Iron-Catalyzed Synthesis of Substituted 3-Arylquinolin-2(1*H*)-ones *via* an Intramolecular Dehydrogenative Coupling of Amido-Alcohols.

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Supporting Information

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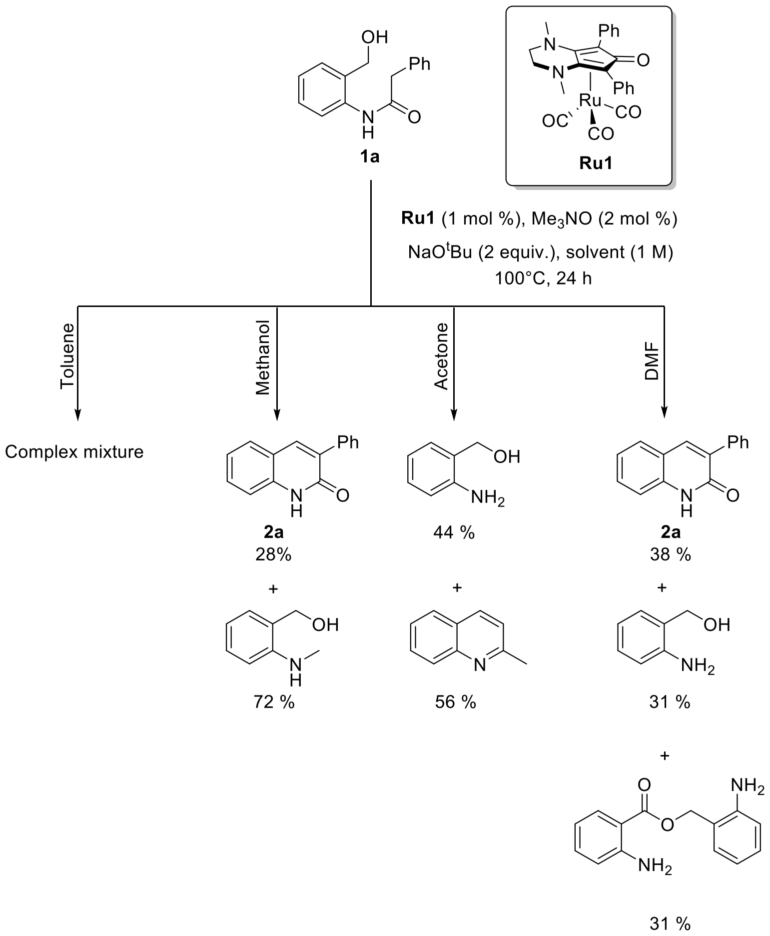
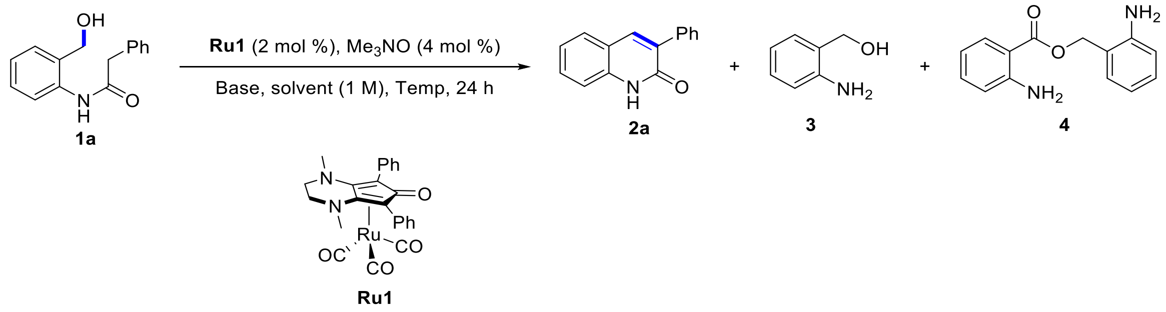
Part 1: Optimization of the condensation of amido-alcohol 1a.

Table S1: Optimization of the reaction conditions with Ruthenium[a]

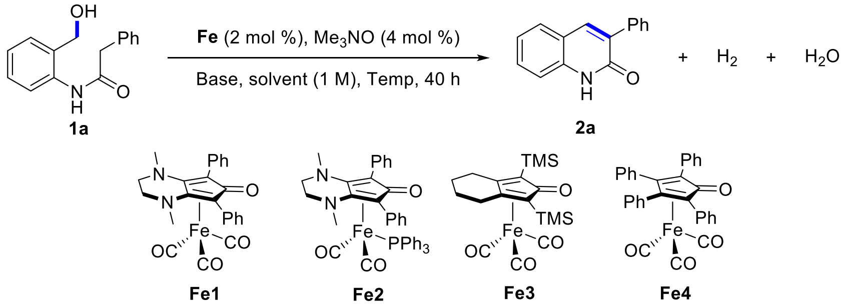




Entry	**Ru**	Base (equiv.)	Solvent	Temp (°C)	**1a/2a/3/4**[b]
1	**Ru1**	NaO^{t}Bu (2.0)	DMF	100	-/38/31/31
2	**Ru1**	NaOH (2.0)	DMF	100	75/25/-/-
3	**Ru1**	Cs_2CO_3 (2.0)	DMF	100	28/72/-/-
4	**Ru1**	K_2CO_3 (2.0)	DMF	100	3/65/17/15
5	**Ru1**	**Na_2CO_3 (2.0)**	**DMF**	**100**	**1/96/3/-**
6	**Ru1**	$NaHCO_3$ (2.0)	DMF	100	24/37/39/-

[a] General Conditions: Amido-alcohol **1a** (0.5 mmol), **Ru** (2 mol %), Me_3NO (4 mol %), base (2 equiv.), DMF (1 M) for 24 h. [b] Conversions and selectivity were determined by ^{1}H-NMR analysis of the crude mixture.

Table S2: Optimization of the reaction conditions with Iron[a]



Entry	Fe	Base (equiv.)	Solvent	Temp (°C)	**1a/2a**[b]
1	**Fe1**	NaO^{t}Bu (1.0)	toluene	90	-/-
2	**Fe1**	NaO^{t}Bu (1.0)	CPME	90	-/-
3	**Fe1**	NaO^{t}Bu (1.0)	MeOH	90	-/17
4	**Fe1**	NaO^{t}Bu (1.0)	^{i}PrOH	90	-/21
5	**Fe1**	NaO^{t}Bu (1.0)	DMF	90	-/29
6	**Fe1**	Na_2CO_3 (1.0)	DMF	90	65/35
7[d]	**Fe2**	Na_2CO_3 (1.0)	DMF	90	72/28
8	**Fe3**	Na_2CO_3 (1.0)	DMF	90	22/78
9	**Fe4**	Na_2CO_3 (1.0)	DMF	90	41/59
10	**Fe3**	Na_2CO_3 (1.0)	toluene	100	-/-
11	**Fe3**	Na_2CO_3 (0.1)	DMF	100	82/18
12	**Fe3**	Na_2CO_3 (0.5)	DMF	100	63/37
13	**Fe3**	Na_2CO_3 (1.0)	DMF	100	14/86
14	**Fe3**	Na_2CO_3 (1.0)	DMF	110	-/77 (48)[c]
15	**Fe3**	**Na_2CO_3 (2.0)**	**DMF**	**100**	**8/92 (78)**[c]
16	**Fe3**	K_2CO_3 (2.0)	DMF	100	26/74
17	**Fe3**	K_3PO_4 (2.0)	DMF	100	28/72
18	**Fe3**	K_2HPO_4 (2.0)	DMF	100	41/59
19	**Fe3**	Cs_2CO_3 (2.0)	DMF	100	28/72
20	**Fe3**	$NaHCO_3$ (2.0)	DMF	100	63/37
21	**Fe3**	NaOH (2.0)	DMF	100	-/25

[a] General Conditions: Amido-alcohol **1a** (0.5 mmol), **Fe** or **Ru** (2 mol %), Me_3NO (4 mol %), base (x equiv.), solvent (1 M) for 40 h. [b] Conversions and selectivity **1a**/**2a** were determined by ^1H-NMR analysis of the crude mixture. [c]Isolated yield. [d] Without Me_3NO.

Part 2: Experimental Part.

General Considerations: All air- and moisture-sensitive manipulations were carried out using standard vacuum line Schlenk tubes techniques. Toluene was dried using a solvent purification system from Innovative Technologies, by passage through towers containing activated alumina. Xylene was purchased from Carlo Erba and was distillated over sodium and stocked over 4Å molecular sieves. Both were degazed prior to use by bubbling argon gas directly in the solvent. Other solvents and chemicals were purchased from different suppliers and used as received. Neutral alumina was purchased from Alfa Aesar (Brockmann Grade I, 58 Angstroms, -60 Mesh Powder, S.A. 150 m^2/g) and silica from Carlo Erba (60Å 40-63µ). Deuterated solvents for NMR spectroscopy were purchased from Sigma Aldrich and used as received. NMR spectra were recorded on a 500 MHz Brücker spectrometer. Proton (^{1}H) NMR information is given in the following format: multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; sept, septet; m, multiplet), coupling constant(s) (*J*) in Hertz (Hz), number of protons. The prefix *app* is occasionally applied when the true signal multiplicity was unresolved and *br* indicates the signal in question broadened. Carbon $^{13}C\{^1H\}$ NMR spectra are reported in ppm (δ) relative to $CDCl_3$ unless noted otherwise. Infrared spectra were recorded over a PerkinElmer Spectrum 100 FT-IR Spectrometer using neat conditions. HRMS analyses were performed by Laboratoire de Chimie Moléculaire et Thioorganique analytical Facilities.

Synthesis of amido-alcohols

General Procedure A: *Step 1*: In a round bottomed flask, the desired phenylacetic acid (10 mmol) was dissolved in thionyl chloride (2.18 mL, 3 equiv.). The mixture was stirred under reflux for 1 hour. After cooling to room temperature, the solvent was evaporated in vacuo to give the desired phenylacetyl chloride, which was directly used for the next step.

Step 2: To a stirred solution of 2-aminobenzyl alcohol (10 mmol, 1 equiv.) in dry THF (15 mL) was added 5 mL of pyridine. A solution of the desired phenylacetyl chloride (10 mmol, 1 equiv.) in dry THF (10 mL) was added dropwise at 0 °C under argon. The mixture was warmed to room temperature and stirred overnight. Solvent was evaporated, water and chloroform were added and the organic phase was washed with aqueous HCl (5 %), brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Depending on the purity of the crude, the product was purified by silica gel chromatography using pentane:ethyl acetate as eluent.

N-[2-(hydroxymethyl)phenyl]-2-phenylacetamide (**1a**). According to general procedure A, **1a** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and phenylacetyl chloride (10 mmol, 1 equiv.), as a white solid (2.19 g, 91 %) without further purification. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 8.37 (br. s, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.43-7.36 (m, 3H), 7.36-7.29 (m, 3H), 7.13 (d, *J* = 6.4 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 4.46 (s, 2H), 3.78 (s, 2H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 169.9, 137.4, 134.8, 129.8, 129.5, 129.2, 129.2, 128.9, 127.6, 124.5, 122.5, 64.3, 45.2. IR (neat): ν 3254, 1652, 1585, 1525, 1451, 1394, 1066, 1028, 968, 754, 699 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{15}H_{15}NO_2Na$ 264.1000; found 264.1001.

N-(2-(hydroxymethyl)phenyl)-N-methyl-2-phenylacetamide (**1b**). According to general procedure A, **1b** was obtained from (2-(methylamino)phenyl)methanol (10 mmol, 1 equiv.) and phenylacetyl chloride (10 mmol, 1 equiv.), after purification by flash column chromatography on silica gel (pentane/ethyl acetate 3:1). Brown solid (1.22 g, 48 %). ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 7.52 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.38-7.35 (m, 2H), 7.20-7.18 (m, 3H), 7.11 (d, *J* = 7.5 Hz, 1H), 6.94-6.93 (m, 2H), 4.38 (d, *J* = 13.2 Hz, 1H), 4.20 (d, *J* = 13.2 Hz, 1H), 3.43 (s, 2H), 3.18 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 171.2, 141.3, 138.8, 135.1, 129.2, 129.2, 129.1, 129.1, 128.6, 128.5, 126.8, 60.7, 41.7, 37.3. IR (neat): ν 2909, 1709, 1584, 1495, 1453, 1231, 1162, 926, 748, 696, 607 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{16}H_{18}NO_2$ 256.1338; found 256.1338.

N-(2-(hydroxymethyl)phenyl)-2-(p-tolyl)acetamide (**1c**). According to general procedure A, **1c** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(p-tolyl)acetic acid (10 mmol, 1 equiv.) as a white solid (2.20 g, 86 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.33 (br. s, 1H), 7.99 (d, *J* = 8.1 Hz, 1H), 7.32-7.29 (m, 1H), 7.26-7.25 (m, 2H), 7.19 (app. d, *J* = 7.9 Hz, 2H), 7.15-7.14 (m, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 4.47 (s, 2H), 3.73 (s, 2H), 2.36 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 170.3, 137.4, 137.4, 131.7, 129.9, 129.8, 129.7, 129.3, 129.1, 124.6, 122.6, 64.3, 44.8, 21.3. IR (neat): ν 3254, 1652, 1587, 1527, 1455, 1341, 1245, 1188, 1035, 763, 702, 493 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_2Na$ 278.1157; found 278.1160.

N-(2-(hydroxymethyl)phenyl)-2-(o-tolyl)acetamide (**1d**). According to general procedure A, **1d** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(o-tolyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.97 g, 77 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.33 (br. s, 1H), 8.03 (dd, *J* = 3.8; 8.1 Hz, 1H), 7.32-7.29 (m, 2H), 7.26-7.24 (m, 2H), 7.10 (app. d, *J* =

7.5 Hz, 2H), 7.03 (t, J = 7.4 Hz, 1H), 4.39 (s, 2H), 3.76 (d, J = 7.5 Hz, 2H), 2.37 (d, J = 2.6 Hz, 3H). $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 169.8, 137.7, 137.3, 133.3, 131.0, 130.9, 129.5, 129.3, 129.0, 128.1, 126.9, 124.5, 122.4, 64.3, 43.2, 19.7. IR (neat): ν 3251, 3047, 1660, 1526, 1489, 1345, 1203, 1032, 967, 757, 745, 661, 501 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_2Na$ 278.1157; found 278.1159.

2-(2-bromophenyl)-N-(2-(hydroxymethyl)phenyl)acetamide (**1e**). According to general procedure A, **1e** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(2-bromophenyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.18 g, 37 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^1H NMR ($CDCl_3$, 500 MHz): δ 8.40 (br. s, 1H), 8.04 (d, J = 8.1 Hz, 1H), 7.64 (dd, J = 1.0; 8.1 Hz, 1H), 7.44 (dd, J = 1.5; 7.5 Hz, 1H), 7.34 (td, J = 1.1; 7.5 Hz, 1H), 7.33-7.30 (m, 1H), 7.19 (td, J = 1.7; 7.8 Hz, 1H), 7.14 (dd, J = 1.0; 7.4 Hz, 1H), 7.05 (td, J = 1.0; 7.4 Hz, 1H), 4.54 (s, 2H), 3.93 (s, 2H). $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 168.4, 137.4, 134.7, 133.4, 132.2, 129.8, 129.5, 129.3, 129.0, 128.3, 125.5, 124.7, 122.8, 64.5, 45.4. IR (neat): ν 3249, 1662, 1532, 1499, 1362, 1253, 1054, 922, 762, 674, 503 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{15}H_{14}NO_2BrNa$ 342.0106; found 342.0111.

N-(2-(hydroxymethyl)phenyl)-2-(2-methoxyphenyl)acetamide (**1f**). According to general procedure A, **1f** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(2-methoxyphenyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.49 g, 55 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^1H NMR ($CDCl_3$, 500 MHz): δ 8.43 (br. s, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.33-7.27 (m, 3H), 7.14 (d, J = 7.4 Hz, 1H), 7.03 (d, J = 7.4 Hz, 1H), 6.96 (d, J = 7.4 Hz, 1H), 6.93 (d, J = 8.1 Hz, 1H), 4.45 (s, 2H), 3.88 (s, 3H), 3.75 (s, 2H), 1.94 (br. s, 1H). $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 170.4, 157.6, 137.3, 131.6, 130.4, 129.2, 129.1, 129.1, 124.6, 123.4, 122.9, 121.2, 110.8, 64.0, 55.6, 40.0. IR (neat): ν 3243, 1653, 1586, 1522, 1453, 1239, 1043, 970, 747, 686, 589, 509 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_3Na$ 294.1106; found 294.1110.

N-(2-(hydroxymethyl)phenyl)-2-(3-methoxyphenyl)acetamide (**1g**).According to general procedure A, **1g** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(3-methoxyphenyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.67 g, 61 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^1H NMR ($CDCl_3$, 500 MHz): δ 8.42 (br. s, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.29 (t, J = 7.9 Hz, 2H), 7.14-7.12 (m, 1H), 7.04 (t, J = 7.3 Hz, 1H), 6.94 (d, J = 7.4 Hz, 1H), 6.90 (s, 1H), 6.88-6.86 (m, 1H), 4.47 (s, 2H), 3.82 (s, 3H), 3.73 (s, 2H), 1.79 (br. s, 1H). $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 169.8, 160.3, 137.4, 136.2, 130.3, 129.7, 129.3, 129.0, 124.6, 122.6, 122.1, 115.2, 113.4, 64.4, 55.4, 45.3. IR (neat): ν 3257, 1655, 1585, 1525, 1491, 1463, 1345, 1263, 1158, 1037, 970, 759, 706, 587 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_3Na$ 294.1106; found 294.1109.

N-(2-(hydroxymethyl)phenyl)-2-(4-methoxyphenyl)acetamide (**1h**).According to general procedure A, **1h** was obtained from2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(3-methoxyphenyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.55 g, 57 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.38 (br. s, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.32-7.29 (m, 1H), 7.27 (d, *J* = 8.6 Hz, 2H), 7.14-7.13 (dd, *J* = 1.0; 7.4 Hz, 1H), 7.07-7.04 (td, *J* = 1.0; 7.4 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 1H), 4.48 (s, 2H), 3.81 (s, 3H), 3.70 (s, 2H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 170.5, 159.2, 137.4, 130.9, 129.7, 129.3, 129.0, 126.7, 124.6, 122.6, 114.6, 64.3, 55.5, 44.31. IR (neat): ν 3259, 1657, 1585, 1512, 1409, 1302, 1243, 1175, 1034, 971, 772, 711, 574, 514, 437 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_3Na$ 294.1106; found 294.1107.

N-(2-(hydroxymethyl)phenyl)-2-(naphthalen-1-yl)acetamide (**1i**). According to general procedure A, **1i** was obtained from2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(naphthalen-1-yl)acetic acid (10 mmol, 1 equiv.) as a light yellow solid (2.36 g, 81 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.30 (br. s, 1H), 8.06 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.90 (dd, *J* = 2.2; 7.1 Hz, 1H), 7.86 (dd, *J* = 2.2; 7.1 Hz, 1H), 7.57-7.49 (m, 4H), 7.28-7.25 (m, 1H), 6.99-6.97 (m, 2H), 4.21 (s, 2H), 4.02 (s, 2H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 169.9, 137.2, 134.0, 132.4, 131.0, 129.5, 129.1, 129.0, 128.9, 128.9, 128.7, 127.1, 126.5, 126.0, 124.5, 124.0, 122.5, 64.0, 43.2. IR (neat): ν 3237, 1650, 1534, 1456, 1399, 1205, 1090, 1045, 886, 779, 529 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{19}H_{17}NO_2Na$ 314.1157; found 314.1160.

2-(4-fluorophenyl)-N-(2-(hydroxymethyl)phenyl)acetamide (**1j**). According to general procedure A, **1j** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(4-fluorophenyl)acetic acid (10 mmol, 1 equiv.) as a light yellow solid (1.84 g, 71 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (br. s, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.34-7.30 (m, 3H), 7.12 (d, *J* = 7.4 Hz, 1H), 7.08-7.04 (m, 3H), 4.51 (s, 2H), 3.72 (s, 2H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ - 114.8. ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ 169.7, 161.5 (d, *J* = 244.5 Hz), 137.4, 131.3 (d, *J* = 8.0 Hz), 130.4 (d, *J* = 3.3 Hz), 129.5, 129.3, 128.9, 116.0 (d, *J* = 21.3 Hz), 64.5, 44.3. IR (neat): ν 3211, 1656, 1588, 1530, 1507, 1354, 1286, 1220, 1157, 1019, 842, 752, 512, 471 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{15}H_{14}NO_2FNa$ 282.0906; found 282.0906.

N-(2-(hydroxymethyl)phenyl)-2-(4-(trifluoromethyl)phenyl)acetamide (**1k**). According to general procedure A, **1k** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(4-(trifluoromethyl)phenyl)acetic acid (10 mmol, 1 equiv.) as a white solid (1.92 g, 62 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (br. s, 1H), 8.06 (d, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.34-7.30 (m, 1H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.05 (t, *J* = 7.4 Hz, 1H), 4.56 (s, 2H), 3.81 (s, 2H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ - 62.5. ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ 168.7, 138.8, 137.5, 130.0, 129.4, 129.3, 128.9, 128.0 (d, *J* = 65.3 Hz) 126.0 (q, *J* = 3.7 Hz), 124.6, 124.2 (d, *J* = 270 Hz), 122.4, 64.7, 44.9. IR (neat): ν 3219, 1663, 1585, 1525, 1486, 1309, 1237, 1198, 1095, 1002, 944, 714, 569 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{14}NO_2F_3Na$ 332.0874; found 332.0874.

N-(2-(hydroxymethyl)phenyl)-2-(thiophen-2-yl)acetamide (**1l**). According to general procedure A, **1l** was obtained from 2-aminobenzyl alcohol (10 mmol, 1 equiv.) and 2-(thiophen-2-yl)acetic acid (10 mmol, 1 equiv.) as a white solid (2.13 g, 86 %) after purification by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.63 (br. s, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.33-7.29 (m, 2H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.08-7.03 (m, 3H), 4.52 (s, 2H), 3.96 (s, 3H), 3.75 (s, 2H), 1.94 (br. s, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 168.8, 137.2, 135.9, 129.7, 129.3, 129.0, 128.1, 127.7, 126.1, 124.7, 122.5, 64.4, 38.8. IR (neat): ν 3250, 1654, 1587, 1532, 1454, 1342, 1248, 1039, 967, 765, 697, 533 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{13}H_{13}NO_2SNa$ 270.0565; found 270.0566.

General Procedure B: *Step 1:* In a round bottomed flask, the desired aniline (15 mmol, 1 equiv.) was dissolved in dichloromethane (24 mL) and triethylamine (2.3 mL, 1.1 equiv.) was added. The mixture was cooled to 0 °C and pivaloyl chloride (1.84 mL, 1 equiv.) was added dropwise. The mixture was stirred at room temperature overnight and then poured into water. The water phase was then washed with dichloromethane and the organic layers were combined. The organic phase was washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure, giving the N-pivaloyl aniline which was directly used for the next step.

Step 2: Under argon, *N*-pivaloyl aniline (1 equiv.) was dissolved in dry diethyl ether (0.25 M) and TMEDA (2.25 equiv.) was added. The mixture was cooled to -5°C. A solution of *n*-butyllithium (2.5 M in hexane, 2.2 equiv.) was added dropwise. The mixture was allowed to warm to room temperature, stirred for 2 hours, and cooled down again to -5°C. DMF (3 equiv.) was added dropwise and the mixture was stirred for 1 hour. Water was added, the water layer was extracted with additional Et_2O and the organic extracts were combined, dried over Na_2SO_4, filtered and concentrated under reduced pressure.

Step 3: The crude *N*-pivaloyl aniline-benzaldehyde (1 equiv.) was dissolved in methanol (0.5 M). Then, sodium borohydride (1.5 equiv.) was added portion wise at 0 °C, the mixture was warmed at room temperature, stirred for 2 hours and quenched with water. The product was extracted with ethyl acetate, washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure.

Step 4: The crude amido-alcohol (1 equiv.) was dissolved in methanol (0.38 M) and sodium hydroxide (5 equiv.) was added. The mixture was stirred and refluxed overnight. After cooling down to room temperature, water was added and the product was extracted with ethyl acetate, washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure.

Step 5: To a stirred solution of 2-aminobenzyl alcohol (1 equiv.) in 15 mL of dry THF was added 5 mL of pyridine. A solution of phenylacetyl chloride (1 equiv.) in 10 mL of dry THF was added dropwise at 0°C under argon. The mixture was warmed to room temperature and stirred overnight. Solvent was evaporated, water and chloroform were added and the organic phase was washed with aqueous HCl (5 %), brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Depending on the purity of the crude, the product was purified on silica gel chromatography using pentane:ethyl acetate as eluent.

N-(2-(hydroxymethyl)-3-methoxyphenyl)-2-phenylacetamide (**1m**). According to the general procedure B, **1m** was obtained over 5 steps from 3-methoxyaniline (15 mmol, 1.85 g) as a white solid (1.052 g, 26 % overall yield) by flash column chromatography on silica gel (pentane/ethyl acetate 1:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.23 (br. s, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.41-7.36 (m, 4H), 7.34-7.31 (m, 1H), 7.22 (t, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 8.2 Hz, 1H), 4.58 (s, 2H), 3.79 (s, 3H), 3.76 (s, 2H), 1.82 (br. s, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 170.2, 157.4, 138.3, 134.8, 129.8, 129.4, 129.3, 127.7, 119.3, 115.6, 107.5, 56.2, 55.9, 45.2. IR (neat): ν 3241, 1655, 1579, 1533, 1476, 1394, 1196, 1039, 968, 744, 576 cm^{-1}. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{20}NO_2$ 318.1494; found 318.1495.

N-(3-(hydroxymethyl)-[1,1'-biphenyl]-2-yl)-2-phenylacetamide (**1n**). According to the general procedure B, **1n** was obtained over 5 steps from [1,1'-biphenyl]-2-amine (15 mmol, 2.54 g) as a white solid (1.57 g, 33 % overall yield) by flash column chromatography on silica gel (pentane/ethyl acetate 1:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.49 (dd, *J* = 1.4; 7.6 Hz, 1H), 7.40-7.38 (m, 3H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.27-7.23 (m, 4H), 7.18-7.17 (m, 2H), 7.01-6.99 (m, 2H), 6.73 (br. s, 1H), 4.50 (s, 2H), 3.61 (s, 2H), 3.51 (br. s, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 172.0, 139.2, 139.2, 138.1, 134.0, 131.9, 130.3, 130.2, 129.6, 129.3, 128.9, 128.8, 127.9, 127.8, 127.7, 62.7, 43.9. IR (neat): ν 3383, 3220, 1662, 1596, 1525, 1435, 1351, 1239, 1096, 1044, 992, 787, 698, 642, 512 cm $^{-1}$. HRMS (ESI-TOF) m/z: [M + Na]$^+$ calcd for $C_{16}H_{17}NO_3Na$ 294.1106; found 294.1106.

N-(2-(hydroxymethyl)-4-(trifluoromethyl)phenyl)-2-phenylacetamide (**1o**). According to the general procedure B, **1o** was obtained over 5 steps from 4-(trifluoromethyl)aniline (15 mmol, 2.42 g) as a white solid (1.62 g, 35 % overall yield) by flash column chromatography on silica gel (pentane/ethyl acetate 1:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.68 (br. s, 1H), 8.31 (d, *J* = 8.5 Hz, 1H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.42-7.40 (m, 2H), 7.37-7.35 (m, 4H), 4.50 (s, 2H), 3.78 (s, 2H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -62.2. ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ 170.0, 134.4, 129.9, 129.3, 128.8, 127.8, 126.8 (d, *J* = 132 Hz), 126.4 (q, *J* = 3.7 Hz) 125.7 (q, *J* = 3.7 Hz), 124.1 (d, *J* = 270 Hz), 121.8, 64.2, 45.4. IR (neat): ν 3256, 1660, 1524, 1408, 1330, 1274, 1166, 1079, 904, 834, 703, 571 cm $^{-1}$. HRMS (ESI-TOF) m/z: [M + Na]$^+$ calcd for $C_{16}H_{15}NO_2F_3$ 310.1055; found 310.1059.

N-(3-(hydroxymethyl)naphthalen-2-yl)-2-phenylacetamide (**1p**). *Step 1:* to a suspension of $LiAlH_4$ (20 mmol, 0.76 g, 2 equiv.) in dry THF (40 mL) under argon at 0°C a solution of 3-amino-2-naphthoic acid (10 mmol, 1.87 g, 1 equiv.) in dry THF (25 mL) was added dropwise. After addition, the reaction was heated to reflux for 16 h. After cooling to room temperature, the reaction was quenched with saturated Na_2SO_4 solution and filtered over celite. The filtrate was then washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure to afford pure (3-aminonaphthalen-2-yl)methanol as a light brown solid (1.54 g, 89 %).

Step 2: To a stirred solution of (3-aminonaphthalen-2-yl)methanol (1.54 g, 8.9 mmol) in dry THF (15 mL) was added 5 mL of pyridine. A solution of phenylacetyl chloride (1.18 mL, 1 equiv.) in dry THF (10 mL) was added dropwise at 0 °C under argon. The mixture was warmed to room temperature and stirred overnight. Solvent was evaporated, water and chloroform were added and the organic phase was washed with aqueous HCl (5 %), brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Crude product was then purified by flash column chromatography on silica gel (pentane/ethyl acetate 1:1) to afford **1p** as a light brown solid

(1.99 g, 77 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.65 (br. s, 1H), 8.61 (s, 1H), 7.79 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.37-7.33 (m, 1H), 4.60 (s, 2H), 3.81 (s, 2H).^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$): δ 170.1, 134.8, 133.9, 130.2, 129.9, 129.3, 129.0, 128.9, 128.1, 127.9, 127.7, 127.5, 126.8, 125.5, 119.3, 64.8, 45.4. IR (neat): ν 3304, 1737, 1645, 1600, 1527, 1496, 1451, 1359, 1166, 1031, 974, 884, 747, 699, 477 cm $^{-1}$. HRMS (ESI-TOF) m/z: [M + Na]$^+$ calcd for $C_{19}H_{17}NO_2Na$ 314.1157; found 314.1164.

General Procedure C: *Step 1:* In a two necks flask, a minimum of diethyl ether was added to small pieces of magnesium (20 mmol, 486 mg, 2 equiv.) and a small amount of iodine. A first part of the halogen derivative (7 mmol, 0.67 equiv.) was added. The mixture was heated until the reaction started. A second part of the halogen derivative (13 mmol, 1.33 equiv.) was added and the reaction mixture was heated at reflux for 30 minutes. After cooling down to room temperature, 2-nitrobenzaldehyde (10 mmol, 1 equiv.) was added dropwise at 0 °C and the mixture was stirred at room temperature overnight. The reaction was quenched with saturated aqueous NH_4Cl solution and the product was extracted with ethyl acetate, washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure.

Step 2: To a stirred solution of the crude nitro-alcohol (1 equiv.) and nickel (II) chloride hexahydrate (1 equiv.) in ethanol (0.33 M) was added portion wise sodium borohydride (10 equiv.) at 0 °C. The mixture was stirred for 2 hours at 0 °C and quenched with a minimum of water, filtered on celite and poured into water. Water phase was then extracted twice with ethyl acetate. The combined organic phases were washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure.

Step 3: To a stirred solution of the crude 2-aminobenzyl alcohol (1 equiv.) in 15 mL of dry THF was added 5 mL of pyridine. A solution of phenylacetyl chloride (1 equiv.) in 10 mL of dry THF was added dropwise at 0 °C under argon. The mixture was warmed to room temperature and stirred overnight. Solvent was evaporated, water and chloroform were added and the organic phase was washed with aqueous HCl (5 %), brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Depending on the purity of the crude, the product was purified on silica gel chromatography using pentane:ethyl acetate as eluent.

N-(2-(hydroxy(phenyl)methyl)phenyl)-2-phenylacetamide (**1q**). According to the general procedure C, **1q** was obtained from bromobenzene (10 mmol, 1.56 g) as a light yellow solid (1.49 g, 47 %) by flash column chromatography on silica gel (pentane/ethyl acetate 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.48 (br. s, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 7.34-7.26 (m, 7H), 7.19-7.15

(m, 4H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.97 (d, *J* = 7.4 Hz, 1H), 5.68 (s, 1H), 3.64-3.55 (m, 2H), 2.48 (br. s, 1H). $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 169.7, 141.3, 136.8, 134.6, 132.0, 129.9, 129.1, 129.0, 128.9, 128.8, 128.7, 128.0, 127.5, 126.6, 124.5, 123.3, 45.2. IR (neat): ν 3340, 1664, 1589, 1520, 1446, 1310, 1019, 868, 755, 722, 695, 543, 495 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{21}H_{19}NO_2Na$ 340.1313; found 340.1313.

N-(2-((4-fluorophenyl)(hydroxy)methyl)phenyl)-2-phenylacetamide (**1r**). According to the general procedure C, **1r** was obtained from 1-bromo-4-fluorobenzene (10 mmol, 1.74 g) as a light yellow solid (1.78 g, 53 %) by flash column chromatography on silica gel (pentane/ethyl acetate 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.46 (br. s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.33-7.26 (m, 4H), 7.17-7.15 (m, 2H), 7.09-7.04 (m, 3H), 6.99-6.95 (m, 3H), 5.65 (s, 1H), 3.63-3.53 (m, 2H), 2.79 (br. s, 1H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -114.5. $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 169.8, 162.4 (d, *J* = 245.0 Hz), 137.0 (d, *J* = 3.1 Hz), 136.6, 134.6, 132.0, 129.8, 129.1, 129.0, 128.8, 128.2 (d, *J* = 8.1 Hz), 127.6, 124.6, 123.4, 115.3 (d, *J* = 21.3 Hz), 74.8, 45.1. IR (neat): ν 3314, 1664, 1588, 1524, 1503, 1449, 1329, 1215, 1152, 1018, 585, 755, 727, 695, 572, 493 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{21}H_{18}NO_2FNa$ 358.1219; found 359.1221.

N-(2-(hydroxy(3-(trifluoromethyl)phenyl)methyl)phenyl)-2-phenylacetamide (**1s**). According to the general procedure C, **1s** was obtained from 1-bromo-3-(trifluoromethyl)benzene (10 mmol, 2.24 g) as a light yellow solid (2.12 g, 55 %) by flash column chromatography on silica gel (pentane/ethyl acetate 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.26 (br. s, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.52 (s, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.26-7.20 (m, 4H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.08 (d, *J* = 6.8 Hz, 2H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 5.65 (s, 1H), 3.56-3.45 (m, 2H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -62.4. $^{13}C\{^1H\}$NMR ($CDCl_3$, 125 MHz): δ 170.0, 142.5, 136.6, 134.3, 132.0, 129.8, 129.4, 129.2, 129.1 (d, *J* = 89.7 Hz), 129.0, 127.7, 126.4 (d, *J* = 256.7 Hz), 124.9, 124.6 (q, *J* = 3.7 Hz), 123.8, 123.2 (q, *J* = 3.7 Hz), 115.3 (d, *J* = 21.3 Hz), 74.7, 45.0. IR (neat): ν 3273, 1664, 1589, 1529, 1445, 1323, 1160, 1109, 1070, 1032, 797, 755, 699, 547 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{22}H_{19}NO_2F_3$ 386.1368; found 386.1365.

N-(2-(1-hydroxyethyl)phenyl)-2-phenylacetamide (**1t**). *Step 1*: 2-aminoacetophenone (10 mmol, 1.35 g, 1 equiv.) was dissolved in methanol (0.5 M). Sodium borohydride (1.5 equiv.) was added portion wise at 0 °C, the mixture was stirred at room temperature for 2 hours and quenched with water. The product was extracted with ethyl acetate, washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure to afforded pure 1-(2-aminophenyl)ethan-1-ol as a light brown oil (1.27 g, 93 %).

Step 2: To a stirred solution of 1-(2-aminophenyl)ethan-1-ol (1.27 g, 9.3 mmol, 1 equiv.) in dry THF (15 mL) was added 5 mL of pyridine. A solution of phenylacetyl chloride (1.23 mL, 1 equiv.) in dry THF (10 mL) was added dropwise at 0 °C under argon. The mixture was warmed to room temperature and stirred overnight. Solvent was evaporated, water and chloroform were added and the organic phase was washed with aqueous HCl (5 %), brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Crude product was then purified by flash column chromatography on silica gel (pentane/ethyl acetate 1:1) to afford **1t** as a brown solid (1.80 g, 76 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.95 (br. s, 1H), 8.13 (d, *J* = 8.2 Hz, 1H), 7.40-7.30 (m, 5H), 7.27-7.24 (m, 1H), 7.08-7.01 (m, 2H), 4.72 (q, *J* = 6.6 Hz, 1H), 3.70 (d, *J* = 2.8 Hz, 2H), 1.31 (d, *J* = 6.6 Hz, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 169.7, 136.6, 134.7, 132.8, 129.9, 129.1, 128.5, 127.5, 126.8, 124.3, 122.5, 70.6, 45.4, 22.6. IR (neat): ν 2967, 1694, 1603, 1497, 1408, 1296, 1239, 1187, 1074, 925, 750, 699, 603, 479 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + Na]^+$ calcd for $C_{16}H_{17}NO_2Na$ 278.1157; found 278.1159.

Synthesis of 3-Arylquinolin-2(1*H*)-ones

General Procedure D: In a 15 mL flame-dried Schlenk tube equipped with a stirring bar, the desired amido-alcohol (0.5 mmol, 1 equiv.), Me_3NO (2.22 mg, 0.02 mmol, 4 mol%), iron complex **Fe3** (4.21 mg, 0.01 mmol, 2 mol %), and Na_2CO_3 (106 mg, 1 mmol, 2 equiv.) were added to a solution of dry DMF (0.5 mL) under an argon atmosphere. The mixture was then placed into a pre-heated oil bath and stirred at 100 °C for 40 h. The mixture was cooled down to room temperature, filtered over a pad of Celite with diethyl ether, and concentrated under reduced pressure. The conversion was determined by ^{1}H NMR spectroscopy and the residue was purified by flash chromatography on silica gel using dichloromethane:diethyl ether as the eluent to afford the desired product.

3-phenylquinolin-2(1H)-one (**2a**).[1] According to the general procedure D, **2a** was obtained from amido-alcohol **1a** (0.5 mmol, 120 mg) as a white solid (86 mg, 78 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.78 (br. s, 1H), 7.93 (s, 1H), 7.83-7.81 (m, 2H), 7.60 (dd, *J* = 1.0; 8.0 Hz, 1H), 7.51-7.48 (m, 3H), 7.44-7.40 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.24-7.21 (m, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 163.2, 138.6, 138.1, 136.3, 132.6, 130.4, 129.1, 128.4, 128.3, 128.0, 122.8, 120.5, 115.6.

