SUPPLEMENTARY INFORMATION

Impact of Mono- and Disubstitution on the Colorimetric Dynamic Covalent Switching Chalcone/Flavanone Scaffold

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GENERAL CONSIDERATIONS

Chemicals were obtained from Sigma-Aldrich and Fisher Scientific. Column chromatography was performed using silica gel from Macherey-Nagel (60 M, 0.04-0.063 mm). ^{1}H and ^{13}C NMR data were recorded in $CDCl_3$ on either a 300 or 500 MHz Bruker Avance III spectrometer at room temperature. Chemical shifts are reported relative to residual $CHCl_3$ (δ 7.24 ppm for ^{1}H, δ 77.23 ppm for ^{13}C). IR data was acquired using an ATI Mattson FTIR. HRMS was performed by the University of Illinois SCS Mass Spectrometry Laboratory; mass was referenced to exact mass of the neutral compound (M). UV/Vis data was recorded on a Shimadzu UV-1800 spectrophotometer using UVProbe software. Buffers for the UV/Vis studies were prepared as described in Robinson and Stokes's "Electrolyte solutions" (1970) and the pH was measured immediately prior to use using a Mettler Toledo FE20 with LE409 probe. Sigmoid fitting was performed using Origin logistic function iteratively until chi^2 was minimized.

SYNTHETIC PROCEDURES

Synthesis of Chalcones (1a-1y)

To a 25 mL round-bottomed flask containing a magnetic stirbar was added sequentially 1 mmol of the appropriate acetophenone, 2 mL of ethanol, 1 mmol of the required benzaldehyde, and 2 mL of 6 M aqueous NaOH. The resulting solution was allowed to stir for 24 hours at a constant temperature, after which the solution was acidified at room temperature with aqueous 1 M HCl. The mixture was extracted with dichloromethane (3 x 20 mL) and the combined organic layers were dried over magnesium sulfate. After filtration and concentration, the chalcones were purified via flash column chromatography using a hexane/ethyl ether eluent. Reported yields are from a single, unoptimized run.

Preparation of Buffer Solution for Flavanone (2) Synthesis

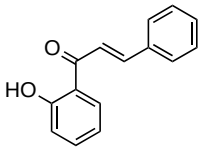
Equal parts of aqueous 0.2 M $NaHCO_3$, 0.2 M Na_2PO_4, and 0.2 M KCl solutions were combined in a large stock bottle. An aqueous solution of 0.2 M NaOH was added to the mixture while stirring to increase the pH of the overall solution to 12.00 as monitored by pH meter.

Synthesis of Flavanones (2a-2y)

To a 250 mL separatory funnel was added 50 mg of the corresponding chalcone dissolved in 100 mL of methanol. The chalcone solution was added dropwise over a period of 10-15 minutes to a 500 mL round-bottomed flask containing a magnetic stirbar and 150 ml of the buffer solution described above, with stirring. 1 M HCl was added in 1 mL portions to the mixture every 5 minutes until the pH was 9.2 ($\approx$ 13 mL total). If precipitate formed in solution before pH 9.2 was reached, an additional 100 mL of methanol was added to redissolve the solid. Methanol was reduced from the solution via rotary evaporator. The remaining solution was extracted with dichloromethane (3 x 50 mL) and the combined organic layers were dried over magnesium sulfate. After filtration and concentration, the flavanones were purified via flash column chromatography using a hexane/ethyl ether eluent. Reported yields are from a single, unoptimized run.

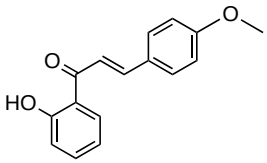
CHARACTERIZATION DATA FOR COMPOUNDS 1a-1y, 2a-2y

(*E*)-1-(2-Hydroxyphenyl)-3-phenylprop-2-en-1-one (1a)



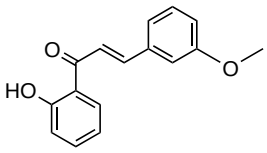
Ambient temperature, 54%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.80 (s, 1H), 7.92 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.92 (d, *J* = 15.5 Hz, 1H), 7.67-7.64 (m, 2H), 7.65 (d, *J* = 15.3 Hz, 1H), 7.49 (ddd, *J* = 8.7, 7.2, 1.6 Hz, 1H), 7.45-7.40 (m, 3H), 7.02 (dd, *J* = 8.5, 1.1 Hz, 1H), 6.94 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.9, 163.8, 145.6, 136.6, 134.8, 131.1, 129.8, 129.2, 128.9, 120.3, 120.2, 119.0, 118.8; IR (neat) 3081, 3027, 1725, 1583, 1574, 1487, 1437, 1363, 1342, 1307, 1268, 1235, 1205, 1161, 1031, 1020, 998, 977, 864, 838, 809, 778, 751, 739, 694, 664 cm^{-1}; HRMS (EI+) *m/z* calculated for $C_{15}H_{12}O_2$ (M) 224.08373, found 224.08289.

(*E*)-1-(2-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1b)



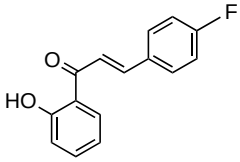
Ambient temperature, 63%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.78 (s, 1H), 7.91 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.87 (d, *J* = 15.5 Hz, 1H), 7.62 (d, *J* = 15.5 Hz, 1H), 7.49 (ddd, *J* = 8.7, 7.1, 1.6 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.17-7.14 (m, 1H), 7.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.98 (dd, *J* = 8.0, 2.6 Hz, 1H), 6.96-6.91 (m, 1H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.9, 163.8, 160.2, 145.6, 136.7, 136.2, 130.3, 129.9, 121.5, 120.7, 120.2, 119.1, 118.9, 116.8, 113.9, 55.6; IR (neat) 3000, 2940, 2835, 1639, 1576, 1486, 1443, 1362, 1351, 1316, 1291, 1273, 1245, 1201, 1158, 1046, 1024, 984, 862, 816, 756, 667 cm-1; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.09430, found 254.09337.

(*E*)-1-(2-Hydroxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1c)



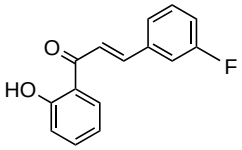
Ambient temperature, 8%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.92 (s, 1H), 7.91 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.89 (d, *J* = 15.4 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.53 (d, *J* = 15.5 Hz, 1H), 7.47 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.01 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.96-6.89 (m, 3H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.9, 163.8, 162.2, 145.6, 136.4, 130.8, 129.8, 127.6, 120.4, 119.0, 118.8, 117.8, 114.8, 55.7; IR (neat) 3006, 2960, 2936, 2839, 2360, 2341, 1683, 1636, 1604, 1579, 1564, 1514, 1487, 1464, 1442, 1424, 1366, 1351, 1321, 1303, 1257, 1236, 1203, 1175, 1157, 1029, 981, 829, 805, 761, 660 cm^{-1}; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.09430, found 254.09475.

(*E*)-1-(2-Hydroxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1d)



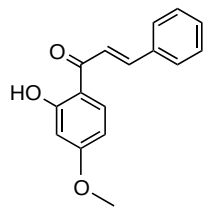
Ambient temperature, 6%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.75 (s, 1H), 7.91-7.89 (m, 1H), 7.87 (d, *J* = 15.7, 1H), 7.67-7.63 (m, 2H), 7.57 (d, *J* = 15.5 Hz, 1H), 7.49 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.13-7.7.10 (m, 2H), 7.02 (dd, *J* = 8.4, 1.1 Hz, 1H), 6.94 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.7, 164.5 (d, J_{CF} = 253.3 H), 163.8, 144.3, 136.6, 131.1 (d, J_{CF} = 3.4 Hz), 130.8 (d, J_{CF} = 8.5 Hz), 129.8, 120.1, 120.0 (d, J_{CF} = 2.4 Hz), 119.1, 118.9, 116.4 (d, J_{CF} = 22.7 Hz); IR (neat) 2955, 2923, 2853, 2361, 2341, 1640, 1598, 1579, 1508, 1492, 1442, 1417, 1369, 1343, 1322, 1299, 1270, 1230, 1206, 1157, 1129, 1026, 983, 913, 868, 828, 813, 761, 752, 713, 662; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 242.0743.

(*E*)-1-(2-Hydroxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1e)



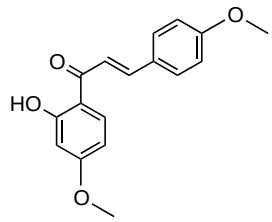
Ambient temperature, 32%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.70 (s, 1H), 7.90 (dd, *J* = 8.1, 2.7 Hz, 1H), 7.86 (d, *J* = 16.5 Hz, 1H), 7.63 (d, *J* = 15.5 Hz, 1H), 7.50 (ddd, *J* = 8.6, 7.2, 1.6 Hz, 1H), 7.43-7.33 (m, 3H), 7.16-7.09 (m, 1H), 7.02 (dd, *J* = 8.4, 1.1 Hz, 1H), 6.94 (ddd, *J* =8.2, 7.2, 1.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.6, 163.8, 163.2 (d, J_{CF} = 248 Hz), 144.1 (d, J_{CF} = 2.66 Hz), 137.0 (d, J_{CF} = 7.5 Hz), 136.8, 130.8 (d, J_{CF} = 8.0 Hz), 129.9, 125.0 (d, J_{CF} = 2.7 Hz), 121.6, 120.1, 119.1, 118.9, 117.9 (d, J_{CF} = 21.5 Hz), 114.8 (d, J_{CF} = 22.1 Hz); IR (neat) 3046, 2924, 2360, 2341, 1965, 1801, 1643, 1611, 1581, 1484, 1439, 1366, 1345, 1319, 1305, 1286, 1235, 1222, 1201, 1148, 1073, 1023, 1001, 969, 944, 900, 859, 846, 819, 800, 788, 749 737, 695, 663, 656; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 272.0742.

(*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-phenylprop-2-en-1-one (1f)



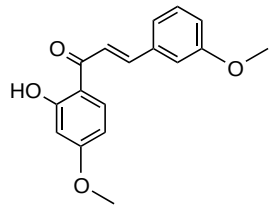
Ambient temperature, 31%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.41 (s, 1H), 7.87 (d, *J* = 15.5 Hz, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.66-7.60 (m, 2H), 7.57 (d, *J* = 15.5 Hz, 1H), 7.45-7.36 (m, 3H), 6.54-6.42 (m, 2H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.1, 166.9, 166.5, 144.6, 135.0, 131.5, 130.9, 129.2, 128.8, 120.6, 114.3, 108.0, 101.3, 55.8; IR (neat) 2961, 2914, 2854, 2369, 1724, 1637, 1573, 1507, 1448, 1359, 1280, 1209, 1154, 1131, 1018, 999, 977, 963, 860, 836, 804, 782, 765, 734, 694, 675 cm^{-1}; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.09430, found 254.09396.

(*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1g)



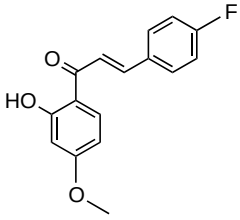
Ambient temperature, 20%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.52 (s, 1H), 7.84 (d, *J* = 15.4, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 15.4 Hz, 1H), 6.93 (d, *J* = 8.7, 2 H), 6.48-6.45 (m, 1H), 6.46 (d, *J* = 8.3 Hz, 1H), 3.843 (s, 3H), 3.838 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.1, 166.9, 166.3, 162.0, 144.5, 131.3, 130.6, 127.7, 118.0, 114.7, 114.4, 107.8, 101.3, 55.8, 55.7; IR (neat) 3726, 3703, 3630, 3600, 3029, 2928, 2842, 2360, 2341, 1627, 1603, 1569, 1509, 1461, 1441, 1422, 1362, 1322, 1310, 1281, 1258, 1214, 1173, 1126, 1019, 980, 958, 888, 832, 813, 797, 752, 720, 678, 669, 656; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1053.

(*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1h)



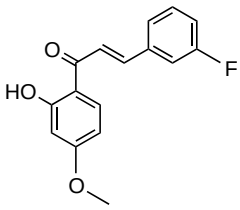
Ambient temperature, 63%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.40 (s, 1H), 7.83 (d, *J* = 15.5 Hz, 1H), 7.83-7.79 (m, 1H), 7.54 (d, *J* = 15.5 Hz, 1H), 7.36-7.30 (m, 1H), 7.25-7.22 (m, 1H), 7.15-7.13 (m, 1H), 6.96 (ddd, *J* = 8.1, 2.5, 1.0 Hz, 1H), 6.50-6.46 (m, 2H), 3.85 (s, 6H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.0, 166.7, 166.5, 160.2, 144.6, 136.4, 131.5, 130.2, 121.4, 120.9, 116.6, 114.3, 113.8, 108.0, 101.3, 55.8, 55.6; IR (neat) 3727, 3702, 3651, 3594, 3051, 3003, 2937, 2912, 2837, 2752, 2694, 2360, 2341, 1634, 1571, 1506, 1492, 1463, 1441, 1358, 1297, 1248, 1215, 1155, 1129, 1091, 1036, 1018, 979, 959, 850, 838, 803, 780, 731, 695, 674; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1049.

(*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1i)



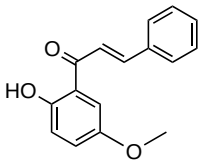
30°C, 15%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.39 (s, 1H), 7.83 (d, *J* = 15.4 Hz, 1H), 7.81-7.78 (m, 1H), 7.65-7.60 (m, 2H), 7.48 (d, *J* = 15.5 Hz, 1H), 7.10 (m, 2H), 6.49-6.45 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.8, 166.9, 166.5, 164.3 (d, J_{CF} = 252.1 Hz), 143.3, 131.4, 131.3 (d, J_{CF} = 3.3 Hz), 130.6 (d, J_{CF} = 14.4 Hz), 120.2 (d, J_{CF} = 2.4 Hz), 116.4 (d, J_{CF} = 21.9 Hz), 114.2, 108.0, 101.3, 55.8; IR (neat) 3728, 3698, 3633, 3593, 3079, 3046, 2980, 2367, 2341, 1639, 1600, 1577, 1506, 1444, 1414, 1365, 1322, 1281, 1220, 1158, 1130, 1098, 1016, 988, 960, 859, 840, 826, 787, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0848.

(*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1j)



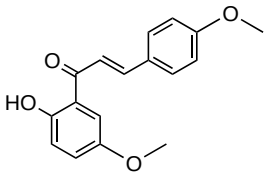
30°C, 55%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.32 (s, 1H), 7.78 (s, 1H), 7.78 (d, *J* = 15.0 Hz), 7.51 (d, *J* = 15.5 Hz), 7.37-7.35 (m, 2H), 7.30-7.29 (m, 1H), 7.10-7.07 (m, 1H), 6.47-6.44 (m, 2H), 3.82 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.6, 167.0, 166.6, 163.2 (d, J_{CF} = 247.0 Hz), 143.0 (d, J_{CF} = 2.7 Hz), 137.2 (d, J_{CF} = 7.6 Hz), 131.4, 130.7 (d, J_{CF} = 8.3 Hz), 124.8 (d, J_{CF} = 2.8 Hz), 121.7, 117.6 (d, J_{CF} = 21.4 Hz), 114.7 (d, J_{CF} = 21.9 Hz), 114.2, 108.1, 101.3, 55.8; IR (neat) 3726, 3703, 3623, 3602, 3059, 2961, 2925, 2846, 2360, 2341, 1641, 1621, 1578, 1509, 1484, 1445, 1415, 1364, 1321, 1295, 1234, 1213, 1181, 1146, 1129, 1094, 1019, 961, 901, 850, 825, 796, 775, 740, 692, 666; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0849.

(*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-phenylprop-2-en-1-one (1k)



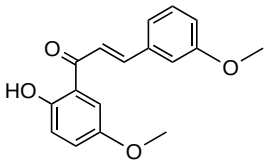
Ambient temperature, 67%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.35 (s, 1H), 7.91 (d, *J* = 15.4 Hz, 1H), 7.69-7.63 (m, 2H), 7.58 (d, *J* = 15.5 Hz, 1H), 7.46-7.41 (m, 2H), 7.35 (d, *J* = 3.2 Hz, 1H), 7.13 (dd, *J* = 9.0, 3.0 Hz, 1H), 6.97 (d, *J* = 9.2 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.6, 158.2, 151.9, 145.8, 134.8, 131.2, 129.3, 128.9, 124.1, 120.4, 119.9, 119.6, 113.1, 56.4; IR (neat) 3080, 3028, 2959, 2835, 2374, 2320, 1720, 1643, 1575, 1486, 1449, 1410, 1355, 1322, 1306, 1286, 1265, 1218, 1174, 1043, 1018, 999, 978, 856, 783, 765, 732, 694, 674 cm^{-1}; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.09430, found 254.09496.

(*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1l)



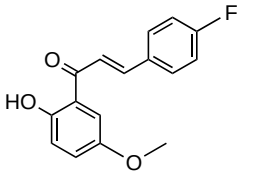
Ambient temperature, 18%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.46 (s, 1H), 7.89 (d, *J* = 15.4 Hz, 1H), 7.61 (m, 2H), 7.46 (d, *J* = 15.4 Hz, 1H), 7.35 (d, *J* = 3.0 Hz, 1H), 7.12 (dd, *J* = 9.1, 3.0 Hz, 1H), 6.97-6.93 (m, 3H), 3.85 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 193.4, 162.2, 158.0, 151.8, 145.7, 130.7, 127.5, 123.7, 119.9, 119.4, 117.7, 114.7, 113.0, 56.3, 55.6; IR (neat) 3001, 2956, 2936, 2836, 2360, 2341, 1640, 1603, 1563, 1511, 1486, 1464, 1442, 1422, 1359, 1322, 1304, 1287, 1254, 1167, 1114, 1022, 981, 934, 827, 806, 783, 770, 750, 734, 683, 670; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1050.

(*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1m)



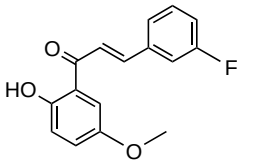
Ambient temperature, 12%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.32 (s, 1H), 7.87 (d, *J* = 15.6 Hz, 1H), 7.55 (d, *J* = 15.5 Hz, 1H), 7.36-7.33 (m, 2H), 7.15 (m, 1H), 7.13 (dd, *J* = 9.1, 3.2 Hz, 1H), 6.98 (dd, *J* = 8.2, 1.0 Hz, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 3.86 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.6, 160.3, 158.2, 152.0, 145.7, 136.2, 130.3, 124.1, 121.5, 120.8, 119.9, 119.6, 116.8, 114.1, 113.3, 56.4, 55.7; IR (neat) 2997, 2936, 2835, 1643, 1577, 1486, 1466, 1413, 1356, 1316, 1271, 1243, 1176, 1044, 1019, 979, 842, 825, 783, 731, 697, 685, 674; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1049.

(*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1n)



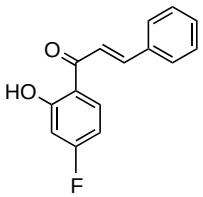
30°C, 46%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.31 (s, 1H), 7.87 (d, *J* = 15.5 Hz, 1H), 7.66-7.63 (m, 2H), 7.50 (d, *J* = 15.5 Hz, 1H), 7.33 (d, *J* = 3.0 Hz, 1H), 7.15-7.10 (m, 3H), 6.97 (d, *J* = 9.1 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.3, 164.5 (d, J_{CF} = 253.3 Hz), 158.1, 151.9, 144.4, 131.0 (d, J_{CF} = 3.4 Hz), 130.8 (d, J_{CF} = 8.6 Hz), 124.1, 120.0 (d, J_{CF} = 1.9 Hz), 119.7, 119.6, 116.4 (d, J_{CF} = 22.24 Hz), 113.1, 56.3; IR (neat) 3009, 2942, 2836, 1644, 1575, 1509, 1486, 1444, 1415, 1356, 1319, 1287, 1265, 1232, 1175, 1158, 1100, 1042, 1017, 980, 934, 829, 785, 772, 740, 685, 671, 656; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0849.

(*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1o)



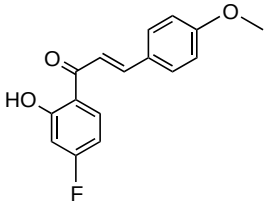
30°C, 12%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.26 (s, 1H), 7.85 (d, *J* = 15.5 Hz, 1H), 7.56 (d, *J* = 15.5 Hz, 1H), 7.42-7.32 (m, 4H), 7.17-7.10 (m, 2H), 6.97 (d, *J* = 9.1 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.3, 163.3 (d, J_{CF} = 247.6 Hz), 158.2, 152.0, 144.2 (d, J_{CF} = 2.6 Hz), 137.0 (d, J_{CF} = 7.5 Hz), 130.8 (d, J_{CF} = 8.3 Hz), 125.0 (d, J_{CF} = 3.0 Hz), 124.4, 121.6, 119.7 (d, J_{CF} = 3.9 Hz), 118.1, 117.9, 114.9 (d, J_{CF} = 21.9 Hz), 113.0, 56.4; IR (neat) 3727, 3695, 3624, 3600, 2360, 2341, 1645, 1582, 1486, 1447, 1414, 1356, 1318, 1272, 1236, 1222, 1180, 1147, 1042, 1019, 1000, 978, 850, 832, 784, 771, 734, 669; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0848.

(*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-phenylprop-2-en-1-one (1p)



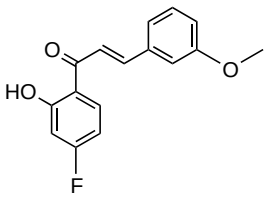
Ambient temperature, 25%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.18 (d, *J* = 1.4 Hz, 1H), 7.93 (dd, *J* = 9.0, 6.3 Hz, 1H), 7.92 (d, *J* = 15.5 Hz, 1H), 7.67-7.64 (m, 2H), 7.56 (d, *J* = 15.5 Hz, 1H), 7.43 (m, 2H), 7.43 (d, *J* = 6.5 Hz, 1H), 6.71-6.62 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.8, 167.7 (d, J_{CF} = 258.7 Hz), 166.4 (d, J_{CF} = 24.0 Hz), 146.0, 134.7, 132.2 (d, J_{CF} = 11.9 H), 131.3, 129.3, 128.7, 120.0, 117.3 (d, J_{CF} = 3.6), 107.4 (d, J_{CF} = 38.0 Hz), 105.4 (d, J_{CF} = 39.0 Hz); IR (neat) 3077, 3026, 2360, 2341, 1638, 1598, 1571, 1508, 1449, 1419, 1370, 1354, 1325, 1302, 1278, 1232, 1208, 1155, 1122, 1081, 1032, 1023, 990, 974, 940, 889, 851, 837, 802, 790, 762, 731, 689, 668, 656; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F$ (M) 241.0665, found 241.0663.

(*E*)-1-(2-Hydroxy-4-Fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1q)



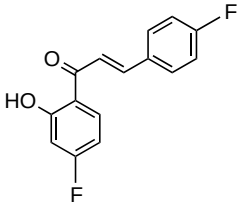
Ambient temperature, 58%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.31 (d, *J* = 1.4 Hz, 1H), 7.91 (dd, *J* = 9.0, 6.4 Hz, 1H), 7.89 (d, *J* = 15.1 Hz, 1H), 7.63-7.60 (m, 2H), 7.43 (d, *J* = 15.4 Hz, 1H), 6.95-6.93 (m, 2H), 6.70-6.60 (m, 2H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.7, 167.5 (d, J_{CF} = 256.9 Hz), 166.4 (d, J_{CF} = 14.23 Hz), 162.4, 145.8, 132.0 (d, J_{CF} = 11.8 Hz), 130.8, 127.4, 117.5, 117.4 (d, J_{CF} = 2.1 Hz), 114.8, 107.2 (d, J_{CF} = 22.8 Hz), 105.3 (d, J_{CF} = 23.5 Hz), 55.7; IR (neat) 2360, 2341, 1638, 1605, 1560, 1514, 1417, 1374, 1355, 1283, 1263, 1234, 1215, 1178, 1125, 1034, 986, 973, 844, 805, 772, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0851.

(*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1r)



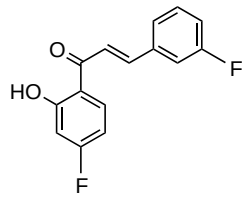
Ambient temperature, 47%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.17 (d, *J* = 1.5 Hz, 1H), 7.91 (dd, *J* = 8.9, 6.4 Hz, 1H), 7.87 (d, *J* = 15.4 Hz, 1H), 7.53 (d, *J* = 15.4 Hz, 1H), 7.37-7.32 (m, 1H), 7.25-7.23 (m, 1H), 7.15-7.14 (m, 1H), 6.98 (ddd, *J* = 8.0, 2.6, 1.0 Hz, 1H), 6.66 (ddd, *J* = 18.9, 10.4, 2.6 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.7, 167.7 (d, J_{CF} = 257.6 Hz), 166.4 (d, J_{CF} = 14.4 Hz), 160.2, 145.9, 136.0, 132.2 (d, J_{CF} = 11.9 Hz), 130.3, 129.2 (d, J_{CF} = 40.2 Hz), 121.5, 120.4, 116.9, 114.0, 107.3 (d, J_{CF} = 22.8 Hz), 105.4 (d, J_{CF} = 23.6 Hz), 55.6; IR (neat) 3739, 3704, 3625, 2978, 2927, 2843, 2360, 2341, 1642, 1603, 1574, 1511, 1495, 1437, 1416, 1374, 1352, 1301, 1264, 1235, 1207, 1160, 1125, 1052, 1030, 979, 851, 836, 807, 773, 745, 737, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0848.

(*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1s)



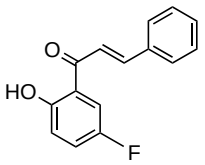
30°C, 41%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.15 (d, *J* = 1.5 Hz, 1H), 7.91 (dd, *J* = 9.0, 6.4 Hz, 1H), 7.87 (d, *J* = 15.8 Hz, 1H), 7.66-7.63 (m, 2H), 7.48 (d, 15.4 Hz, 1H), 7.12 (m, 2H), 6.69 (dd, *J* = 10.3, 2.5 Hz, 1H), 6.66-6.63 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.5, 167.1 (d, J_{CF} = 239.5 Hz), 166.4 (d, J_{CF} = 8.7 Hz), 165.1 (d, J_{CF} = 236.8 Hz), 144.6, 132.1 (d, J_{CF} = 11.8 Hz), 130.9 (d, J_{CF} = 3.4 Hz), 130.9 (d, J_{CF} = 8.7 Hz), 119.8 (d, J_{CF} = 1.9 Hz), 117.2 (d, J_{CF} = 1.9 Hz), 116.5 (d, J_{CF} = 13.2 Hz), 107.37 (d, J_{CF} = 22.9 Hz), 105.41 (d, J_{CF} = 23.6 Hz); IR (neat) 3083, 2980, 2927, 2360, 2341, 1885, 1639, 1595, 1567, 1508, 1415, 1373, 1354, 1322, 1300, 1278, 1229, 1212, 1156, 1121, 1096, 1027, 973, 934, 831, 798, 743, 669; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0649.

(*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1t)



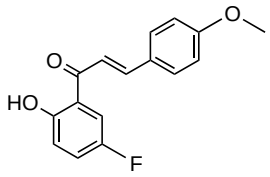
30°C, 18%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.08 (d, *J* = 1.4 Hz, 1H), 7.91 (dd, *J* = 9.0, 6.4 Hz, 1H), 7.86 (d, *J* = 15.5 Hz, 1H), 7.54 (d, *J* = 15.5 Hz, 1H), 7.42-7.38 (m, 2H), 7.37-7.32 (m, 1H), 7.18-7.10 (m, 1H), 6.72-6.63 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.5, 167.8 (d, J_{CF} = 257.8 Hz), 166.5 (d, J_{CF} = 14.5 Hz), 163.3 (d, J_{CF} = 248.0 Hz), 144.4 (d, J_{CF} = 2.6 Hz),136.9 (d, J_{CF} = 7.8 Hz), 132.2 (d, J_{CF} = 12.0 Hz), 130.9 (d, J_{CF} = 8.2 Hz), 125.0 (d, J_{CF} = 2.7 Hz), 121.4, 118.1 (d, J_{CF} = 21.6 Hz), 117.2, (d, J_{CF} = 1.7 Hz), 114.9 (d, J_{CF} = 22.0 Hz), 107.5 (d, J_{CF} = 22.8 Hz), 105.5 (d, J_{CF} = 23.6 Hz); IR (neat) 2980, 2928, 2894, 2360, 2340, 1643, 1605, 1580, 1507, 1484, 1452, 1420, 1369, 1356, 1321, 1297, 1273, 1239, 1204, 1153, 1125, 1030, 1002, 973, 851, 813, 798, 783, 736, 689, 662; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0649.

(*E*)-1-(2-Hydroxy-5-flurorphenyl)-3-phenylprop-2-en-1-one (1u)



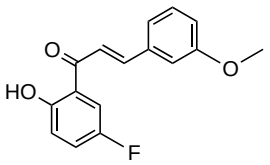
Ambient temperature, 16%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.52 (s, 1H), 7.93 (d, *J* = 15.5 Hz, 1H), 7.67-7.65 (m, 2H), 7.57 (dd, *J* = 9.1, 3.1 Hz, 1H), 7.53 (d, *J* = 15.5 Hz, 1H), 7.45-7.42 (m, 3H), 7.23 (ddd, *J* = 16.8, 9.1, 6.8 Hz, 1H), 6.98 (dd, *J* = 9.2, 4.6 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.1 (d, J_{CF} = 2.6 Hz), 160.0, 155.1 (d, J_{CF} = 238.6 Hz), 146.6, 134.6, 131.4, 129.3, 129.0, 124.1 (d, J_{CF} = 23.6 Hz), 120.1 (d, J_{CF} = 7.3 Hz), 119.8, 119.7 (d, J_{CF} = 6.4 Hz), 114.8 (d, J_{CF} = 23.5 Hz); IR (neat) 3061, 3031, 2918, 2850, 2366, 1965, 1643, 1573, 1507, 1480, 1449, 1420, 1347, 1308, 1259, 1247, 1198, 1166, 1114, 1071, 1020, 995, 979, 943, 857, 828, 787, 770, 732, 692, 680; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 242.0742.

(*E*)-1-(2-Hydroxy-5-Fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1v)



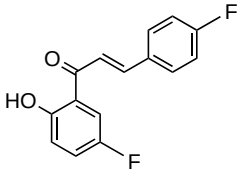
Ambient temperature, 56%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.63 (s, 1H), 7.91 (d, 15.4 Hz, 1H), 7.64-7.61 (m, 2H), 7.56 (dd, *J* = 9.2, 3.0 Hz, 2H), 7.41 (d, *J* = 15.3 Hz, 1H), 6.99-6.93 (m, 3H), 3.86 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 193.0 (d, J_{CF} = 2.7 Hz), 162.5, 159.9 (d, J_{CF} = 1.0 Hz), 155.0 (d, J_{CF} = 239.6 Hz), 146.5, 130.9, 127.3, 123.8 (d, J_{CF} = 23.6 Hz), 120.0 (d, J_{CF} = 7.3 Hz), 119.8 (d, J_{CF} = 6.15 Hz), 117.2, 114.78, 114.5, 55.7; IR (neat) 3071, 2842, 2360, 2340, 1642, 1606, 1569, 1535, 1486, 1440, 1420, 1353, 1312, 1303, 1276, 1260, 1241, 1203, 1187, 1167, 1113, 1025, 988, 944, 873, 851, 821, 806, 782, 751, 735, 716, 676; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0849.

(*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1w)



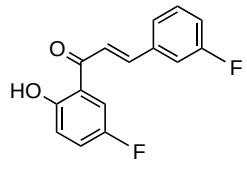
Ambient temperature, 3%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.50 (s, 1H), 7.89 (d, *J* = 15.4 Hz, 1H), 7.56 (dd, *J* = 9.1, 3.1 Hz, 1H), 7.50 (d, *J* = 15.4 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 7.26-7.21 (m, 2H), 7.16 (m, 1H), 7.00-6.97 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 193.1 (d, J_{CF} = 2.7 Hz), 160.1 (d, J_{CF} = 35.3 Hz), 155.1 (d, J_{CF} = 238.4 Hz), 146.5, 135.9, 130.3, 124.2 (d, J_{CF} = 23.6 Hz), 121.7, 120.1, 120.1, 119.7 (d, J_{CF} = 6.0 Hz), 117.2, 114.9, 114.7, 114.0, 55.6; IR (neat) 2838, 2361, 1646, 1579, 1485, 1453, 1438, 1422, 1351, 1316, 1293, 1272, 1245, 1229, 1203, 1174, 1051, 1023, 979, 924, 849, 825, 801, 783, 743, 733, 693, 677; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0851.

(*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1x)



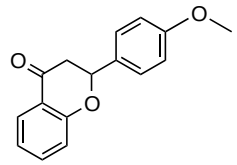
30°C, 19%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.47 (s, 1H), 7.89 (d, *J* = 15.5 Hz, 1H), 7.67-7.65 (m, 2H), 7.55 (dd, *J* = 9.1, 3.0 Hz, 1H), 7.45 (d, *J* = 15.4 Hz, 1H), 7.13 (m, 2H), 6.99 (dd, *J* = 9.2, 4.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.8 (d, J_{CF} = 2.7 Hz), 164.7 (d, J_{CF} = 253.4 Hz), 160.0, 155.0 (d, J_{CF} = 238.7 Hz), 145.2, 131.0 (d, J_{CF} = 8.5 Hz), 130.8 (d, J_{CF} = 3.5 Hz), 124.4 (d, J_{CF} = 23.6 Hz), 120.1 (d, J_{CF} = 7.3 Hz), 119.6 (d, J_{CF} = 6.0 Hz), 119.5 (d, J_{CF} = 2.4 Hz), 116.5 (d, J_{CF} = 22.3 Hz), 114.7 (d, J_{CF} = 23.4 Hz), IR (neat) 2980, 2877, 2360, 2341, 1646, 1583, 1550, 1511, 1485, 1423, 1356, 1323, 1303, 1270, 1249, 1232, 1206, 1170, 1023, 979, 945, 830, 784, 744, 669; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0647.

(*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1y)



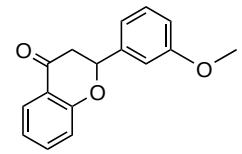
30°C, 56%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.42 (s, 1H), 7.87 (d, *J* = 15.4 Hz, 1H), 7.55 (dd, *J* = 9.1, 3.1 Hz, 1H), 7.51 (d, *J* = 15.3 Hz, 1H), 7.43-7.34 (m, 3H), 7.17-7.11 (m, 1H), 6.99 (dd, *J* = 9.1, 4.6 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.8 (d, J_{CF} = 2.7 Hz), 163.3 (d, J_{CF} = 249.1 Hz), 160.0 (d, J_{CF} = 1.5 Hz), 155.1 (d, J_{CF} = 240.2 Hz), 145.0 (d, J_{CF} = 2.7 Hz), 136.8 (d, J_{CF} = 7.7 Hz), 130.9 (d, J_{CF} = 8.3 Hz), 125.0 (d, J_{CF} = 3.0 Hz), 124.4 (d, J_{CF} = 23.8 Hz), 121.0, 120.2 (d, J_{CF} = 7.3 Hz), 119.5 (d, J_{CF} = 6.2 Hz), 118.3 (d, J_{CF} = 21.5 Hz), 115.0 (d, J_{CF} = 21.7 Hz), 114.7 (d, J_{CF} = 23.2 Hz);IR (neat) 2980, 2891, 2360, 2341, 1649, 1592, 1490, 1451, 1424, 1358, 1321, 1285, 1242, 1225, 1201, 1177, 1161, 1025, 1001, 976, 938, 847, 824, 785, 738, 691, 678, 668; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0648.

2-(4-Methoxyphenyl)chroman-4-one (2b)



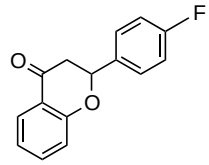
18%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.51-7.46 (m, 1H), 7.42-7.37 (m, 2H), 7.06-7.00 (m, 2H), 6.97-6.92 (m, 2H), 5.42 (dd, *J* = 13.3, 2.9 Hz, 1H), 3.82 (s, 3H), 3.10 (dd, *J* = 16.8, 13.3 Hz, 2H), 2.85 (dd, *J* = 16.9, 2.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.4, 161.8, 160.2, 136.3, 131.0, 127.9, 127.2, 121.7, 121.1, 118.3, 114.4, 79.5, 55.5, 44.6; IR (neat) 3726, 3632, 3362, 3063, 2999, 2959, 2930, 2854, 2360, 2341, 1688, 1603, 1576, 1514, 1462, 1426, 1400, 1371, 1301, 1249, 1224, 1177, 1148, 1114, 1066, 1027, 984, 956, 936, 905, 861, 845, 824, 763, 718, 668, 656; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.0943, found 254.0947.

2-(3-Methoxyphenyl)chroman-4-one (2c)



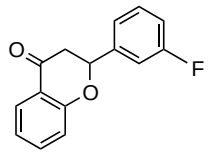
53%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.51-7.48 (m, 1H), 7.33 (t, *J* = 8.2 Hz, 1H), 7.06-7.02 (m, 4H), 6.92-6.89 (m, 1H), 5.44 (dd, *J* = 13.4, 2.9 Hz, 1H), 3.83 (s, 3H), 3.06 (dd, *J* = 16.9, 13.4 Hz, 1H), 2.88 (dd, *J* = 16.9, 3.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.2, 161.7, 160.2, 140.5, 136.4, 130.2, 127.3, 121.9, 121.1, 118.5, 118.4, 114.3, 112.1, 79.7, 55.5, 44.9; IR (neat) 3062, 2999, 2961, 2938, 2836, 2360, 2341, 1688, 1640, 1605, 1588, 1489, 1462, 1437, 1400, 1362, 1341, 1303, 1267, 1224, 1199, 1180, 1151, 1115, 1067, 1046, 1028, 993, 949, 930, 881, 847, 763, 738, 720, 696, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.09430, found 254.09386.

2-(4-Fluorophenyl)chroman-4-one (2d)



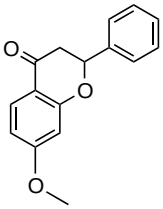
>99%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.53-7.43 (m, 3H), 7.14-7.02 (m, 4H), 5.45 (dd, *J* = 13.2, 3.0 Hz, 1H), 3.05 (dd, *J* = 16.9, 13.2 Hz, 1H), 2.86 (dd, *J* = 16.8, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.9, 163.0 (d, J_{CF} = 249.4 Hz), 161.6, 136.5, 134.8 (d, J_{CF} = 3.2 Hz), 128.2 (d, J_{CF} = 8.3 Hz), 127.3, 122.0, 121.1, 118.3, 116.0 (d, J_{CF} = 21.6 Hz), 79.1, 44.9; IR (neat) 3073, 2980, 2899, 2360, 2341, 1687, 1604, 1577, 1511, 1463, 1422, 1401, 1367, 1304, 1225, 1158, 1150, 1115, 1068, 1028, 1016, 990, 957, 908, 863, 850, 830, 797, 764, 720, 668, 656; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 242.0744.

2-(3-Fluorophenyl)chroman-4-one (2e)



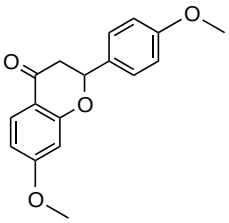
73%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.51 (ddd, *J* = 8.6, 7.2, 1.8 Hz, 1H), 7.42-7.35 (m, 1H), 7.23-7.20 (m, 2H), 7.09-7.02 (m, 3H), 5.47 (dd, *J* = 12.9, 3.3 Hz, 1H), 3.02 (dd, *J* = 16.9, 12.9 Hz, 1H), 2.88 (dd, *J* = 16.9, 3.3 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.6, 163.2 (d, J_{CF} = 248.7 Hz), 161.4, 141.5 (d, J_{CF} = 7.4 Hz), 136.5, 130.7 (d, J_{CF} = 8.3 Hz), 127.3, 122.0, 121.8 (d, J_{CF} = 3.1 Hz), 121.1, 118.3, 115.8 (d, J_{CF} = 21.3 Hz), 113.4 (d, J_{CF} = 22.8 Hz), 78.9(d, J_{CF} = 1.7 Hz), 44.8; IR (neat) 3368, 3067, 3040, 2970, 2906, 2360, 2341, 1939, 1689, 1606, 1578, 1487, 1463, 1451, 1400, 1364, 1303, 1275, 1260, 1223, 1186, 1147, 1114, 1066, 1028, 993, 970, 946, 886, 849, 784, 763, 739, 720, 692, 668; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 242.0742.

7-Methoxy-2-phenylchroman-4-one (2f)



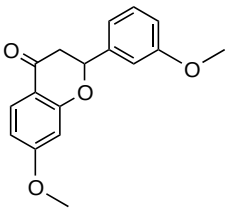
71%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.8 Hz, 1H), 7.47-7.35 (m, 5H), 6.60 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.49 (d, *J* = 2.4 Hz, 1H), 5.46 (dd, *J* = 13.3, 2.9 Hz, 1H), 3.82 (s, 3H), 3.03 (dd, *J* = 16.9, 13.3 Hz, 1H), 2.82 (dd, *J* = 16.9, 3.0 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.8, 166.4, 163.7, 139.0, 129.1, 129.0, 126.4, 115.0, 110.5, 101.1, 80.2, 55.9, 44.6; IR (neat) 3750, 3725, 3628, 3566, 3031, 2967, 2874, 2840, 2360, 2341, 1682, 1653, 1606, 1573, 1541, 1520, 1497, 1456, 1442, 1397, 1363, 1336, 1315, 1295, 1275, 1258, 1216, 1199, 1159, 1131, 1115, 1060, 1023, 999, 954, 884, 862, 838, 815, 768, 747, 699, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.0943, found 254.0937.

7-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2g)



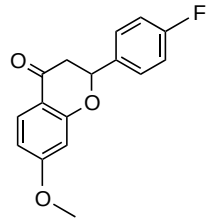
41%**;** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.9 Hz, 1H), 7.40-7.37 (m, 2H), 6.95-6.23 (m, 2H), 6.59 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 5.40 (dd, *J* = 13.3, 2.8 Hz, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.04 (dd, *J* = 16.9, 13.3 Hz, 1H), 2.78 (dd, *J* = 16.9, 2.9 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.9, 166.2, 163.7, 160.0, 130.9, 128.8, 127.8, 114.9, 114.2, 110.2, 101.0, 79.8, 55.7, 55.4, 44.1; IR (neat) 2837, 2360, 2341, 2250, 1677, 1603, 1573, 1514, 1497, 1442, 1368, 1354, 1333, 1306, 1274, 1251, 1198, 1176, 1156, 1131, 1112, 1060, 1025, 992, 953, 909, 884, 830, 813, 727, 668; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1044.

7-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2h)



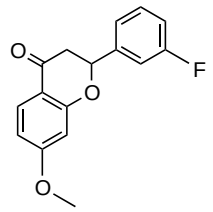
26%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 1H), 7.36-7.30 (m, 1H), 7.03-7.01 (m, 2H), 6.92-6.88 (m, 1H), 6.60 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.49 (d, *J* = 2.4 Hz), 5.42 (dd, *J* = 13.2, 3.0 Hz, 1H), 3.82 (s, 3H), 3.82 (s, 3H), 3.01 (dd, *J* = 16.9, 13.1 Hz, 1H), 2.81 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.8, 166.4, 163.7, 160.1, 140.6, 130.2, 129.0, 118.5, 115.0, 114.3, 112.1, 110.5, 101.1, 80.1, 55.9, 55.5, 44.6; IR (neat) 3003, 2962, 2944, 2838, 2360, 2341, 1681, 1606, 1574, 1490, 1441, 1361, 1335, 1293, 1256, 1203, 1158, 1131, 1114, 1046, 1023, 996, 956, 838, 809, 784, 740, 728, 694, 669, 656; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1042.

2-(4-Fluorophenyl)-7-methoxychroman-4-one (2i)



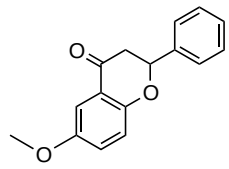
42%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 1H), 7.46-7.42 (m, 2H), 7.13-7.07 (m, 2H), 6.61 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 5.43 (dd, *J* = 13.1, 3.0 Hz, 1H), 3.82 (s, 3H), 2.99 (dd, *J* = 16.9, 13.1 Hz, 1H), 2.79 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.5, 166.4, 163.6, 163.0 (d, J_{CF} = 249.4 Hz), 134.9 (d, J_{CF} = 3.3 Hz), 129.0, 128.3 (d, J_{CF} = 8.3 Hz), 116.0 (d, J_{CF} = 21.6 Hz), 115.0, 110.6, 101.1, 79.5, 55.9, 44.5; IR (neat) 2971, 2948, 2898, 2842, 2359, 2341, 1681, 1608, 1575, 1542, 1512, 1445, 1420, 1362, 1336, 1301, 1275, 1258, 1227, 1199, 1157, 1133, 1116, 1061, 1023, 998, 954, 887, 836, 744, 731, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0846.

2-(3-Fluorophenyl)-7-methoxychroman-4-one (2j)



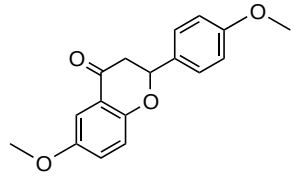
88%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 1H), 7.40-7.35 (m, 1H), 7.21-7.20 (m, 2H), 7.01-7.03 (m, 1H), 6.61 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.49 (d, *J* = 2.4 Hz, 1H), 5.45 (dd, *J* = 13.1, 3.0 Hz, 1H), 3.82 (s, 3H), 2.96 (dd, *J* = 16.8, 13.1 Hz, 1H), 2.82 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.2, 166.5, 163.4, 163.2 (d, J_{CF} = 247.5 Hz), 141.5 (d, J_{CF} = 7.3 Hz), 130.7 (d, J_{CF} = 8.2 Hz), 129.0, 121.8 (d, J_{CF} = 2.8 Hz), 115.8 (d, J_{CF} = 21.3 Hz), 115.0, 113.4 (d, J_{CF} = 22.7 Hz), 110.6, 101.1, 79.3 (d, J_{CF} = 1.5 Hz), 55.9, 44.5; IR (neat) 3065, 2967, 2945, 2842, 2360, 2341, 1681, 1605, 1574, 1489, 1441, 1354, 1336, 1294, 1275, 1257, 1202, 1159, 1129, 1114, 1061, 1023, 1002, 973, 949, 865, 838, 820, 786, 742, 728, 689, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0848.

6-Methoxy-2-phenylchroman-4-one (2k)



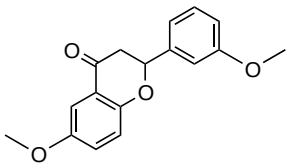
98%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49-7.34 (m, 6H), 7.11 (dd, *J* = 9.0, 3.2 Hz, 1H), 6.98 (d, *J* = 9.0 Hz, 1H), 5.43 (dd, *J* = 13.3, 3.0 Hz, 1H), 3.81 (s, 3H), 3.06 (dd, *J* = 17.0, 13.3 Hz, 1H), 2.86 (dd, *J* = 17.0, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.3, 156.5, 154.4, 139.0, 129.0, 128.9, 126.3, 125.6, 121.0, 119.6, 107.5, 79.9, 56.0, 44.8; IR (neat) 3734, 3648, 3009, 2959, 2937, 2905, 2834, 2360, 2341, 1673, 1616, 1584, 1558, 1541, 1484, 1460, 1432, 1400, 1383, 1350, 1320, 1284, 1226, 1211, 1168, 1123, 1063, 1034, 992, 948, 929, 911, 895, 864, 824, 792, 770, 712, 698, 669, 656; HRMS (EI+) *m/z* calculated for $C_{16}H_{14}O_3$ (M) 254.0943, found 254.0942.

6-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2l)



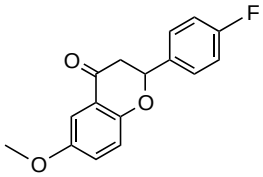
55%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.38 (m, 2H), 7.33 (d, *J* = 3.2 Hz, 1H), 7.10 (dd, *J* = 9.0, 3.2 Hz, 1H), 6.97-6.92 (m, 3H), 5.37 (dd, *J* = 13.4, 2.9 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.07 (dd, *J* = 16.9, 13.4 Hz, 1H), 2.83 (16.9, 2.9 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.5, 160.2, 156.6, 154.4, 131.1, 127.9, 125.6, 120.9, 119.7, 114.4, 107.5, 79.7, 56.0, 55.6, 44.6; IR (neat) 3735, 3648, 2959, 2937, 2705, 2836, 2360, 2341, 1686, 1653, 1615, 1586, 1558, 1541, 1515, 1486, 1464, 1431, 1397, 1373, 1341, 1307, 1281, 1249, 1221, 1206, 1178, 1120, 1061, 1032, 992, 911, 895, 866, 830, 761, 721, 699, 668; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.10486, found 284.10531

6-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2m)



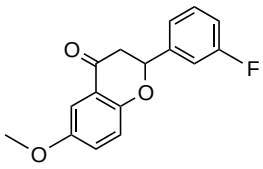
62%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.30 (m, 2H), 7.11 (dd, *J* = 9.0, 3.2 Hz, 1H), 7.04-7.02 (m, 2H), 6.98 (d, *J* = 9.0 Hz, 1H), 6.90 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H), 5.40 (dd, *J* = 13.2, 3.0 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.04 (dd, *J* = 17.0, 13.2 Hz, 1H), 2.86 (dd, *J* = 17.0, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.2, 160.2, 156.4, 154.5, 140.6, 130.2, 125.6, 121.0, 119.7, 118.5, 114.3, 112.1, 107.5, 79.8, 56.0, 55.5, 44.9; IR (neat) 3001, 2956, 2939, 2836, 2360, 2341, 1686, 1614, 1586, 1486, 1465, 1431, 1362, 1341, 1280, 1212, 1172, 1121, 1061, 1034, 996, 949, 931, 864, 830, 784, 754, 707, 694, 669; HRMS (EI+) *m/z* calculated for $C_{17}H_{16}O_4$ (M) 284.1049, found 284.1051.

2-(4-Fluorophenyl)-6-methoxychroman-4-one (2n)



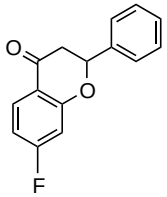
99%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.42 (m, 2H), 7.33 (d, *J* = 3.2 Hz, 1H), 7.13-7.07 (m, 3H), 6.96 (d, *J* = 9.0 Hz, 1H), 5.40 (dd, *J* = 13.3, 3.1 Hz, 1H), 3.80 (s, 3H), 3.02 (dd, *J* = 16.9, 13.2 Hz, 1H), 2.84 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 192.1, 163.0 (d, J_{CF} = 249.2 Hz), 156.3, 154.5, 134.9 (d, J_{CF} = 3.2 Hz), 128.2 (d, J_{CF} = 8.3 Hz), 125.7, 120.9, 119.6, 116.0 (d, J_{CF} = 21.6 Hz), 107.6, 79.2, 56.0, 44.8; IR (neat) 3002, 2940, 2905, 2836, 2360, 2341, 1686, 1647, 1609, 1559, 1511, 1485, 1430, 1366, 1341, 1279, 1223, 1204, 1160, 1121, 1099, 1063, 1033, 996, 940, 912, 896, 864, 832, 769, 729, 700, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0850.

2-(3-Fluorophenyl)-6-methoxychroman-4-one (2o)



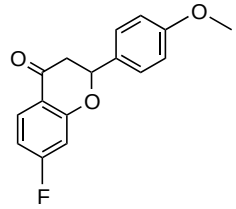
81%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.35 (m, 1H), 7.33 (d, *J* = 3.2 Hz, 1H), 7.22-7.20 (m, 2H), 7.11 (dd, *J* = 9.0, 3.2 Hz, 1H), 7.07-7.03 (m, 1H), 6.98 (d, *J* = 9.0 Hz, 1H), 5.42 (dd, *J* = 13.2, 3.0 Hz, 1H), 3.80 (s, 3H), 2.99 (dd, *J* = 17.0, 13.2 Hz, 1H), 2.87 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.7, 163.2 (d, J_{CF} = 247.4 Hz), 156.1, 154.6, 141.6 (d, J_{CF} = 7.2 Hz), 130.6 (d, J_{CF} = 8.3 Hz), 125.7, 121.8 (d, J_{CF} = 3.2 Hz), 121.0, 119.6, 115.7 (d, J_{CF} = 21.4 Hz), 113.4 (d, J_{CF} = 22.6 Hz), 107.6, 79.1, 56.0, 44.8; IR (neat) 2999, 2963, 2904, 2836, 2360, 2341, 1686, 1653, 1617, 1592, 1559, 1541, 1486, 1450, 1431, 1399, 1363, 1341, 1280, 1261, 1210, 1172, 1142, 1121, 1082, 1062, 1033, 1001, 971, 946, 867, 834, 786, 760, 707, 690, 669; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0847.

7-Fluoro-2-phenylchroman-4-one (2p)



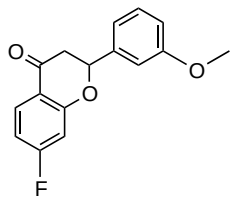
53%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.8, 6.6 Hz, 1H), 7.47-7.36 (m, 5H), 6.78-6.72 (m, 2H), 5.49 (dd, *J* = 13.2, 2.9 Hz, 1H), 3.06 (dd, *J* = 16.9, 13.2 Hz, 1H), 2.88 (dd, *J* = 17.0, 3.0 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.7, 167.8 (d, J_{CF} = 258.2 Hz), 163.4 (d, J_{CF} = 13.6 Hz), 138.5, 129.8 (d, J_{CF} = 11.4 hz), 129.2, 129.1, 126.3, 118.1 (d, J_{CF} = 2.5 Hz), 110.3 (d, J_{CF} = 22.7 Hz), 105.1 (d, J_{CF} = 24.4 Hz), 80.4, 44.5; IR (neat) 3726, 3628, 3567, 3368, 3066, 3036, 2903, 2360, 2341, 1689, 1609, 1584, 1486, 1439, 1403, 1368, 1333, 1315, 1282, 1252, 1221, 1176, 1139, 1106, 1061, 1031, 998, 963, 917, 886, 850, 812, 764, 749, 726, 698, 670; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.07431, found 242.07394.

7-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2q)



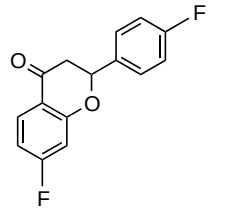
44%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.7, 6.6 Hz, 1H), 7.39-7.35 (m, 2H), 6.97-6.92 (m, 2H), 6.78-6.68 (m, 2H), 5.43 (dd, *J* = 13.1, 2.9 Hz, 1H), 3.82 (s, 3H), 3.08 (dd, *J* = 16.9, 13.1 Hz, 1H), 2.84 (dd, *J* = 16.9, 3.0 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.0, 167.8 (d, J_{CF} = 258.1 Hz), 163.5 (d, J_{CF} = 13.8 Hz), 160.3, 130.5, 129.8 (d, J_{CF} = 11.4 Hz), 128.0, 118.1 (d, J_{CF} = 2.5 Hz), 114.5, 110.2 (d, J_{CF} = 22.9 Hz), 105.1 (d, J_{CF} = 24.6 Hz), 80.2, 55.6, 44.3; IR (neat) 3076, 3003, 2960, 2935, 2908, 2838, 2360, 2341, 1690, 1613, 1586, 1515, 1442, 1371, 1335, 1307, 1283, 1253, 1222, 1179, 1139, 1108, 1063, 1032, 995, 966, 886, 852, 831, 813, 792, 730, 655; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0847.

7-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2r)



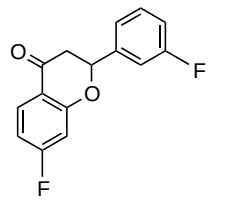
83%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.8, 6.7 Hz, 1H), 7.35-7.32 (m, 1H), 6.92-6.90 (m, 1H), 6.75 (ddd, *J* = 17.3, 8.3, 2.4 Hz, 2H), 5.45 (dd, *J* = 13.2, 2.9 Hz, 1H), 3.82 (s, 3H), 3.04 (dd, *J* = 17.0, 13.2 Hz, 1H), 2.87 (dd, *J* = 17.0, 3.0 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.7, 167.8 (d, J_{CF} = 258.2 Hz), 163.3 (d, J_{CF} = 13.7 Hz), 160.2, 140.0, 130.2, 129.8 (d, J_{CF} = 11.4 Hz), 118.5, 118.1 (d, J_{CF} = 2.4 Hz), 114.4, 112.1, 110.3 (d, J_{CF} = 22.8 Hz), 105.2 (d, J_{CF} = 24.6 Hz), 80.3, 55.5, 44.5; IR (neat) 3070, 3002, 2986, 2837, 2360, 2341, 1689, 1609, 1585, 1489, 1438, 1360, 1336, 1283, 1233, 1221, 1198, 1183, 1139, 1107, 1062, 1042, 997, 965, 927, 851, 815, 781 743, 727, 703, 691, 669; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0849.

7-Fluoro-2-(4-fluorophenyl)chroman-4-one (2s)



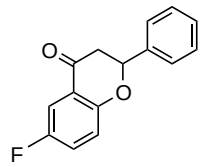
23%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.8, 6.6 Hz, 1H), 7.45-7.42 (m, 2H), 7.13-7.10 (m, 2H), 6.77 (dt, *J* = 8.4, 2.4 Hz, 1H), 6.72 (dd, *J* = 9.7, 2.4 Hz, 1H), 5.47 (dd, *J* = 13.2, 2.9 Hz, 1H), 3.03 (dd, *J* = 16.9, 13.2 Hz, 1H), 2.86 (dd, *J* = 16.9, 3.0 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.4, 164.6 (d, J_{CF} = 226.6 Hz), 163.3, 163.1 (d, J_{CF} = 249.8 Hz), 134.3 (d, J_{CF} = 3.2 Hz), 129.8 (d, J_{CF} = 11.3 Hz), 128.3 (d, J_{CF} = 8.4 Hz), 118.0 (d, J_{CF} = 2.4 Hz), 116.1 (d, J_{CF} = 21.7 Hz), 110.4 (d, J_{CF} = 22.7 Hz), 105.1 (d, J_{CF} = 24.5 Hz), 79.7, 44.5; IR (neat) 3098, 3068, 2980, 2906, 2360, 2342, 1909, 1679, 1620, 1607, 1584, 1511, 1481, 1448, 1428, 1401, 1372, 1341, 1304, 1289, 1251, 1221, 1183, 1161, 1144, 1112, 1066, 1018, 999, 965, 956, 888, 864, 834, 812, 748, 729, 681, 656; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0646.

7-Fluoro-2-(3-fluorophenyl)chroman-4-one (2t)



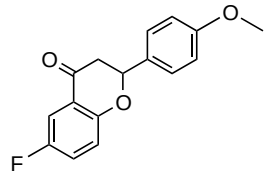
50%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.8, 6.6 Hz, 1H), 7.41-7.37 (dt, *J* = 8.1, 6.0 Hz, 1H), 7.21-7.18 (m, 2H), 7.07 (ddd, *J* = 8.5, 2.5, 1.0 Hz, 1H), 6.79-6.73 (m, 2H), 5.49 (dd, *J* = 13.0, 3.1 Hz, 1H), 3.01 (dd, *J* = 16.9, 13.0 Hz, 1H), 2.88 (dd, *J* = 16.9, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 190.2, 167.8 (d, J_{CF} = 258.6 Hz), 163.2 (d, J_{CF} = 248.9 Hz), 163.1 (d, J_{CF} = 13.7 Hz), 141.0 (d, J_{CF} = 7.3 Hz), 130.8 (d, J_{CF} = 8.2 Hz), 129.9 (d, J_{CF} = 11.6 Hz), 121.8 (d, J_{CF} = 3.2 Hz), 118.1 (d, J_{CF} = 1.8 Hz), 116.0 (d, J_{CF} = 21.0 Hz), 113.4 (d, J_{CF} = 22.8 Hz), 110.5 (d, J_{CF} = 22.8 Hz), 105.2 (d, J_{CF} = 24.7 Hz), 79.5, 44.5; IR (neat) 3073.46, 2958.92, 2924.50, 2854.86, 2359.99, 2340.79, 1690.47, 1609.31, 1585.78, 1487.40, 1439.33, 1360.74, 1337.29, 1284.40, 1252.42, 1224.80, 1187.08, 1139.04, 1107.80, 1063.48, 1025.44, 1001.60, 956.89, 854.59, 820.76, 803.11, 785.44, 744.10, 727.51, 702.42, 686.78, 668.36; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.06489, found 260.06521.

6-Fluoro-2-phenylchroman-4-one (2u)



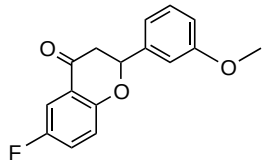
66%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.2, 3.2 Hz, 1H), 7.47-7.36 (m, 5H), 7.24-7.20 (m, 1H), 7.02 (dd, *J* = 9.1, 4.2 Hz, 1H), 5.45 (dd, *J* = 13.4, 2.9 Hz, 1H), 3.06 (dd, *J* = 17.0, 13.4 Hz, 1H), 2.89 (dd, *J* = 17.0, 2.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.4, 158.0 (d, J_{CF} = 1.5 Hz), 157.6 (d, J_{CF} = 242.9 Hz), 138.6, 129.1, 126.3, 123.9 (d, J_{CF} = 24.6 Hz), 121.6 (d, J_{CF} = 6.5 Hz), 120.0 (d, J_{CF} = 7.3 Hz), 112.3, 112.1, 80.0, 44.5; IR (neat) 3066, 3038, 3011, 2886, 2360, 2341, 1692, 1619, 1480, 1454, 1435, 1400, 1370, 1340, 1314, 1270, 1237, 1218, 1187, 1162, 1117, 1081, 1058, 1032, 995, 923, 900, 886, 863, 824, 788, 760, 724, 697, 656; HRMS (EI+) *m/z* calculated for $C_{15}H_{11}O_2F$ (M) 242.0743, found 272.0743.

6-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2v)



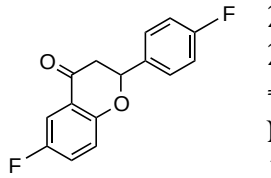
29%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.2, 3.2 Hz, 1H), 7.40-7.37 (m, 2H), 7.23-7.17 (m, 1H), 7.00 (dd, *J* = 9.1, 4.2 Hz, 1H), 6.97-6.93 (m, 2H), 5.39 (dd, *J* = 13.3, 2.9 Hz, 1H), 3.82 (s, 3H), 3.08 (dd, *J* = 17.0, 13.3 Hz, 1H), 2.85 (dd, *J* = 17.0, 2.9 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.7 (d, J_{CF} = 1.9 Hz), 160.3, 158.1, 157.5 (d, J_{CF} = 243.9 Hz), 130.6, 128.0, 123.9 (d, J_{CF} = 24.6 Hz), 121.5 (d, J_{CF} = 6.5 Hz), 120.0 (d, J_{CF} = 7.4 Hz), 114.4, 112.2 (d, J_{CF} = 23.4 Hz), 79.8, 55.6, 44.3; IR (neat) 3068, 2999, 2969, 2904, 2838, 2360, 2341, 1694, 1615, 1587, 1515, 1481, 1436, 1372, 1340, 1307, 1271, 1256, 1218, 1183, 1162, 1116, 1060, 1033, 990, 902, 864, 830, 804, 761, 705, 668; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0849.

6-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2w)



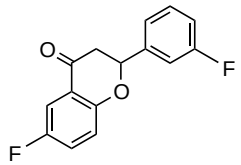
53%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.2, 3.2 Hz, 1H), 7.36-7.31 (m, 1H), 7.25-7.18 (m, 1H), 7.05-7.00 (m, 3H), 6.93-6.89 (m, 1H), 5.44 (dd, *J* = 13.1, 3.1 Hz, 1H), 3.82 (s, 3H), 3.05 (dd, *J* = 17.0, 13.1 Hz, 1H), 2.88 (dd, *J* = 17.0, 3.1 Hz, 1H); ^{13}C NMR (76 MHz, $CDCl_3$) δ 191.3 (d, J_{CF} = 1.9 Hz), 160.2, 157.9 (d, J_{CF} = 1.7 Hz), 157.6 (d, J_{CF} = 243.9 Hz), 140.2, 130.2, 123.9 (d, J_{CF} = 24.5 Hz), 121.6 (d, J_{CF} = 6.5 Hz), 120.0 (d, J_{CF} = 7.4 Hz), 118.5, 114.3, 112.2 (d, J_{CF} = 23.3Hz), 112.1, 79.9, 55.5, 44.6; IR (neat) 3067, 2961, 2837, 2360, 2341, 1691, 1614, 1603, 1586, 1479, 1434, 1401, 1363, 1341, 1321, 1291, 1266, 1219, 1199, 1187, 1167, 1116, 1091, 1043, 994, 948, 917, 870, 822, 781, 754, 726, 711, 693, 666; HRMS (EI+) *m/z* calculated for $C_{16}H_{13}O_3F$ (M) 272.0849, found 272.0846.

6-Fluoro-2-(4-fluorophenyl)chroman-4-one (2x)



22%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.2, 3.2 Hz, 1H), 7.45-7.43 (m, 2H), 7.23-7.20 (m, 1H), 7.13-7.09 (m, 2H), 7.01 (dd, *J* = 9.1, 4.2 Hz, 1H), 5.43 (dd, *J* = 13.3, 2.9 Hz, 1H), 3.03 (dd, *J* = 17.0, 13.3 Hz, 1H), 2.87 (dd, *J* = 17.0, 2.9 Hz); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.1 (d, J_{CF} = 1.6 Hz), 163.1 (d, J_{CF} = 248.4 Hz), 157.8, 157.7 (d, J_{CF} = 243.0 Hz), 134.5 (d, J_{CF} = 3.5 Hz), 128.3 (d, J_{CF} = 8.5 Hz), 124.0 (d, J_{CF} = 24.6 Hz), 121.6 (d, J_{CF} = 6.5 Hz), 120.0 (d, J_{CF} = 7.3 Hz), 116.1 (d, J_{CF} = 21.6 Hz), 112.3 (d, J_{CF} = 23.6 Hz), 79.4, 44.6; IR ($CDCl_3$) 2360, 2341, 1694, 1648, 1608, 1512, 1481, 1437, 1368, 1341, 1301, 1272, 1228, 1187, 1160, 1117, 1099, 1072, 1016, 996, 904, 888, 866, 834, 784, 769, 703, 668; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0653.

