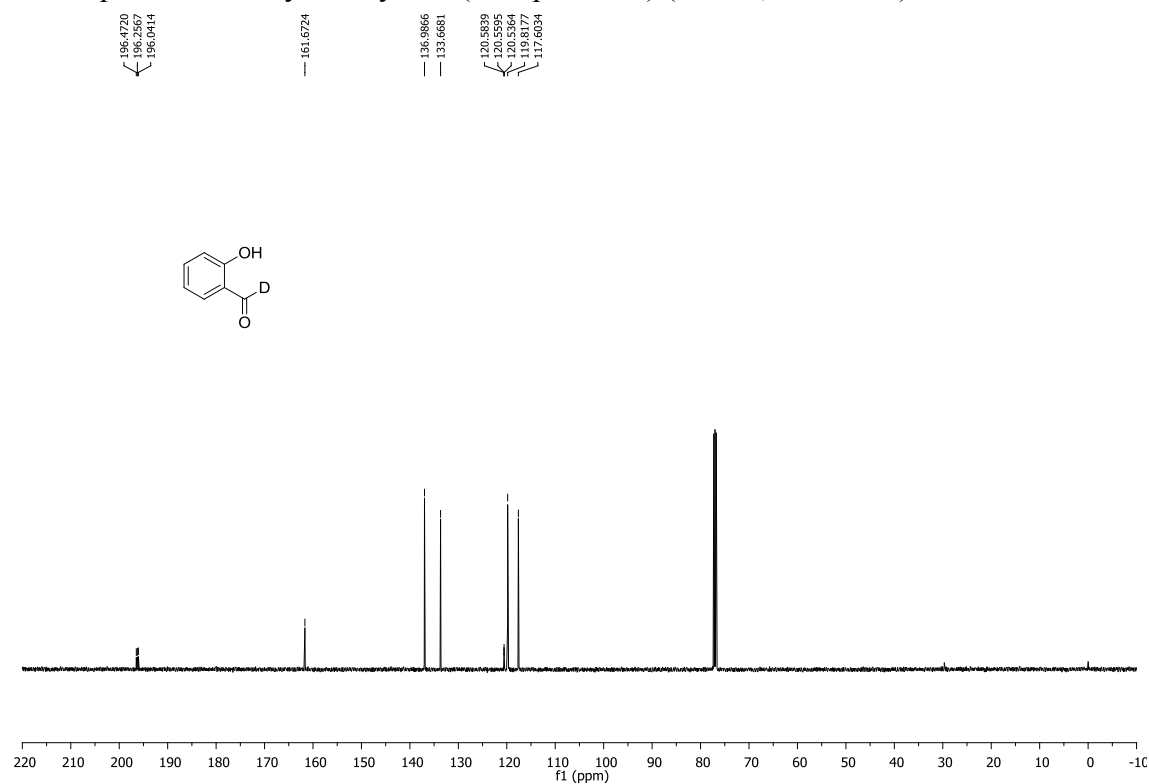
¹³C NMR spectra of compound **B** (CDCl₃, 125 MHz)



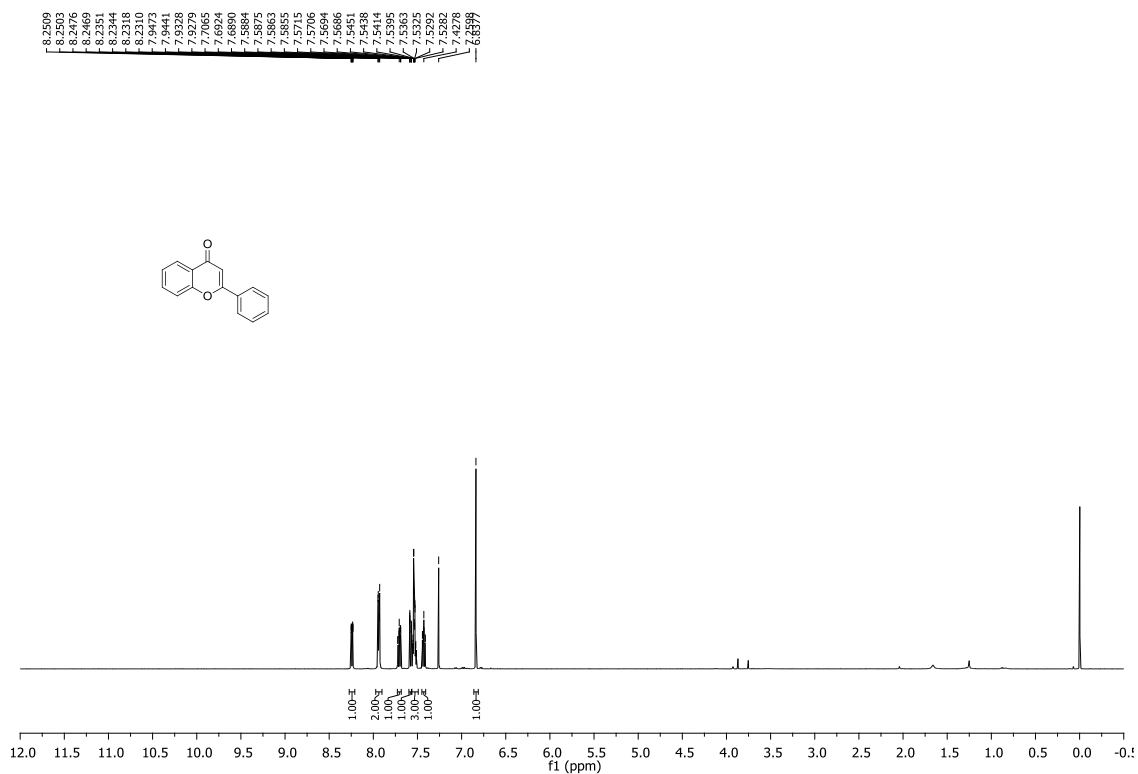
¹H NMR spectra of Salicylaldehyde-*d* (Compound-C) (CDCl₃, 125 MHz)