Scale up for **2a**. In a 30 mL flame-dried Schlenk tube equipped with a stirring bar, amido-alcohol **1a** (5 mmol, 1.2 g), iron complex **Fe3** (42.1 mg, 2 mol %), Me_3NO (22.2 mg, 4 mol %), Na_2CO_3 (1.06 g, 2 equiv.) were added to a solution of dry DMF (5 mL) under an argon atmosphere. The mixture was rapidly stirred at room temperature for 2 min and then placed into a pre-heated oil bath at 100 °C and stirred over 40 hours. The mixture was cooled-down to room temperature, filtrated over a pad of Celite with diethyl ether. The conversion was determined by ^{1}H-NMR spectroscopy and the residue was purified by flash chromatography on silica gel using dichloromethane:diethyl ether (3:1) as eluent to afford the pure product **2a** as a white solid (829 mg, 75 %). ^{1}H-NMR data were comparable with the previous NMR data.

1-methyl-3-phenylquinolin-2(1H)-one (**2b**).[2] According to the general procedure D, **2b** was obtained from amido-alcohol **1b** (0.5 mmol, 128 mg) as a yellow solid (105 mg, 89 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.81 (s, 1H), 7.73-7.71 (m, 2H), 7.61 (dd, *J* = 1.4; 7.7 Hz, 1H), 7.56 (ddd, *J* = 1.4; 7.3; 8.7 Hz, 1H), 7.45-7.42 (m, 2H), 7.39-7.36 (m, 2H), 7.27-7.24 (m, 1H), 3.81 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 161.7, 139.8, 136.9, 132.7, 130.4, 129.1, 129.0, 128.3, 128.2, 122.3, 120.9, 114.1, 30.1.

3-(p-tolyl)quinolin-2(1H)-one (**2c**).[1] According to the general procedure D, **2c** was obtained from amido-alcohol **1c** (0.5 mmol, 128 mg) as a white solid (86 mg, 73 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.60 (br. s, 1H), 7.90 (s, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.59 (dd, *J* = 1.1; 7.8 Hz, 1H), 7.46 (ddd, *J* = 1.1; 7.3; 8.1 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.23-7.0 (m, 1H), 2.43 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 163.2, 138.6, 138.1, 136.3, 132.6, 130.4, 129.1, 128.4, 128.3, 128.0, 122.8, 120.5, 115.6, 21.5.

3-(o-tolyl)quinolin-2(1H)-one (**2d**).[3] According to the general procedure D, **2d** was obtained from amido-alcohol **1d** (0.5 mmol, 128 mg) as a white solid (91 mg, 77 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 12.45 (br. s, 1H), 7.76 (s, 1H), 7.56 (dd, *J* = 1.1; 7.8 Hz, 1H), 7.45-7.42 (m, 1H), 7.36-7.30 (m, 5H), 7.22-7.20 (m, 1H), 2.36 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 163.2, 140.0, 138.5, 137.4, 136.6, 134.2, 130.4, 130.2, 130.2, 128.3, 127.7, 125.9, 122.7, 120.1, 116.2, 20.3.

3-(2-bromophenyl)quinolin-2(1H)-one (**2e**). According to the general procedure D, **2e** was obtained from amido-alcohol **1e** (0.5 mmol, 160 mg) as a white solid (103 mg, 69 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.74 (br. s, 1H), 7.80 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.57 (dd, *J* = 1.0; 7.8 Hz, 1H), 7.51-7.48 (m, 1H), 7.45-7.40 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.31-7.27 (m, 1H), 7.24-7.21 (m, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 162.4, 140.6, 138.6, 137.5, 133.30, 133.1, 131.8, 130.8, 129.8, 128.1, 127.5, 124.2, 122.8, 119.8, 116.1. IR (neat): ν 2842, 1651, 1568, 1497, 1431, 1230, 1055, 1026, 904, 829, 754, 739, 596, 560, 470 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{15}H_{11}NOBr$ 300.0024; found 300.0028.

3-(2-methoxyphenyl)quinolin-2(1H)-one (**2f**).[4] According to the general procedure D, **2f** was obtained from amido-alcohol **1f** (0.5 mmol, 136 mg) as a white solid (68 mg, 54 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 11.80 (br. s, 1H), 7.83 (s, 1H), 7.64 (dd, *J* = 1.0; 7.8 Hz, 1H), 7.49-7.46 (m, 1H), 7.37-7.33 (m, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.25 (dd, *J* = 1.7; 7.4 Hz, 1H), 7.18-7.14 (m, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.99-6.96 (m, 1H), 3.71 (s, 3H). ^{13}C{^{1}H}NMR (DMSO-d_6, 125 MHz): δ 160.8, 157.1, 138.7, 138.5, 130.9, 130.9, 130.0, 129.2, 127.8, 125.8, 121.7, 120.0, 119.2, 114.7, 111.3, 55.5.

3-(3-methoxyphenyl)quinolin-2(1H)-one (**2g**).[3] According to the general procedure D, **2g** was obtained from amido-alcohol **1g** (0.5 mmol, 136 mg) as a white solid (77 mg, 61 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 12.48 (br. s, 1H), 7.94 (s, 1H), 7.60 (dd, *J* = 1.0; 7.9 Hz, 1H), 7.50-7.46 (m, 1H), 7.44-7.38 (m, 4H), 7.24-7.21 (m, 1H), 6.99-6.97 (m, 1H), 3.90 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 163.4, 159.6, 138.7, 138.2, 137.7, 132.3, 130.4, 129.4, 127.9, 122.8, 121.5, 120.4, 115.9, 114.6, 114.2, 55.5.

3-(4-methoxyphenyl)quinolin-2(1H)-one (**2h**).[1] According to the general procedure D, **2h** was obtained from amido-alcohol **1h** (0.5 mmol, 136 mg) as a white solid (104 mg, 83 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 11.90 (br. s, 1H), 8.04 (s, 1H), 7.72 (d, *J* = 8.8 Hz, 2H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.48-7.45 (m, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.19-7.15 (m, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H). ^{13}C{^{1}H}NMR (DMSO-d_6, 125 MHz): δ 161.2, 159.1, 138.1, 136.4, 131.0, 129.9, 129.9, 128.5, 127.9, 121.8, 119.7, 114.6, 113.4, 55.2.

3-(naphthalen-1-yl)quinolin-2(1H)-one (**2i**).[3] According to the general procedure D, **2i** was obtained from amido-alcohol **1i** (0.5 mmol, 146 mg) as a white solid (80 mg, 59 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 12.01 (br. s, 1H), 8.00 (s, 1H), 7.95 (dd, *J* = 4.1; 8.0 Hz, 2H), 7.71 (d, *J* = 7.4 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.57-7.50 (m, 3H), 7.46-7.42 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.19 (t, *J* = 7.4 Hz, 1H). ^{13}C{^{1}H}NMR (DMSO-d_6, 125 MHz): δ 161.3, 139.8, 138.8, 135.0, 133.1, 132.6, 131.6, 130.3, 128.1, 128.1, 128.1, 127.4, 126.0, 125.9, 125.8, 125.4, 121.9, 119.3, 114.9.

3-(4-fluorophenyl)quinolin-2(1H)-one (**2j**).[3] According to the general procedure D, **2j** was obtained from amido-alcohol **1j** (0.5 mmol, 130 mg) as a white solid (74 mg, 62 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d$_6$, 500 MHz): δ 11.98 (br. s, 1H), 8.12 (s, 1H), 7.84-7.82 (m, 2H), 7.72 (dd, *J* = 1.0; 7.8 Hz, 1H), 7.52-7.50 (m, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.28-7.25 (m, 2H), 7.22-7.19 (m, 1H). ^{19}F NMR (DMSO-d$_6$, 500 MHz): δ -114.1. ^{13}C{^{1}H}NMR (DMSO-d$_6$, 125 MHz): δ 161.8 (d, *J* = 243.5 Hz), 161.0, 138.3, 137.5 (d, *J* = 5.8 Hz), 132.5 (d, *J* = 3.2 Hz), 130.7 (d, *J* = 7.9 Hz), 130.3, 130.2, 128.1, 121.9, 119.5, 114.8, 114.7 (d, *J* = 1.9 Hz).

3-(4-(trifluoromethyl)phenyl)quinolin-2(1H)-one (**2k**).[3] According to the general procedure D, **2k** was obtained from amido-alcohol **1k** (0.5 mmol, 155 mg) as a white solid (94 mg, 65 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d$_6$, 500 MHz): δ 12.06 (br. s, 1H), 8.24 (s, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.74 (d, *J* = 7.4 Hz, 1H), 7.55-7.51 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.23-7.0 (m, 1H). ^{19}F NMR (DMSO-d$_6$, 500 MHz): δ -60.9. ^{13}C{^{1}H}NMR (DMSO-d$_6$, 125 MHz): δ 160.7, 140.3, 138.8 (d, *J* = 21.6 Hz), 130.7, 129.9, 129.4, 128.4, 128.0 (d, *J* = 31.7 Hz), 124.7 (q, *J* = 3.7 Hz), 122.0, 121.5 (q, *J* = 267.6 Hz), 119.3, 114.8.

3-(thiophen-2-yl)quinolin-2(1H)-one (**2l**).[1] According to the general procedure D, **2l** was obtained from amido-alcohol **1l** (0.5 mmol, 124 mg) as a white solid (54 mg, 48 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 12.30 (br. s, 1H), 8.27 (s, 1H), 7.84 (dd, *J* = 1.0; 3.7 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.55 (ddd, *J* = 1.2; 7.2; 8.2 Hz, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.46 (dd, *J* = 1.0; 5.1 Hz, 1H), 7.33-7.30 (m, 1H), 7.16 (dd, *J* = 3.7; 5.1 Hz, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 161.5, 136.8, 136.7, 135.2, 130.8, 128.0, 127.9, 127.2, 126.3, 125.0, 123.8, 120.7, 116.2.

5-methoxy-3-phenylquinolin-2(1H)-one (**2m**). According to the general procedure D, **2m** was obtained from amido-alcohol **1m** (0.5 mmol, 136 mg) as a light yellow solid (85 mg, 68 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.42 (br. s, 1H), 8.34 (s, 1H), 7.84-7.82 (m, 2H), 7.48-7.46 (m, 2H), 7.41-7.38 (m, 2H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.63 (d, *J* = 8.1 Hz, 1H), 3.96 (s, 3H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 163.1, 156.3, 139.3, 136.7, 133.3, 131.2, 130.9, 129.1, 128.3, 128.1, 111.4, 108.1, 102.8, 55.9. IR (neat): ν 2851, 1656, 1563, 1522, 1499, 1412, 1352, 1254, 1049, 912, 833, 752, 598, 471 cm^{-1}. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{16}H_{14}NO_2$ 252.1025; found 252.1027.

3,8-diphenylquinolin-2(1H)-one (**2n**). According to the general procedure D, **2n** was obtained from amido-alcohol **1n** (0.5 mmol, 159 mg) as a white solid (83 mg, 56 %) by flash column chromatography on silica gel (pentane/ethyl acetate 6:4). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.89 (br. s, 1H), 7.93 (s, 1H), 7.76-7.74 (m, 2H), 7.61 (dd, *J* = 1.3; 7.9 Hz, 1H), 7.57-7.54 (m, 2H), 7.51-7.48 (m, 1H), 7.47-7.44 (m, 4H), 7.42 (dd, *J* = 1.3; 7.4 Hz, 1H), 7.38 (ddd, *J* = 1.3; 3.9; 7.4 Hz, 1H). ^{13}C{^{1}H}NMR ($CDCl_3$, 125 MHz): δ 161.6, 138.5, 136.1, 136.0, 135.0, 133.0, 131.1, 129.8, 129.3, 128.8, 128.8, 128.5, 128.4, 128.3, 127.6, 122.6, 120.6. IR (neat): ν 2853, 1736, 1654, 1559, 1492, 1456, 1315, 1222, 1193, 1057, 907, 824, 766, 597 cm $^{-1}$. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for $C_{21}H_{16}NO$ 298.1232; found 298.1237.

3-phenyl-6-(trifluoromethyl)quinolin-2(1H)-one (**2o**).[1] According to the general procedure D, **2o** was obtained from amido-alcohol **1o** (0.5 mmol, 155 mg) as a white solid (103 mg, 71 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 11.80 (br. s, 1H), 7.83 (s, 1H), 7.64 (dd, *J* = 1.0; 7.8 Hz, 1H), 7.49-7.46 (m, 1H), 7.37-7.33 (m, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.25 (dd, *J* = 1.7; 7.4 Hz, 1H), 7.18-7.14 (m, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.99-6.96 (m, 1H), 3.71 (s, 3H). ^{19}F NMR (DMSO-d_6, 500 MHz): δ -60.1. ^{13}C{^{1}H}NMR (DMSO-d_6, 125 MHz): δ 161.1, 140.7, 137.1, 135.7, 133.0, 128.7, 128.1, 128.0, 126.1 (q, *J* = 3.4 Hz), 125.5 (q, *J* = 4.2 Hz), 124.4 (d, *J* = 269.8 Hz), 121.8 (q, *J* = 32.2 Hz), 119.1, 115.6.

3-phenylbenzo[g]quinolin-2(1H)-one (**2p**). According to the general procedure D, **2p** was obtained from amido-alcohol **1p** (0.5 mmol, 146 mg) as a light yellow solid (80 mg, 59 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 11.93 (br. s, 1H), 8.32 (s, 1H), 8.20 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.76-7.74 (m, 2H), 7.67 (s, 1H), 7.52-7.48 (m, 1H), 7.44-7.37 (m, 4H). ^{13}C{^{1}H}NMR (DMSO-d_6, 125 MHz): δ 161.4, 137.4, 136.1, 135.8, 133.6, 132.3, 128.9, 128.7, 128.3, 128.0, 128.0, 127.8, 127.4, 126.8, 124.4, 120.6, 109.6. IR (neat): ν 3029, 1662, 1568, 1497, 1431, 1230, 1055, 1026, 904, 829, 754, 739, 596, 560, 470 cm $^{-1}$. IR (neat): ν 2851, 1663, 1557, 1530, 1446, 1334, 1232, 1031, 888, 742, 693, 589, 570, 474 cm $^{-1}$. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for $C_{19}H_{14}NO$ 272.1075; found 272.1078.

3,4-diphenylquinolin-2(1H)-one (**2q**).[4] According to the general procedure D, **2q** was obtained from amido-alcohol **1q** (0.5 mmol, 159 mg) as a white solid (114 mg, 77 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 12.07 (br. s, 1H), 8.32 (s, 1H), 8.20 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.76-7.74 (m, 2H), 7.67 (s, 1H), 7.52-7.48 (m, 1H), 7.44-7.37 (m, 4H). $^{13}C\{^{1}H\}$NMR (DMSO-d_6, 125 MHz): δ 161.1, 148.0, 138.2, 136.1, 135.7, 131.9, 130.6, 130.1, 129.4, 127.9, 127.4, 127.0, 126.8, 126.5, 121.7, 119.9, 115.1.

4-(4-fluorophenyl)-3-phenylquinolin-2(1H)-one (**2r**). According to the general procedure D, **2r** was obtained from amido-alcohol **1r** (0.5 mmol, 168 mg) as a light yellow solid (124 mg, 79 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 12.37 (br. s, 1H), 7.40-7.37 (m, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.22-7.17 (m, 4H), 7.16-7.12 (m, 2H), 7.07-7.03 (m, 3H), 6.97-6.93 (m, 2H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -113.8. $^{13}C\{^{1}H\}$NMR ($CDCl_3$, 125 MHz): δ 163.4, 162.2 (d, *J* = 246.0 Hz), 148.9, 138.1, 135.3, 132.4, 132.3, 131.6 (d, *J* = 8.0 Hz), 131.0, 130.5, 127.8, 127.2 (d, *J* = 8.8 Hz), 122.5, 120.9, 116.4, 115.2 (d, *J* = 21.4 Hz). IR (neat): ν 2848, 1640, 1598, 1496, 1430, 1376, 1219, 1154, 1013, 904, 754, 702, 690, 641, 560, 510, 462 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{21}H_{15}NOF$ 316.1138; found 316.1142.

3-phenyl-4-(3-(trifluoromethyl)phenyl)quinolin-2(1H)-one (**2s**). According to the general procedure D, **2s** was obtained from amido-alcohol **1s** (0.5 mmol, 192 mg) as a light yellow solid (135 mg, 74 %) by flash column chromatography on silica gel (dichloromethane/diethyl ether 3:1). ^{1}H NMR (DMSO-d_6, 500 MHz): δ 12.14 (br. s, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.55-7.49 (m, 3H), 7.48 (s, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.14-7.08 (m, 4H), 7.07-7.05 (m, 2H), 6.94 (d, *J* = 8.2 Hz, 1H). ^{19}F NMR (DMSO-d_6, 500 MHz): δ -61.2. $^{13}C\{^{1}H\}$NMR (DMSO-d_6, 125 MHz): δ 161.0, 146.6, 138.4, 137.2, 135.4, 133.7, 132.7, 130.6, 130.4, 129.1, 128.8 (q, *J* = 31.6 Hz), 127.2, 126.7 (d, *J* = 45.8 Hz), 126.4 (q, *J* = 3.9 Hz), 124.3 (q, *J* = 3.2 Hz), 123.9 (q, *J* = 270.8 Hz), 122.0, 119.5, 115.3. IR (neat): ν 2849, 1644, 1598, 1443, 1327, 1290, 1164, 1123, 1074, 907, 759, 697, 683, 604, 559, 509, 463 cm $^{-1}$. HRMS (ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{22}H_{15}NOF_3$ 366.1106; found 366.1106.

4-methyl-3-phenylquinolin-2(1H)-one (**2t**).[5] According to the general procedure D, **2t** was obtained from amido-alcohol **1t** (0.5 mmol, 128 mg) as a white solid (68 mg, 58 %) by flash column chromatography on silica gel (pentane/ethyl acetate 1:1). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.34 (br. s, 1H), 7.74 (dd, *J* = 1.0; 8.1 Hz, 1H), 7.50-7.44 (m, 3H), 7.42-7.39 (m, 1H), 7.35-7.33 (m, 2H), 7.26-7.22 (m, 1H), 2.36 (s, 3H). $^{13}C\{^{1}H\}$NMR ($CDCl_3$, 125 MHz): δ 163.0, 144.9, 137.5, 136.1, 132.4, 130.5, 130.2, 128.4, 127.7, 125.1, 122.5, 121.0, 116.2, 17.1.

Part 3: Computational Details.

All calculations were conducted at the DFT level with the Gaussian16 set of programs,[6] using the BP86 functional.[7] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O and F (SVP keyword in Gaussian).[8] For Fe, the quasi-relativistic Stuttgart/Dresden effective core potential[9] with an associated valence basis set (standard SDD keyword in Gaussian16) was used. Geometry optimizations were carried out without symmetry constraints and normal mode analysis were computed to confirm minima and transition states on the potential energy surface. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298 K and 1 atm by using the standard statistical mechanics relationships for an ideal gas. Accurate electronic energies were obtained via single-point calculation using the M06 functional of Zhao and Truhlar,[10] on the BP86-optimized geometries. In these calculations, the cc-pVTZ basis set was used for the description of H, C, N, O and F,[11] whereas for Fe the SDD basis set (and pseudopotential) has been employed, together with the solvent effects of ethanol estimated with the polarizable continuous solvation model (PCM).[12-13] On top of the M06/cc-pVTZ~SDD(PCM-EtOH) electronic energies, we added the thermal and entropy corrections obtained at the BP86/SVP~SDD level in gas phase.

Table S1. Absolute energies (in a.u.) of all computed species.

	E_{gas}	G_{gas}	E_{solv}	G_{solv}
H_2O	-76.3597377	-76.356792	-76.4233898	-76.4204441
H_2	-1.1724038	-1.174212	-1.1708874	-1.1726956
Me_3NO	-249.4270678	-249.335358	-249.5457603	-249.4540505
Me_3N	-174.3373394	-174.248791	-174.3931084	-174.30456
CO	-113.2244893	-113.238737	-113.2934742	-113.3077219
CO_2	-188.4544418	-188.463802	-188.5706702	-188.5800304
Na_2CO3	-588.2045568	-588.218274	-588.5477194	-588.5614366
NaHCO3	-426.5207693	-426.521557	-426.7827288	-426.7835165
NaOH	-238.0061853	-238.018488	-238.1666436	-238.1789463
I	-1704.901903	-1704.576623	-1705.108639	-1704.783359
I-II	-1954.330686	-1953.890193	-1954.646042	-1954.205549
II	-1591.605583	-1591.287388	-1591.750328	-1591.432133
III-IV	-2538.608355	-2538.06457	-2539.087564	-2538.543779
III	-2538.619207	-2538.080748	-2539.09577	-2538.557311
IV	-1754.521928	-1754.19628	-1754.744869	-1754.419221
V	-1592.821039	-1592.482368	-1592.967452	-1592.628781
V-VI	-1669.179175	-1668.823811	-1669.364454	-1669.009091
VI	-1592.806229	-1592.47115	-1592.950907	-1592.615827
VI-VII	-1592.777729	-1592.451602	-1592.923643	-1592.597516
SUBSTa	-785.2680352	-785.052357	-785.5406224	-785.3249442
SUBSTaNa	-946.9585255	-946.754551	-947.2960429	-947.0920684
SUBSTaNa	-946.9585255	-946.754551	-947.2960429	-947.0920684
SUBST1a	-784.0690802	-783.876427	-784.336141	-784.1434878
SUBST1-2a	-783.9700273	-783.779417	-784.2228356	-784.0322253
SUBST2a	-784.085488	-783.886354	-784.3558985	-784.1567645

SUBST2-3a	-784.0161714	-783.823138	-784.2693354	-784.076302
PRODa	-707.7279766	-707.552291	-707.937133	-707.7614474
SUBST1Na	-945.7408377	-945.560781	-946.0860568	-945.9060001
SUBST1aNaISOMER	-945.7621523	-945.576491	-946.1105473	-945.924886
SUBST1-2aNa	-945.7426428	-945.55996	-946.1134261	-945.9307433
SUBST2aNa	-945.7621522	-945.576483	-946.1105147	-945.9248455
SUBST2aNaISOMER	-945.7507321	-945.566061	-946.1087403	-945.9240692
SUBST2-3aNa	-945.711679	-945.531001	-946.0573998	-945.8767218

Table S3. Xyz coordinates and absolute energies in gas phase (in a.u.) of all computed species.

2

H2 SCF Done: -1.17240382647 A.U.

H 0.000000 0.000000 0.383727

H 0.000000 0.000000 -0.383727

Table S4. Xyz coordinates and absolute energies (in a.u.) of all computed species.

3

CO2 SCF Done: -188.454441841 A.U.
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.175258
O 0.000000 0.000000 -1.175258

2

CO SCF Done: -113.224489253 A.U.
C 0.000000 0.000000 -0.652873
O 0.000000 0.000000 0.489655

3

H2O SCF Done: -76.3597377176 A.U.
O -0.000000 0.000000 0.122683
H -0.000000 0.759080 -0.490731
H -0.000000 -0.759080 -0.490731

82

KNO-III-IVpost1 SCF Done: -2538.61868854 A.U.
Fe -2.110026 -0.151448 -0.623218
C -3.182213 0.641496 1.274597
O -3.060717 0.334860 2.507954
C -2.380361 1.638673 0.533320
C -2.946994 1.752923 -0.807138
C -2.671061 2.785447 -1.874955
H -1.582319 2.968183 -1.977010
H -3.117381 3.756278 -1.550873
C -4.890136 0.694990 -2.163825

H	-5.941741	0.598719	-1.816631
H	-4.687820	-0.221823	-2.756653
C	-3.982352	0.761484	-0.948922
C	-4.046686	-0.024796	0.272218
Si	-1.192275	2.833362	1.437233
C	-2.264008	4.113314	2.387636
H	-2.875613	4.722517	1.689310
H	-1.632939	4.808615	2.981418
H	-2.957053	3.593598	3.081337
C	0.002273	3.753376	0.247657
H	-0.534214	4.444491	-0.434314
H	0.594056	3.049111	-0.373094
H	0.719410	4.363230	0.838282
C	-0.104258	1.899864	2.727113
H	0.510300	1.100407	2.259146
H	-0.734601	1.465976	3.531363
H	0.607385	2.604622	3.207939
Si	-5.205760	-1.461439	0.762639
C	-6.686240	-0.743943	1.757235
H	-7.363338	-1.549692	2.113351
H	-7.288177	-0.044002	1.140012
H	-6.317364	-0.185143	2.642335
C	-5.866132	-2.411864	-0.771441
H	-6.458795	-3.292199	-0.441689
H	-5.037804	-2.783159	-1.409713
H	-6.528464	-1.785231	-1.403604
C	-4.261664	-2.709322	1.881501
H	-4.905188	-3.575634	2.145399
H	-3.953799	-2.208899	2.823000
H	-3.360926	-3.101387	1.362363
C	-0.453866	0.128740	-1.035290
O	0.695527	0.275379	-1.269897
C	-2.345969	-1.363256	-1.857269
O	-2.497626	-2.176218	-2.687046
C	-3.283219	2.376288	-3.227227
H	-3.208438	3.221427	-3.943878
H	-2.693955	1.536947	-3.660319
C	-4.749662	1.946228	-3.057433
H	-5.317345	2.790583	-2.603255
H	-5.219624	1.752557	-4.044833
Na	-1.266486	-0.925838	2.410116
C	4.052442	-4.496424	-0.761500
C	4.215436	-3.151468	-1.118878
C	3.438707	-2.141073	-0.502727
C	2.487248	-2.529225	0.496124
C	2.311743	-3.900741	0.810576
C	3.092698	-4.882076	0.199143

H	4.663107	-5.262441	-1.265549
H	1.556934	-4.157021	1.570113
H	2.959341	-5.943884	0.456125
C	1.728065	-1.522315	1.248027
H	2.047739	-0.457293	1.102818
H	-1.645939	-1.280150	0.283827
O	0.798727	-1.783894	2.024801
N	3.531337	-0.795478	-0.899281
C	4.645578	-0.010758	-1.227021
O	4.474950	1.100092	-1.712222
C	6.045650	-0.565569	-0.912397
H	5.987791	-1.451348	-0.250135
H	6.467823	-0.918011	-1.880915
C	6.969397	0.475491	-0.304062
C	7.411099	0.338395	1.028860
C	7.400050	1.594992	-1.049690
C	8.266846	1.292726	1.606542
H	7.083241	-0.531079	1.623279
C	8.253079	2.549809	-0.472707
H	7.048306	1.722383	-2.084231
C	8.690399	2.402419	0.856064
H	8.603432	1.166624	2.648076
H	8.579654	3.418023	-1.067315
H	9.361729	3.151664	1.305155
H	2.641761	-0.288263	-1.041507
H	4.913753	-2.880717	-1.923470

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KNO-III-IVpost2 SCF Done: -2538.61856594 A.U.

Fe	-2.047188	-0.296998	-0.592521
C	-2.942297	0.749736	1.275246
O	-2.674487	0.643485	2.519069
C	-2.272993	1.642289	0.304895
C	-2.986901	1.530148	-0.963424
C	-2.876914	2.391716	-2.199653
H	-1.815419	2.588978	-2.451718
H	-3.331018	3.387333	-1.977636
C	-5.014172	0.217244	-1.913523
H	-6.016648	0.146158	-1.438380
H	-4.835136	-0.774456	-2.379933
C	-3.983927	0.498492	-0.834394
C	-3.877980	-0.090126	0.491041
Si	-1.048296	2.993475	0.878169
C	-2.063855	4.368530	1.754758
H	-2.780185	4.847426	1.054477
H	-1.403082	5.163849	2.161131
H	-2.646906	3.937307	2.594823

C	-0.041453	3.761442	-0.565844
H	-0.684379	4.326184	-1.271706
H	0.509399	2.990846	-1.144000
H	0.707844	4.474282	-0.159091
C	0.220897	2.293198	2.149374
H	0.807241	1.446423	1.731435
H	-0.292535	1.970904	3.079333
H	0.955299	3.077777	2.430902
Si	-4.909393	-1.464474	1.324174
C	-6.307309	-0.642870	2.356816
H	-6.902926	-1.401575	2.908265
H	-7.004763	-0.068908	1.710814
H	-5.872512	0.060935	3.096654
C	-5.682993	-2.666810	0.040400
H	-6.194498	-3.500891	0.567340
H	-4.910451	-3.109761	-0.621670
H	-6.438067	-2.169649	-0.602720
C	-3.794432	-2.491334	2.509269
H	-4.364119	-3.326897	2.969253
H	-3.416459	-1.841690	3.325803
H	-2.934026	-2.930337	1.960005
C	-0.466243	-0.033783	-1.243579
O	0.637994	0.110285	-1.639949
C	-2.362372	-1.696553	-1.586695
O	-2.568131	-2.635244	-2.256797
C	-3.611637	1.758830	-3.395657
H	-3.654265	2.483687	-4.236023
H	-3.034138	0.879874	-3.760628
C	-5.029426	1.317556	-2.996560
H	-5.583415	2.205348	-2.613934
H	-5.593857	0.958668	-3.883109
Na	-0.857855	-0.581960	2.419744
C	4.296713	-4.364497	-0.803243
C	4.342584	-3.071710	-1.342368
C	3.579613	-2.025011	-0.772532
C	2.758799	-2.320073	0.362306
C	2.697041	-3.644175	0.865573
C	3.467100	-4.661234	0.299816
H	4.892446	-5.163531	-1.272748
H	2.039684	-3.832602	1.728557
H	3.422918	-5.685029	0.701427
C	2.017781	-1.254843	1.050425
H	2.255041	-0.207767	0.726822
H	-1.423376	-1.250374	0.414878
O	1.188494	-1.449306	1.949919
N	3.555861	-0.739313	-1.347410
C	4.601682	0.062022	-1.819784

O	4.348088	1.065956	-2.476327
C	6.035392	-0.271047	-1.385661
H	6.153263	-1.323759	-1.069198
H	6.669996	-0.111006	-2.282616
C	6.492672	0.646895	-0.255291
C	6.911961	0.106325	0.978697
C	6.507062	2.049716	-0.423273
C	7.343663	0.945191	2.021622
H	6.906471	-0.986917	1.123780
C	6.935882	2.887123	0.619227
H	6.161803	2.475971	-1.378106
C	7.357162	2.338923	1.844635
H	7.671260	0.504888	2.977086
H	6.942216	3.979155	0.472450
H	7.695935	2.997909	2.659894
H	2.625794	-0.320922	-1.518204
H	4.933208	-2.874400	-2.249299

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KNO-III-IVpre SCF Done: -2538.60922469 A.U.

Fe	1.350210	0.556381	-0.626217
C	1.410029	-1.168057	0.922850
O	0.531381	-1.651876	1.702758
C	1.649516	-1.564896	-0.482521
C	2.840728	-0.861492	-0.933421
C	3.661658	-1.083144	-2.181557
H	3.009852	-1.205903	-3.069484
H	4.206500	-2.050560	-2.066871
C	4.546281	0.850534	0.017116
H	5.073267	0.781174	0.993485
H	4.331869	1.930258	-0.129434
C	3.255053	0.057417	0.099541
C	2.314946	-0.024895	1.202145
Si	0.850165	-3.129996	-1.251001
C	1.761708	-4.630185	-0.460784
H	2.847179	-4.616991	-0.694794
H	1.346622	-5.591571	-0.832384
H	1.653170	-4.611807	0.643758
C	1.055841	-3.212611	-3.160675
H	2.111958	-3.344012	-3.473251
H	0.656706	-2.304735	-3.658604
H	0.484476	-4.082571	-3.550191
C	-1.016092	-3.265940	-0.857862
H	-1.615208	-2.484369	-1.369666
H	-1.187544	-3.192778	0.234523
H	-1.402065	-4.249376	-1.203010
Si	2.498985	0.812805	2.916475

C	3.836460	-0.172395	3.891735
H	3.972063	0.246544	4.912017
H	4.823772	-0.145449	3.384369
H	3.542087	-1.237869	3.996520
C	3.056093	2.645126	2.769613
H	3.134854	3.093290	3.783426
H	2.327962	3.247518	2.188923
H	4.046197	2.751561	2.281484
C	0.866203	0.777695	3.924140
H	0.975004	1.389040	4.845634
H	0.625634	-0.260714	4.235977
H	0.027809	1.190302	3.323454
C	0.757973	0.563707	-2.268655
O	0.354622	0.558069	-3.370856
C	1.651413	2.281731	-0.609385
O	1.889554	3.426916	-0.623968
C	4.683169	0.047616	-2.402445
H	5.377575	-0.231541	-3.222735
H	4.152478	0.968087	-2.734832
C	5.465981	0.339832	-1.112116
H	5.973837	-0.595474	-0.782539
H	6.271284	1.081066	-1.299340
Na	-1.406570	-1.037991	2.472868
C	-2.813618	4.419872	-1.862364
C	-3.016230	3.139120	-2.398836
C	-2.583734	1.994511	-1.696386
C	-1.930740	2.133458	-0.445955
C	-1.767908	3.424592	0.095669
C	-2.194270	4.561006	-0.605833
H	-3.149692	5.307980	-2.420484
H	-1.294836	3.507341	1.086716
H	-2.043520	5.563347	-0.174396
C	-1.461920	0.931431	0.360410
H	-1.740798	-0.037772	-0.133543
H	-0.157620	0.848079	-0.034014
O	-1.528030	1.004445	1.644936
N	-2.800866	0.698318	-2.274744
C	-3.678082	-0.287492	-1.871705
O	-3.659662	-1.407756	-2.387551
C	-4.696295	0.066142	-0.772740
H	-4.725938	1.154611	-0.572318
H	-5.682116	-0.220782	-1.200790
C	-4.484962	-0.697190	0.530465
C	-4.518200	-0.017916	1.768409
C	-4.264005	-2.095106	0.533961
C	-4.339692	-0.711464	2.980550
H	-4.671842	1.072174	1.786717

C	-4.065788	-2.788141	1.741450
H	-4.232243	-2.625303	-0.430096
C	-4.105558	-2.101262	2.973471
H	-4.384914	-0.160342	3.933966
H	-3.894343	-3.876296	1.721609
H	-3.984875	-2.651489	3.921602
H	-2.157617	0.396894	-3.018510
H	-3.520856	3.004901	-3.368489

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KNO-III-IV SCF Done: -2538.60835491 A.U.

Fe	-1.363045	-0.504178	-0.686482
C	-1.465618	1.052355	1.025787
O	-0.600921	1.493299	1.852179
C	-1.733153	1.580848	-0.328428
C	-2.906085	0.886849	-0.843627
C	-3.740855	1.202841	-2.062502
H	-3.097970	1.432782	-2.935623
H	-4.320079	2.134331	-1.855002
C	-4.542343	-0.971105	-0.063404
H	-5.067521	-1.015002	0.915653
H	-4.292013	-2.023438	-0.315529
C	-3.279056	-0.143717	0.090924
C	-2.332052	-0.138006	1.194753
Si	-0.982858	3.232436	-0.942676
C	-1.916532	4.630790	-0.004555
H	-3.003604	4.616425	-0.231025
H	-1.525183	5.632587	-0.283750
H	-1.798003	4.506978	1.092161
C	-1.203207	3.499404	-2.834023
H	-2.264782	3.630607	-3.127725
H	-0.782754	2.655718	-3.419646
H	-0.658786	4.419206	-3.138481
C	0.885125	3.374425	-0.551223
H	1.495346	2.665349	-1.148417
H	1.065028	3.187153	0.526190
H	1.245762	4.397925	-0.791310
Si	-2.484994	-1.141870	2.815744
C	-3.855418	-0.314401	3.887555
H	-3.970787	-0.837987	4.860960
H	-4.842708	-0.329684	3.379652
H	-3.603559	0.746492	4.097416
C	-2.962320	-2.974608	2.496849
H	-3.020019	-3.522264	3.462066
H	-2.211661	-3.485153	1.859564
H	-3.948034	-3.073955	1.998382
C	-0.858730	-1.139712	3.841559

H	-0.960896	-1.820476	4.713910
H	-0.650762	-0.122059	4.234942
H	-0.001640	-1.491010	3.229816
C	-0.728033	-0.327733	-2.295336
O	-0.267357	-0.204087	-3.370757
C	-1.565972	-2.232368	-0.824486
O	-1.711996	-3.389817	-0.930393
C	-4.721696	0.062390	-2.391596
H	-5.431043	0.394368	-3.178983
H	-4.158355	-0.800481	-2.812894
C	-5.485917	-0.384417	-1.134667
H	-6.023919	0.495334	-0.712610
H	-6.266259	-1.131234	-1.392902
Na	1.311512	0.840744	2.600052
C	2.849860	-4.129388	-2.321794
C	3.001016	-2.794718	-2.731002
C	2.631989	-1.739999	-1.872108
C	2.088946	-2.029693	-0.592599
C	1.976437	-3.374959	-0.182073
C	2.345768	-4.419591	-1.039291
H	3.136547	-4.945835	-3.003230
H	1.577633	-3.572101	0.825092
H	2.235771	-5.465729	-0.713044
C	1.679963	-0.935985	0.348531
H	1.797210	0.096838	-0.063255
H	0.091654	-0.768838	-0.156723
O	1.657028	-1.126167	1.594192
N	2.787139	-0.386722	-2.316355
C	3.664568	0.580084	-1.864920
O	3.593220	1.742095	-2.269617
C	4.744684	0.158380	-0.852841
H	4.859015	-0.942208	-0.802186
H	5.690745	0.573890	-1.264054
C	4.523906	0.723435	0.547497
C	4.707523	-0.094161	1.684136
C	4.133938	2.069720	0.741250
C	4.500405	0.409412	2.981098
H	5.000978	-1.147943	1.553488
C	3.912238	2.573358	2.035918
H	3.992684	2.711714	-0.141641
C	4.094342	1.746025	3.164751
H	4.656170	-0.247604	3.851711
H	3.612451	3.626079	2.164226
H	3.954359	2.151319	4.181009
H	2.103451	-0.038961	-3.003013
H	3.415906	-2.550619	-3.721310

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KNO-I-II SCF Done: -1954.33068579 A.U.

Fe	0.349519	0.011392	-1.036369
C	0.063783	0.009626	1.357807
O	-0.816897	-0.347526	2.165464
C	1.162226	-0.833934	0.762752
C	2.096750	0.067537	0.123785
C	3.525459	-0.191702	-0.297835
H	3.620876	-1.166566	-0.816683
H	4.130941	-0.283489	0.634472
C	2.281043	2.597952	-0.427260
H	2.103053	3.445904	0.268249
H	1.892445	2.934053	-1.412231
C	1.508884	1.385631	0.062820
C	0.200782	1.338895	0.689801
Si	1.510336	-2.630764	1.338686
C	2.591620	-2.494141	2.926542
H	3.558433	-1.986299	2.725749
H	2.818948	-3.500507	3.339256
H	2.060301	-1.915230	3.710669
C	2.455297	-3.655770	0.014619
H	3.496649	-3.305102	-0.138447
H	1.935590	-3.627190	-0.965569
H	2.509238	-4.718536	0.335022
C	-0.110734	-3.549759	1.780040
H	-0.676183	-3.810930	0.862535
H	-0.741392	-2.896501	2.415644
H	0.113402	-4.489549	2.328335
Si	-0.832485	2.858903	1.236476
C	-0.045807	3.464484	2.886430
H	-0.602138	4.334372	3.296914
H	1.012100	3.773655	2.751030
H	-0.067617	2.653472	3.643917
C	-0.806329	4.296140	-0.040762
H	-1.473849	5.111802	0.312112
H	-1.173930	3.965463	-1.033772
H	0.203093	4.733291	-0.180902
C	-2.658192	2.391523	1.548742
H	-3.220726	3.244642	1.983920
H	-2.705041	1.524817	2.237894
H	-3.123605	2.106787	0.585034
C	1.245432	-0.770919	-2.330943
O	1.845070	-1.270371	-3.199956
C	-0.391109	1.198423	-2.111122
O	-0.854435	1.999238	-2.821713
C	4.093808	0.951058	-1.158916
H	5.188320	0.812374	-1.285321
H	3.651726	0.906867	-2.179170

C	3.795731	2.318525	-0.523926
H	4.240954	2.343299	0.497142
H	4.288484	3.132495	-1.096592
C	-1.017518	-1.264198	-1.088667
O	-1.269302	-2.409211	-1.246349
O	-2.683025	-0.304021	-0.831590
N	-3.813417	-1.033351	-0.406906
C	-3.490454	-1.792726	0.857666
H	-2.827482	-2.633460	0.596207
H	-2.937927	-1.099926	1.522228
H	-4.427357	-2.166218	1.315666
C	-4.272387	-1.962647	-1.500515
H	-4.496986	-1.342989	-2.387128
H	-3.444115	-2.655201	-1.723445
H	-5.173888	-2.515590	-1.169079
C	-4.892190	-0.029000	-0.125422
H	-5.832658	-0.552706	0.138944
H	-4.548777	0.610402	0.705490
H	-5.022234	0.580752	-1.037059

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KNO-III SCF Done: -2538.61920670 A.U.