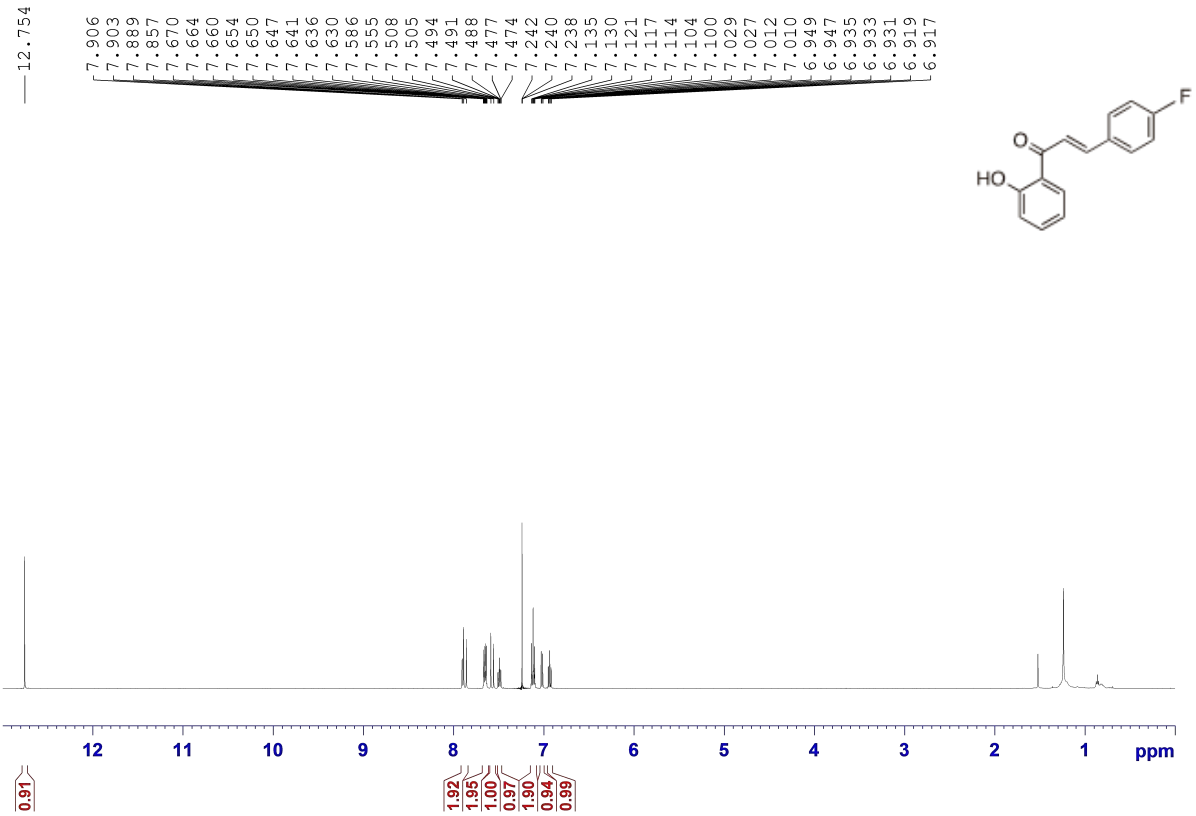
6-Fluoro-2-(3-fluorophenyl)chroman-4-one (2y)



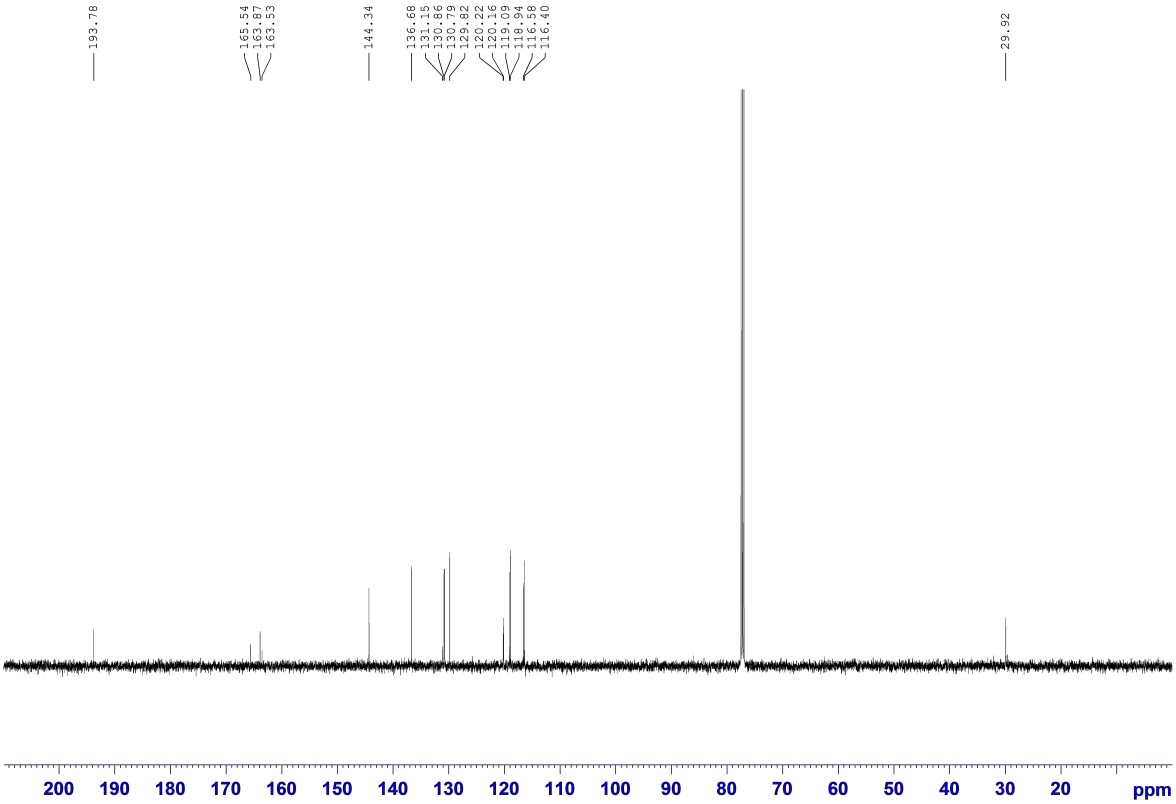
91%; ^{1}H NMR (500 MHz, CDCl3) δ 7.56 (dd, *J* = 4.9, 1.9 Hz, 1H), 7.41-7.37 (dt, *J* = 7.8, 5.4 Hz, 1H), 7.25-7.20 (m, 3H), 7.09-7.02 (m, 2H), 5.45 (dd, *J* = 7.8, 1.9 Hz, 1H), 3.01 (dd, *J* = 10.2, 7.8 Hz, 1H), 2.90 (dd, *J* = 10.2, 1.9 Hz, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 190.8 (d, J_{CF} = 1.7 Hz), 164.8, 161.5, 159.3, 157.6 (d, J_{CF} = 1.7 Hz), 156.0, 114.1 (d, J_{CF} = 7.3 Hz), 130.7 (d, J_{CF} = 8.2 Hz), 124.0 (d, J_{CF} = 24.6 Hz), 121.8 (d, J_{CF} = 3.1 Hz), 121.5 (d, J_{CF} = 6.5 Hz), 120.0 (d, J_{CF} = 7.5 Hz), 115.9 (d, J_{CF} = 20.1 Hz), 113.4 (d, J_{CF} = 22.7 Hz), 112.3 (d, J_{CF} = 23.5 Hz), 79.2 (d, J_{CF} = 1.8 Hz), 44.5; IR ($CDCl_3$) 3070, 2899, 2360, 2341, 1692, 1619, 1593, 1479, 1449, 1432, 1401, 1363, 1341, 1322, 1269, 1240, 1219, 1193, 1168, 1141, 1116, 1082, 1061, 1000, 972, 946, 919, 872, 833, 822, 786, 759, 726, 711, 690, 667; HRMS (EI+) *m/z* calculated for $C_{15}H_{10}O_2F_2$ (M) 260.0649, found 260.0651.

^{1}H NMR AND ^{13}C NMR SPECTRA FOR COMPOUNDS **1a-1y, 2a-2y**

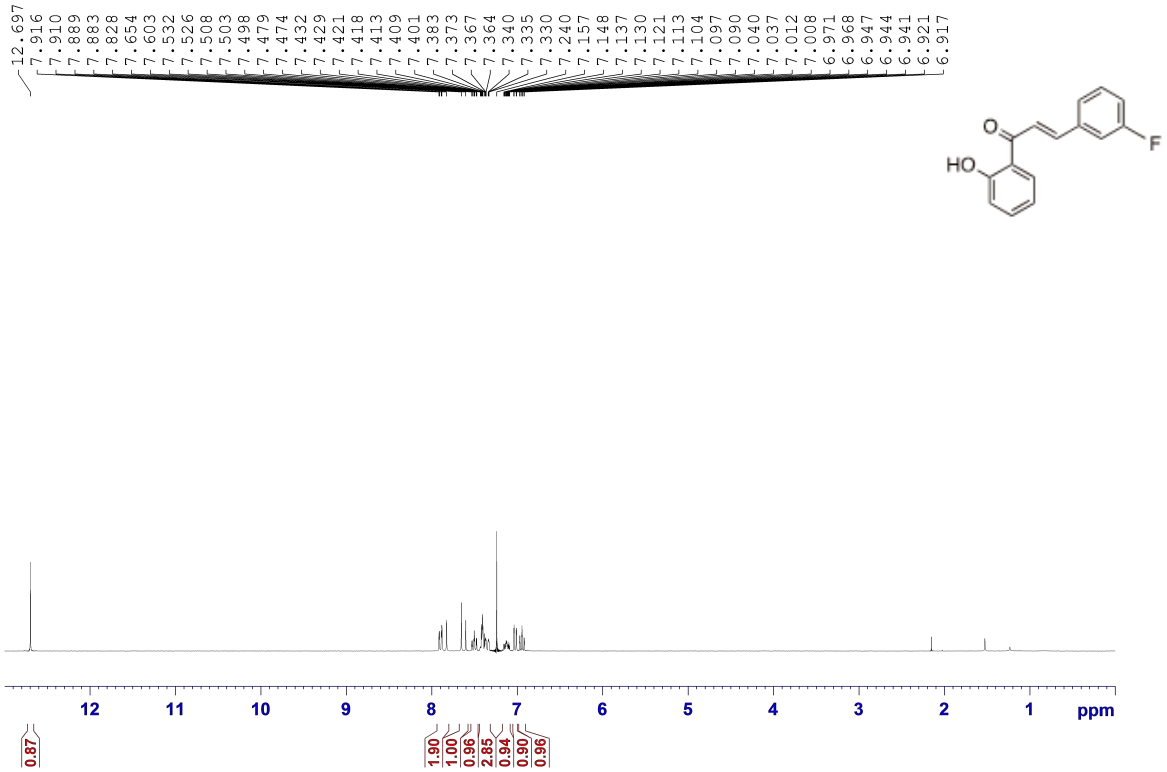
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1d)



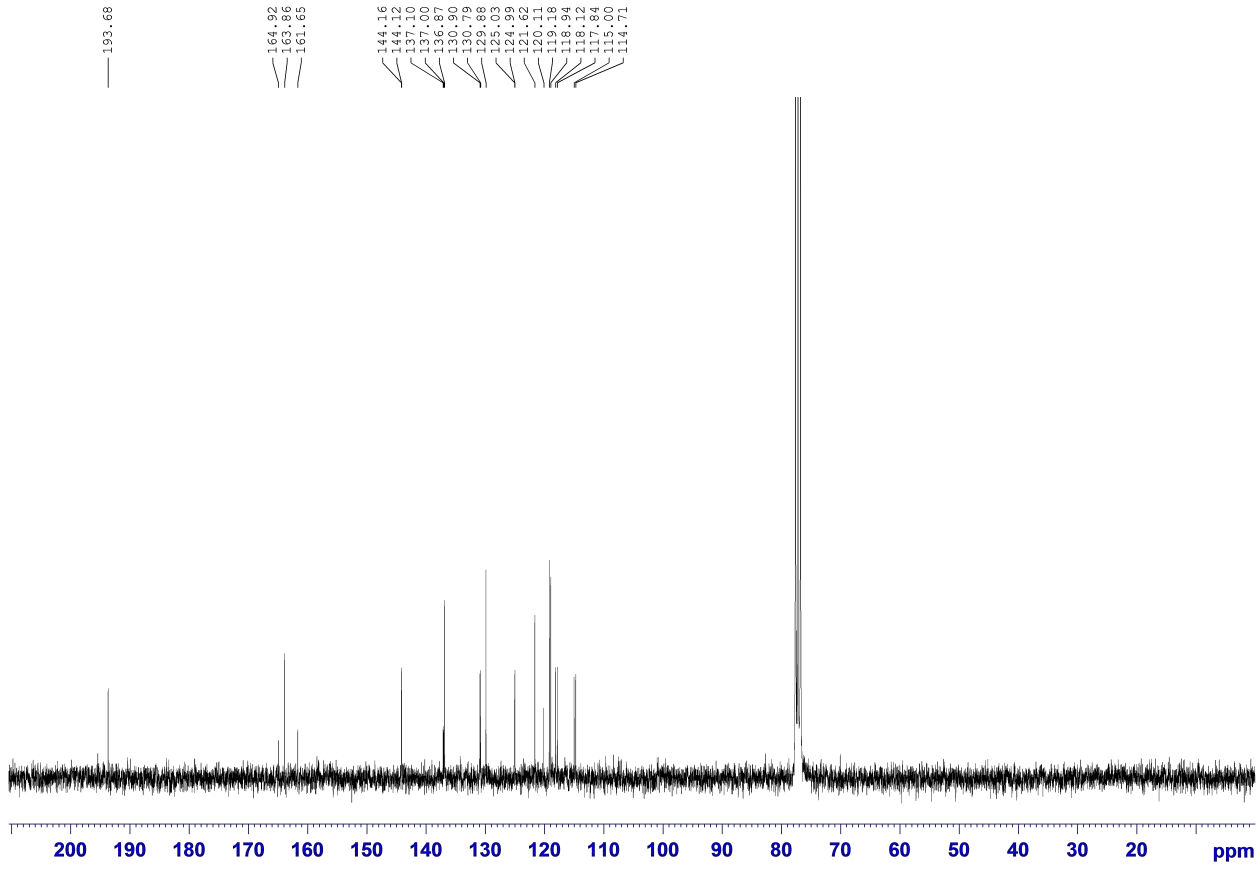
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1d)



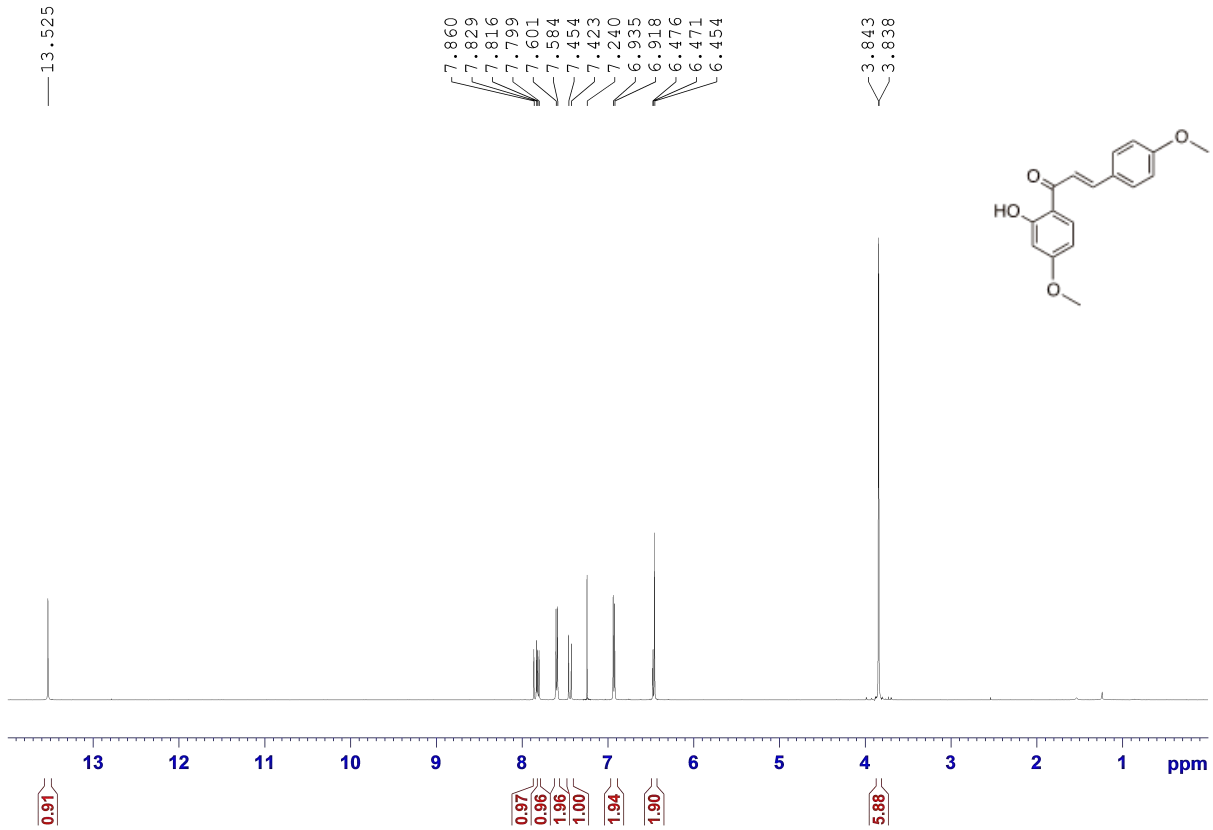
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1e)



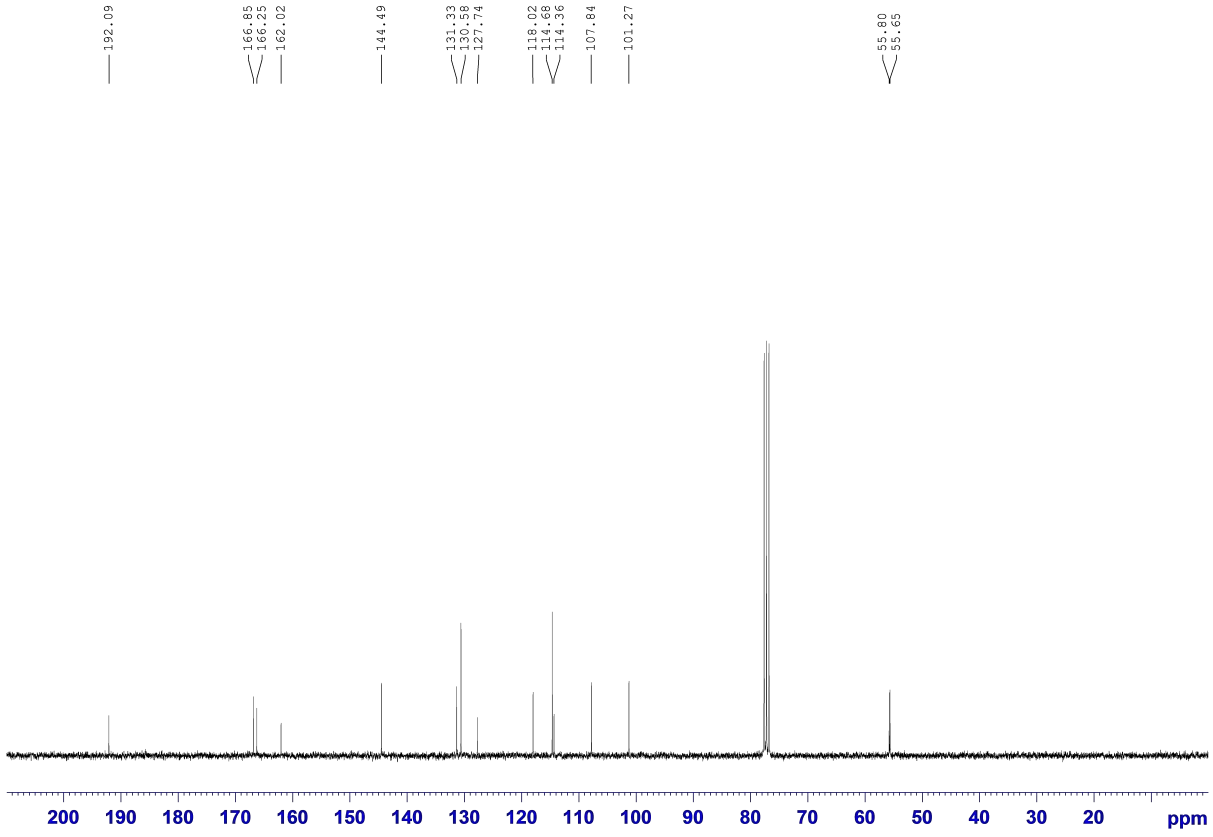
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1e)



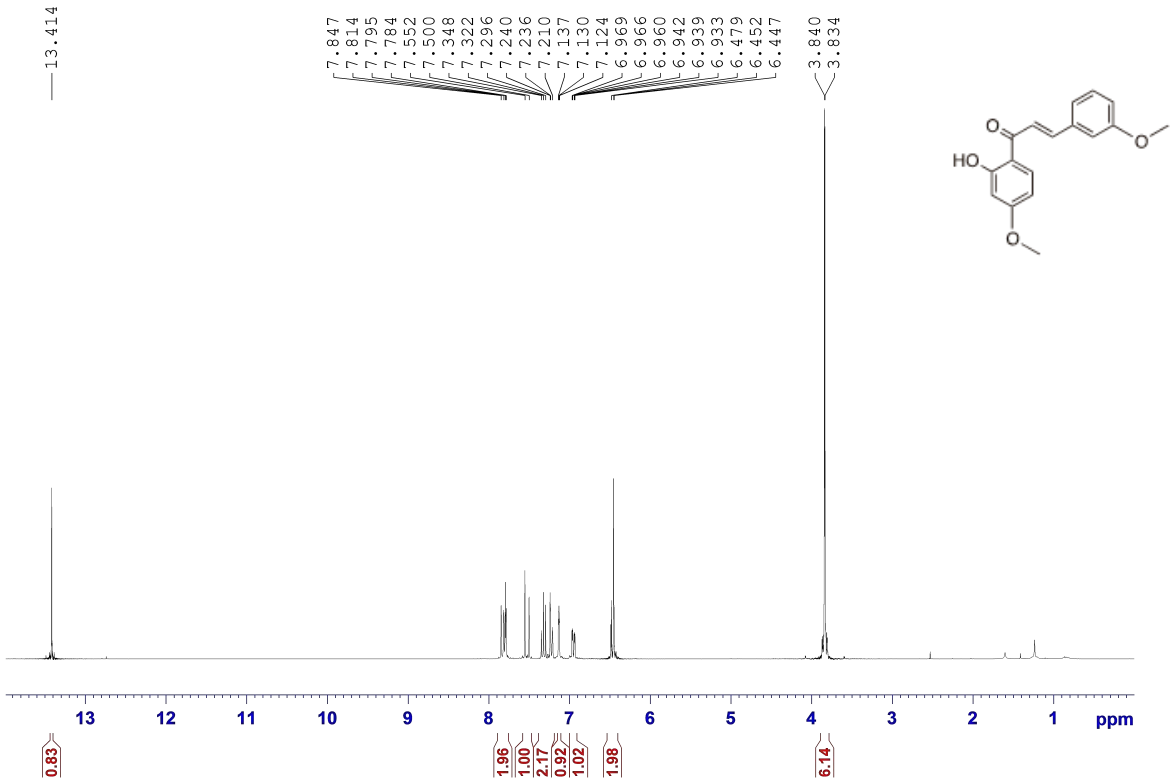
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1g)



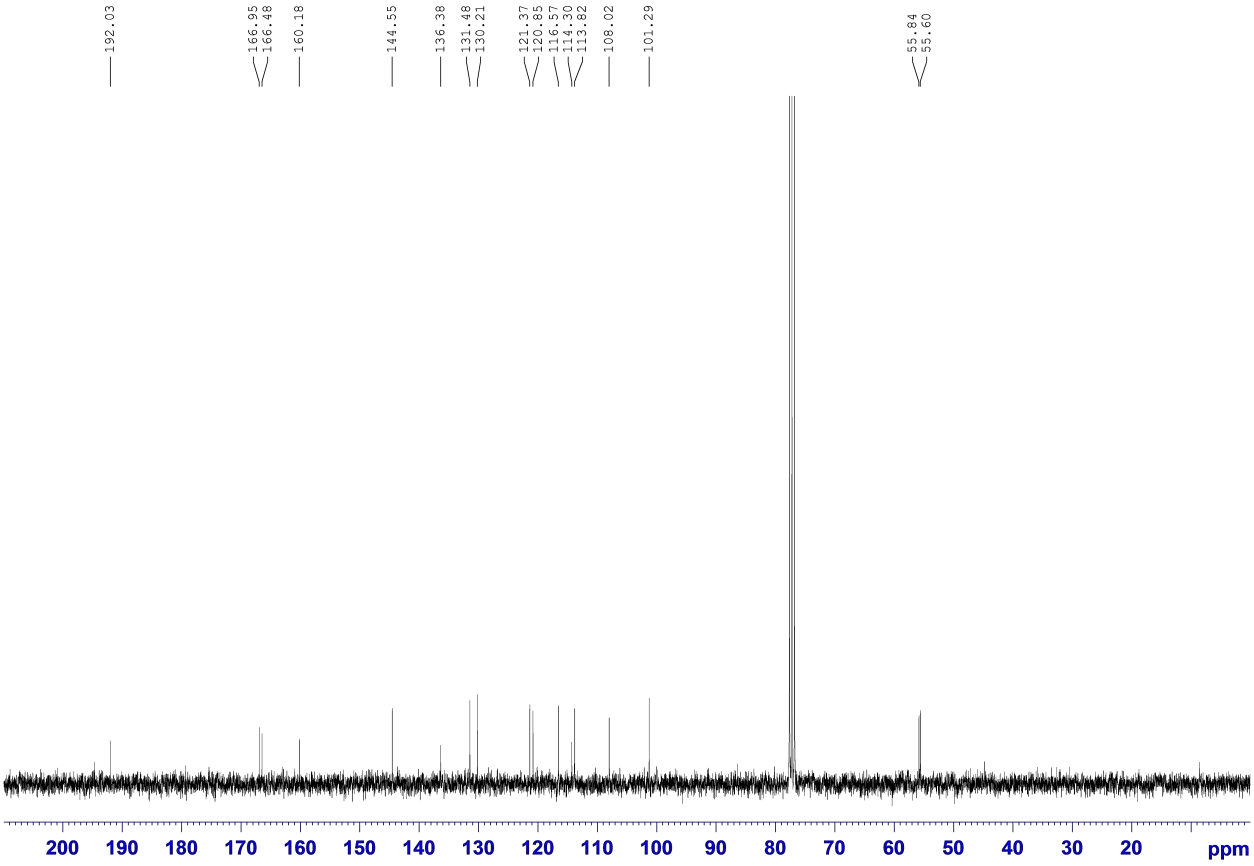
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1g)



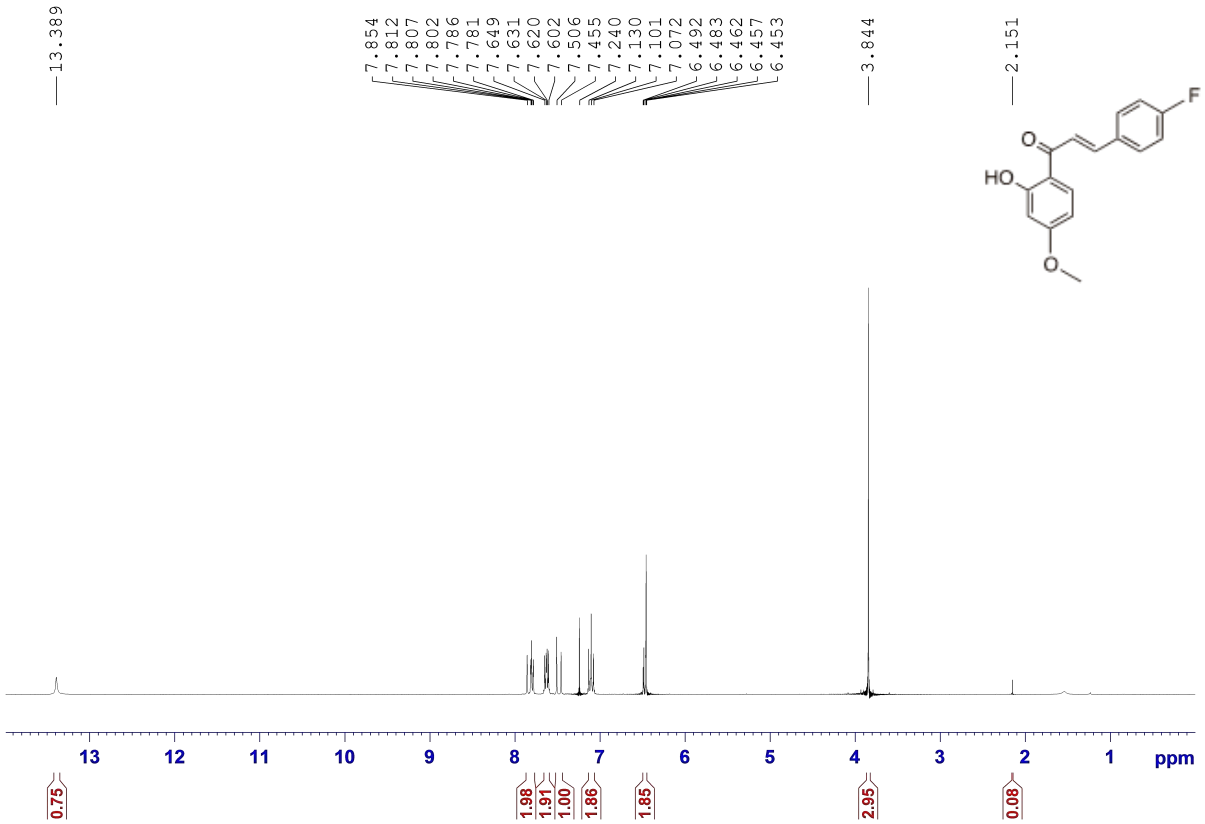
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1h)



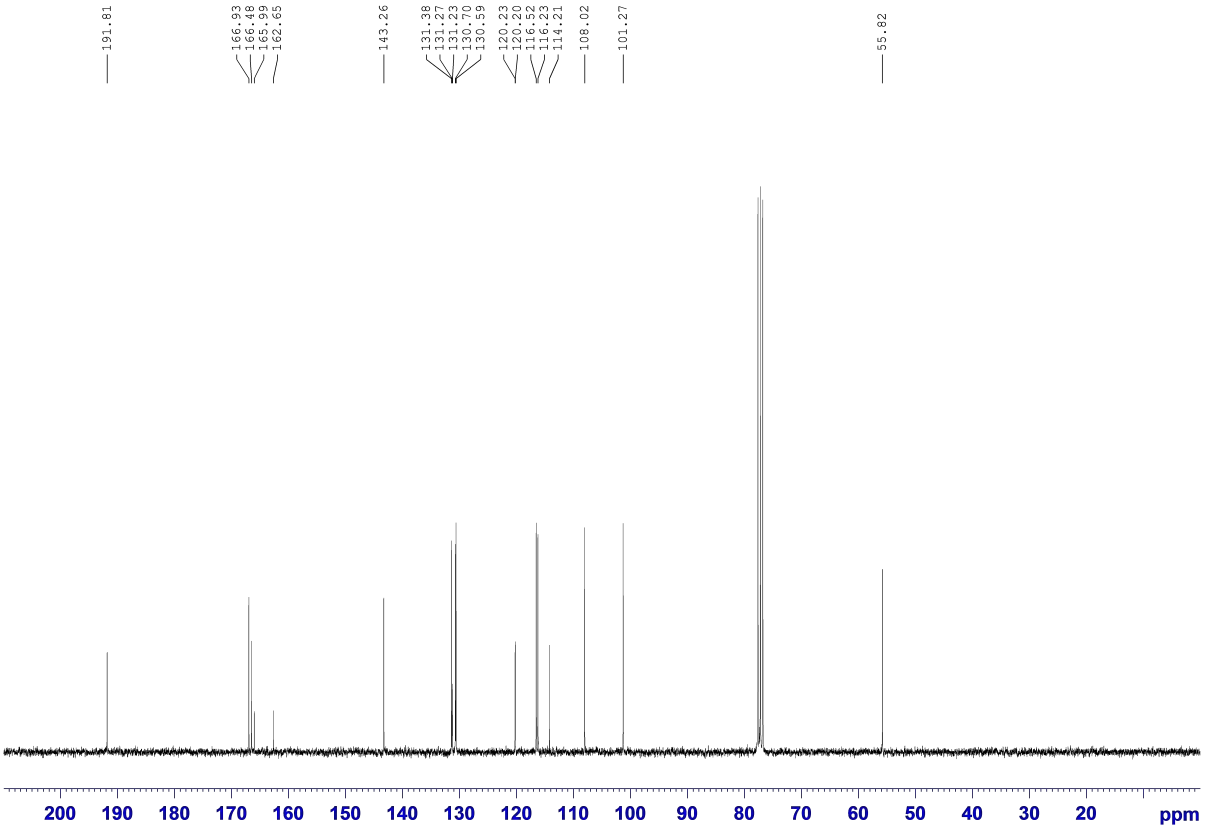
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1h)



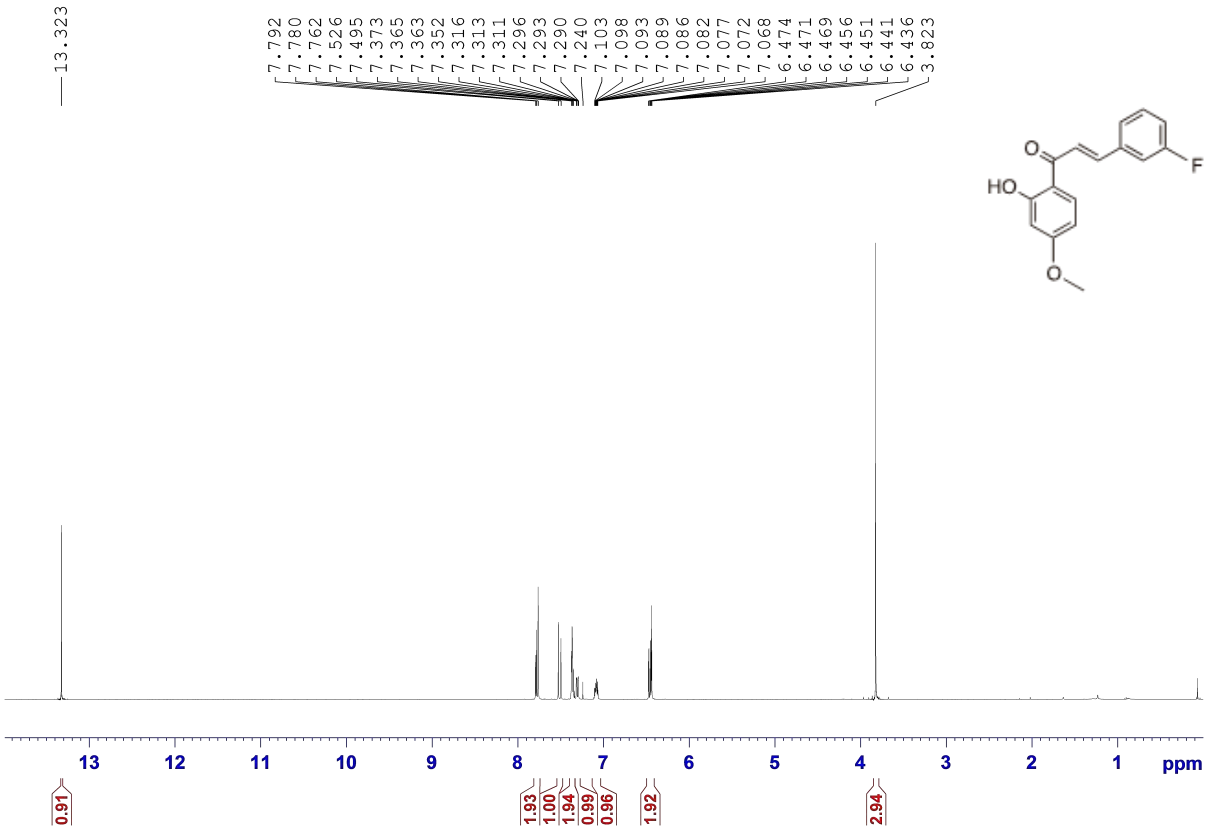
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1i)



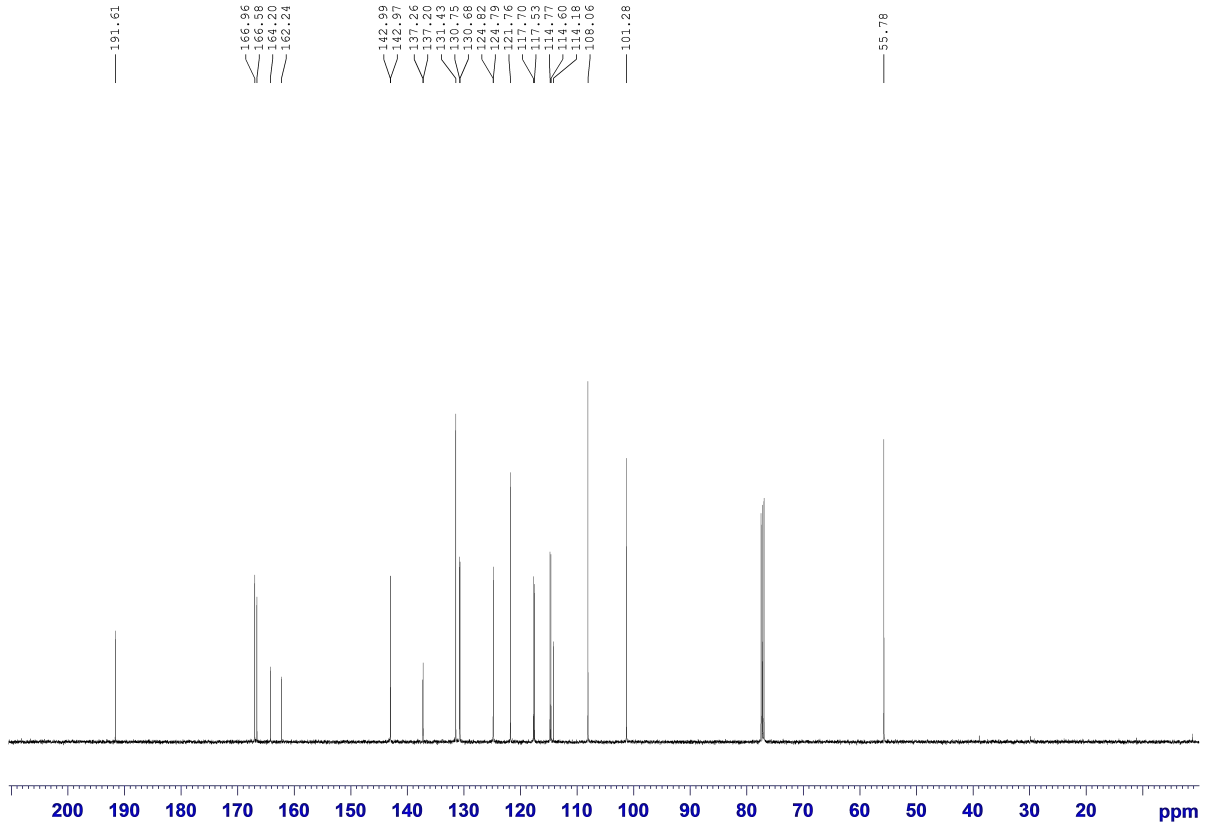
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1i)



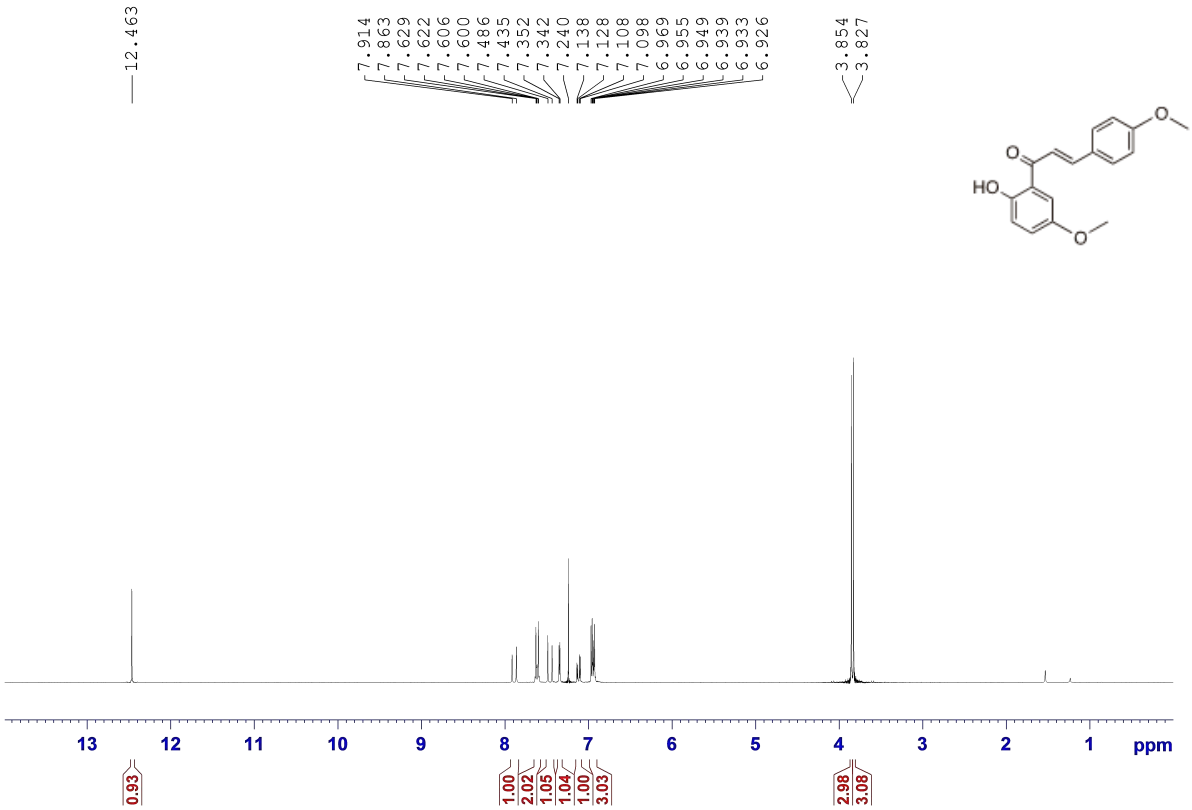
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1j)



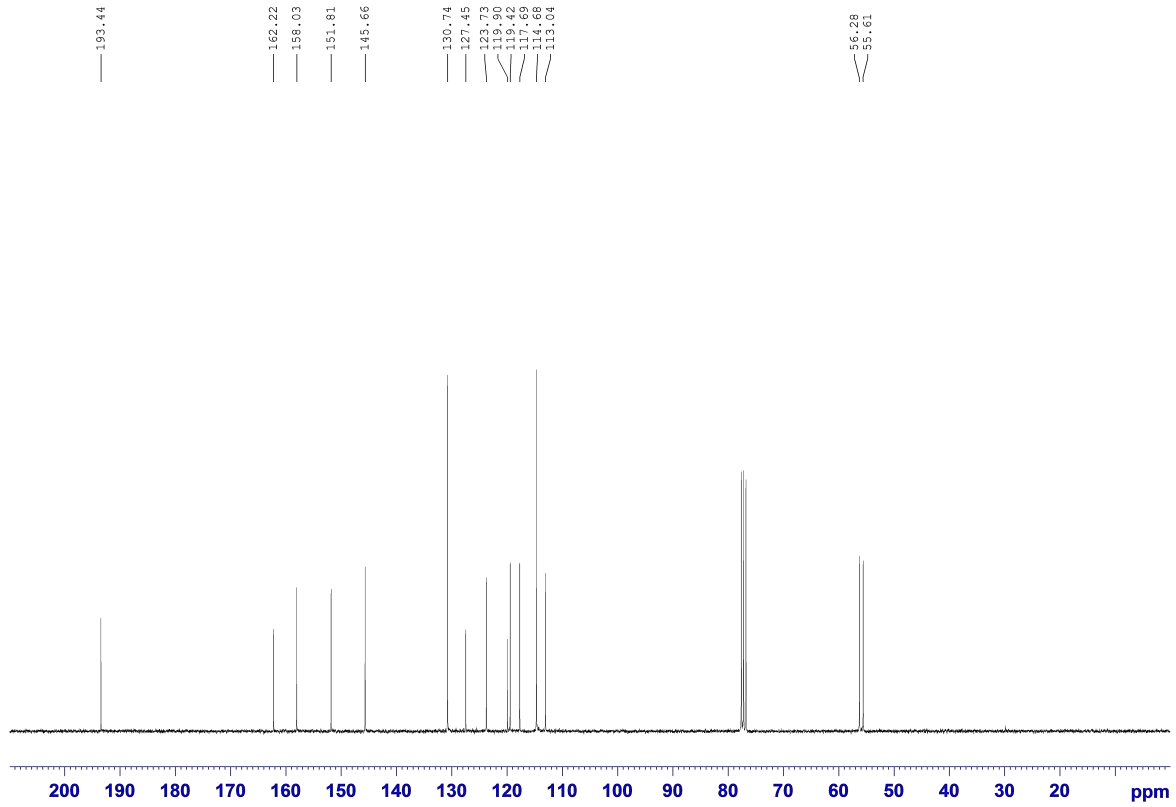
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1j)



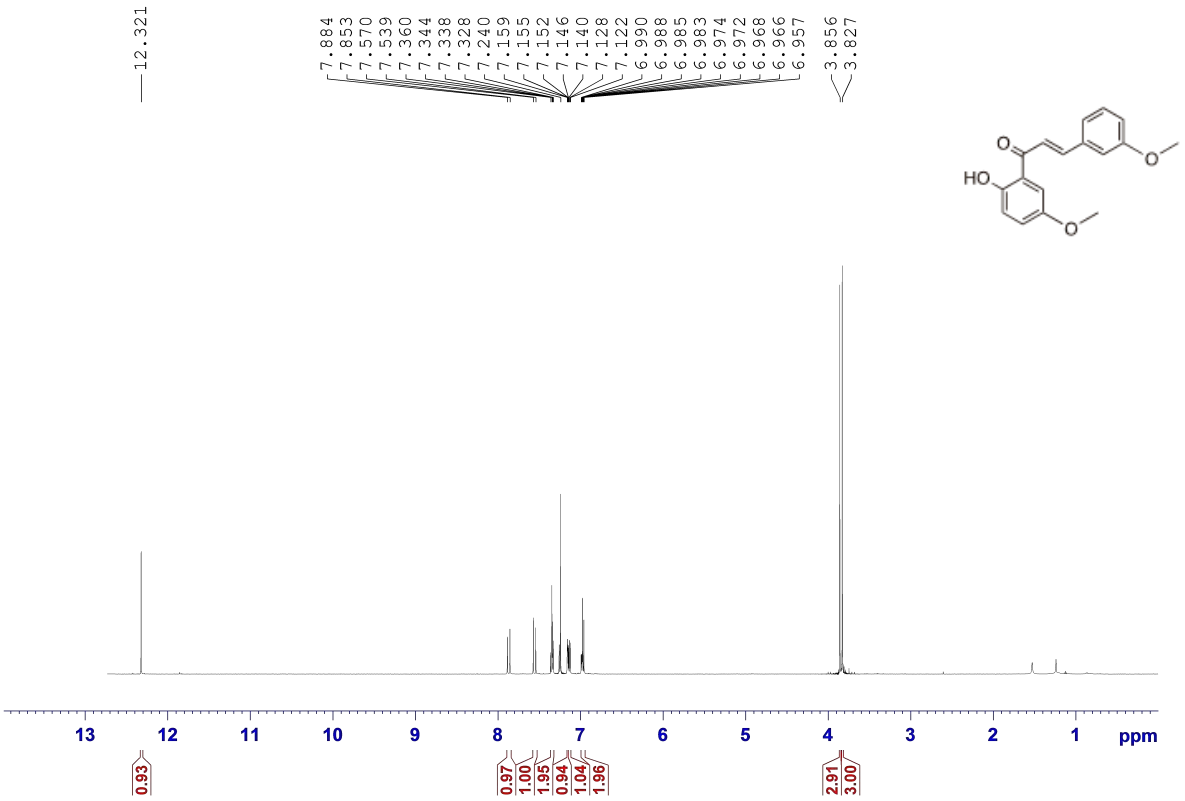
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1l)



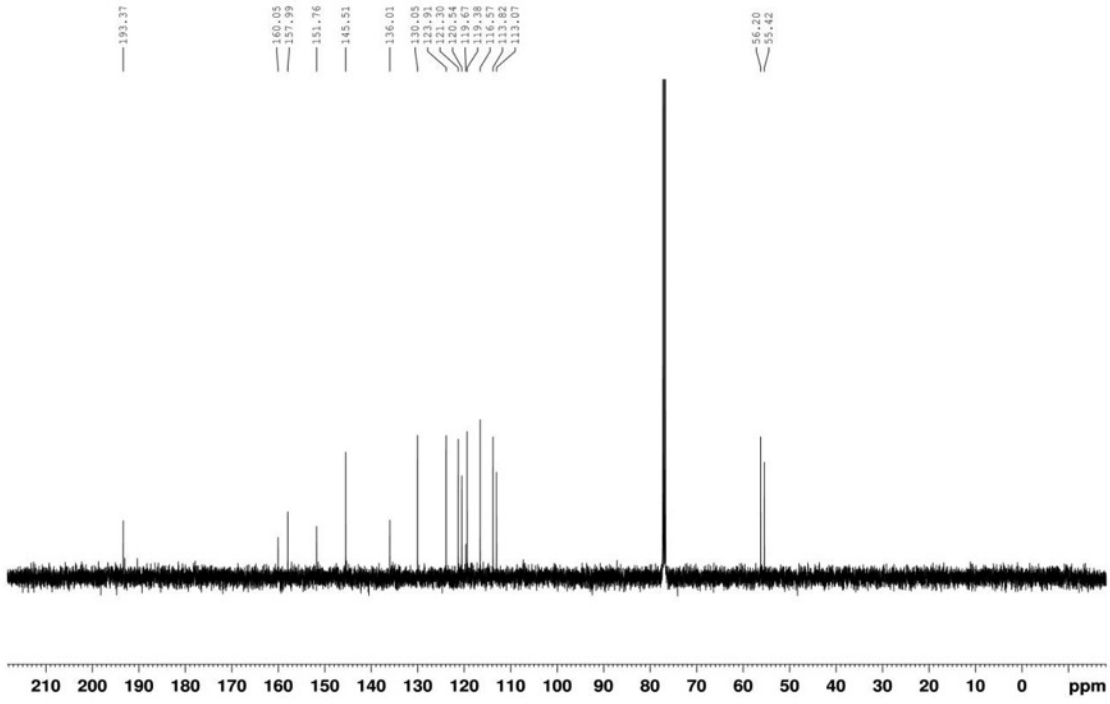
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1l)



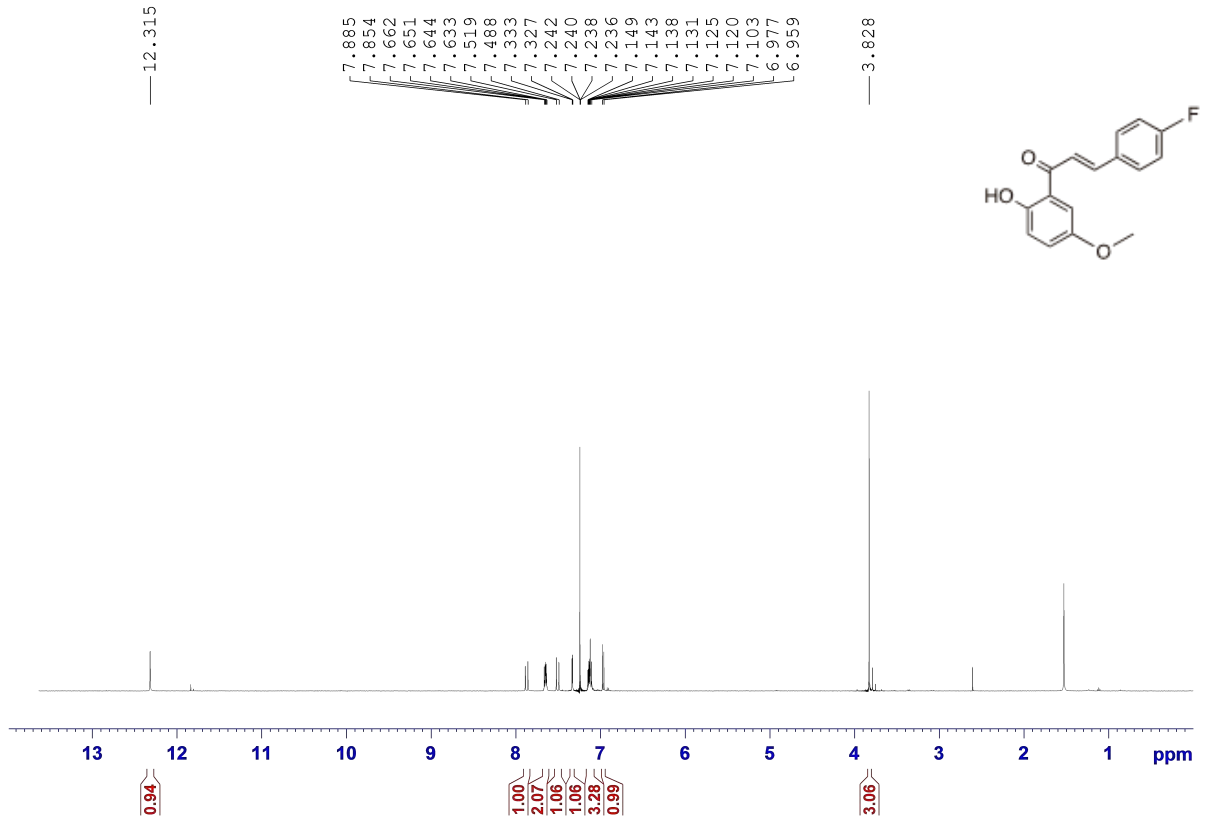
[1]H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1m)



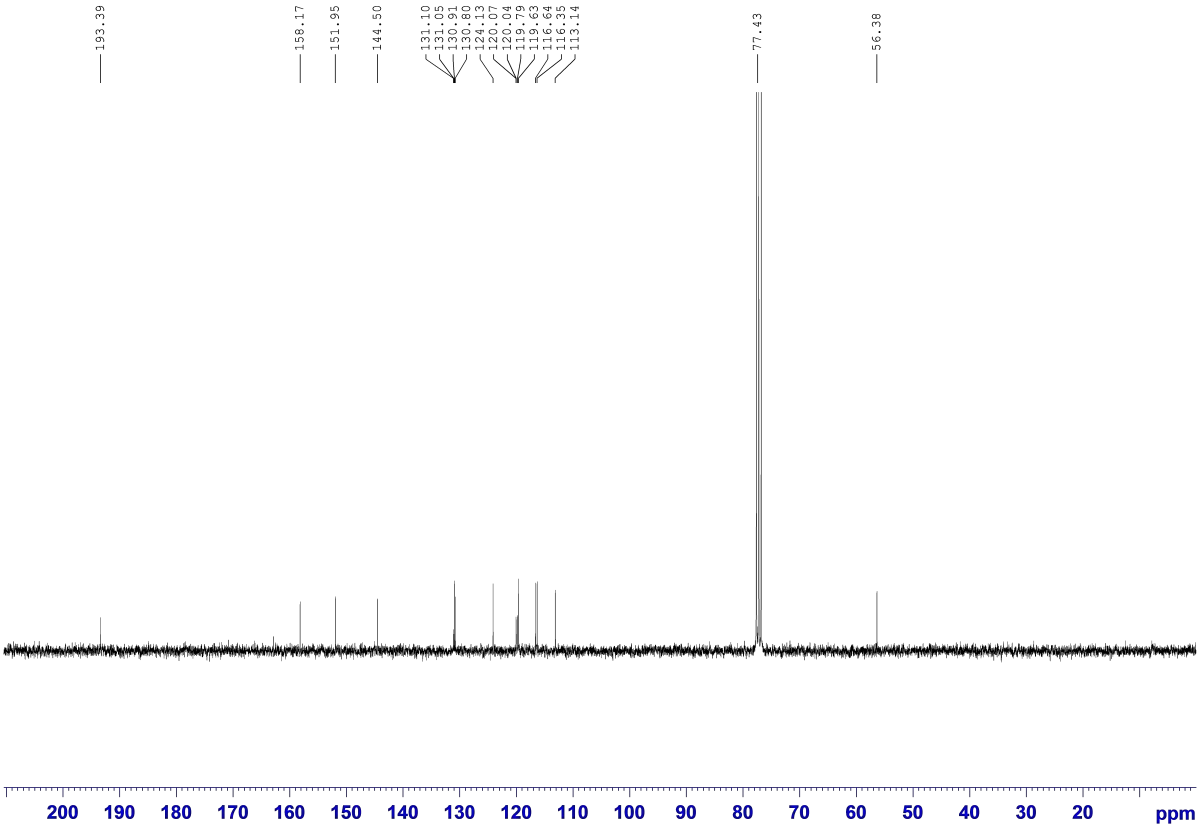
[13]C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1m)



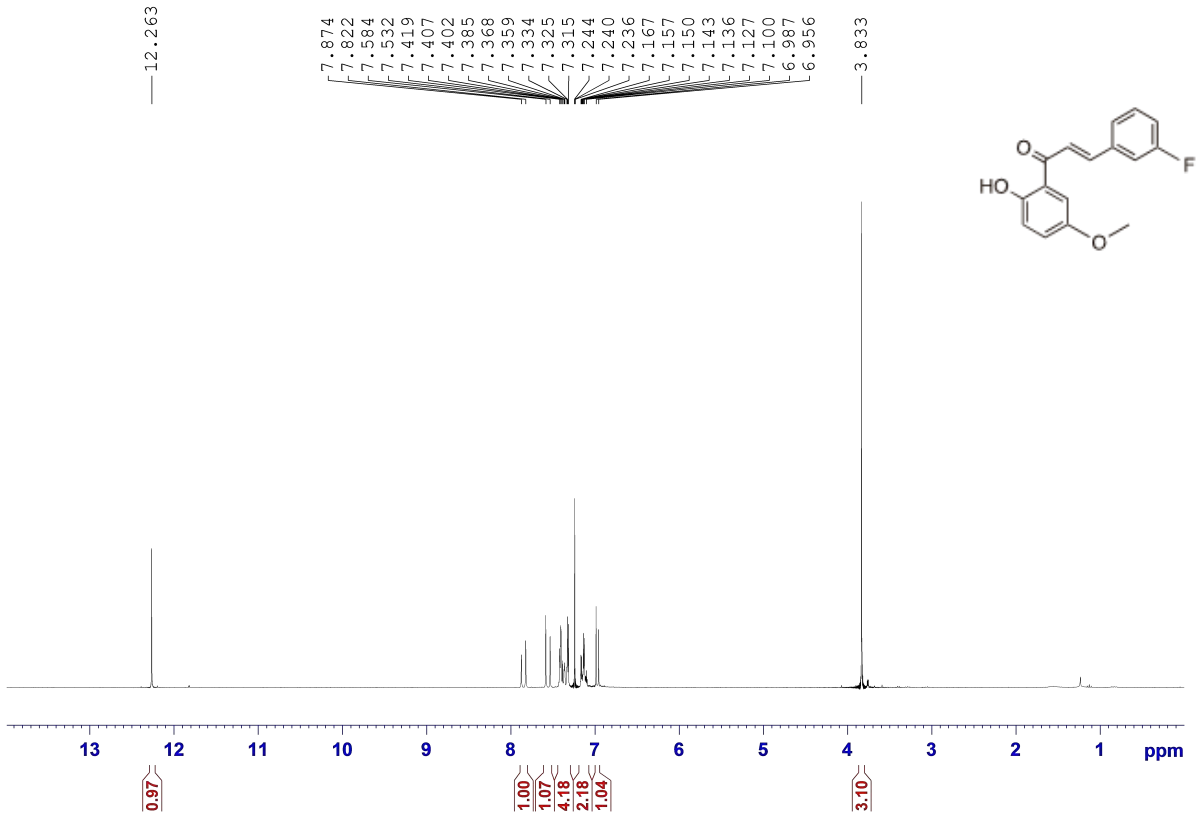
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1n)



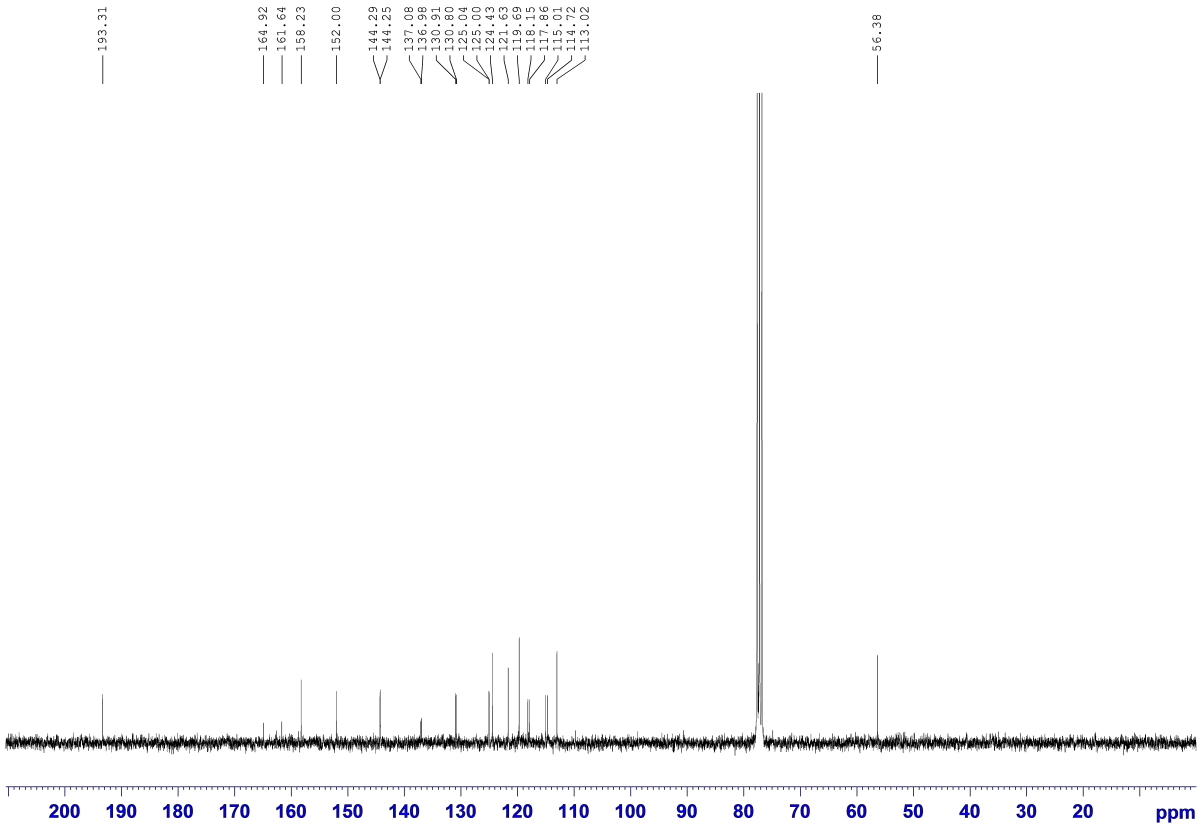
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1n)



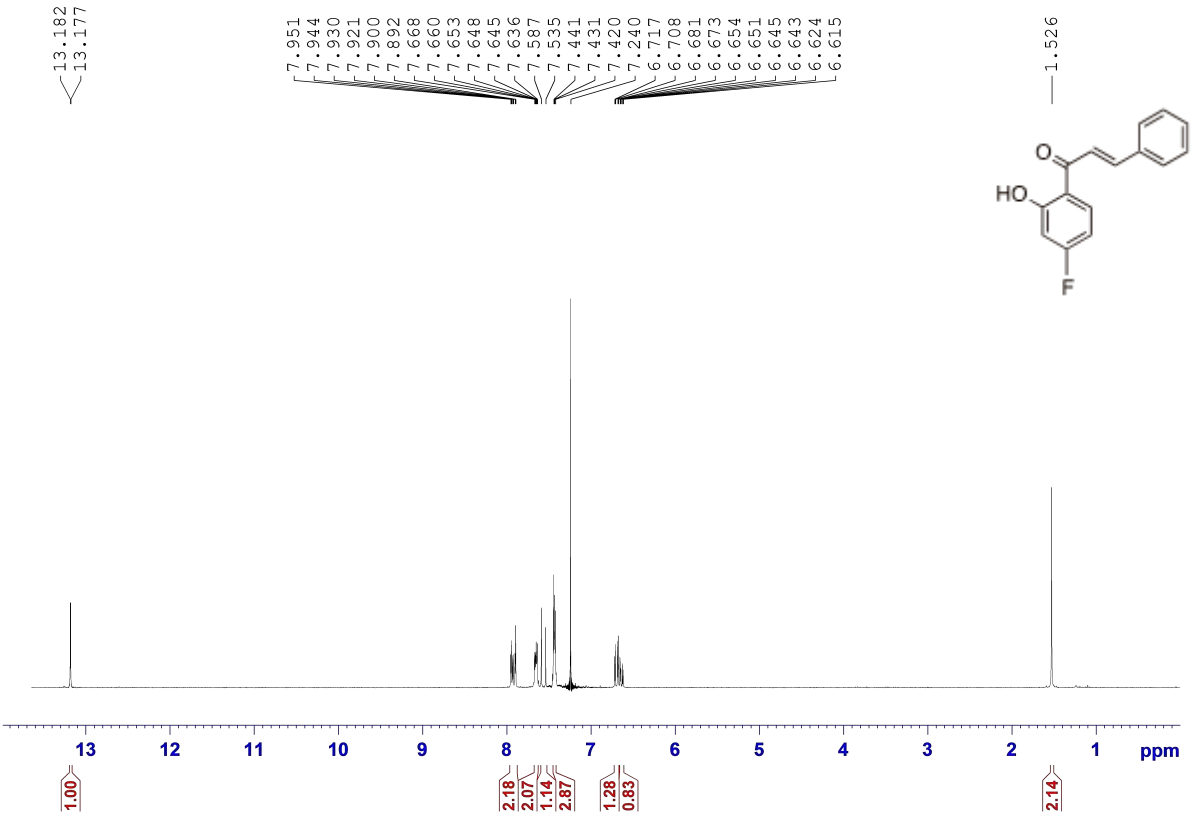
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1o)