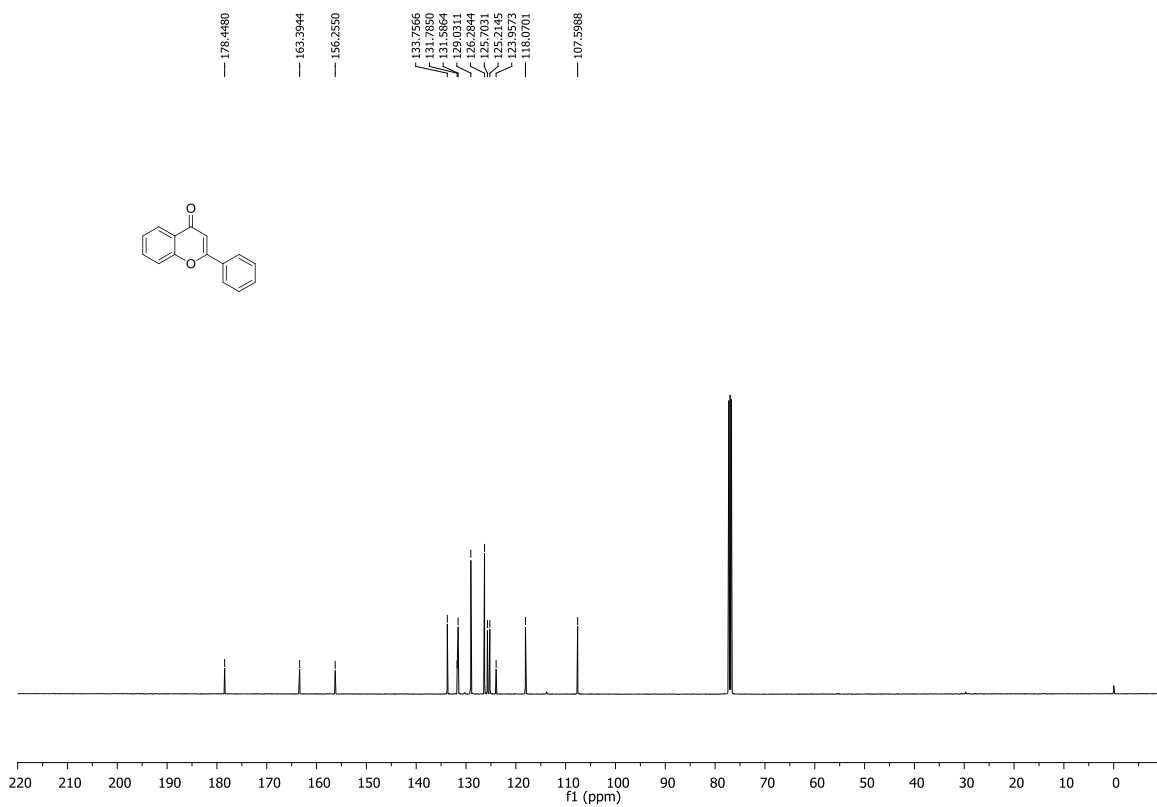
¹³C NMR spectra of Salicylaldehyde-*d* (Compound-C) (CDCl₃, 125 MHz)



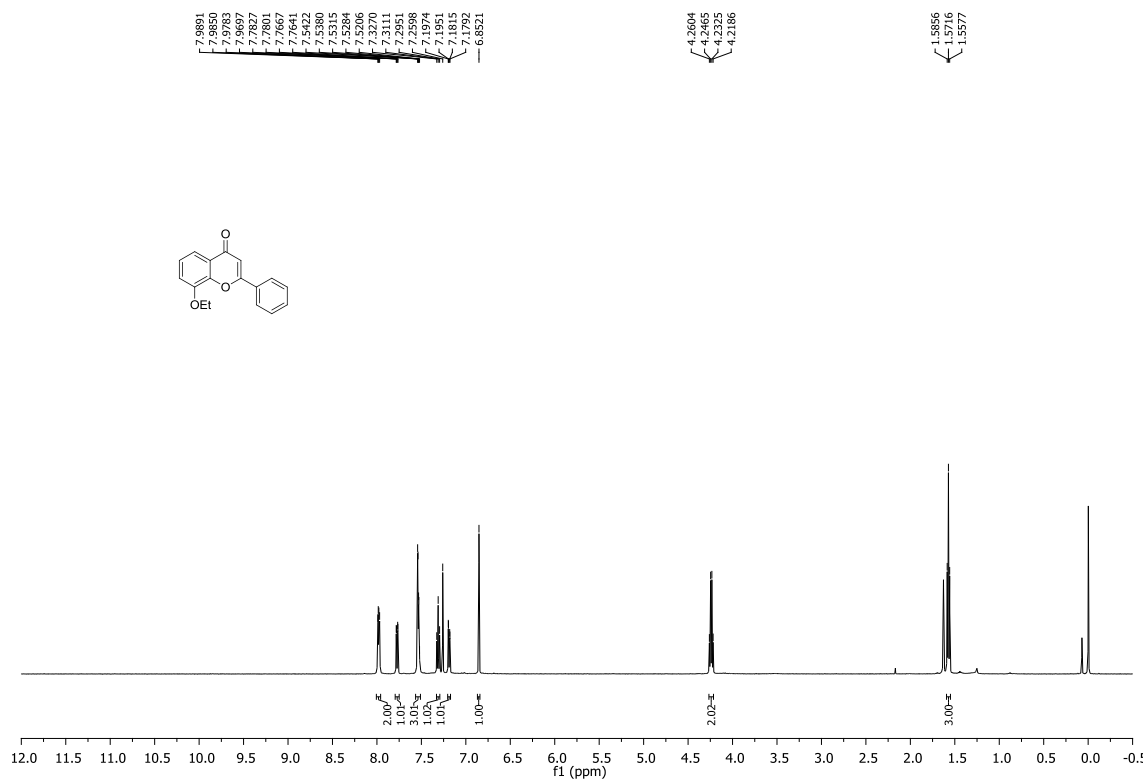
¹H NMR spectra of compound **4aa** (CDCl₃, 500 MHz)