Fe	-2.646830	-0.408107	-1.091617
C	-2.148760	0.410886	1.017752
O	-1.038415	0.607073	1.624337
C	-2.832212	1.352264	0.108697
C	-4.129343	0.772447	-0.227157
C	-5.314161	1.416055	-0.909492
H	-4.992370	2.015974	-1.784505
H	-5.778139	2.138384	-0.195956
C	-5.450860	-1.404276	0.275057
H	-5.629839	-1.838094	1.282836
H	-5.314717	-2.272588	-0.404091
C	-4.191418	-0.557851	0.319368
C	-2.927438	-0.843635	0.987176
Si	-2.136556	3.103879	-0.183349
C	-2.250596	4.095181	1.459412
H	-3.307685	4.244386	1.765251
H	-1.779888	5.097293	1.365709
H	-1.738104	3.540189	2.272170
C	-3.071249	4.061442	-1.562625
H	-4.130496	4.255227	-1.295075
H	-3.052953	3.514550	-2.528112
H	-2.585019	5.047578	-1.725338
C	-0.284149	3.011542	-0.713164
H	-0.151376	2.317353	-1.570719
H	0.354619	2.683658	0.133925

H	0.084854	4.009250	-1.034000
Si	-2.377095	-2.376698	1.978567
C	-2.589538	-2.014052	3.854651
H	-2.212086	-2.852585	4.478361
H	-3.656881	-1.851971	4.114914
H	-2.031432	-1.094999	4.129338
C	-3.375011	-3.952607	1.516371
H	-2.957942	-4.830979	2.054637
H	-3.320157	-4.165452	0.428799
H	-4.445795	-3.871608	1.794978
C	-0.518164	-2.751845	1.638221
H	-0.205568	-3.697750	2.130168
H	0.116581	-1.935733	2.041707
H	-0.328964	-2.860077	0.548749
C	-2.692235	0.354803	-2.659038
O	-2.717985	0.877630	-3.708349
C	-2.819740	-2.020047	-1.732808
O	-2.940874	-3.106414	-2.158002
C	-6.364904	0.369860	-1.324188
H	-7.288451	0.882098	-1.668456
H	-5.982423	-0.215326	-2.190520
C	-6.682685	-0.580784	-0.158398
H	-7.044472	0.024322	0.704596
H	-7.514146	-1.266961	-0.426018
Na	0.467876	0.032863	0.135951
C	6.760435	-2.791003	-2.148388
C	7.084910	-1.447315	-1.904675
C	6.099816	-0.544997	-1.451396
C	4.760145	-1.004878	-1.284561
C	4.458801	-2.371380	-1.502817
C	5.449079	-3.261247	-1.929847
H	7.542924	-3.483221	-2.497605
H	3.417099	-2.698190	-1.358679
H	5.203830	-4.319438	-2.108672
C	3.655849	-0.059842	-1.007463
H	3.919471	1.027664	-1.052209
H	-1.132212	-0.556341	-1.252760
O	2.492309	-0.411162	-0.794815
N	6.449248	0.808440	-1.185773
C	6.531924	1.469269	0.044551
O	6.872555	2.646094	0.086283
C	6.206712	0.662722	1.305526
H	6.459244	-0.408918	1.171769
H	6.887392	1.073462	2.081705
C	4.762950	0.794821	1.778663
C	4.080682	-0.327906	2.294546
C	4.089349	2.037559	1.733833

C	2.750678	-0.219998	2.736863
H	4.595884	-1.301416	2.344987
C	2.756169	2.141623	2.165862
H	4.622333	2.924890	1.355721
C	2.074851	1.013122	2.663785
H	2.235785	-1.106964	3.139348
H	2.243297	3.115515	2.121009
H	1.021873	1.090455	2.978767
H	6.857078	1.356938	-1.952277
H	8.116129	-1.086244	-2.042036

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KNO-II SCF Done: -1591.60558316 A.U.

Fe	-0.007047	0.385896	1.028341
C	-0.003617	-1.332773	-0.294892
O	-0.009279	-2.487040	0.196540
C	-1.202469	-0.465581	-0.483265
C	-0.723427	0.825801	-0.893349
C	-1.506478	2.031232	-1.347945
H	-2.416506	2.163344	-0.729551
H	-1.871295	1.819567	-2.381031
C	1.545766	2.006727	-1.376196
H	2.352033	1.646564	-2.049430
H	2.070218	2.467210	-0.511746
C	0.737999	0.815512	-0.905691
C	1.203221	-0.472627	-0.476570
Si	-2.964050	-1.219037	-0.313967
C	-3.135829	-2.526303	-1.708655
H	-3.046520	-2.065287	-2.714793
H	-4.121318	-3.036063	-1.654210
H	-2.342656	-3.295647	-1.609604
C	-4.333080	0.114516	-0.510775
H	-4.302512	0.614290	-1.501107
H	-4.270522	0.894550	0.276457
H	-5.329466	-0.368428	-0.415670
C	-3.140941	-2.059295	1.397530
H	-3.077607	-1.320839	2.223805
H	-2.332583	-2.805446	1.534487
H	-4.120696	-2.576415	1.479431
Si	2.964904	-1.218184	-0.274618
C	3.203373	-2.479107	-1.701841
H	4.193343	-2.977659	-1.628352
H	3.143051	-1.988211	-2.695937
H	2.418841	-3.262336	-1.656201
C	4.322311	0.138158	-0.372400
H	5.315222	-0.324423	-0.185204
H	4.175863	0.926349	0.394942

H	4.370349	0.627328	-1.367233
C	3.087530	-2.108037	1.416196
H	4.068207	-2.619983	1.517338
H	2.279793	-2.862118	1.503470
H	2.989518	-1.393853	2.260336
C	-1.295575	1.218846	1.898461
O	-2.148456	1.828019	2.412765
C	1.268139	1.225459	1.913992
O	2.109549	1.845482	2.434569
C	-0.648940	3.309499	-1.365912
H	-1.214755	4.129796	-1.854809
H	-0.450694	3.640509	-0.321717
C	0.681258	3.063512	-2.094609
H	0.464550	2.722972	-3.132850
H	1.257440	4.007122	-2.192976

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KNO-IV SCF Done: -1754.52192835 A.U.

Fe	-0.004834	0.473455	1.033745
C	-0.003136	-1.175750	-0.623225
O	-0.009809	-2.454423	-0.571663
C	-1.182439	-0.289051	-0.587433
C	-0.709707	1.069854	-0.831261
C	-1.505429	2.309629	-1.166792
H	-2.403478	2.393273	-0.521755
H	-1.886191	2.204267	-2.210629
C	1.557487	2.280184	-1.202972
H	2.344137	1.977888	-1.927917
H	2.102075	2.665141	-0.314736
C	0.731591	1.059944	-0.837948
C	1.185279	-0.300614	-0.577829
Si	-2.940597	-1.031325	-0.559559
C	-3.268382	-1.920397	-2.229265
H	-3.267724	-1.200082	-3.074349
H	-4.249809	-2.441012	-2.227717
H	-2.473281	-2.670383	-2.420188
C	-4.304498	0.284104	-0.250651
H	-4.368542	1.019202	-1.079458
H	-4.134348	0.842311	0.693064
H	-5.294677	-0.214531	-0.173772
C	-3.063829	-2.340267	0.857716
H	-2.737224	-1.905492	1.828078
H	-2.455048	-3.236212	0.609153
H	-4.110962	-2.685977	0.991692
Si	2.941858	-1.044016	-0.513466
C	3.325699	-1.901459	-2.188014
H	4.309855	-2.416404	-2.165553

H	3.346399	-1.166810	-3.020393
H	2.542311	-2.653112	-2.417435
C	4.285261	0.273346	-0.132239
H	5.275228	-0.219473	-0.023171
H	4.071511	0.816175	0.811419
H	4.377108	1.023959	-0.944081
C	3.024384	-2.378603	0.882221
H	4.065537	-2.736658	1.029620
H	2.410524	-3.263031	0.606943
H	2.684621	-1.955946	1.853533
C	-1.288659	1.232516	1.941829
O	-2.154806	1.739815	2.545577
C	1.260548	1.244304	1.957086
O	2.112033	1.769668	2.566550
H	-0.007248	-0.659834	2.078106
C	-0.641450	3.580495	-1.069112
H	-1.201669	4.446604	-1.480625
H	-0.440494	3.810675	0.001353
C	0.689112	3.398789	-1.818043
H	0.467417	3.151165	-2.881523
H	1.263489	4.349122	-1.834369
Na	-0.022894	-2.684774	1.571961

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KNO-I SCF Done: -1704.90190276 A.U.

Fe	-0.010988	0.451910	1.032879
C	0.000950	-1.301601	-0.681756
O	-0.001195	-2.531503	-0.778484
C	-1.186644	-0.382819	-0.560896
C	-0.715129	0.949551	-0.876193
C	-1.505636	2.165227	-1.299709
H	-2.415982	2.286235	-0.679011
H	-1.870623	1.975152	-2.336448
C	1.555128	2.140469	-1.326769
H	2.344287	1.784742	-2.023116
H	2.099974	2.585676	-0.468033
C	0.737211	0.941925	-0.880034
C	1.193223	-0.388871	-0.545657
Si	-2.957925	-1.133966	-0.575635
C	-3.213995	-1.885535	-2.324117
H	-3.166461	-1.109178	-3.116585
H	-4.203410	-2.385300	-2.398080
H	-2.427211	-2.639750	-2.530498
C	-4.314446	0.184693	-0.239336
H	-4.383651	0.939751	-1.049627
H	-4.152194	0.719182	0.719482
H	-5.303657	-0.317485	-0.173580

C	-3.061688	-2.507730	0.751001
H	-2.984494	-2.093174	1.777529
H	-2.236996	-3.234246	0.604672
H	-4.027670	-3.050890	0.676595
Si	2.968050	-1.130650	-0.524457
C	3.300889	-1.798545	-2.294503
H	4.296944	-2.287244	-2.351196
H	3.278046	-0.988042	-3.053143
H	2.531123	-2.549109	-2.568234
C	4.290640	0.185976	-0.068607
H	5.287566	-0.300902	-0.005853
H	4.088822	0.654566	0.916630
H	4.366911	0.995718	-0.823144
C	3.031611	-2.564027	0.739454
H	4.003112	-3.098560	0.675332
H	2.215900	-3.285150	0.530040
H	2.914680	-2.197730	1.780402
C	-1.307759	1.380021	1.808886
O	-2.158690	1.989974	2.316815
C	1.256450	1.398071	1.836192
O	2.084524	2.027329	2.358457
C	-0.647139	3.442870	-1.290116
H	-1.210024	4.272936	-1.765806
H	-0.453076	3.756281	-0.239527
C	0.686300	3.212187	-2.019888
H	0.469863	2.892812	-3.064720
H	1.260195	4.159026	-2.098973
C	-0.011808	-0.958506	2.144227
O	-0.013014	-1.837111	2.900494

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Me3NO SCF Done: -249.427067795 A.U.

O	0.000007	0.000071	1.439458
N	-0.000003	0.000006	0.104909
C	0.135108	-1.418759	-0.424127
H	1.076496	-1.814587	-0.002697
H	-0.713965	-1.985223	-0.001327
H	0.138762	-1.467298	-1.534136
C	1.161192	0.826329	-0.424239
H	1.033237	1.839535	-0.002813
H	2.076240	0.374316	-0.001292
H	1.201048	0.853881	-1.534240
C	-1.296256	0.592364	-0.424185
H	-1.340561	0.612378	-1.534198
H	-2.109643	-0.024485	-0.001779
H	-1.361915	1.611272	-0.002239

13

Me3N SCF Done: -174.337339352 A.U.

N	-0.000038	-0.000045	-0.354187
C	1.047782	-0.919136	0.056777
H	0.845455	-1.934593	-0.344827
H	2.028318	-0.585511	-0.344028
H	1.153529	-1.012568	1.174675
C	-1.319951	-0.447741	0.056752
H	-2.097991	0.235759	-0.344351
H	-1.521767	-1.463435	-0.344486
H	-1.453657	-0.493151	1.174686
C	0.272203	1.366880	0.056762
H	0.299879	1.505202	1.174674
H	1.253011	1.699129	-0.344552
H	-0.506709	2.049471	-0.344231

6

Na2CO3 SCF Done: -588.204556841 A.U.

C	0.000028	0.568173	0.000566
O	1.136052	1.168183	0.000043
O	-0.000046	-0.804218	0.001446
Na	2.163054	-0.712159	-0.000659
O	-1.135936	1.168281	-0.000261
Na	-2.163120	-0.712114	-0.000543

6

NaHCO3 SCF Done: -426.520769269 A.U.

C	0.563439	0.043807	0.000147
O	1.934961	0.097739	-0.000051
O	0.025652	-1.117835	0.000346
H	2.210477	-0.842050	0.000016
O	-0.049787	1.150988	0.000078
Na	-1.897975	-0.042538	-0.000354

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PRODa SCF Done: -707.727976592 A.U.

C	4.629468	-0.209016	0.016520
C	3.735767	0.857240	-0.127627
C	2.342758	0.614608	-0.080553
C	1.847854	-0.712656	0.111572
C	2.782126	-1.771363	0.258499
C	4.156645	-1.527972	0.211079
H	5.712864	-0.014388	-0.021730
H	2.400650	-2.794166	0.409667
H	4.870651	-2.357914	0.324665
C	0.421664	-0.899902	0.148269
H	0.051055	-1.924579	0.317696
N	1.415278	1.629064	-0.208356
C	0.013596	1.519749	-0.162331

O	-0.671890	2.540286	-0.262659
C	-0.491423	0.128876	0.005959
C	-1.954512	-0.124708	0.003629
C	-2.464520	-1.345292	-0.509283
C	-2.878990	0.817489	0.523230
C	-3.838402	-1.625525	-0.484943
H	-1.774344	-2.074709	-0.962373
C	-4.253056	0.531583	0.549055
H	-2.506832	1.779323	0.899086
C	-4.740873	-0.688227	0.049136
H	-4.208300	-2.577460	-0.898467
H	-4.951787	1.275569	0.964196
H	-5.821037	-0.904504	0.065511
H	1.740985	2.593363	-0.334900
H	4.105650	1.884415	-0.276859

31

SUBST1-2aNa SCF Done: -945.742642759 A.U.

C	4.514382	-0.182779	1.104390
C	3.631317	0.898909	0.975828
C	2.437335	0.760053	0.223661
C	2.211133	-0.483615	-0.460170
C	3.083121	-1.578211	-0.270810
C	4.237184	-1.433678	0.509519
H	5.429397	-0.056657	1.705756
H	2.857338	-2.521024	-0.794090
H	4.931094	-2.277523	0.643289
C	1.124027	-0.506068	-1.440828
H	0.925296	0.516038	-1.875404
O	0.512672	-1.497507	-1.891451
N	1.494602	1.768211	0.126983
C	0.034975	1.624035	0.015695
O	-0.557637	2.443176	-0.725333
C	-0.528213	0.531871	0.734021
H	0.135605	-0.064837	1.377170
C	-1.925124	0.154508	0.721244
C	-2.956612	0.902947	0.047039
C	-2.339731	-1.068570	1.350133
C	-4.284453	0.437026	0.003529
H	-2.677321	1.873610	-0.392597
C	-3.666336	-1.511217	1.304714
H	-1.583690	-1.666877	1.885462
C	-4.656741	-0.770479	0.622753
H	-5.046897	1.048267	-0.508471
H	-3.936811	-2.454374	1.807795
H	-5.698947	-1.123743	0.589038
H	1.806284	2.735266	0.251769

H	3.837471	1.850317	1.492055
Na	-1.507172	-0.404516	-1.707335

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SUBST1-2a SCF Done: -783.970027272 A.U.

C	4.520141	-0.143948	0.692560
C	3.626725	0.937412	0.605181
C	2.347895	0.745184	0.041834
C	1.998688	-0.538173	-0.461626
C	2.875568	-1.628175	-0.306642
C	4.145151	-1.430739	0.258955
H	5.517633	0.018233	1.131019
H	2.547265	-2.614047	-0.671600
H	4.844747	-2.274603	0.359879
C	0.711889	-0.680779	-1.178514
H	0.525558	0.124968	-1.938838
O	0.084257	-1.833290	-1.301788
N	1.396434	1.772216	-0.018964
C	-0.011141	1.658595	0.040381
O	-0.693506	2.663743	-0.138245
C	-0.540199	0.283264	0.337463
H	-0.505224	-0.950528	-0.541632
H	-0.027806	-0.169555	1.209658
C	-2.002289	0.027496	0.310184
C	-2.884802	0.699010	-0.579940
C	-2.538632	-0.993161	1.142011
C	-4.248408	0.376930	-0.605369
H	-2.493544	1.495558	-1.227662
C	-3.903510	-1.312726	1.107247
H	-1.867783	-1.531644	1.831729
C	-4.766698	-0.627187	0.234580
H	-4.918569	0.918385	-1.292230
H	-4.295676	-2.102021	1.768199
H	-5.839439	-0.875604	0.206173
H	1.719101	2.744631	-0.004155
H	3.910421	1.929076	0.992639

31

SUBST1aNaISOMER SCF Done: -945.762152279 A.U.

C	4.735601	0.348802	-0.246949
C	3.961491	-0.823451	-0.178195
C	2.570590	-0.728111	0.029911
C	1.954324	0.537934	0.189124
C	2.737336	1.695480	0.093144
C	4.125795	1.610235	-0.124499
H	5.822641	0.270383	-0.409434
H	2.212230	2.657379	0.207307
H	4.734313	2.526192	-0.194607

C	0.456148	0.605147	0.509355
H	0.364022	0.137899	1.549352
O	-0.105392	1.817529	0.410661
N	1.756460	-1.878455	0.093416
C	0.376921	-1.901833	-0.054443
O	-0.266888	-2.938491	0.109266
C	-0.213185	-0.544940	-0.436904
H	0.124739	-0.300210	-1.469425
C	-1.705797	-0.463751	-0.368499
C	-2.426114	0.226344	-1.376046
C	-2.421206	-0.891925	0.779324
C	-3.799881	0.512733	-1.231884
H	-1.891270	0.552538	-2.282900
C	-3.790146	-0.605848	0.928337
H	-1.889722	-1.454272	1.561331
C	-4.487582	0.108267	-0.069810
H	-4.336412	1.043159	-2.035907
H	-4.323183	-0.949252	1.829812
H	-5.562134	0.322257	0.045444
H	2.188989	-2.793503	0.251430
H	4.433653	-1.813232	-0.295125
Na	-2.149147	2.164276	0.525235

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SUBST1aNa SCF Done: -945.740837685 A.U.

C	-2.915970	-2.402968	0.628796
C	-1.890694	-1.451508	0.637263
C	-2.130909	-0.114174	0.216873
C	-3.456926	0.222338	-0.224408
C	-4.477903	-0.758598	-0.198556
C	-4.222920	-2.067264	0.212949
H	-2.695261	-3.426123	0.974832
H	-5.476092	-0.439329	-0.539049
H	-5.023179	-2.823180	0.215994
C	-3.806198	1.555860	-0.766379
H	-2.940978	2.272803	-0.902552
O	-4.936356	1.902603	-1.092411
N	-1.150457	0.869285	0.286305
C	0.274079	0.858044	0.261935
O	0.789034	1.968818	0.665976
C	0.996591	-0.277395	-0.164913
H	0.444486	-1.197553	-0.397734
C	2.434645	-0.340331	-0.360992
C	3.284823	0.805392	-0.559376
C	3.095638	-1.613455	-0.386728
C	4.679247	0.674397	-0.712301
H	2.809911	1.794590	-0.673321

C	4.479701	-1.731210	-0.546813
H	2.483300	-2.523643	-0.272893
C	5.296504	-0.588291	-0.692731
H	5.285667	1.579876	-0.885413
H	4.936935	-2.734620	-0.555102
H	6.386256	-0.686200	-0.814292
H	-1.470537	1.836565	0.382820
H	-0.896533	-1.723373	1.016667
Na	2.504504	1.308073	1.799062

31

SUBST1a SCF Done: -784.069080204 A.U.

C	2.966251	-2.317514	-0.068996
C	1.937005	-1.612199	0.570870
C	1.894033	-0.198669	0.524589
C	2.928420	0.496857	-0.172982
C	3.973880	-0.235847	-0.781745
C	3.995884	-1.632826	-0.745198
H	2.977851	-3.417787	-0.014143
H	4.753918	0.345199	-1.299247
H	4.809651	-2.192120	-1.231906
C	2.933925	1.977659	-0.331853
H	2.025525	2.517671	0.066992
O	3.832563	2.603343	-0.876525
N	0.884913	0.521045	1.202064
C	-0.492223	0.307042	1.332223
O	-1.137663	1.030140	2.082013
C	-1.136757	-0.809715	0.496030
H	-0.469500	-1.119910	-0.331999
H	-1.235867	-1.691158	1.169833
C	-2.501928	-0.428144	-0.047522
C	-2.689127	-0.252352	-1.434685
C	-3.603787	-0.238526	0.815122
C	-3.947698	0.100017	-1.952970
H	-1.837325	-0.396014	-2.120529
C	-4.860898	0.115052	0.298695
H	-3.467263	-0.356291	1.900552
C	-5.038054	0.284761	-1.086383
H	-4.074816	0.230331	-3.039602
H	-5.710710	0.259800	0.984922
H	-6.025822	0.559984	-1.489267
H	1.167815	1.369792	1.703987
H	1.179394	-2.158258	1.150887

31

SUBST2-3a SCF Done: -784.016171447 A.U.

C	4.534672	0.064063	0.641424
C	3.676171	-0.973662	0.264667

C	2.306556	-0.707243	0.013388
C	1.818800	0.627149	0.137188
C	2.707665	1.655437	0.531970
C	4.056241	1.385510	0.786010
H	5.595822	-0.159545	0.835197
H	2.317743	2.681670	0.630656
H	4.737850	2.193219	1.092276
C	0.405792	0.889934	-0.162494
H	-0.002928	1.803920	0.300439
O	0.269189	1.411488	-1.852825
N	1.420845	-1.710896	-0.324308
C	0.005057	-1.616473	-0.373711
O	-0.634791	-2.663769	-0.488014
C	-0.541947	-0.242850	-0.337321
H	1.137364	1.229618	-2.281738
H	-0.331044	0.307556	-1.633283
C	-1.990040	0.003186	-0.014005
C	-2.836957	-1.003130	0.513542
C	-2.550085	1.290772	-0.224014
C	-4.173462	-0.720473	0.839481
H	-2.437513	-2.016609	0.650346
C	-3.885868	1.569100	0.105743
H	-1.941304	2.085706	-0.684548
C	-4.707902	0.564806	0.644949
H	-4.805784	-1.522671	1.253774
H	-4.289007	2.579049	-0.073548
H	-5.757772	0.779538	0.900424
H	1.754486	-2.678932	-0.364168
H	4.052836	-2.004757	0.170139

31

SUBST2aNa SCF Done: -945.762152155 A.U.

C	4.735475	-0.349458	0.247578
C	3.961674	0.823004	0.178629
C	2.570809	0.727957	-0.029766
C	1.954329	-0.538001	-0.189095
C	2.736989	-1.695755	-0.092889
C	4.125426	-1.610767	0.125134
H	5.822504	-0.271326	0.410279
H	2.211702	-2.657529	-0.207218
H	4.733812	-2.526799	0.195445
C	0.456269	-0.604784	-0.510278
H	0.364832	-0.136519	-1.549894
O	-0.105678	-1.816959	-0.412935
N	1.756768	1.878306	-0.093424
C	0.377106	1.901930	0.054076
O	-0.266396	2.938675	-0.110007

C	-0.213108	0.545135	0.436736
H	0.125261	0.300298	1.469070
C	-1.705618	0.463814	0.368918
C	-2.422083	0.893279	-0.777722
C	-2.424880	-0.228166	1.376011
C	-3.791057	0.606723	-0.926054
H	-1.891529	1.456997	-1.559358
C	-3.798601	-0.514950	1.232556
H	-1.889147	-0.555469	2.281930
C	-4.487420	-0.109124	0.071555
H	-4.324862	0.951216	-1.826664
H	-4.334188	-1.046851	2.036227
H	-5.561974	-0.323373	-0.043172
H	2.189230	2.793326	-0.251856
H	4.434024	1.812686	0.295626
Na	-2.150210	-2.162141	-0.527749

31

SUBST2a SCF Done: -784.085488044 A.U.

C	-4.624832	-0.047555	-0.124859
C	-3.704460	1.011647	-0.177660
C	-2.327302	0.755573	-0.012114
C	-1.871528	-0.567353	0.217638
C	-2.807184	-1.613678	0.261053
C	-4.180632	-1.364291	0.086924
H	-5.698163	0.161799	-0.256603
H	-2.435539	-2.632860	0.450207
H	-4.902117	-2.195001	0.125199
C	-0.385028	-0.791435	0.465738
H	-0.167099	-0.569424	1.537793
O	0.010118	-2.139461	0.293524
N	-1.385753	1.797179	-0.056258
C	-0.010922	1.654699	-0.201862
O	0.728771	2.630202	-0.218635
C	0.458094	0.196172	-0.400179
H	-0.148135	-2.370539	-0.643988
H	0.206719	-0.034467	-1.465061
C	1.951236	0.016239	-0.210486
C	2.600770	0.482253	0.953024
C	2.711626	-0.678212	-1.172844
C	3.972492	0.255389	1.147128
H	2.031842	1.043273	1.711020
C	4.085100	-0.907764	-0.982466
H	2.220967	-1.042062	-2.091413
C	4.719814	-0.441759	0.180813
H	4.463805	0.631095	2.058899
H	4.661182	-1.451355	-1.748296

H	5.796668	-0.617226	0.333454
H	-1.714361	2.767809	-0.041095
H	-4.050076	2.043229	-0.354504

33

SUBSTaNa SCF Done: -946.958525523 A.U.

C	4.099135	-1.142221	-1.138305
C	3.125427	-1.517705	-0.196011
C	2.308667	-0.540938	0.400105
C	2.445081	0.834217	0.082464
C	3.428662	1.183987	-0.864918
C	4.248737	0.214977	-1.471104
H	4.737437	-1.907216	-1.608166
H	3.547605	2.248823	-1.130045
H	5.007112	0.521174	-2.210108
C	1.540668	1.890020	0.746060
H	1.877812	1.926883	1.834837
H	1.876158	2.889021	0.337618
O	0.204212	1.649841	0.588653
N	1.324320	-0.942048	1.378896
C	-0.027465	-0.907402	1.134333
O	-0.852807	-0.804466	2.066177
C	-0.475479	-1.230193	-0.301833
H	0.273545	-0.850349	-1.021401
H	-0.469303	-2.341265	-0.380407
C	-1.857010	-0.699266	-0.619323
C	-2.013868	0.576033	-1.213706
C	-3.015387	-1.432445	-0.277335
C	-3.298717	1.098653	-1.458212
H	-1.109851	1.171642	-1.422542
C	-4.298588	-0.911747	-0.524288
H	-2.907982	-2.423274	0.192605
C	-4.445242	0.356481	-1.115266
H	-3.402571	2.090634	-1.927576
H	-5.189536	-1.501163	-0.254077
H	-5.450017	0.762976	-1.313527
H	1.528411	-0.668244	2.348762
H	2.988947	-2.572019	0.092970
Na	-1.634270	1.259001	1.497653

33

SUBSTa SCF Done: -785.268035244 A.U.

C	4.187921	-0.575195	-0.972710
C	3.158916	-1.341769	-0.405906
C	2.098500	-0.724649	0.292786
C	2.077659	0.686981	0.442528
C	3.103729	1.444033	-0.160762
C	4.151238	0.825606	-0.860286

H	5.008255	-1.071495	-1.514809
H	3.060809	2.539804	-0.068313
H	4.943541	1.439489	-1.317217
C	1.016176	1.394567	1.261359
H	0.103491	0.764071	1.345441
H	1.408098	1.519887	2.303739
O	0.732952	2.658710	0.666418
H	0.106377	3.121346	1.253489
N	1.076839	-1.550966	0.864712
C	-0.222244	-1.778477	0.423327
O	-0.930428	-2.613624	0.978874
C	-0.704115	-0.972082	-0.795067
H	0.053702	-0.235315	-1.123940
H	-0.795712	-1.720954	-1.613446
C	-2.046314	-0.294995	-0.575720
C	-2.143007	1.113613	-0.538861
C	-3.220514	-1.061476	-0.401449
C	-3.387114	1.741219	-0.343589
H	-1.232708	1.727370	-0.649362
C	-4.460677	-0.433067	-0.202864
H	-3.148465	-2.159470	-0.405330
C	-4.550234	0.970631	-0.177353
H	-3.446460	2.841771	-0.324853
H	-5.366863	-1.045783	-0.069285
H	-5.525279	1.461805	-0.028555
H	1.359189	-2.217561	1.592683
H	3.154449	-2.438523	-0.508166

Part 4: References.

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Part 5: NMR spectra of the amido-alcohols.

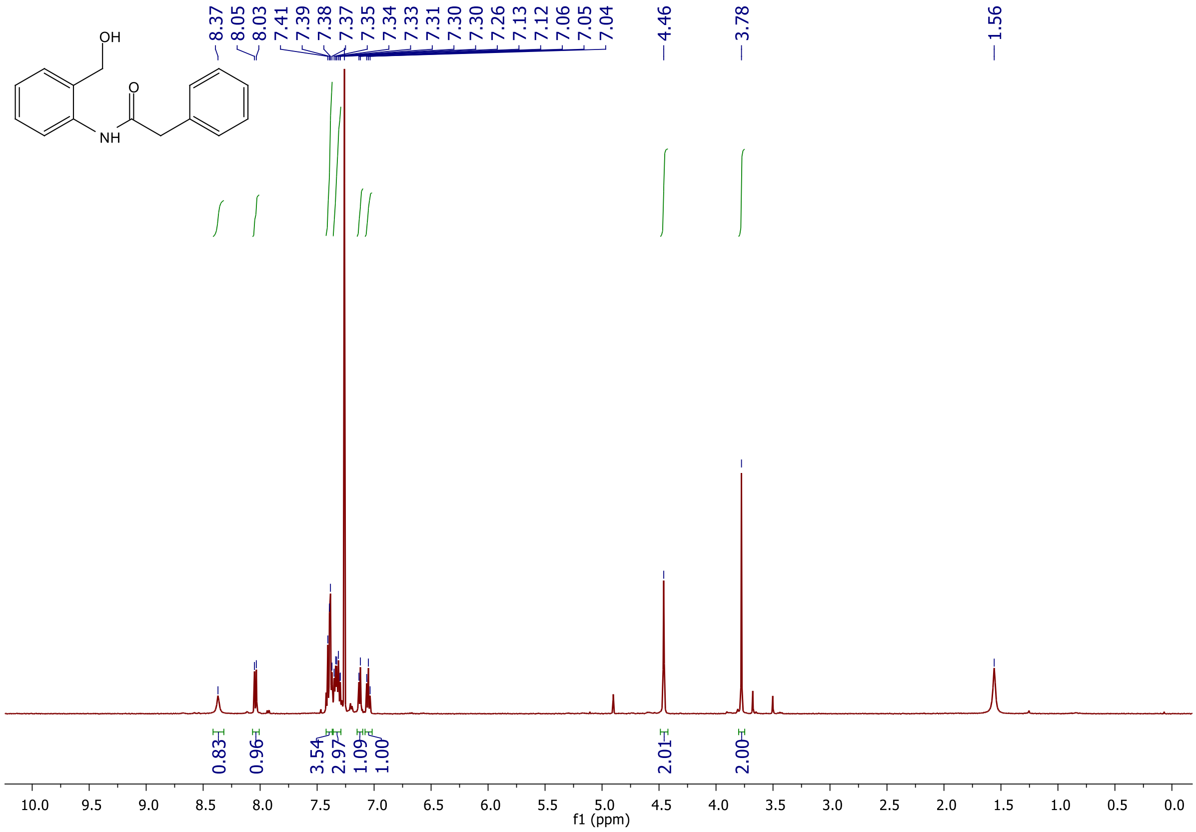


Figure S1: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1a.

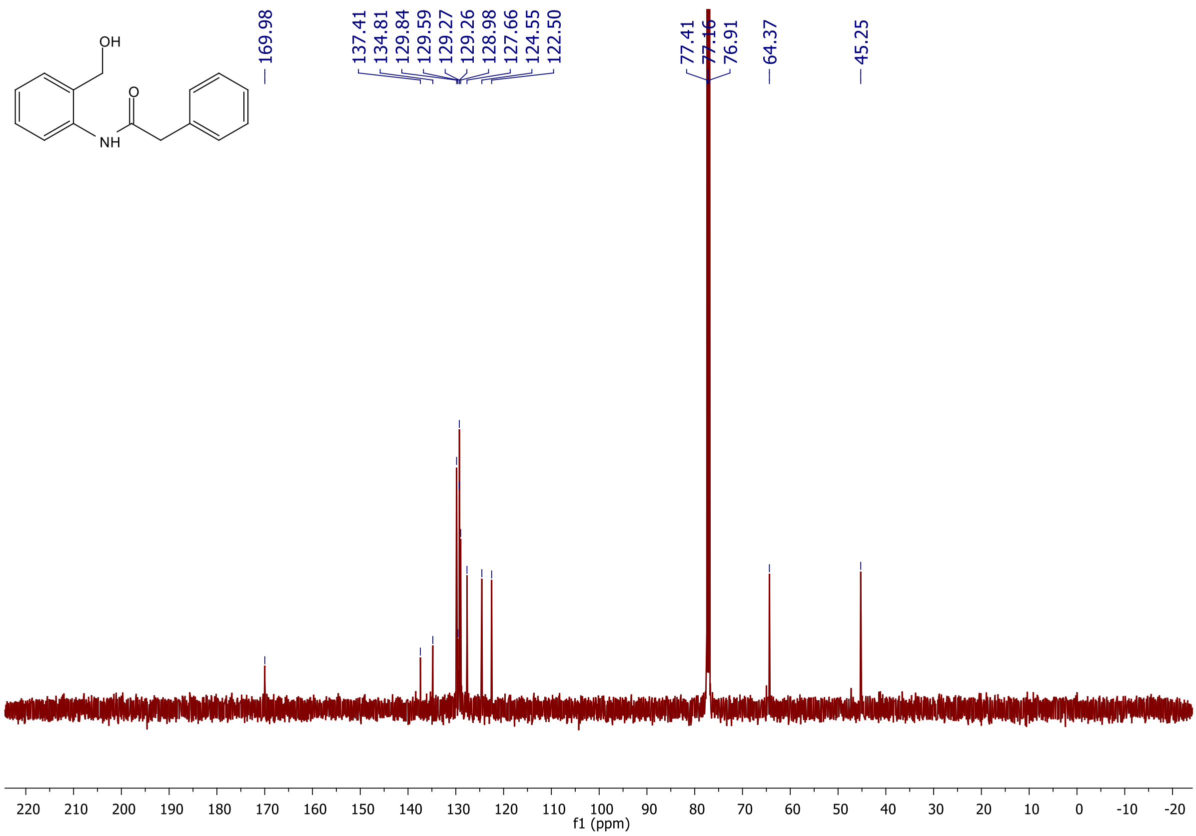


Figure S2: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1a.

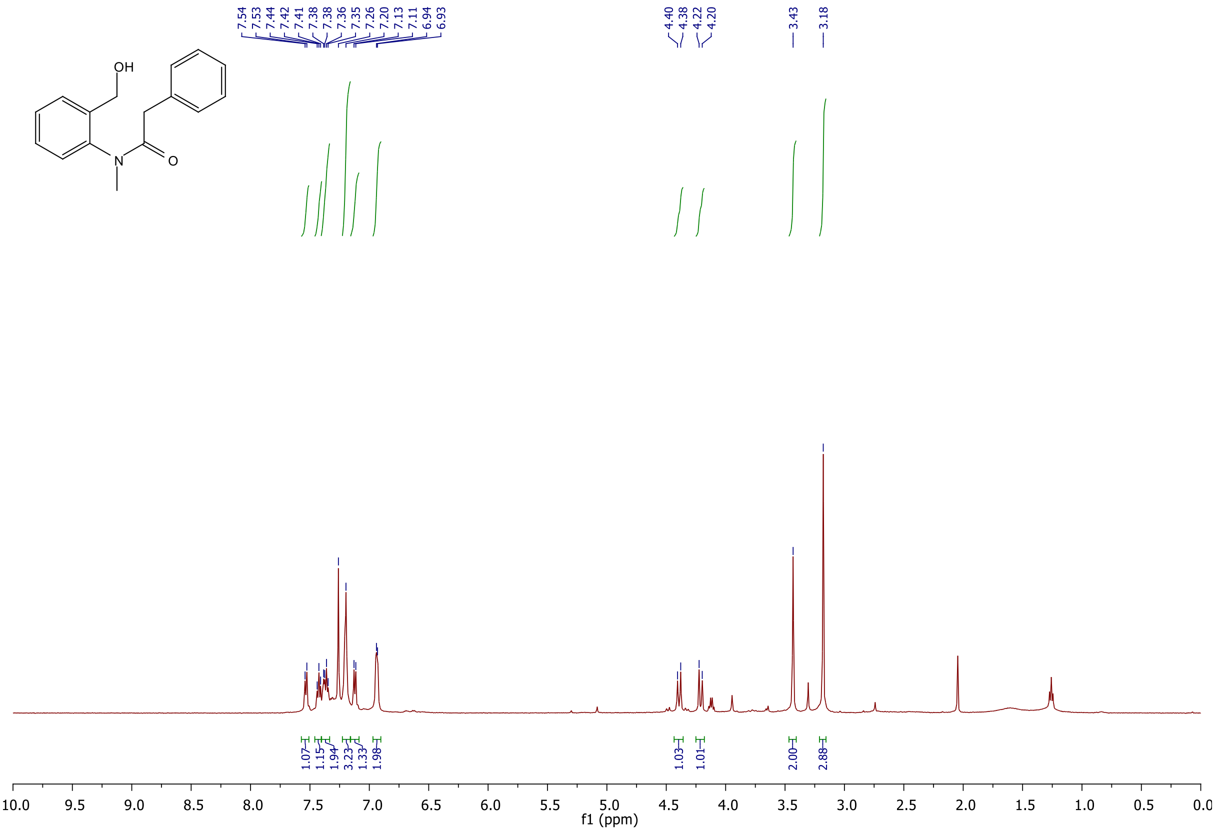


Figure S3: ^1H-NMR (500 MHz) in $CDCl_3$ of 1b.