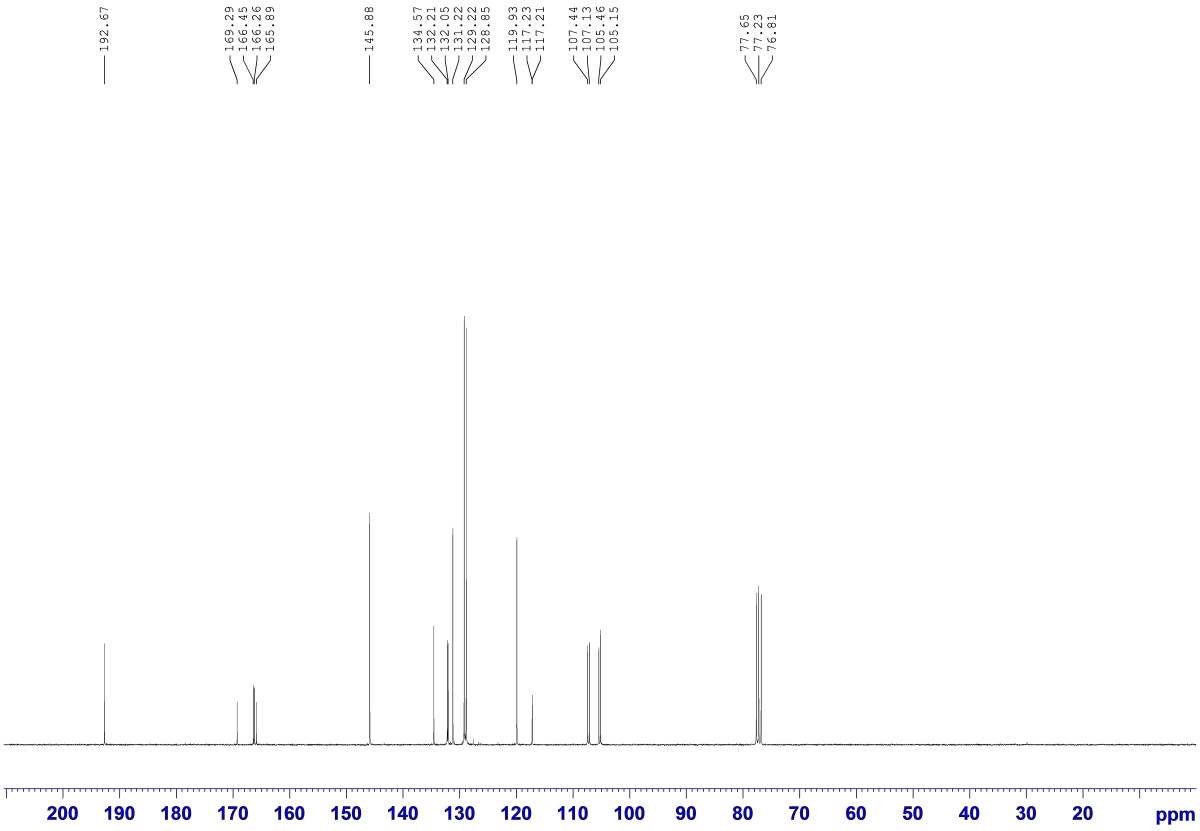
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-methoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1o)



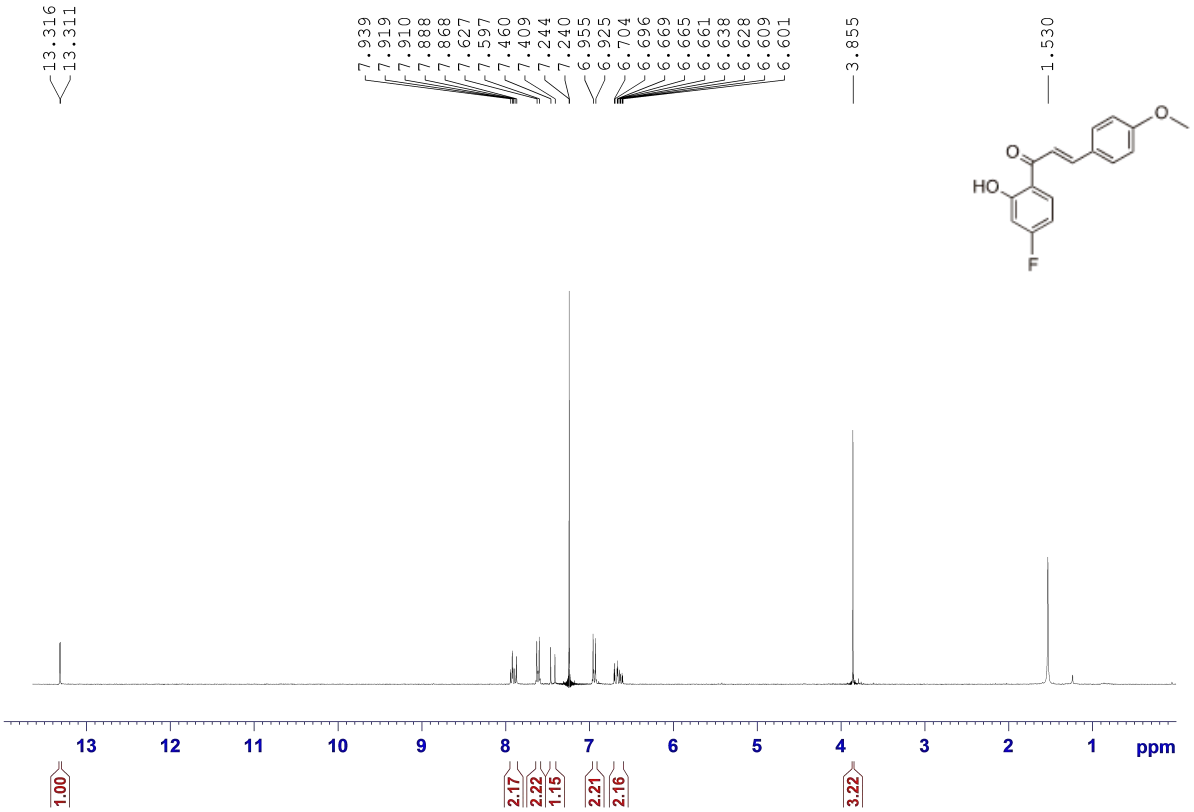
[1]H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-phenylprop-2-en-1-one (1p)



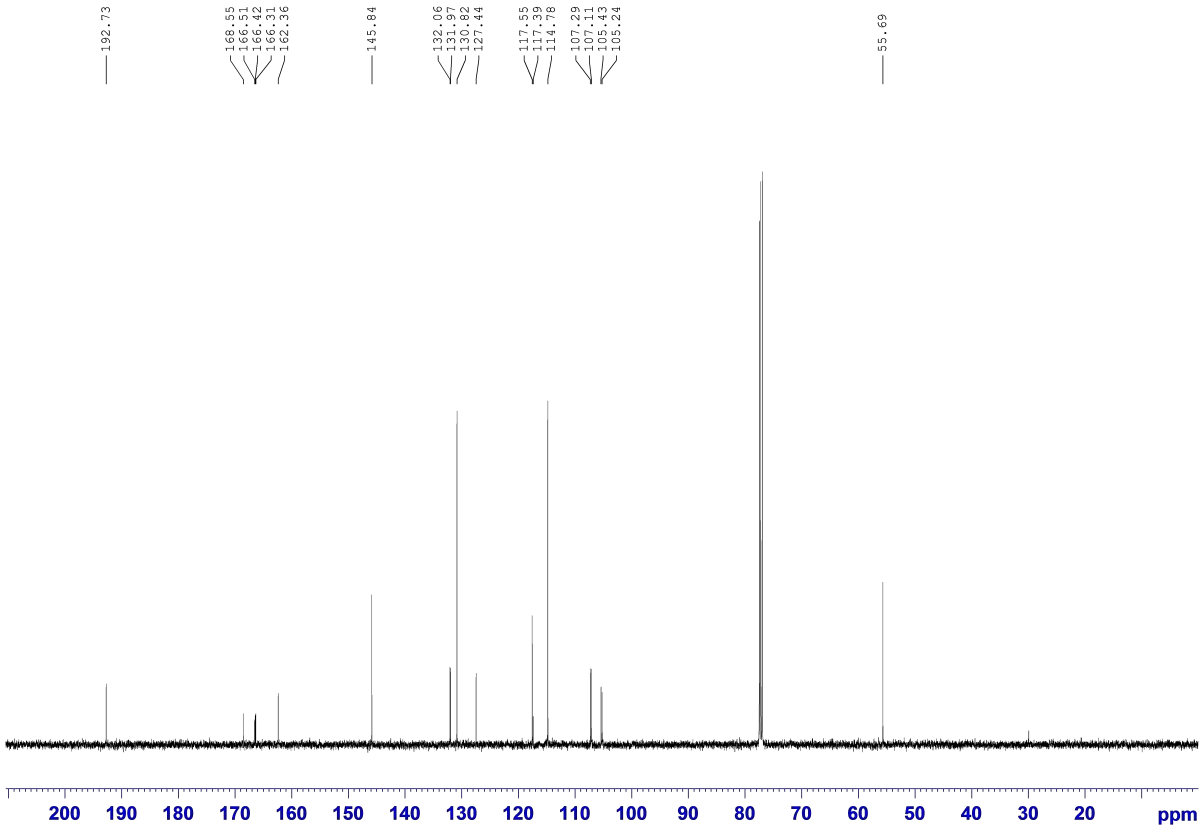
[13]C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-phenylprop-2-en-1-one (1p)



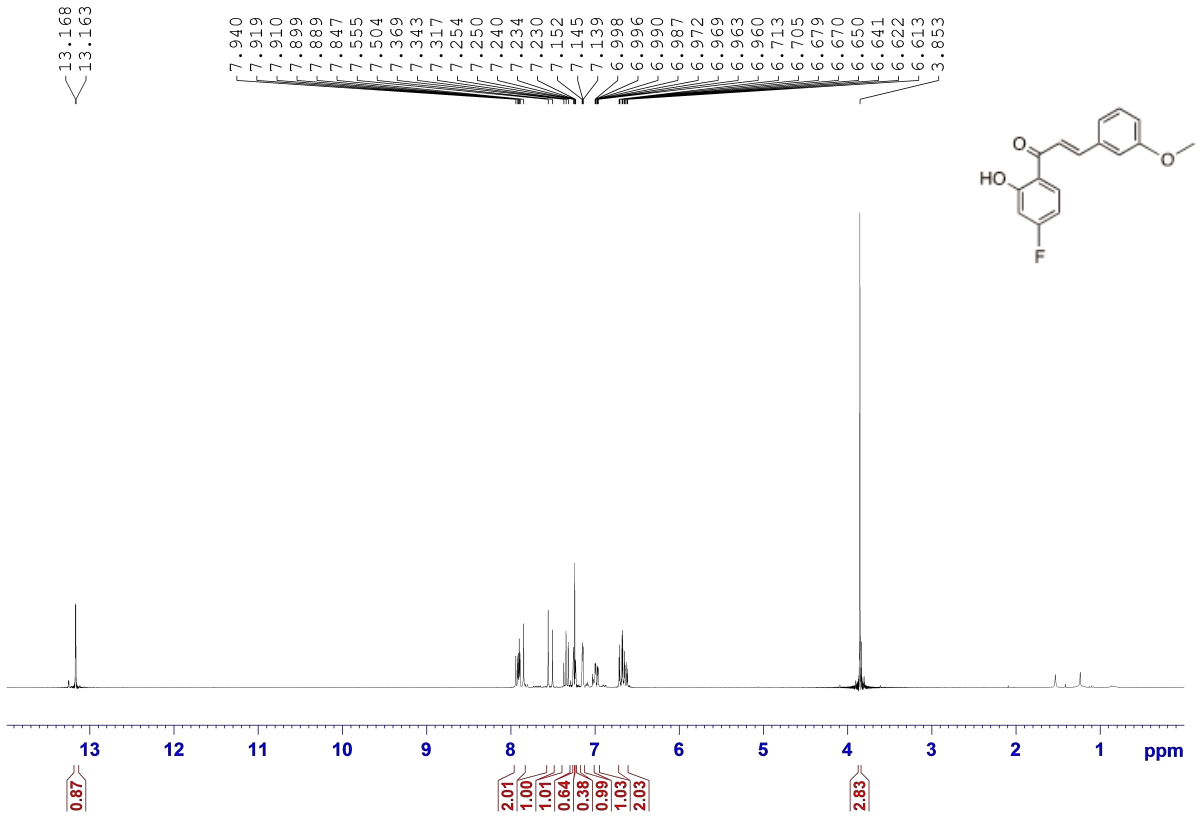
[1]H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1q)



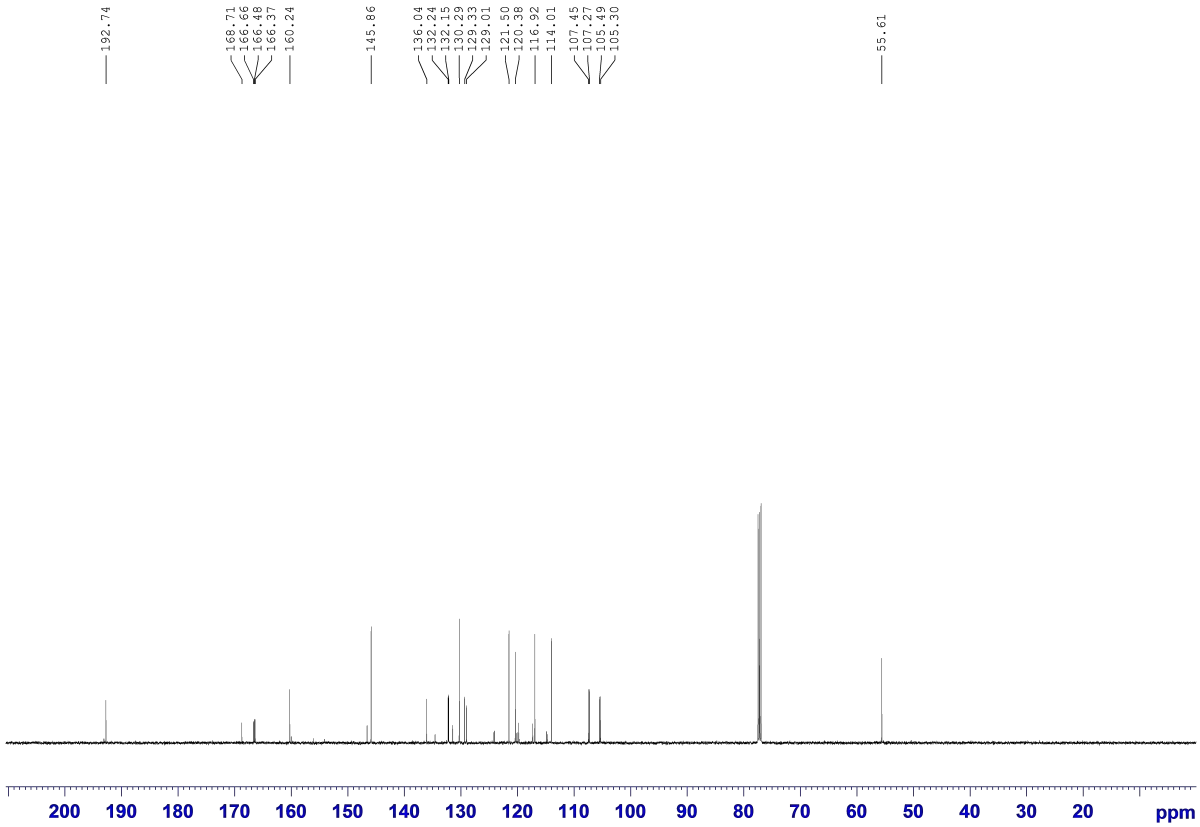
[13]C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1q)



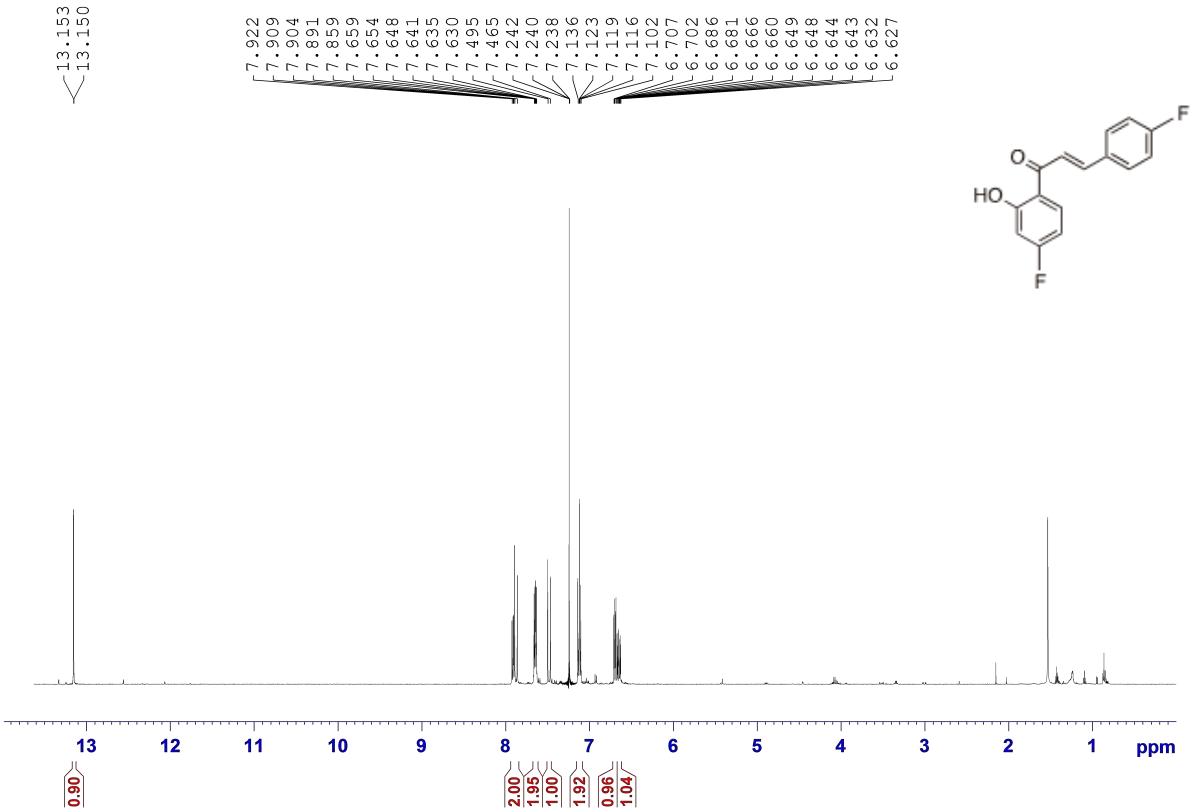
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1r)



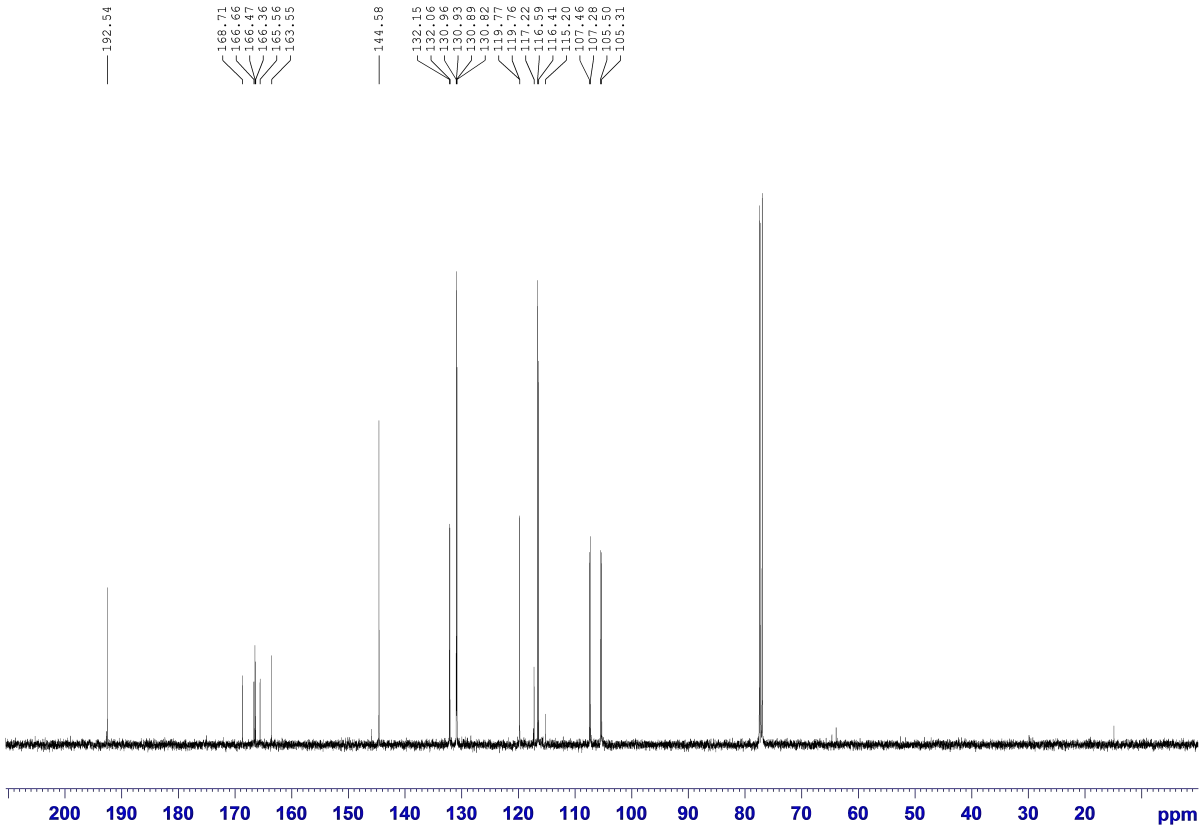
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1r)



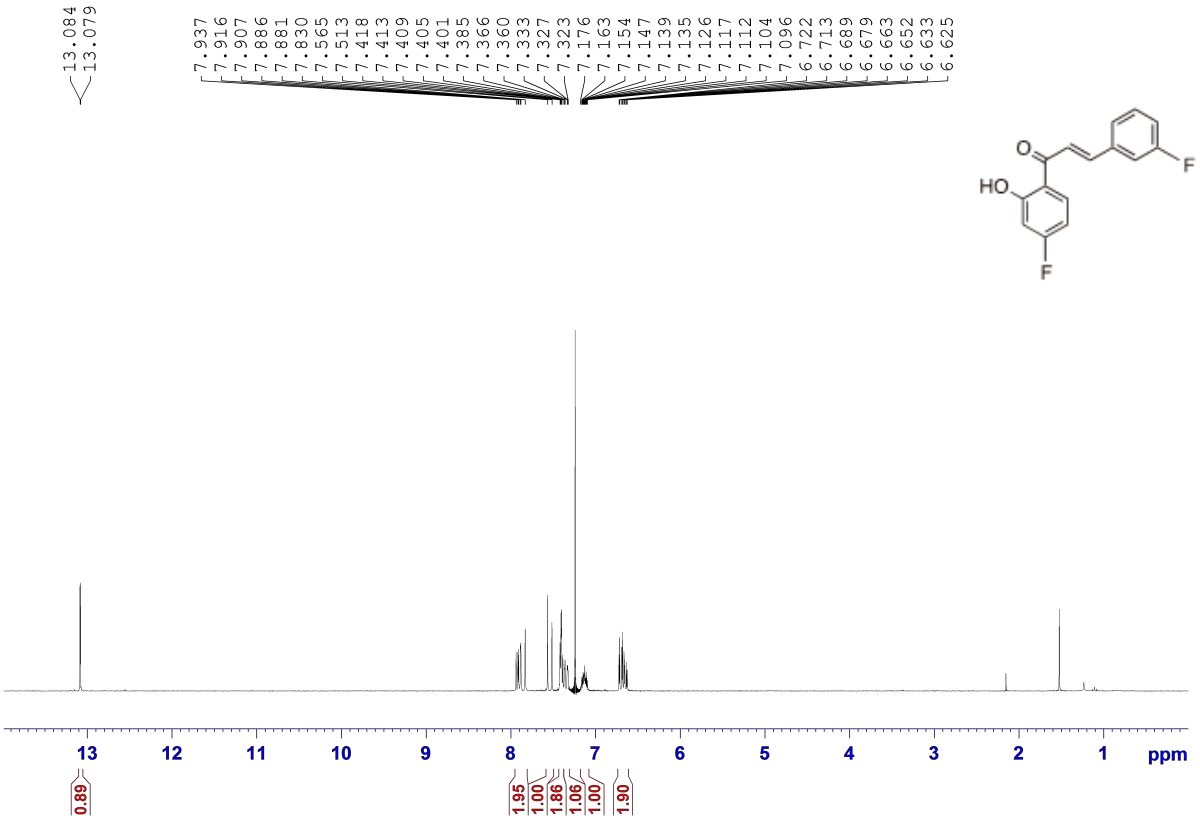
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1s)



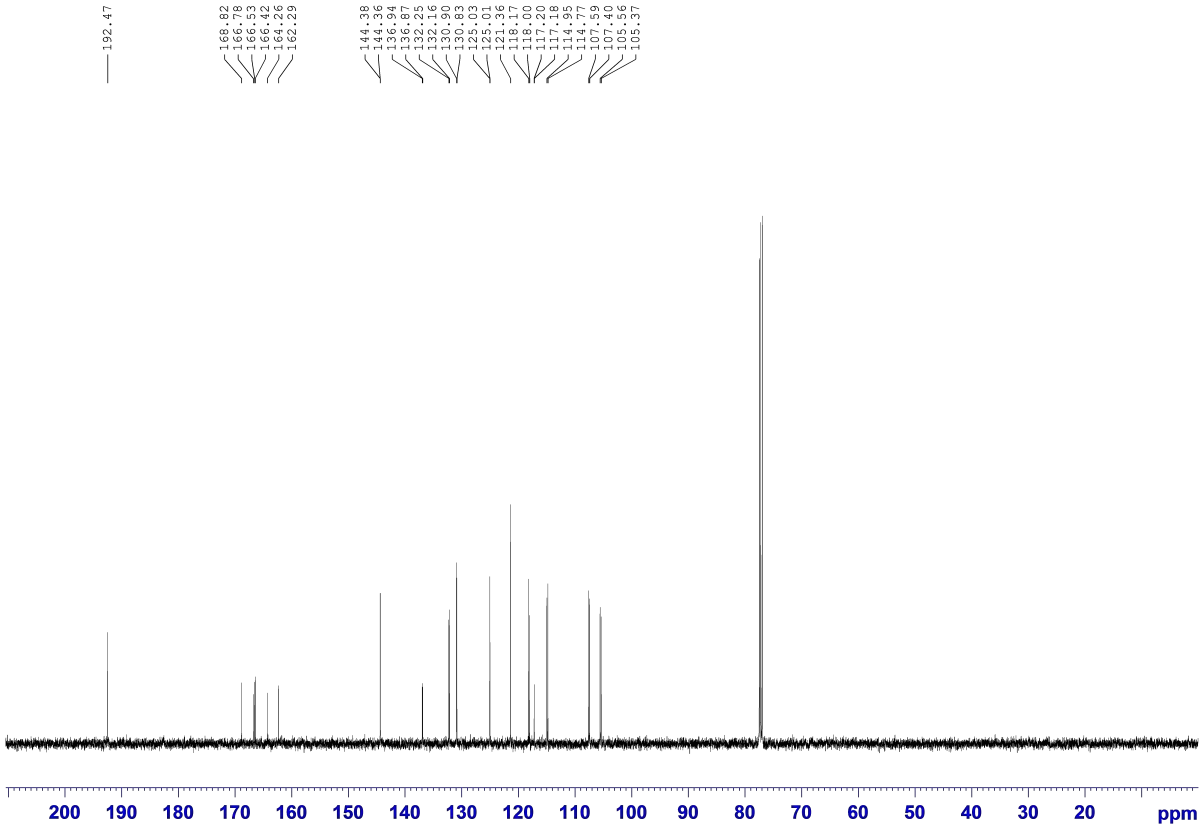
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1s)



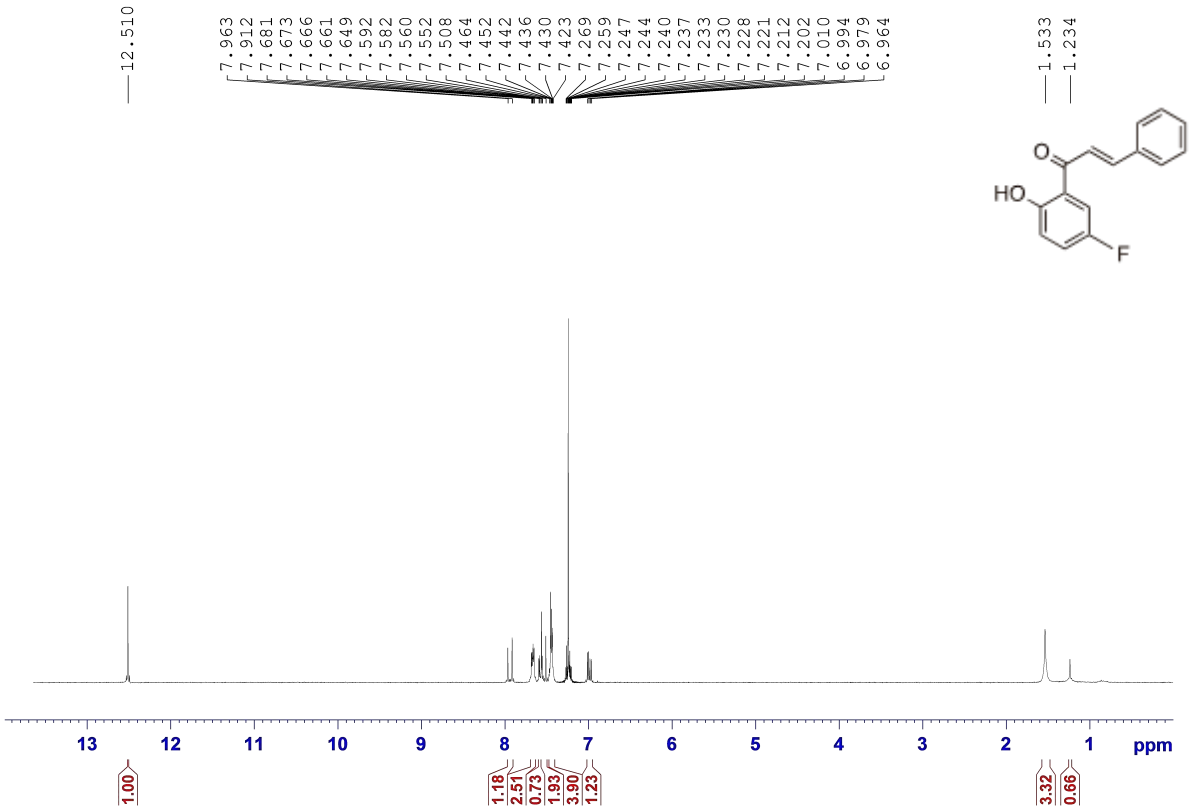
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1t)



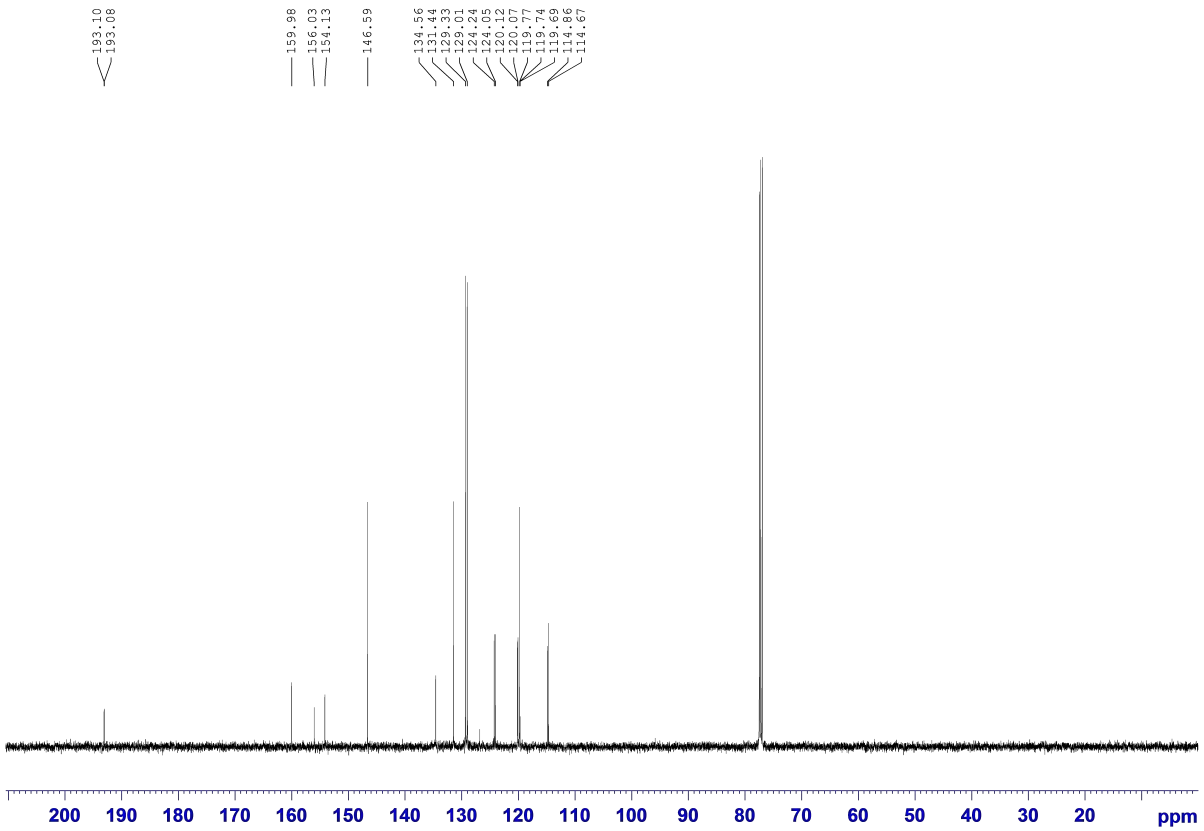
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-4-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1t)



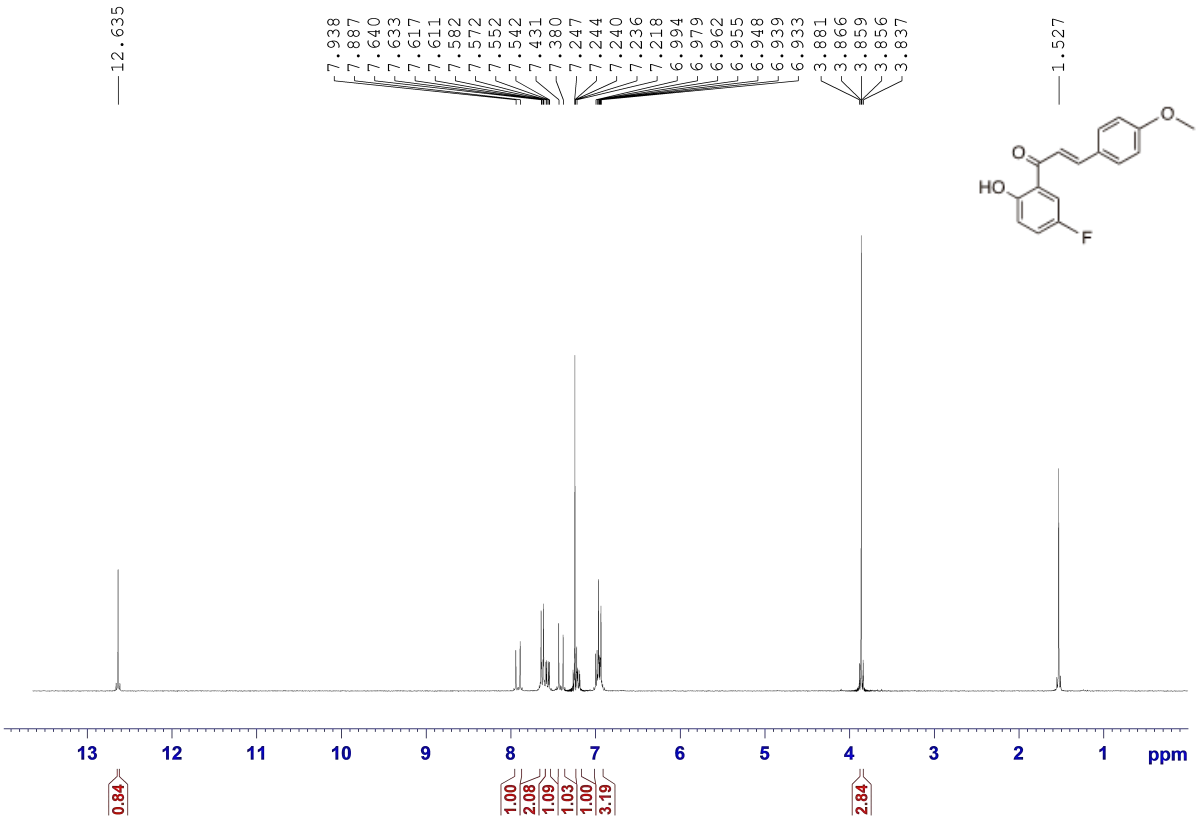
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-phenylprop-2-en-1-one (1u)



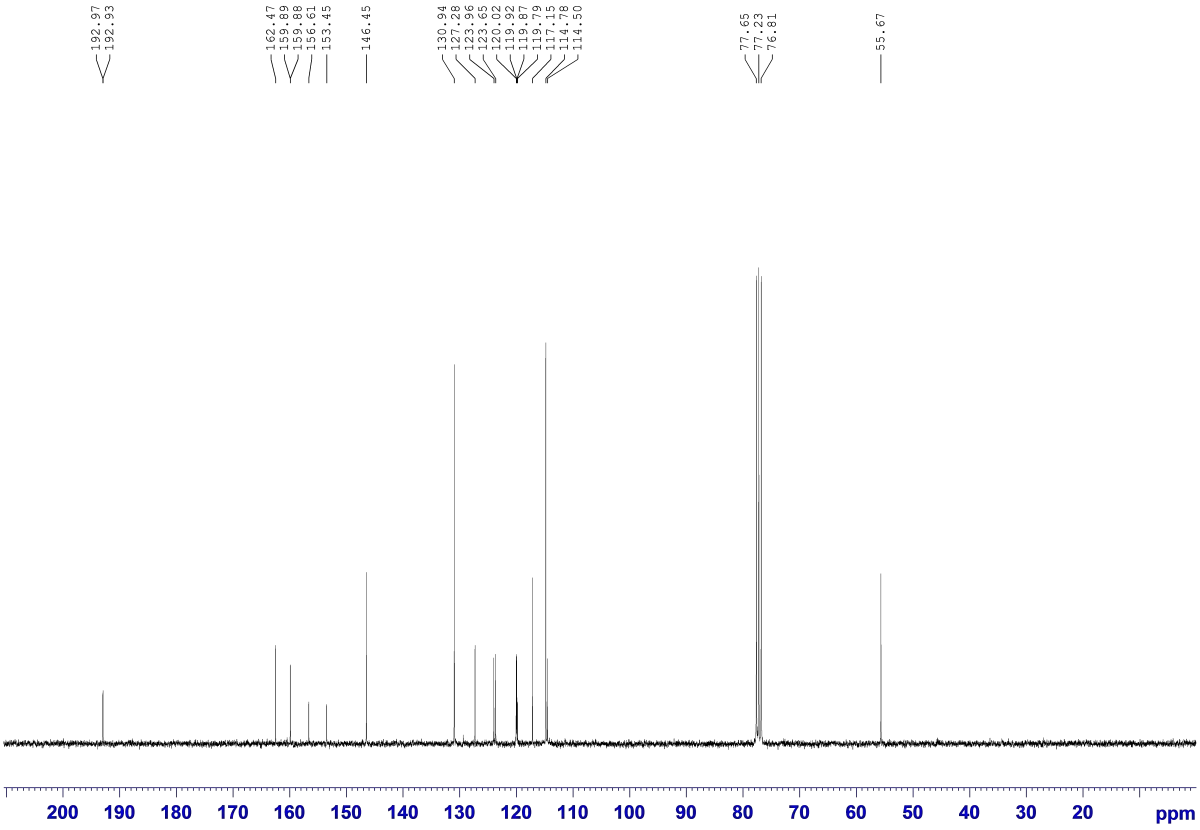
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-phenylprop-2-en-1-one (1u)



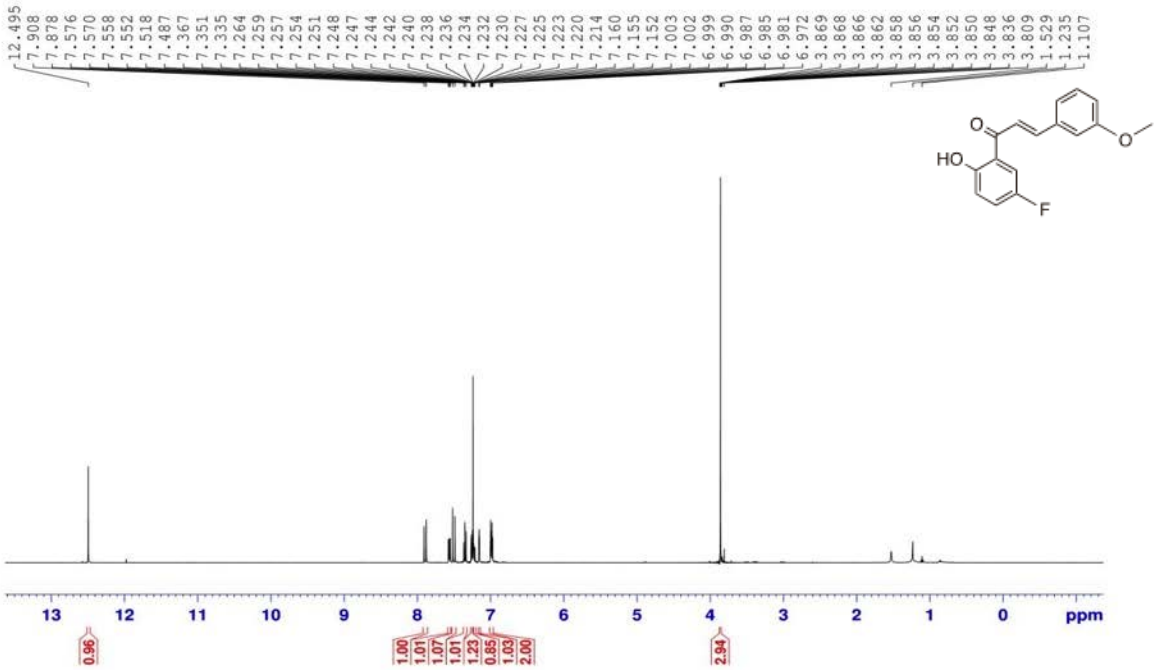
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1v)



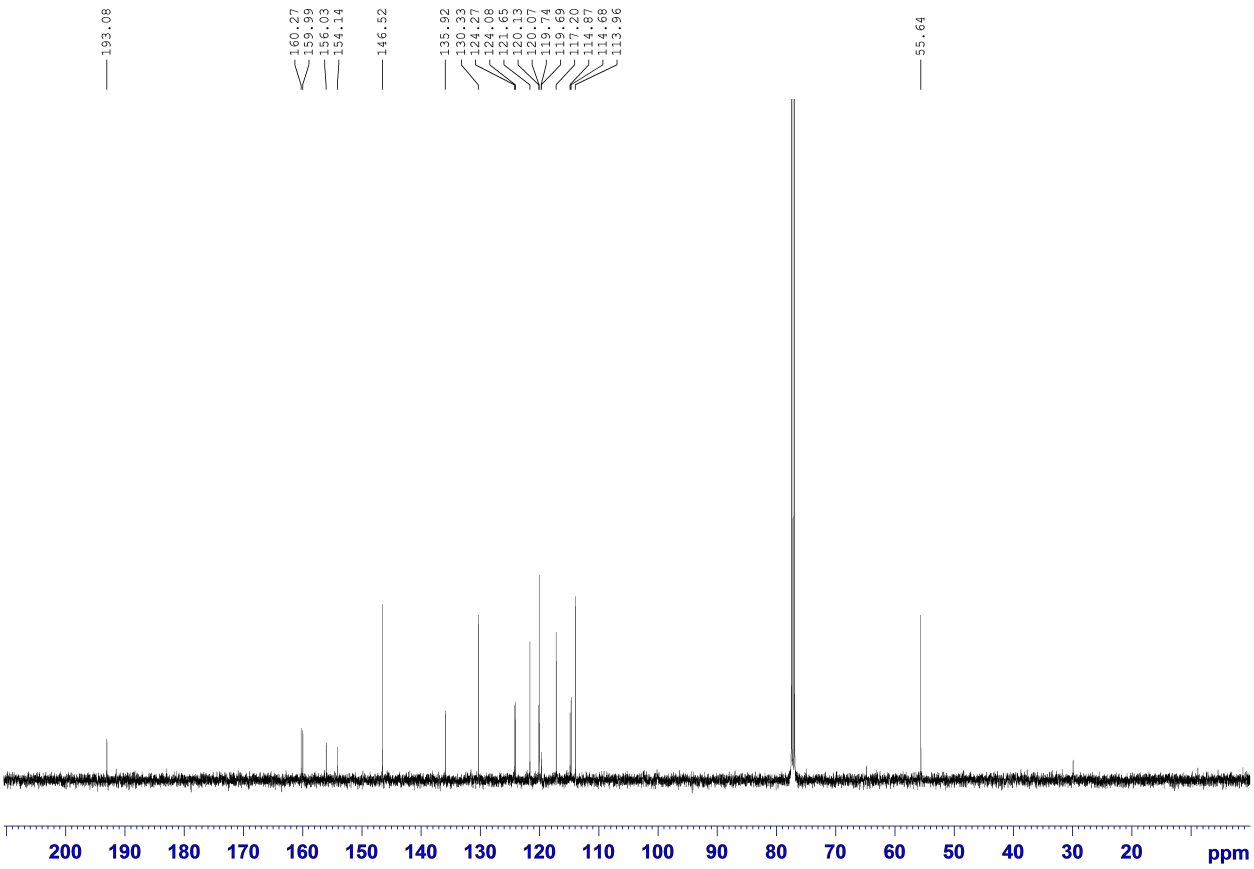
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1v)



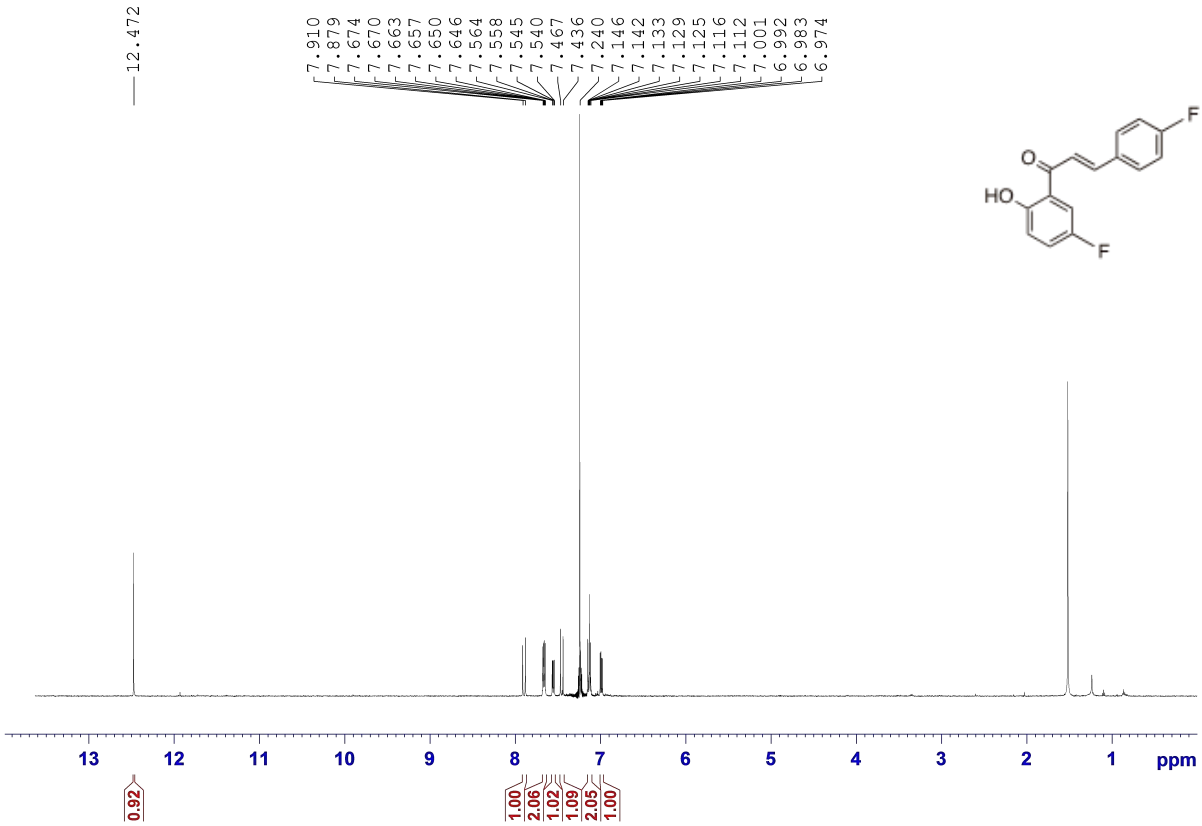
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1w)



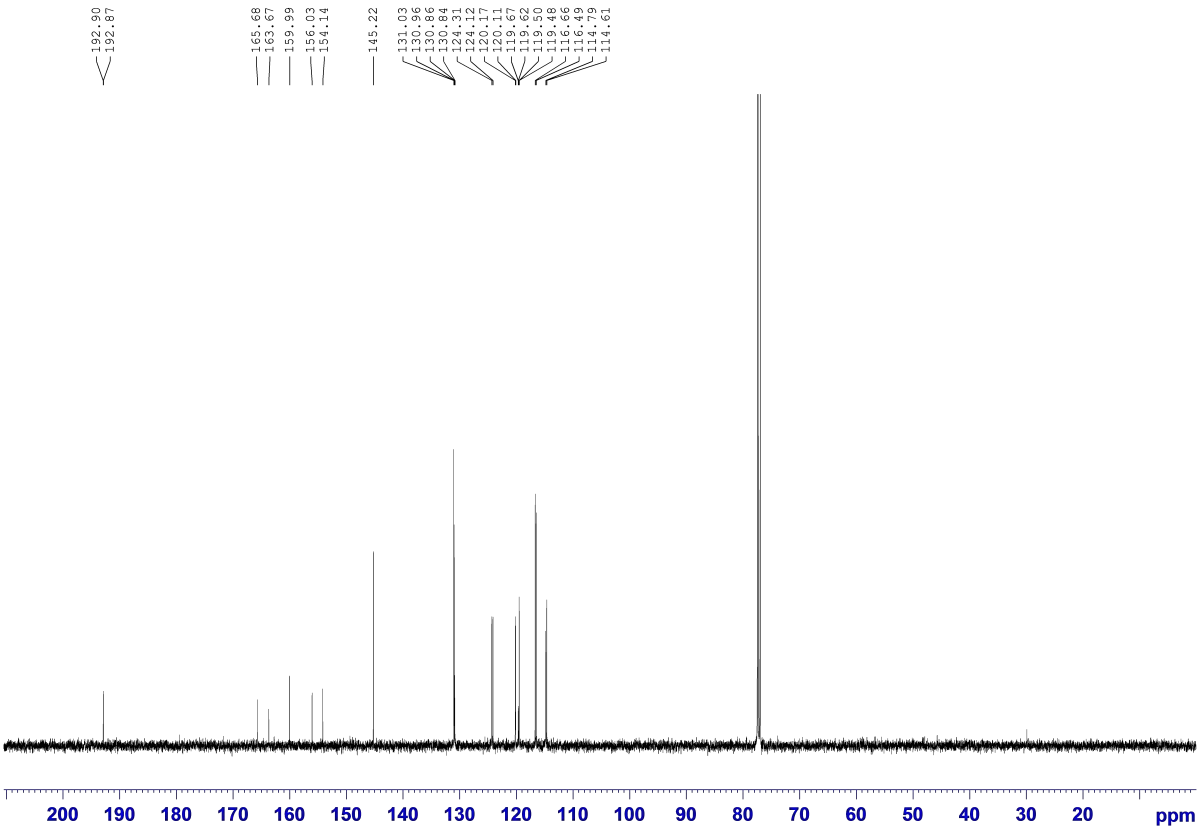
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (1w)



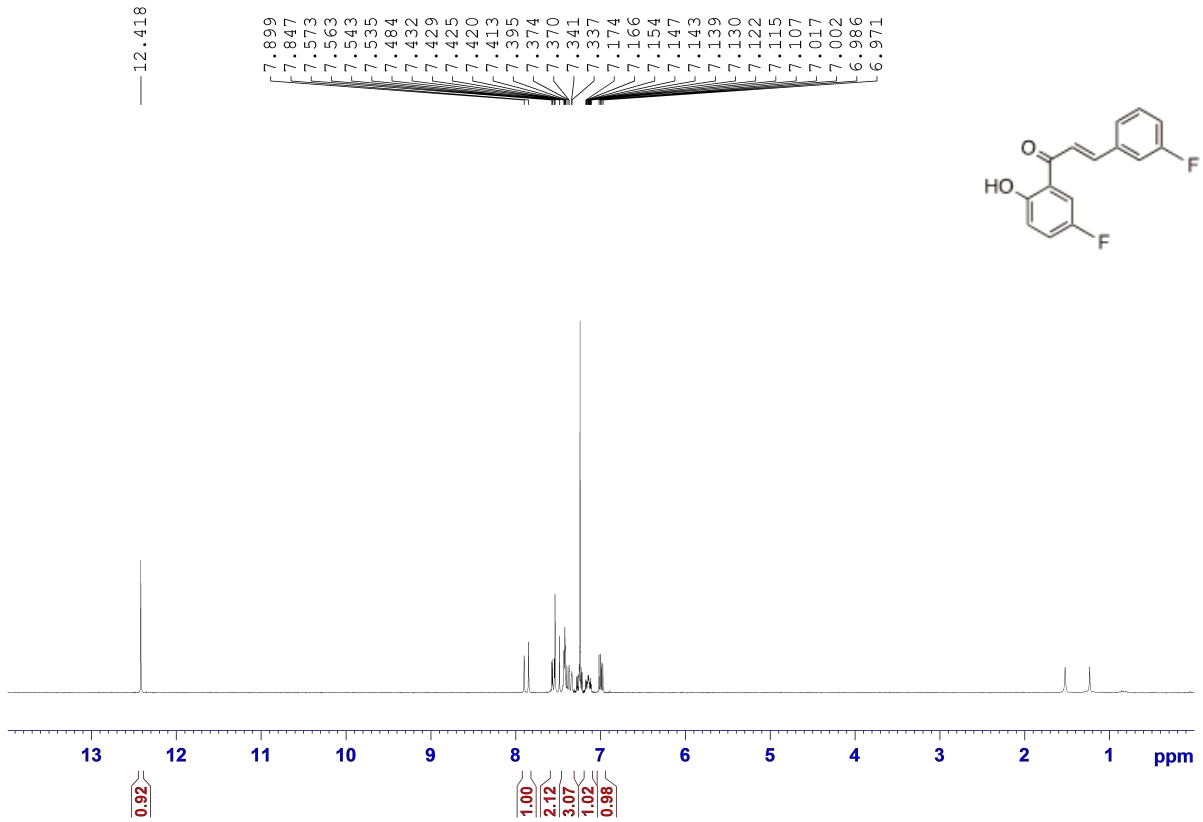
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1x)



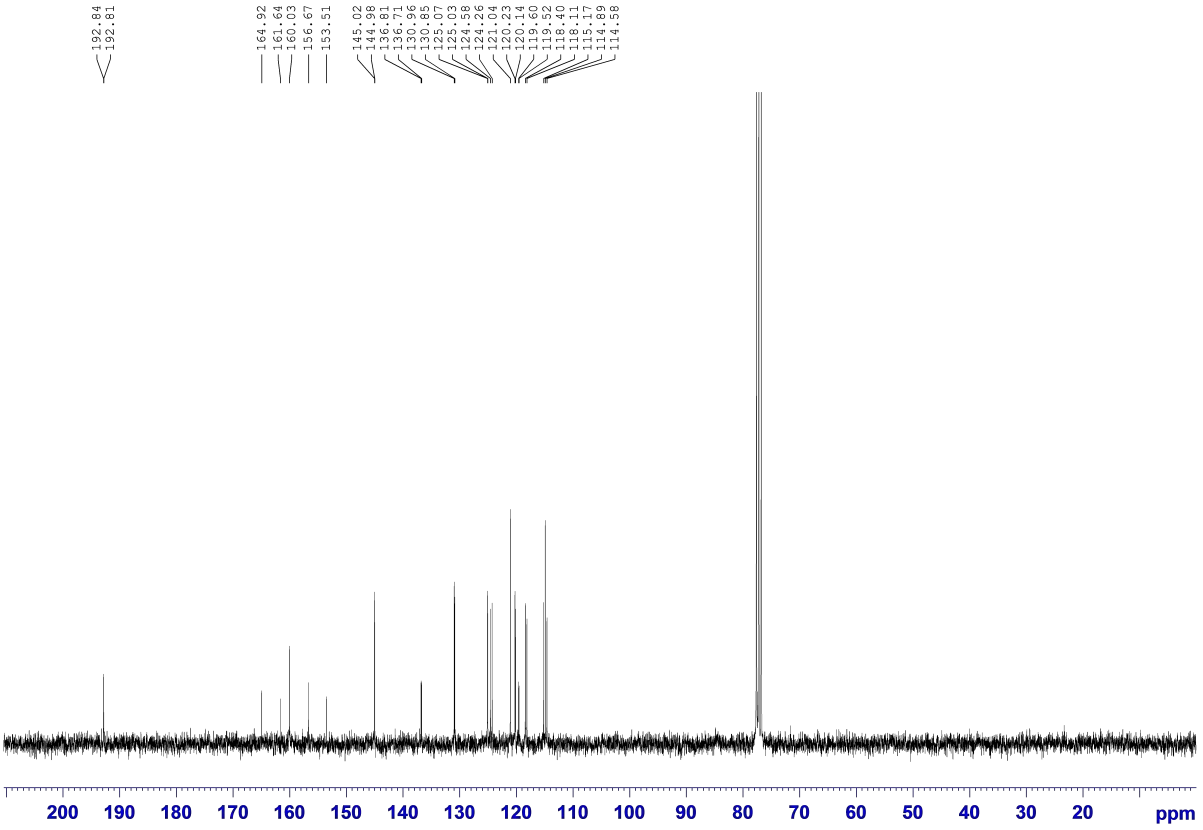
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (1x)



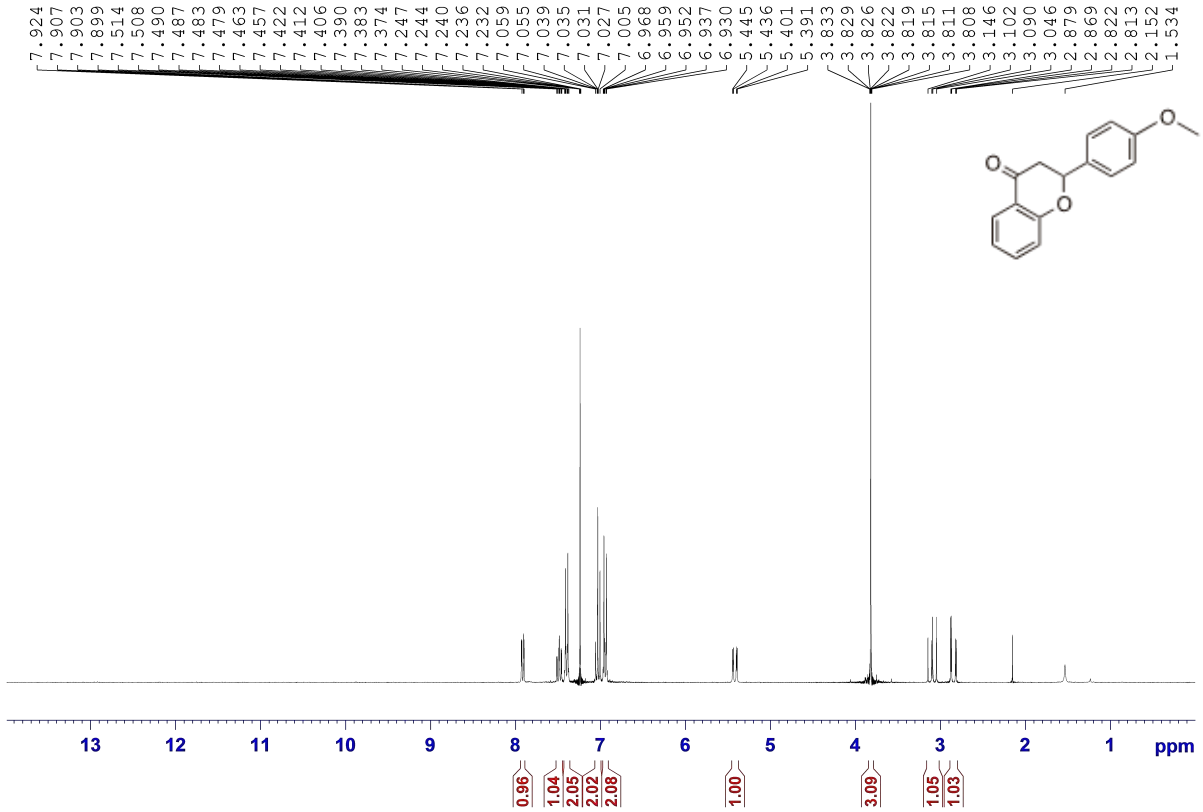
^{1}H NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1y)



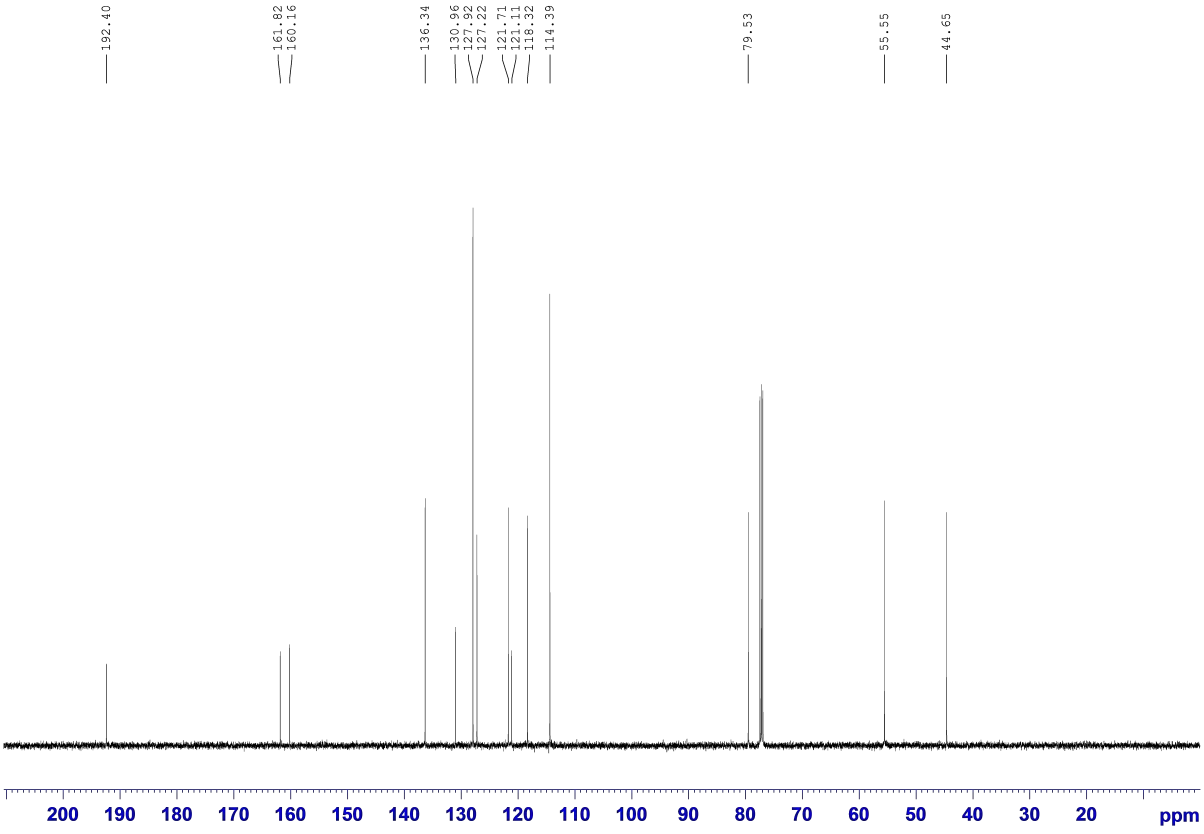
^{13}C NMR Spectrum of (*E*)-1-(2-Hydroxy-5-fluorophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (1y)



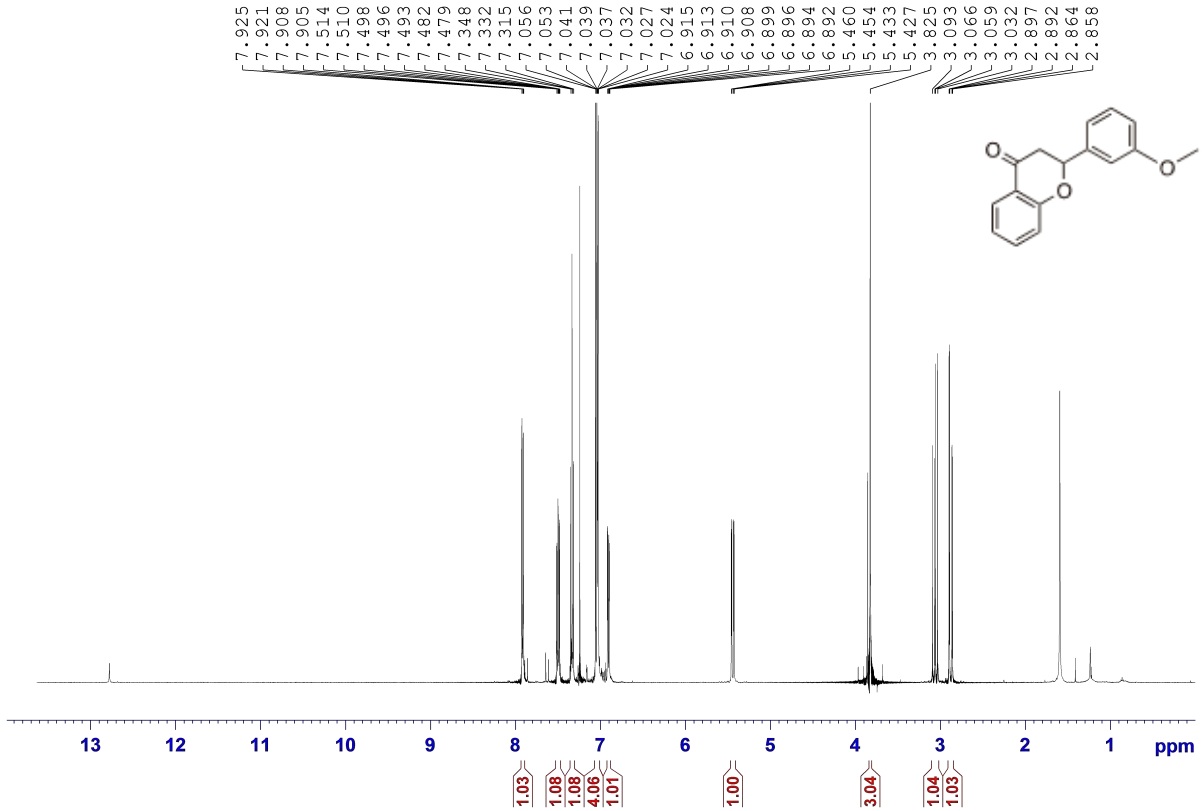
^{1}H NMR Spectrum of 2-(4-Methoxyphenyl)chroman-4-one (2b)