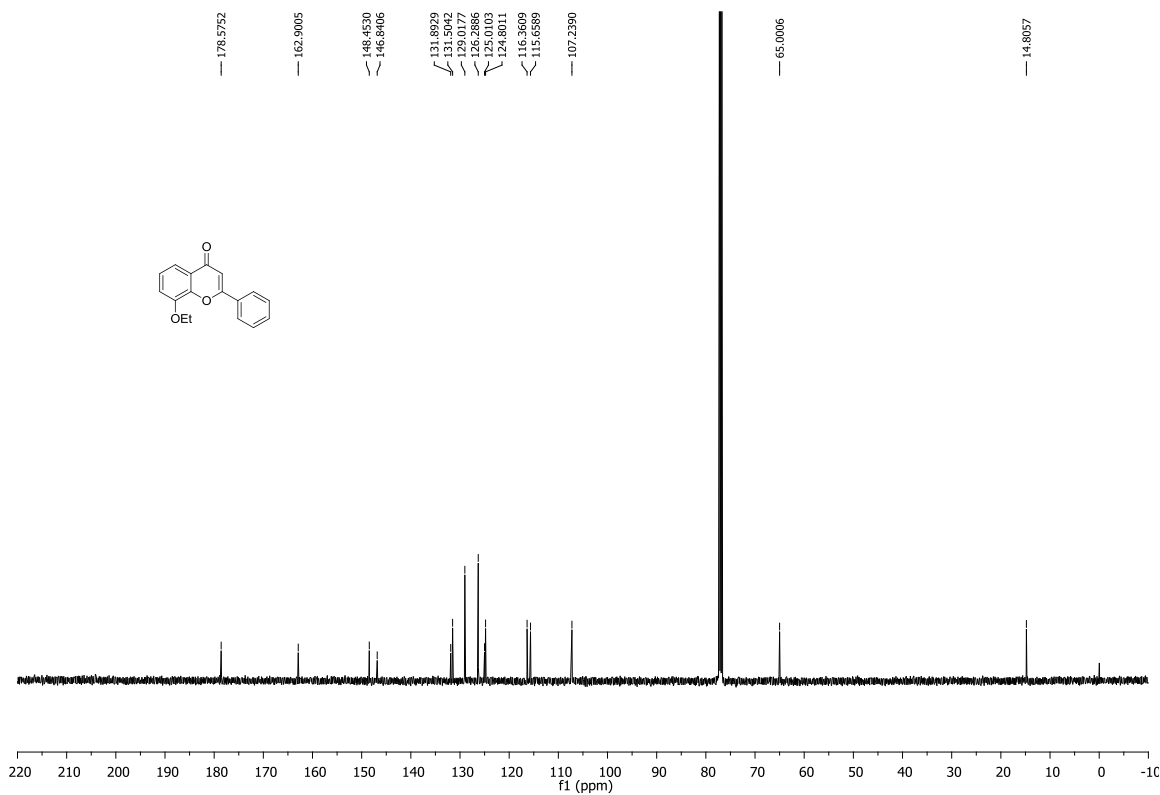
¹³C NMR spectra of compound **4aa** (CDCl₃, 125 MHz)