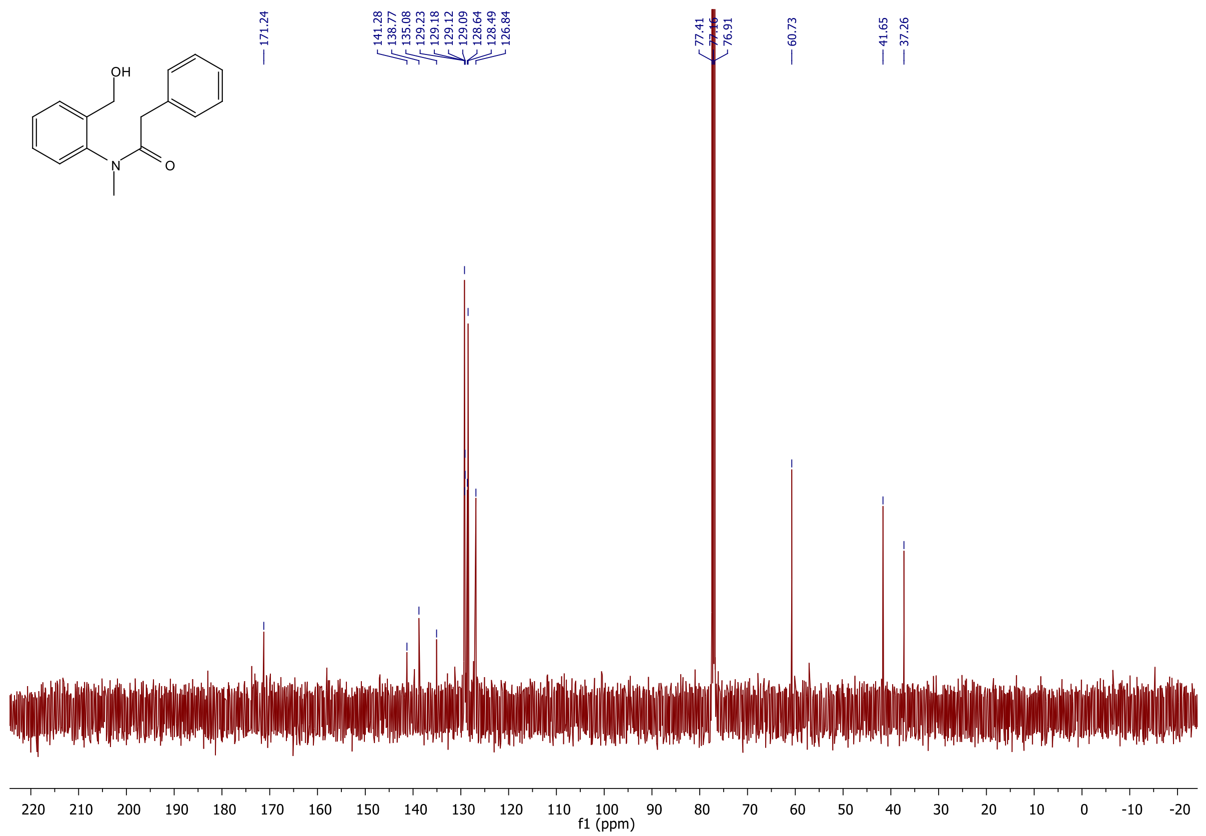


Figure S4: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1b.

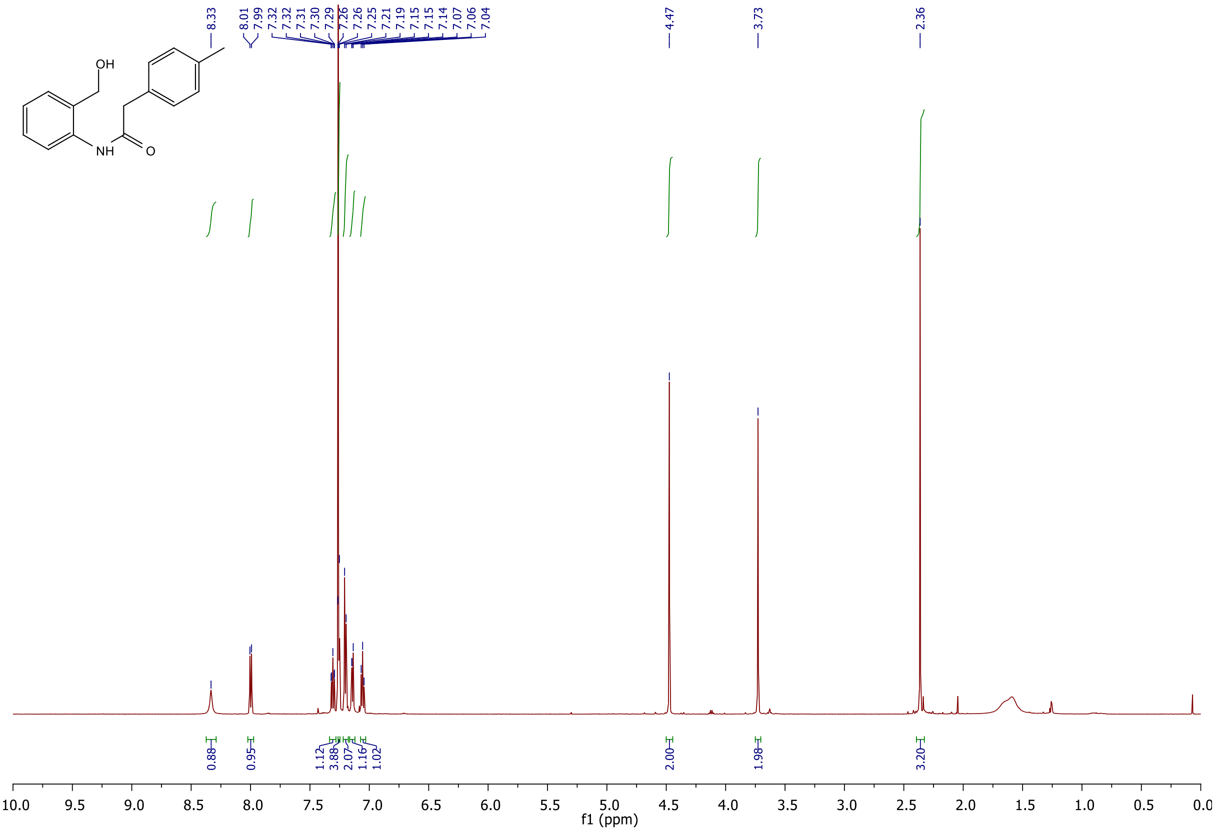


Figure S5: ^1H-NMR (500 MHz) in $CDCl_3$ of 1c.

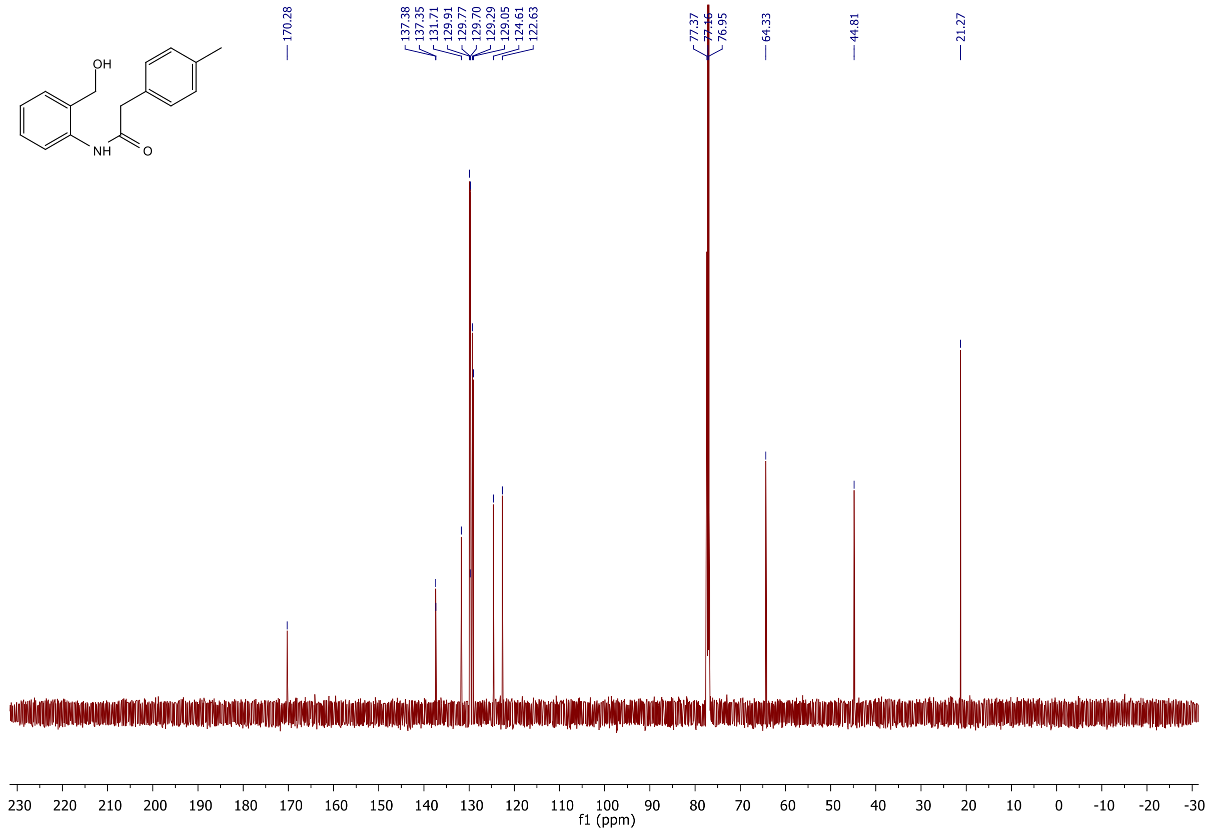


Figure S6: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1c.

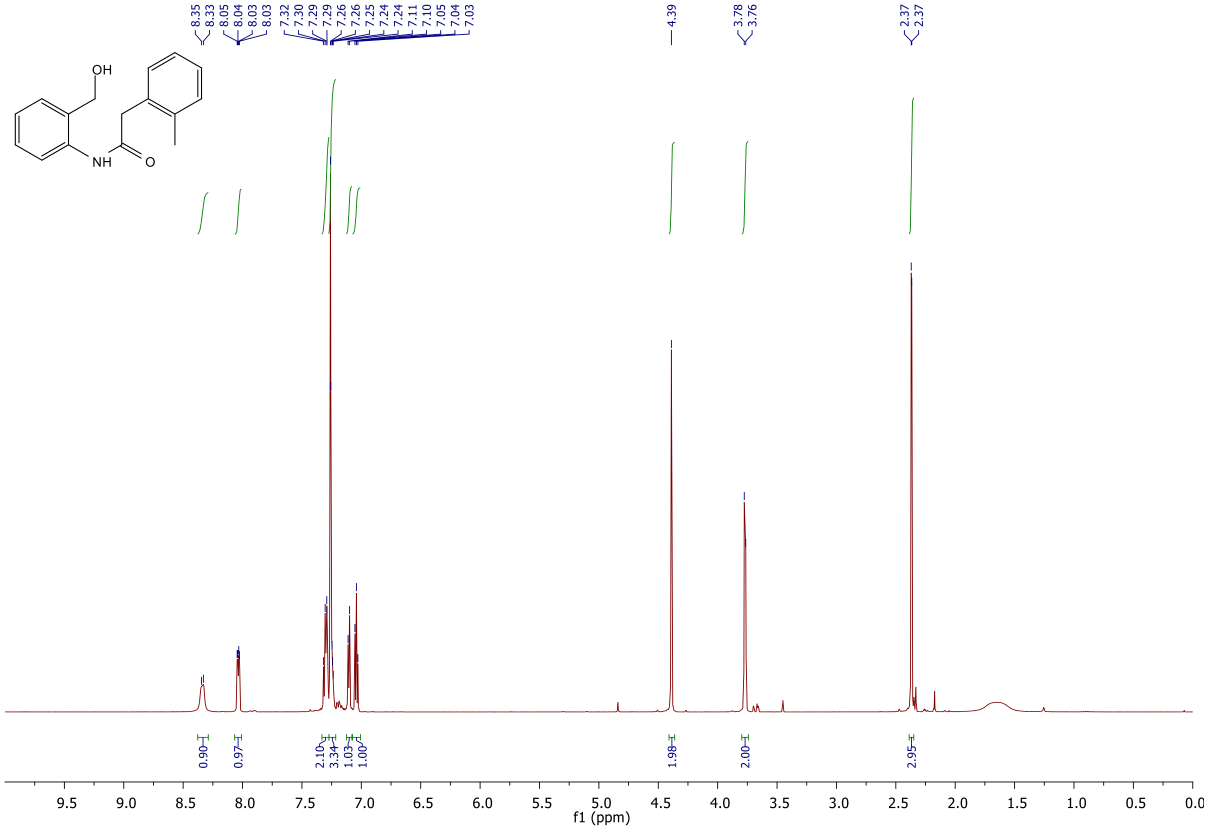


Figure S7: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1d.

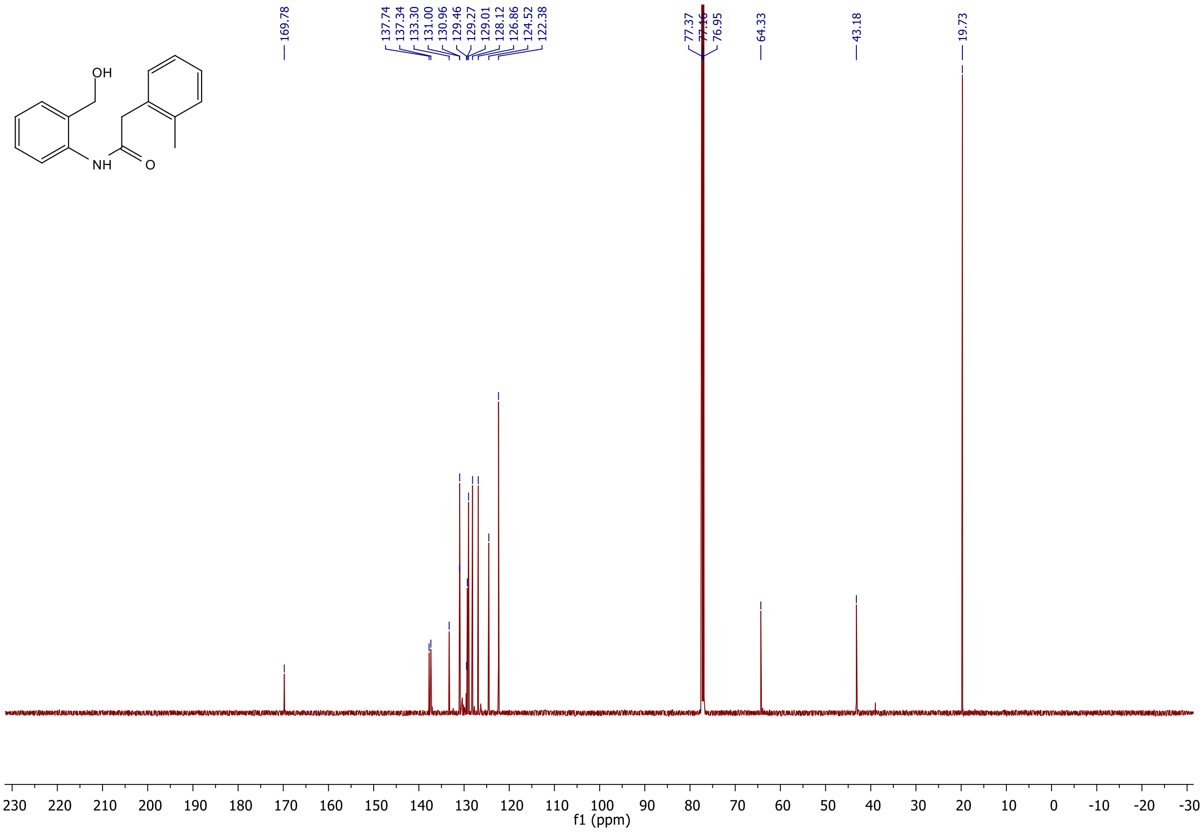


Figure S8: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1d.

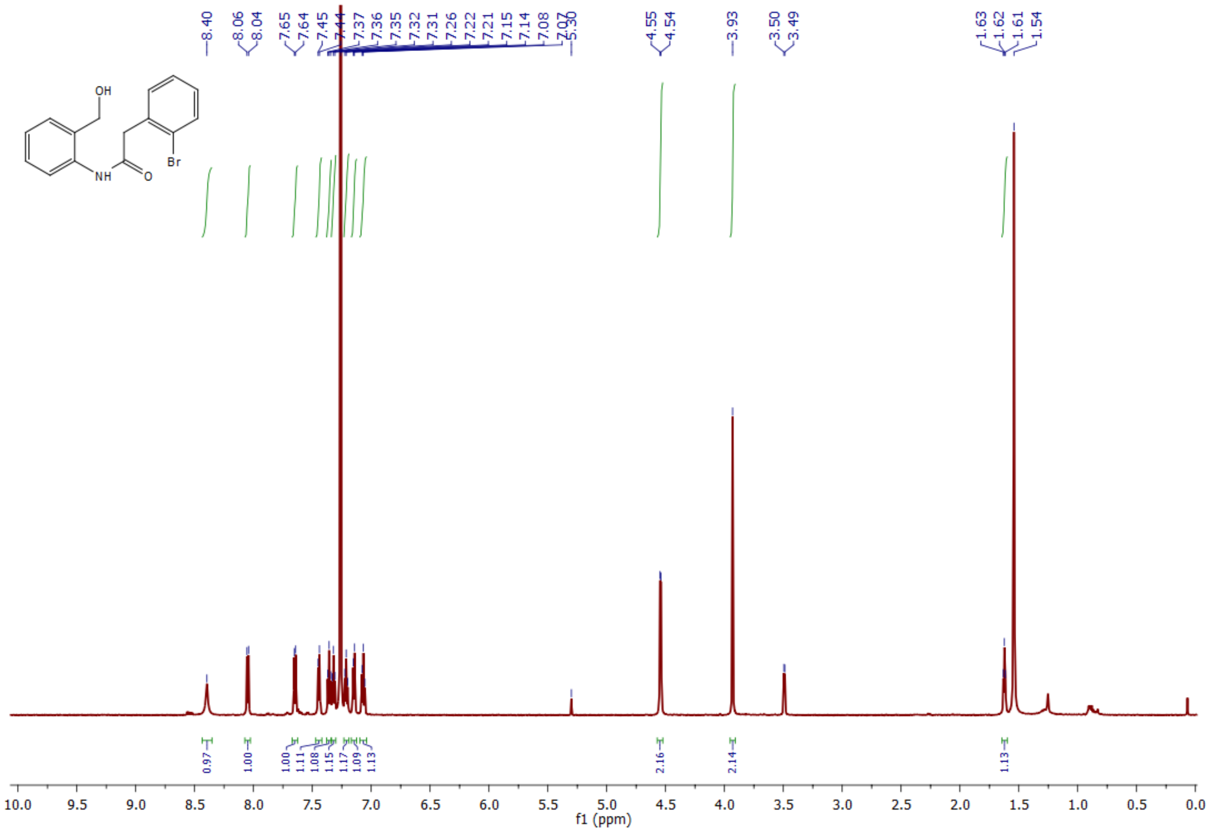


Figure S9: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1e.

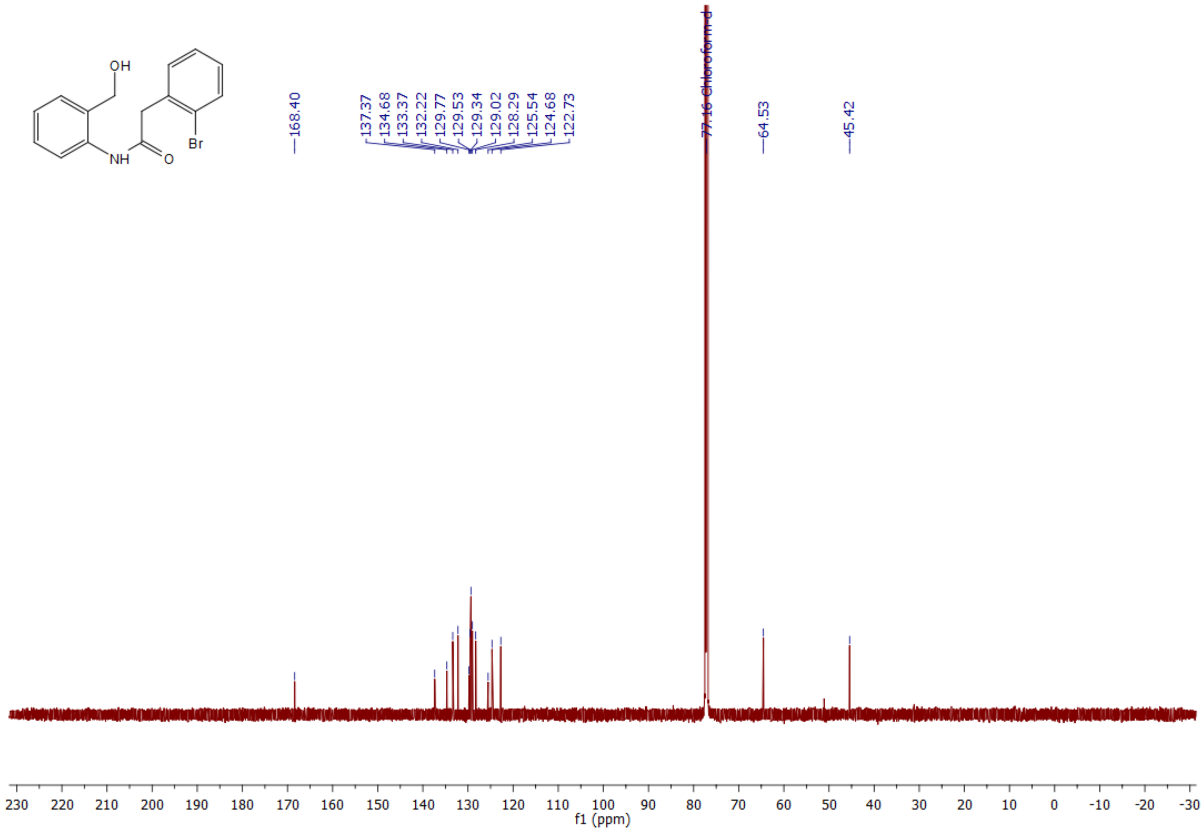


Figure S10: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1e.

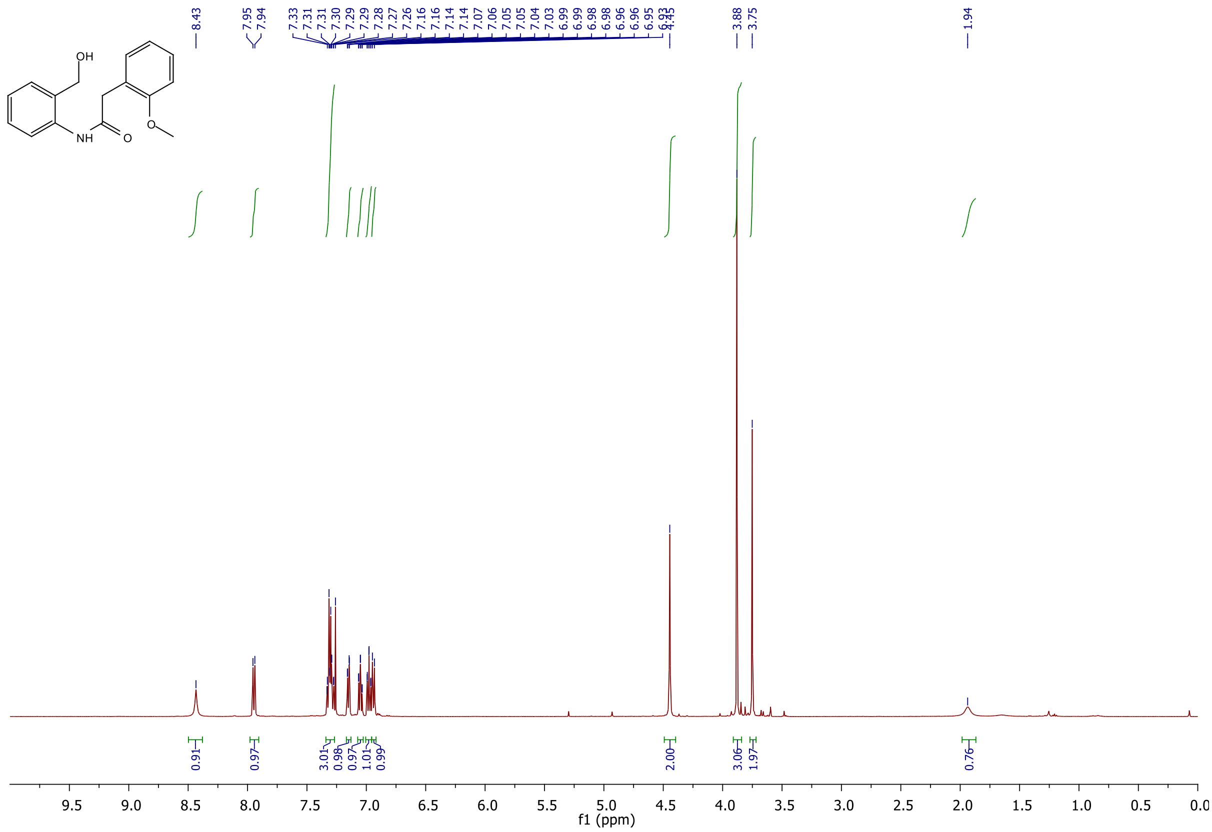


Figure S11: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1f.

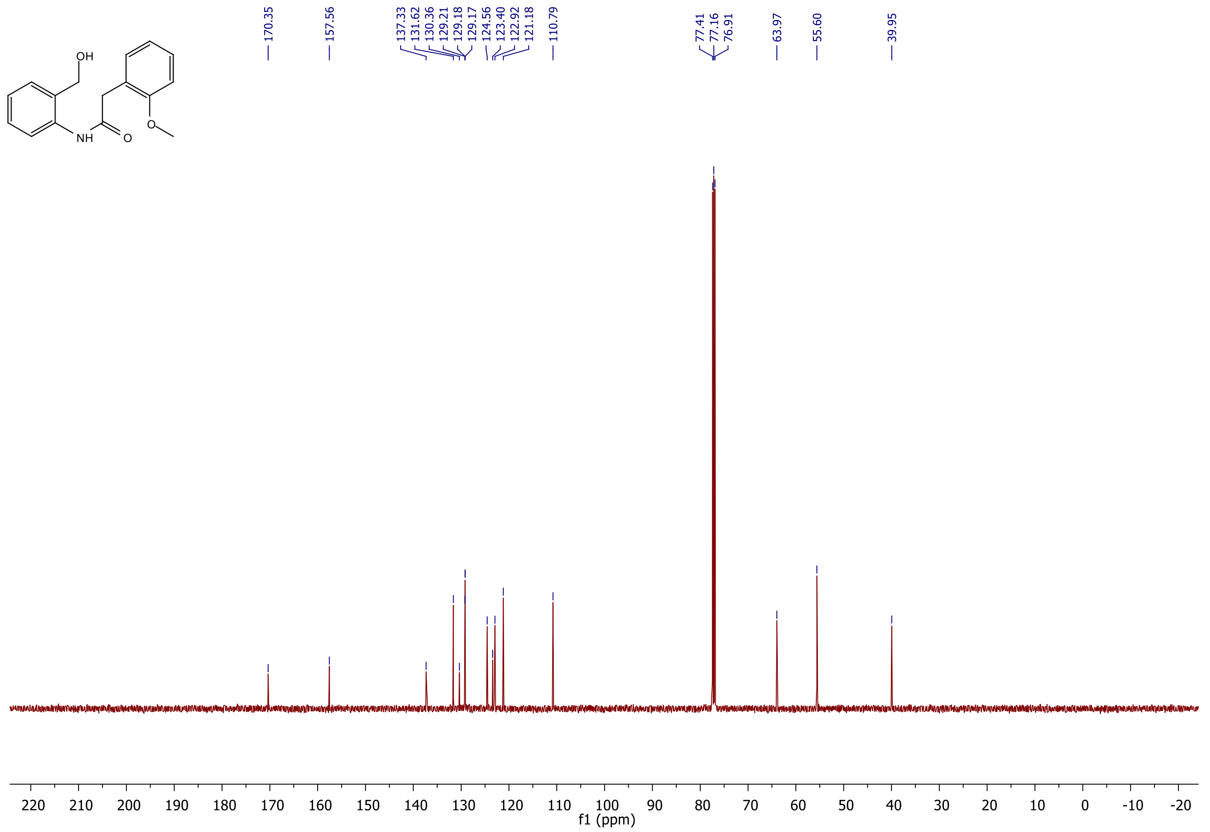


Figure S12: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1f.

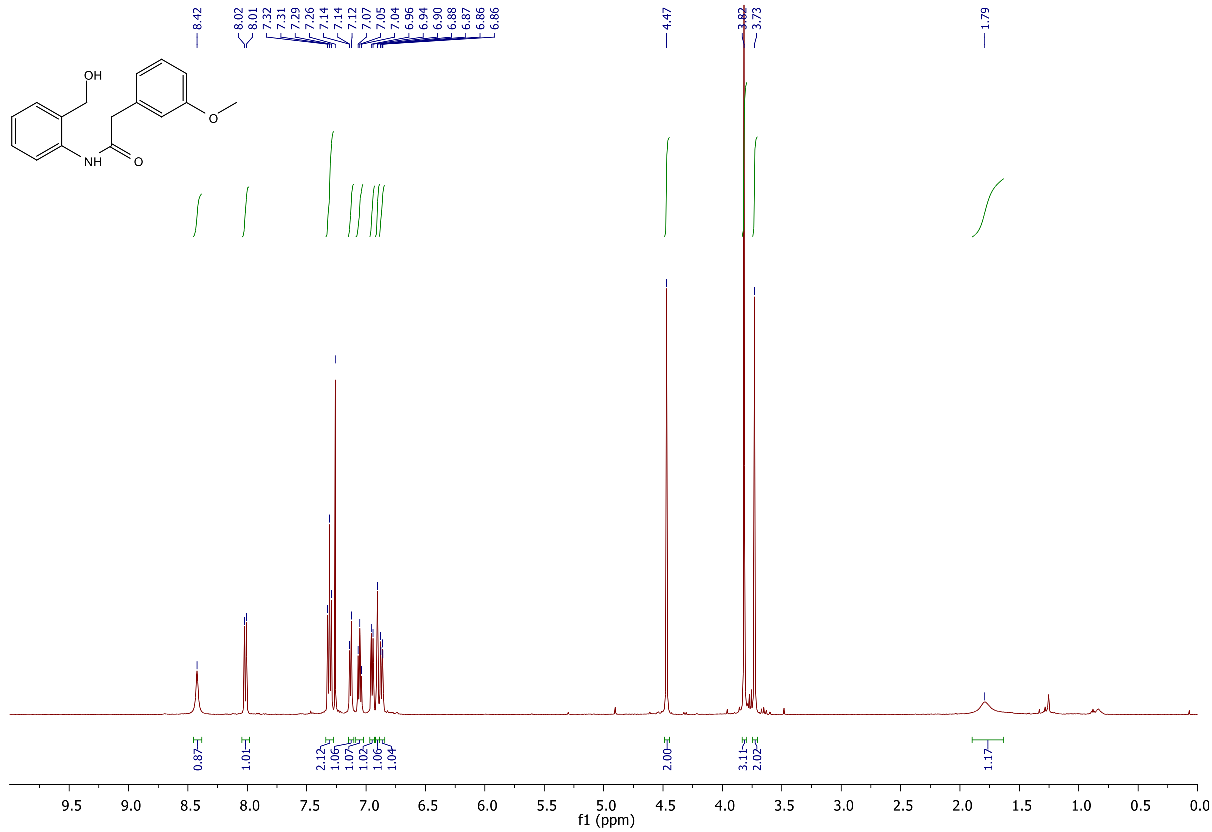


Figure S13: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1g.

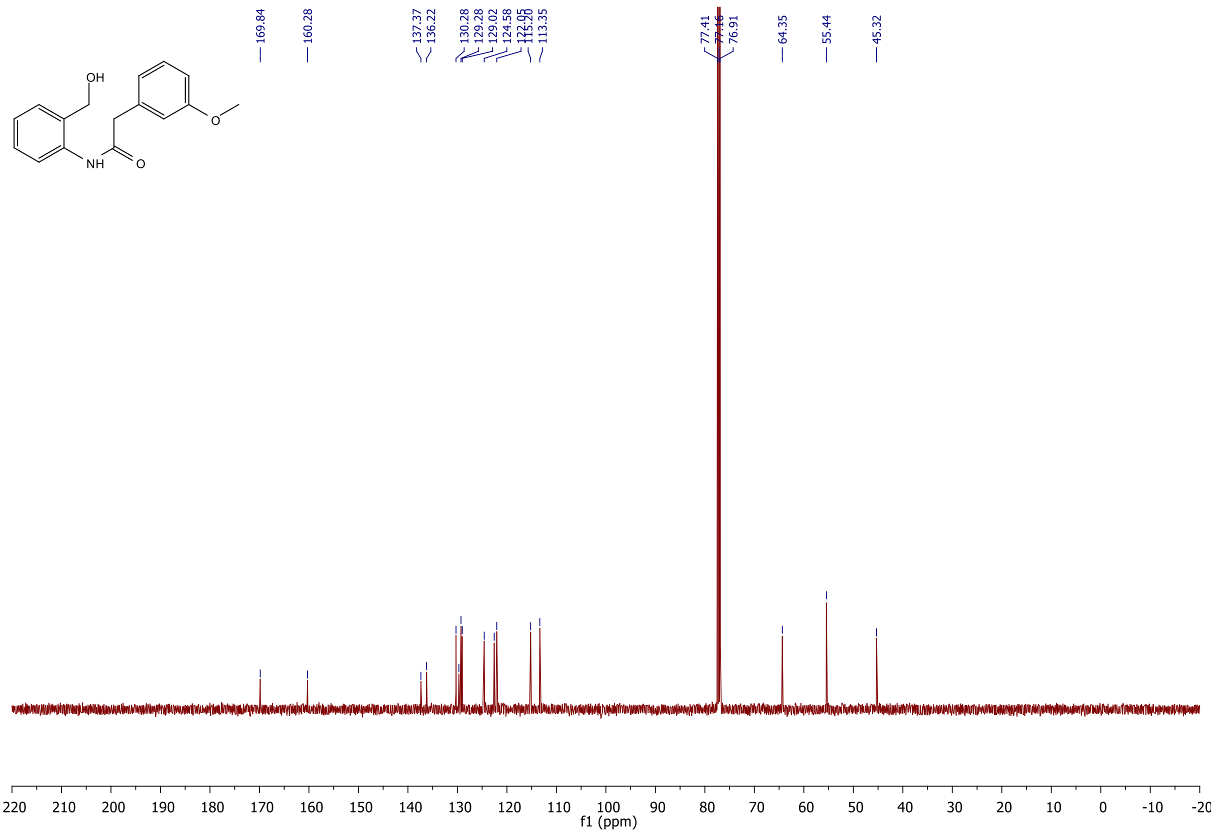


Figure S14: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1g.

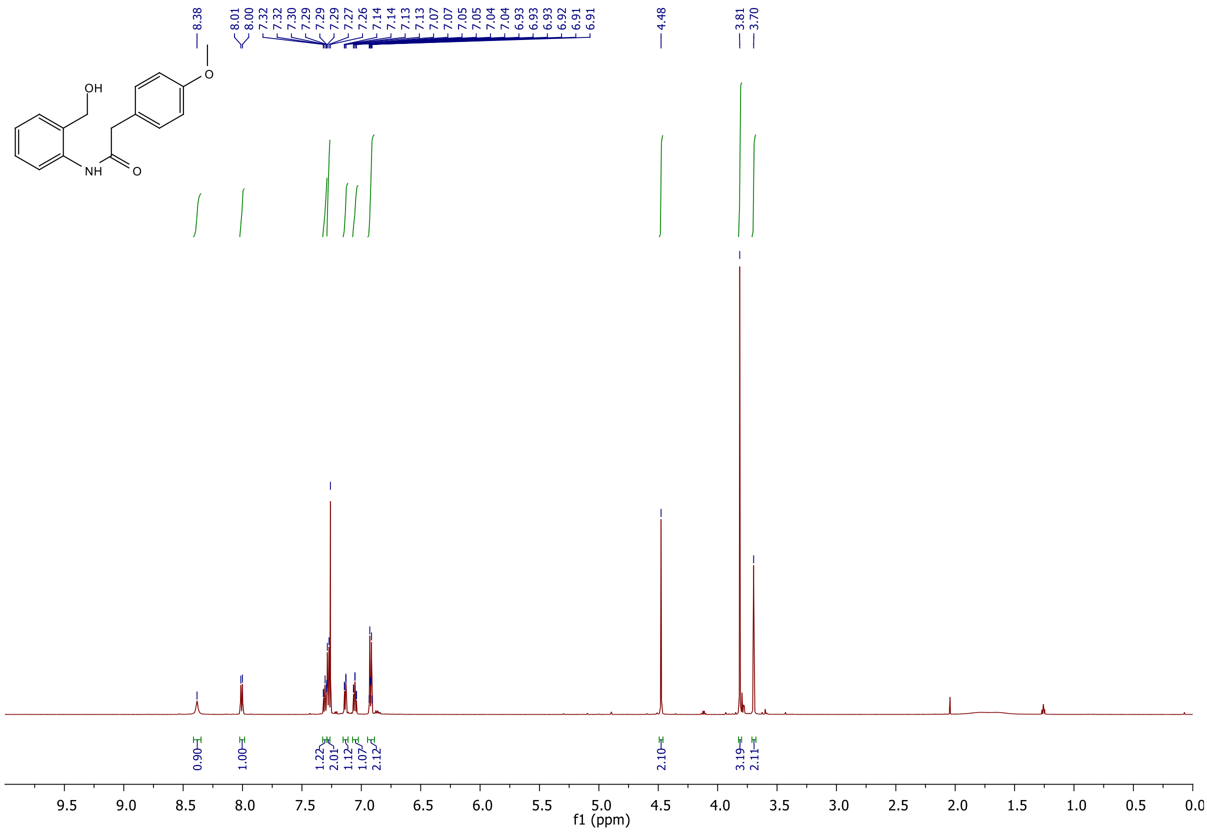


Figure S15: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1h.