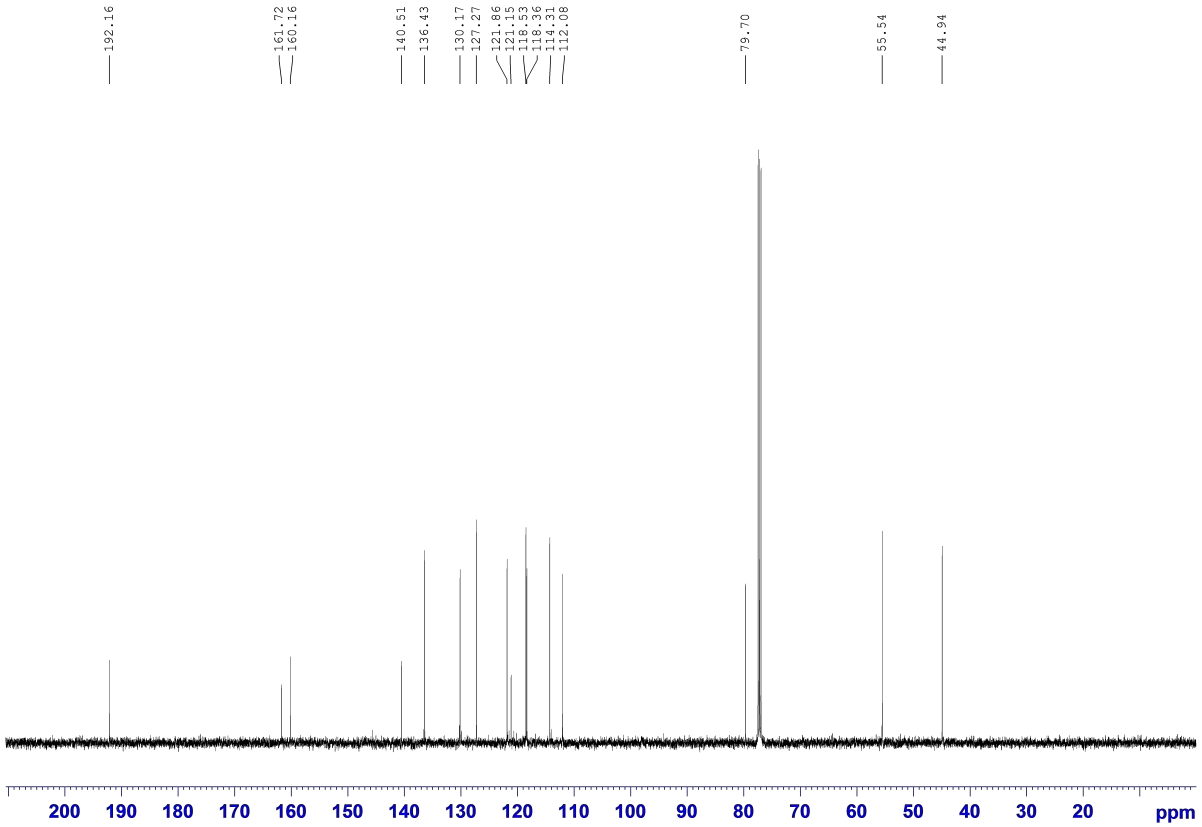
^{13}C NMR Spectrum of 2-(4-Methoxyphenyl)chroman-4-one (2b)



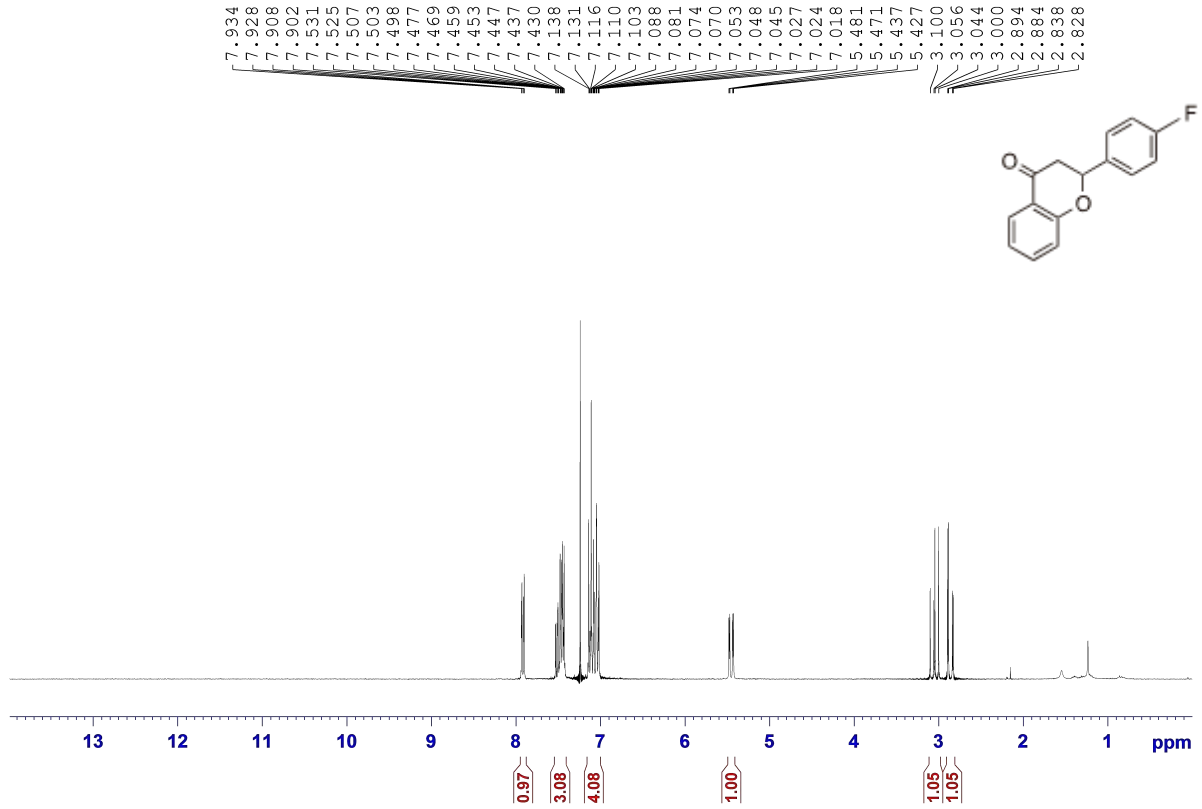
[1]H NMR Spectrum of 2-(3-Methoxyphenyl)chroman-4-one (2c)



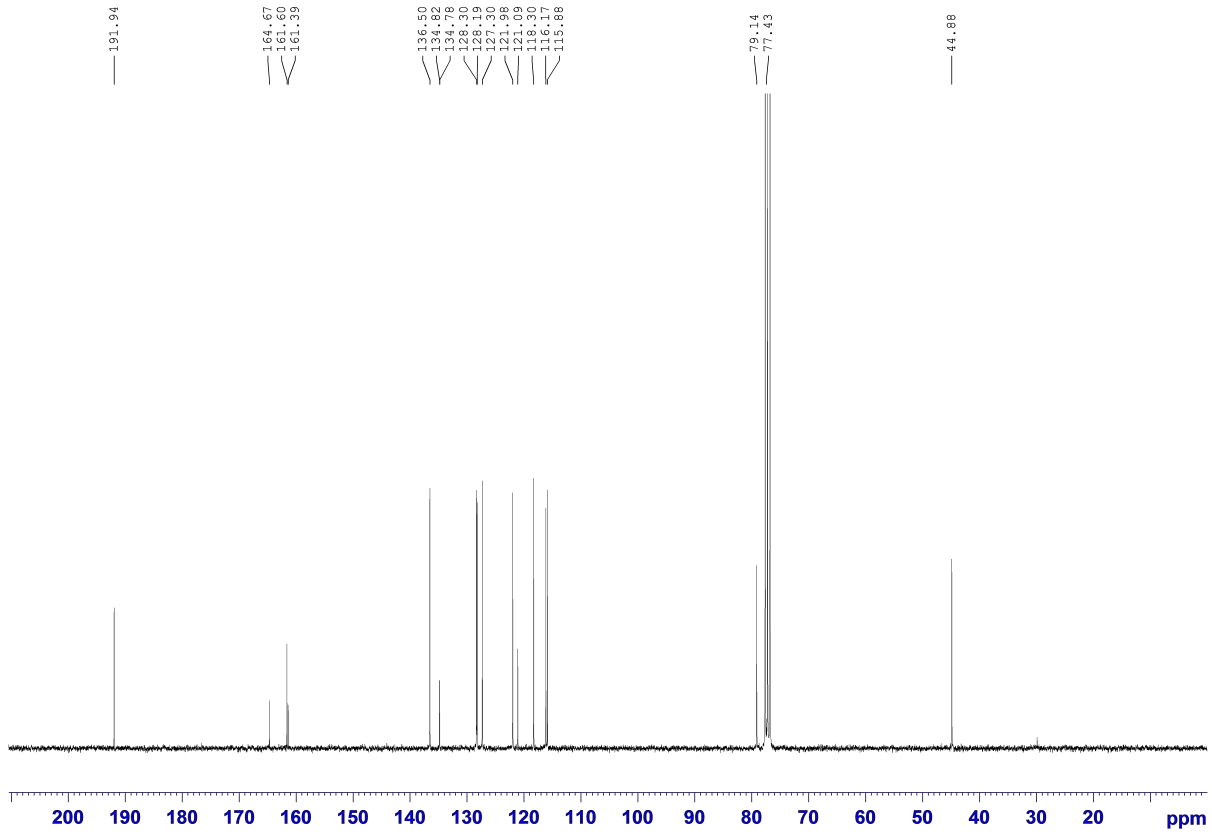
[13]C NMR Spectrum of 2-(3-Methoxyphenyl)chroman-4-one (2c)



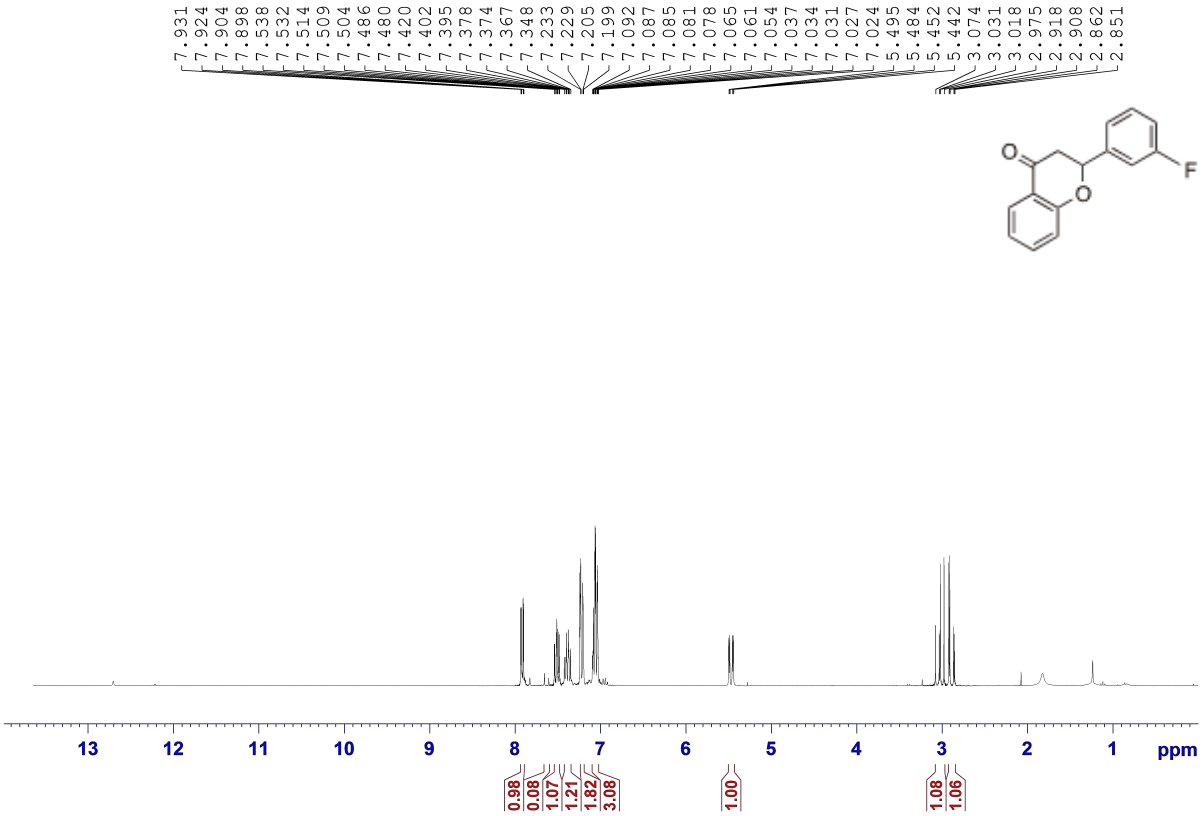
^{1}H NMR Spectrum of 2-(4-Fluorophenyl)chroman-4-one (2d)



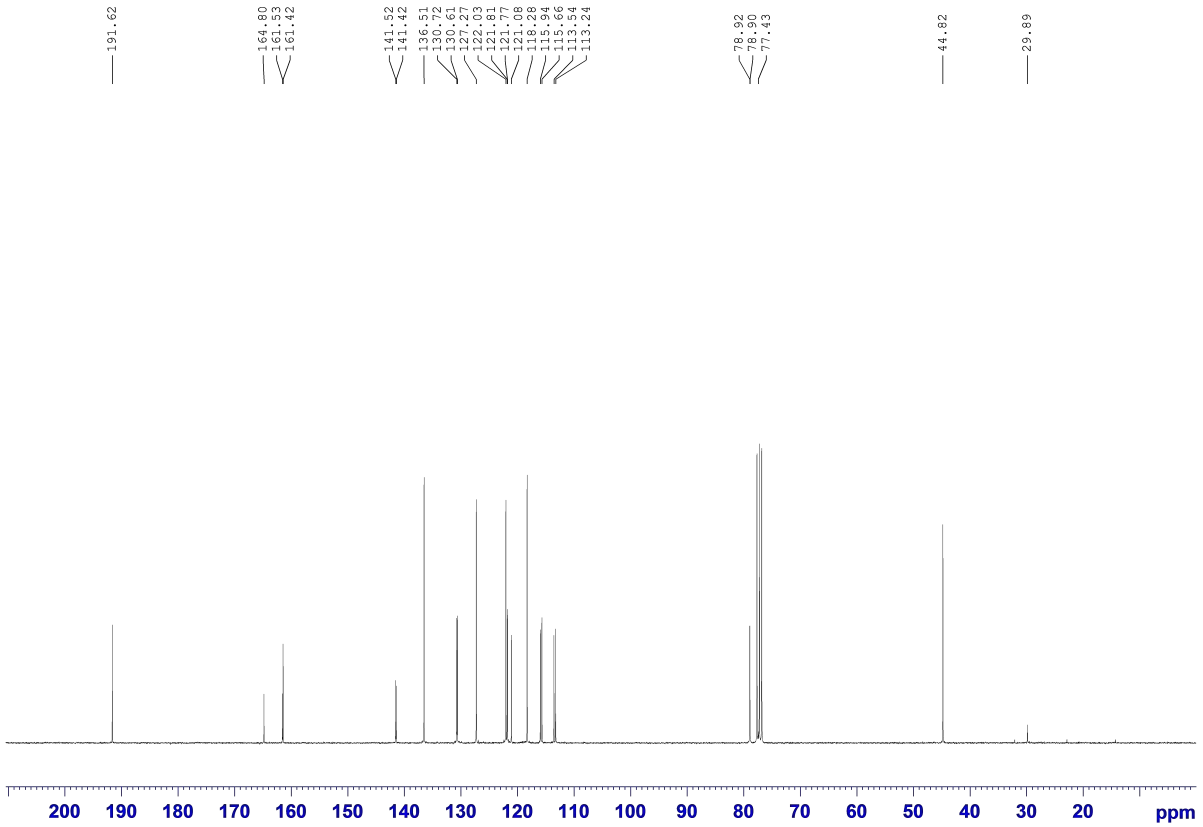
^{13}C NMR Spectrum of 2-(4-Fluorophenyl)chroman-4-one (2d)



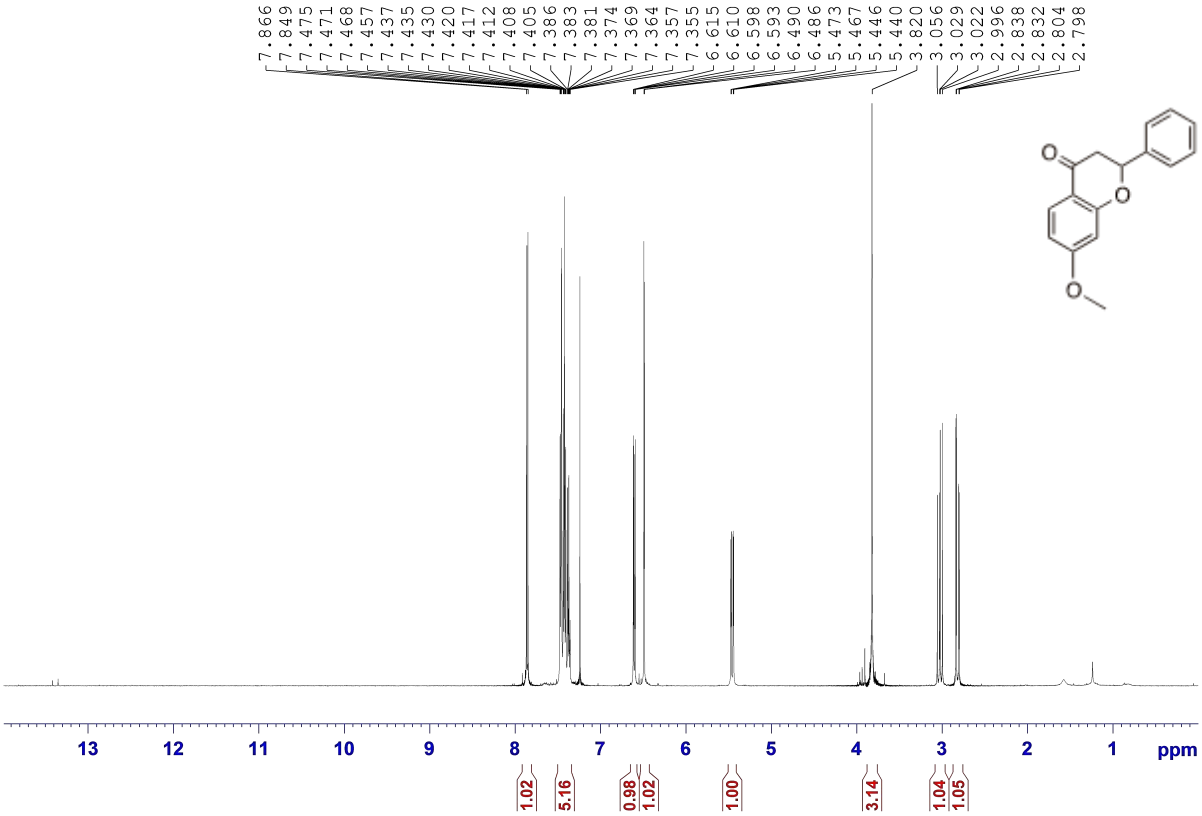
[1]H NMR Spectrum of 2-(3-Fluorophenyl)chroman-4-one (2e)



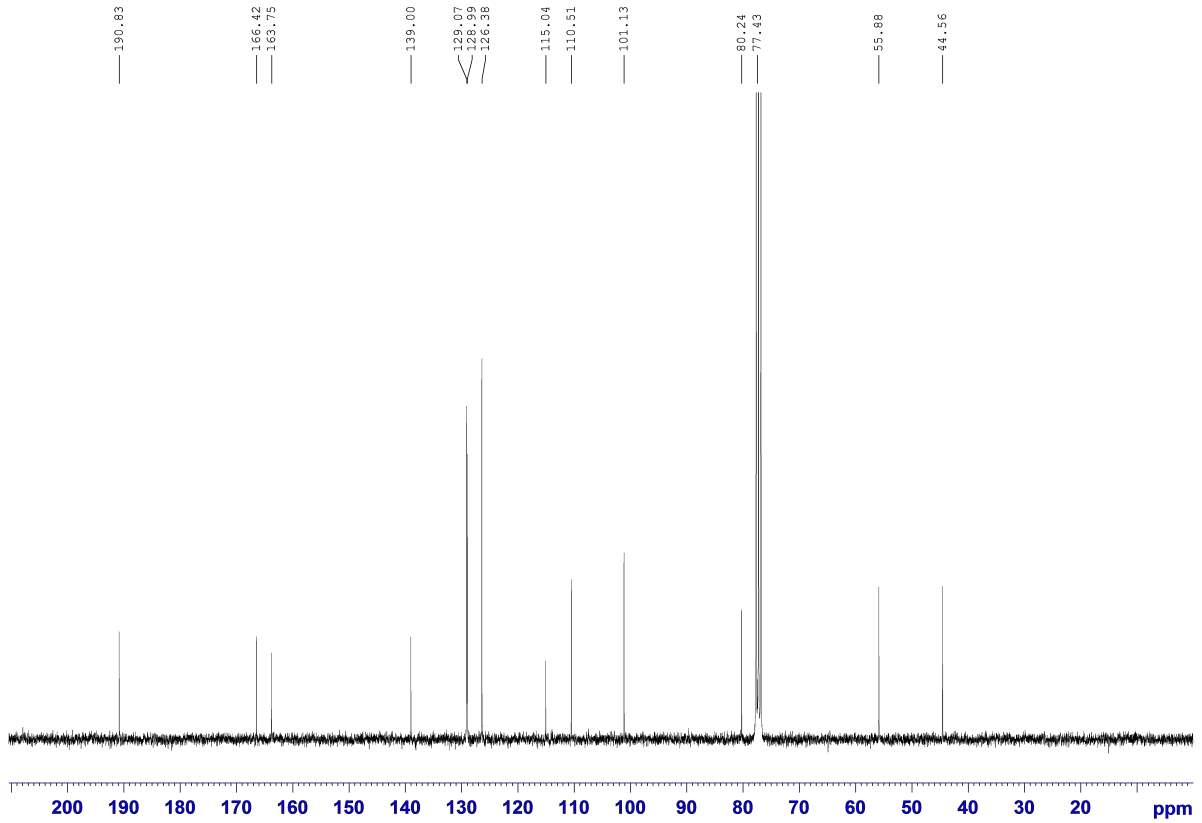
[13]C NMR Spectrum of 2-(3-Fluorophenyl)chroman-4-one (2e)



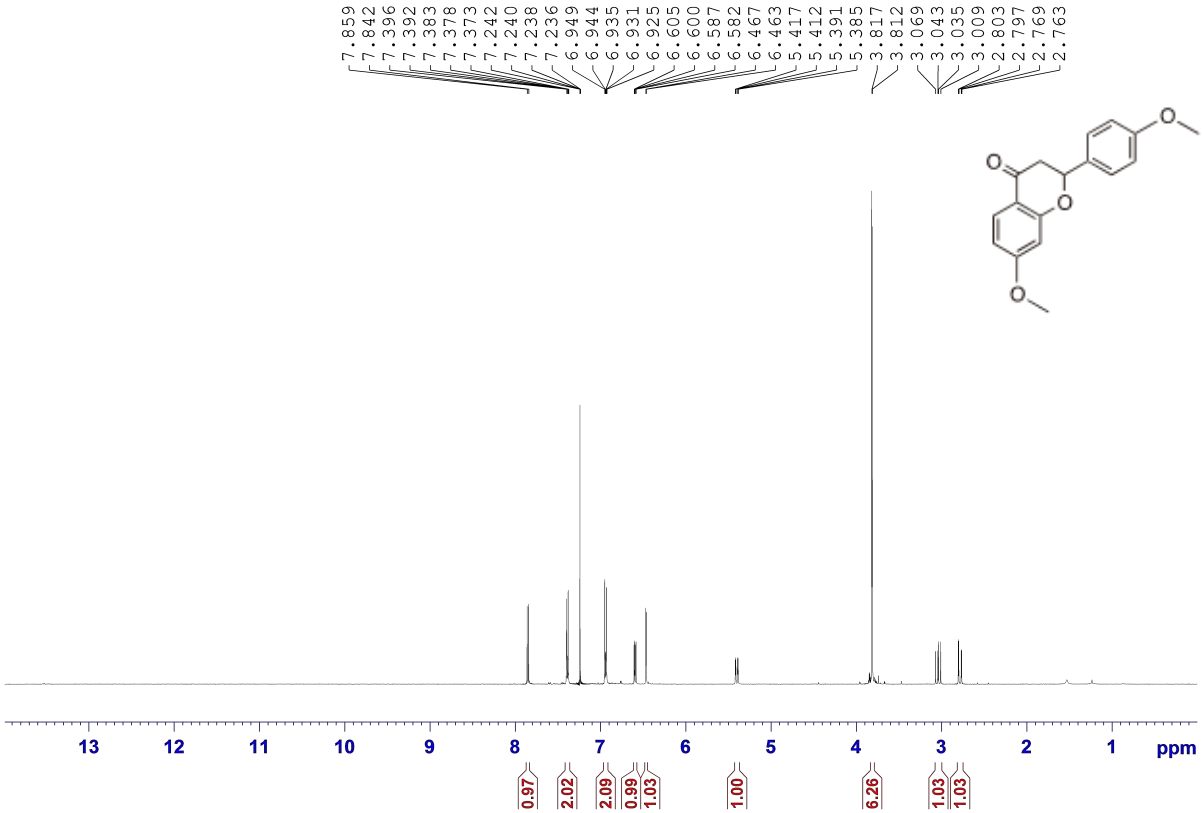
^{1}H NMR Spectrum of 7-Methoxy-2-phenylchroman-4-one (2f)



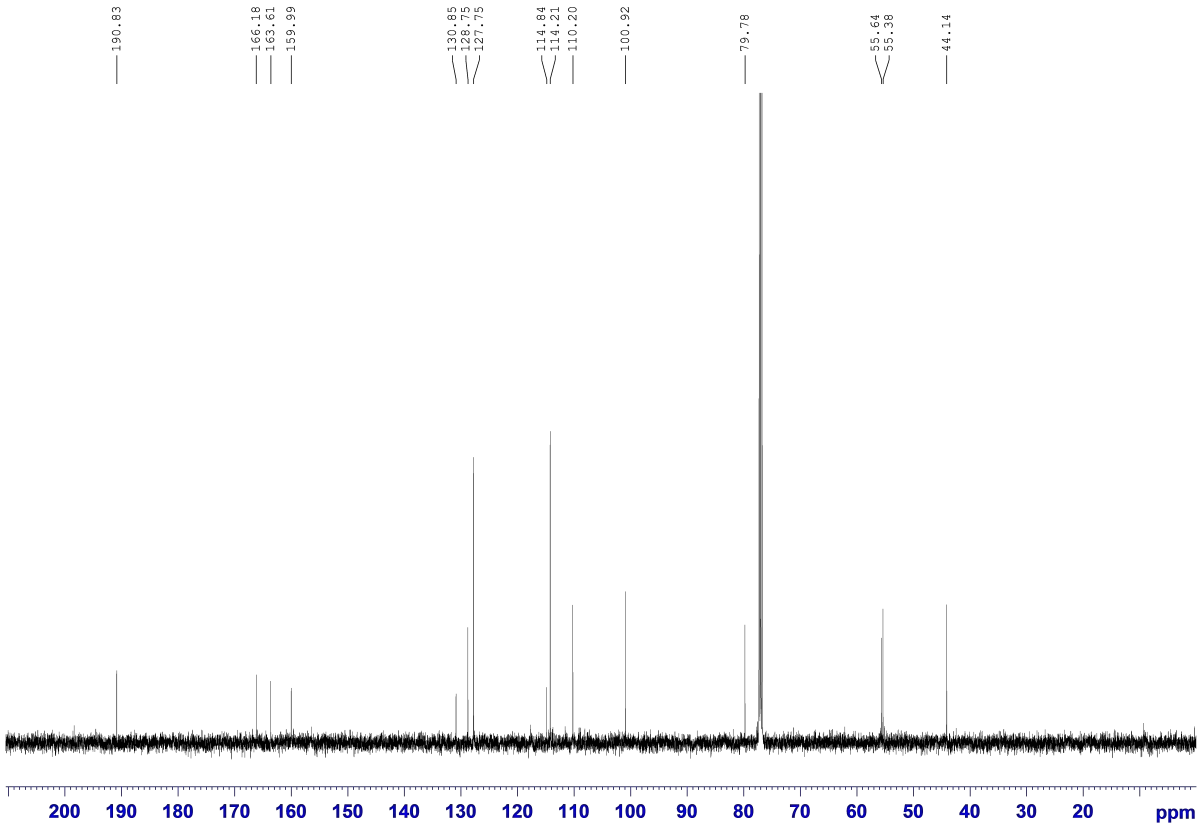
^{13}C NMR Spectrum of 7-Methoxy-2-phenylchroman-4-one (2f)



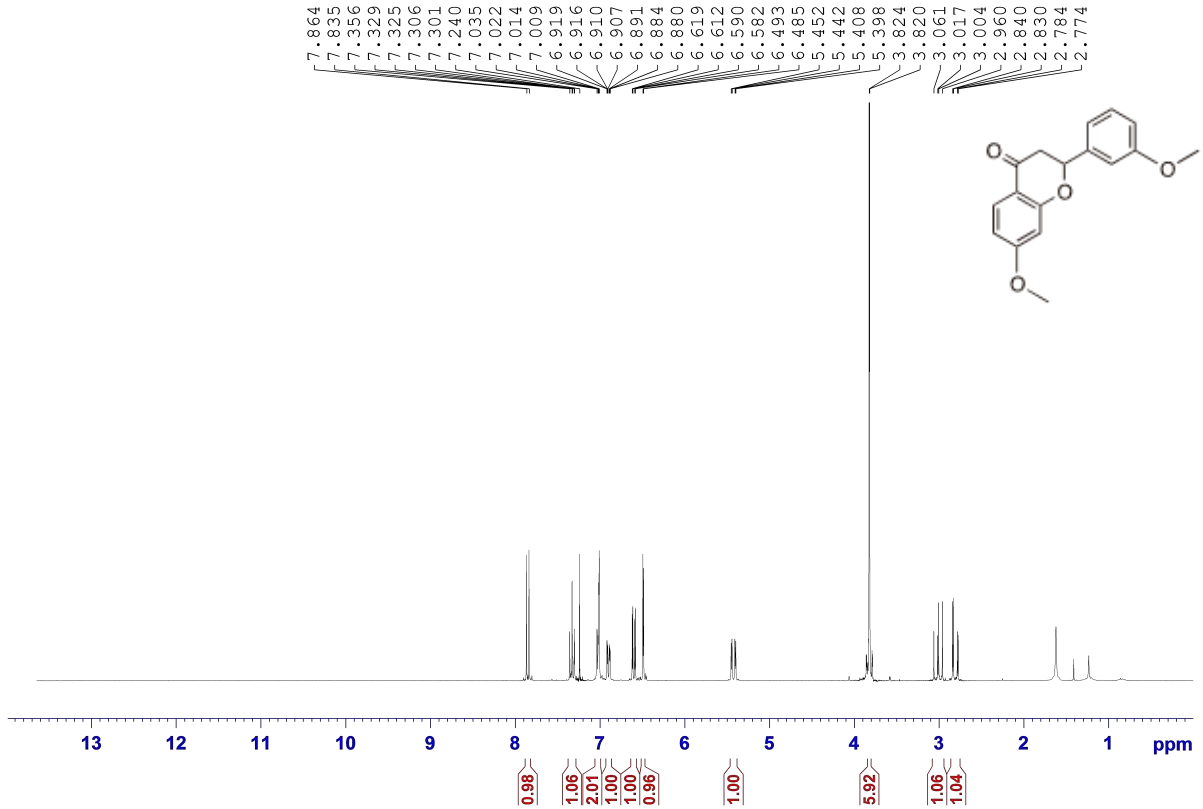
^{1}H NMR Spectrum of 7-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2g)



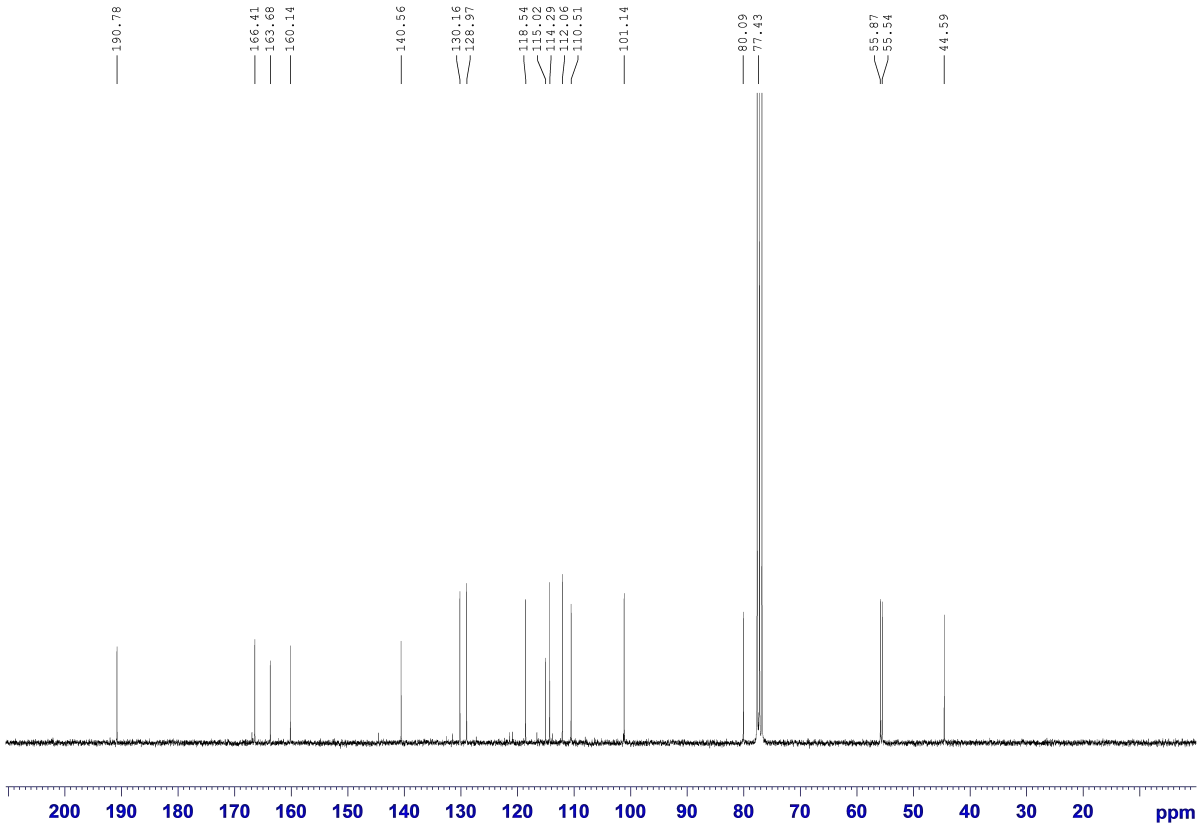
^{13}C NMR Spectrum of 7-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2g)



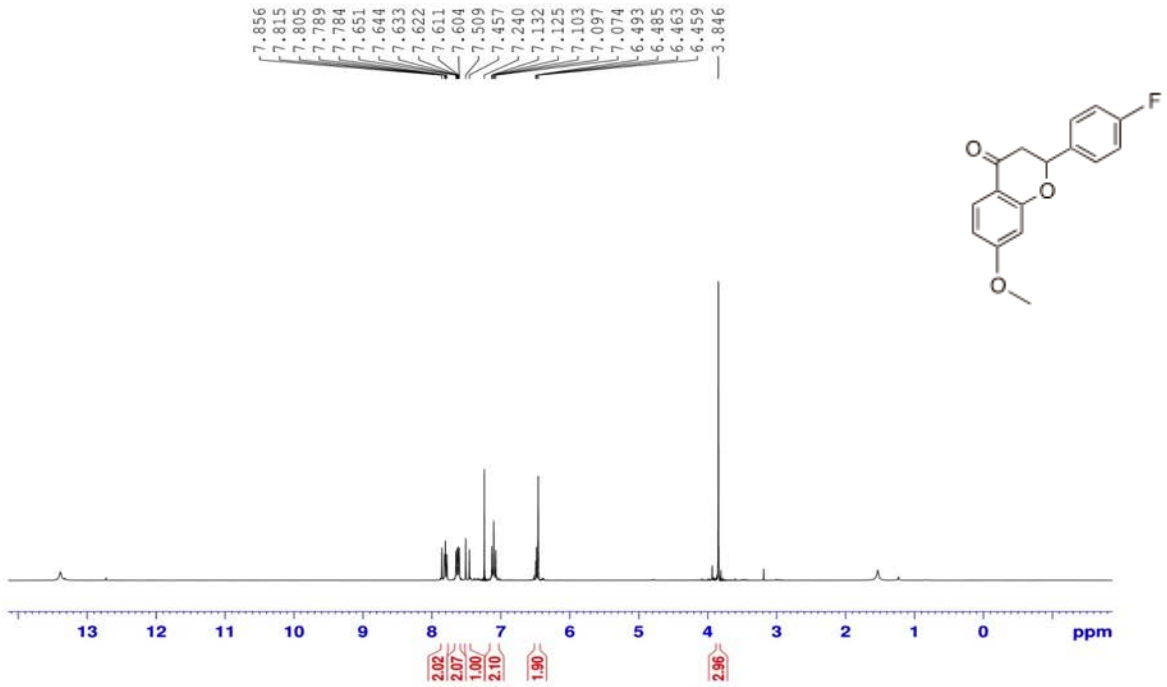
^{1}H NMR Spectrum of 7-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2h)



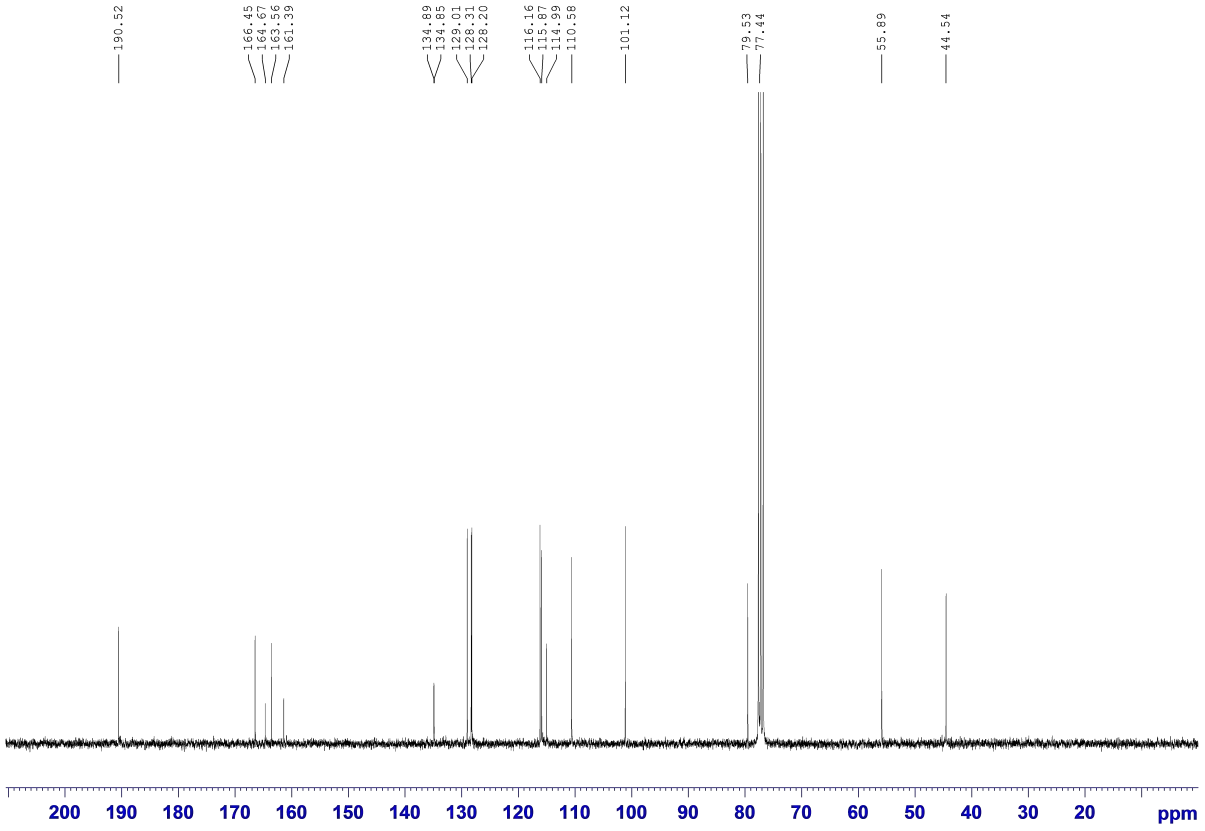
^{13}C NMR Spectrum of 7-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2h)



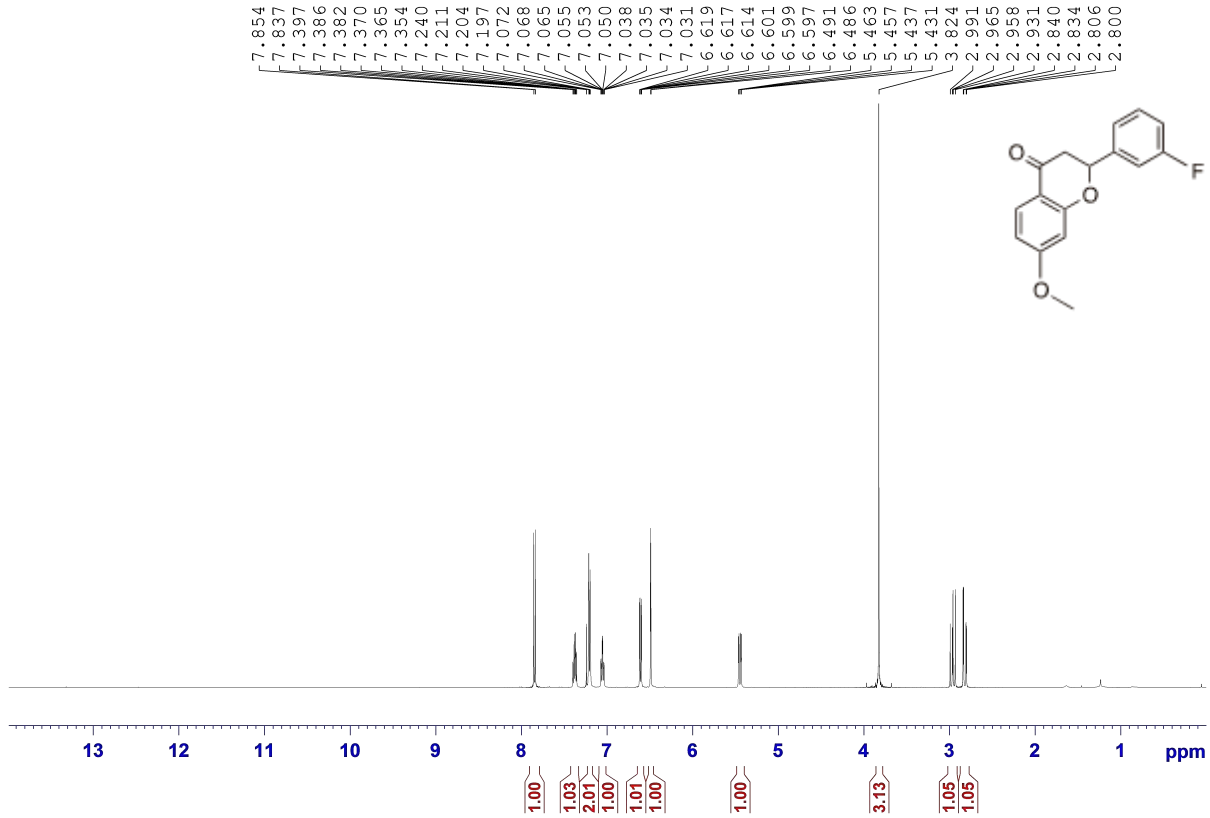
^{1}H NMR Spectrum of 2-(4-Fluorophenyl)-7-methoxychroman-4-one (2i)



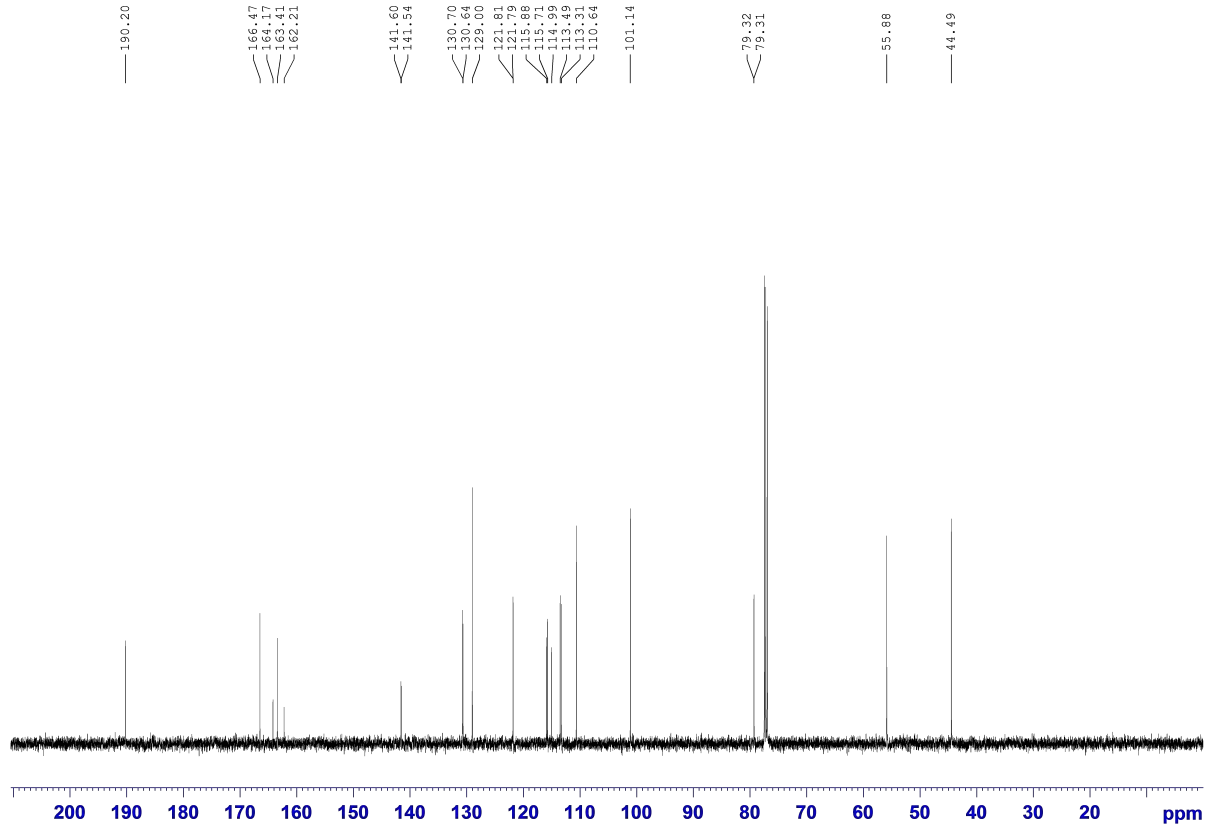
^{13}C NMR Spectrum of 2-(4-Fluorophenyl)-7-methoxychroman-4-one (2i)



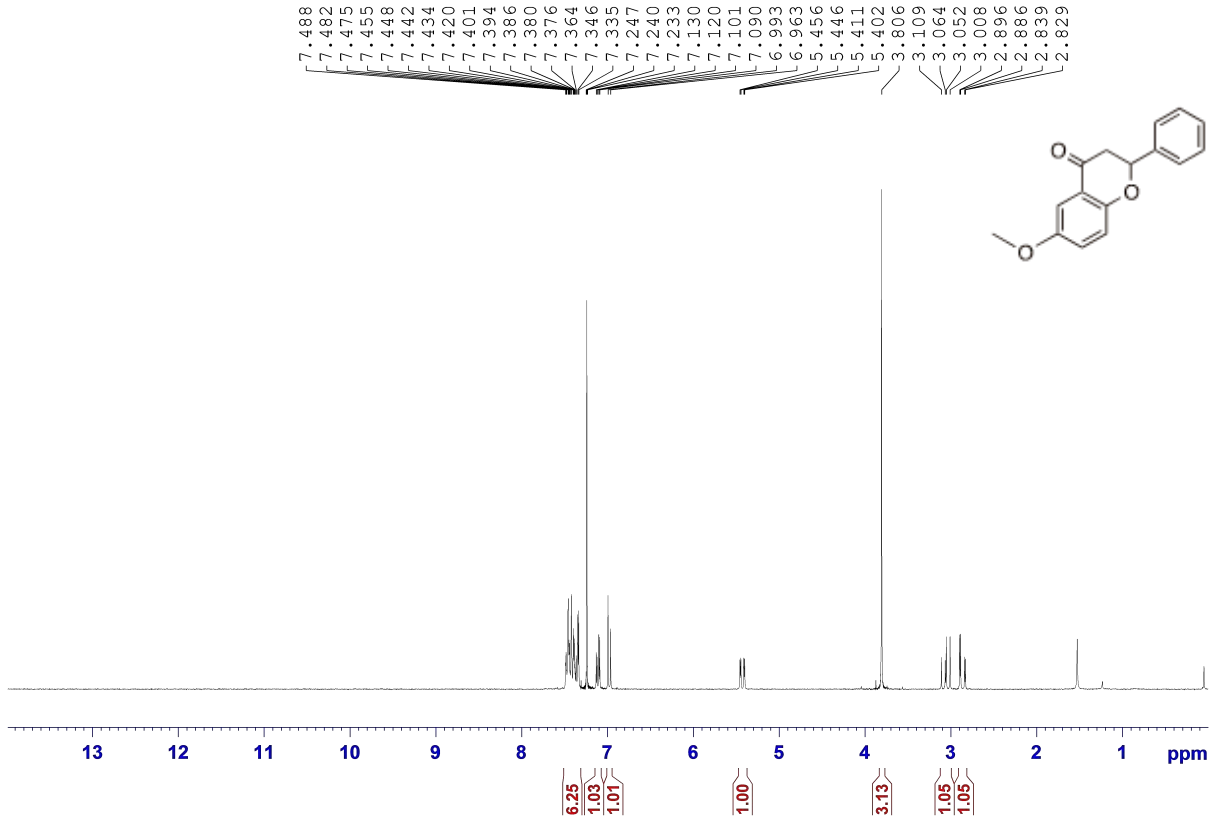
^{1}H NMR Spectrum of 2-(3-Fluorophenyl)-7-methoxychroman-4-one (2j)



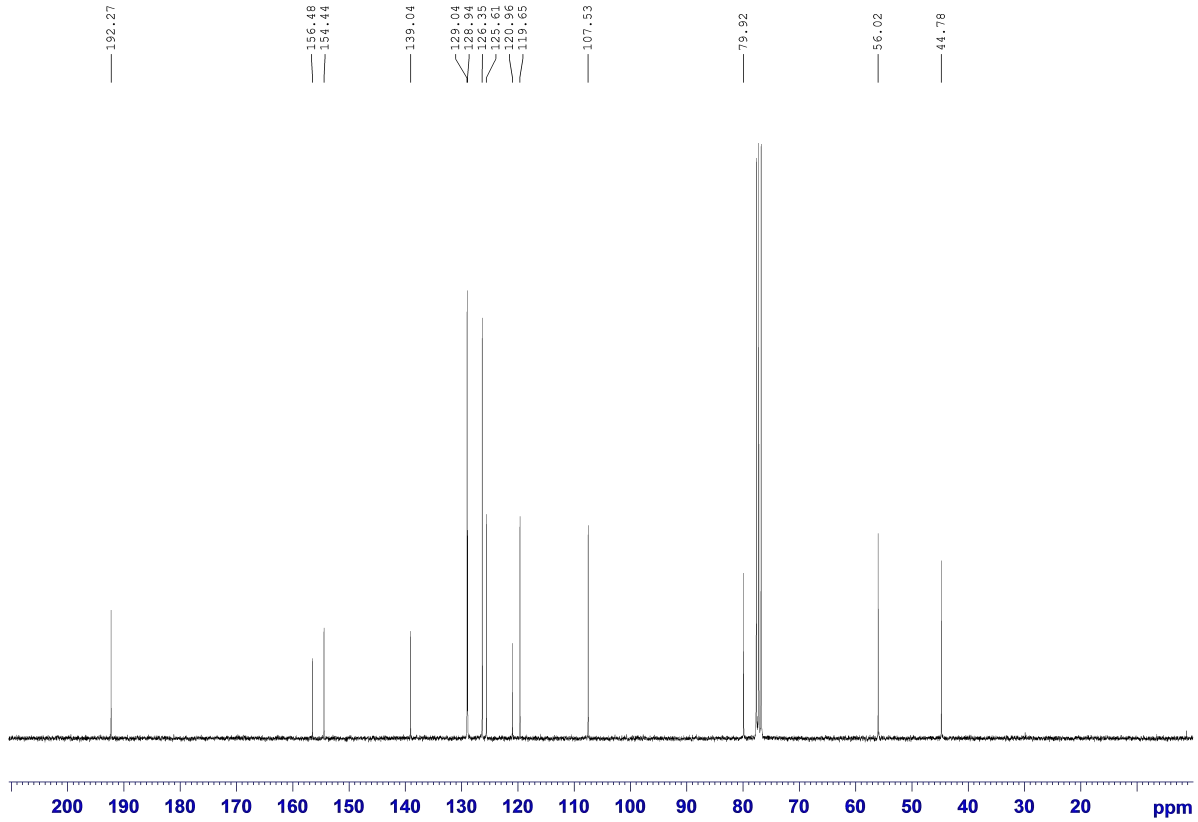
^{13}C NMR Spectrum of 2-(3-Fluorophenyl)-7-methoxychroman-4-one (2j)



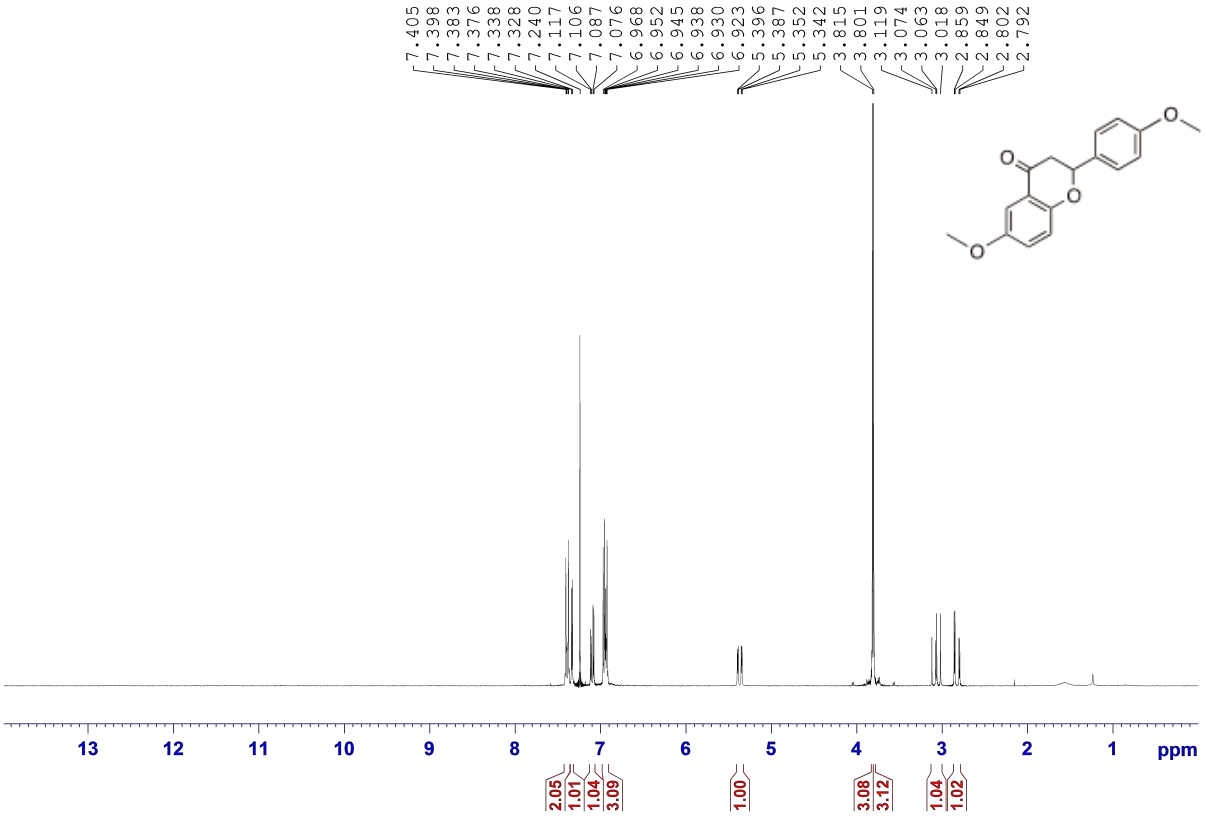
^{1}H NMR Spectrum of 6-Methoxy-2-phenylchroman-4-one (2k)



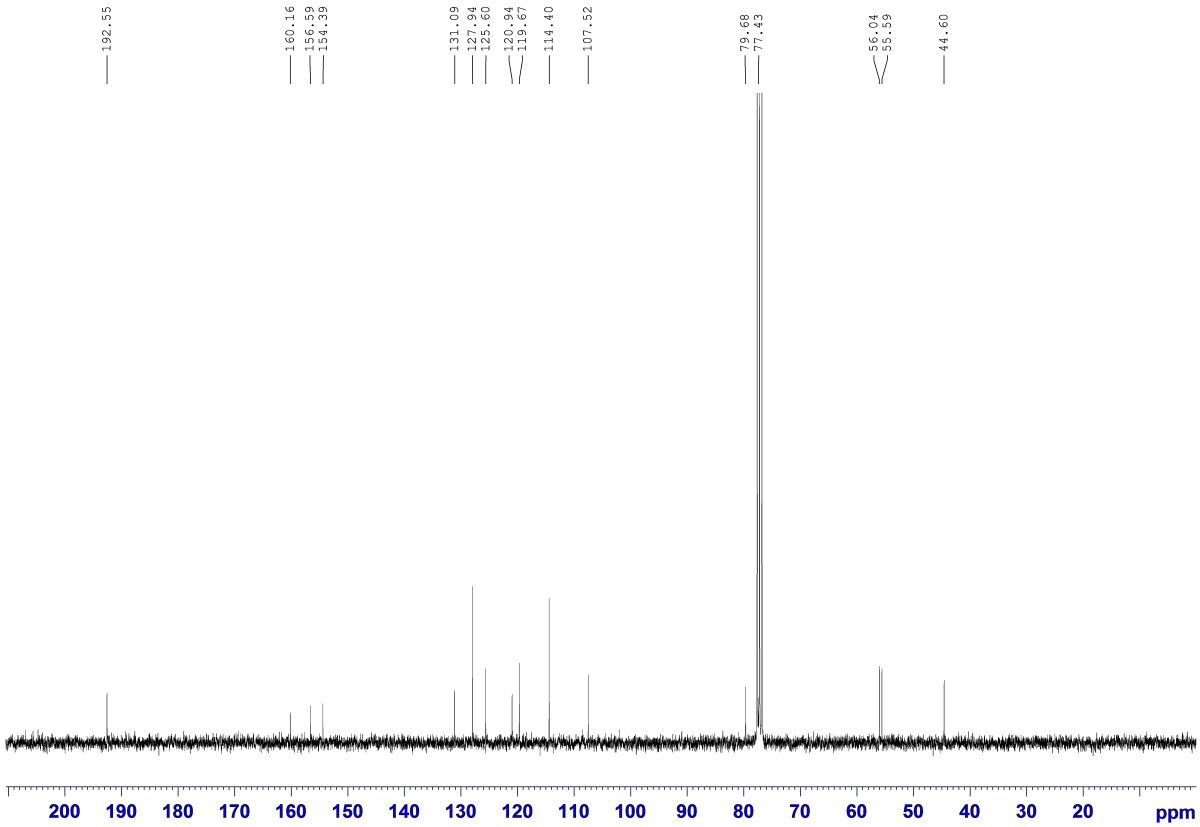
^{13}C NMR Spectrum of 6-Methoxy-2-phenylchroman-4-one (2k)



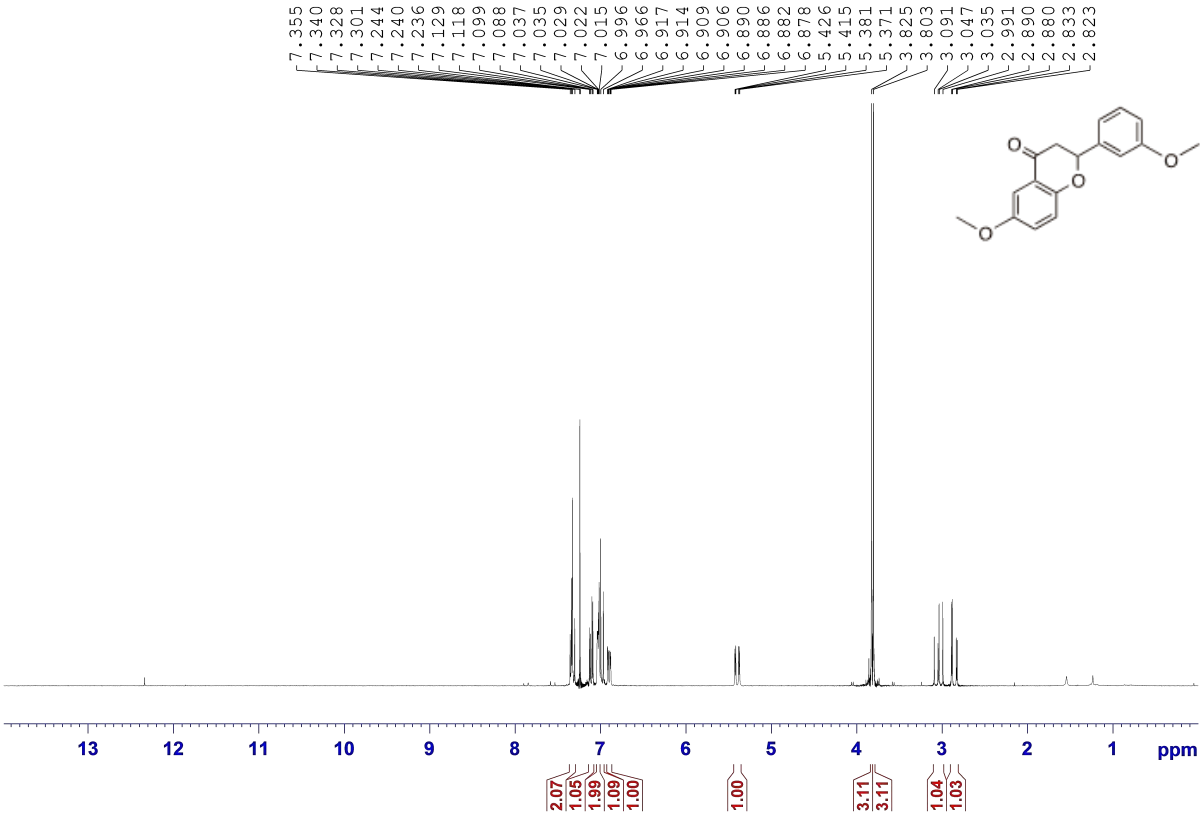
^{1}H NMR Spectrum of 6-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2l)



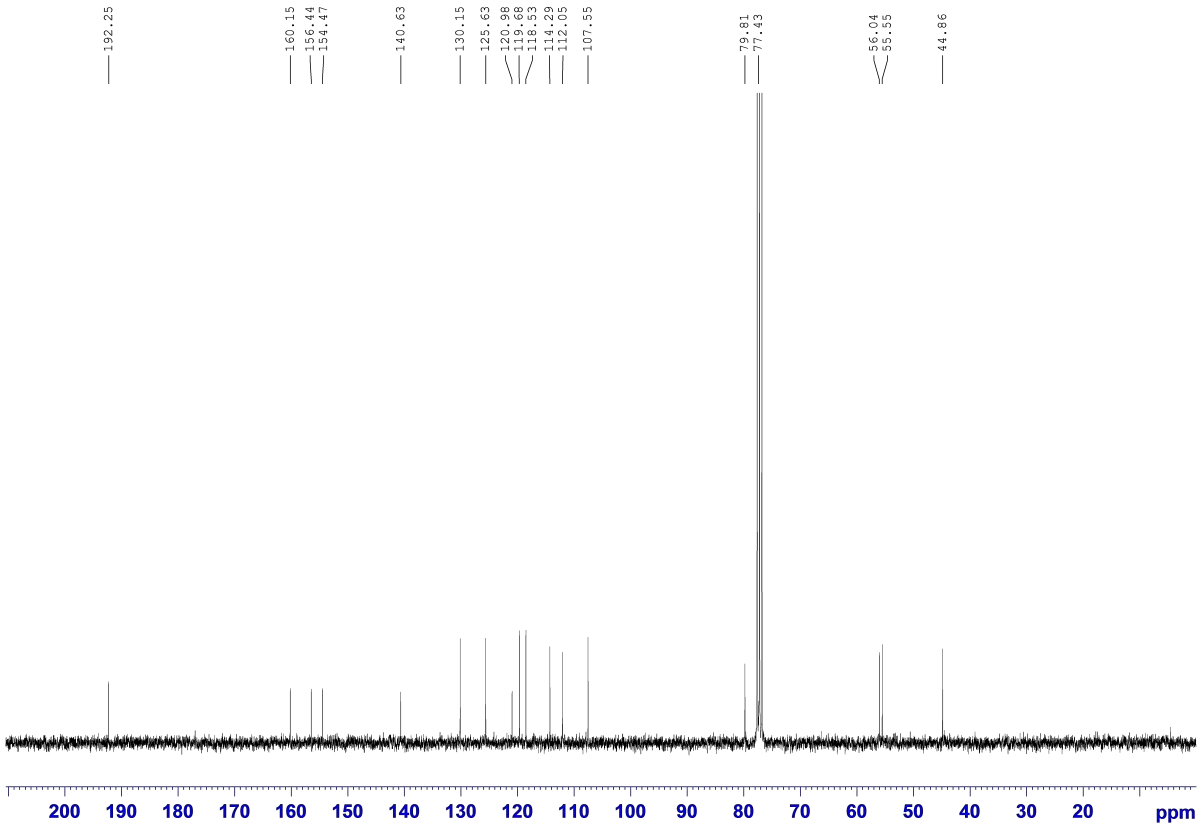
^{13}C NMR Spectrum of 6-Methoxy-2-(4-methoxyphenyl)chroman-4-one (2l)