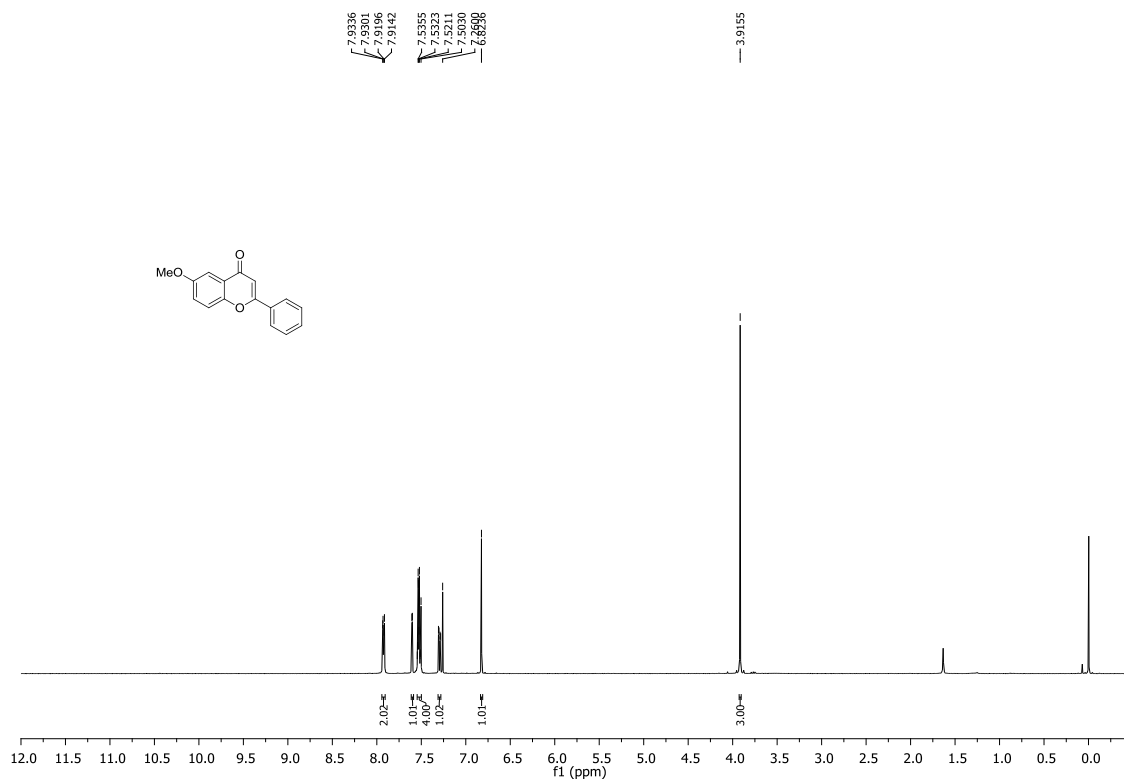
¹H NMR spectra of compound **4ba** (CDCl₃, 500 MHz)



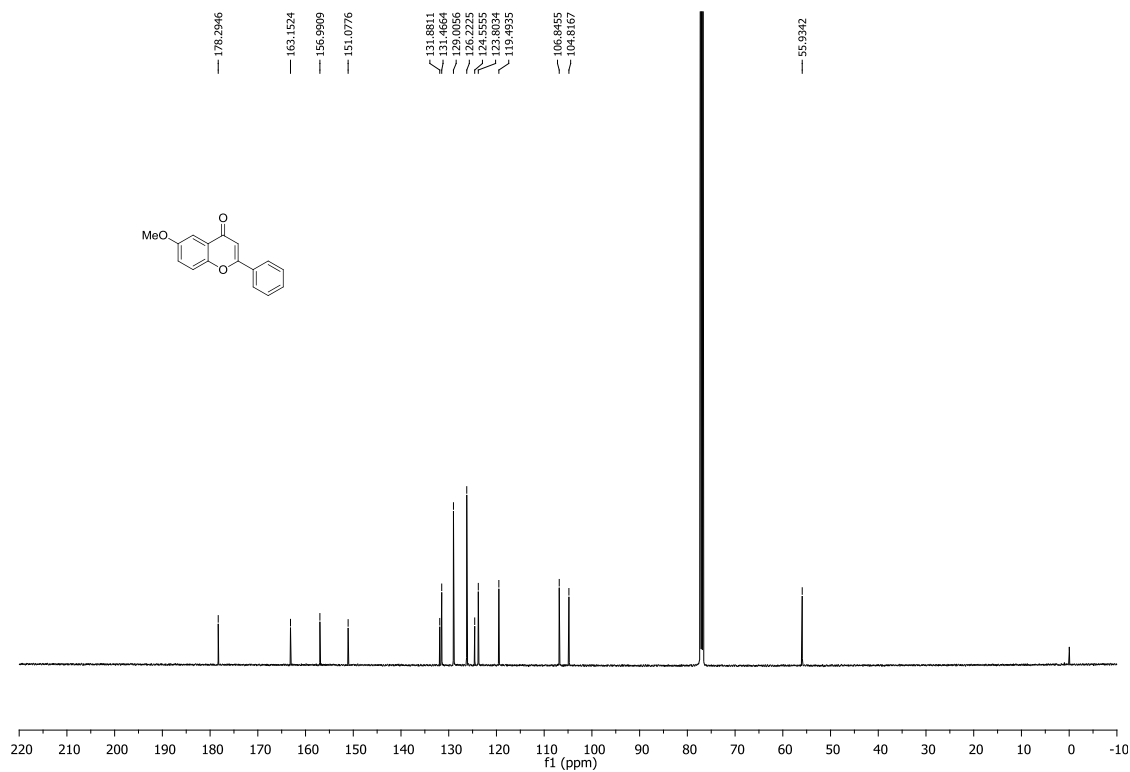
¹³C NMR spectra of compound **4ba** (CDCl₃, 125 MHz)