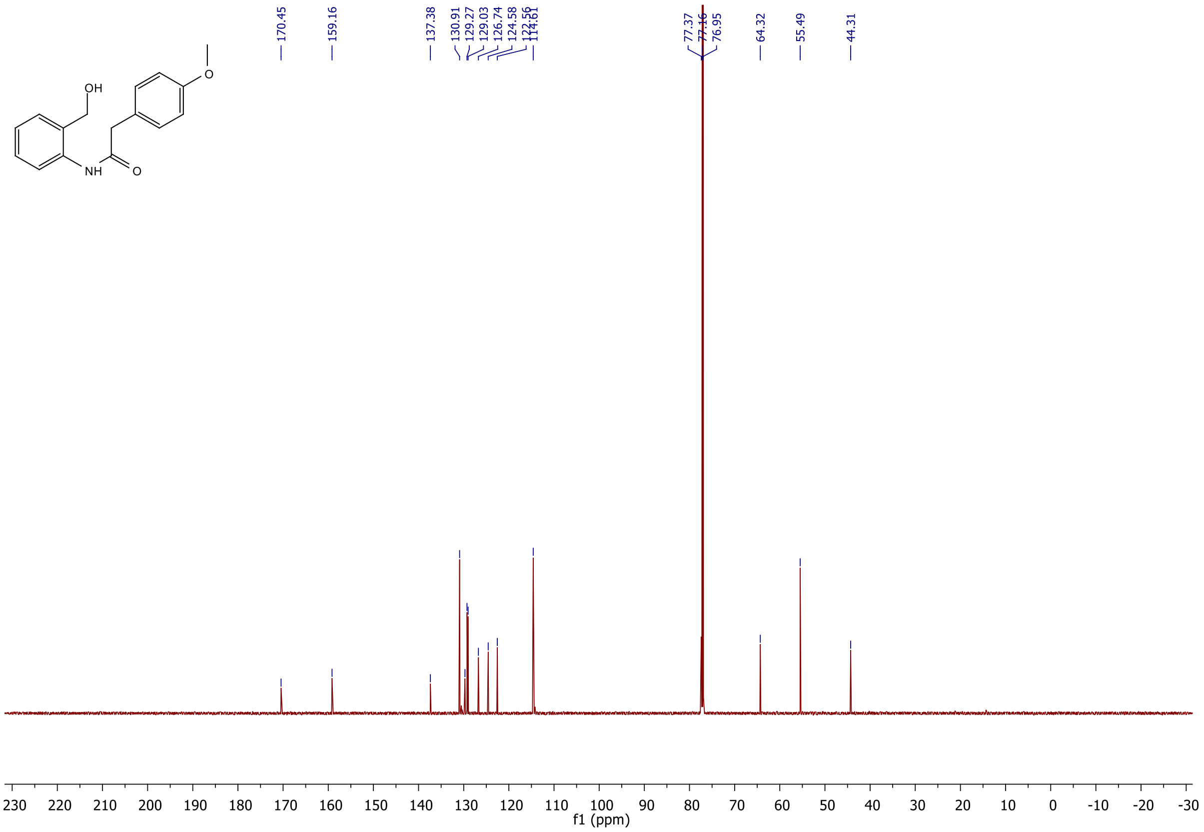


Figure S16: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1h.

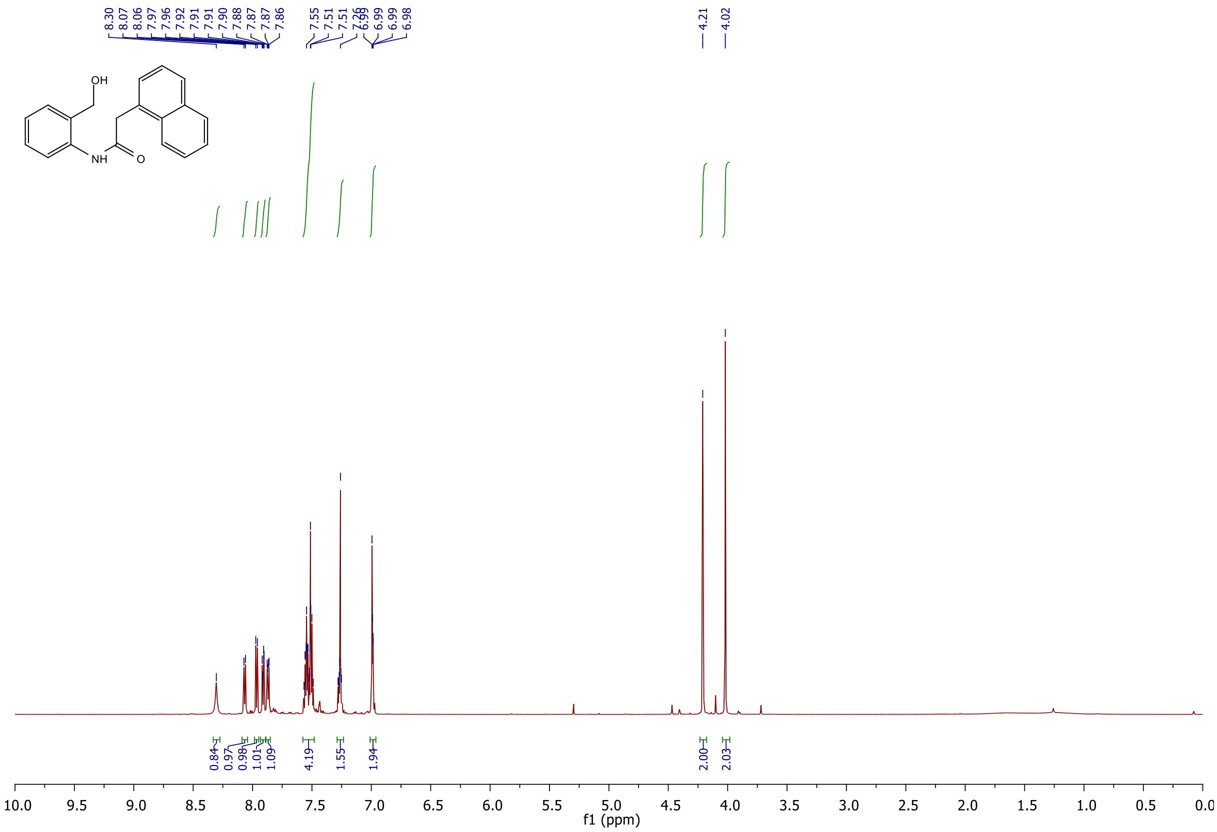


Figure S17: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1i.

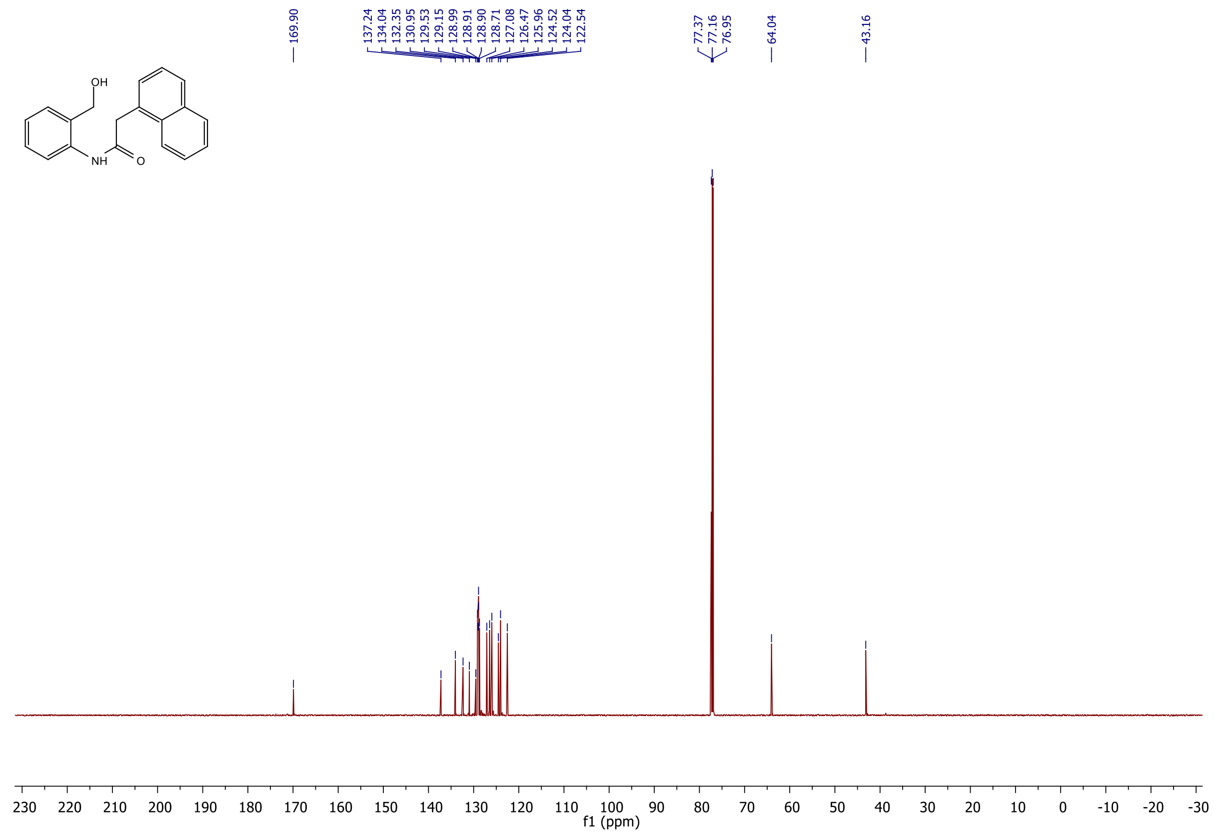


Figure S18: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1i.

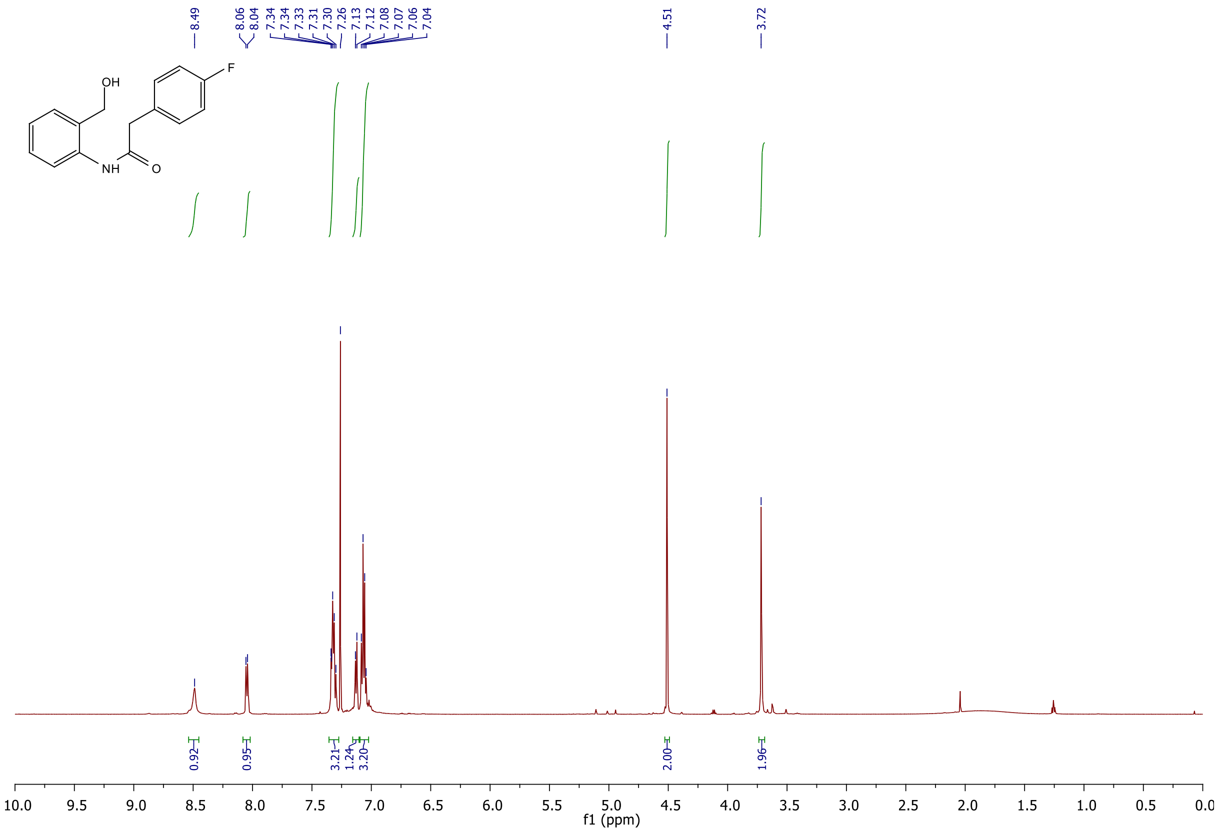


Figure S19: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1j.

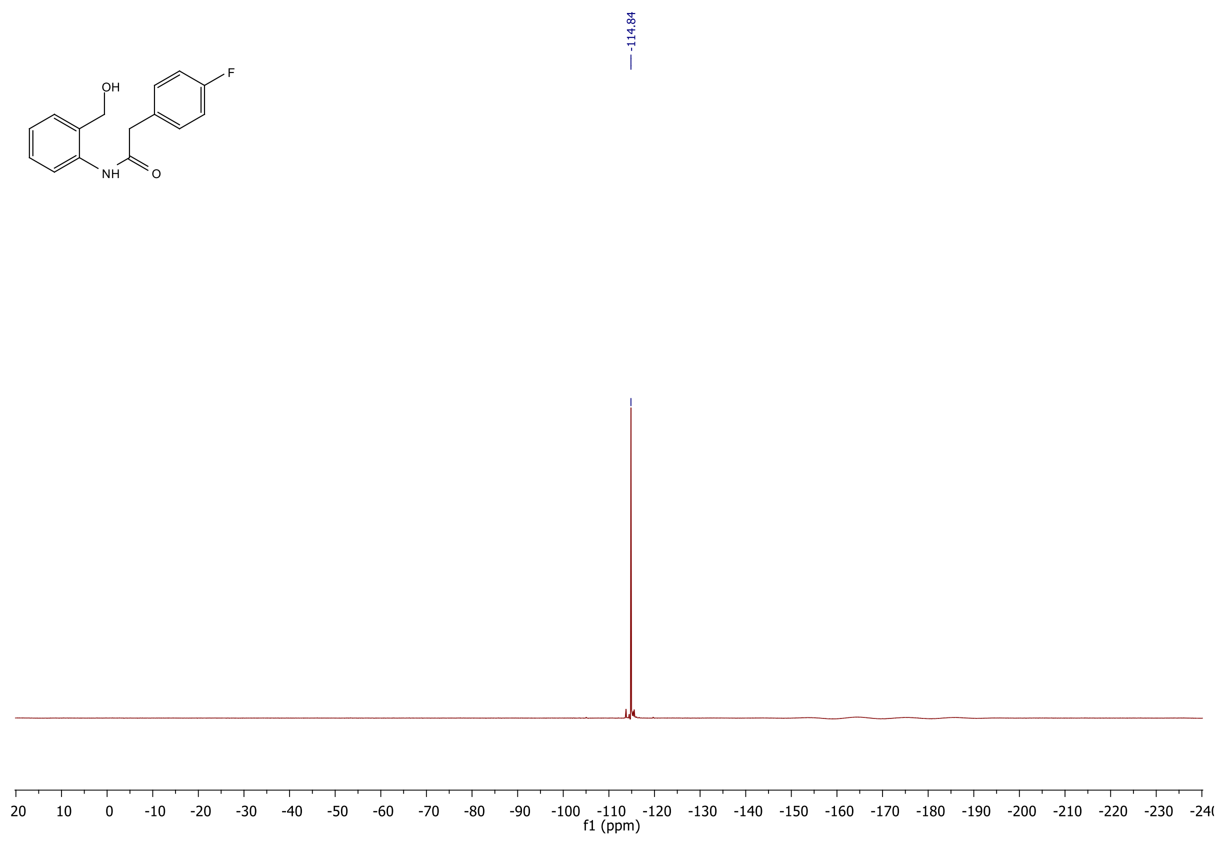


Figure S20: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 1j.

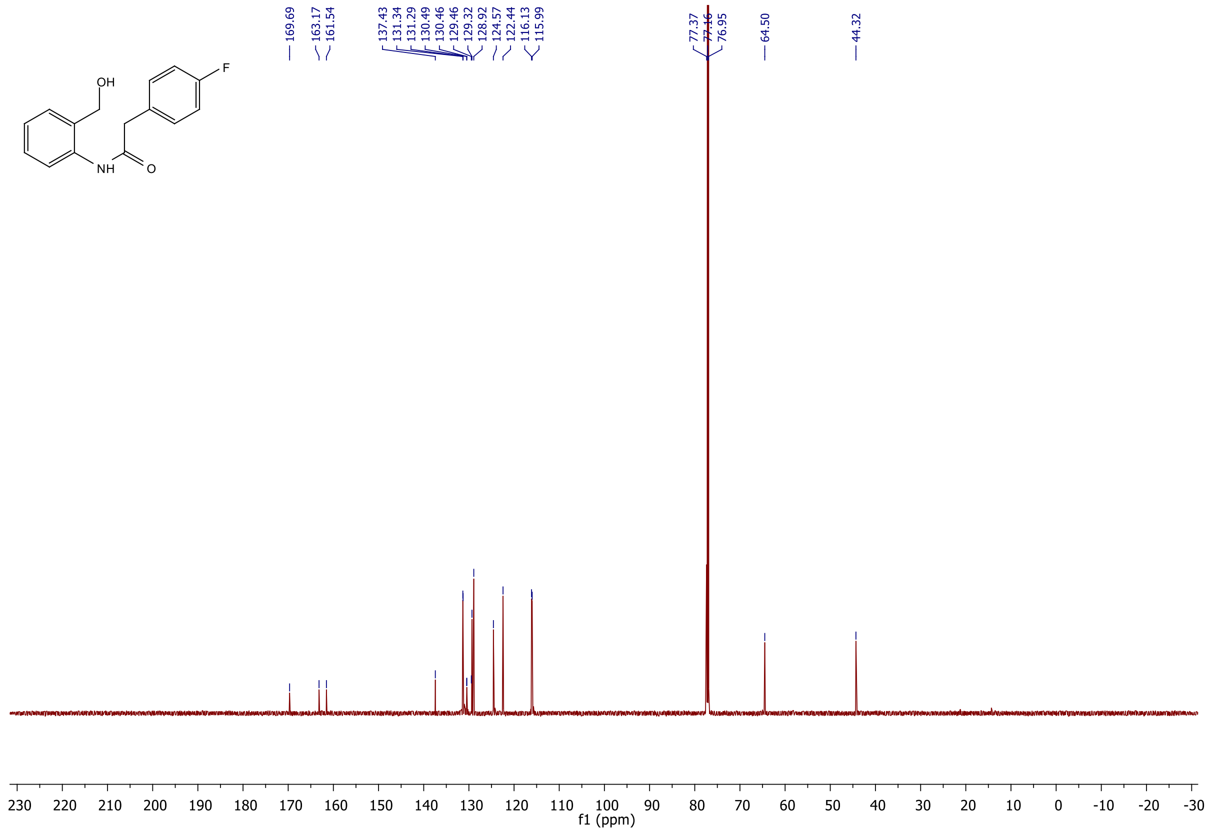


Figure S21: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1j.

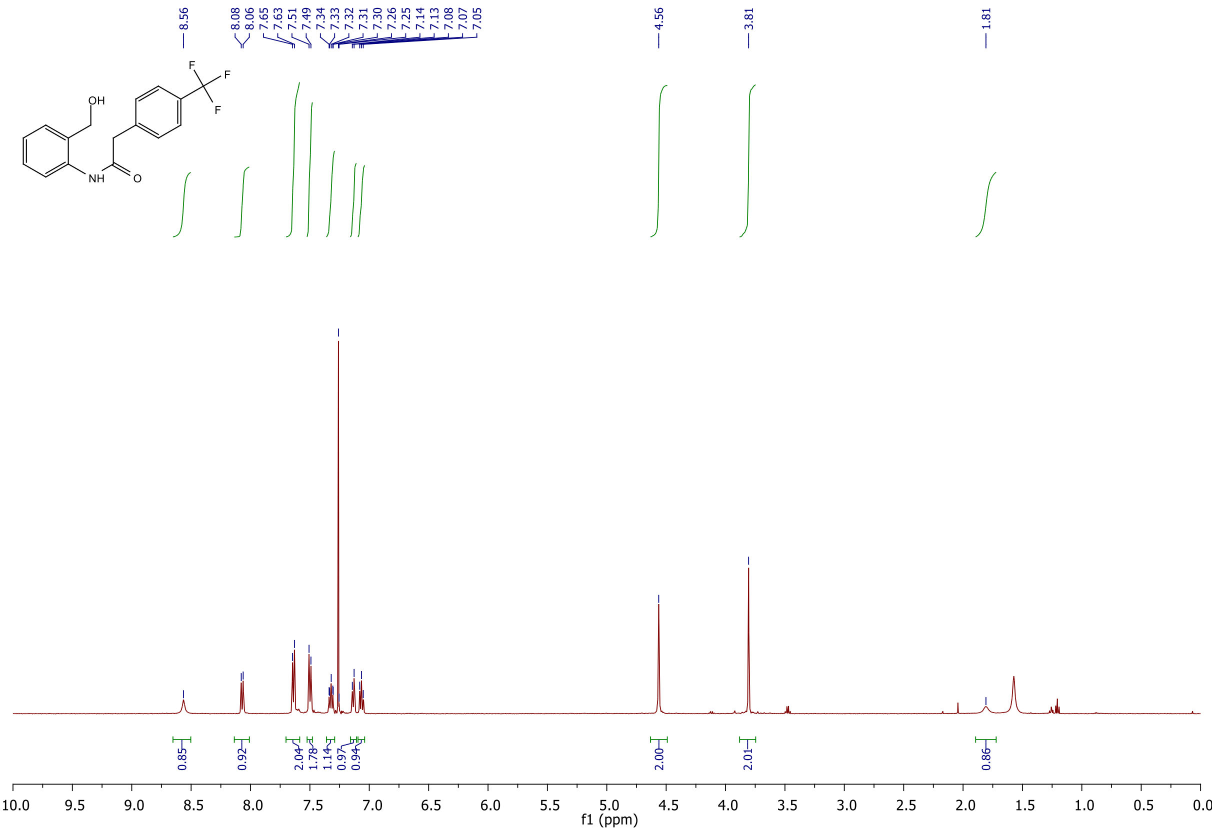


Figure S22: ^1H-NMR (500 MHz) in $CDCl_3$ of 1k.

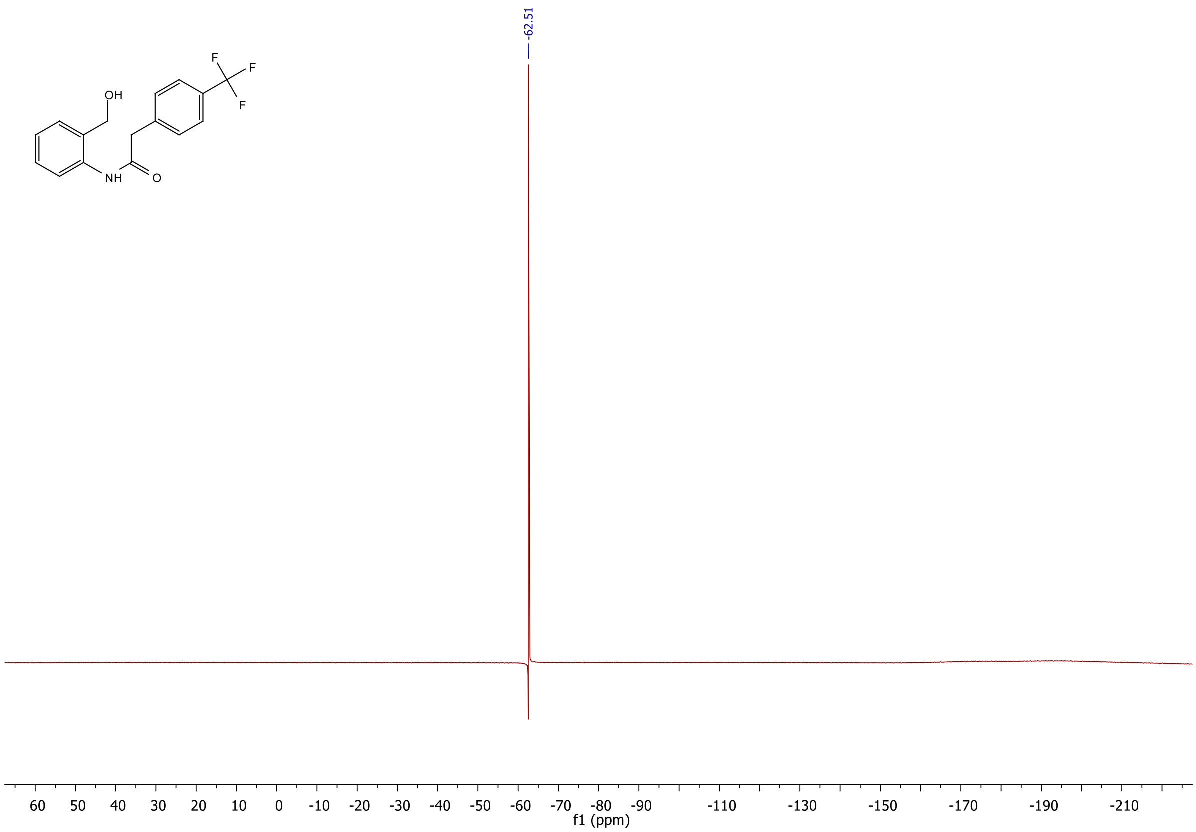


Figure S23: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 1k.

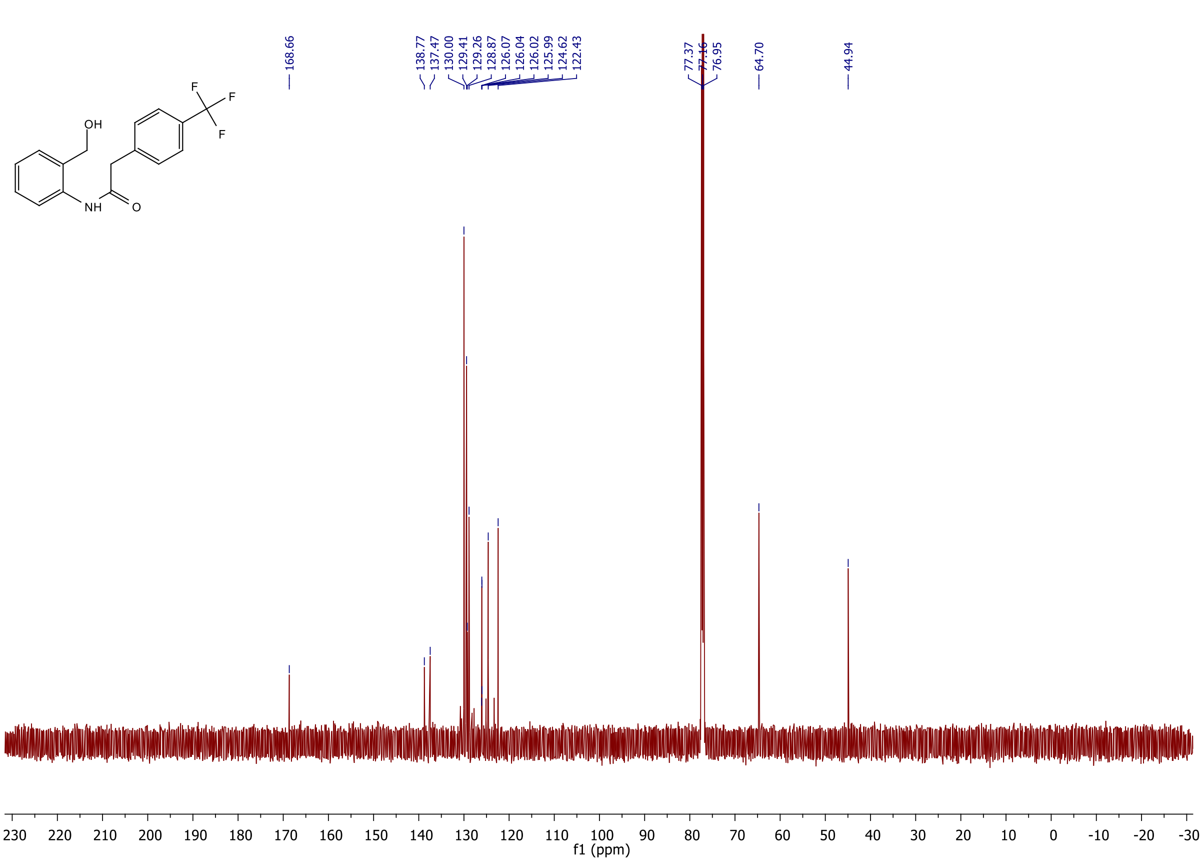


Figure S24: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1k.

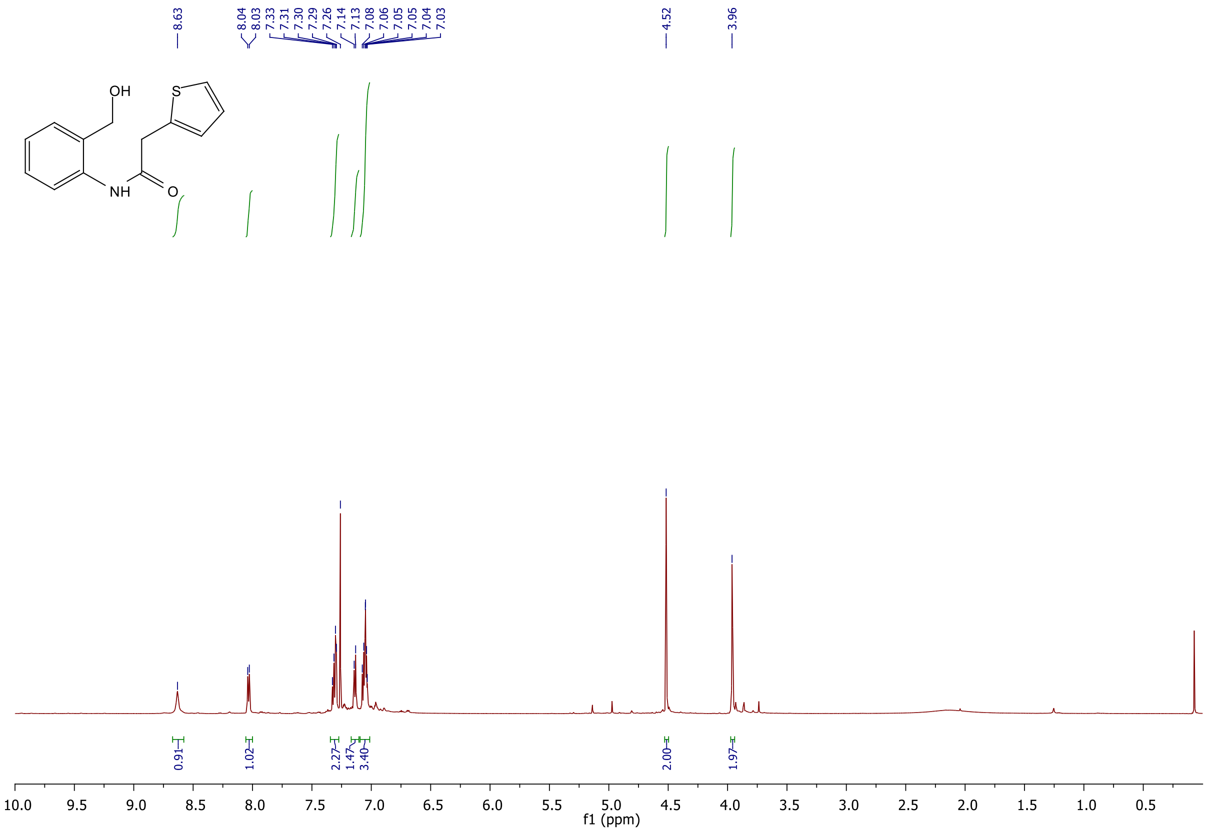


Figure S25: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1l.

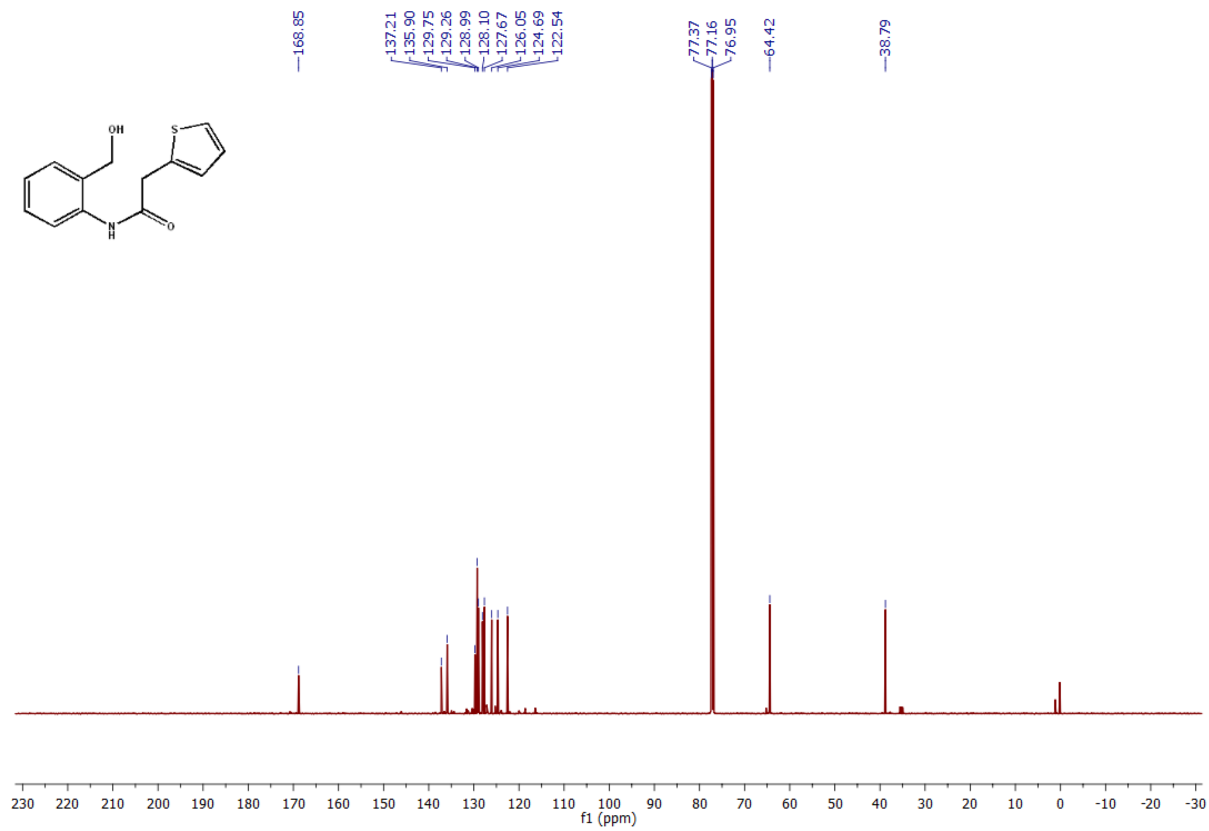


Figure S26: ^{13}C{^{1}H} NMR (125 MHz) in $CDCl_3$ of 1l.

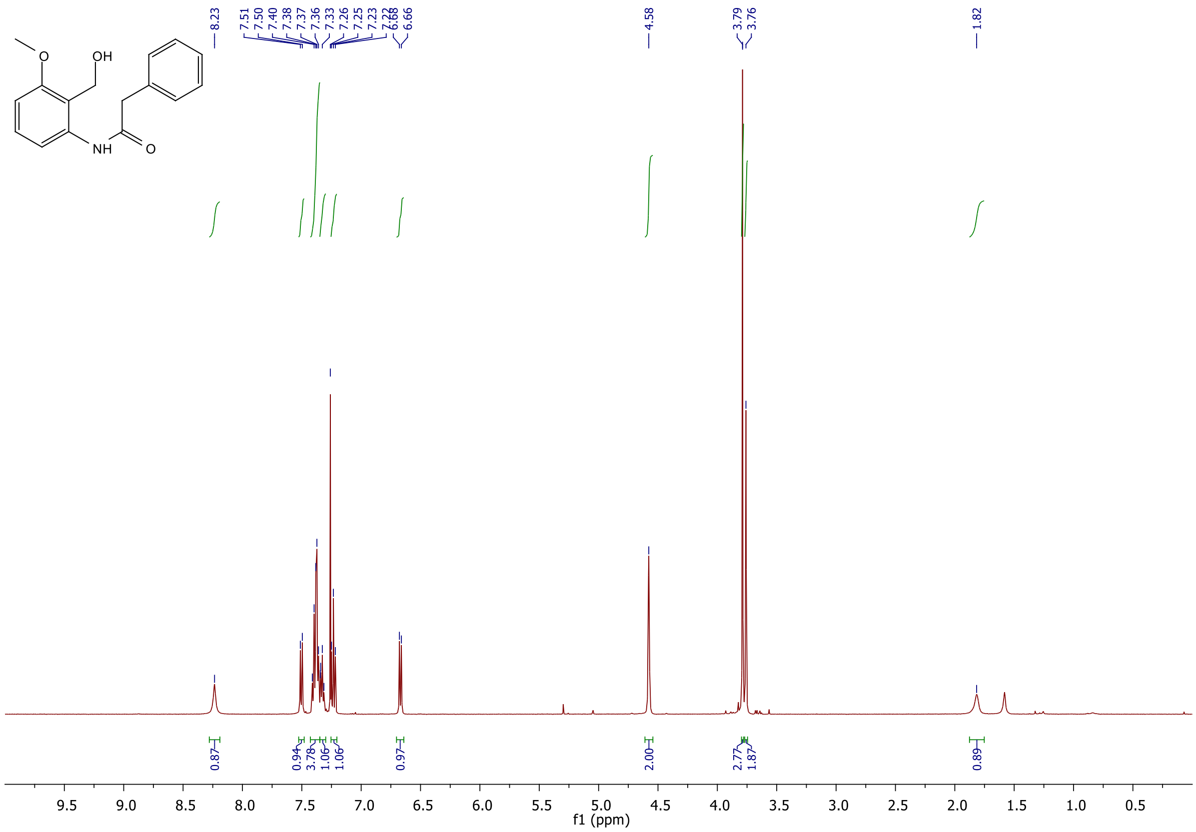


Figure S27: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1m.