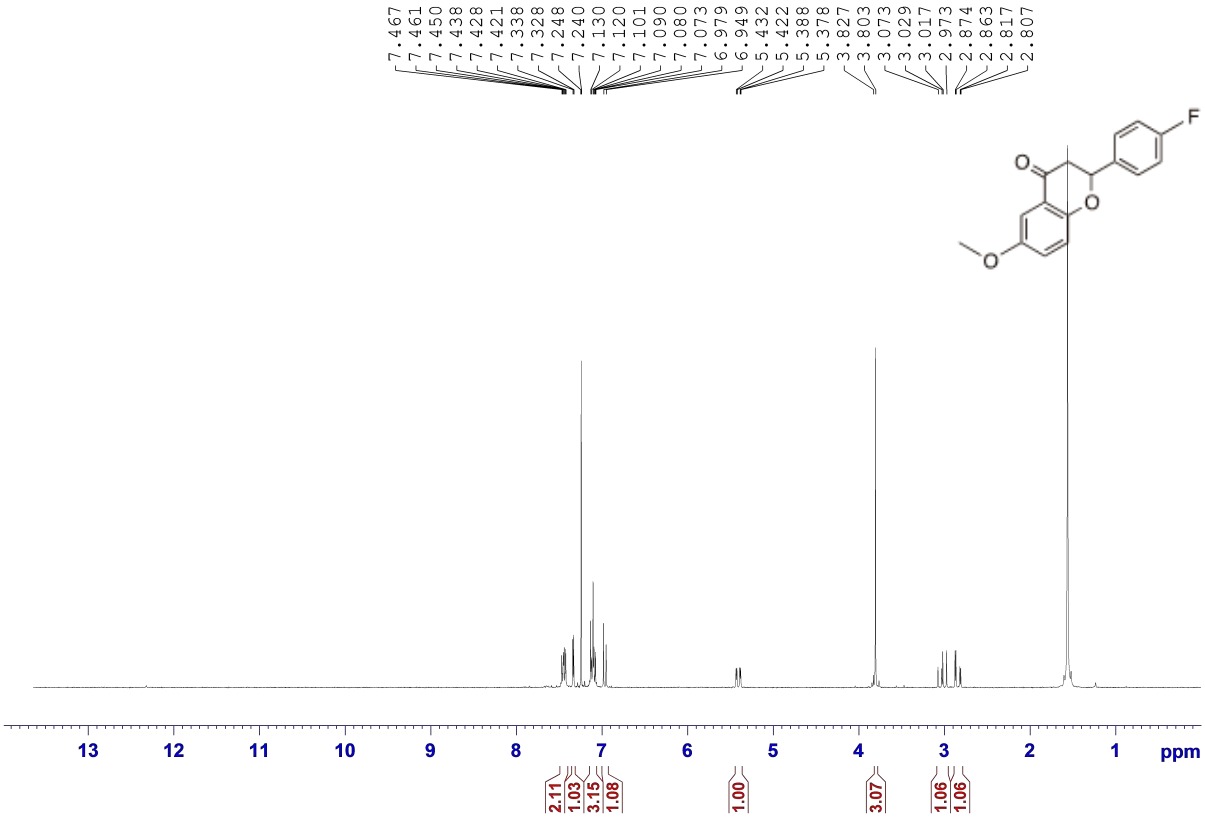
^{1}H NMR Spectrum of 6-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2m)



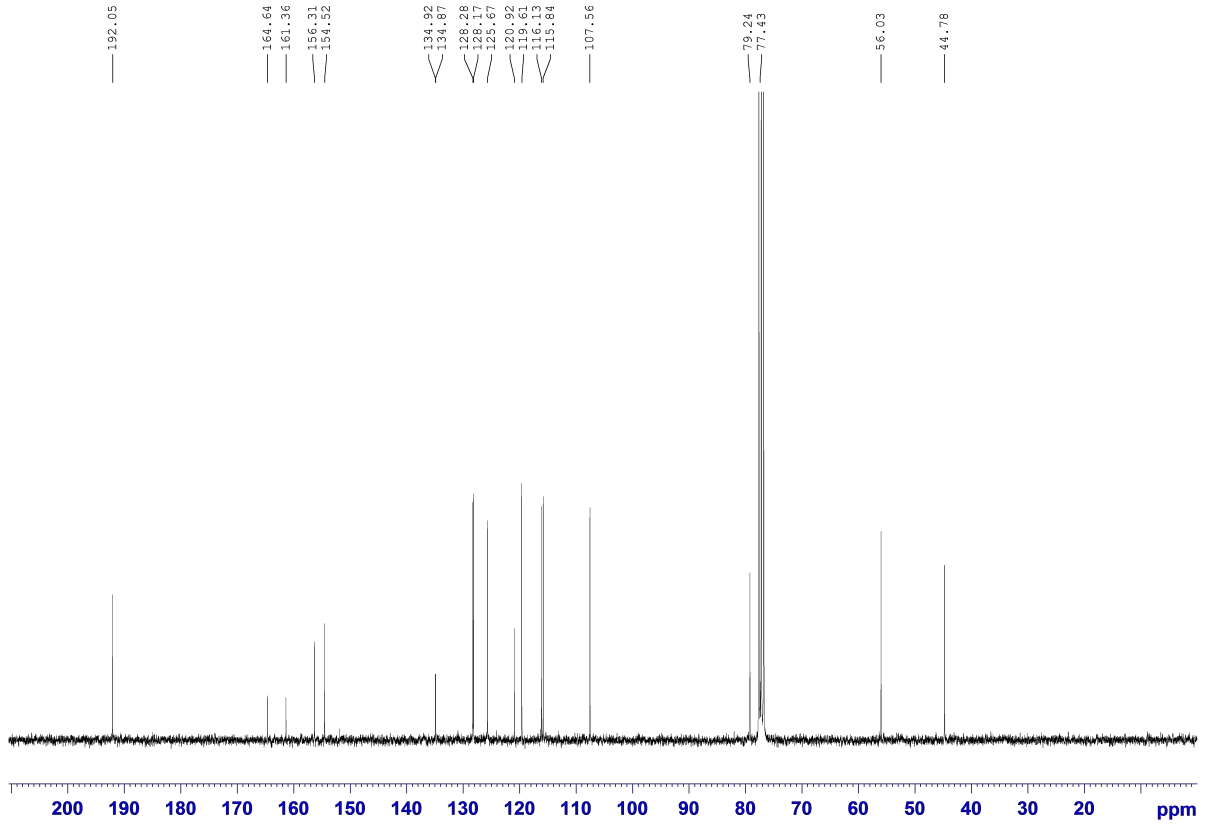
^{13}C NMR Spectrum of 6-Methoxy-2-(3-methoxyphenyl)chroman-4-one (2m)



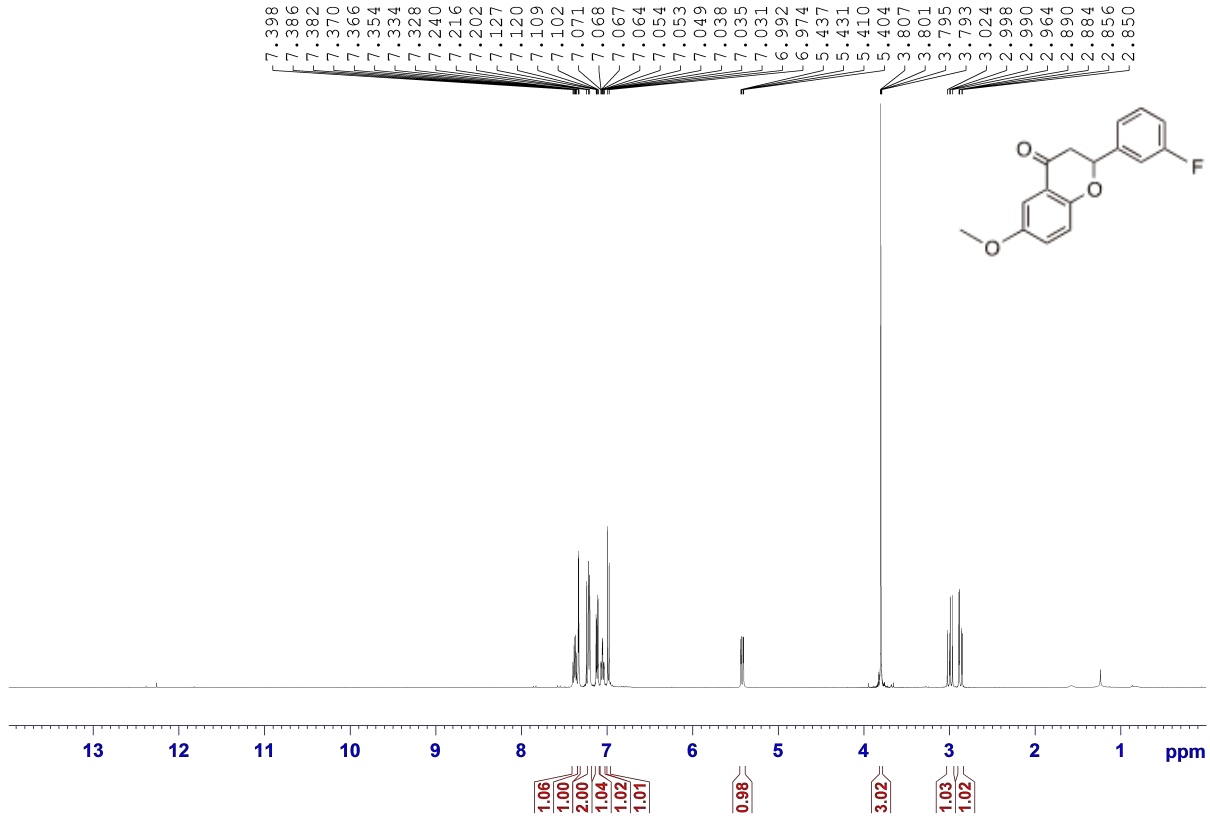
^{1}H NMR Spectrum of 2-(4-Fluorophenyl)-6-methoxychroman-4-one (2n)



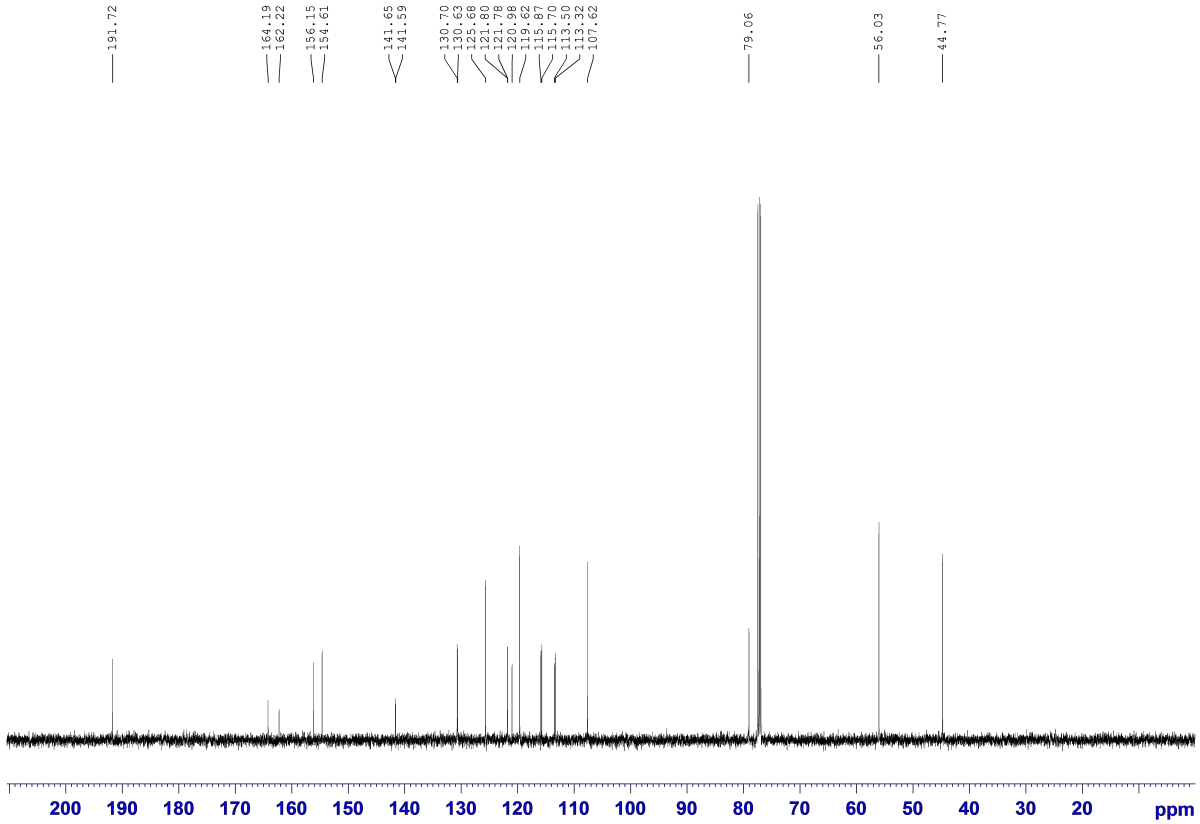
^{13}C NMR Spectrum of 2-(4-Fluorophenyl)-6-methoxychroman-4-one (2n)



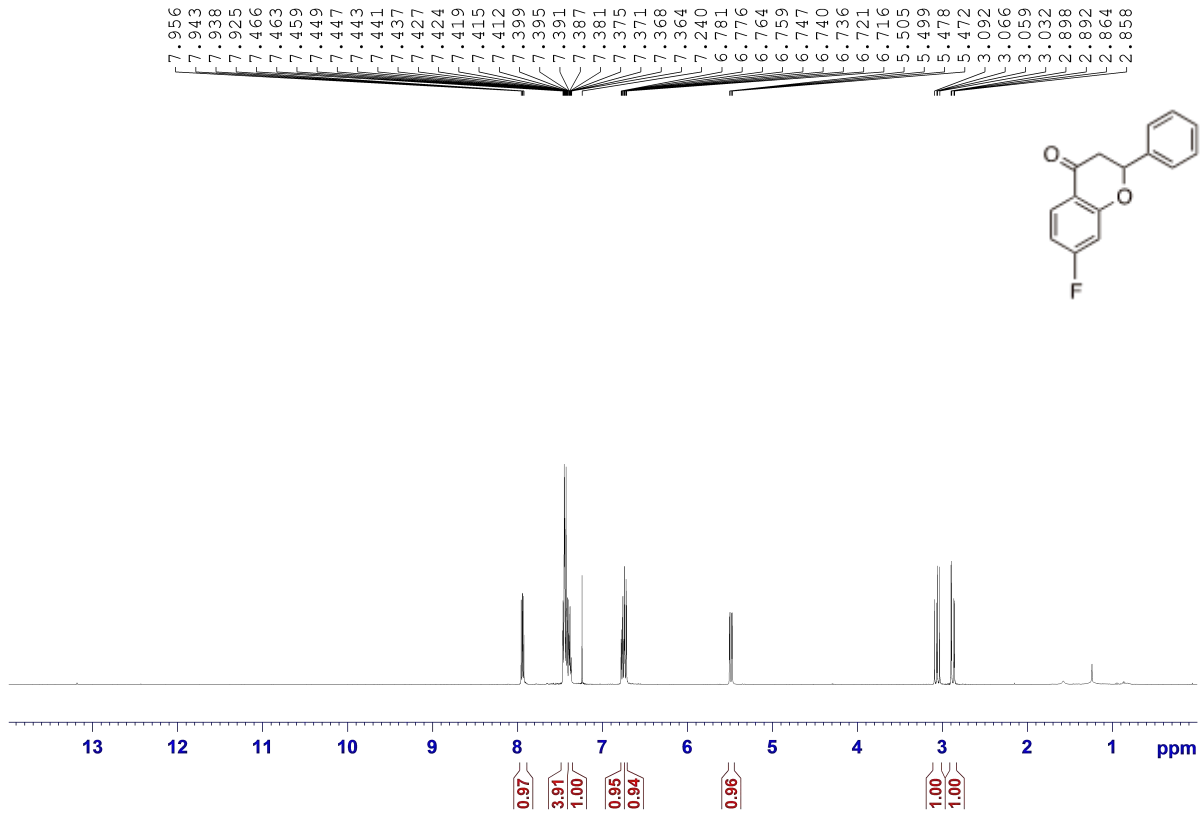
^{1}H NMR Spectrum of 2-(3-Fluorophenyl)-6-methoxychroman-4-one (2o)



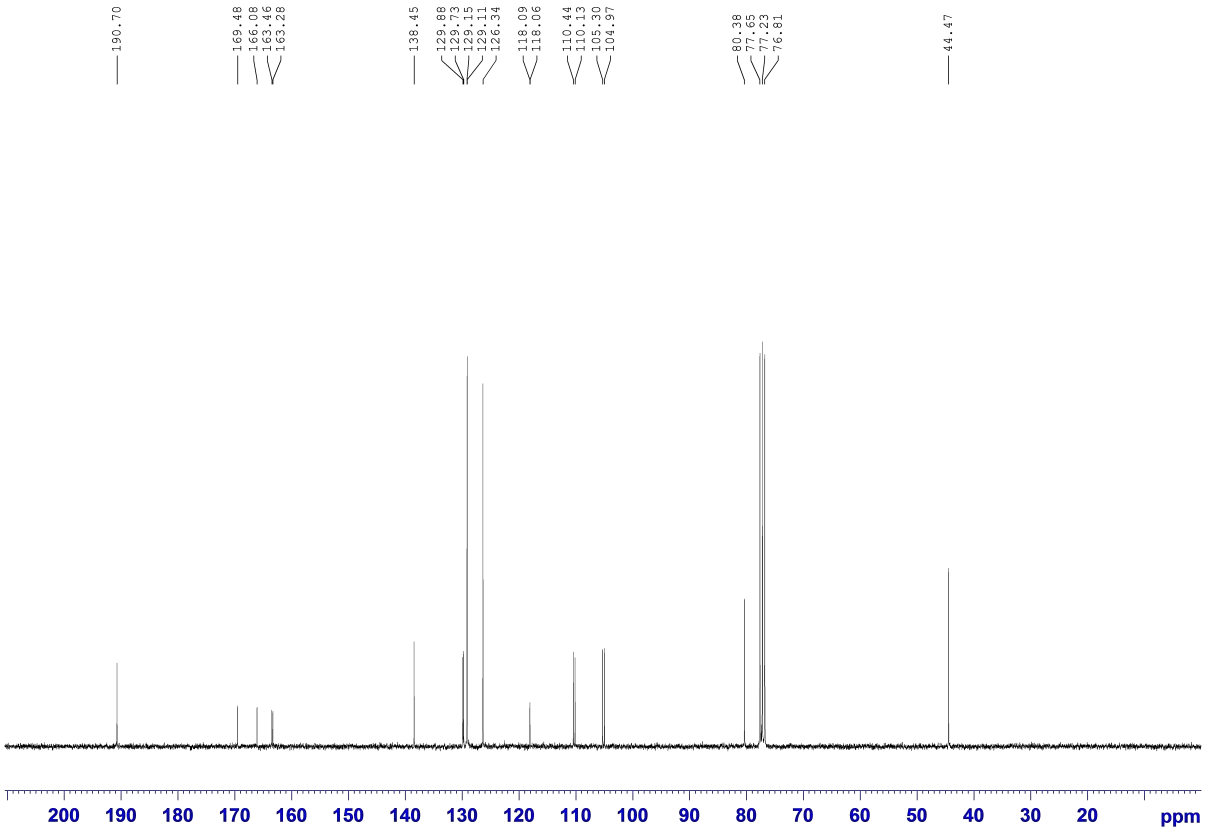
^{13}C NMR Spectrum of 2-(3-Fluorophenyl)-6-methoxychroman-4-one (2o)



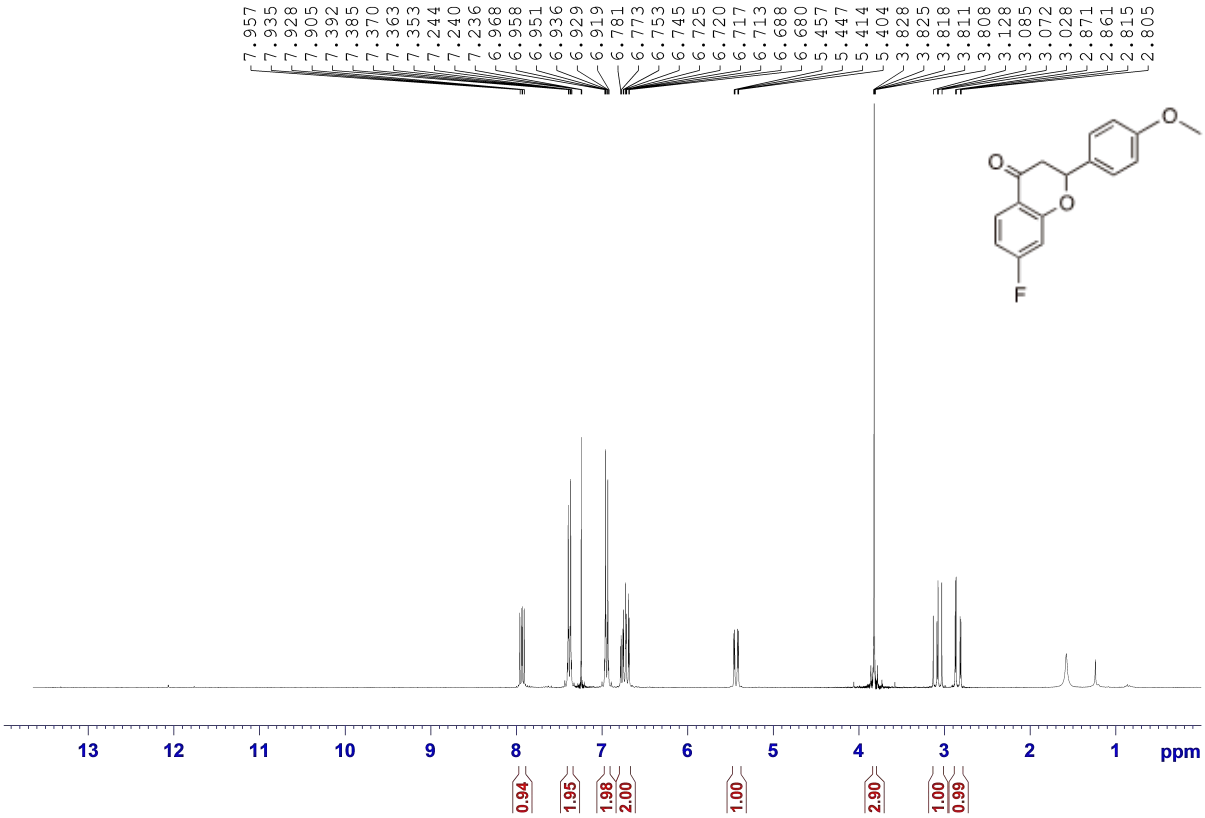
^{1}H NMR Spectrum of 7-Fluoro-2-phenylchroman-4-one (2p)



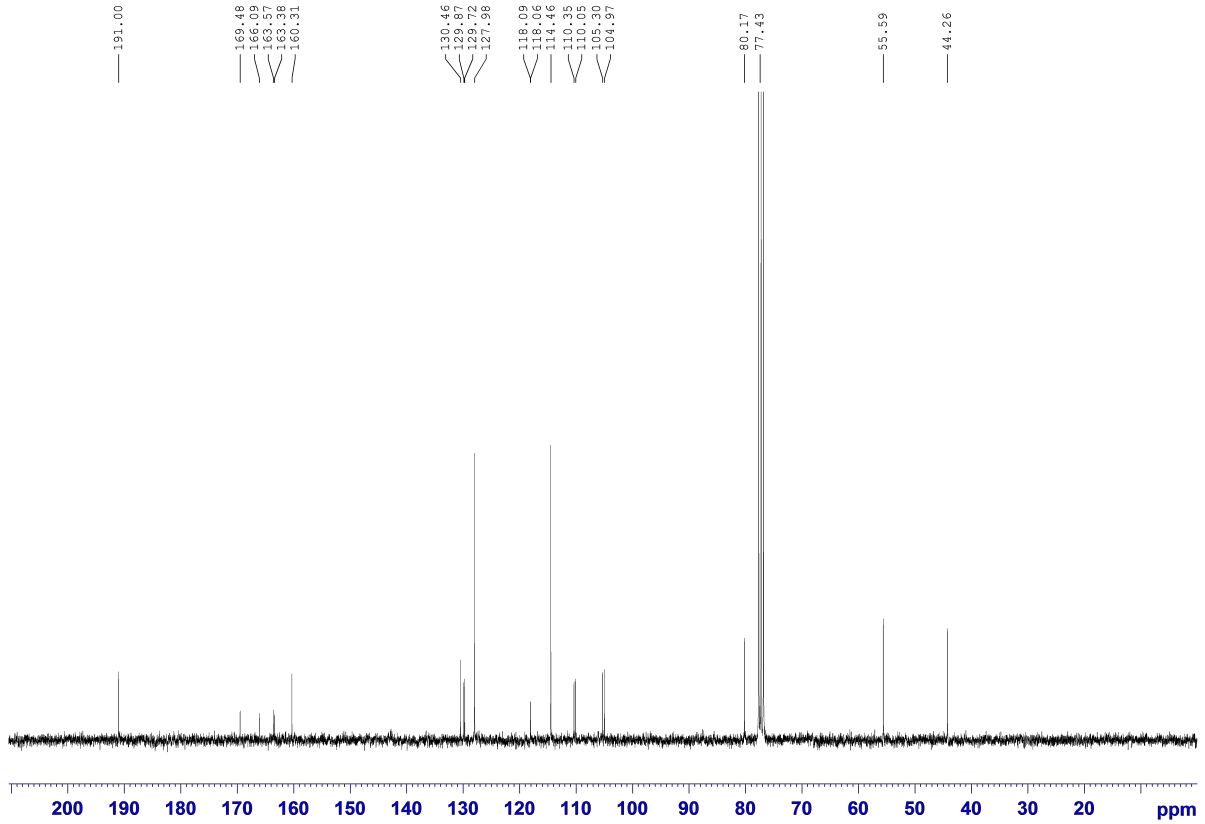
^{13}C NMR Spectrum of 7-Fluoro-2-phenylchroman-4-one (2p)



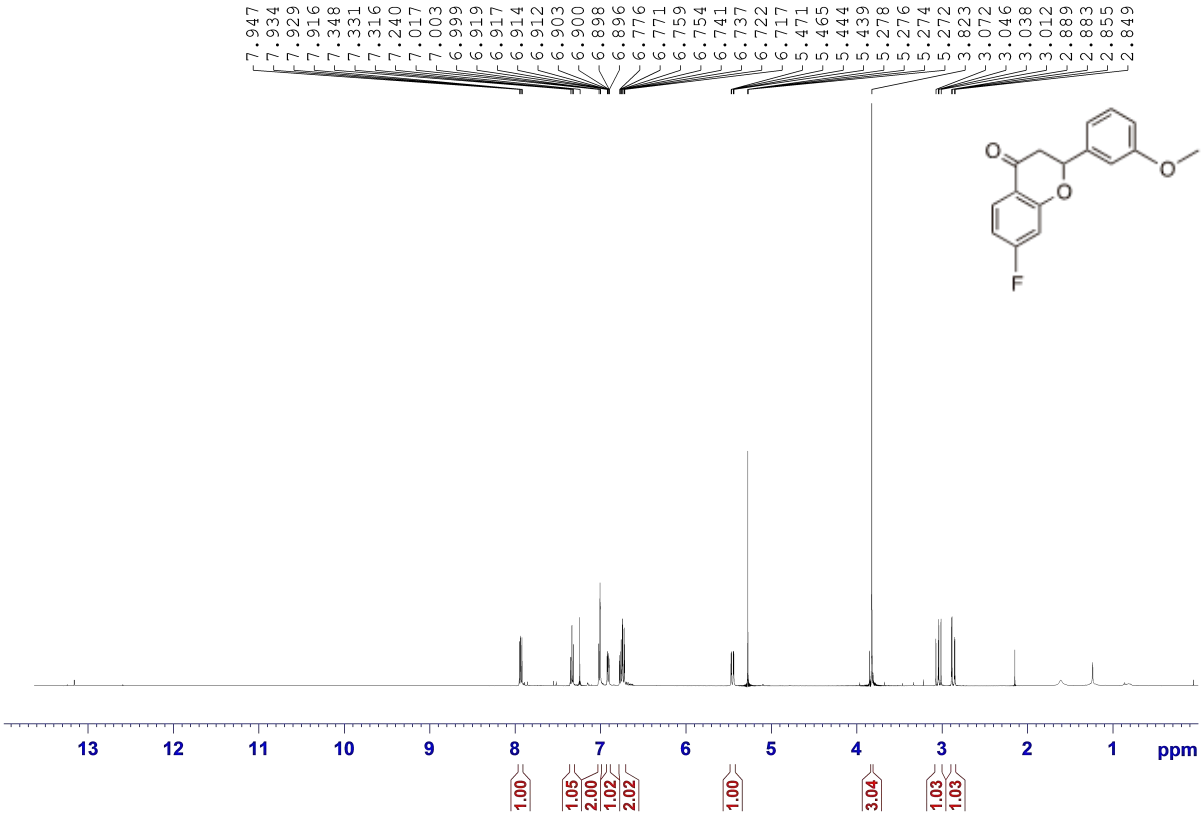
^{1}H NMR Spectrum of 7-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2q)



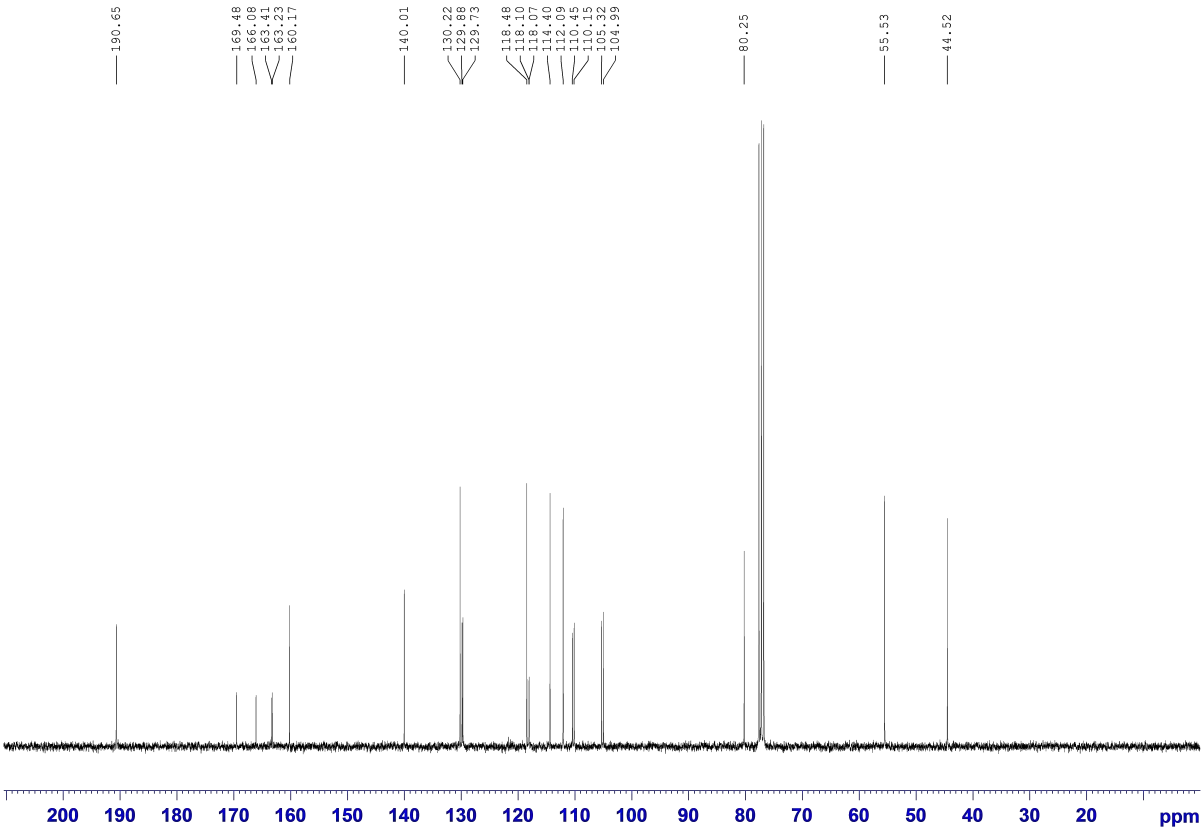
^{13}C NMR Spectrum of 7-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2q)



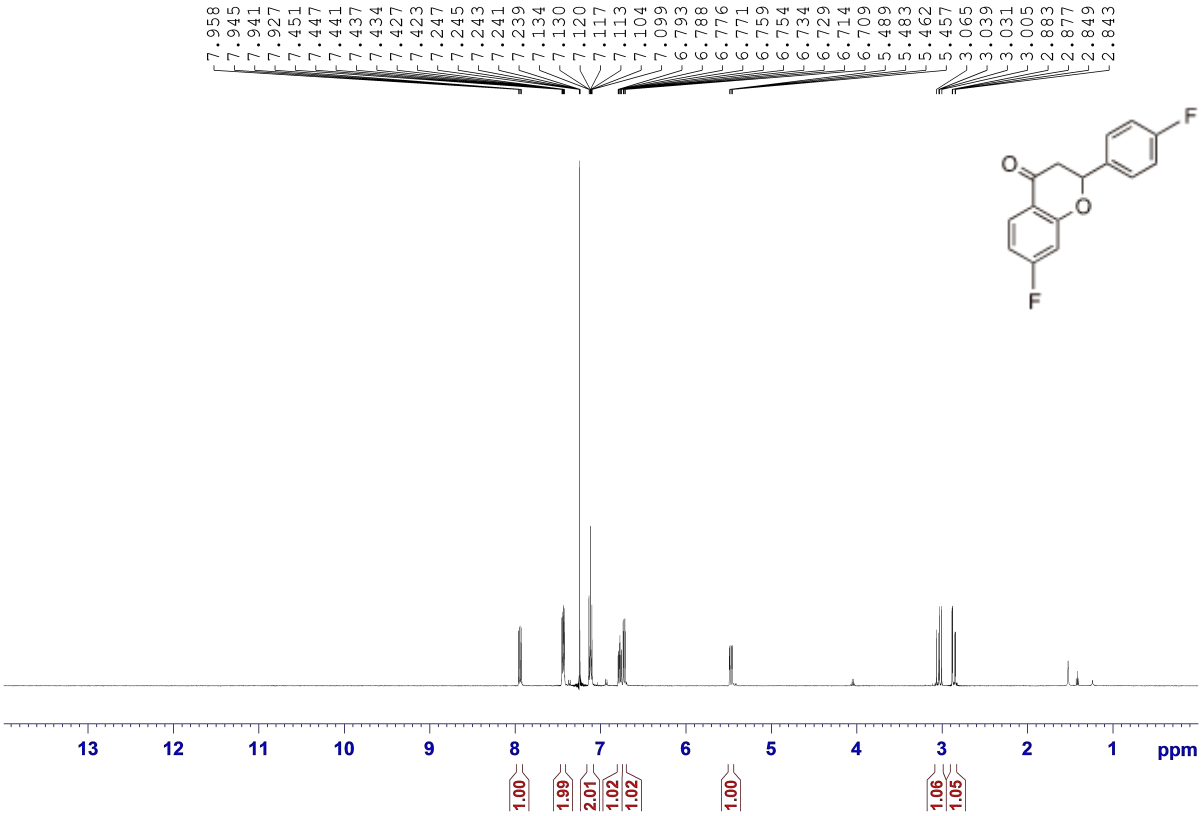
^{1}H NMR Spectrum of 7-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2r)



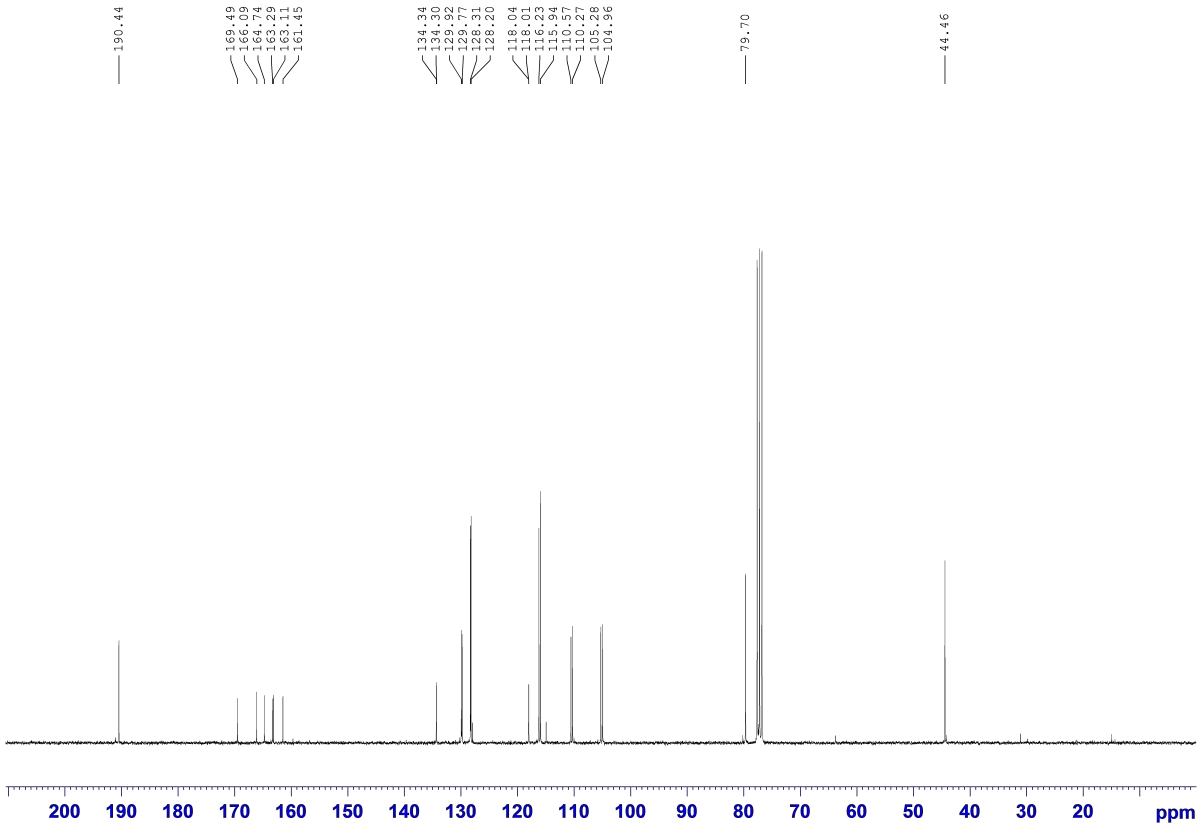
^{13}C NMR Spectrum of 7-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2r)



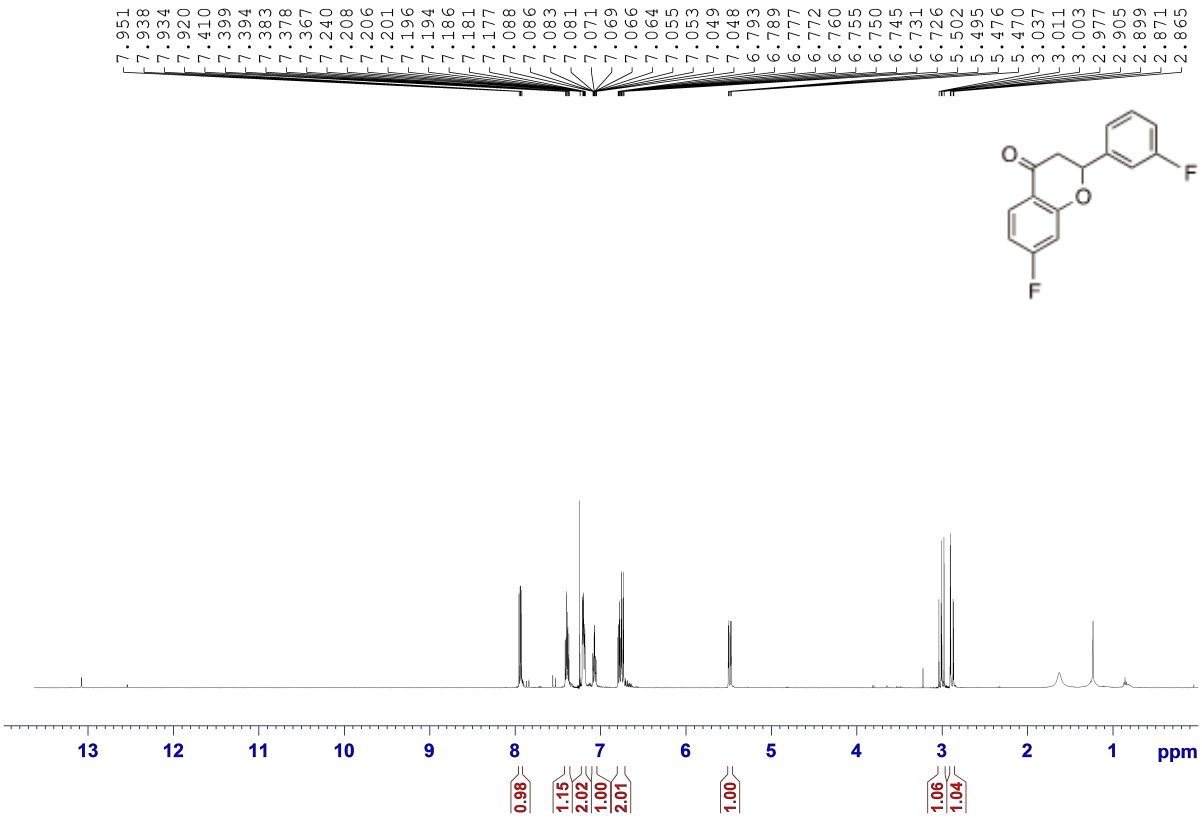
[1]H NMR Spectrum of 7-Fluoro-2-(4-fluorophenyl)chroman-4-one (2s)



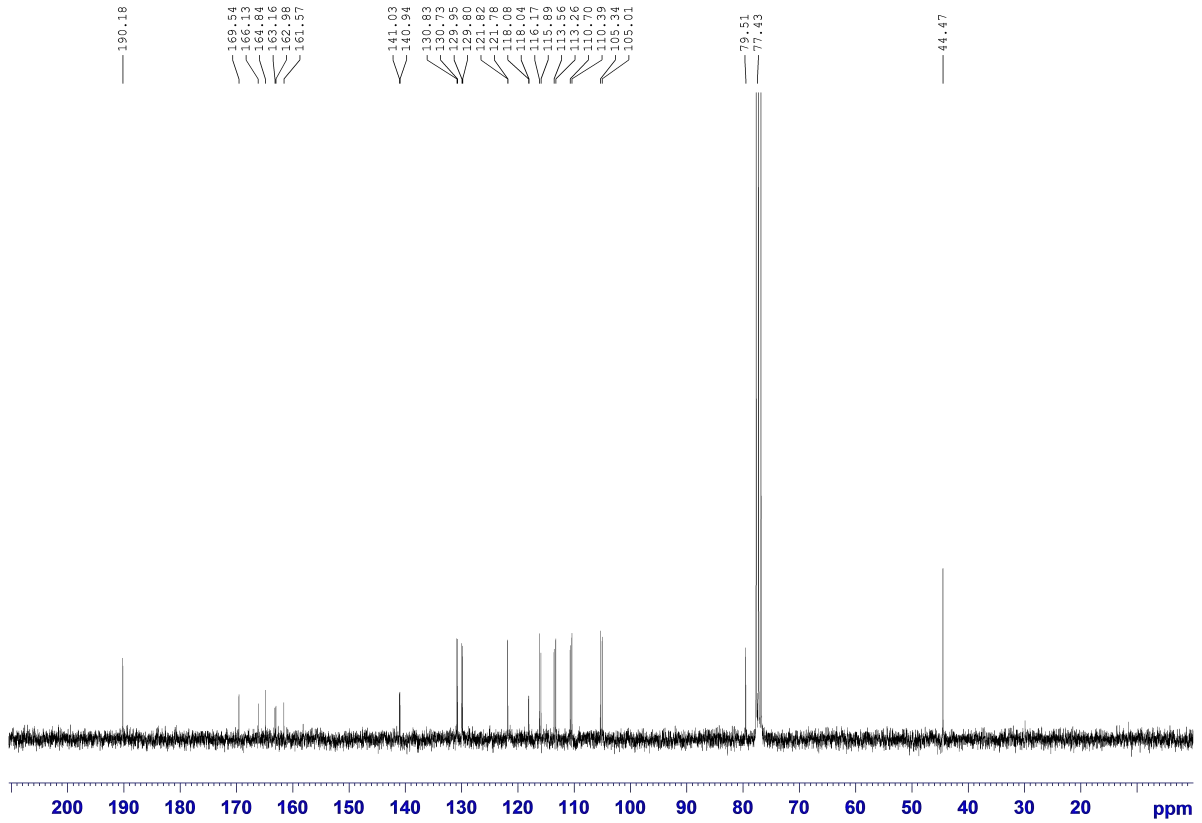
[13]C NMR Spectrum of 7-Fluoro-2-(4-fluorophenyl)chroman-4-one (2s)



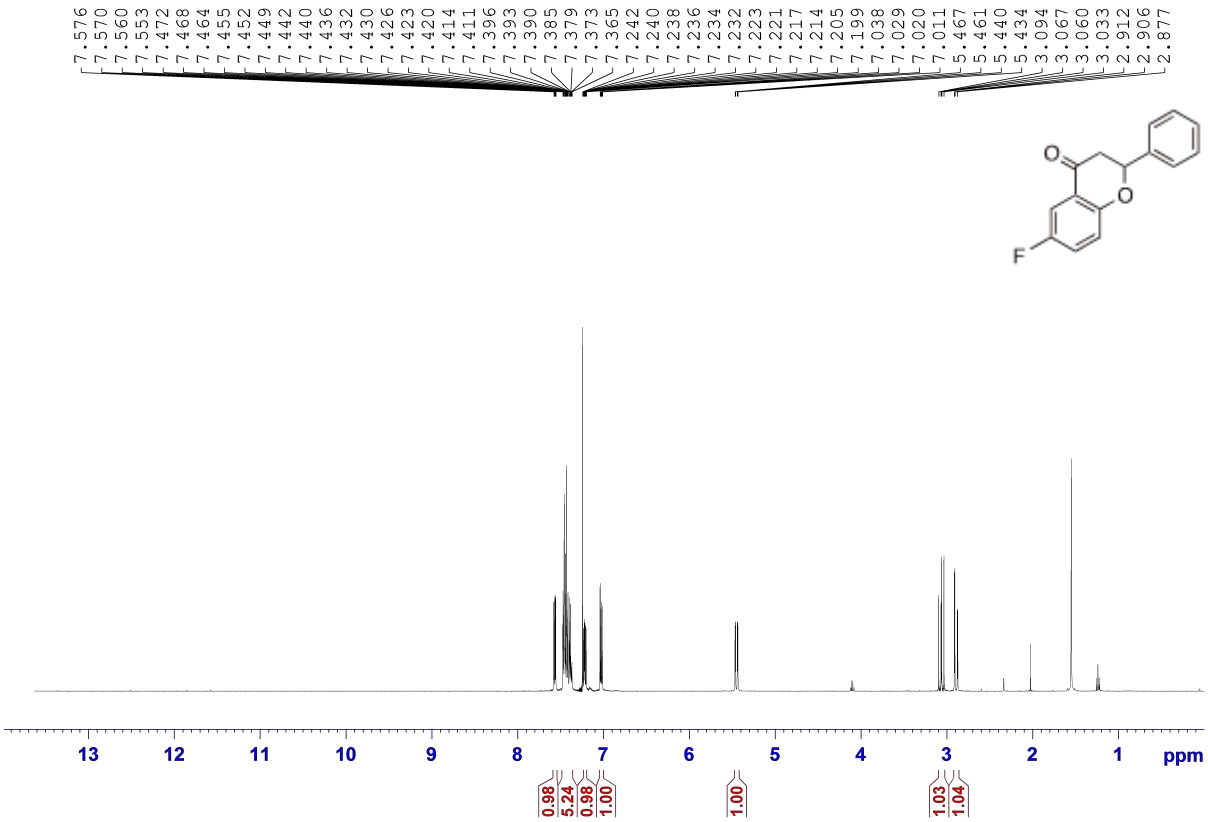
[1]H NMR Spectrum of 7-Fluoro-2-(3-fluorophenyl)chroman-4-one (2t)



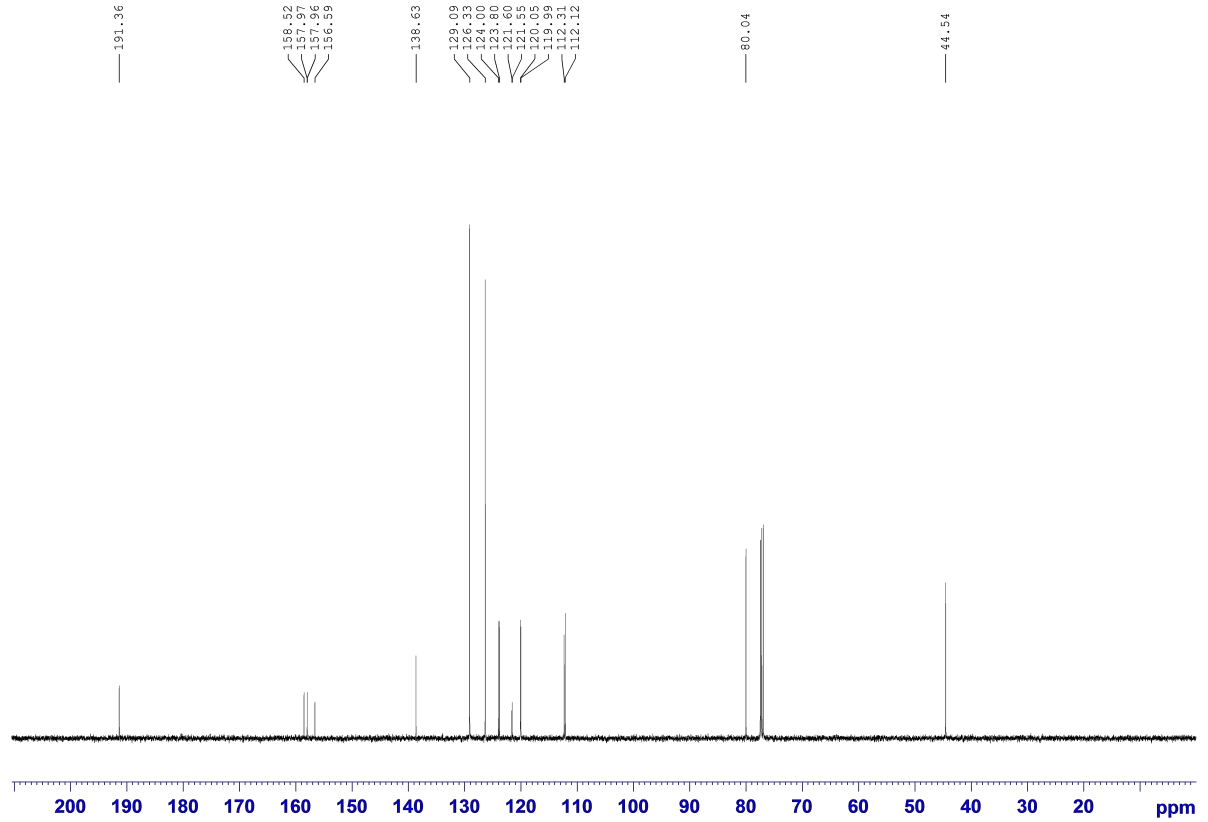
[13]C NMR Spectrum of 7-Fluoro-2-(3-fluorophenyl)chroman-4-one (2t)



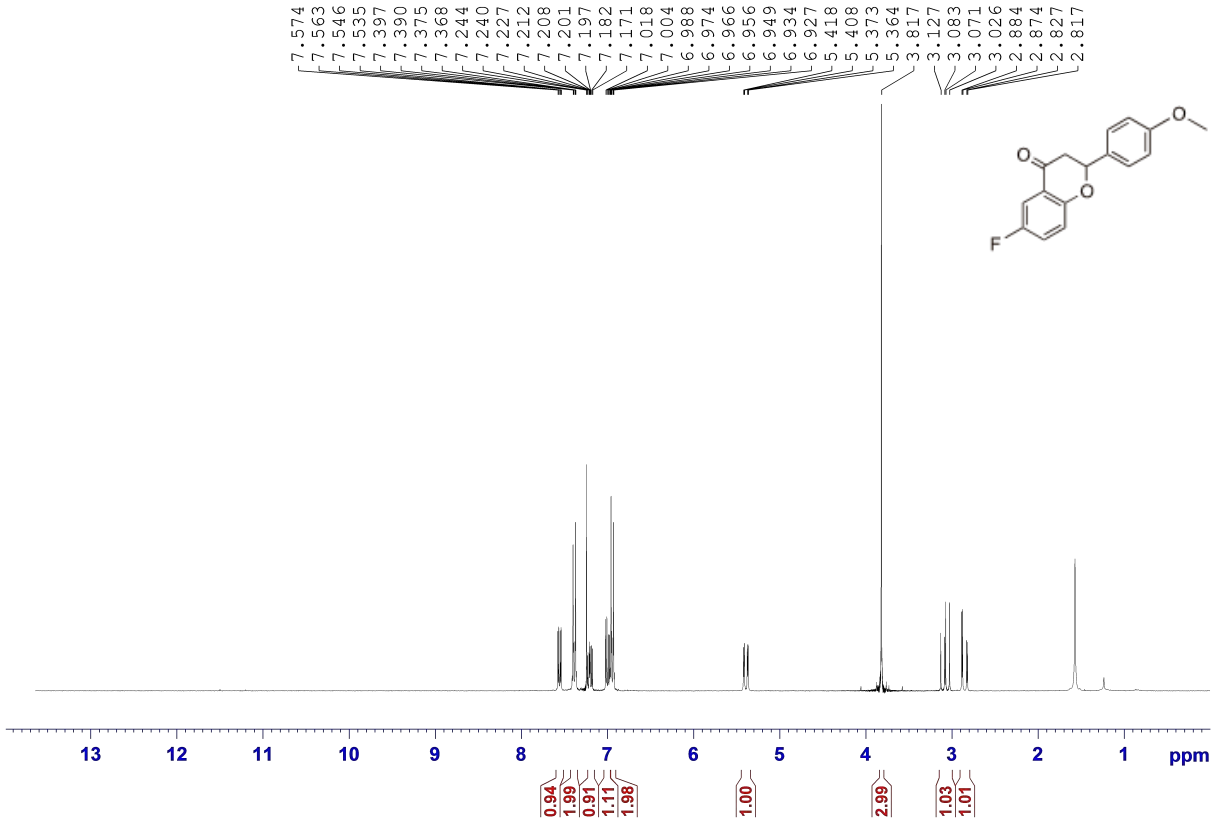
^{1}H NMR Spectrum of 6-Fluoro-2-phenylchroman-4-one (2u)



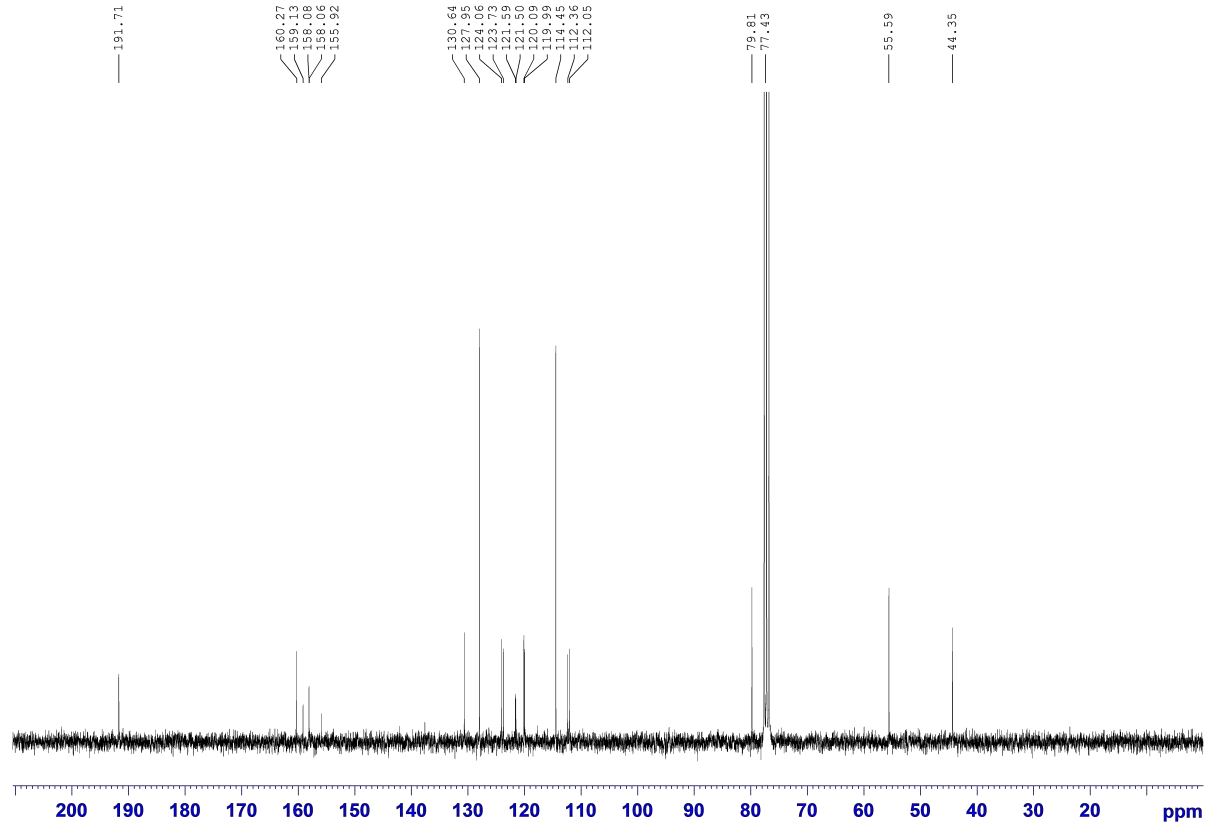
^{13}C NMR Spectrum of 6-Fluoro-2-phenylchroman-4-one (2u)



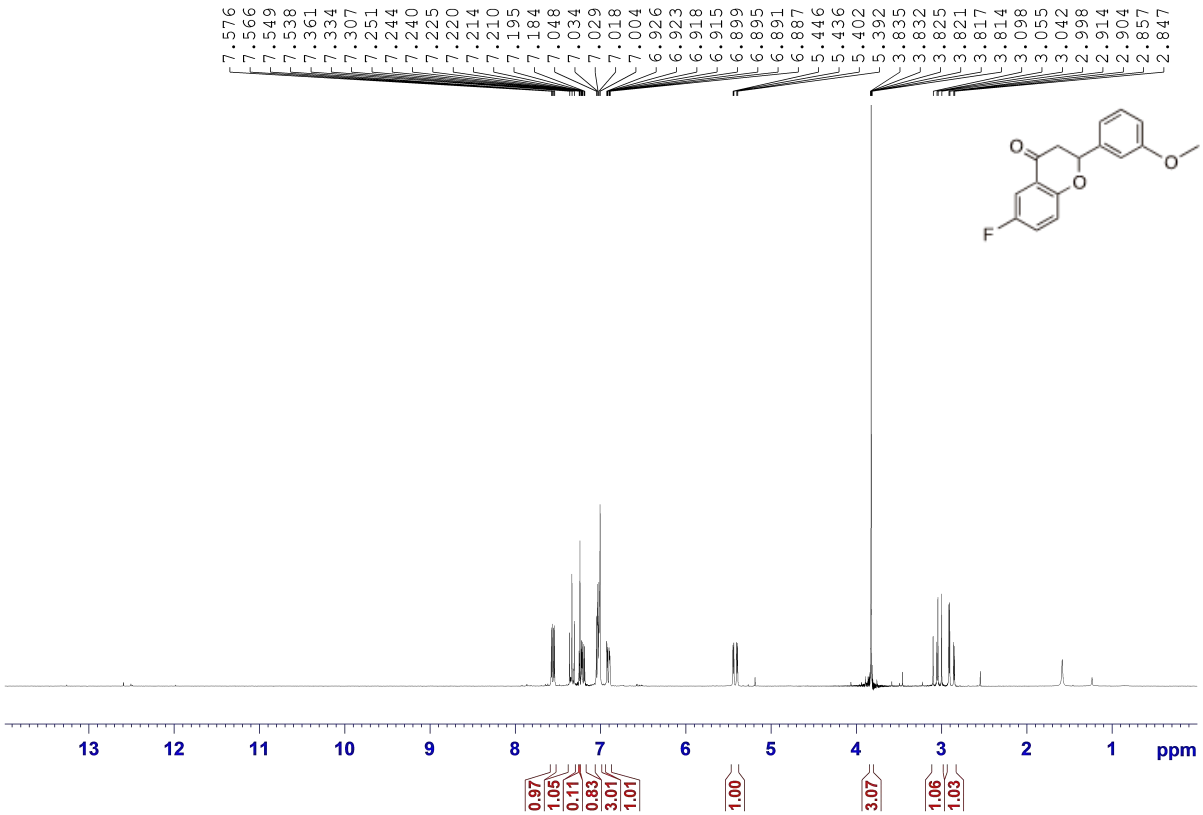
^{1}H NMR Spectrum of 6-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2v)



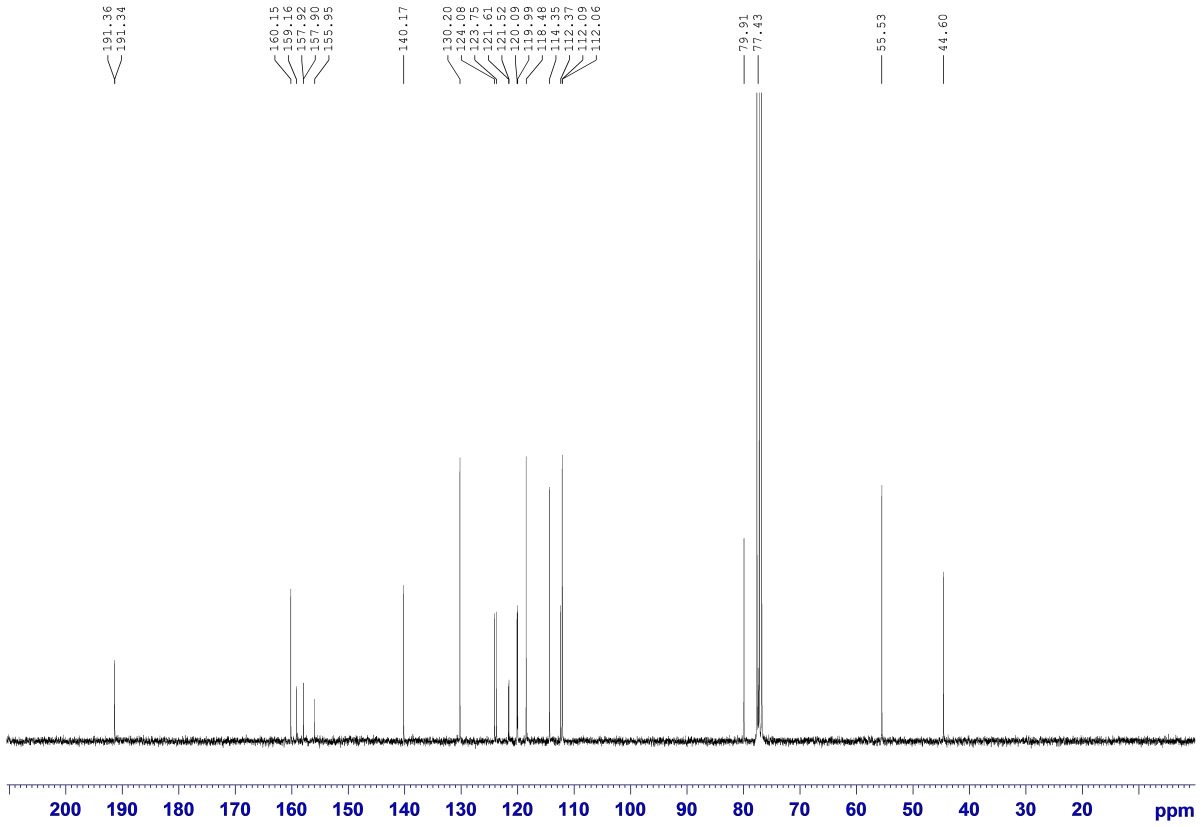
^{13}C NMR Spectrum of 6-Fluoro-2-(4-methoxyphenyl)chroman-4-one (2v)



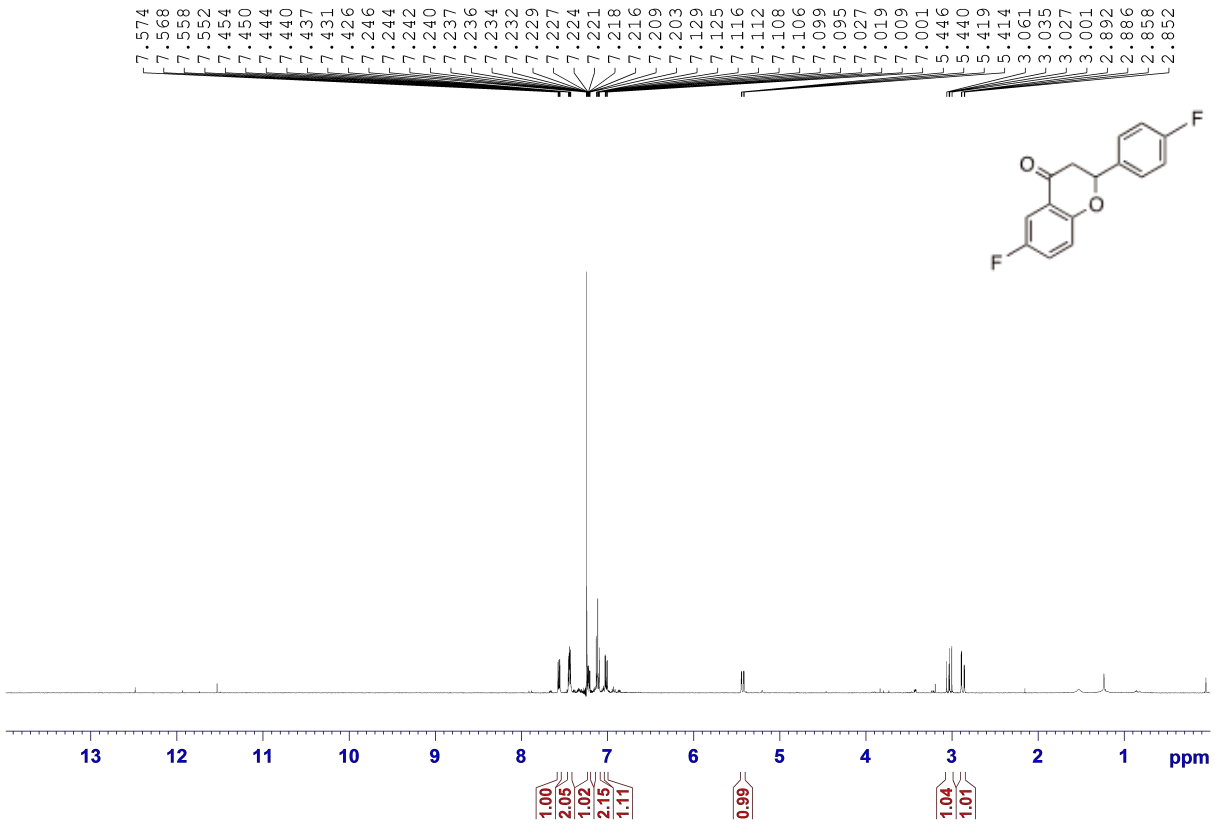
^{1}H NMR Spectrum of 6-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2w)