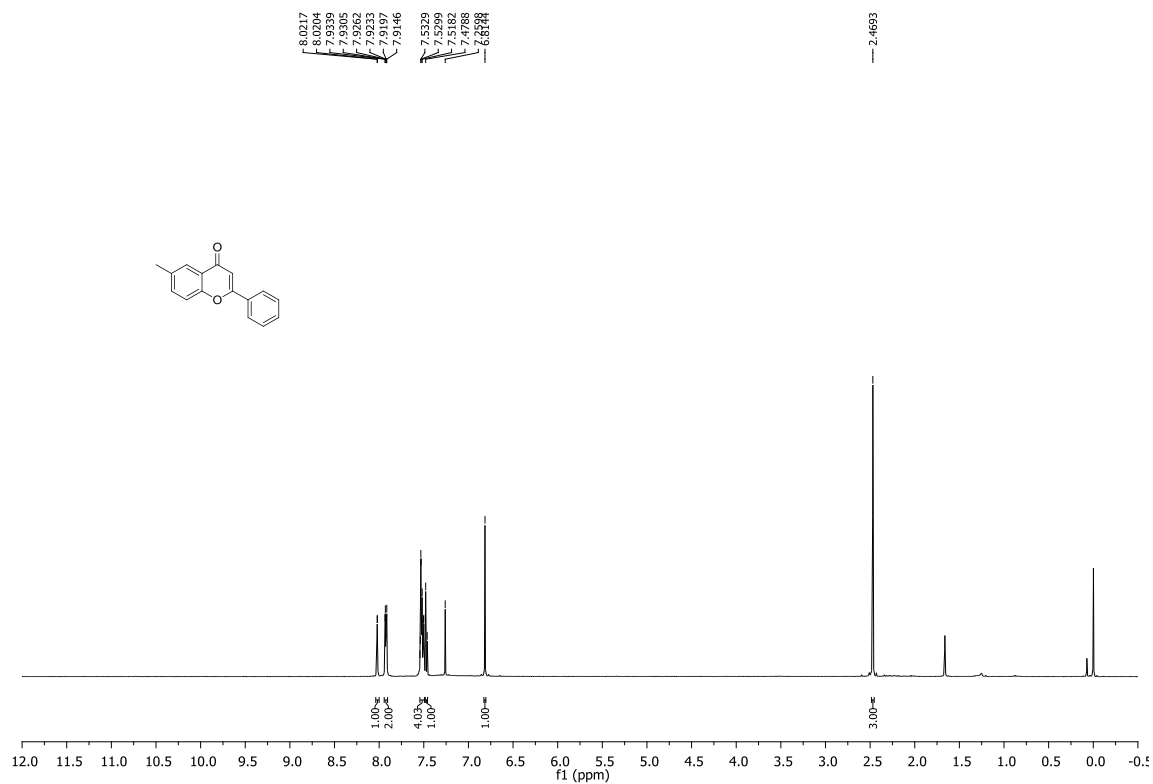
¹H NMR spectra of compound **4da** (CDCl₃, 500 MHz)



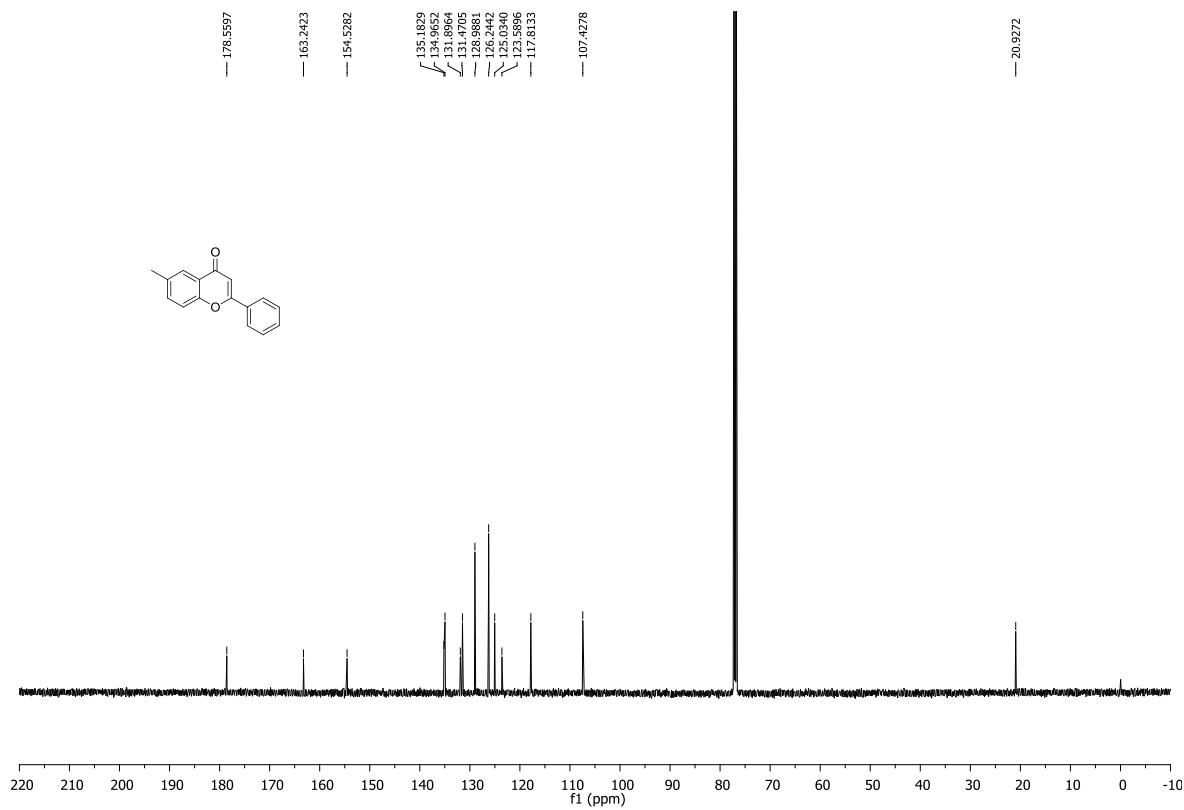
¹³C NMR spectra of compound **4da** (CDCl₃, 125 MHz)