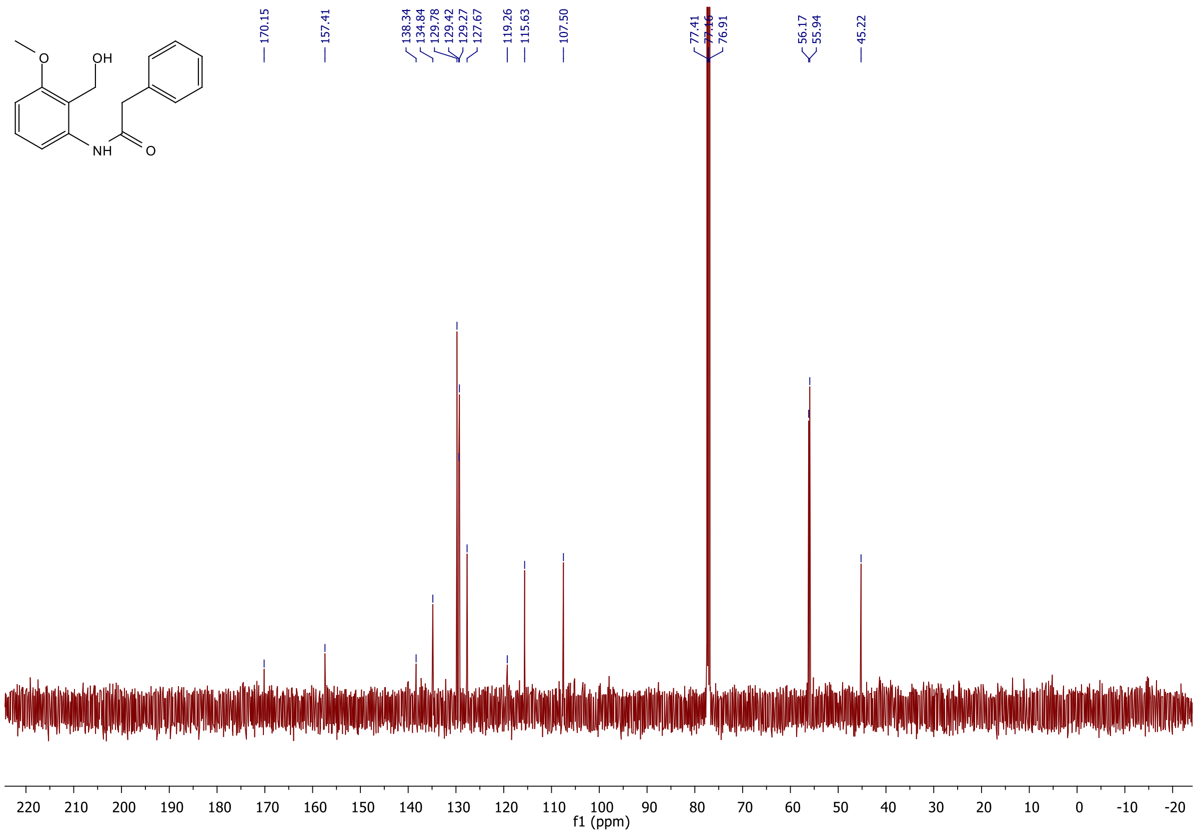


Figure S28: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1m.

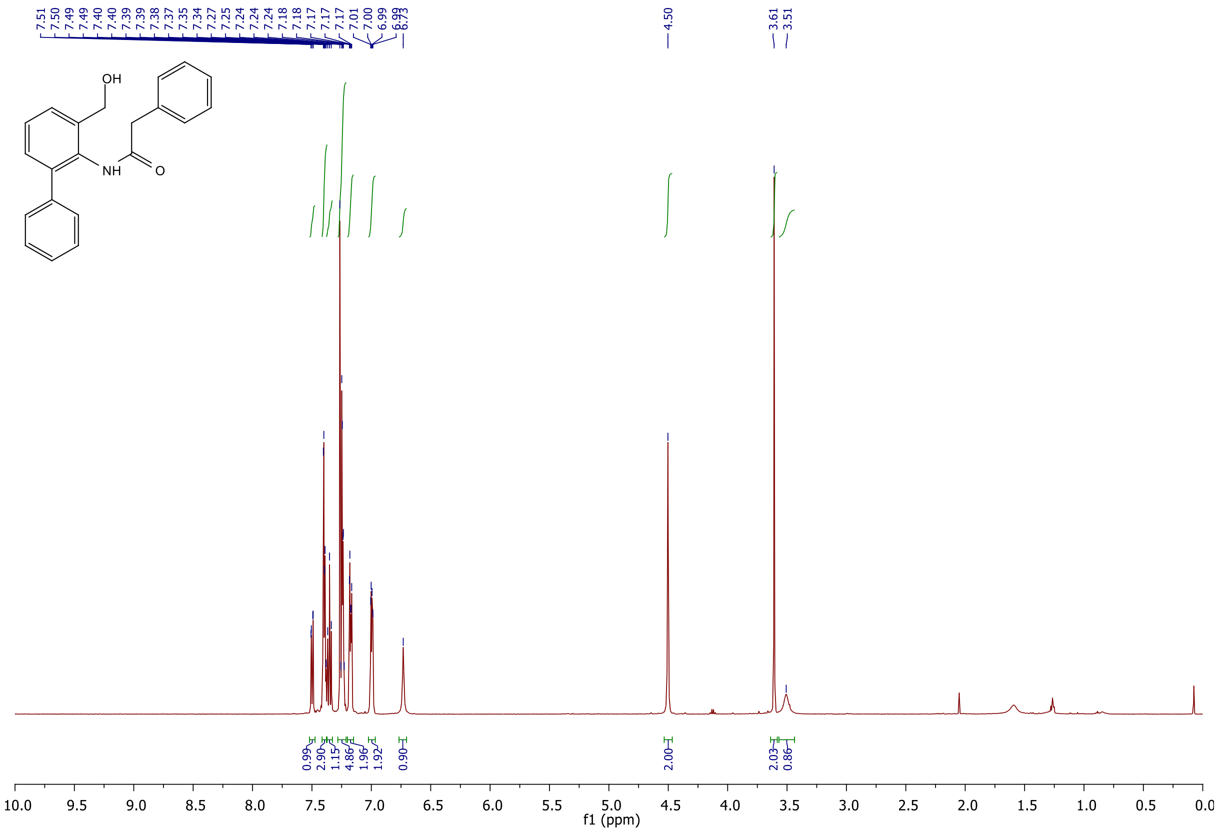


Figure S29: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1n.

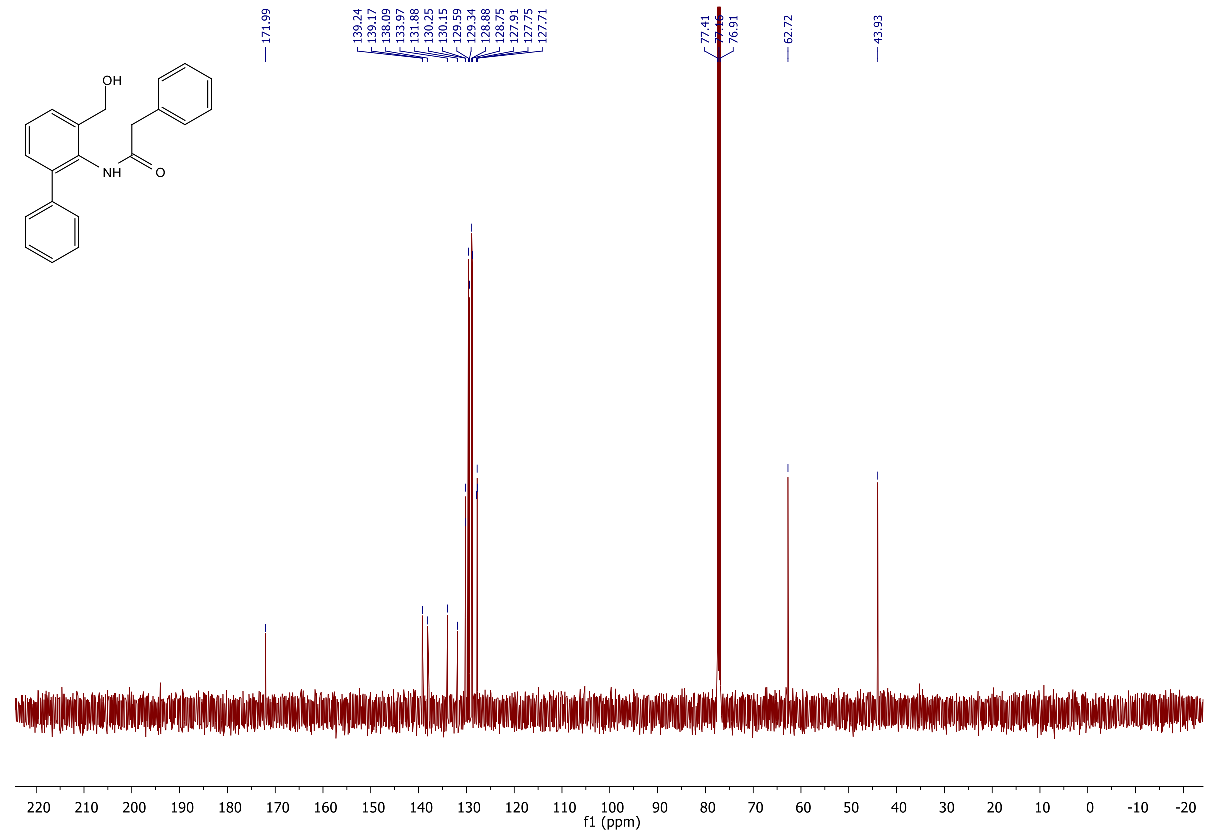


Figure S30: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1n.

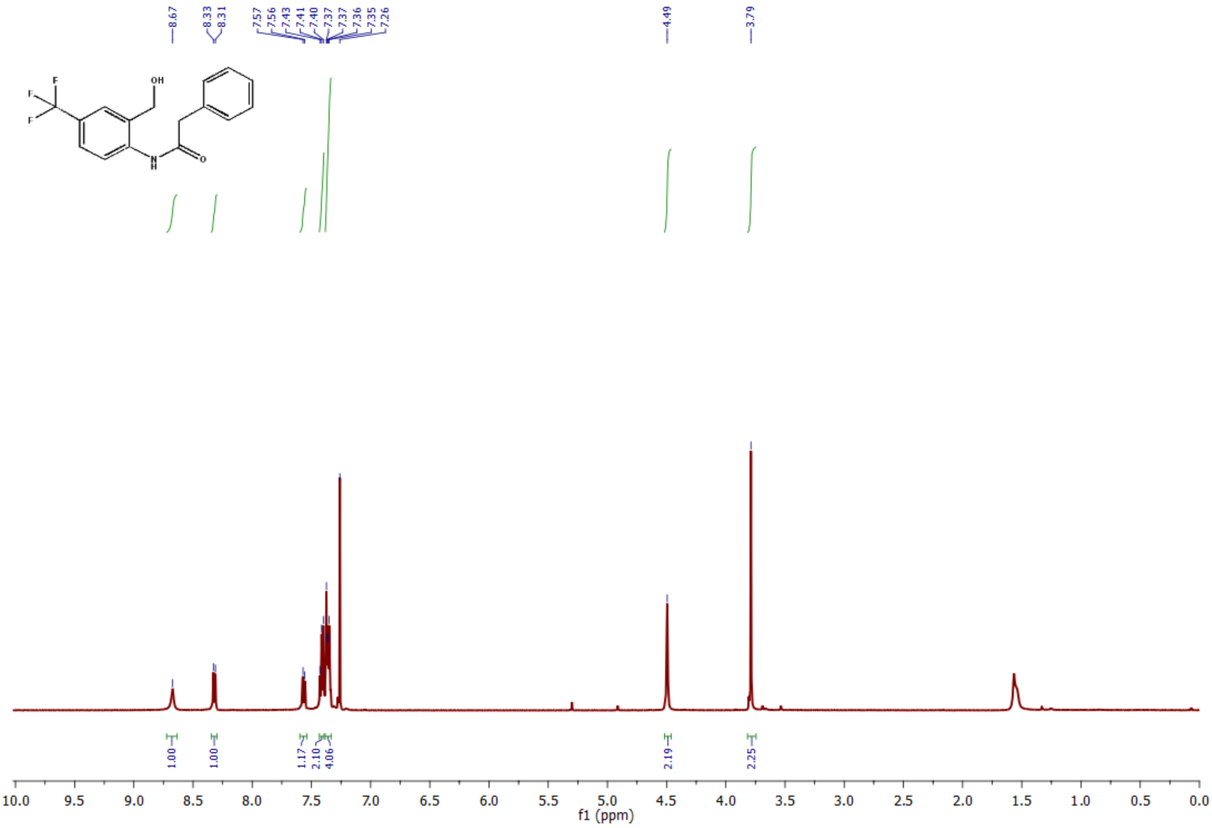


Figure S31: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1o.

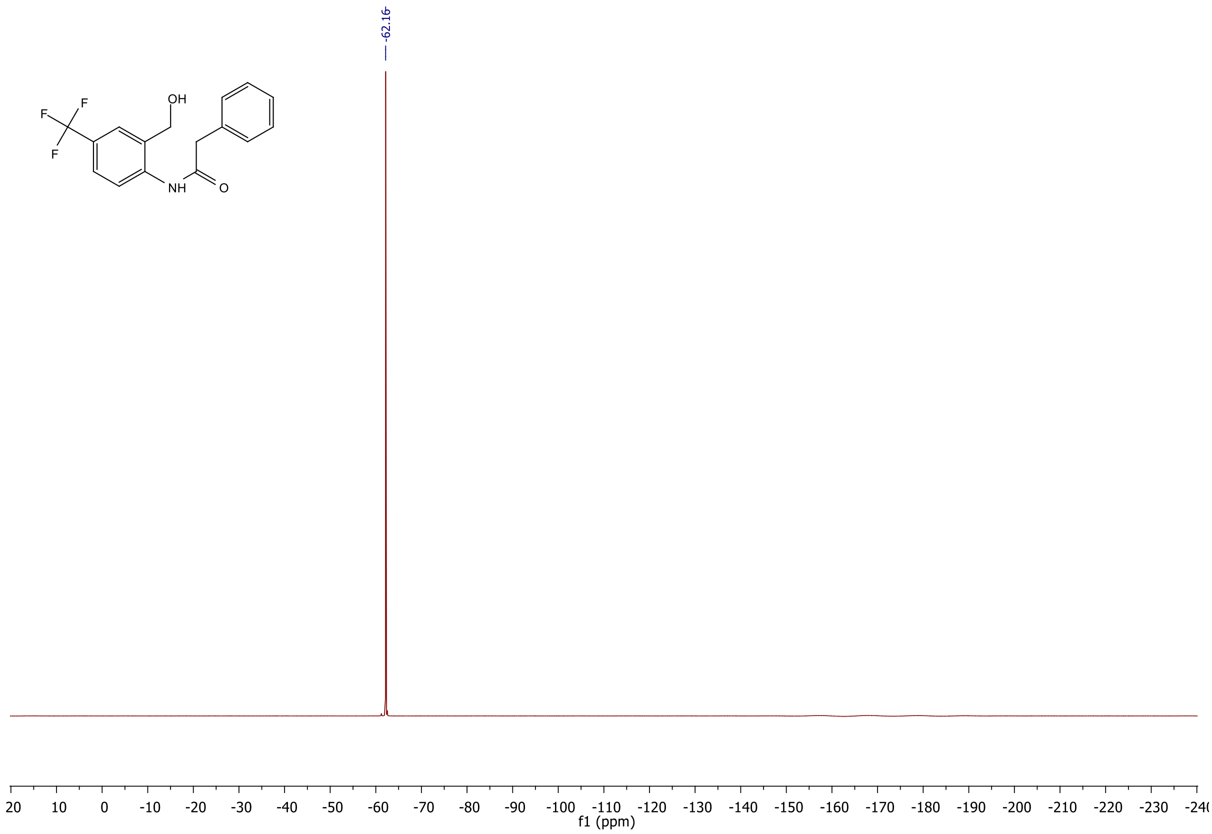


Figure S32: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 1o.

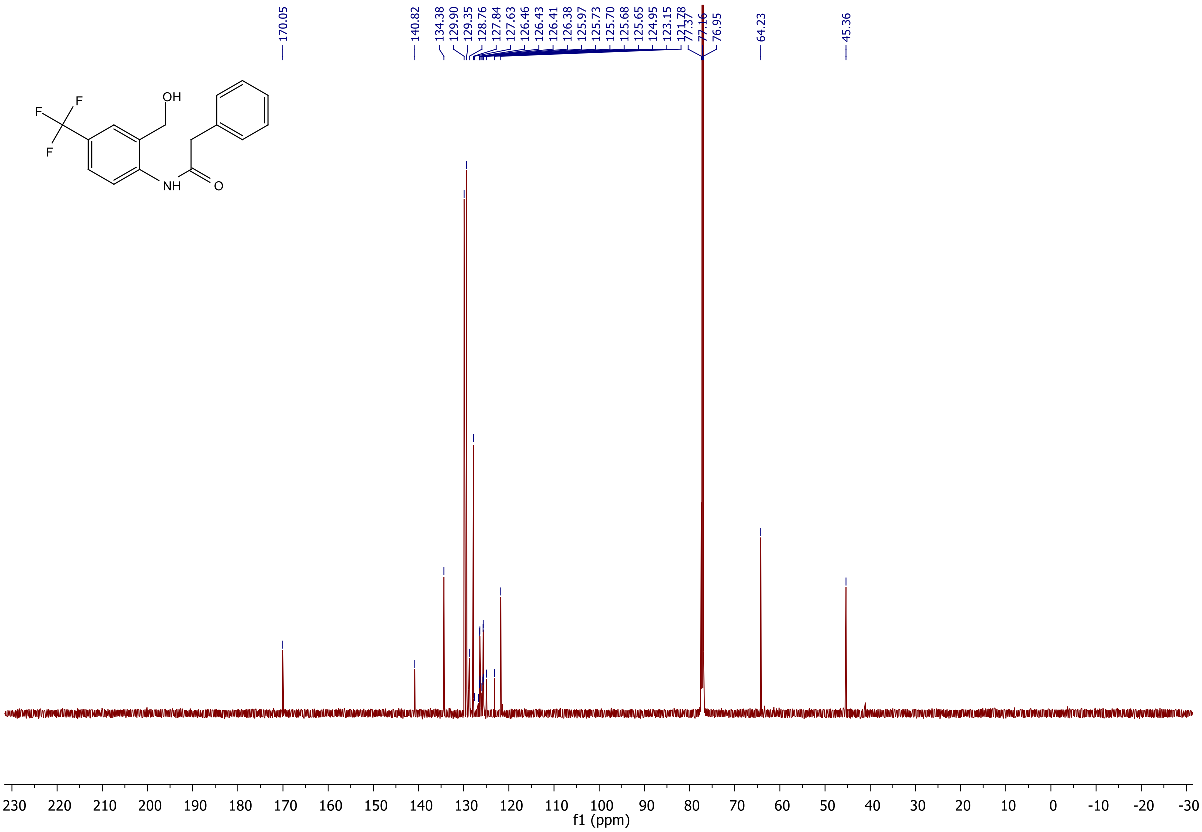


Figure S33: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1o.

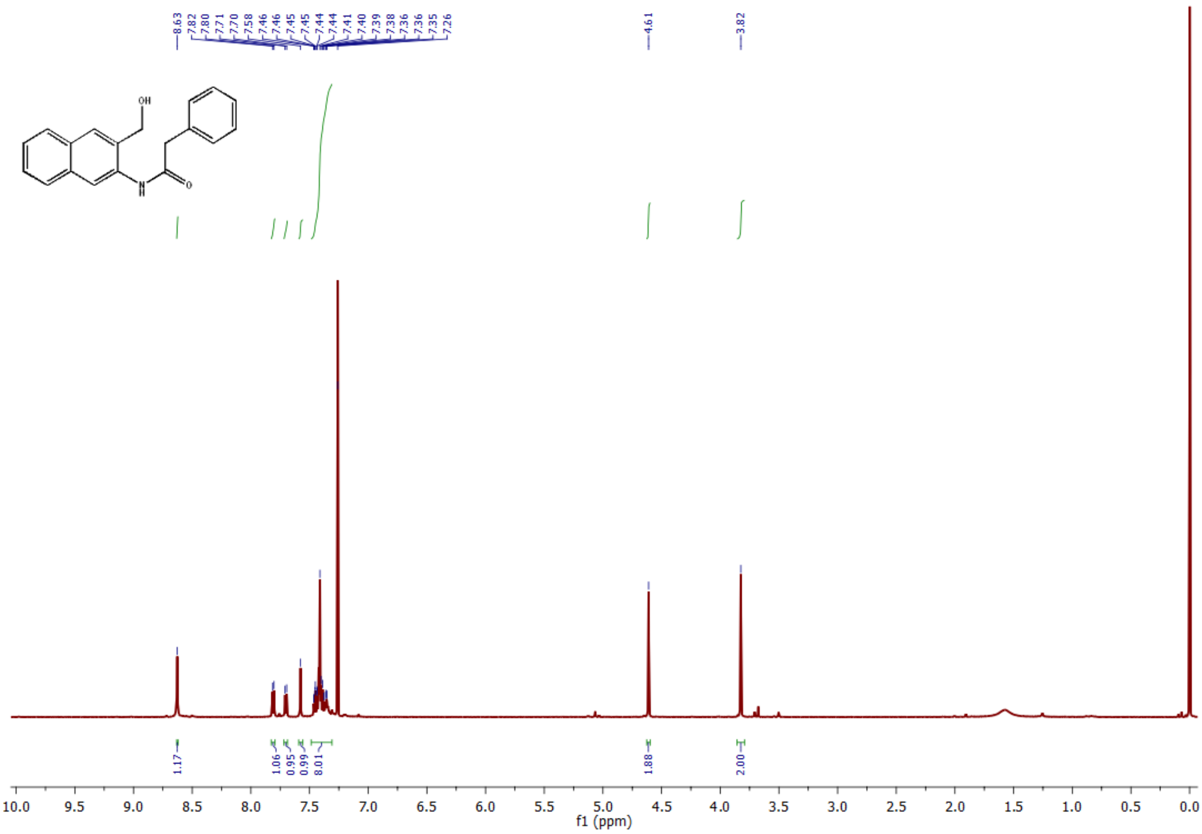


Figure S34: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1p.

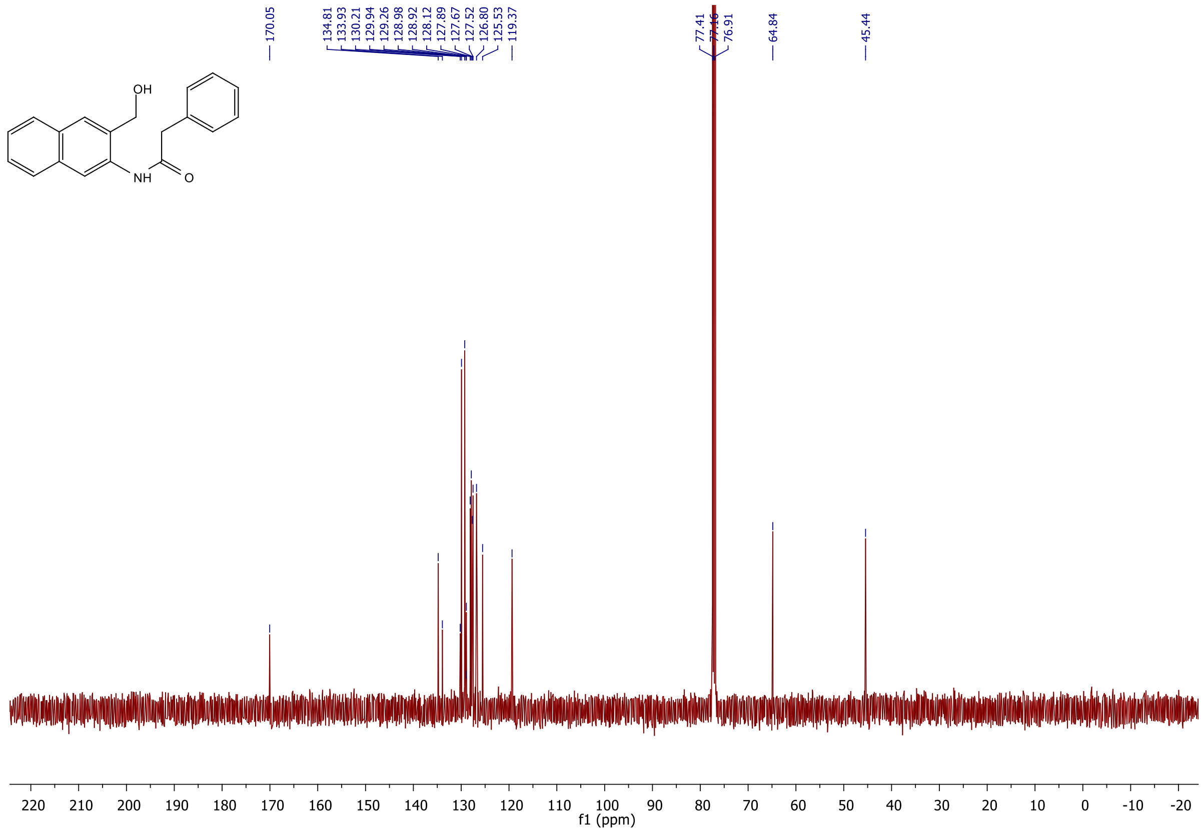


Figure S35: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 1p.

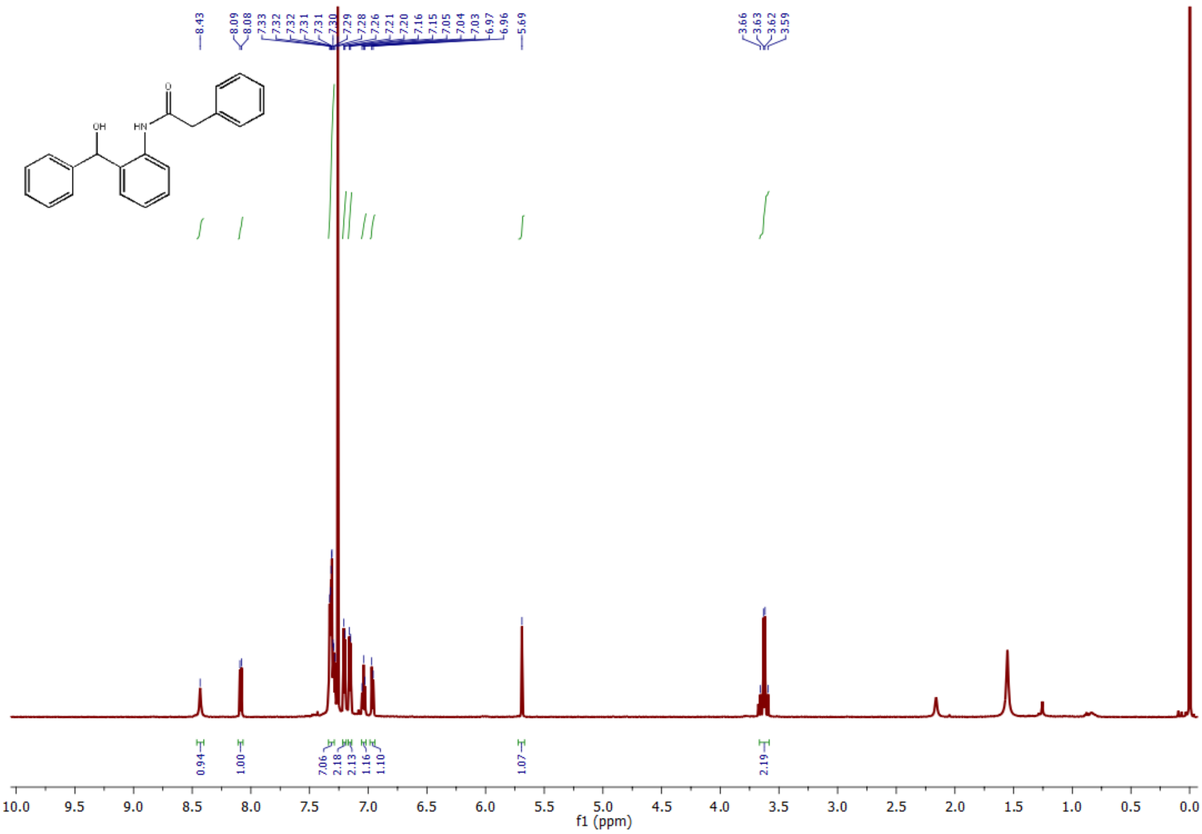


Figure S36: ^1H-NMR (500 MHz) in $CDCl_3$ of 1q.

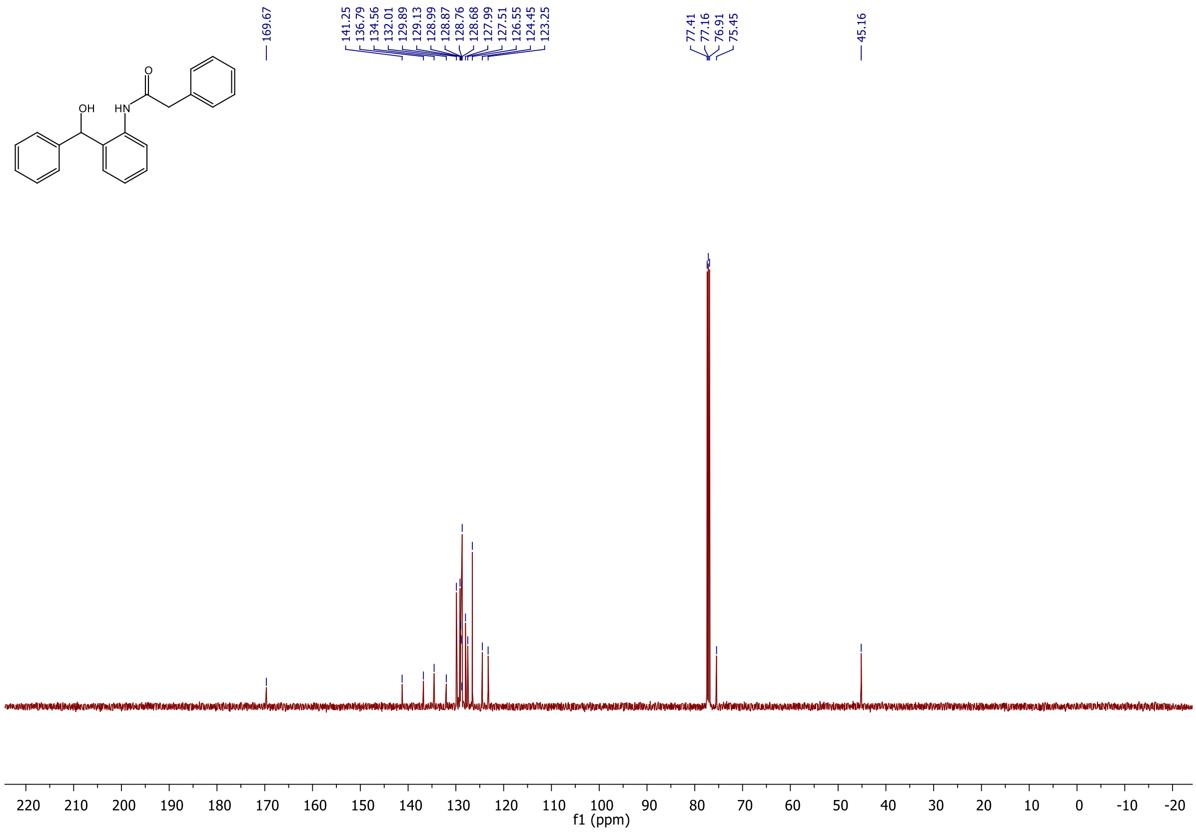


Figure S37: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1q.

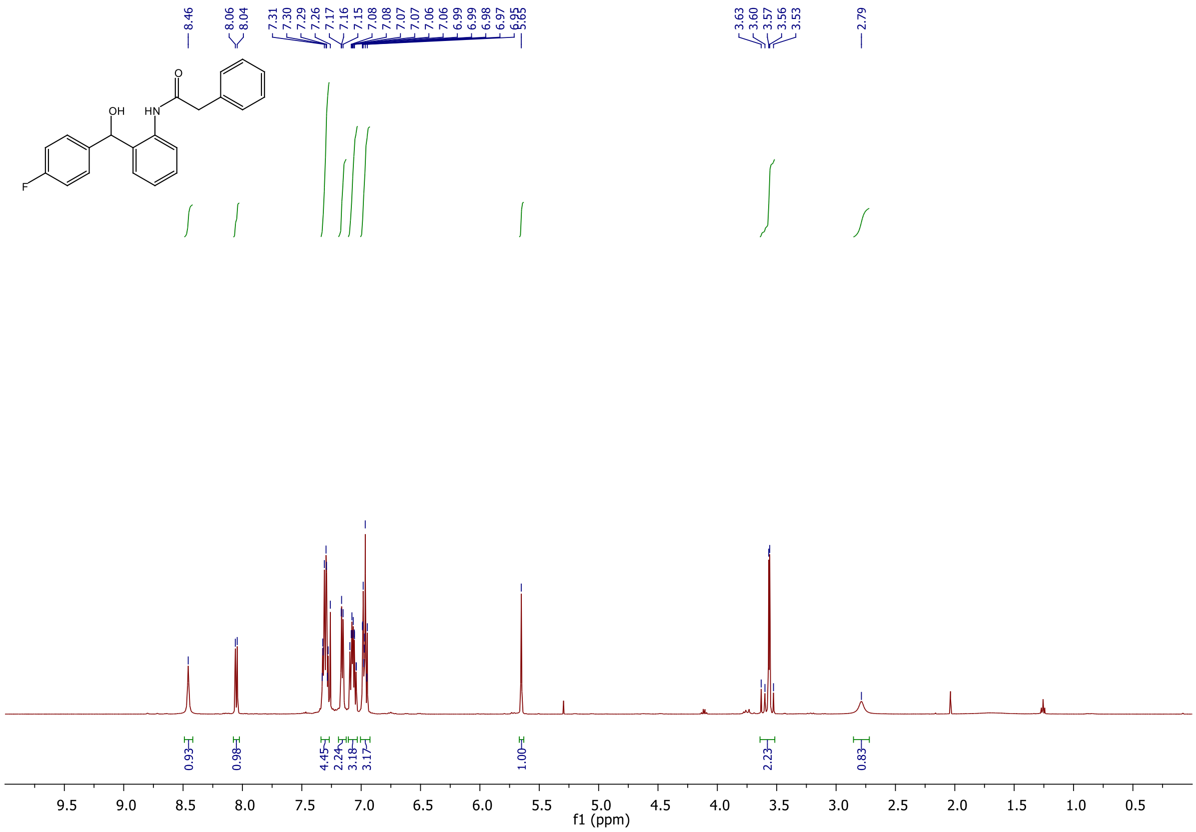


Figure S38: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1r.

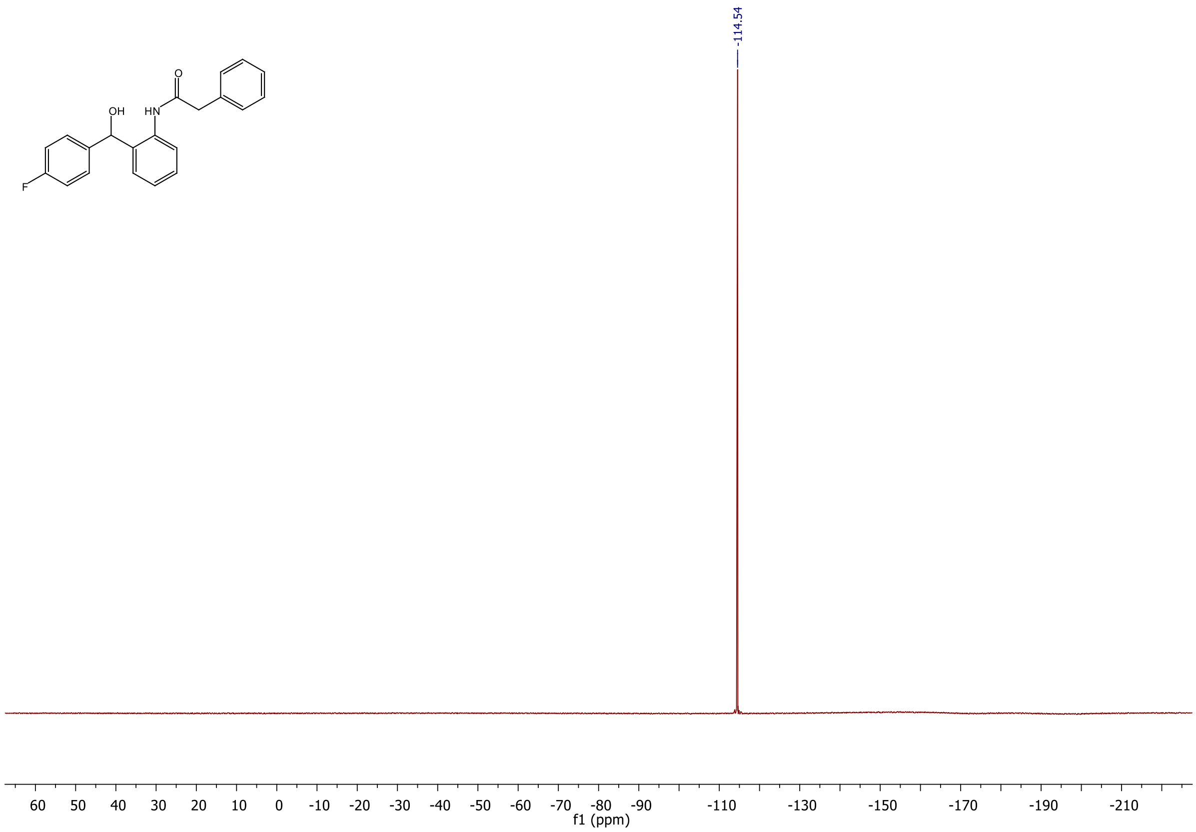


Figure S39: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 1r.