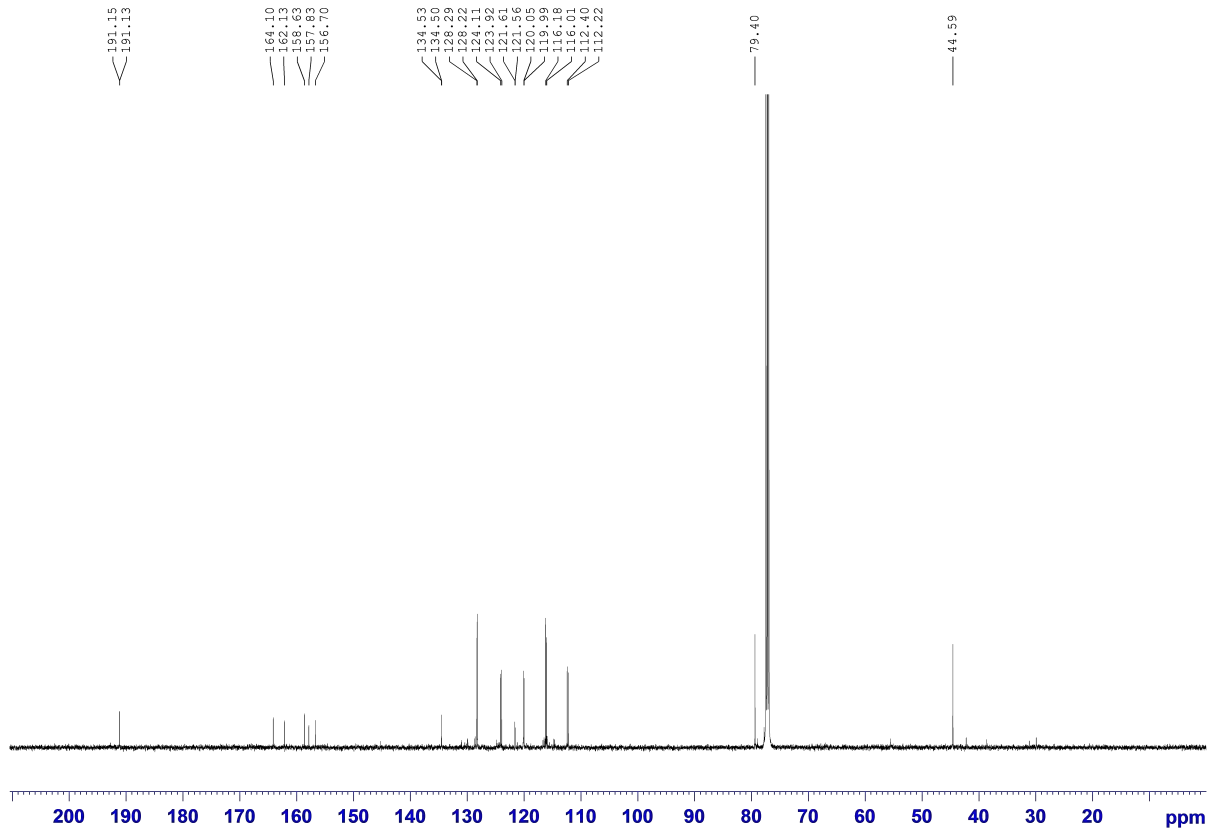
^{13}C NMR Spectrum of 6-Fluoro-2-(3-methoxyphenyl)chroman-4-one (2w)



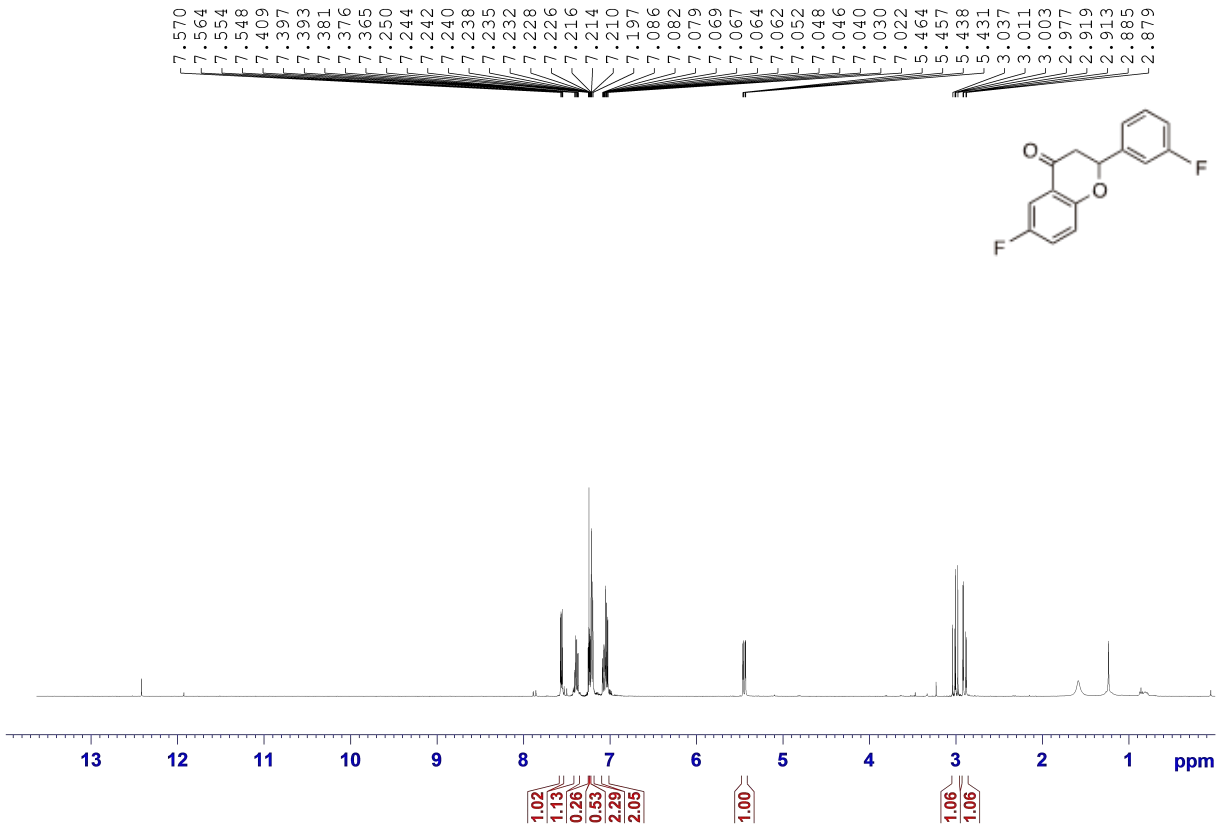
[1]H NMR Spectrum of 6-Fluoro-2-(4-fluorophenyl)chroman-4-one (2x)



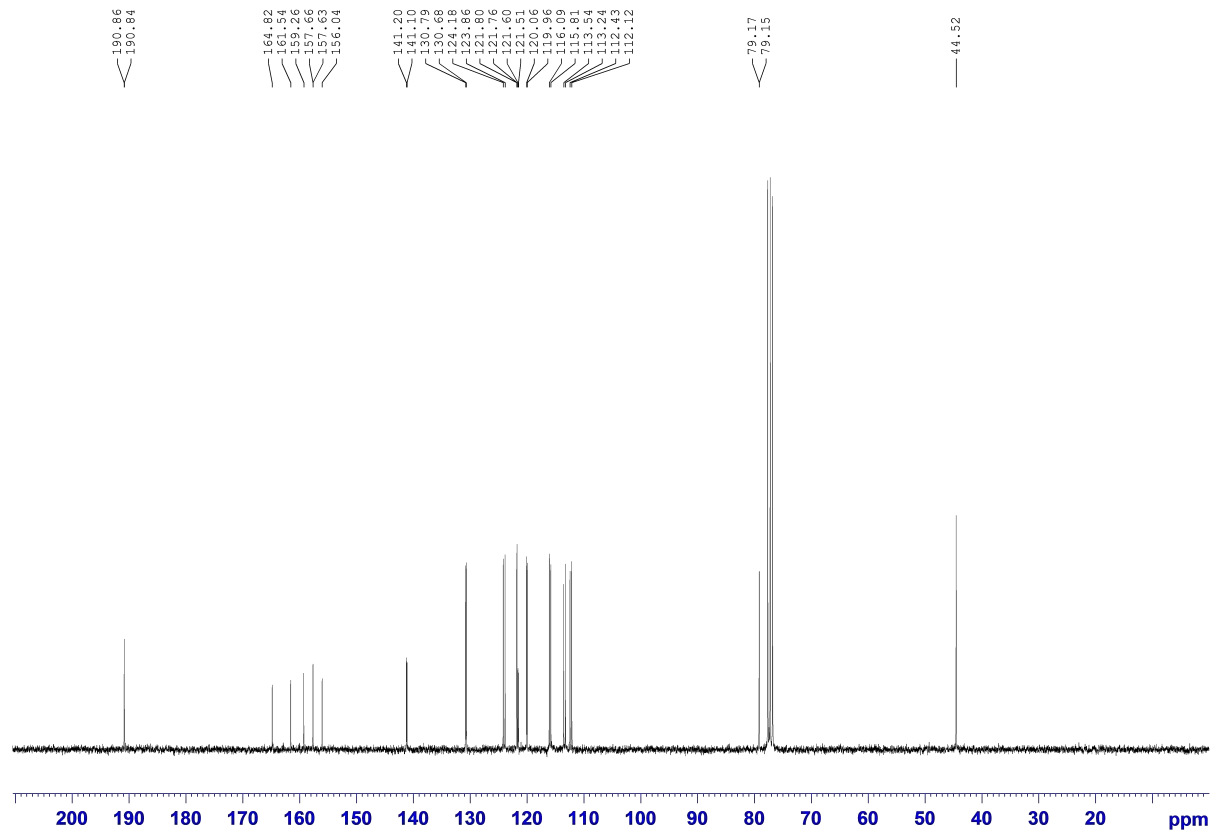
[13]C NMR Spectrum of 6-Fluoro-2-(4-fluorophenyl)chroman-4-one (2x)



^{1}H NMR Spectrum of 6-Fluoro-2-(3-fluorophenyl)chroman-4-one (2y)

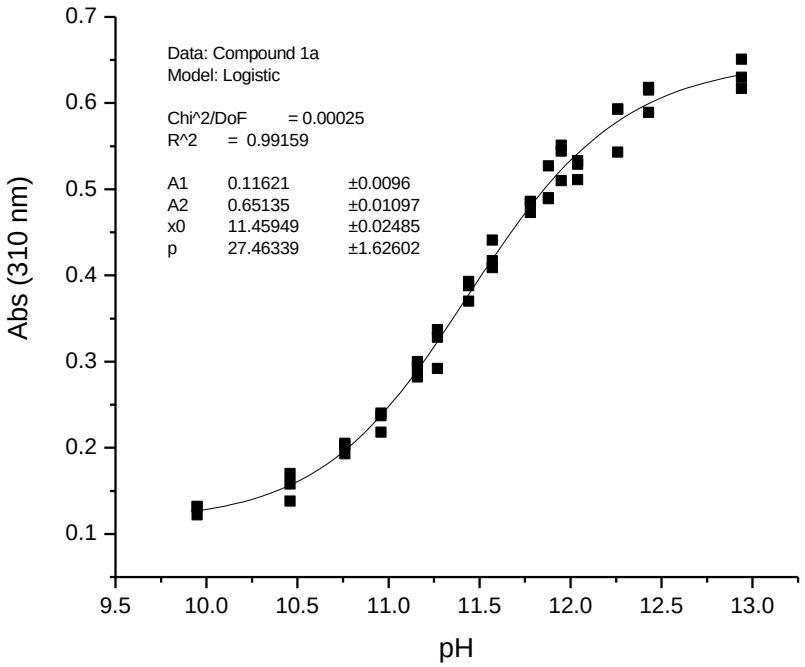


^{13}C NMR Spectrum of 6-Fluoro-2-(3-fluorophenyl)chroman-4-one (2y)

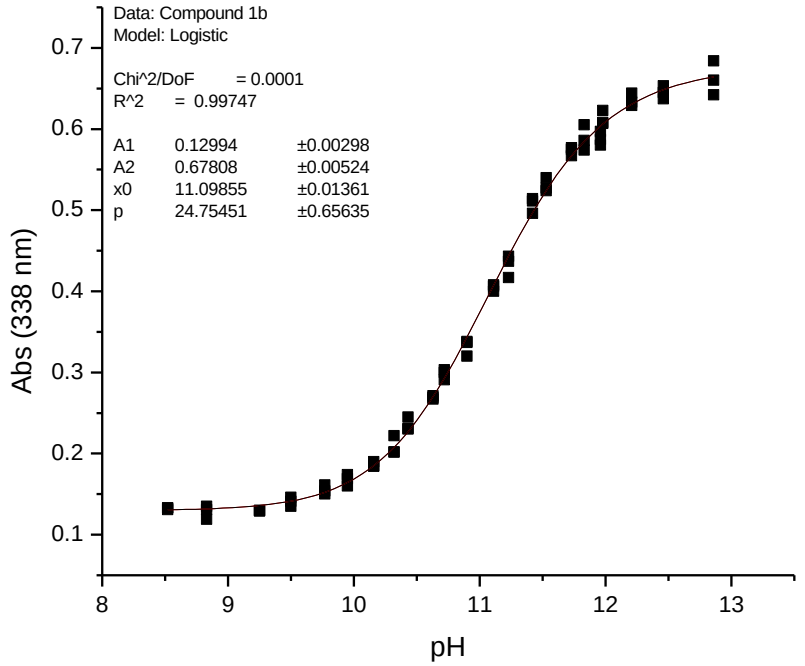


SIGMOIDAL CURVES DERIVED FROM UV/VIS MIDPOINT pH DATA

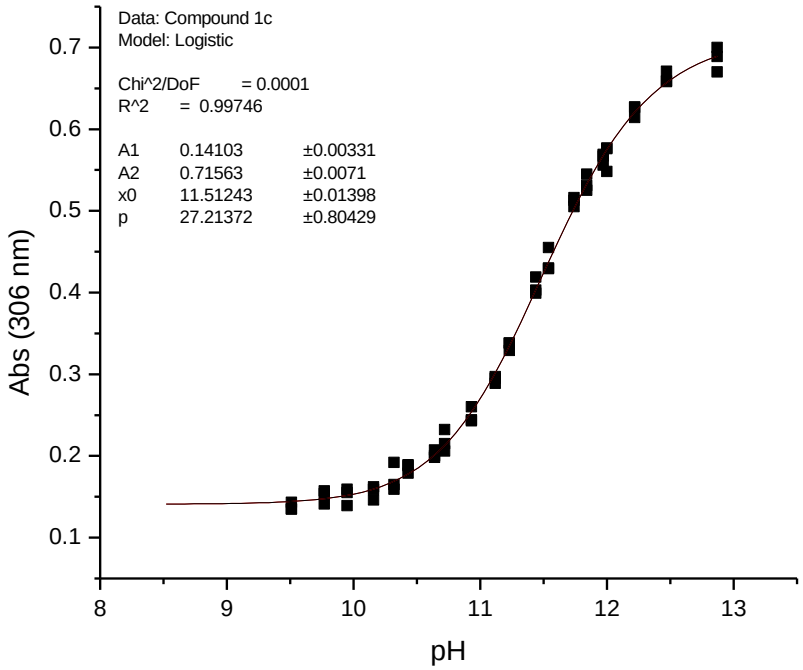
pH vs. Absorbance Plot for 1a/2a



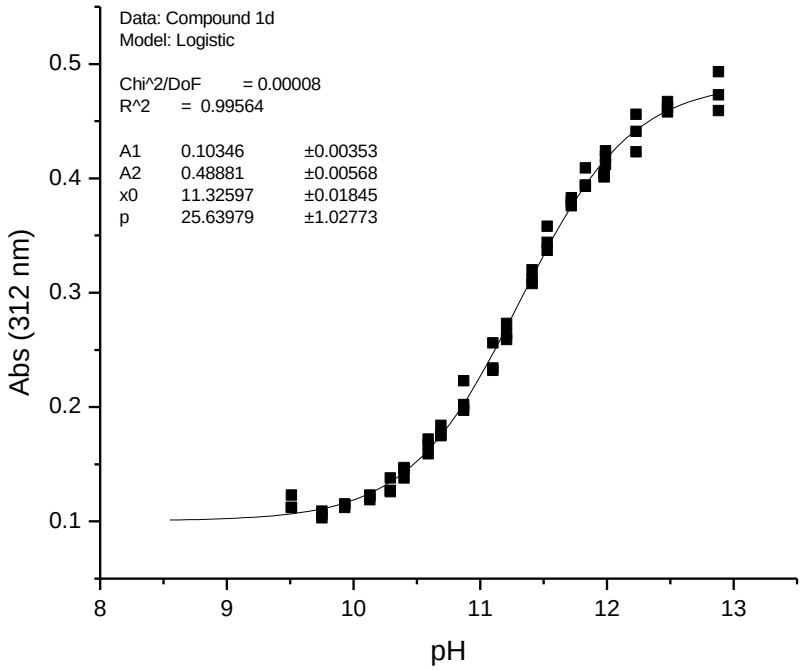
pH vs. Absorbance Plot for 1b/2b



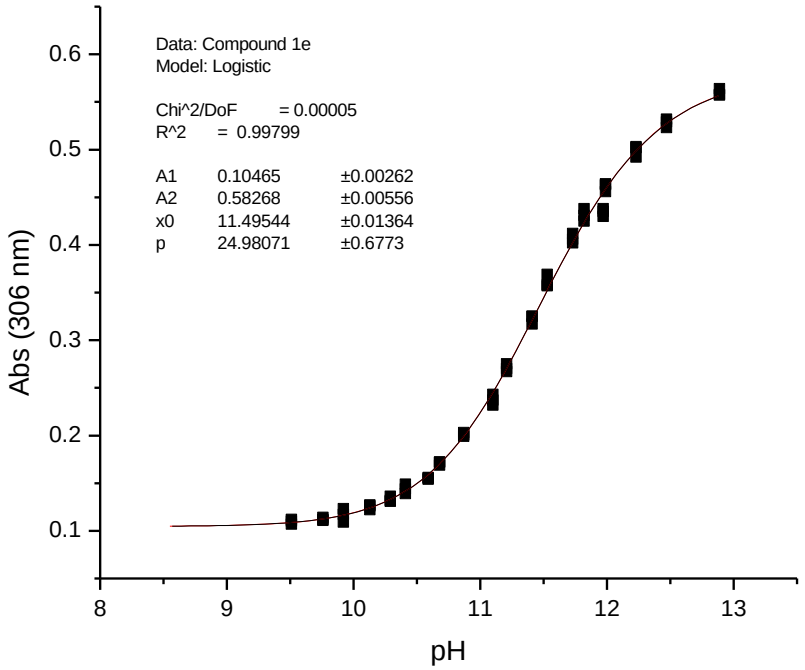
pH vs. Absorbance Plot for 1c/2c



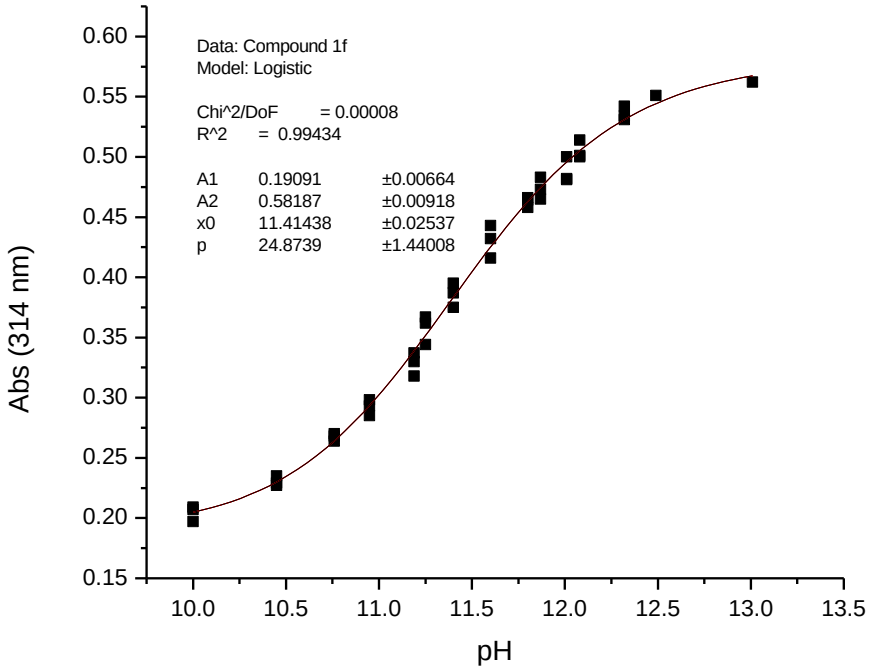
pH vs. Absorbance Plot for 1d/2d



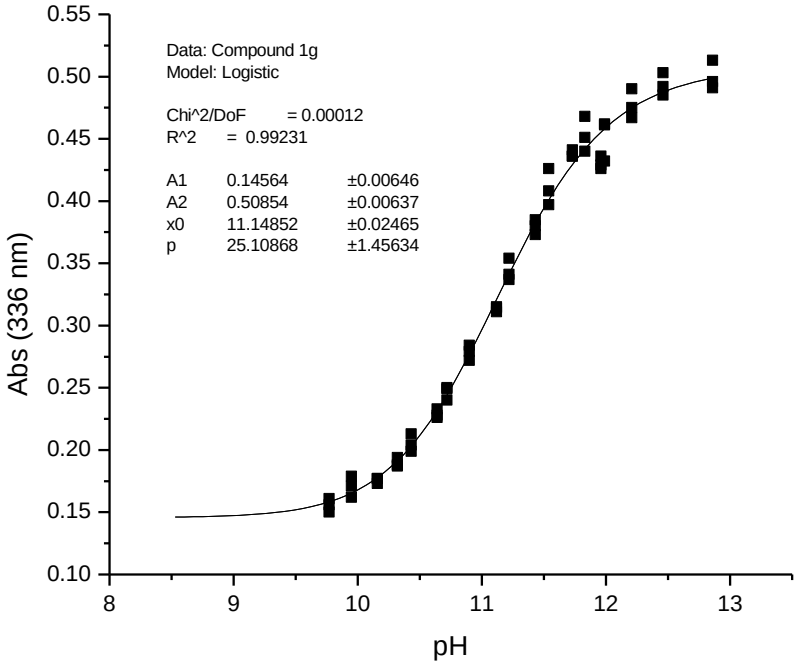
pH vs. Absorbance Plot for 1e/2e



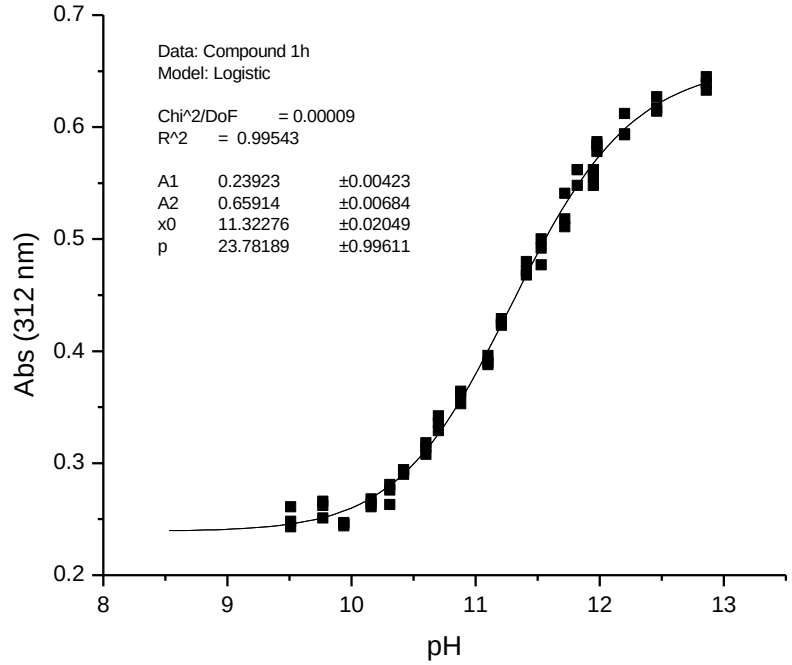
pH vs. Absorbance Plot for 1f/2f



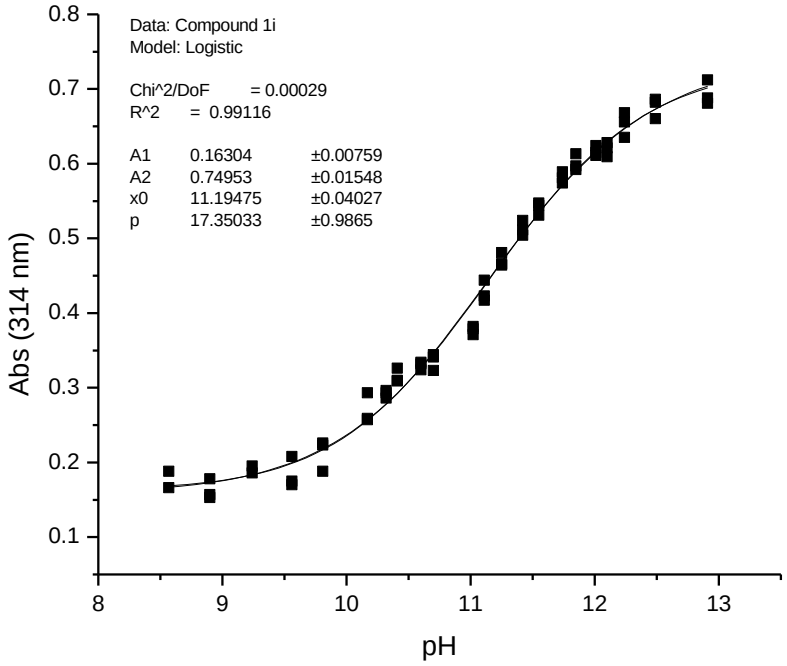
pH vs. Absorbance Plot for 1g/2g



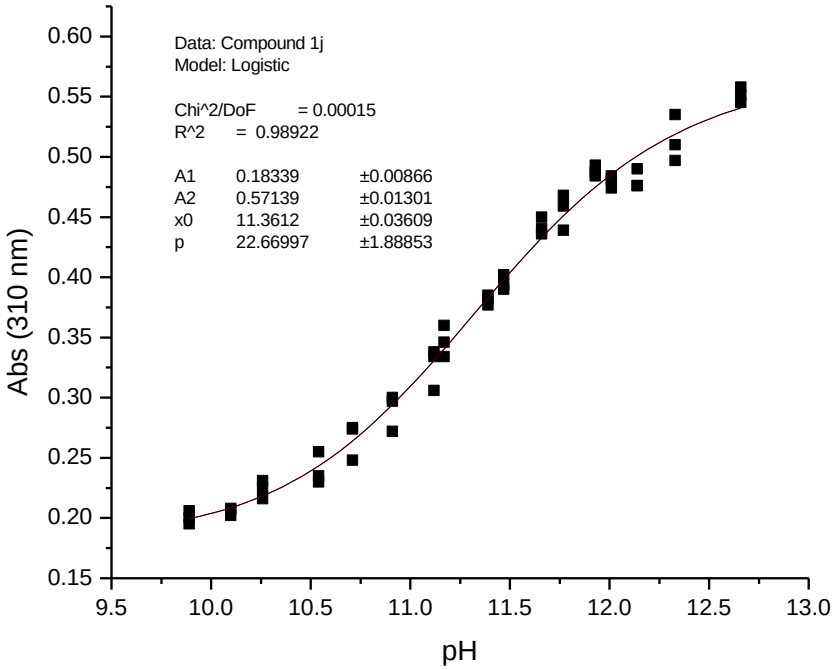
pH vs. Absorbance Plot for 1h/2h



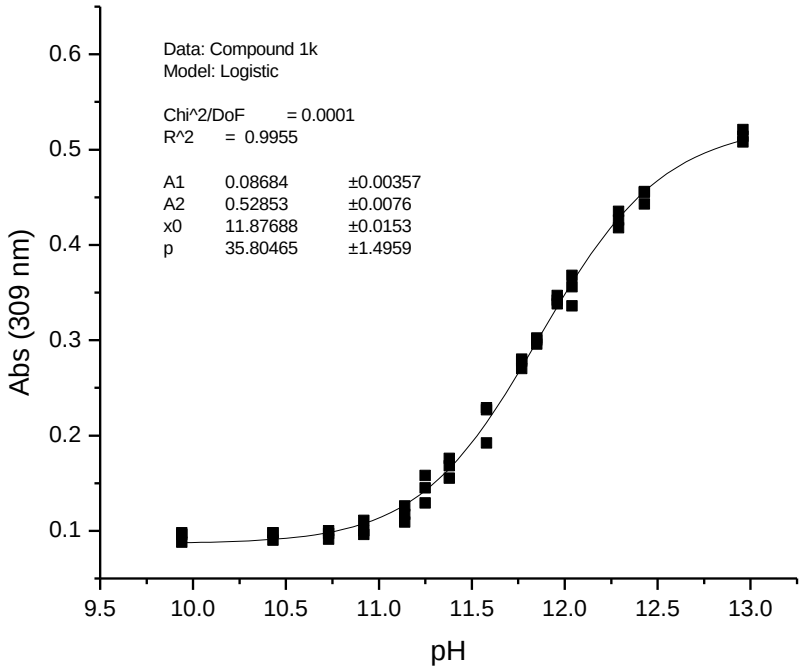
pH vs. Absorbance Plot for 1i/2i



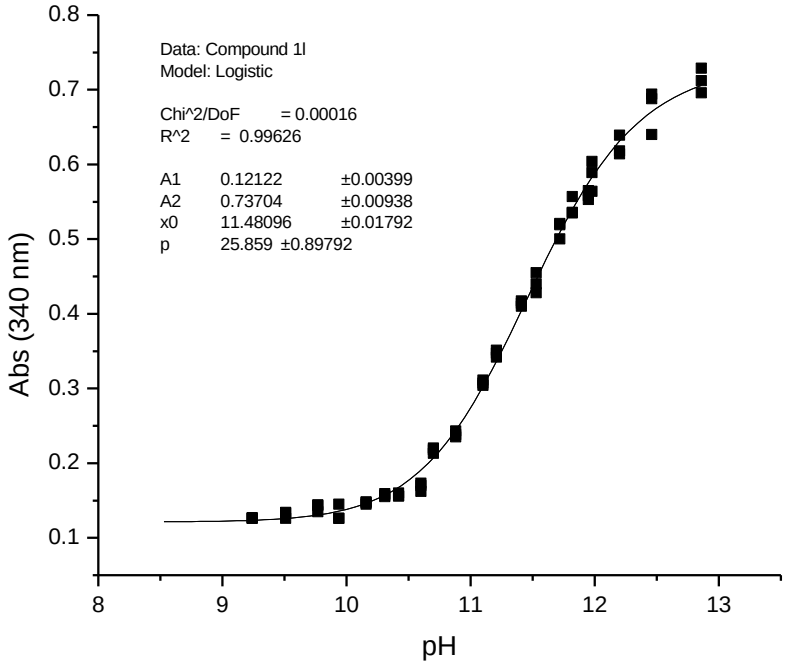
pH vs. Absorbance Plot for 1j/2j



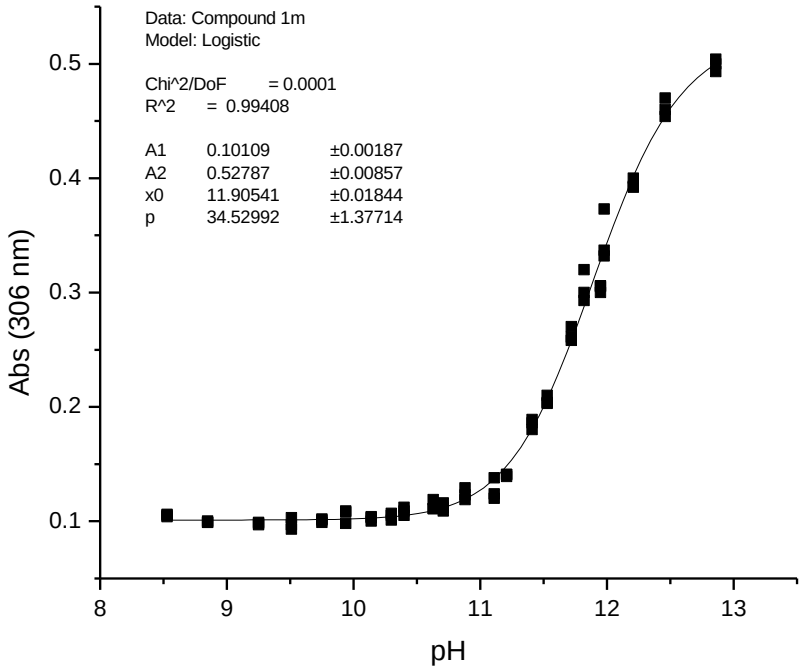
pH vs. Absorbance Plot for 1k/2k



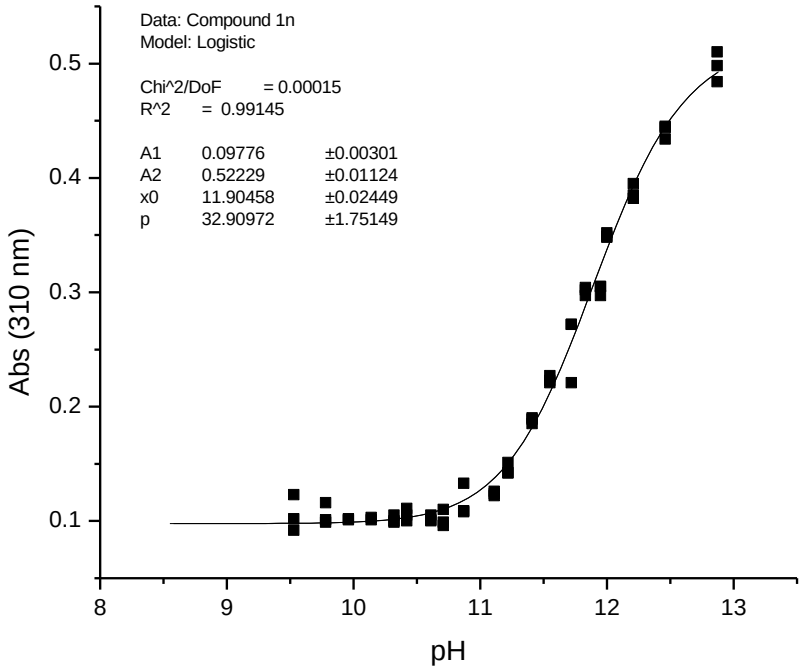
pH vs. Absorbance Plot for 1l/2l



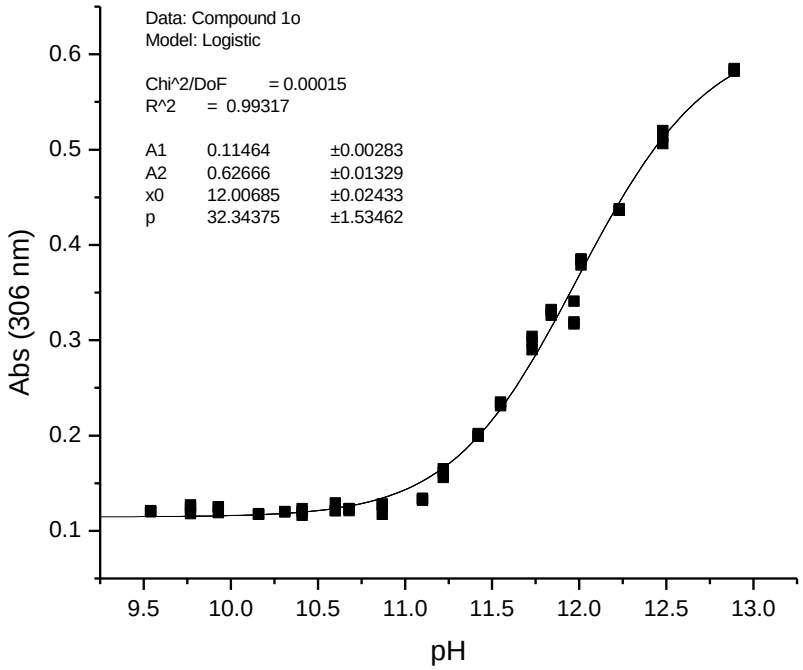
pH vs. Absorbance Plot for 1m/2m



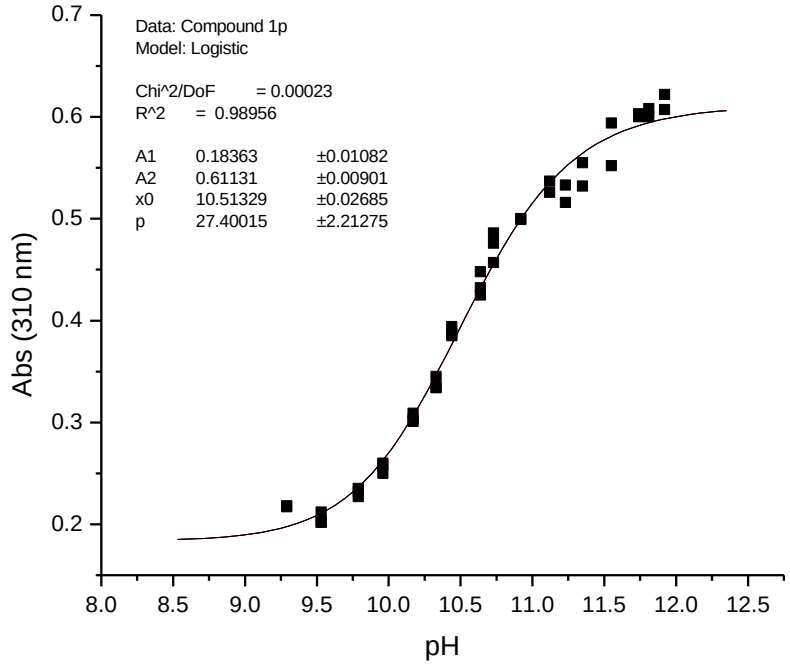
pH vs. Absorbance Plot for 1n/2n



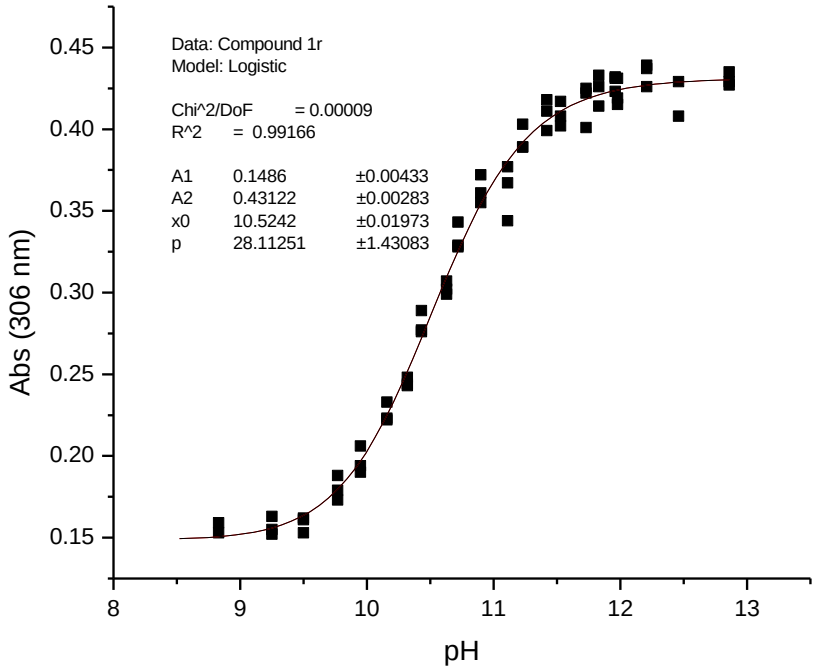
pH vs. Absorbance Plot for 1o/2o



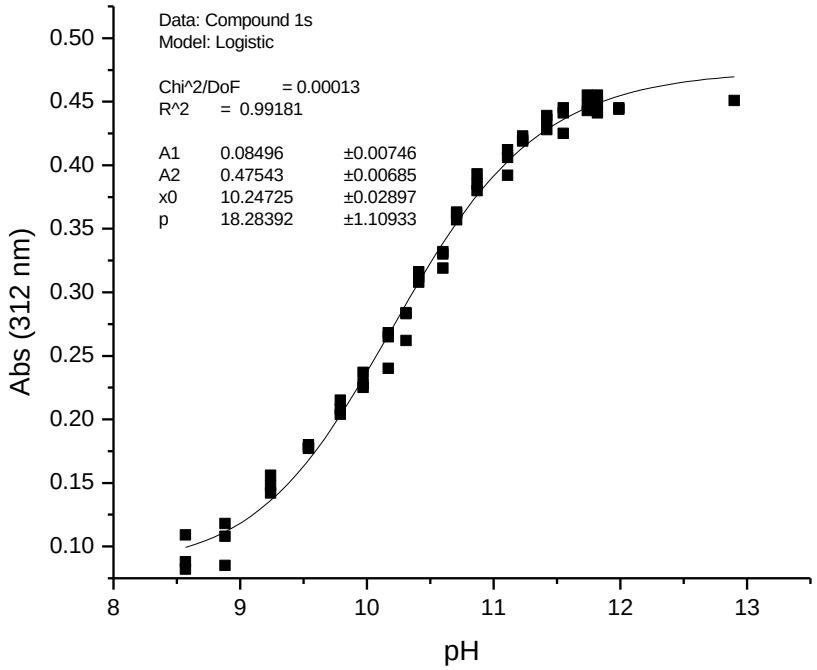
pH vs. Absorbance Plot for 1p/2p



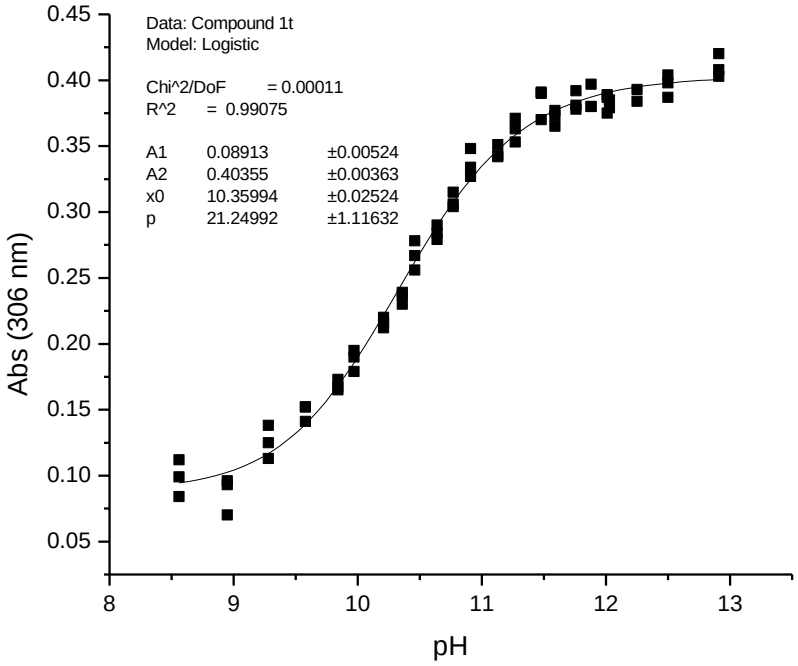
pH vs. Absorbance Plot for 1r/2r



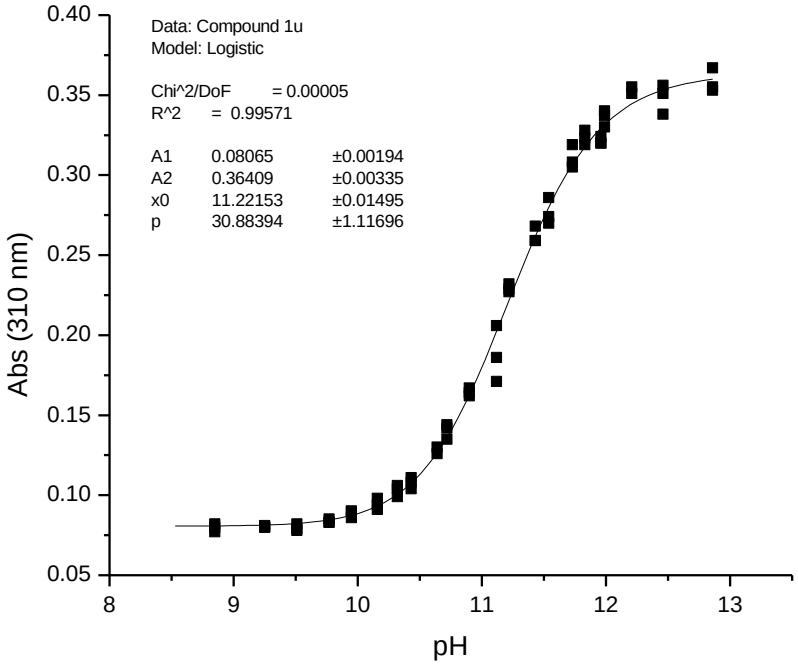
pH vs. Absorbance Plot for 1s/2s



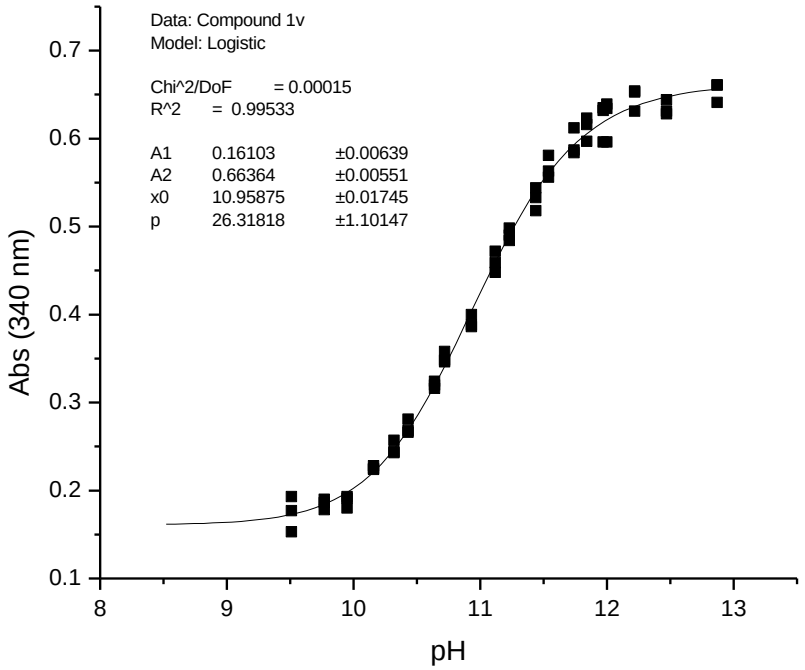
pH vs. Absorbance Plot for 1t/2t



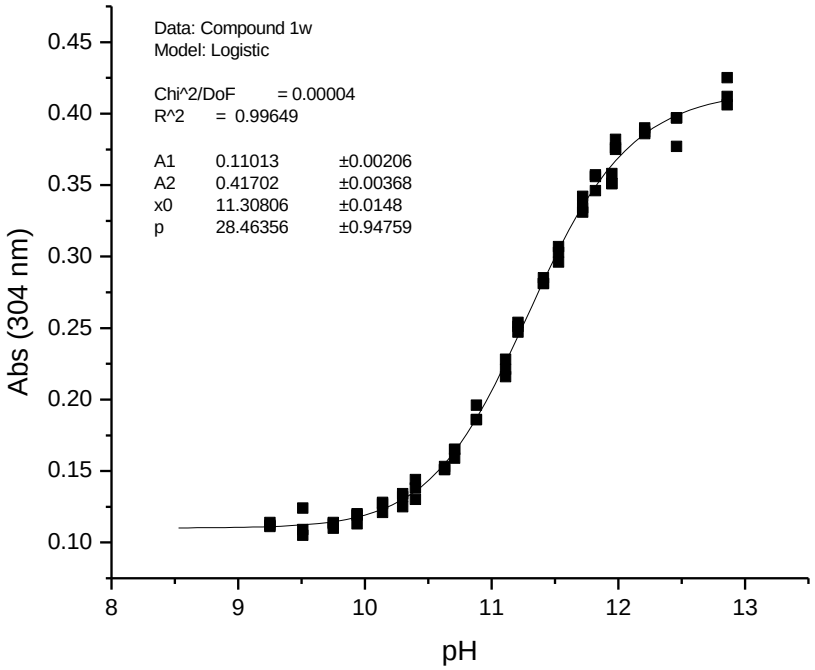
pH vs. Absorbance Plot for 1u/2u



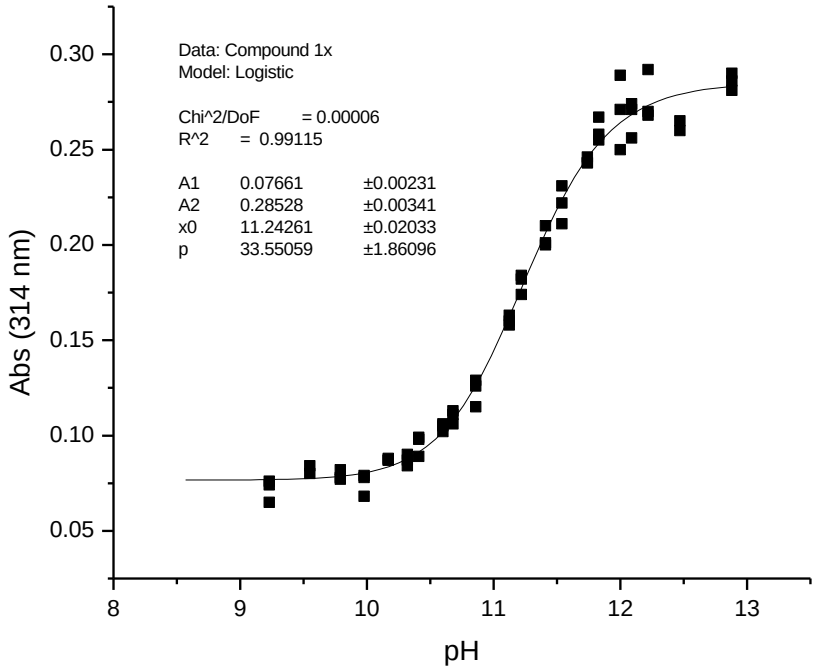
pH vs. Absorbance Plot for 1v/2v



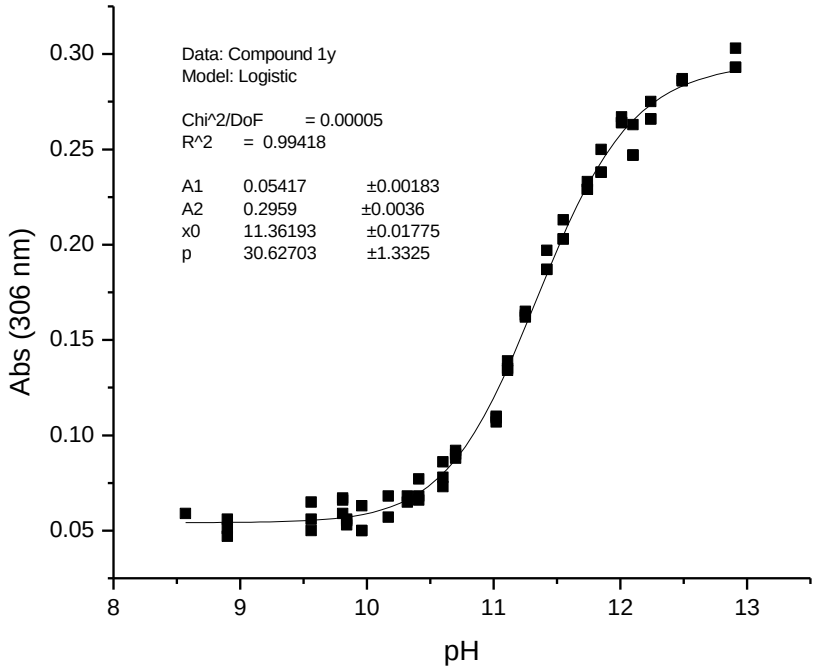
pH vs. Absorbance Plot for 1w/2w



pH vs. Absorbance Plot for 1x/2x



pH vs. Absorbance Plot for 1y/2y



PROCEDURES FOR THE VERIFICATION STUDIES OF UV/VIS RATE ASSAYS

Kinetic Verification Study for Chalcone (1) to Flavanone (2)

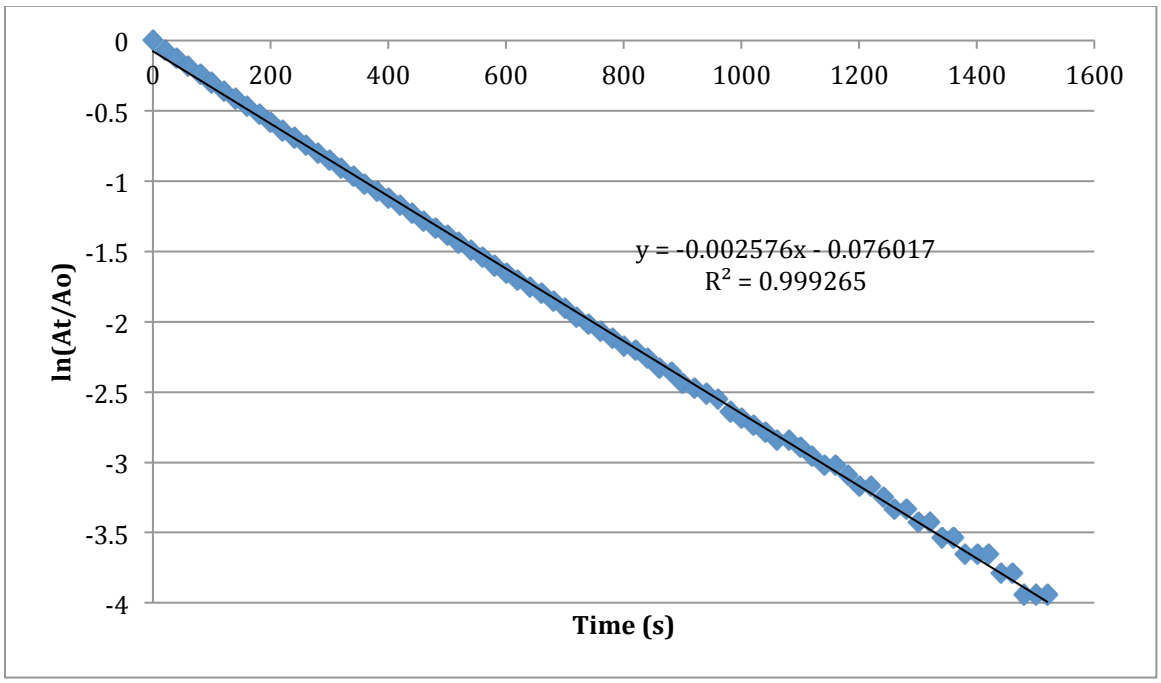
A 4 x 10^{-4} M stock solution using 3.0 mg of chalcone in methanol was prepared in a 100 mL round-bottomed flask. Into a 500 mL round-bottomed flask was added 411.19 mL of 9.25 pH $NaHCO_3$ buffer solution. The chalcone solution was added at once to the buffer solution. The mixture was stirred at ambient temperature for 1 hour after which the solution was quenched with excess 6 M HCl. The mixture was extracted with dichloromethane (3x75 mL), and the combined organic layers were dried over magnesium sulfate. After filtration and concentration, the mass of the solid was taken followed by NMR.

Kinetic Verification Study for Flavanone (2) to Chalcone (1)

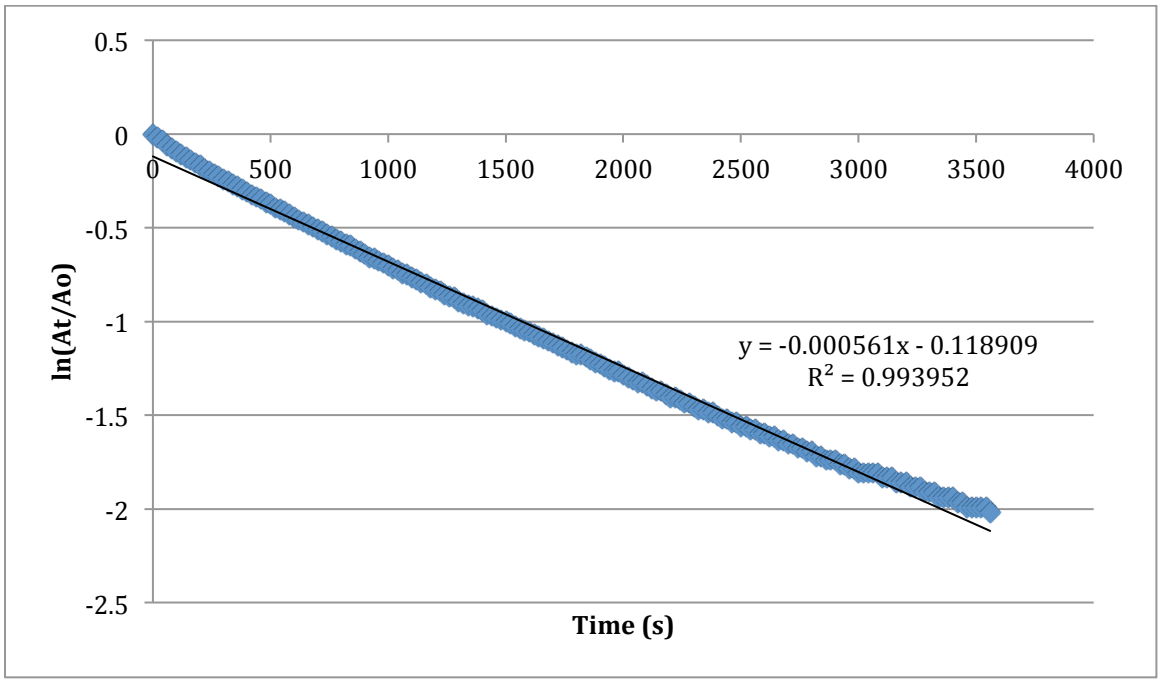
A 4 x 10^{-4} M stock solution using 3.0 mg of flavanone in methanol was prepared in a 100 mL round-bottomed flask. Into a 500 mL round-bottomed flask was added 411.19 mL of 12.5 pH KCl buffer solution. The flavanone solution was added at once to the buffer solution. The mixture was stirred at ambient temperature for 1 hour after which the solution was quenched with excess 6 M HCl. The mixture was extracted with dichloromethane (3x75 mL), and the combined organic layers were dried over magnesium sulfate. After filtration and concentration, the mass of the solid was taken followed by NMR.