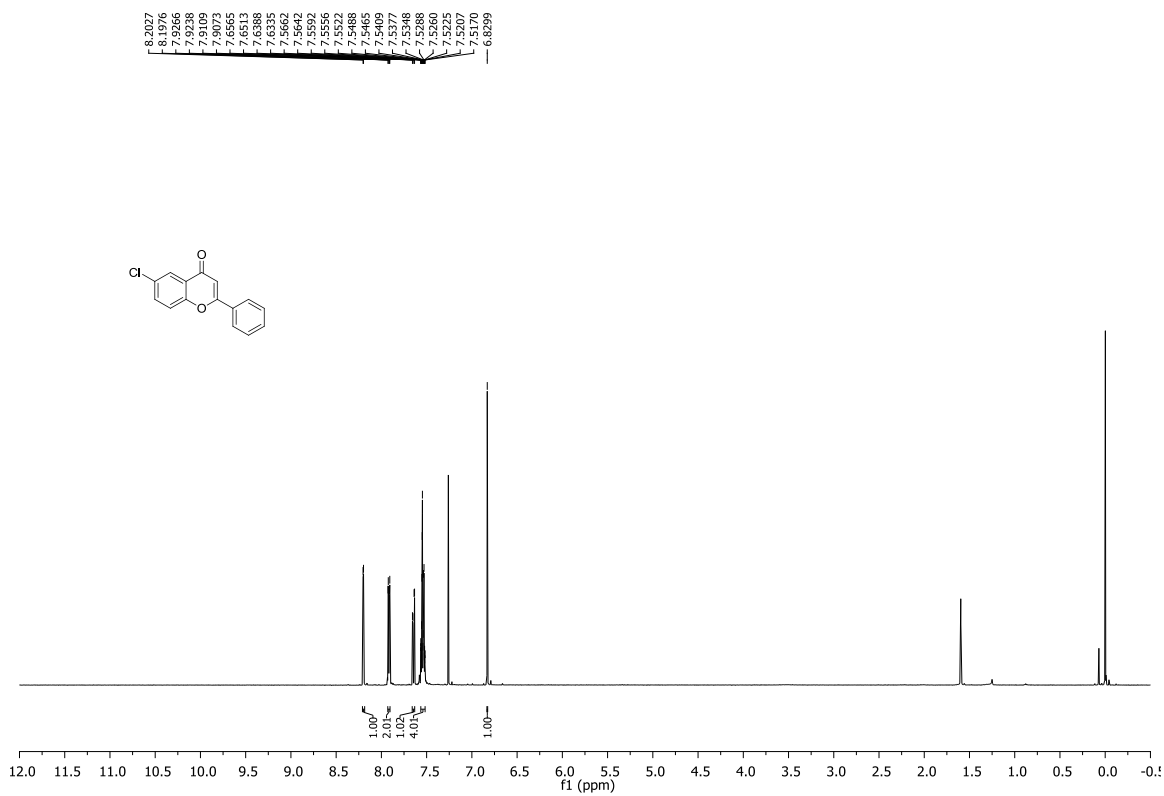
¹H NMR spectra of compound **4ea** (CDCl₃, 500 MHz)



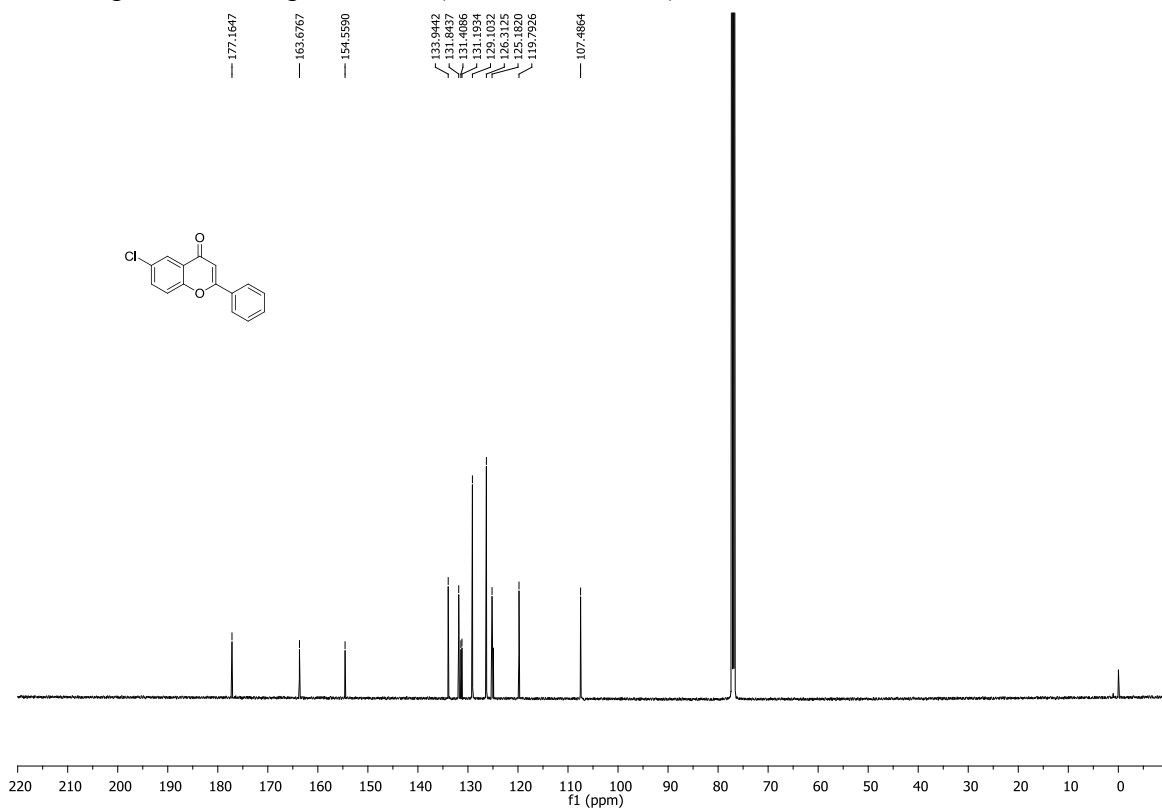
¹³C NMR spectra of compound **4ea** (CDCl₃, 125 MHz)