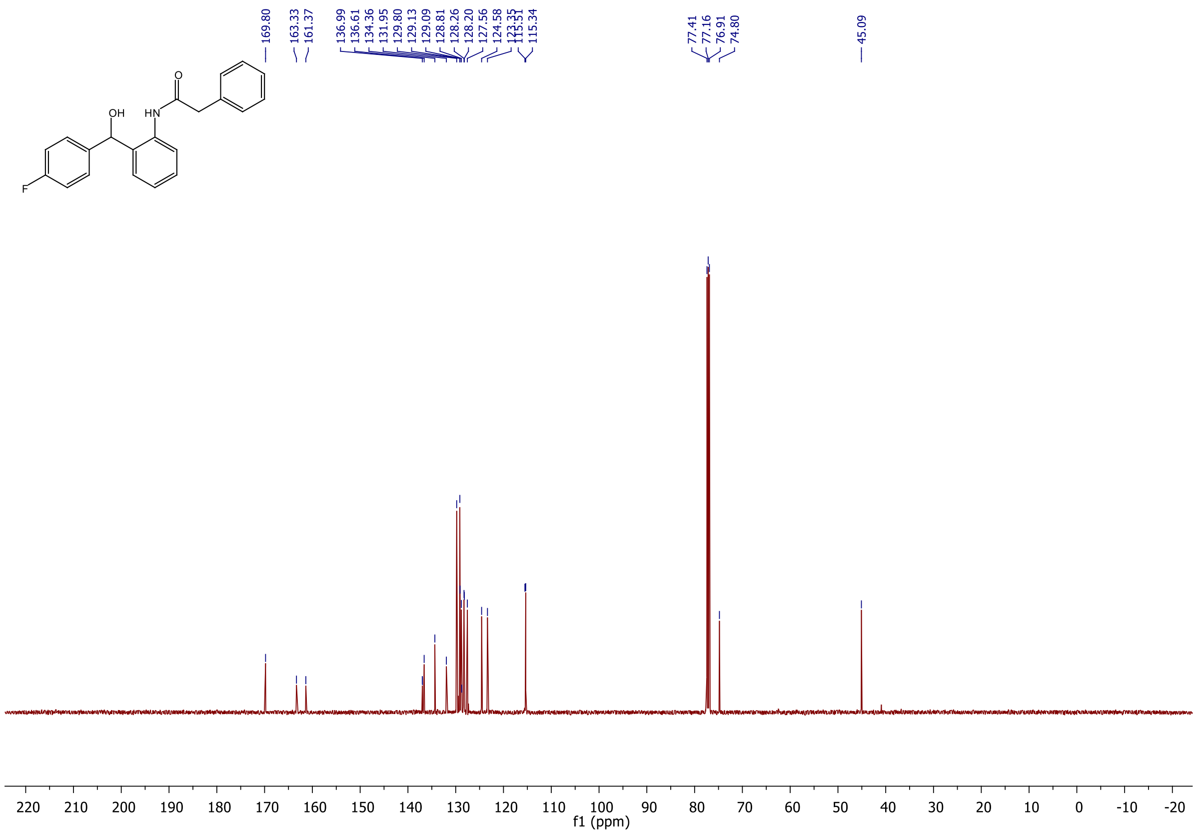


Figure S40: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1r.

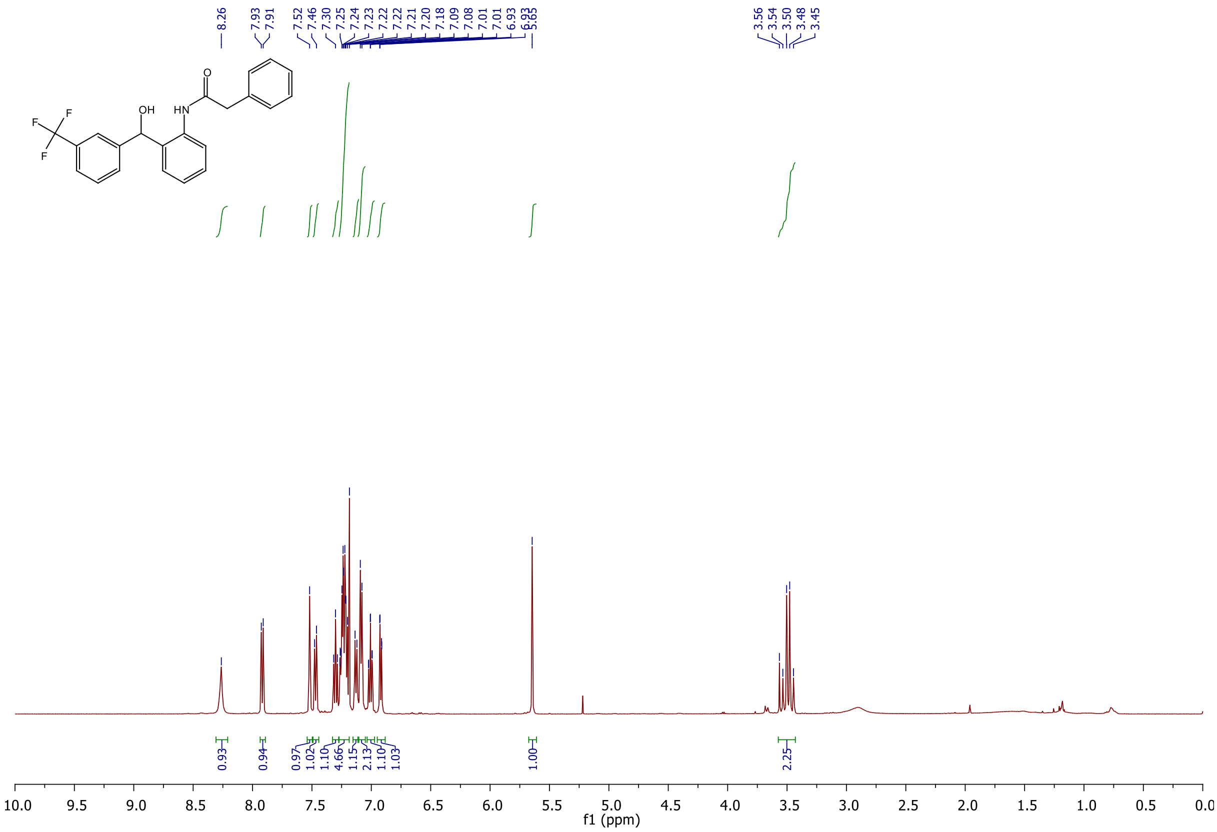


Figure S41: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1s.

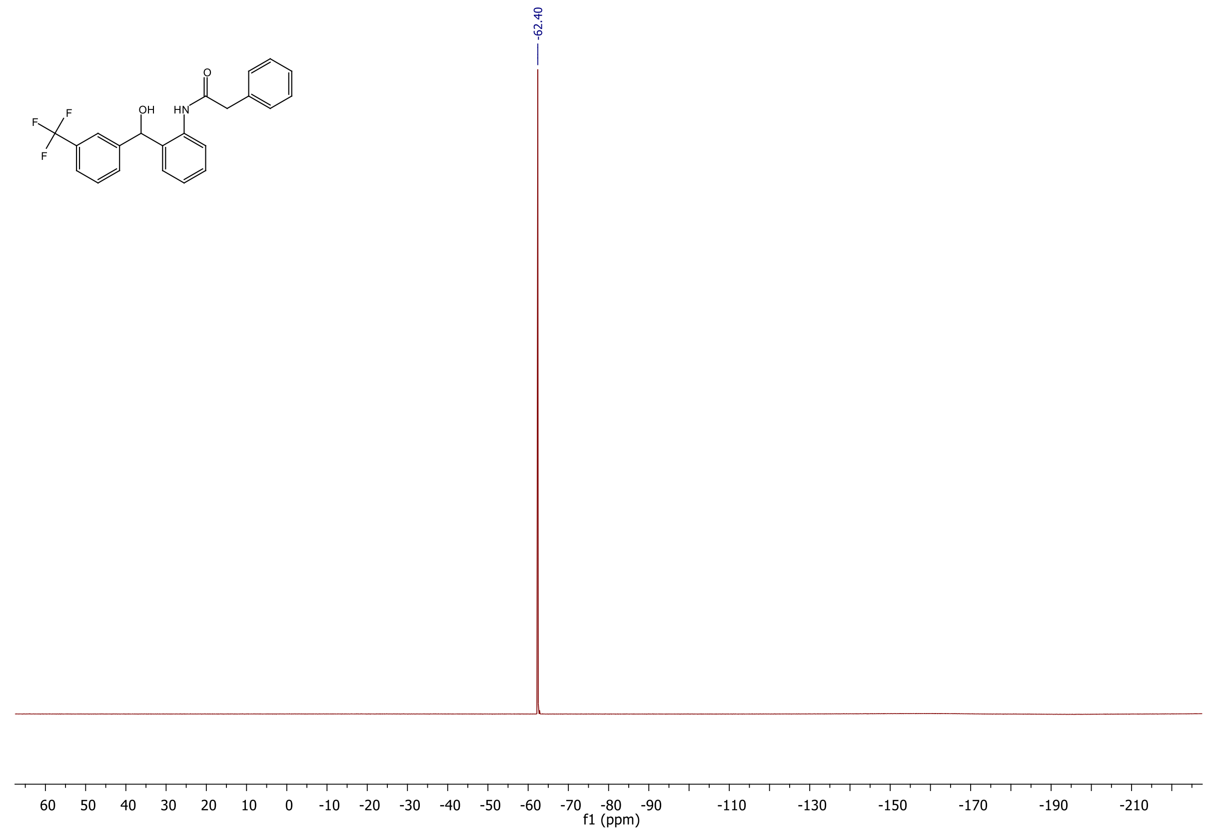


Figure S42: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 1s.

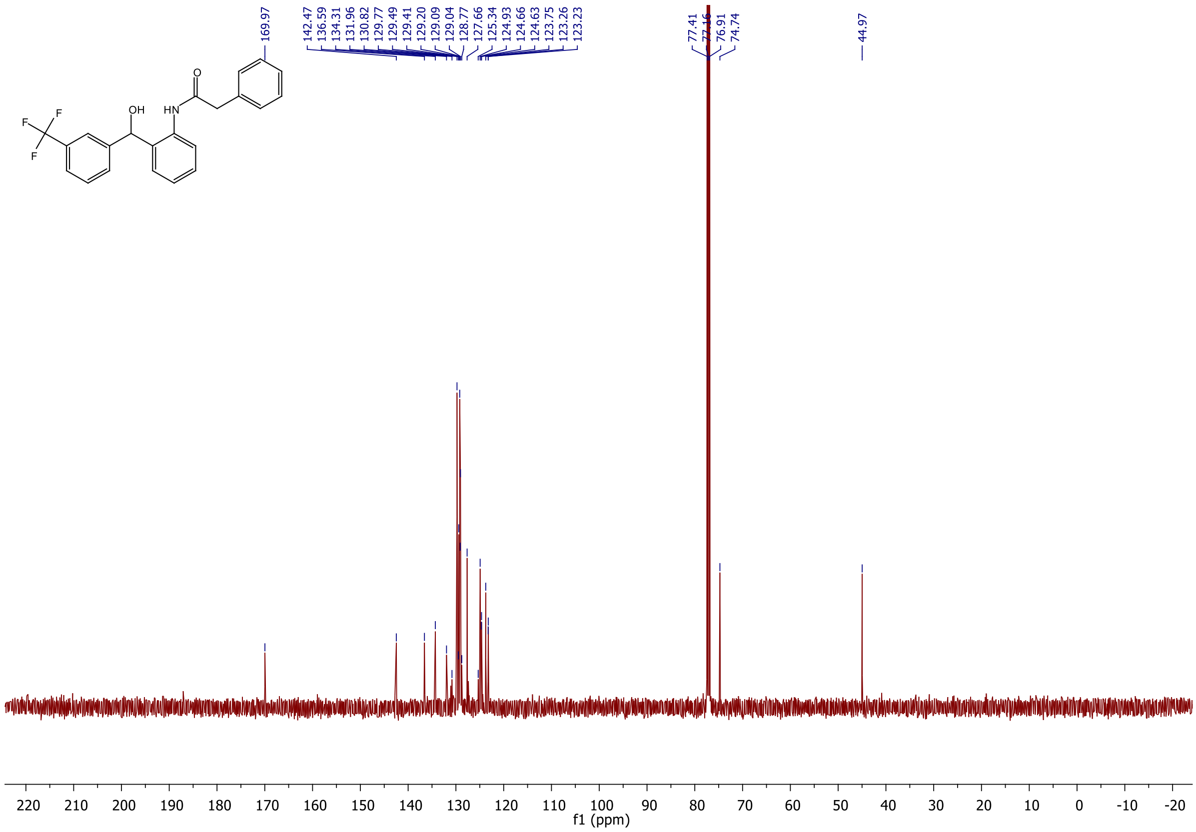


Figure S43: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1s.

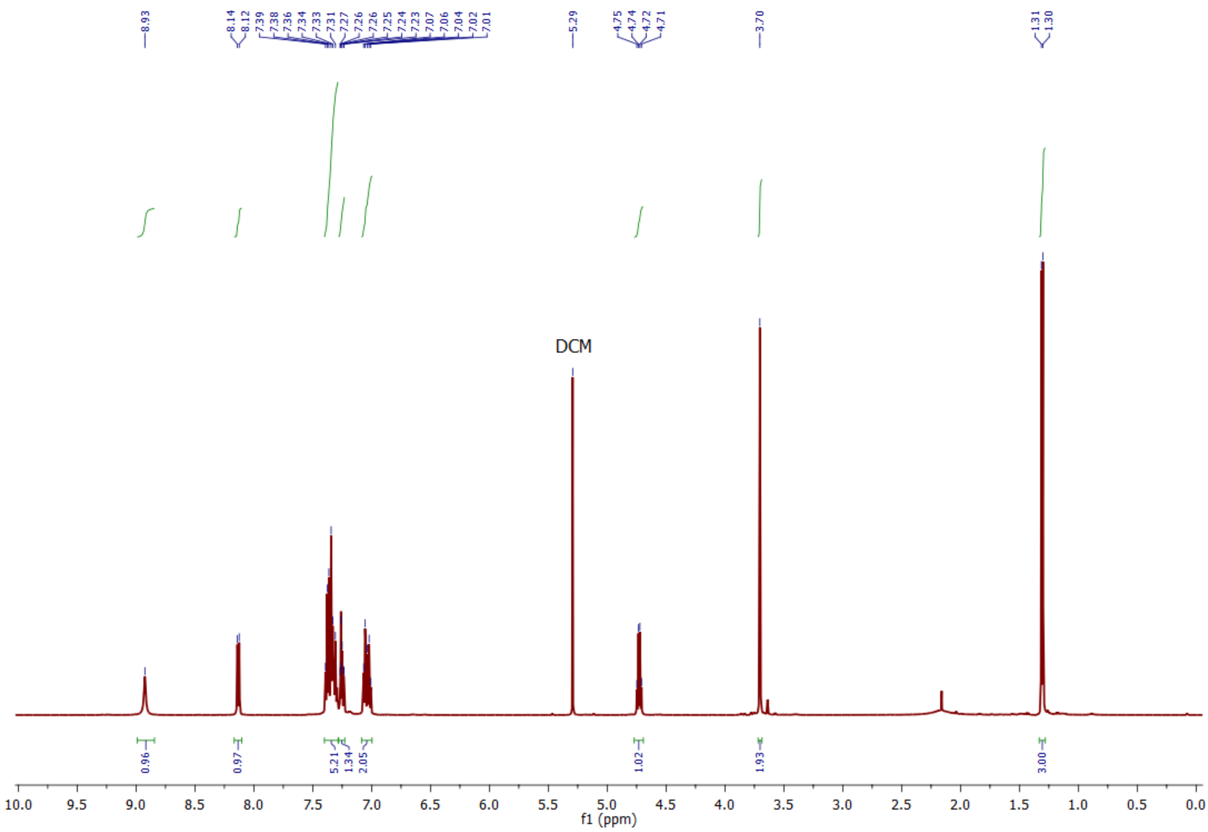


Figure S44: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 1t.

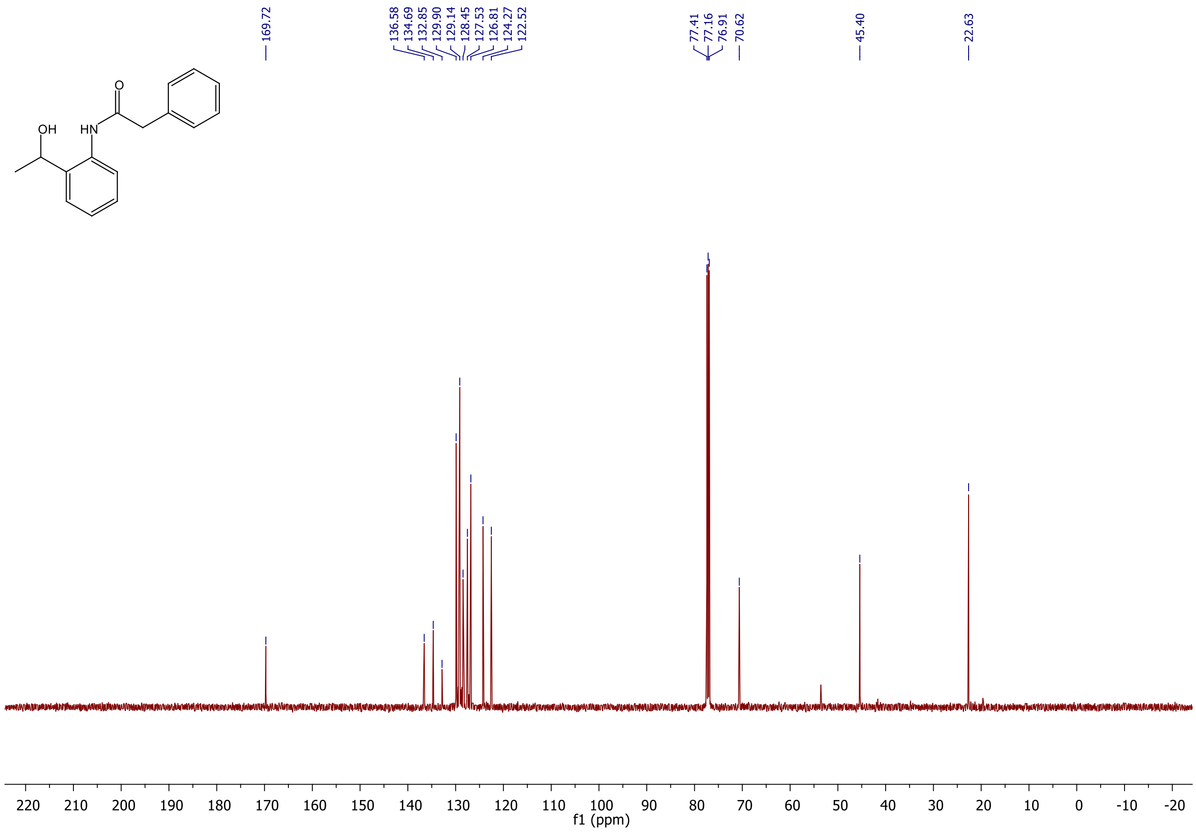


Figure S45: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 1t.

Part 6: NMR spectra of the quinolinones.

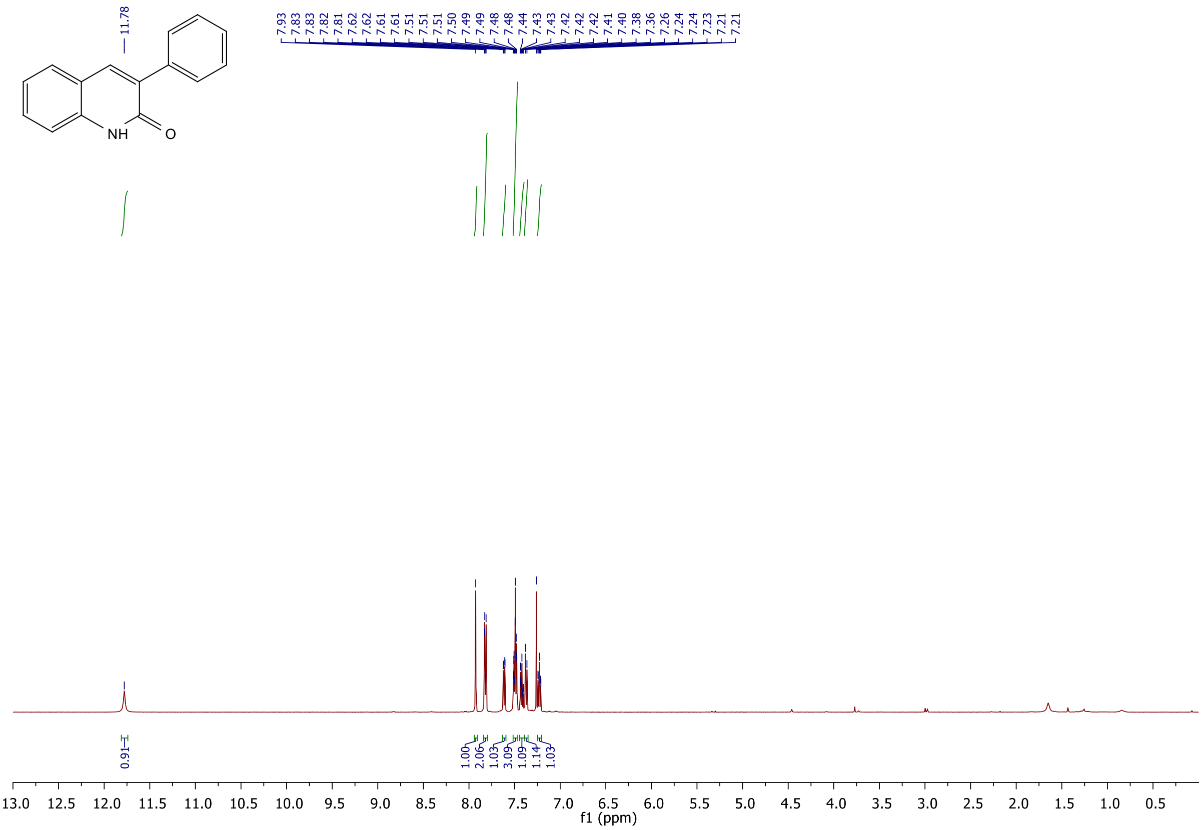


Figure S46: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2a.

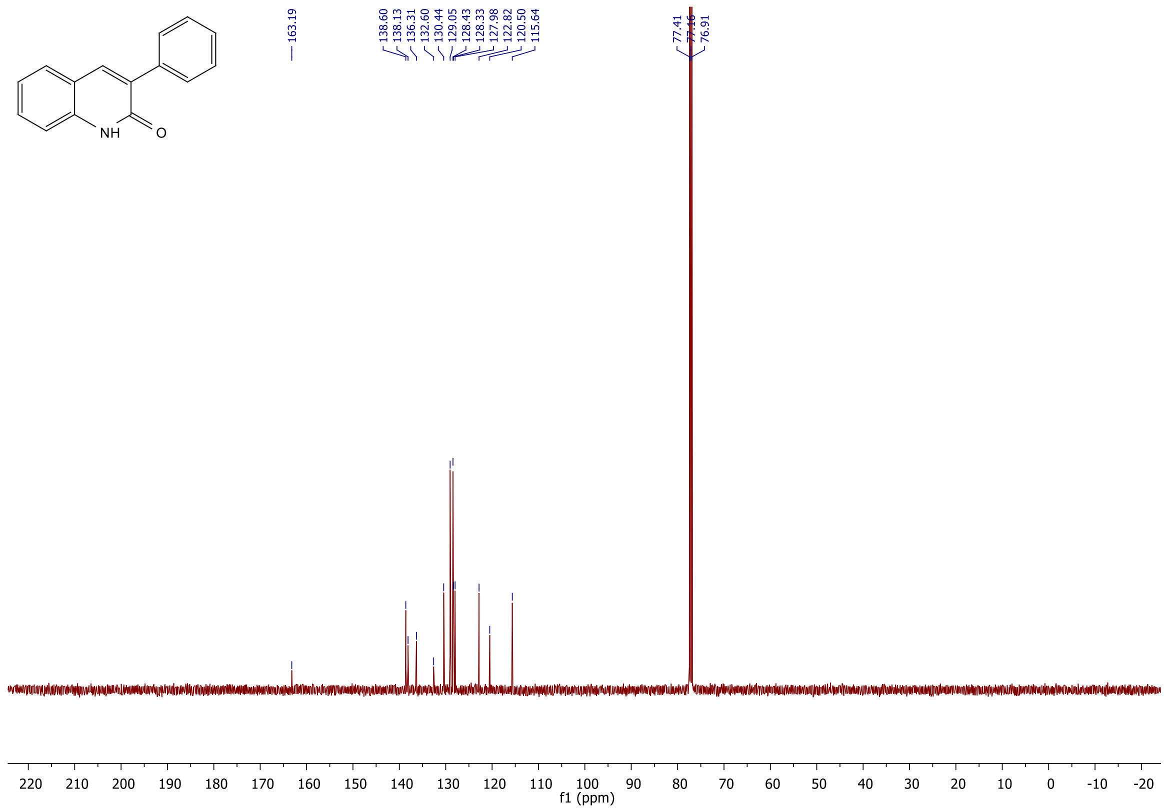


Figure S47: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2a.

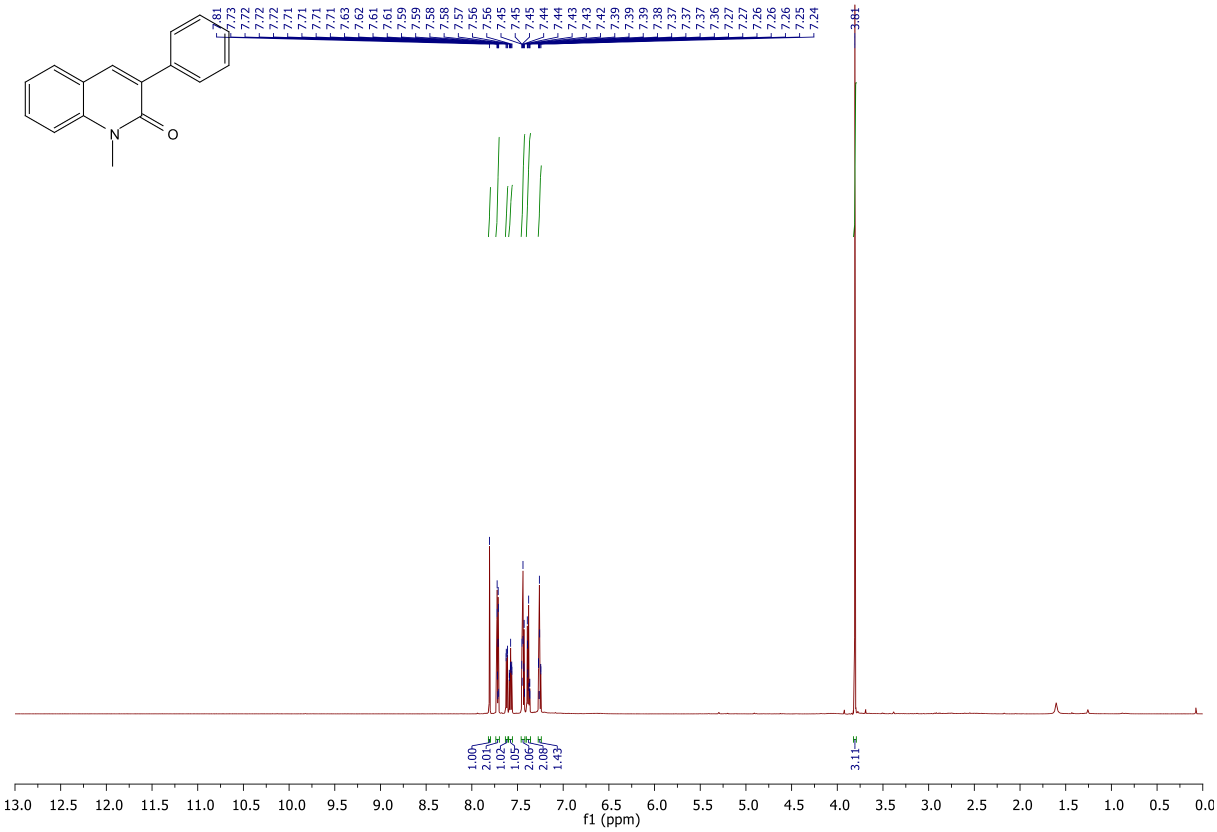


Figure S48: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2b.

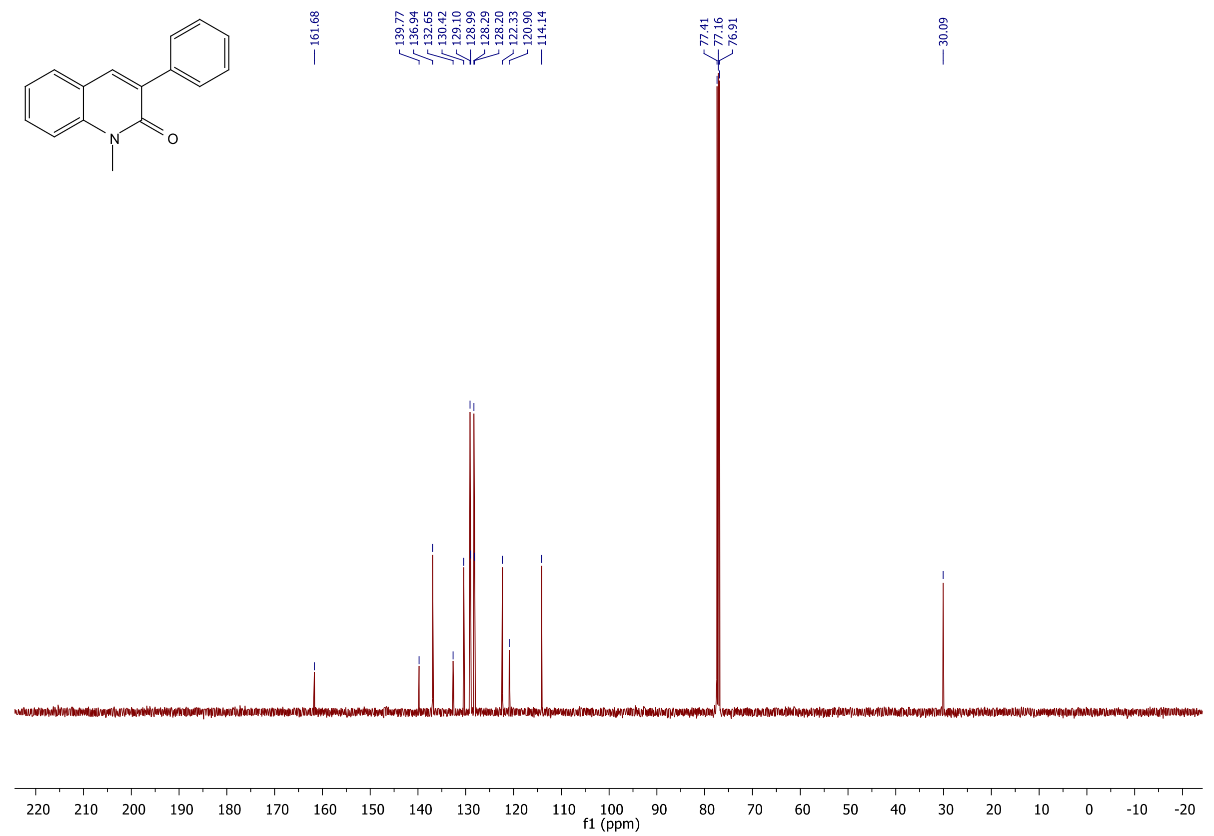


Figure S49: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2b.

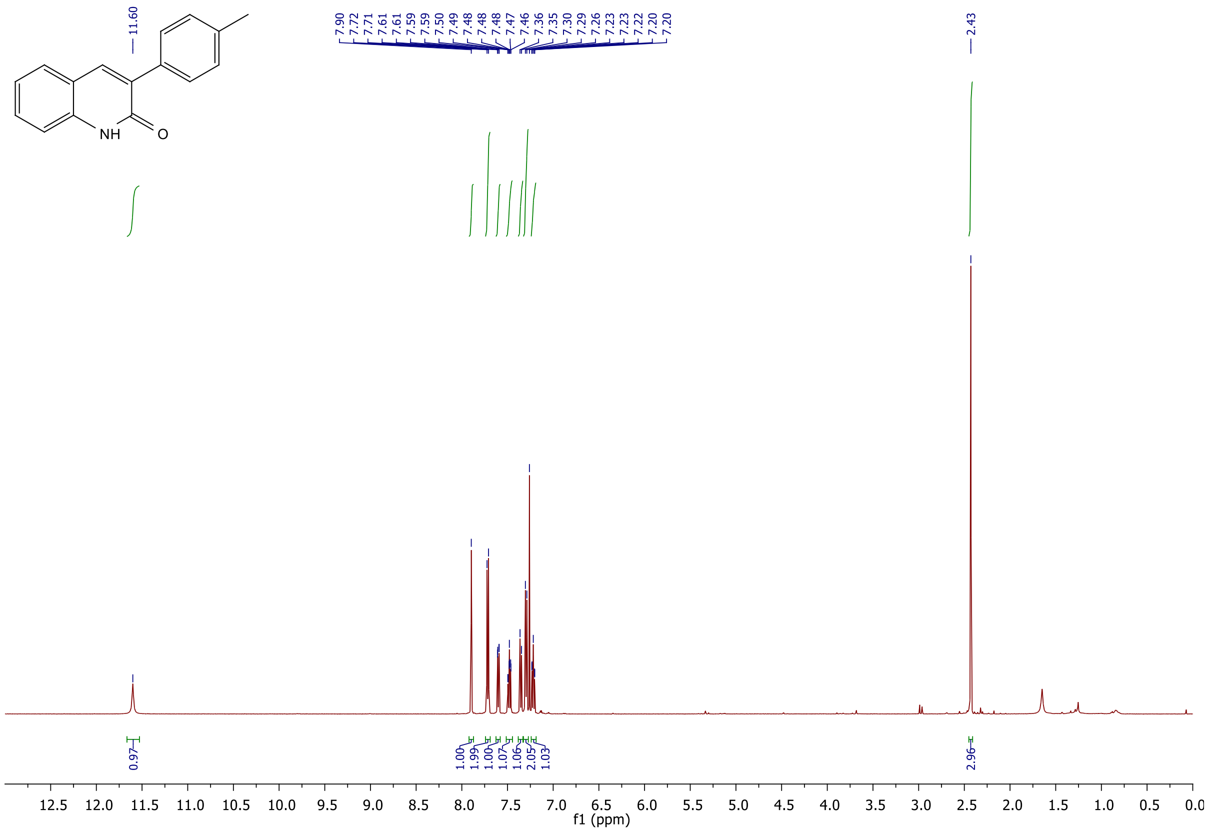


Figure S50: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2c.

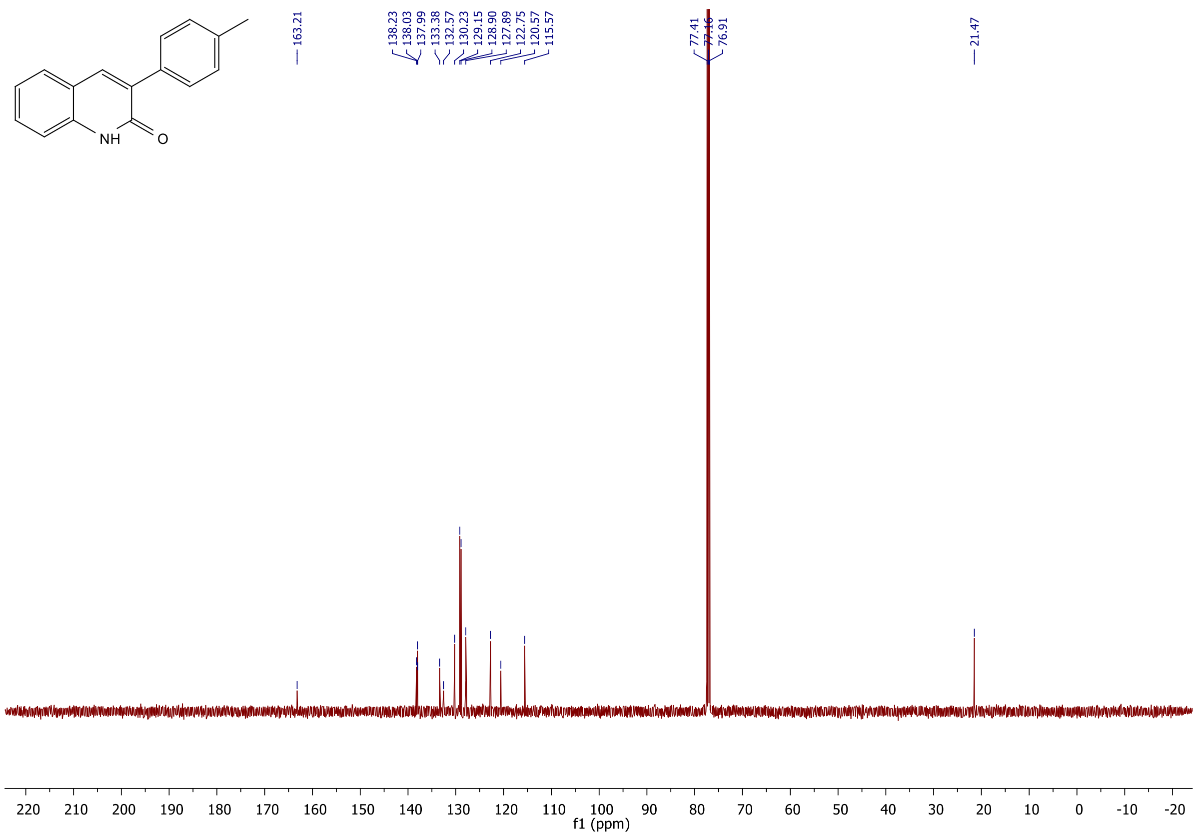


Figure S51: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2c.

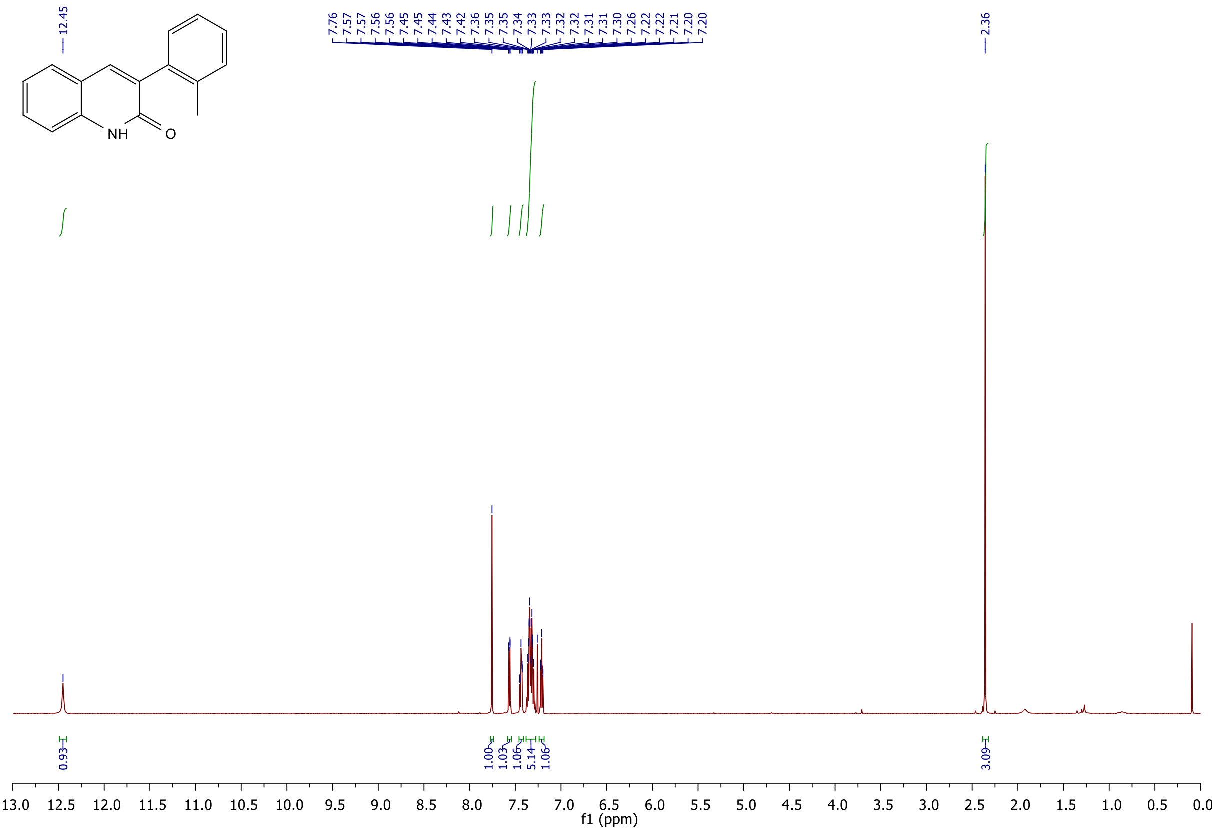


Figure S52: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2d.