RAW DATA PLOTS FROM CHALCONE TO FLAVANONE RATE DETERMINATION ASSAY

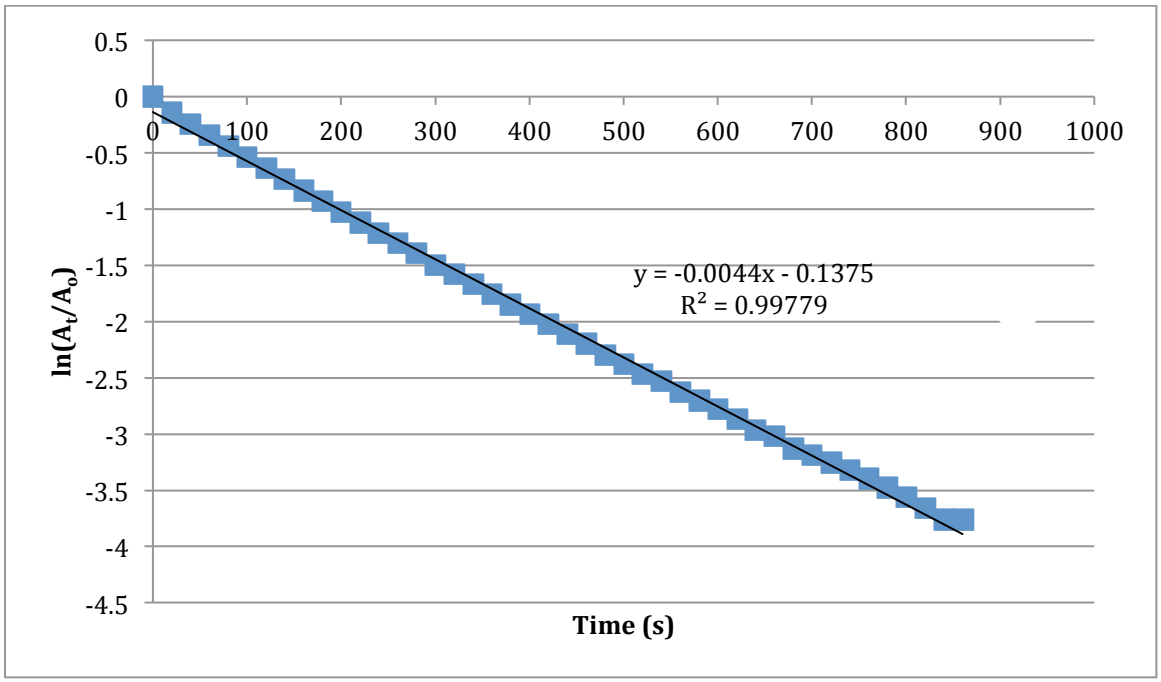
Rate Data for Conversion of 1a to 2a at pH 9.25



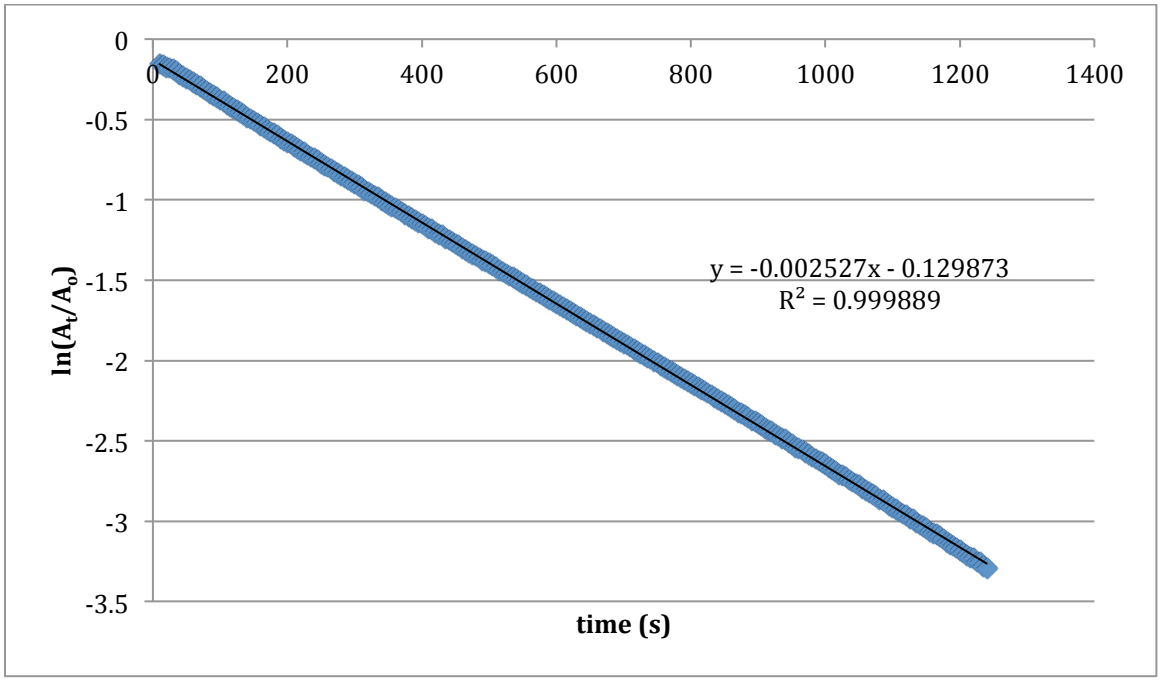
Rate Data for Conversion of 1b to 2b at pH 9.25



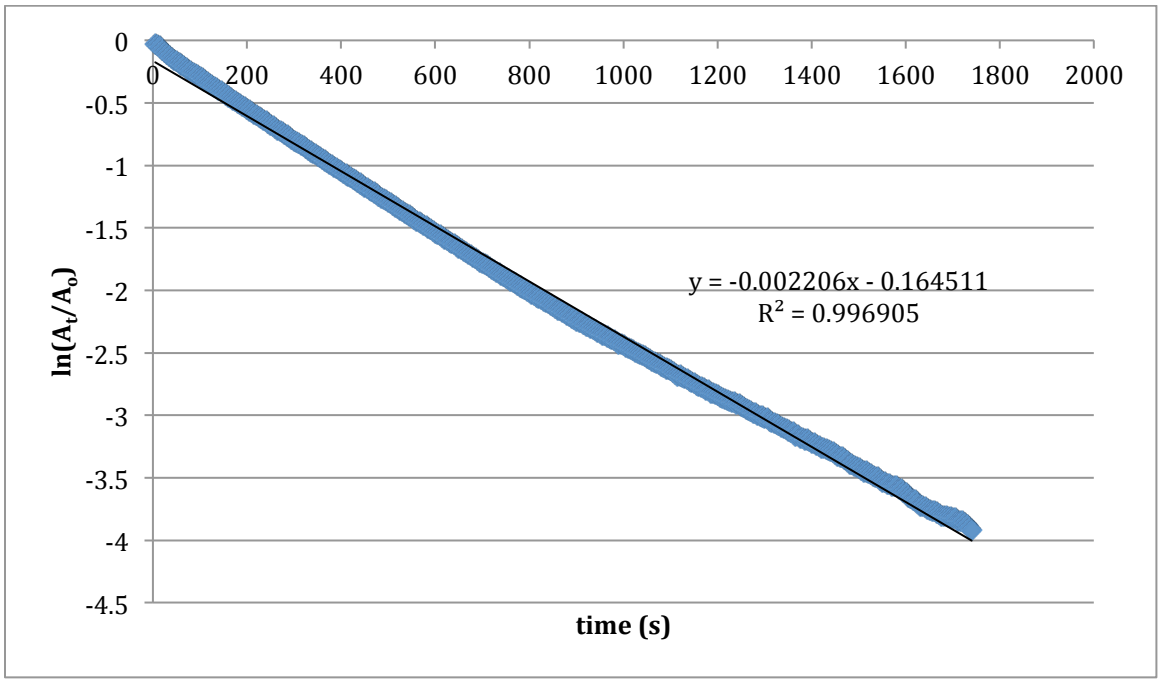
Rate Data for Conversion of 1c to 2c at pH 9.25



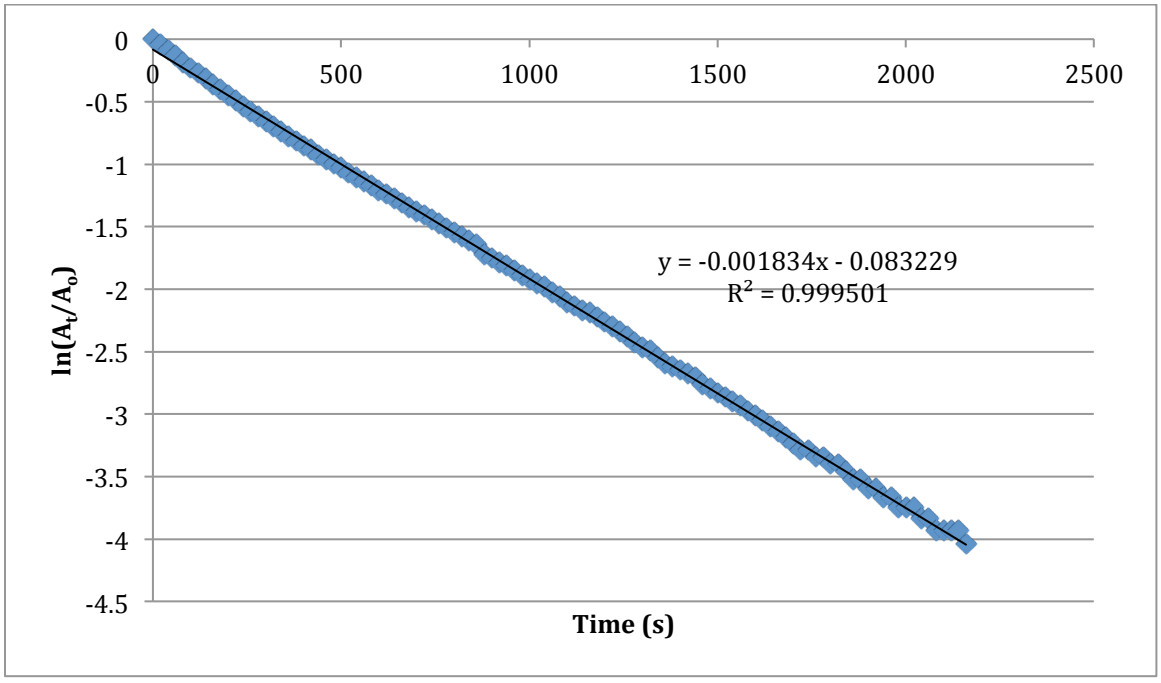
Rate Data for Conversion of 1d to 2d at pH 9.25



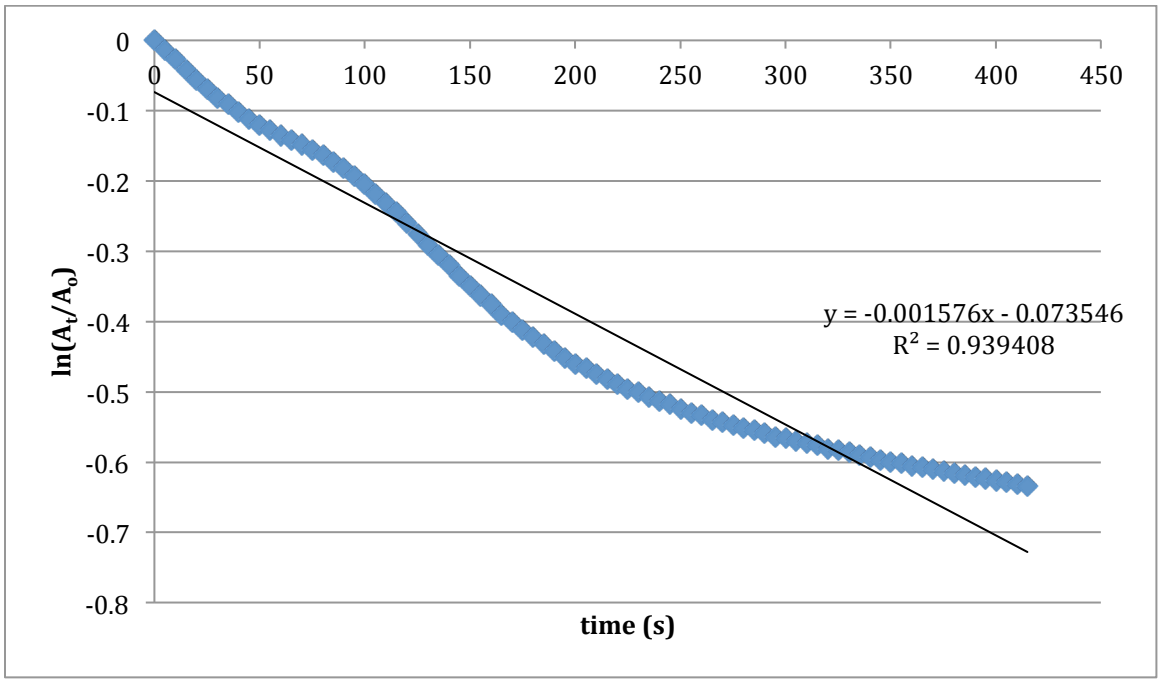
Rate Data for Conversion of 1e to 2e at pH 9.25



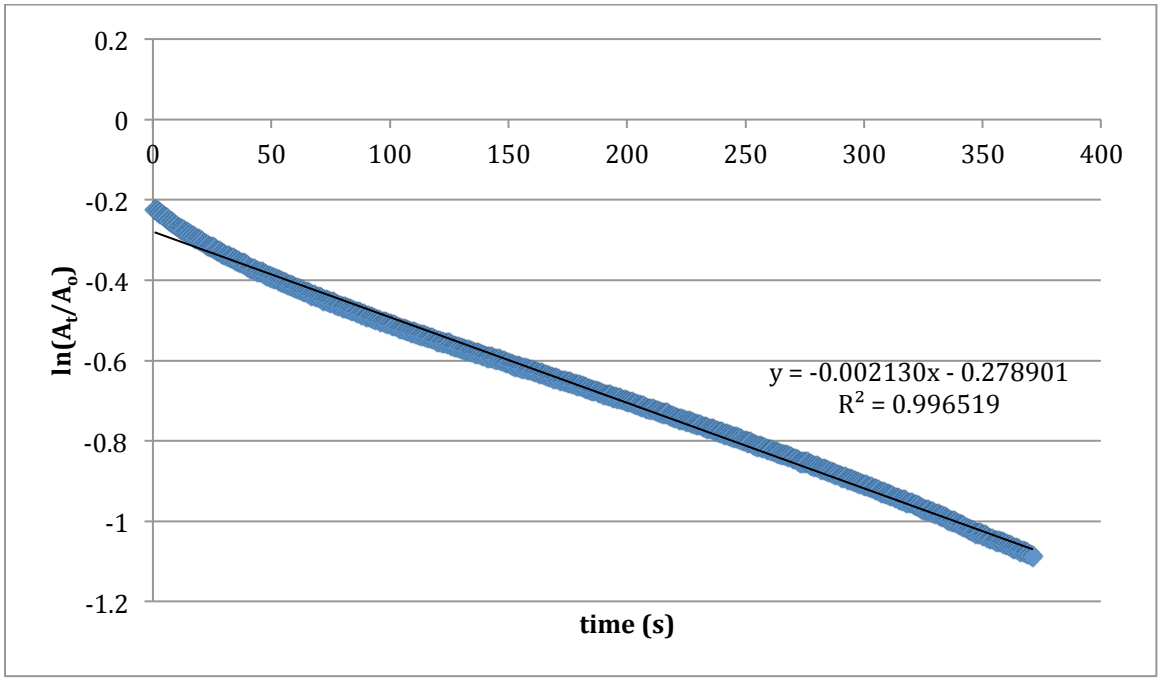
Rate Data for Conversion of 1f to 2f at pH 9.25



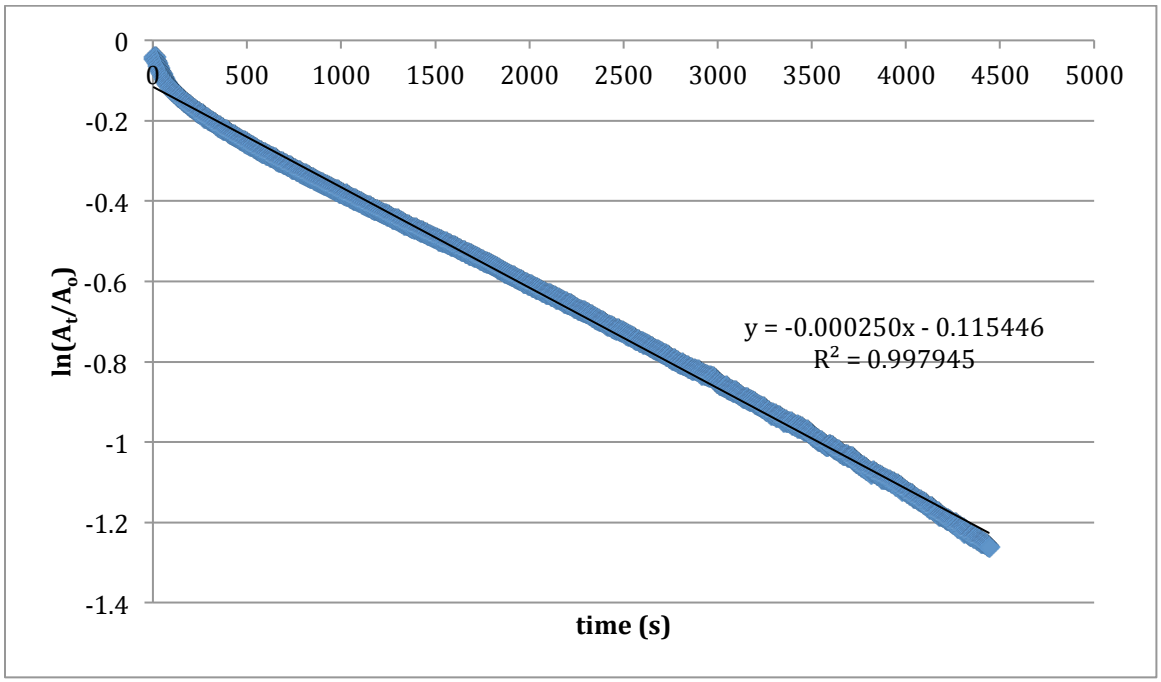
Rate Data for Conversion of 1g to 2g at pH 9.25



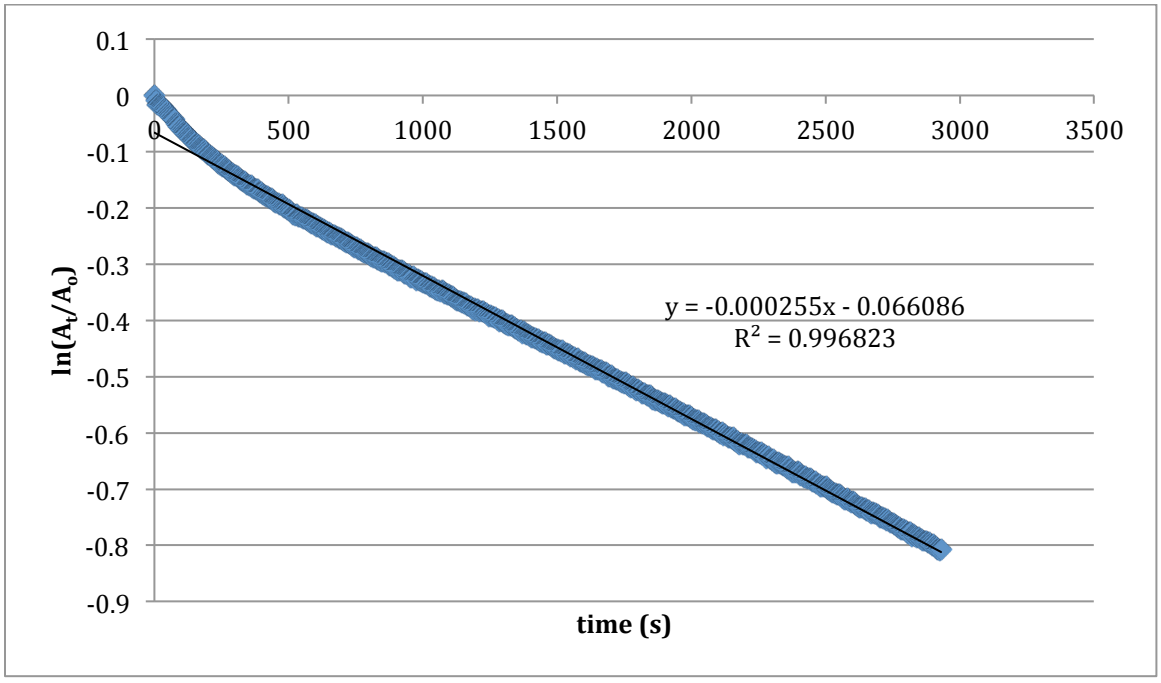
Rate Data for Conversion of 1h to 2h at pH 9.25



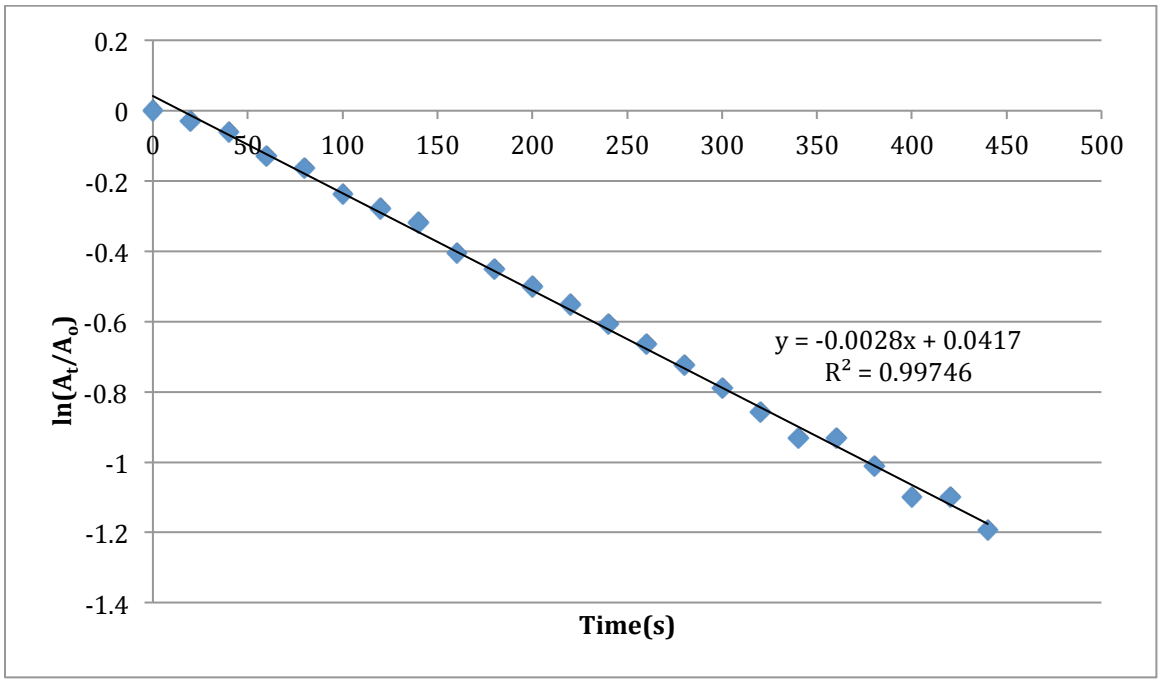
Rate Data for Conversion of 1i to 2i at pH 9.25



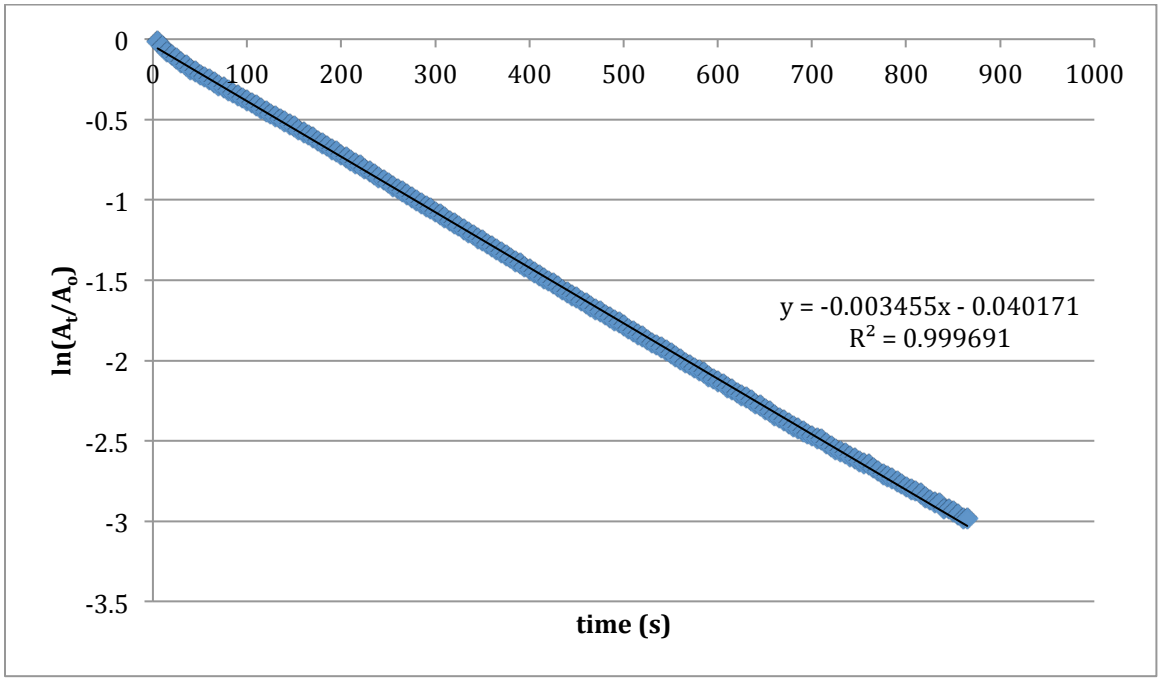
Rate Data for Conversion of 1j to 2j at pH 9.25



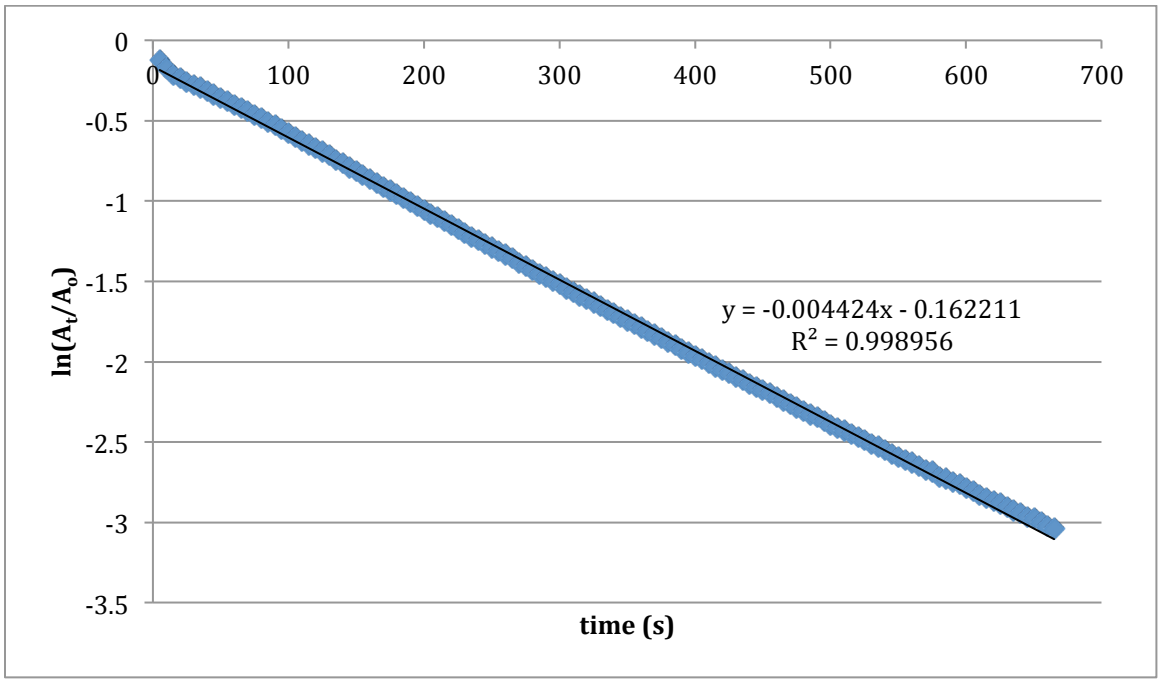
Rate Data for Conversion of 1k to 2k at pH 9.25



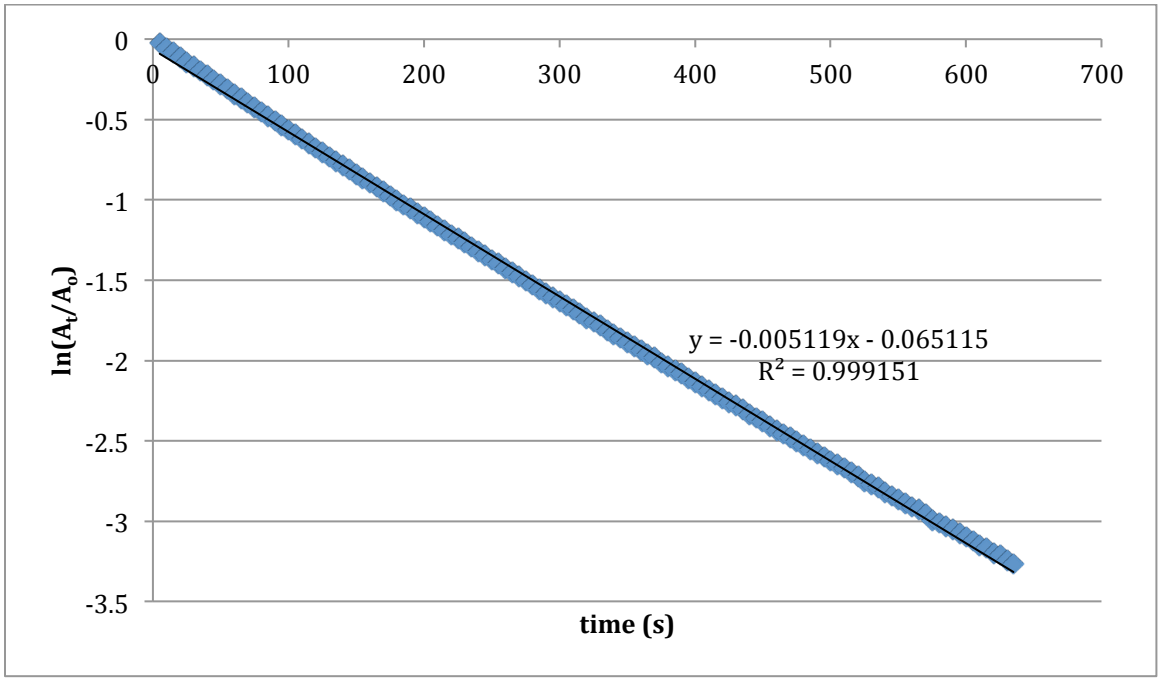
Rate Data for Conversion of 1l to 2l at pH 9.25



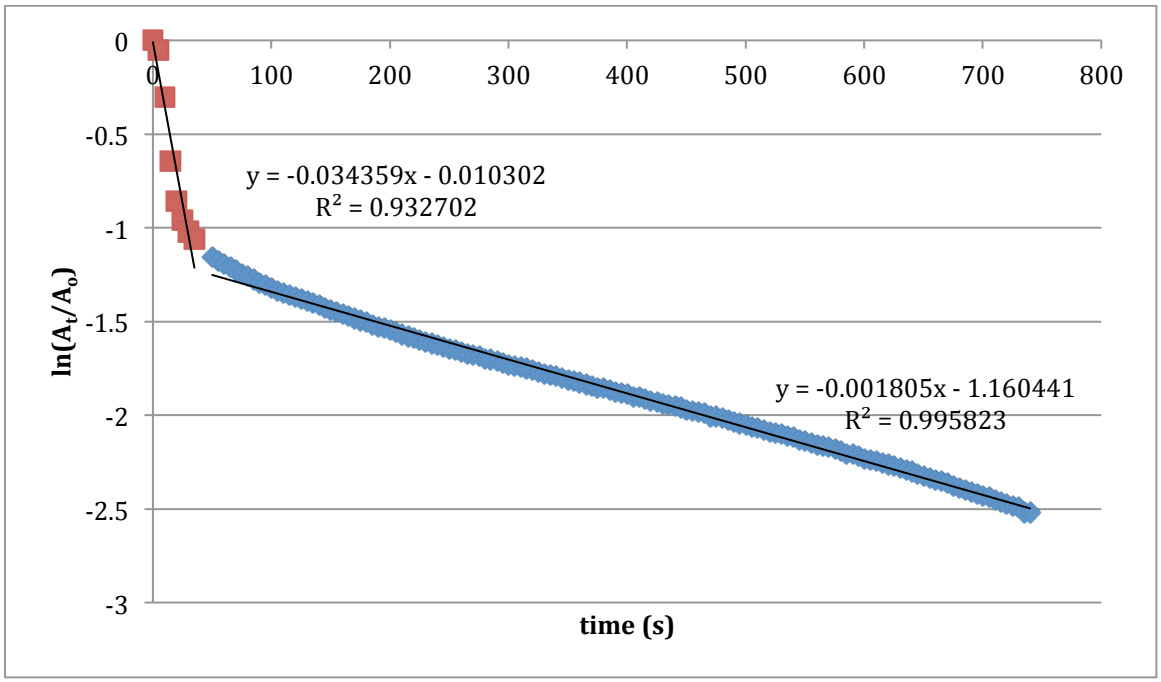
Rate Data for Conversion of 1m to 2m at pH 9.25



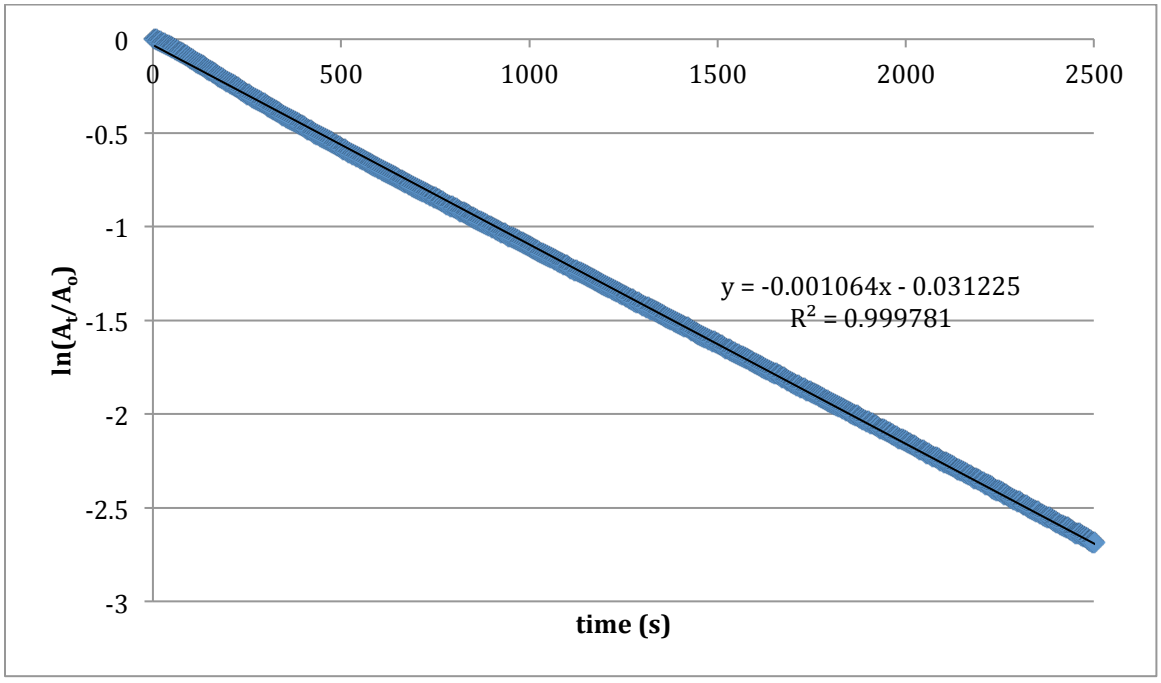
Rate Data for Conversion of 1n to 2n at pH 9.25



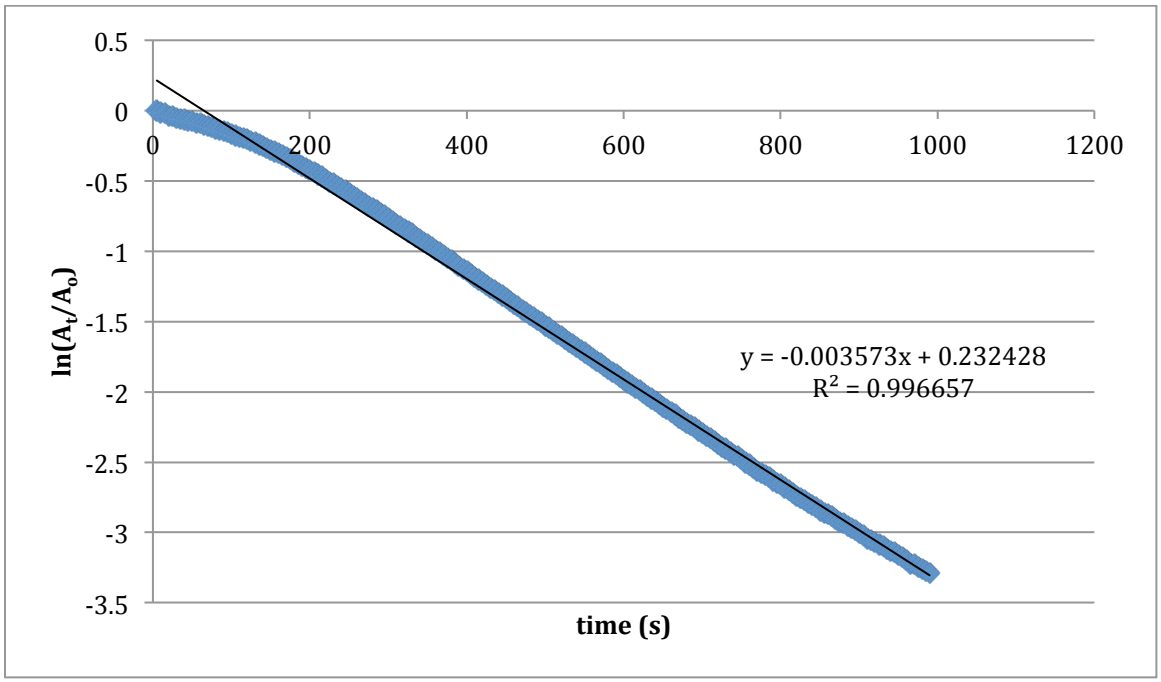
Rate Data for Conversion of 1o to 2o at pH 9.25



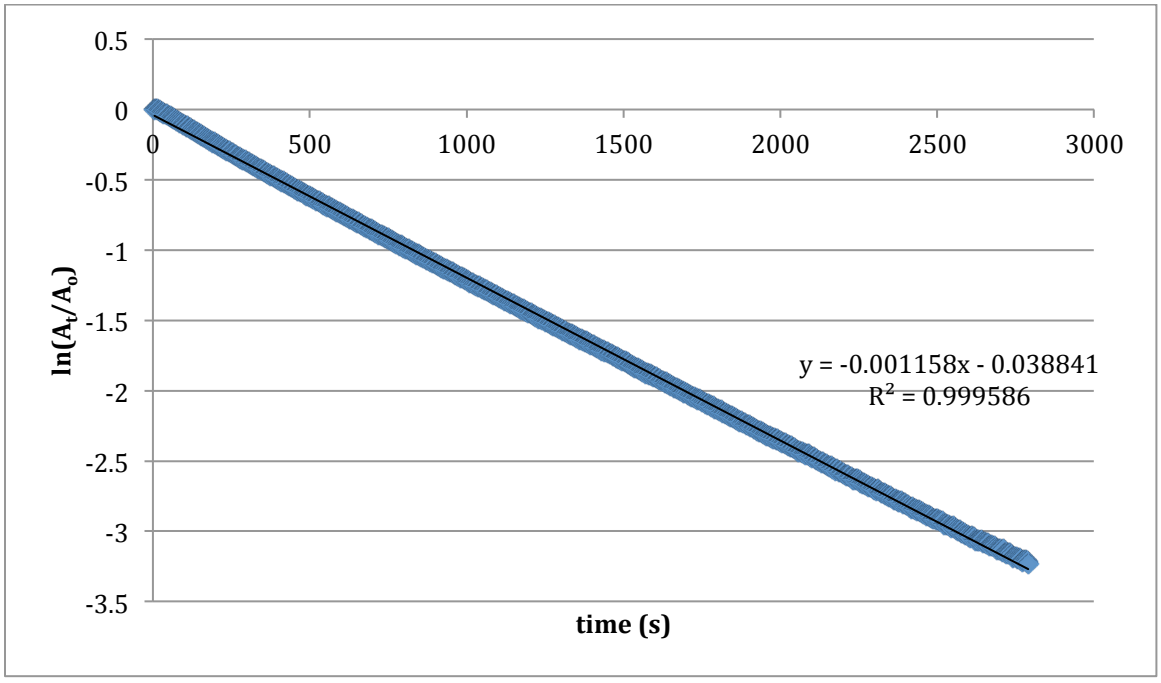
Rate Data for Conversion of 1p to 2p at pH 9.25



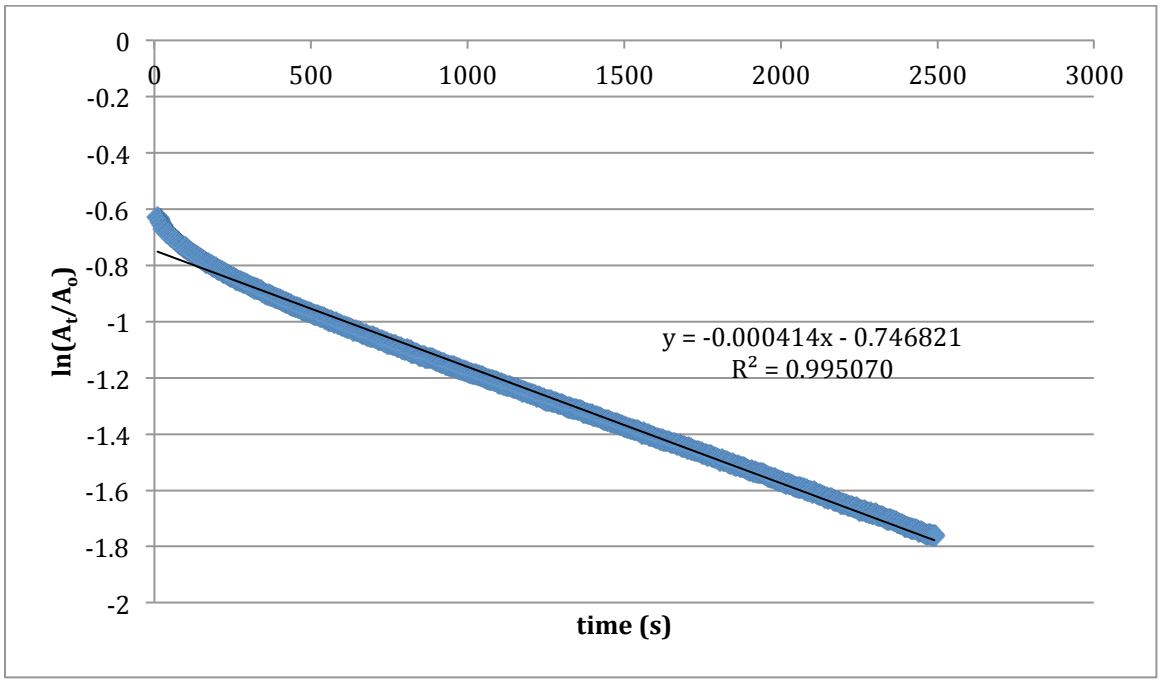
Rate Data for Conversion of 1r to 2r at pH 9.25



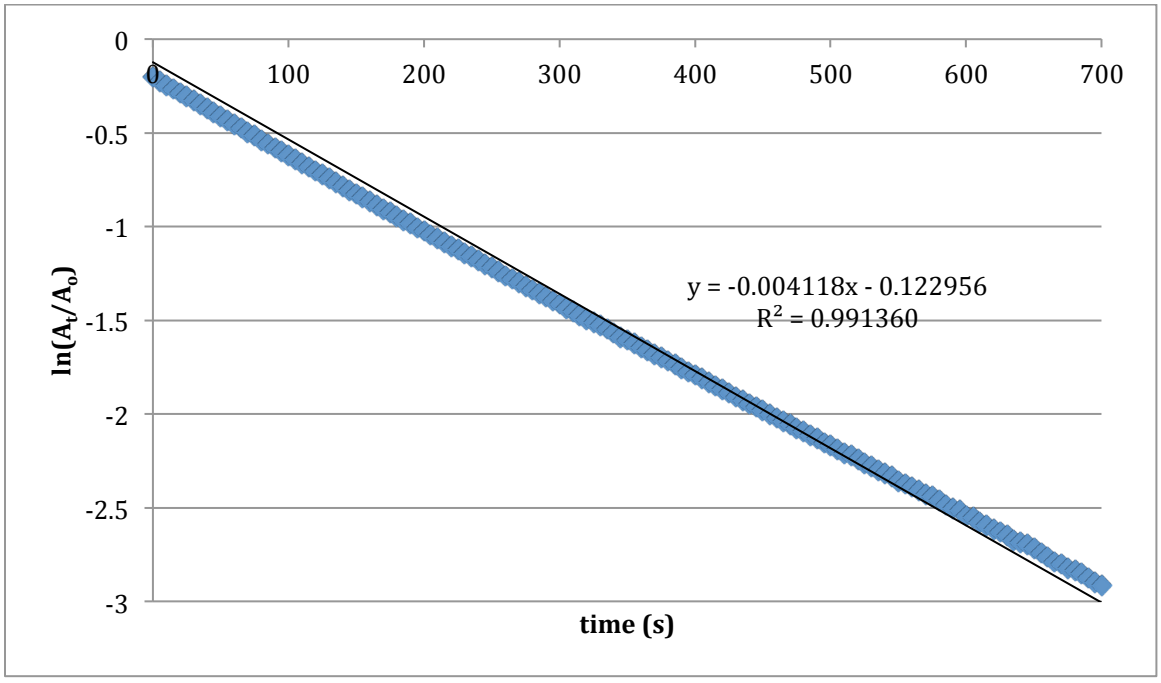
Rate Data for Conversion of 1s to 2s at pH 9.25



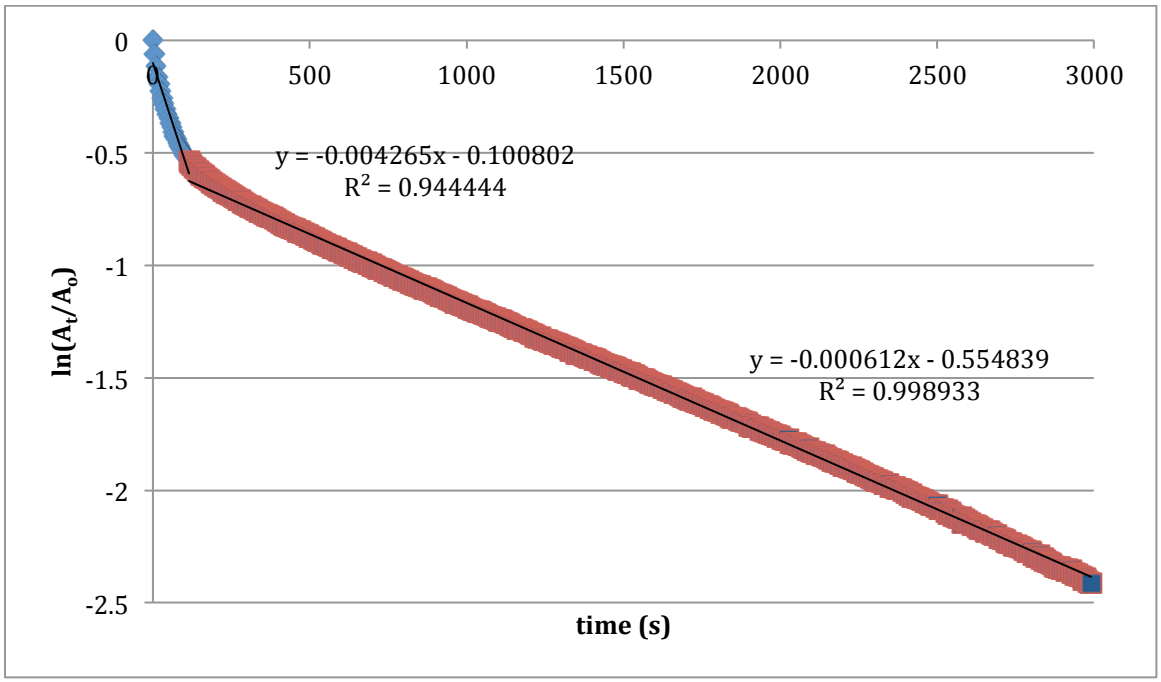
Rate Data for Conversion of 1t to 2t at pH 9.25



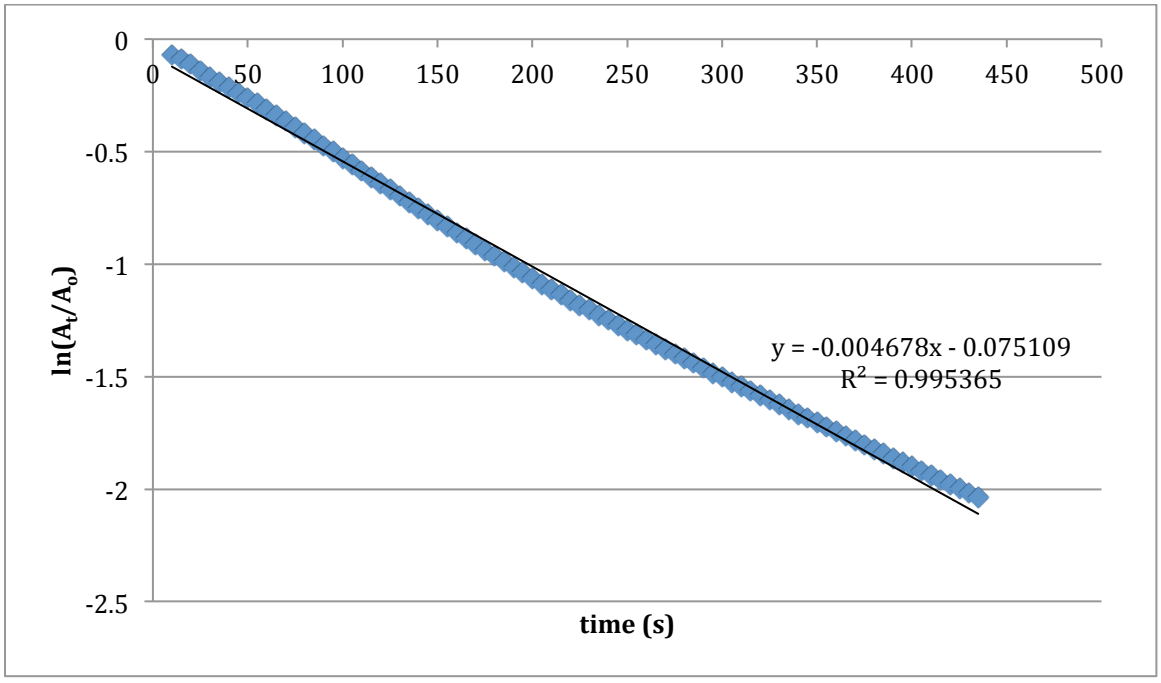
Rate Data for Conversion of 1u to 2u at pH 9.25



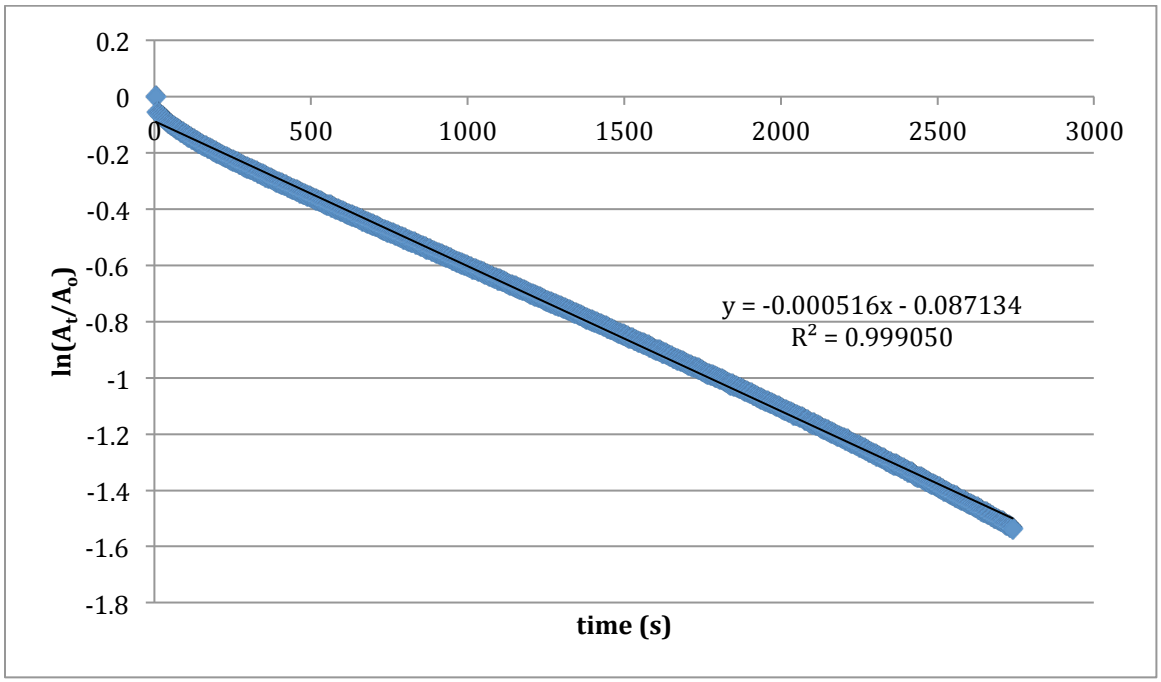
Rate Data for Conversion of 1v to 2v at pH 9.25



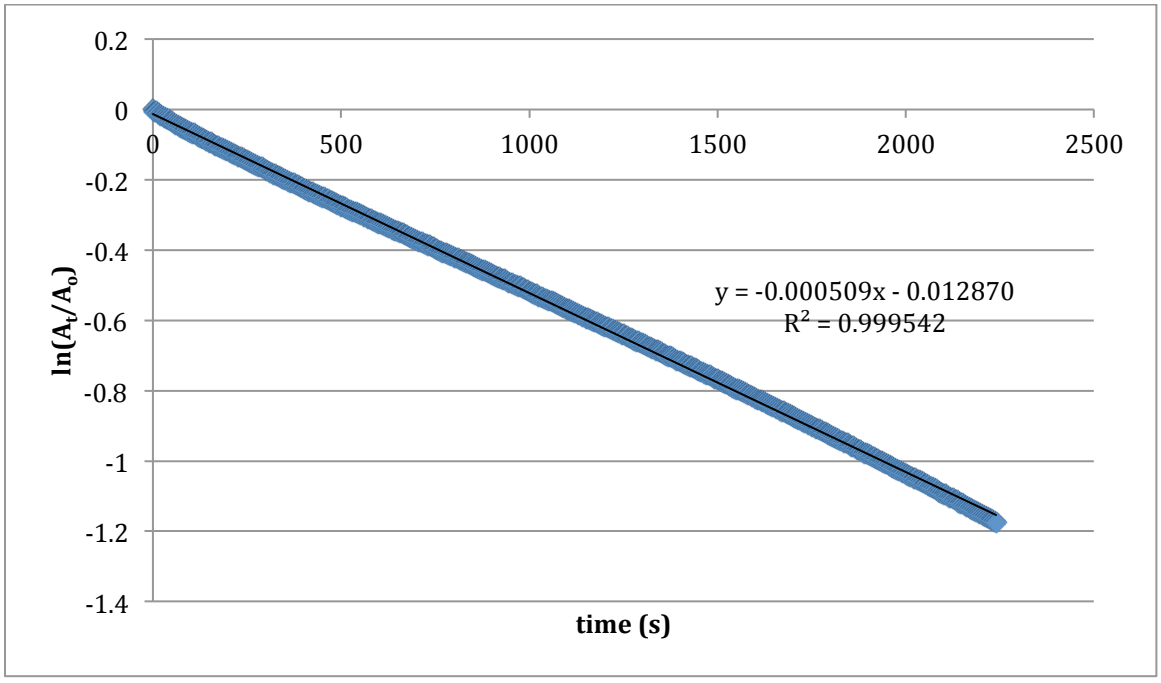
Rate Data for Conversion of 1w to 2w at pH 9.25



Rate Data for Conversion of 1x to 2x at pH 9.25

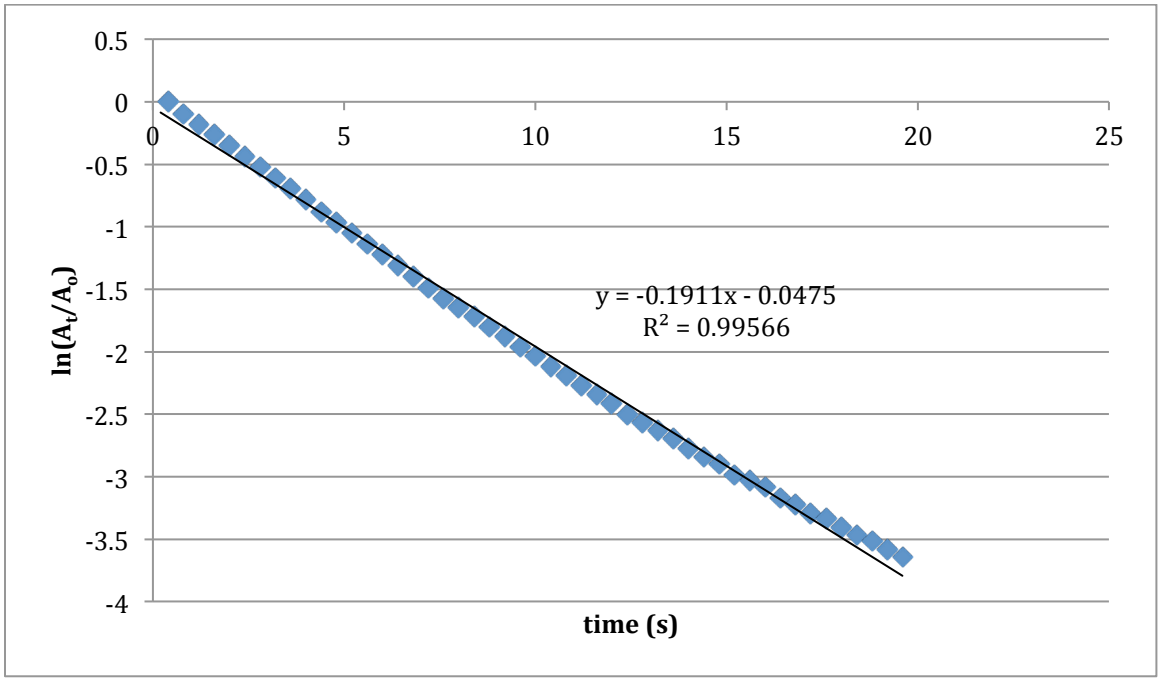


Rate Data for Conversion of 1y to 2y at pH 9.25

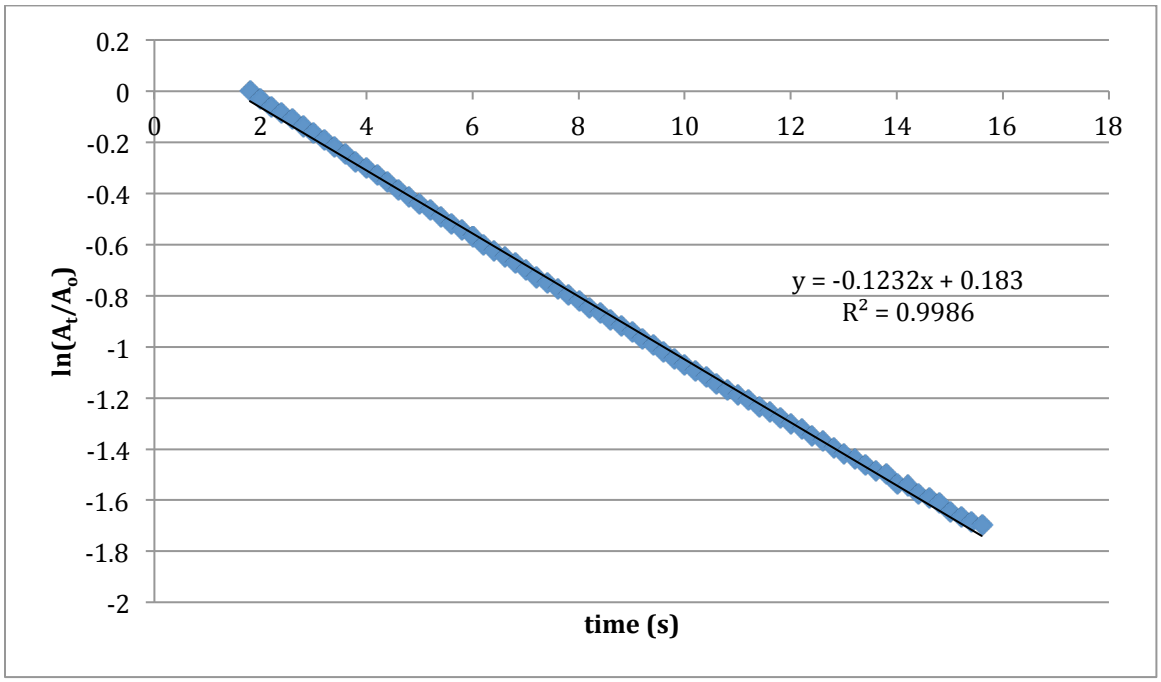


RAW DATA PLOTS FROM FLAVANONE TO CHALCONE RATE DETERMINATION ASSAY

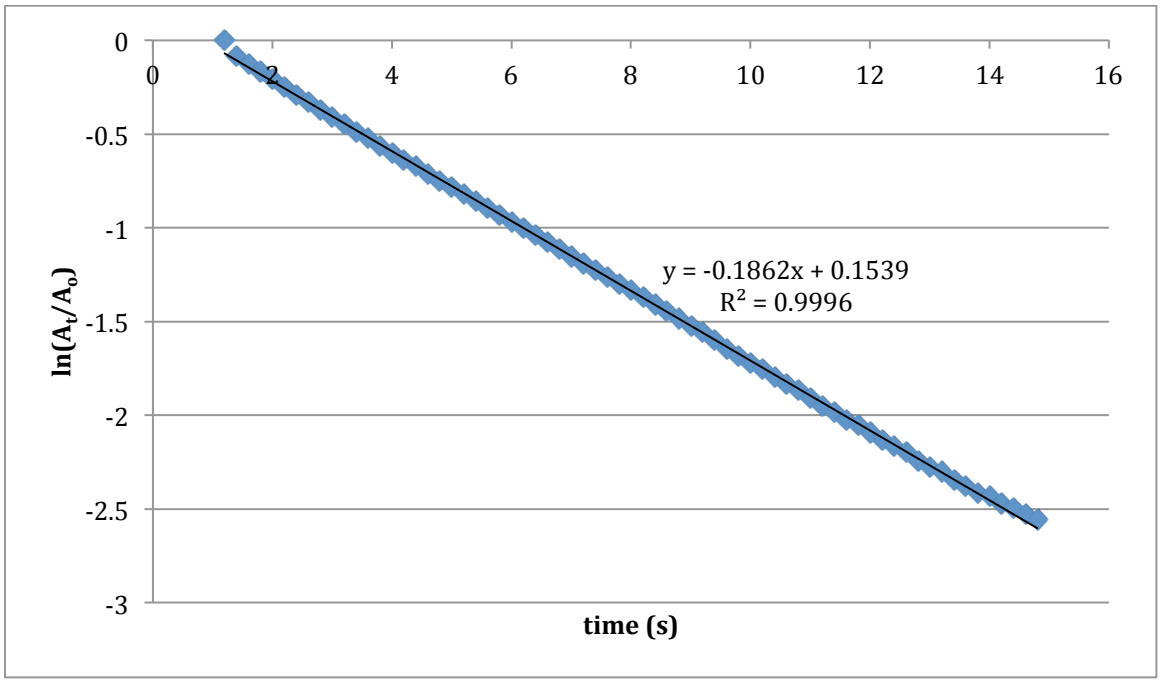
Rate Data for Conversion of 2a to 1a at pH 13



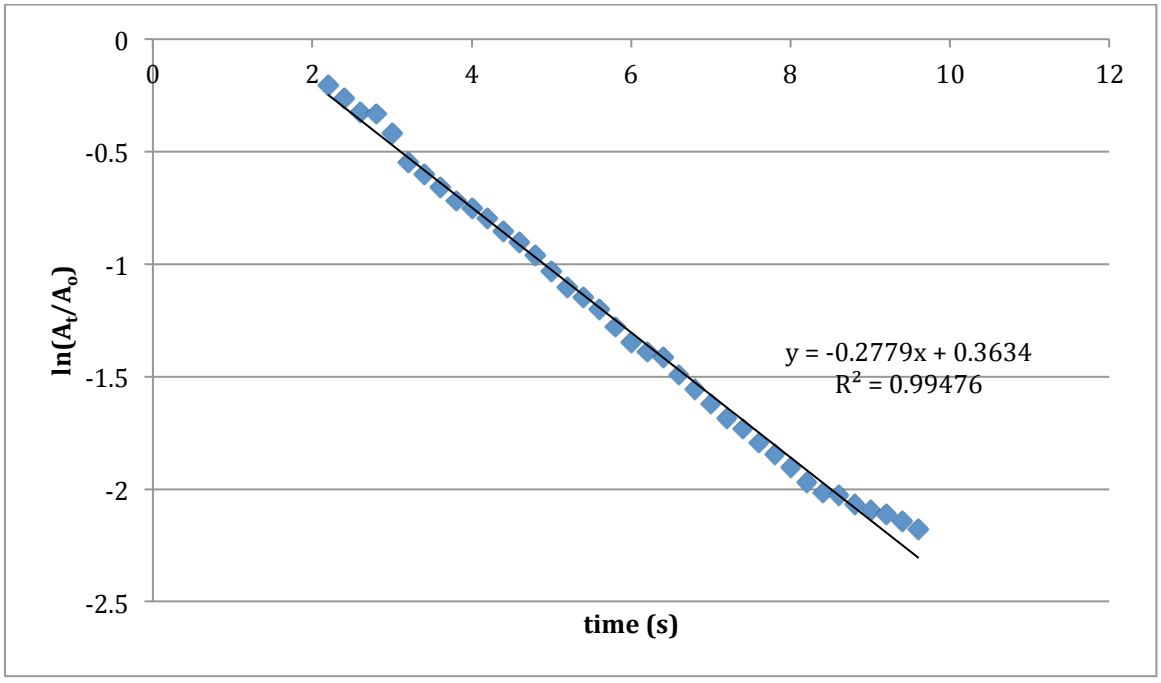
Rate Data for Conversion of 2b to 1b at pH 13



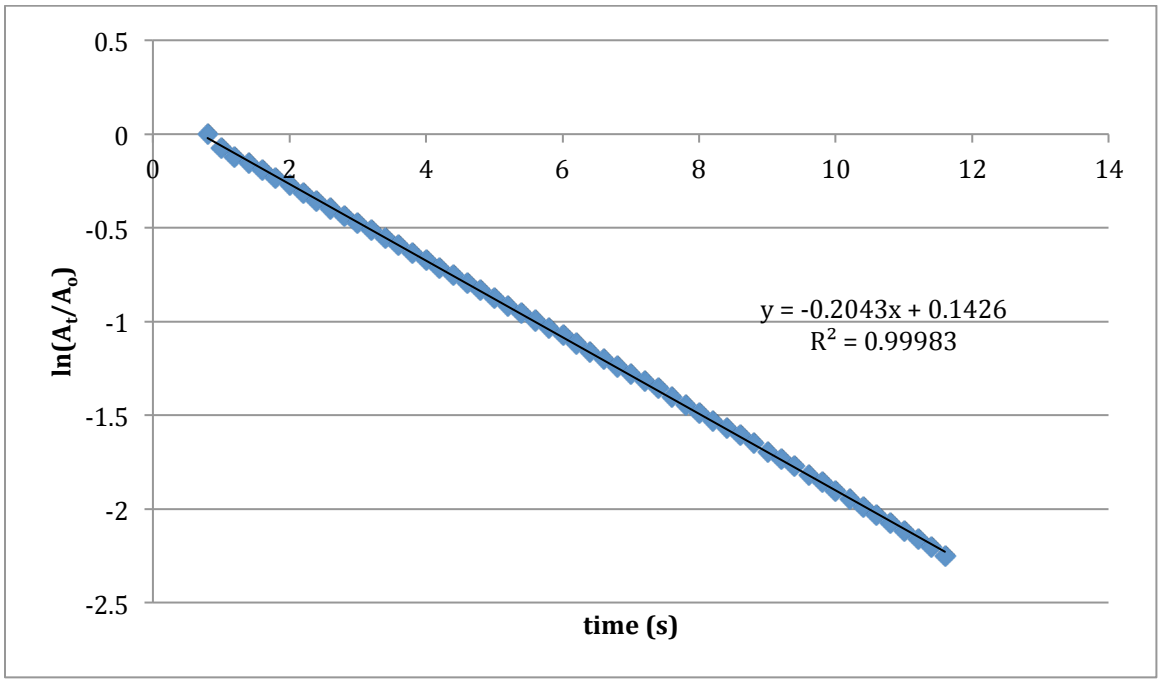
Rate Data for Conversion of 2c to 1c at pH 13



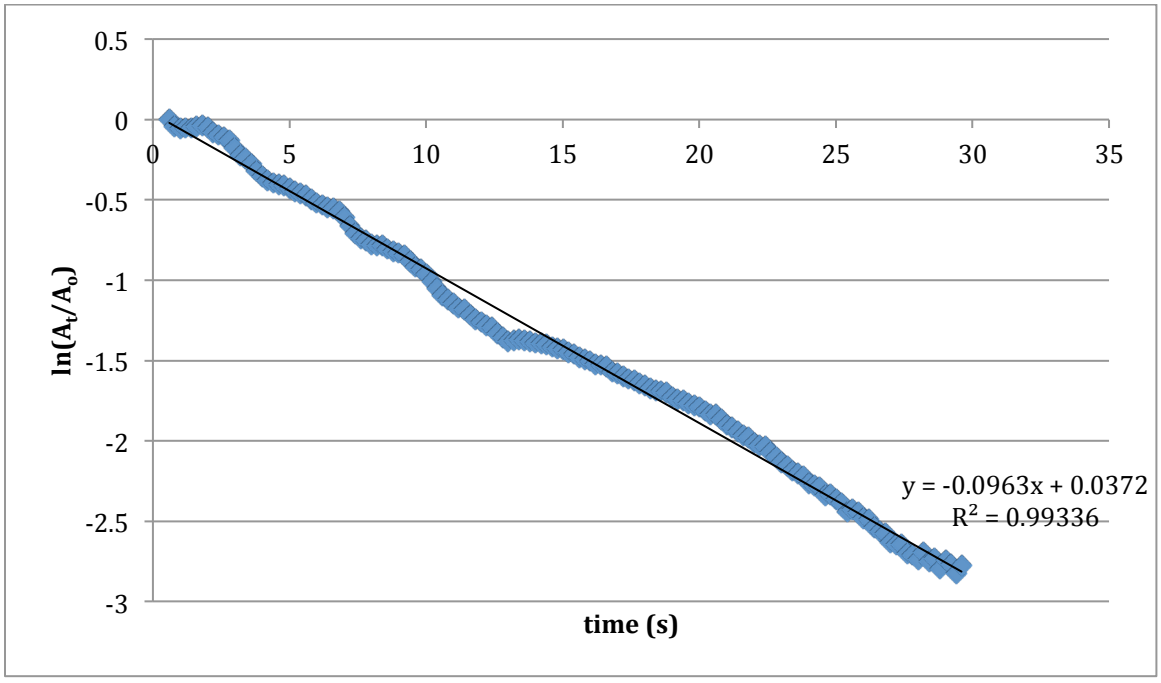
Rate Data for Conversion of 2d to 1d at pH 13



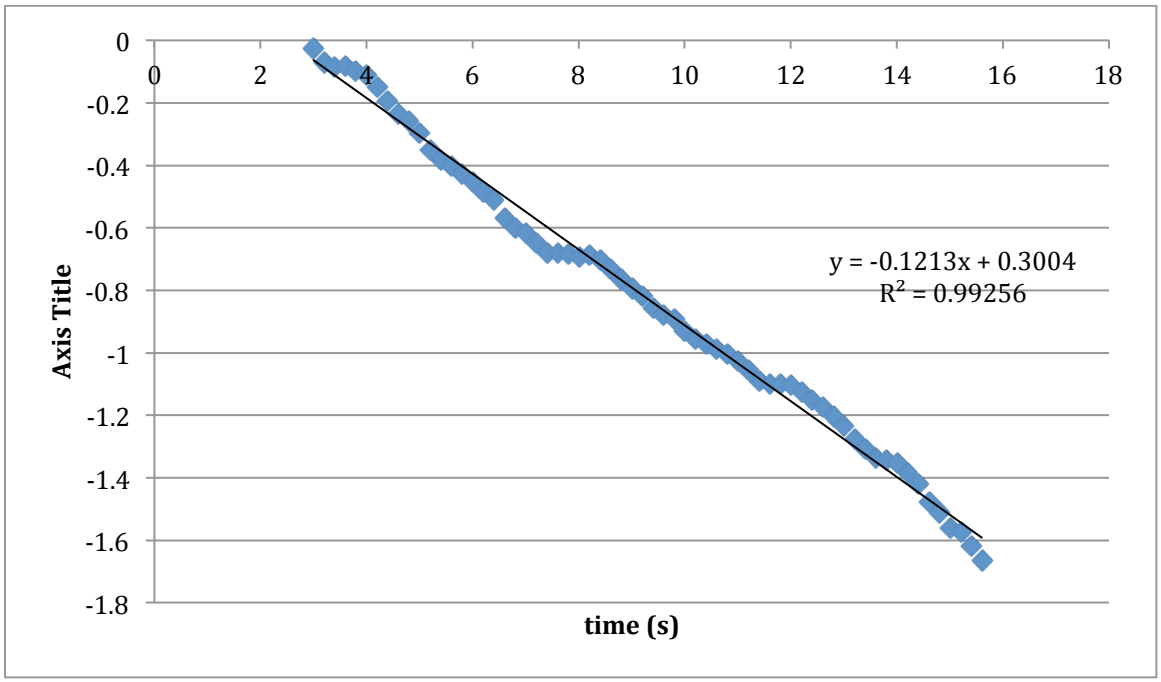
Rate Data for Conversion of 2e to 1e at pH 13