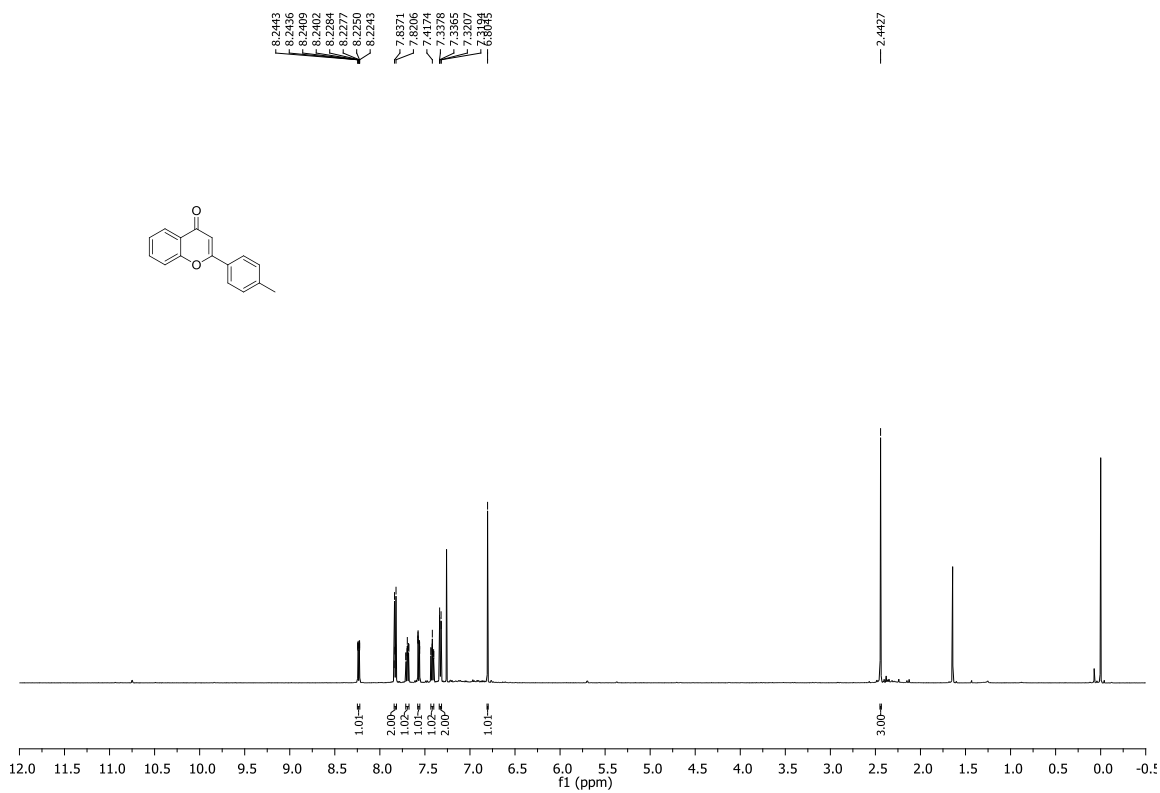
¹H NMR spectra of compound **4ha** (CDCl₃, 500 MHz)



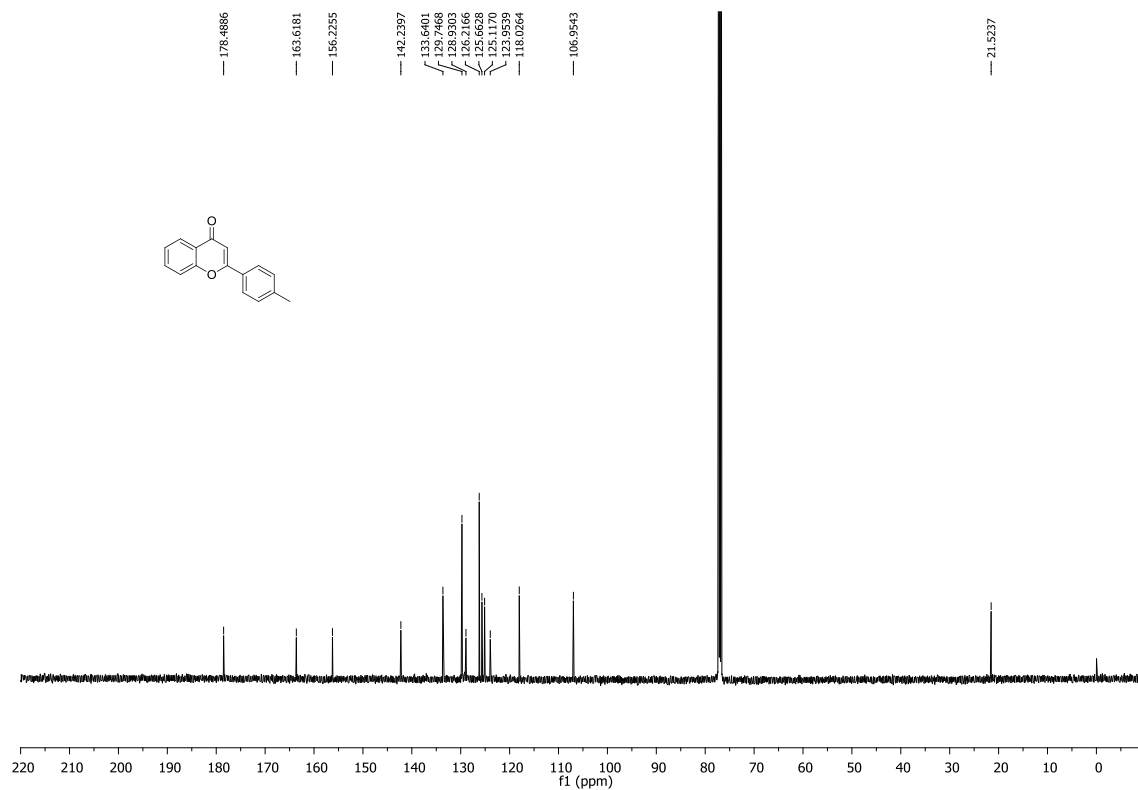
¹³C NMR spectra of compound **4ha** (CDCl₃, 125 MHz)



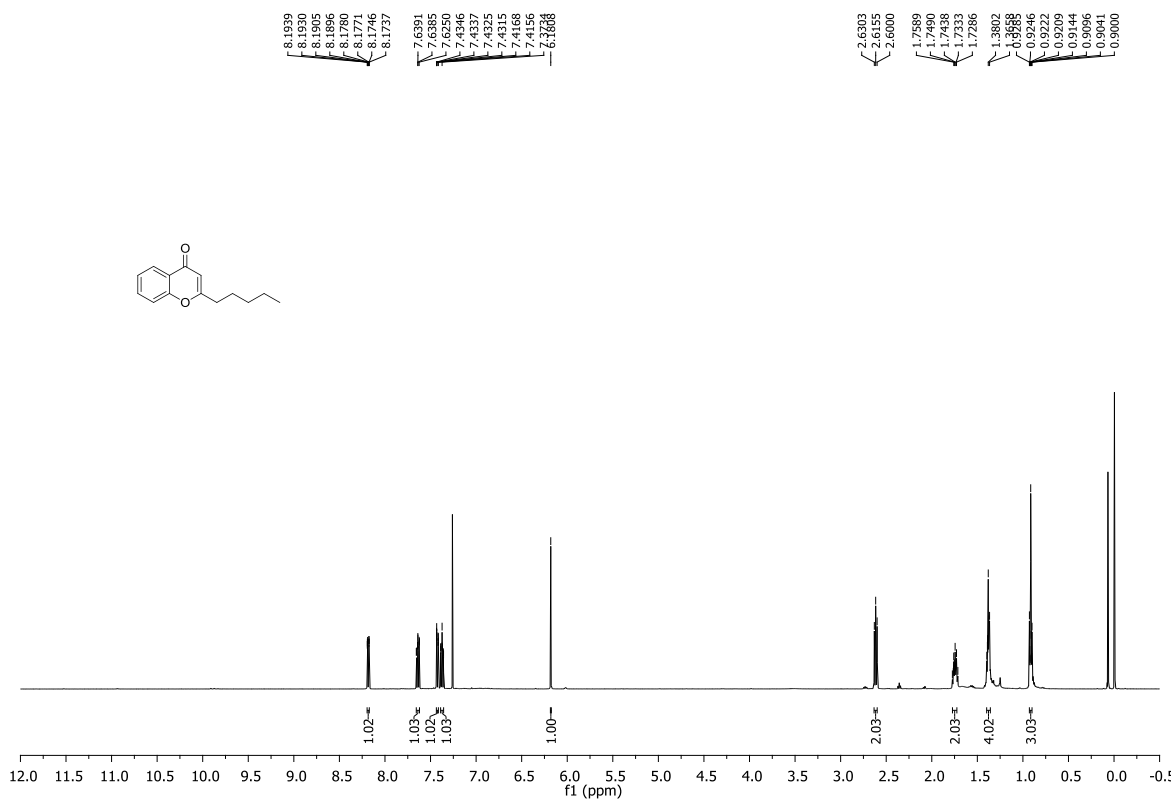
¹H NMR spectra of compound **4ad** (CDCl₃, 500 MHz)



¹³C NMR spectra of compound **4ad** (CDCl₃, 125 MHz)



¹H NMR spectra of compound **4am** (CDCl₃, 500 MHz)



¹³C NMR spectra of compound **4am** (CDCl₃, 125 MHz)