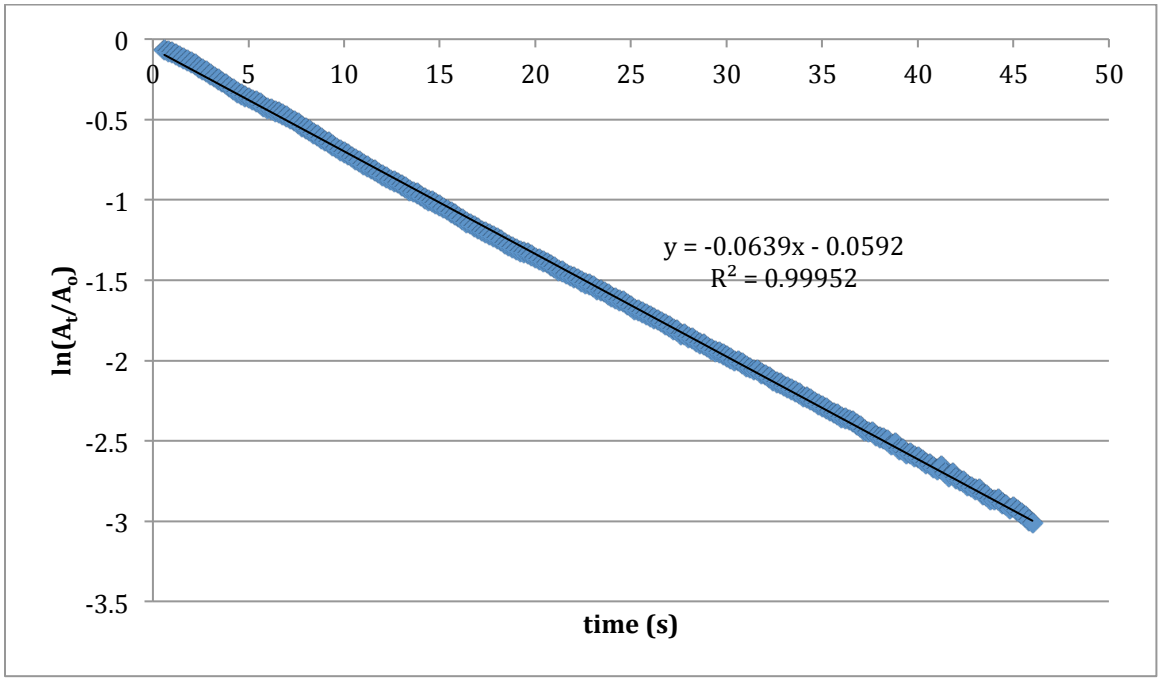
Rate Data for Conversion of 2f to 1f at pH 13



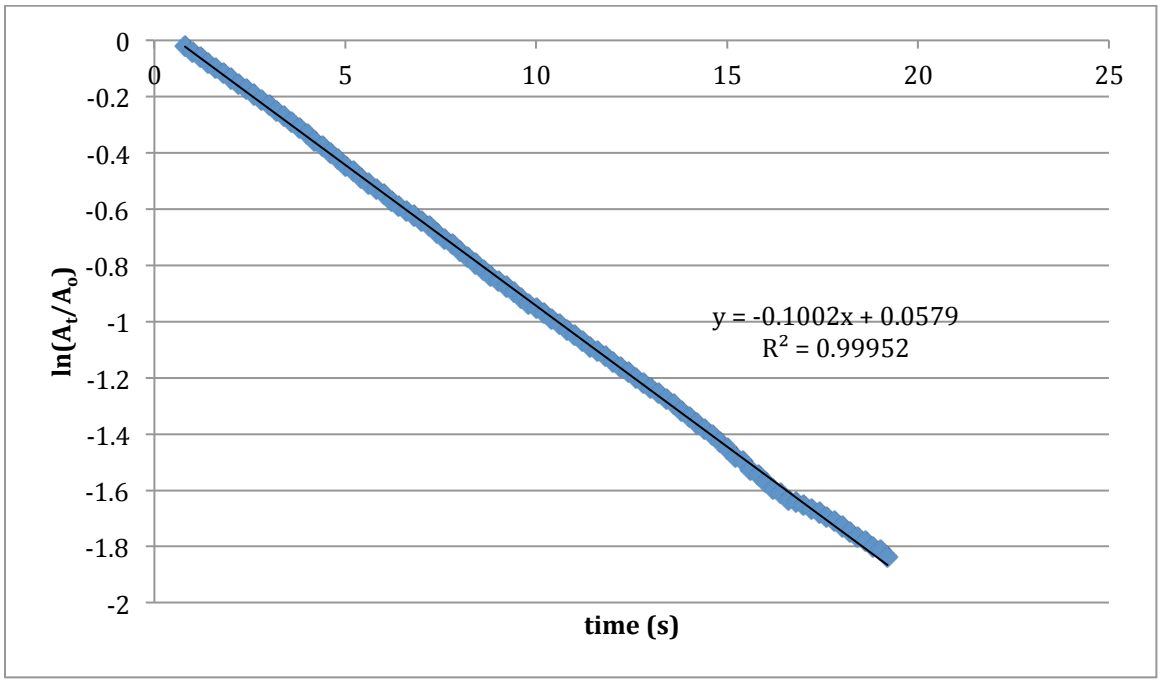
Rate Data for Conversion of 2g to 1g at pH 13



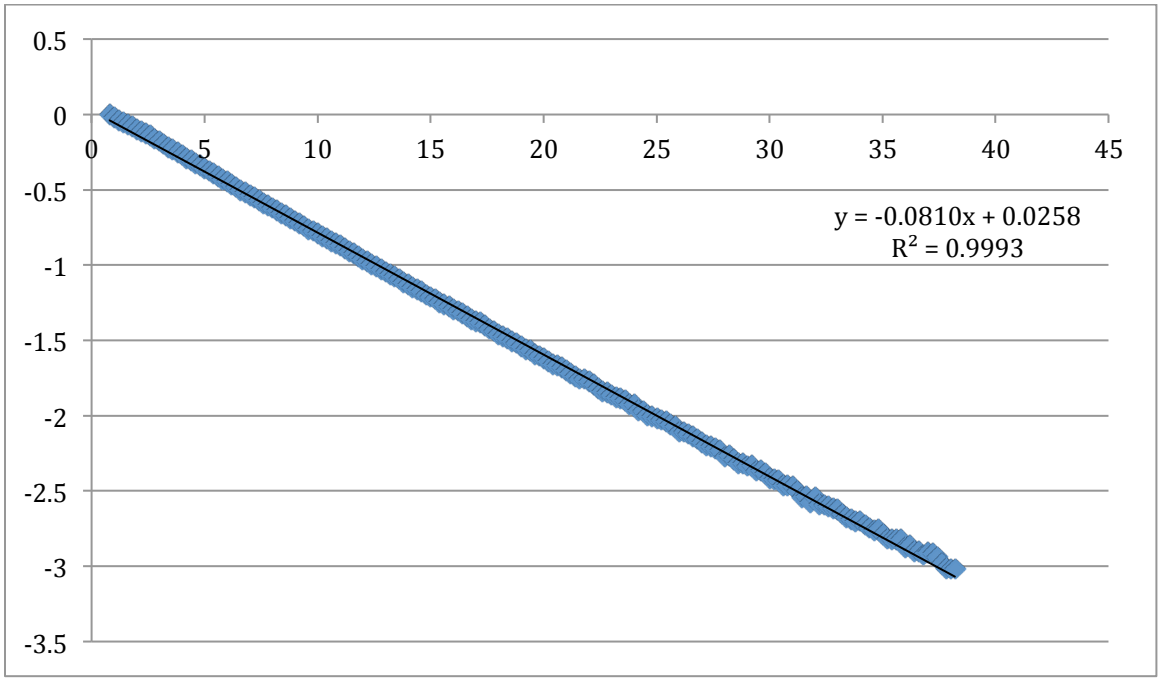
Rate Data for Conversion of 2h to 1h at pH 13



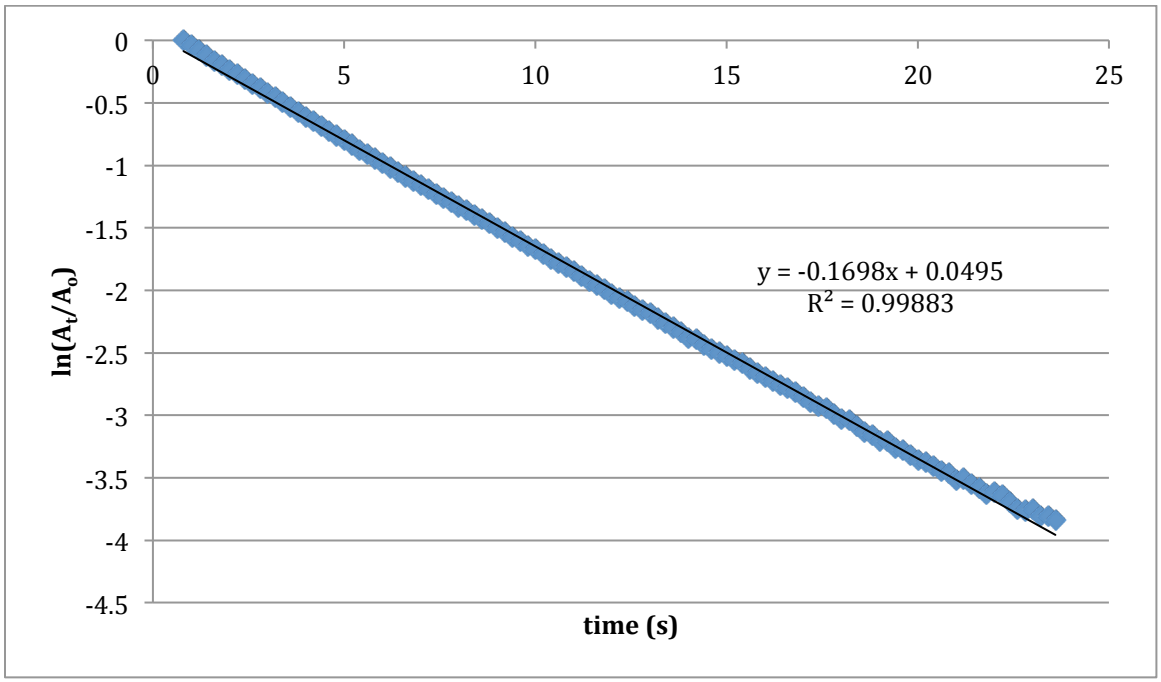
Rate Data for Conversion of 2i to 1i at pH 13



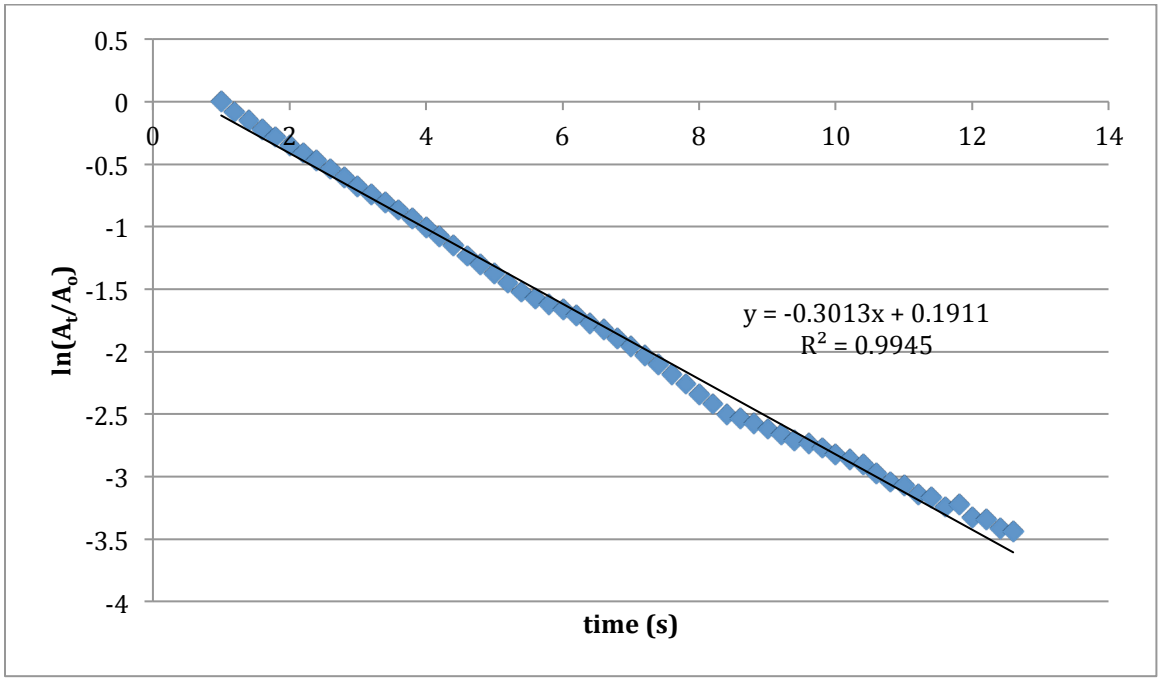
Rate Data for Conversion of 2j to 1j at pH 13



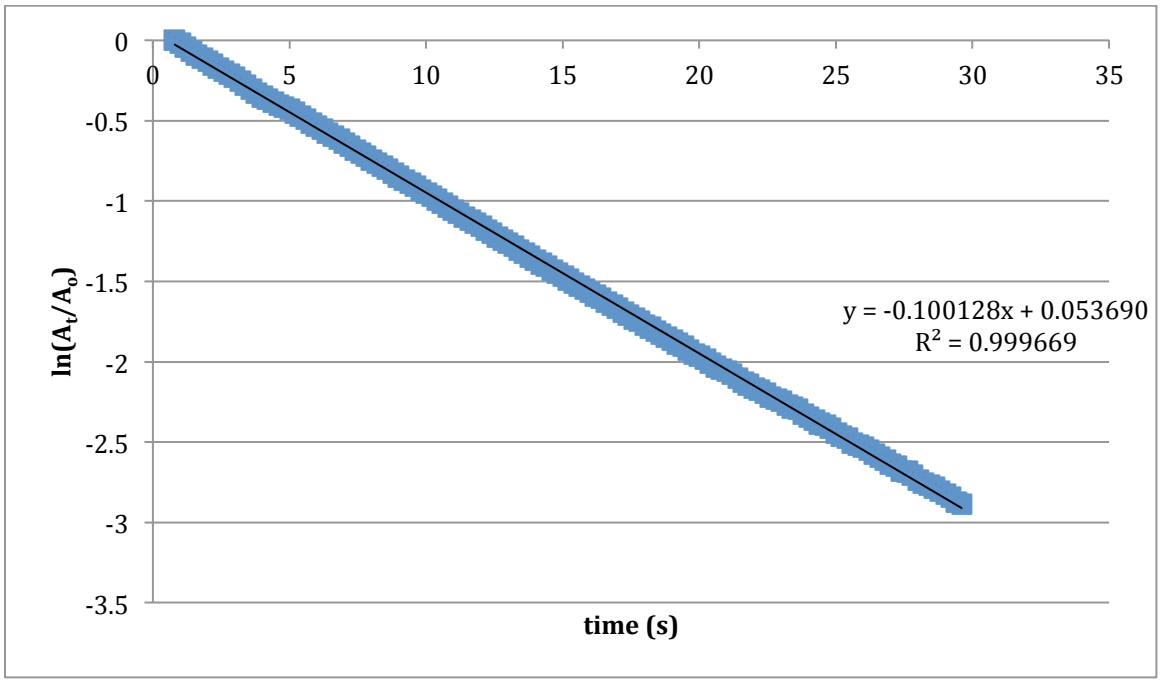
Rate Data for Conversion of 2k to 1k at pH 13



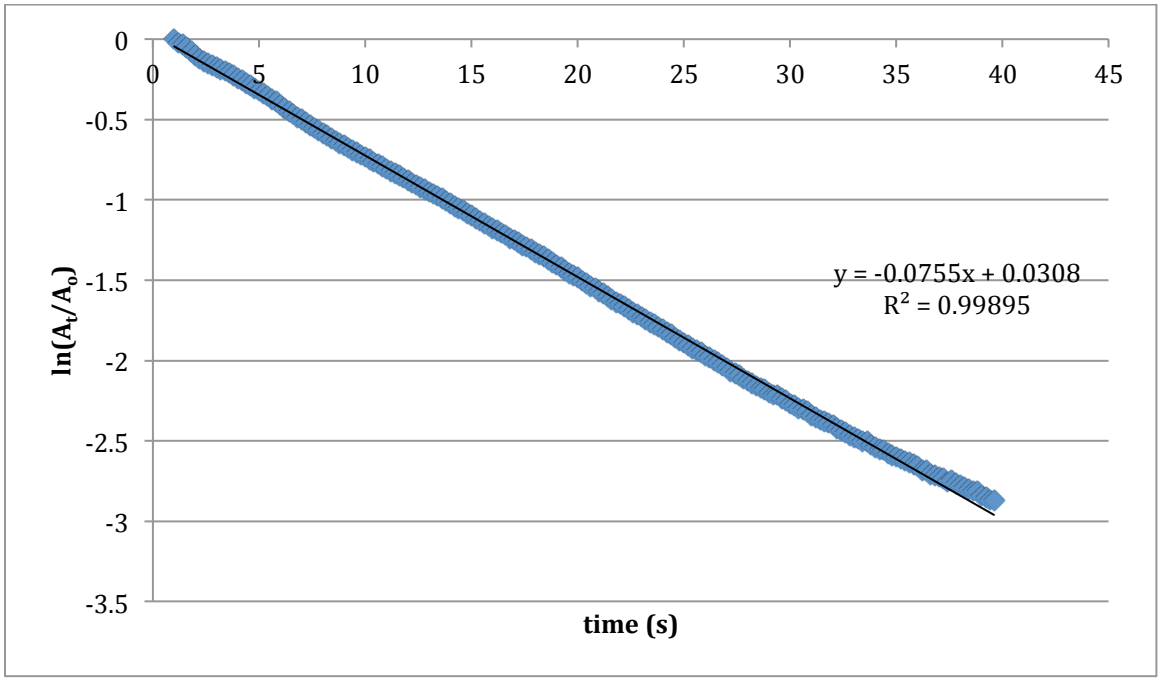
Rate Data for Conversion of 2l to 1l at pH 13



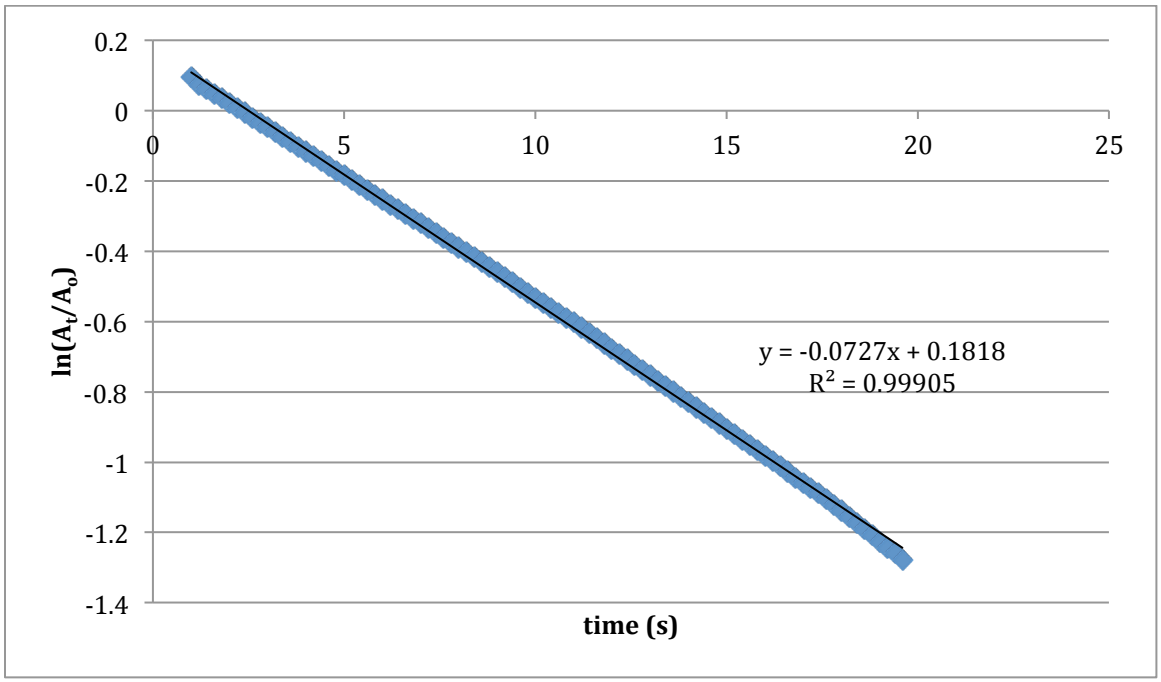
Rate Data for Conversion of 2m to 1m at pH 13



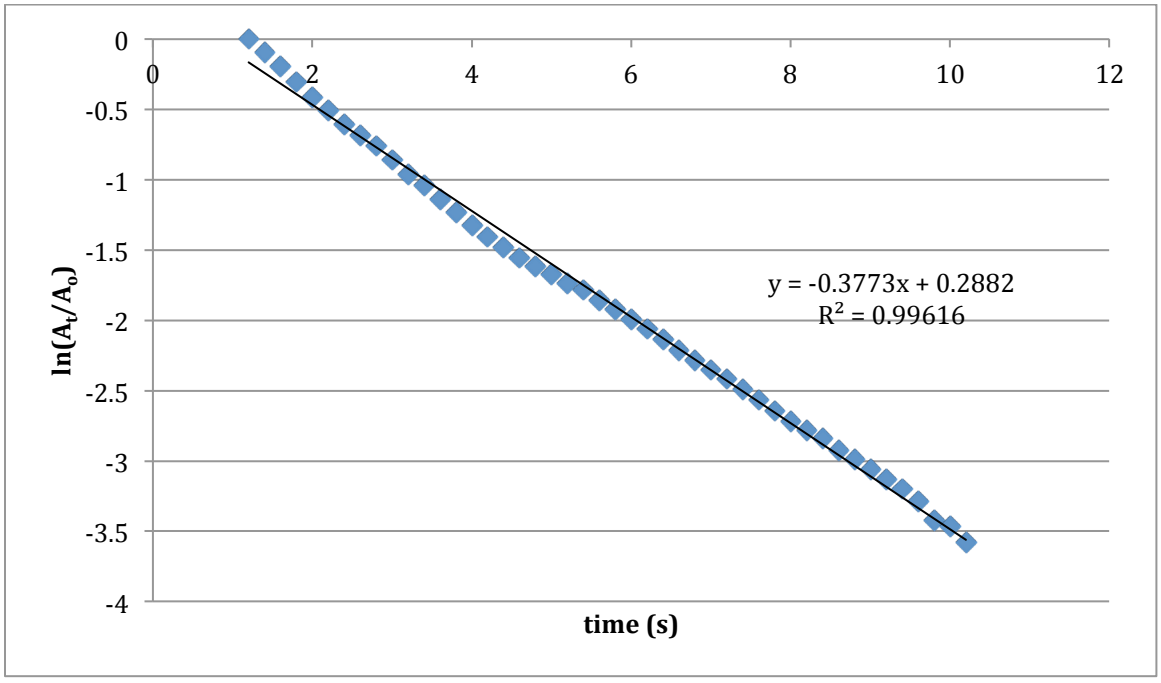
Rate Data for Conversion of 2n to 1n at pH 13



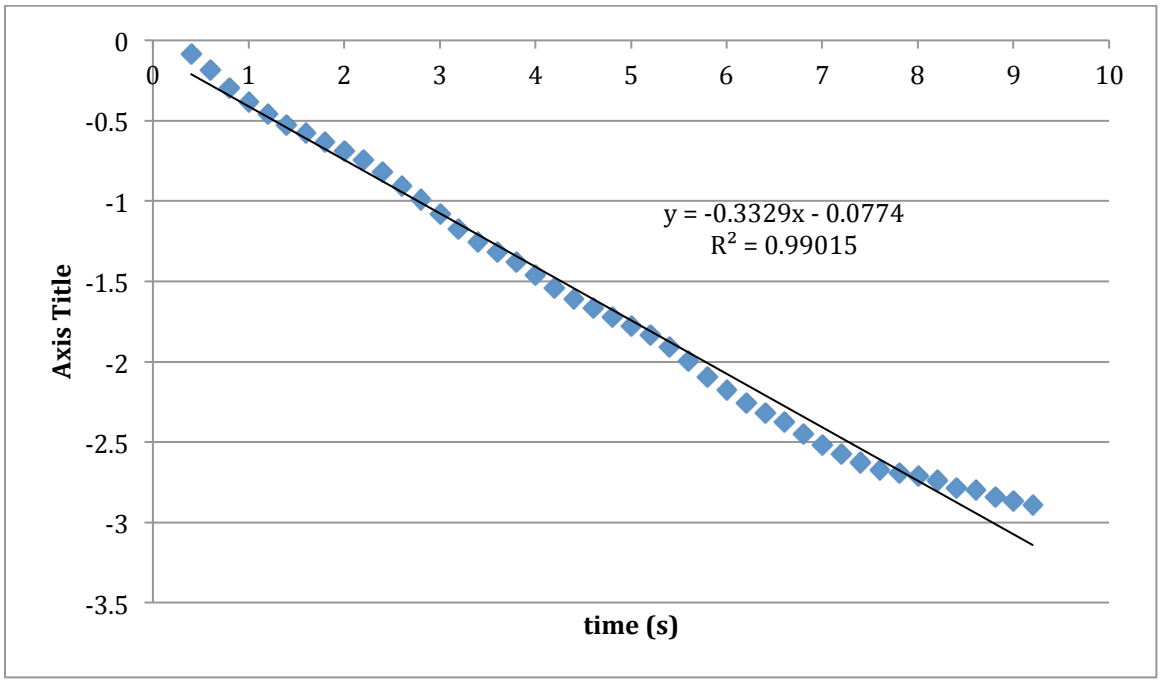
Rate Data for Conversion of 2o to 1o at pH 13



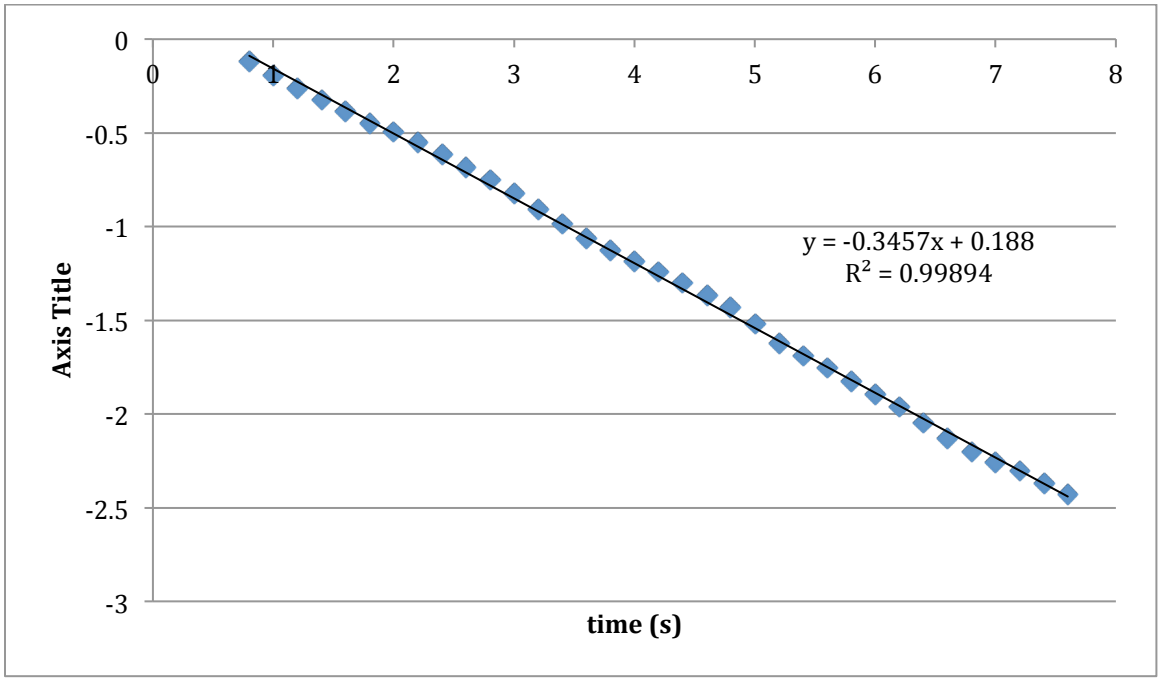
Rate Data for Conversion of 2p to 1p at pH 13



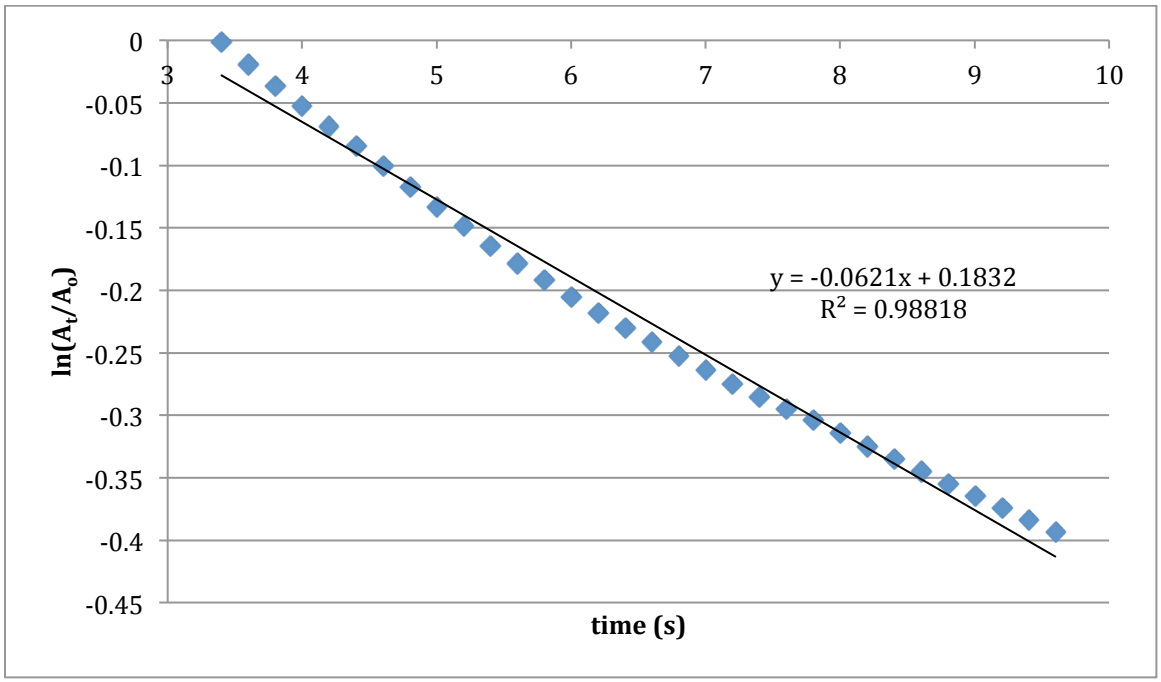
Rate Data for Conversion of 2q to 1q at pH 13



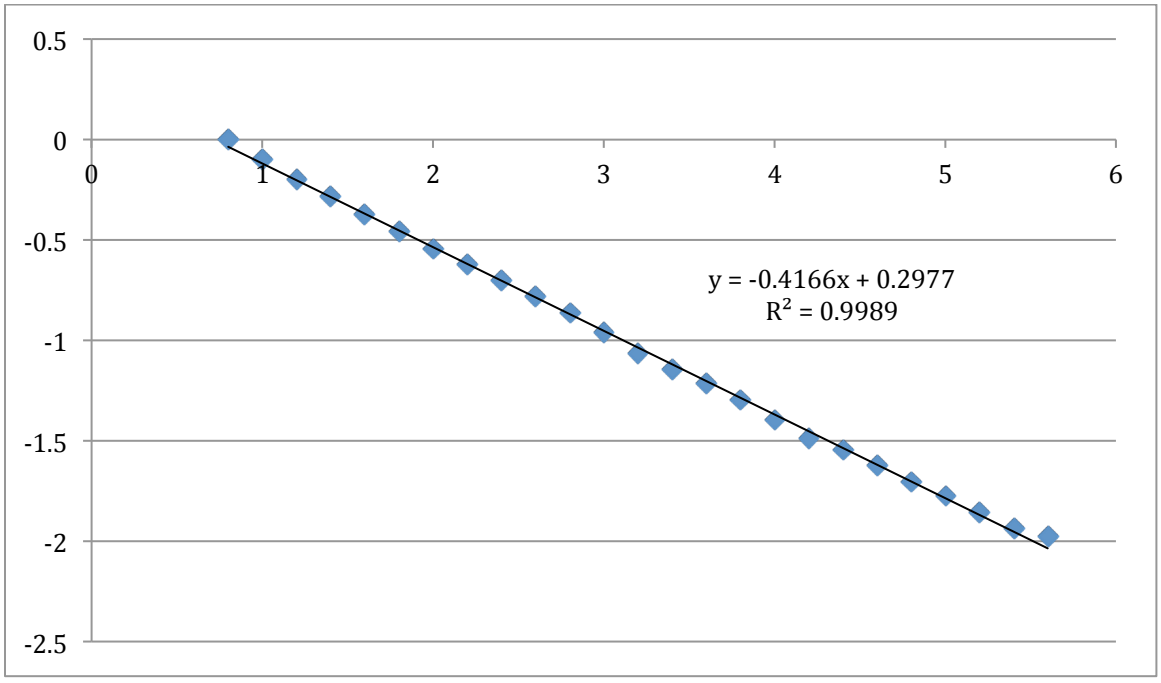
Rate Data for Conversion of 2r to 1r at pH 13



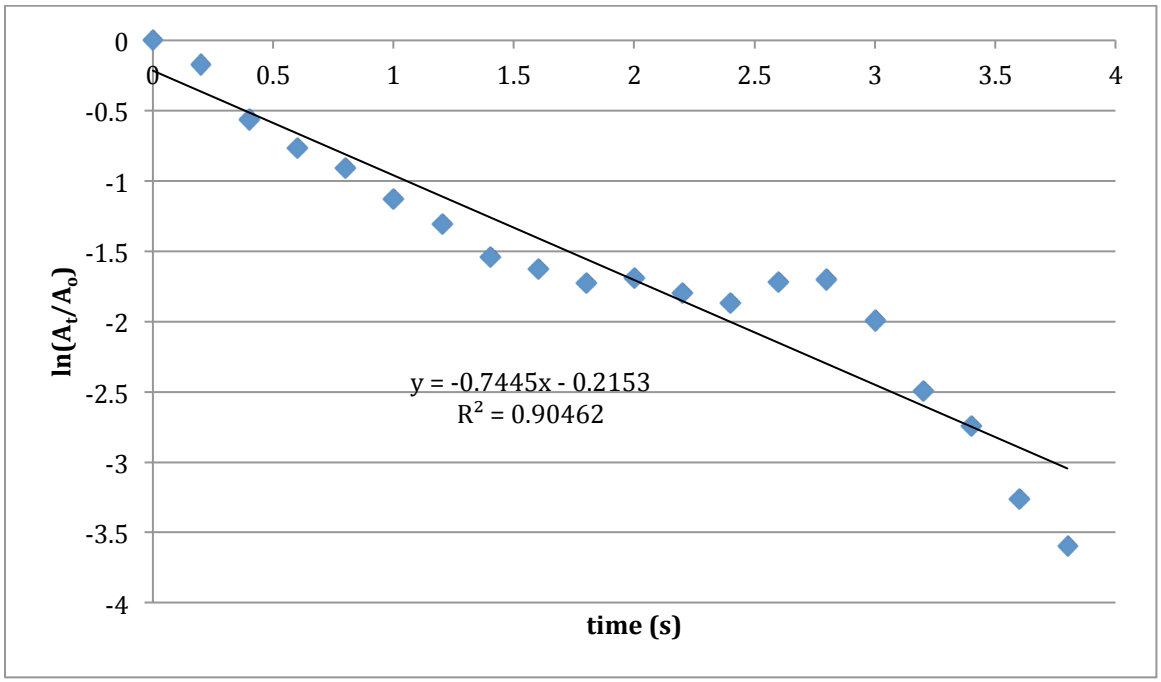
Rate Data for Conversion of 2s to 1s at pH 13



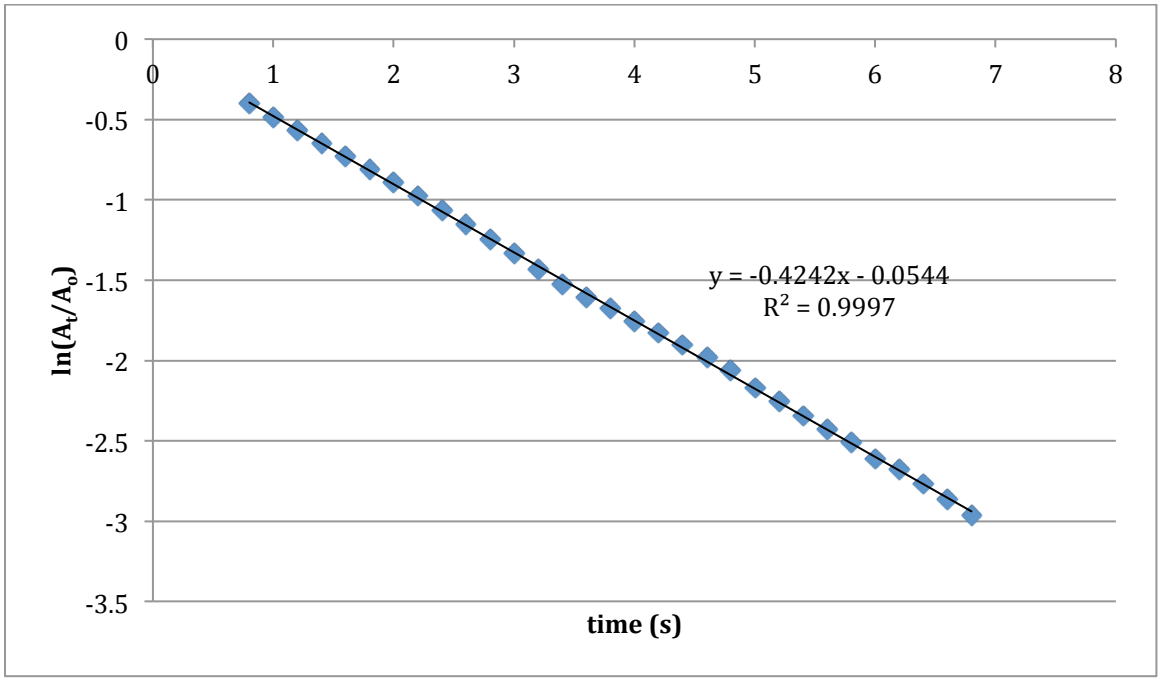
Rate Data for Conversion of 2t to 1t at pH 13



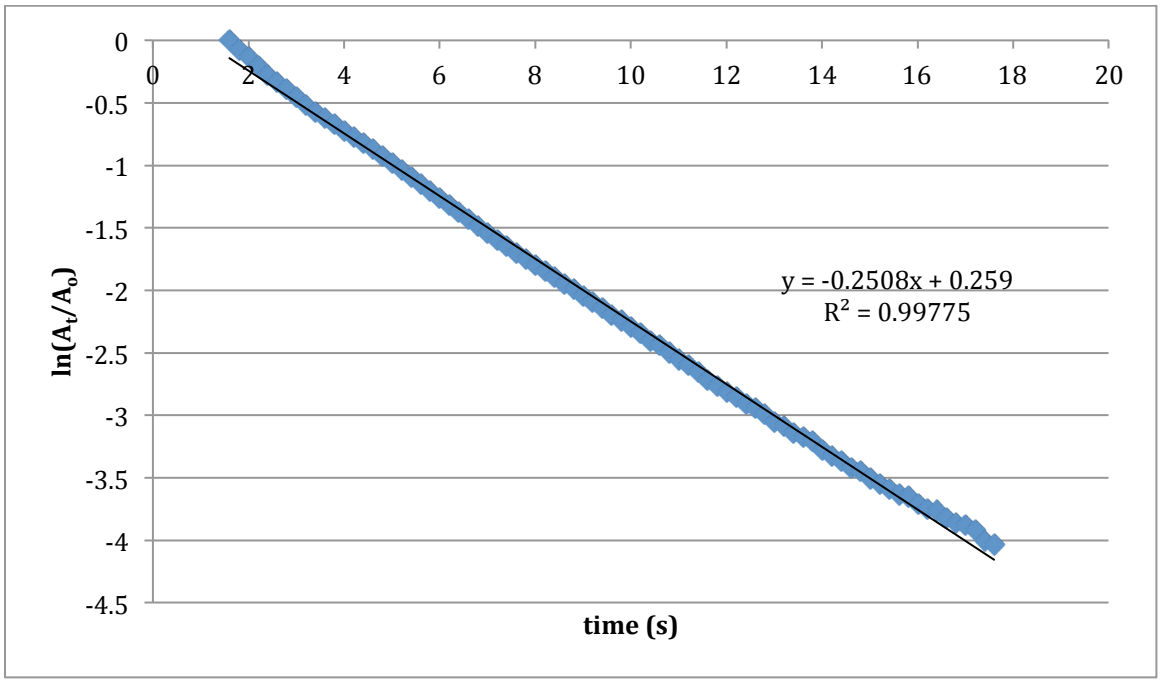
Rate Data for Conversion of 2u to 1u at pH 13



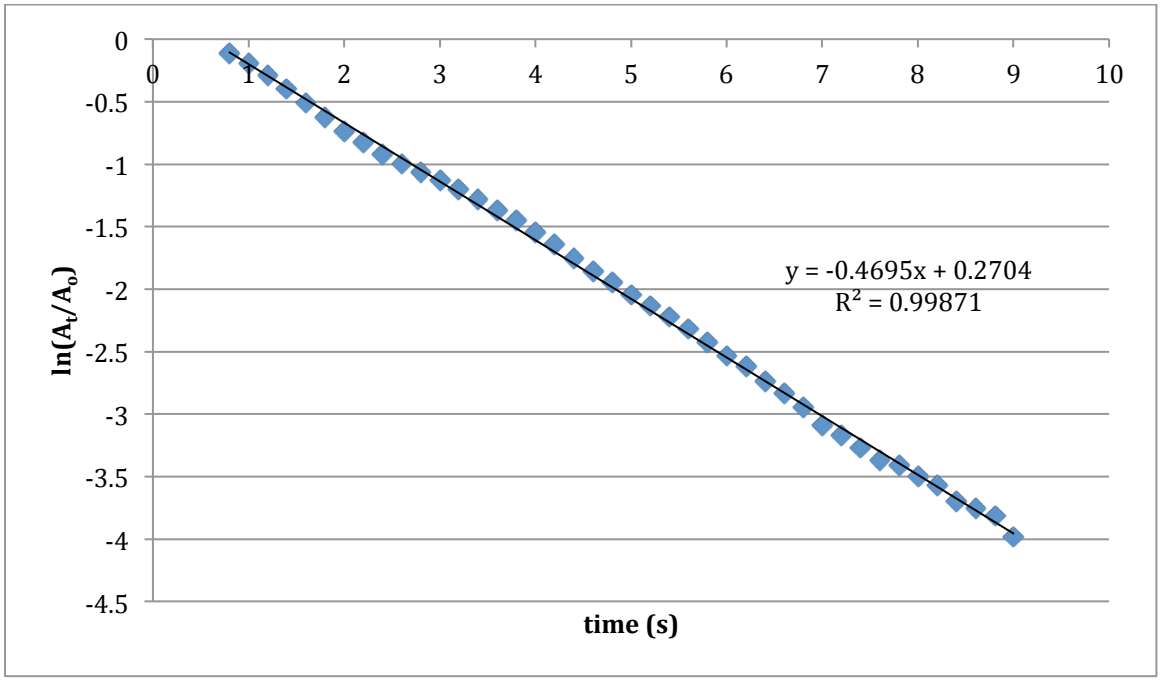
Rate Data for Conversion of 2v to 1v at pH 13



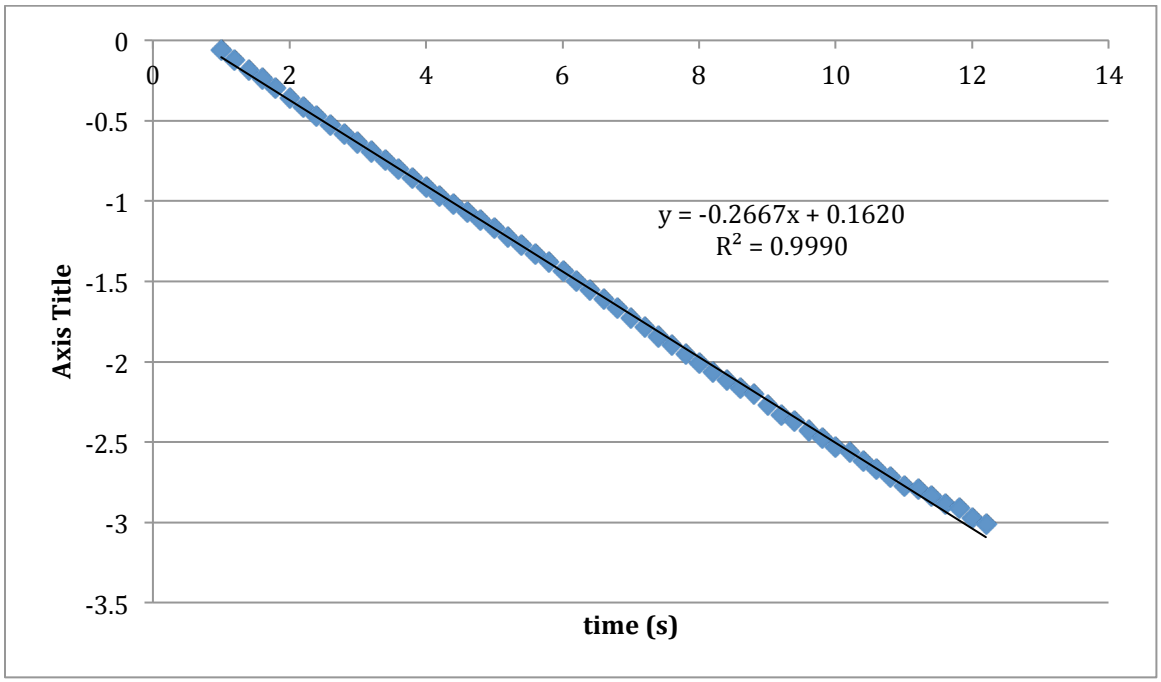
Rate Data for Conversion of 2w to 1w at pH 13



Rate Data for Conversion of 2x to 1x at pH 13



Rate Data for Conversion of 2y to 1y at pH 13

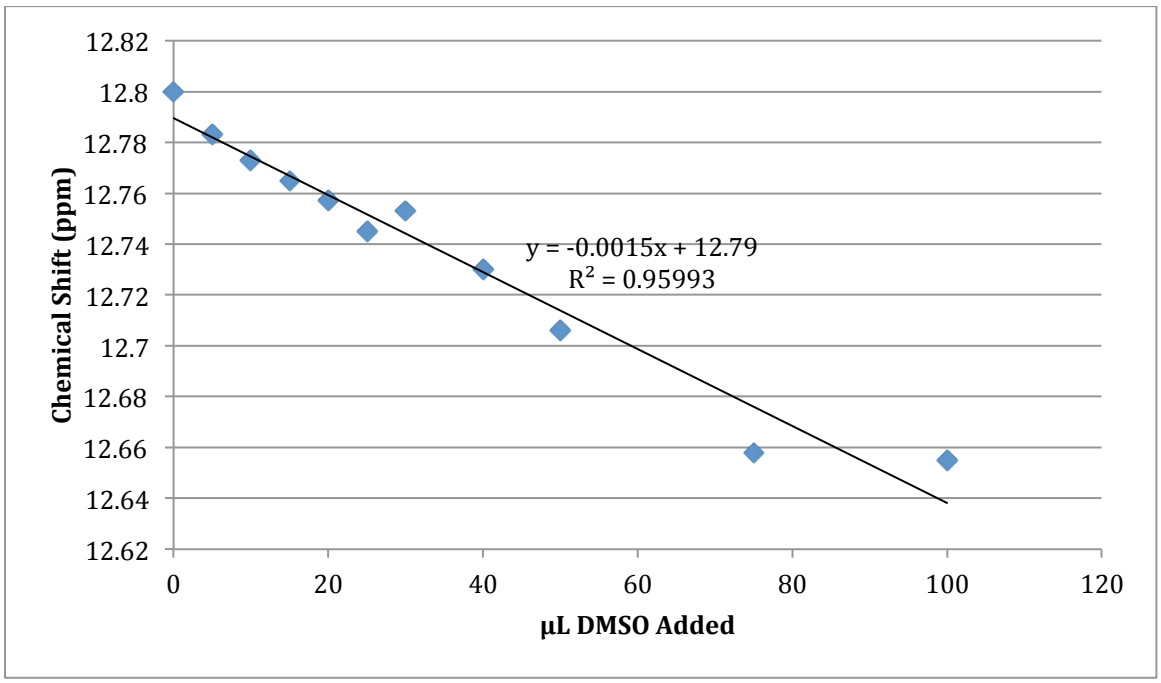


PROCEDURE FOR ^{1}H NMR d_6-DMSO TITRATION STUDIES

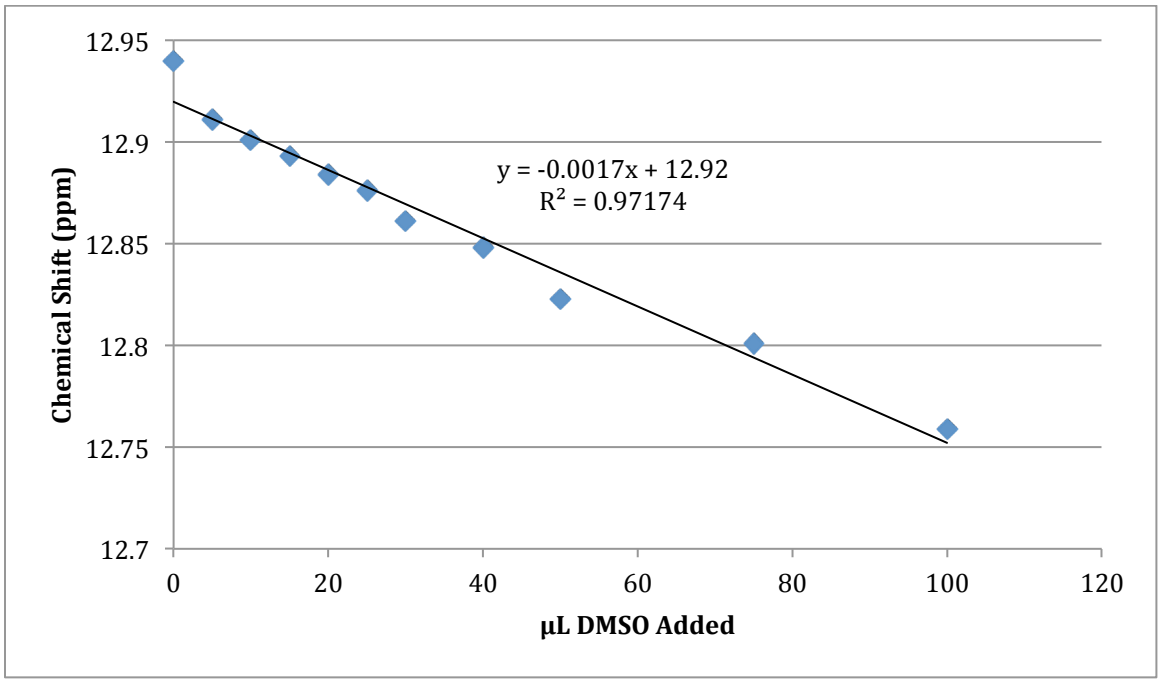
A total of 12 mL of a 10 mM solution of chalcone in $CDCl_3$ was prepared. Into 10 different NMR tubes was added 1 mL of chalcone solution via autopipette. To each NMR tube was added a different volume (5, 10, 15, 20, 25, 30, 40, 50, 75, and 100 µL) of d_6-DMSO via autopipette. The NMR spectrum of each sample was acquired and the shift of the phenolic proton (H_A) was recorded for each and plot against the volume of d_6-DMSO added.

RAW DATA PLOTS FROM d_6-DMSO TITRATION STUDIES

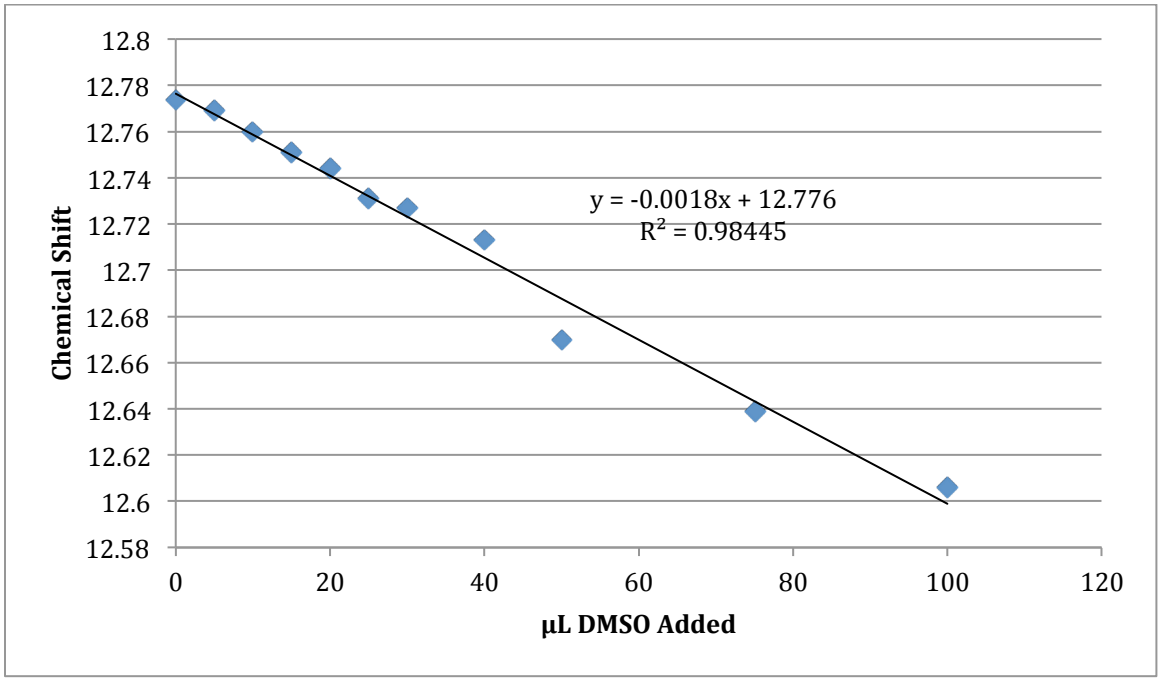
DMSO-Titration Data for 1a



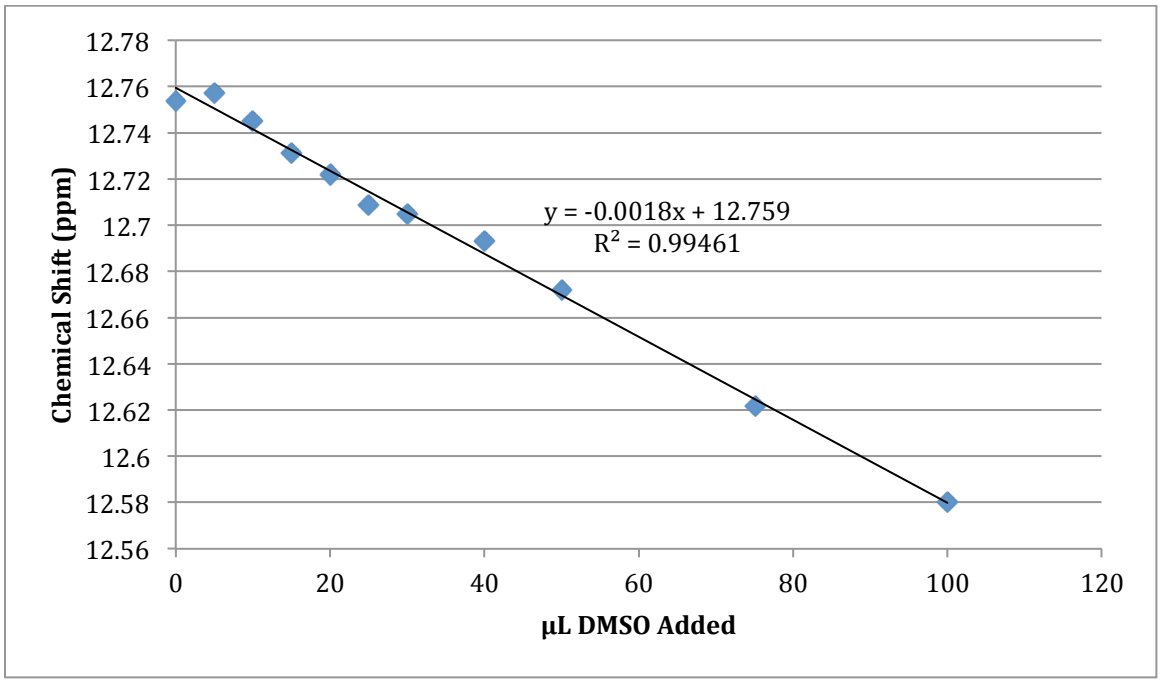
DMSO-Titration Data for 1b



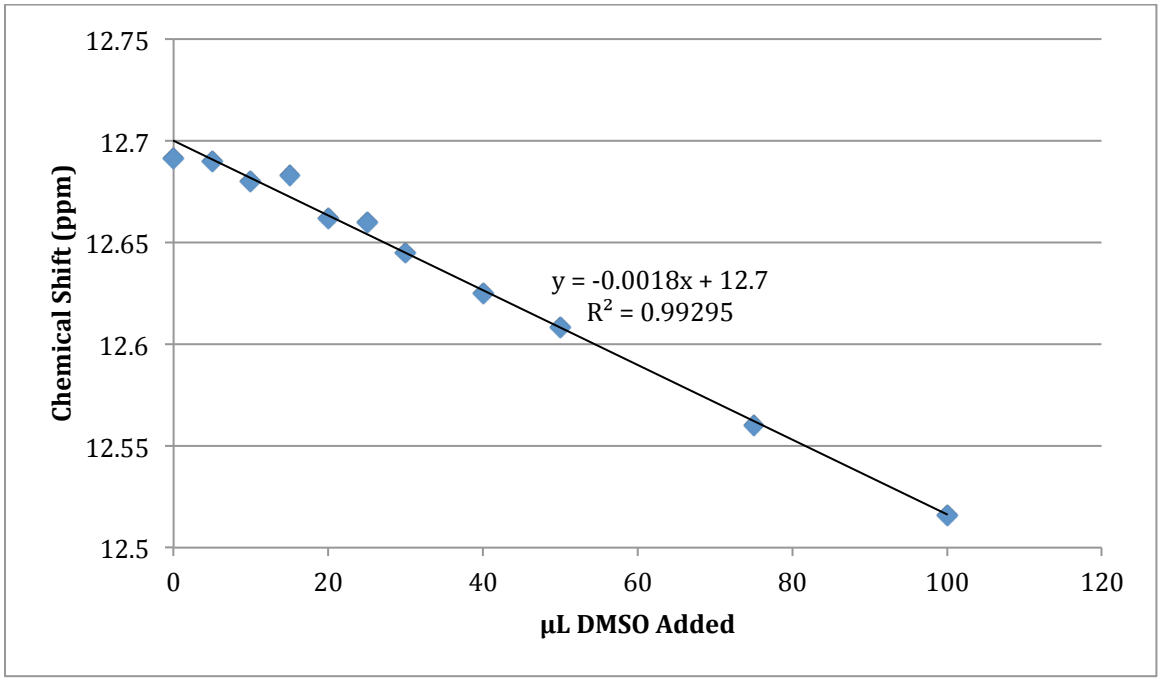
DMSO-Titration Data for 1c



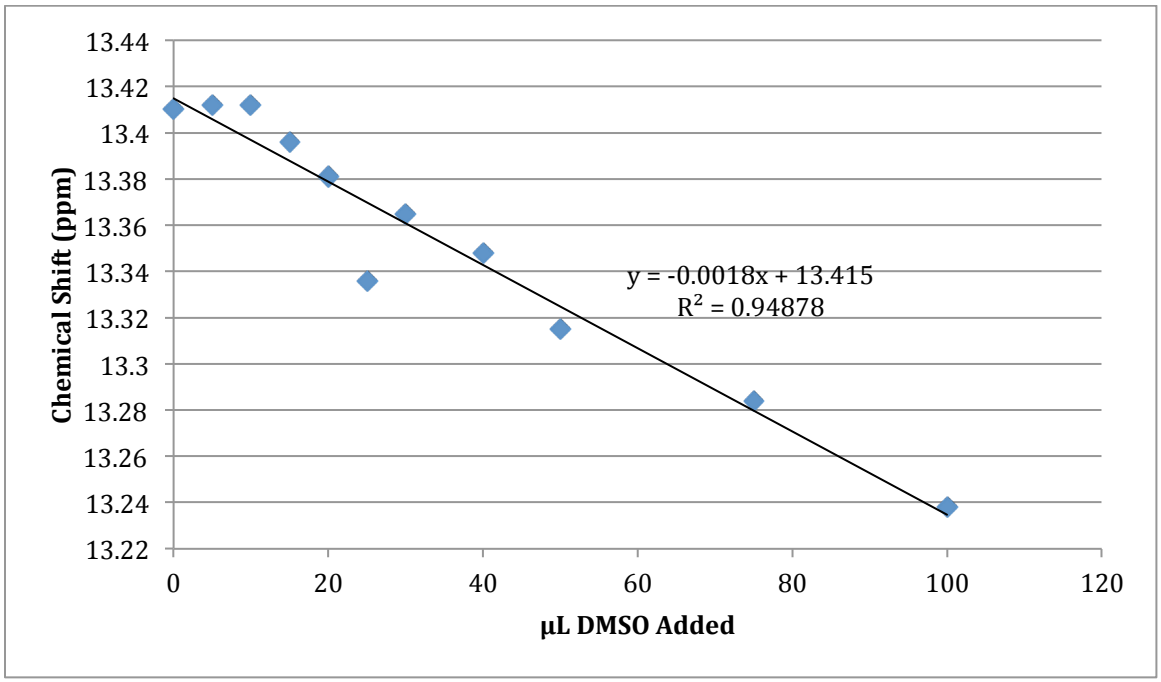
DMSO-Titration Data for 1d



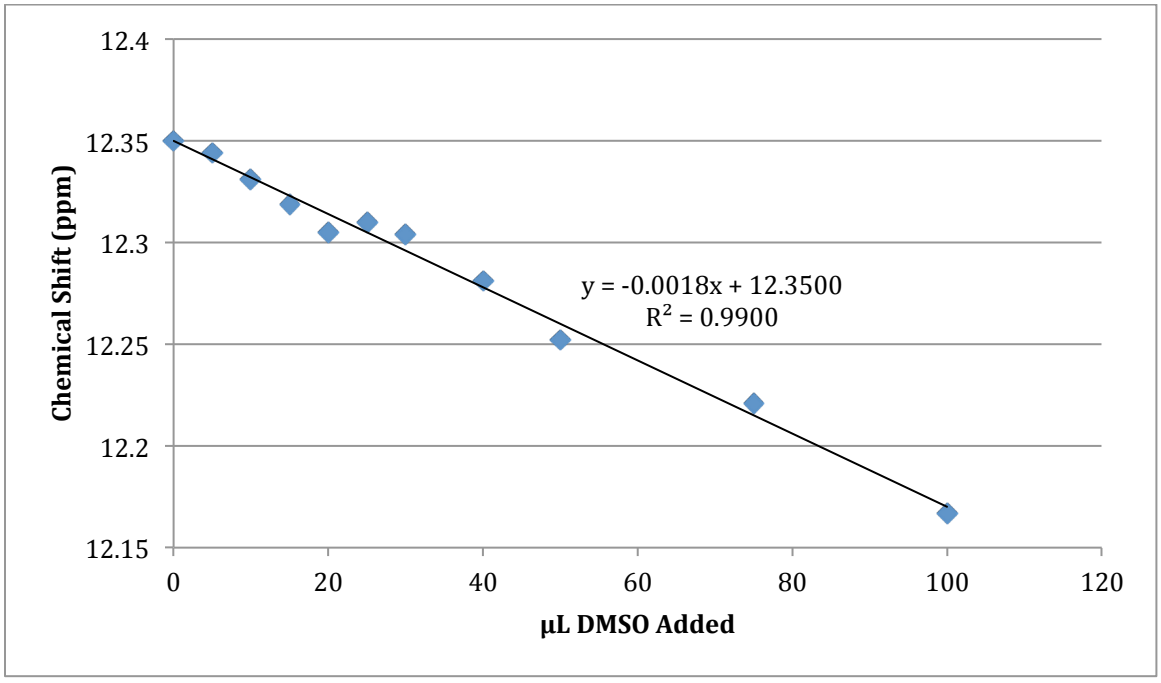
DMSO-Titration Data for 1e



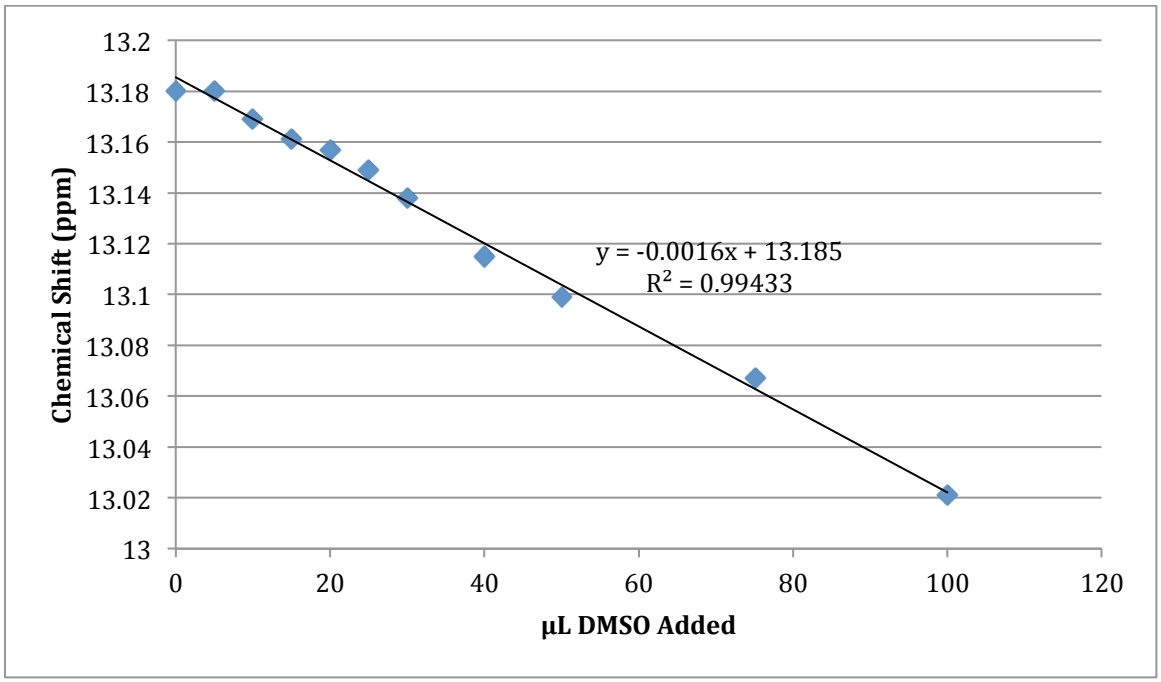
DMSO-Titration Data for 1f



DMSO-Titration Data for 1k



DMSO-Titration Data for 1p



DMSO-Titration Data for 1u