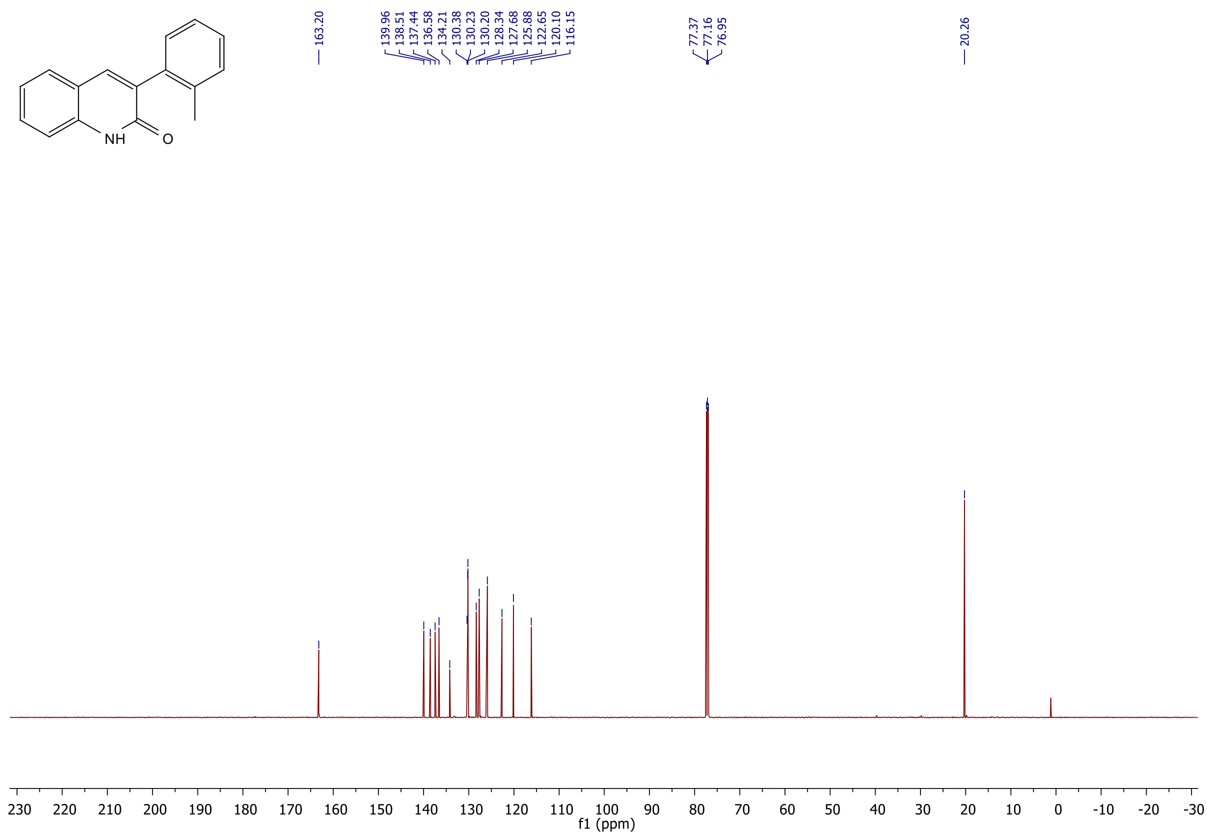


Figure S53: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 2d.

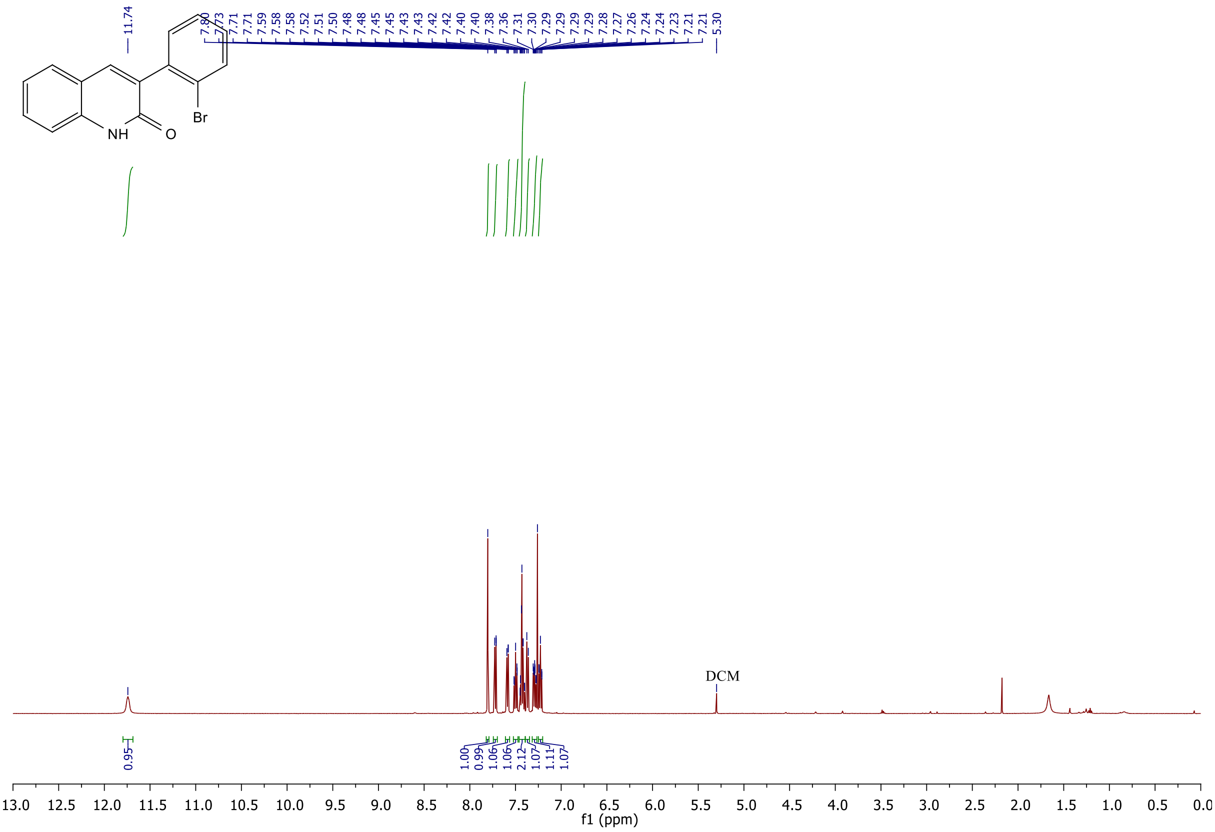


Figure S54: ^1H-NMR (500 MHz) in $CDCl_3$ of 2e.

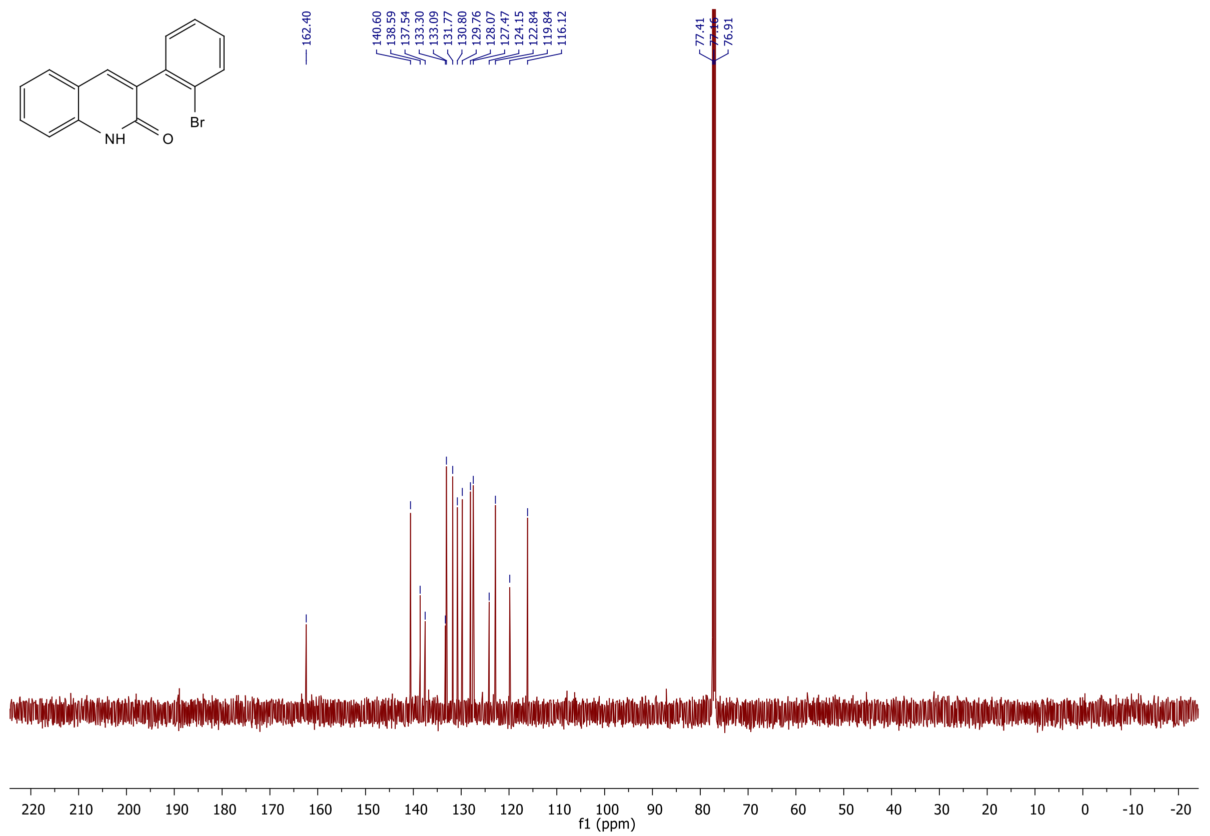
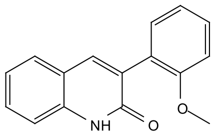


Figure S55: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2e.



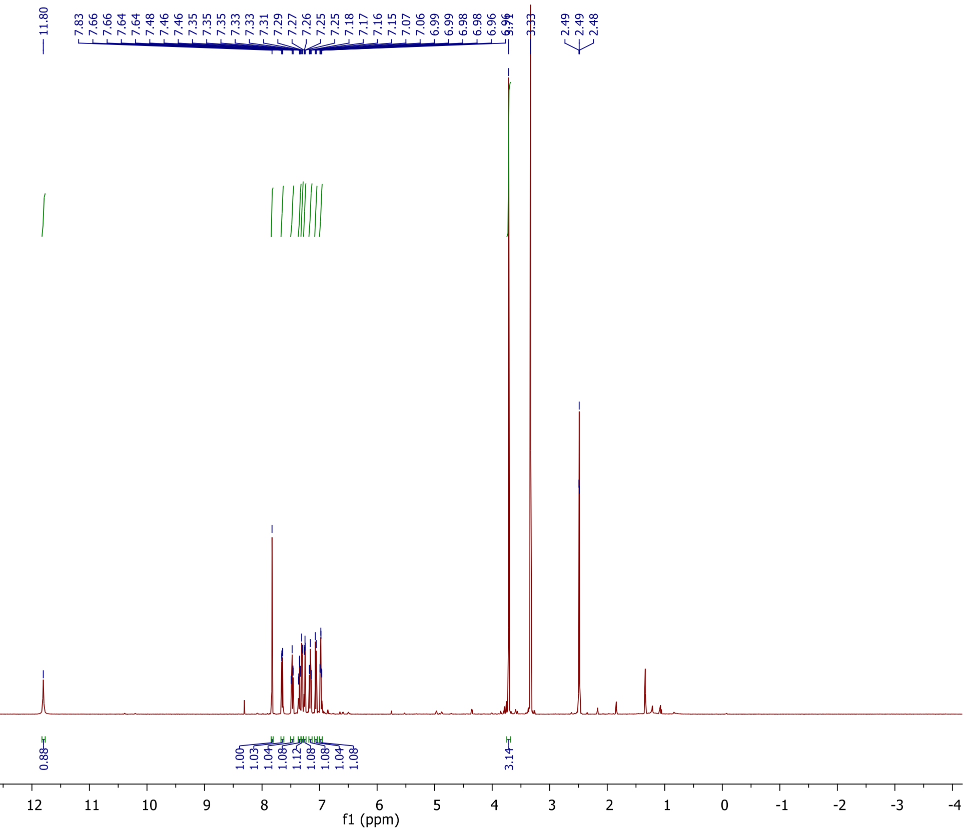
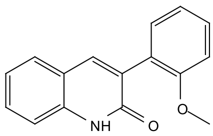


Figure S56: ^{1}H-NMR (500 MHz) in DMSO-d_6 of 2f.



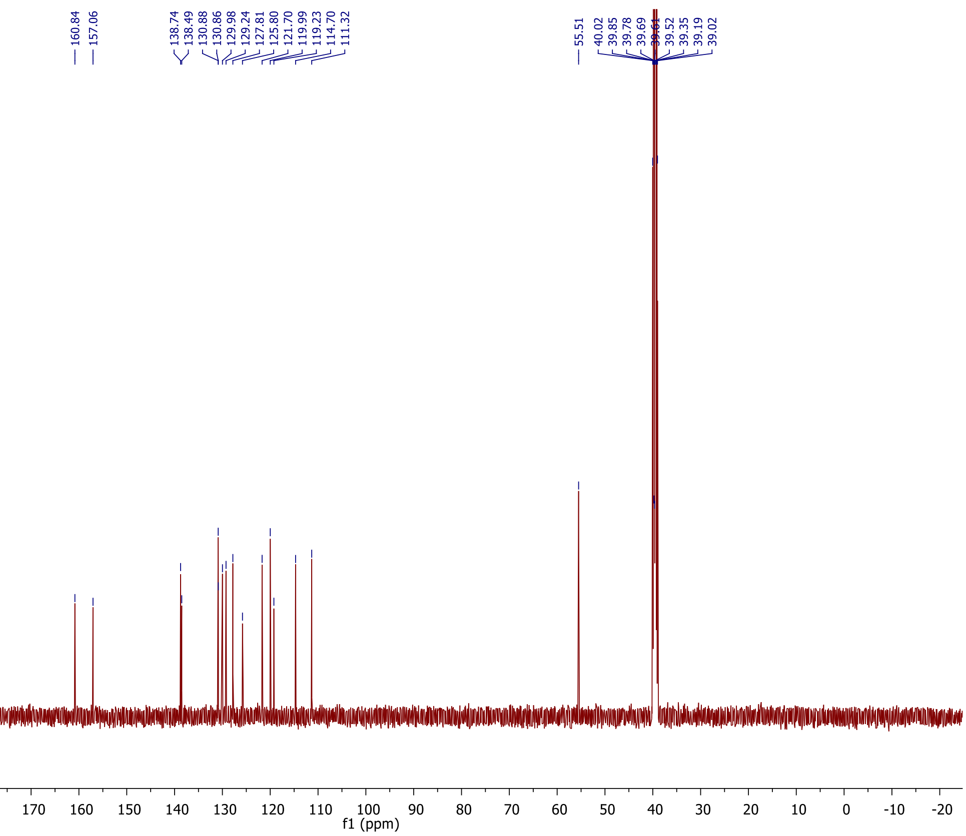


Figure S57: $^{13}C\{^1H\}$ NMR (125 MHz) in DMSO-d_6 of 2f.

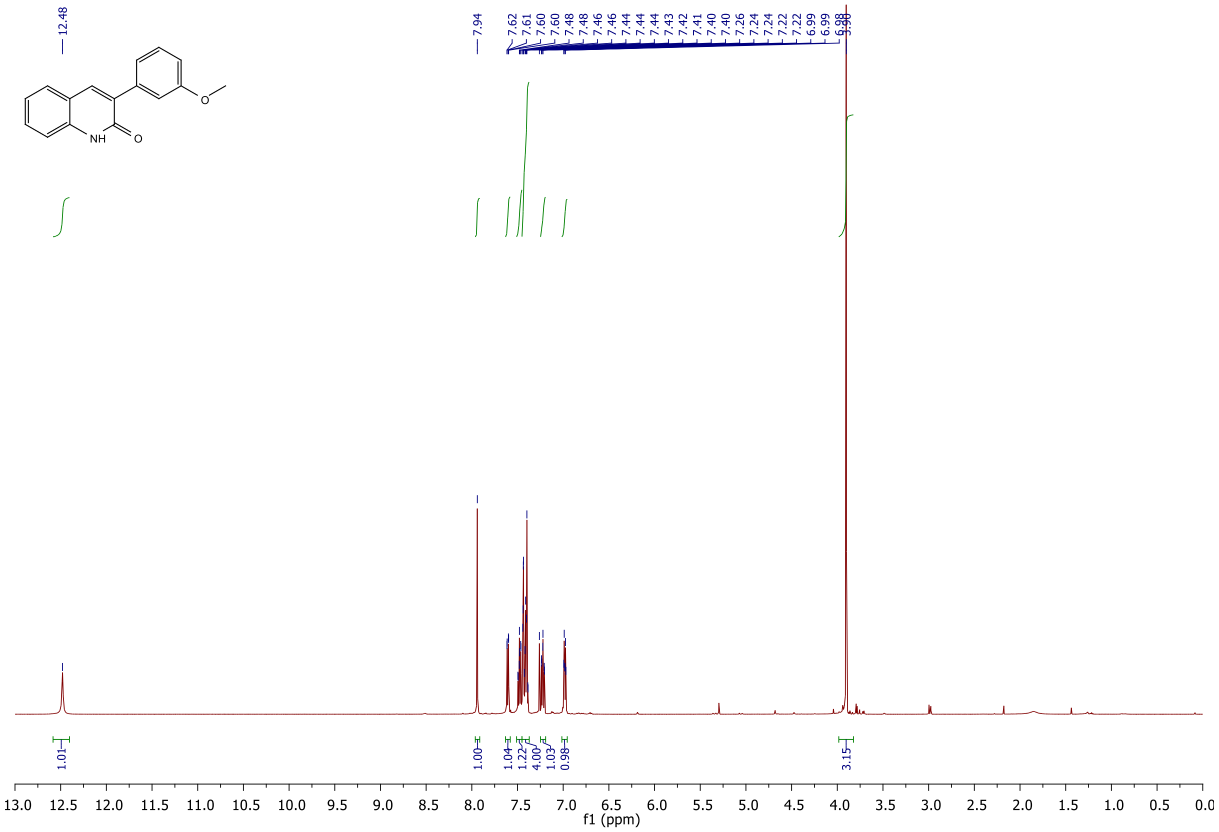


Figure S58: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2g.

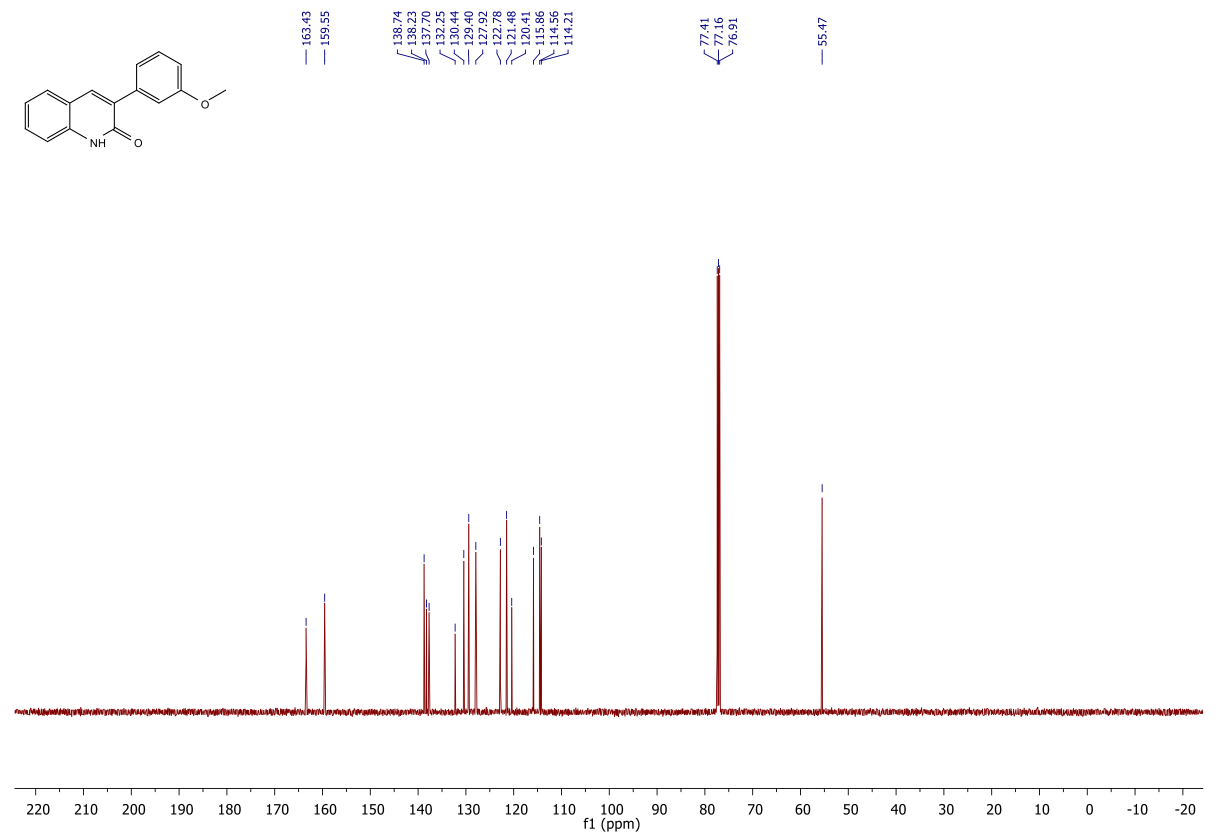


Figure S59: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2g.

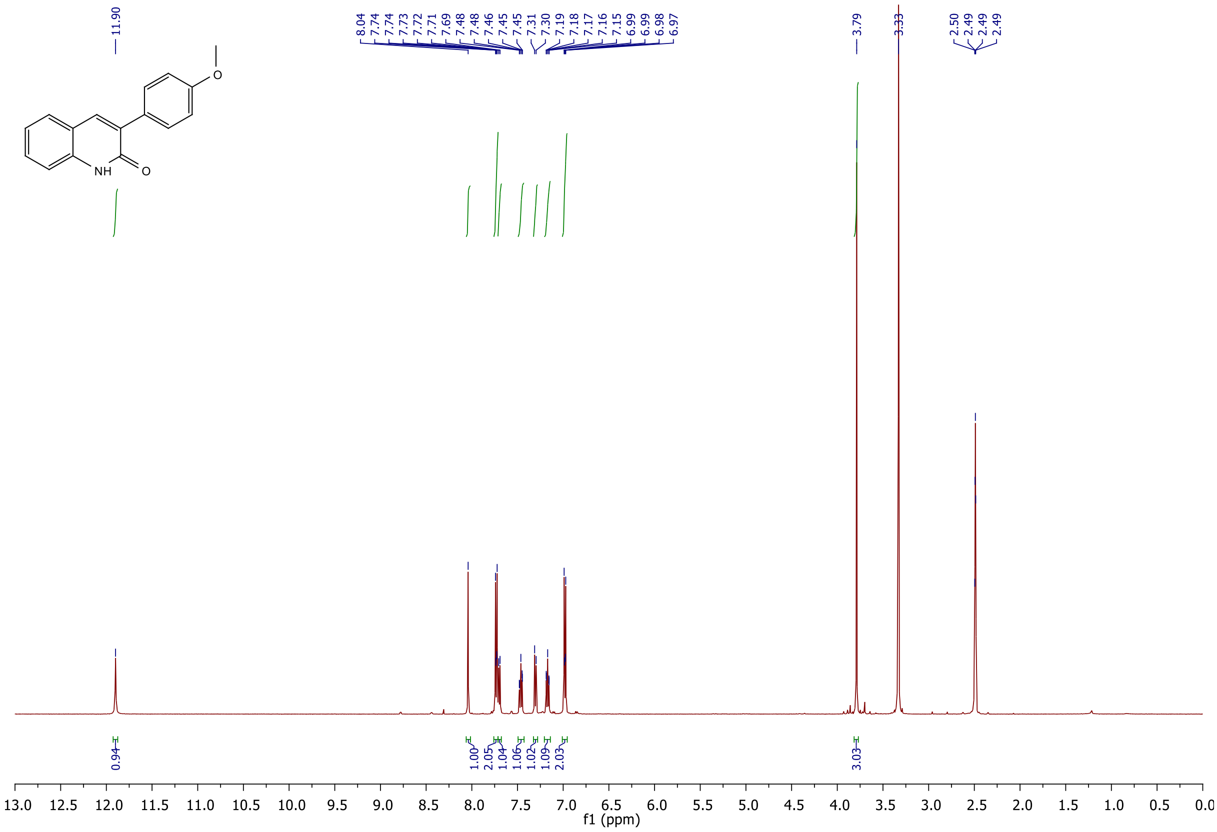


Figure S60: ^{1}H-NMR (500 MHz) in DMSO-d_6 of 2h.

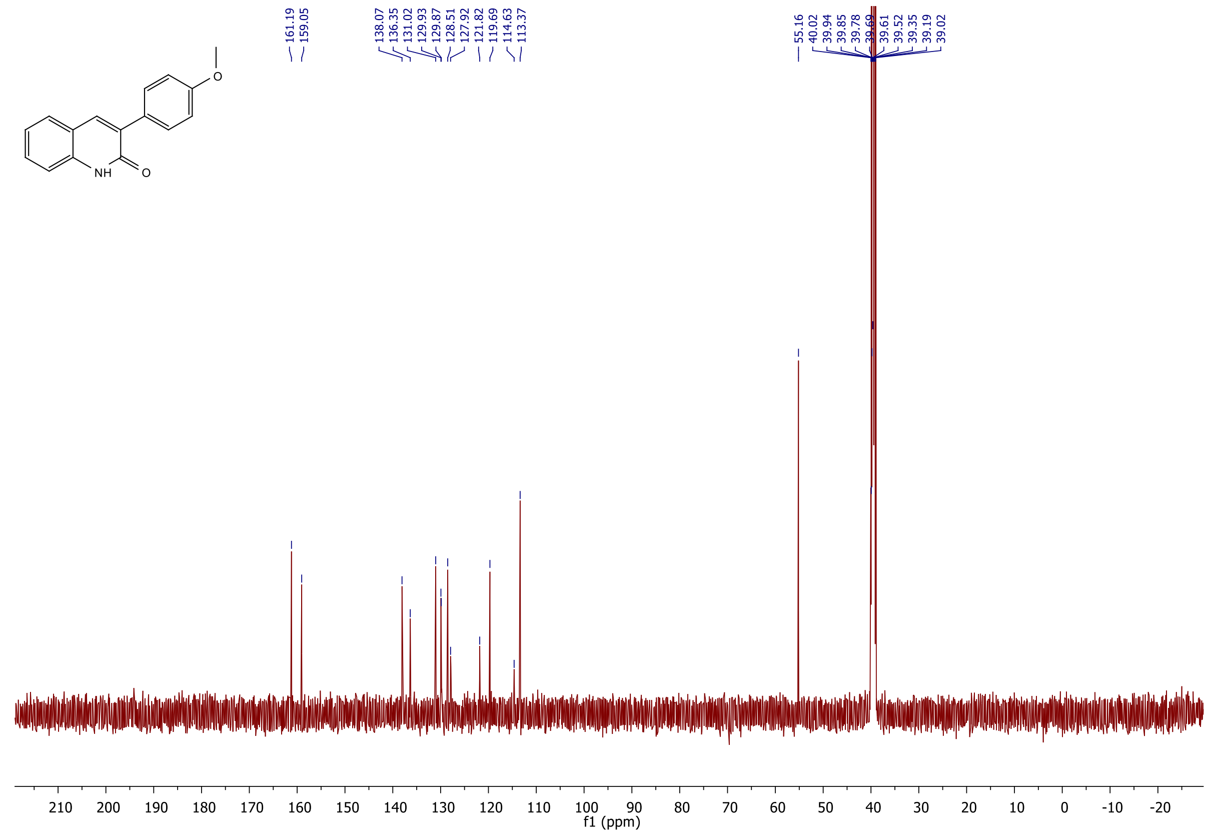


Figure S61: $^{13}C\{^{1}H\}$ NMR (125 MHz) in DMSO-d$_6$ of 2h.

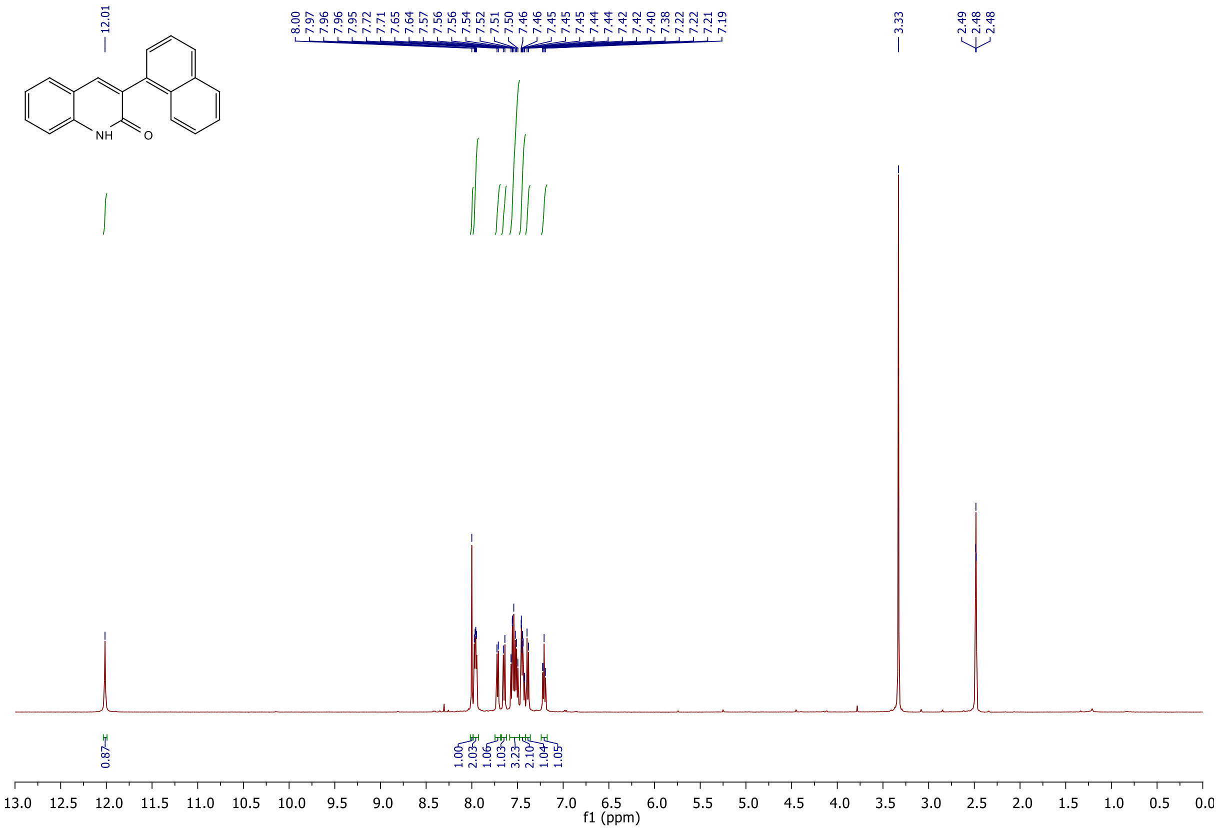


Figure S62: ^{1}H-NMR (500 MHz) in DMSO-d$_6$ of 2i.

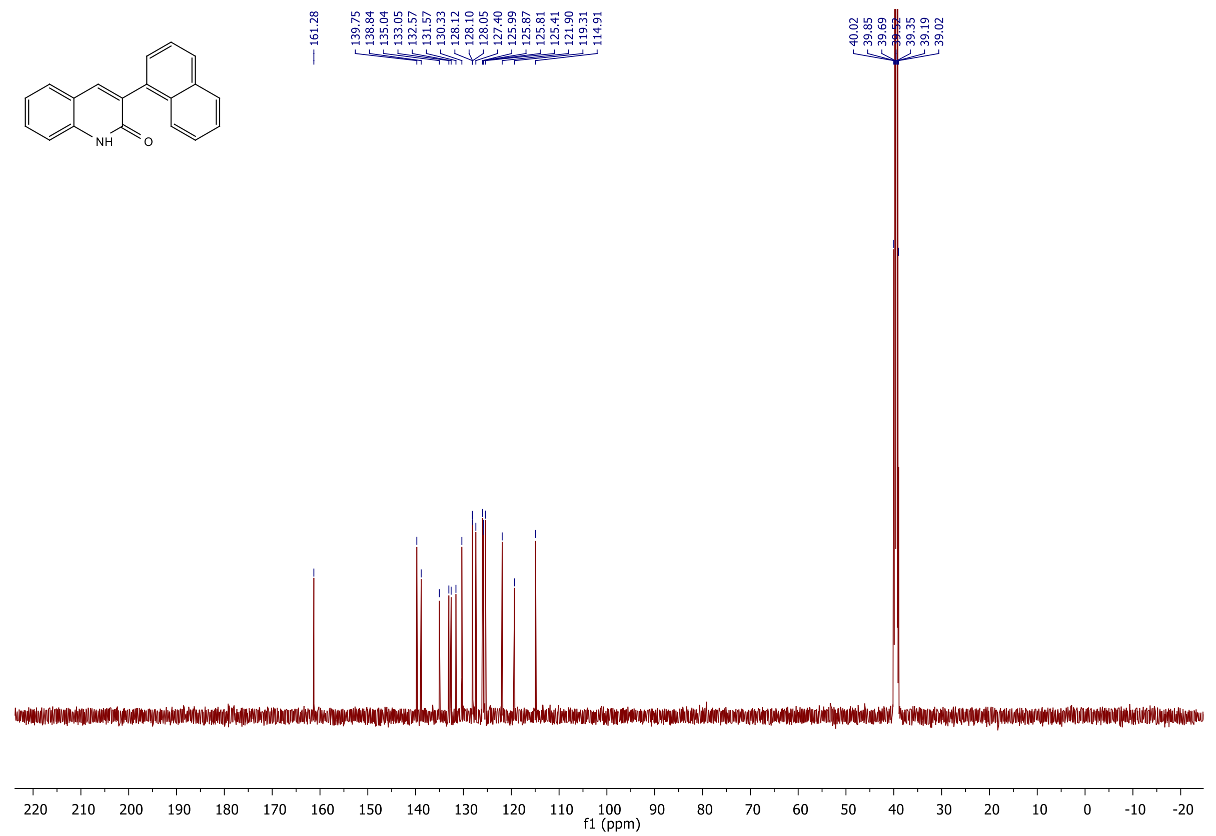


Figure S63: $^{13}C\{^{1}H\}$ NMR (125 MHz) in DMSO-d_6 of 2i.

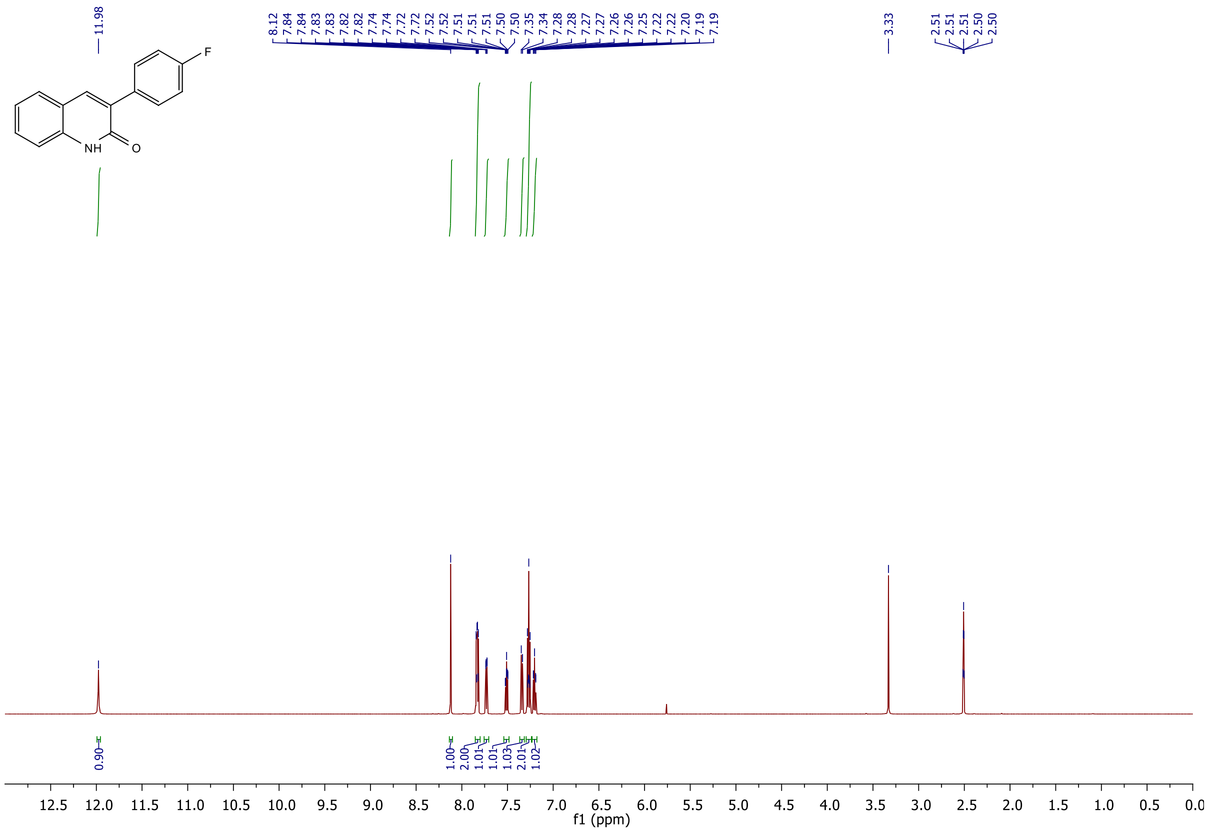


Figure S64: ^{1}H-NMR (500 MHz) in DMSO-d_6 of 2j.

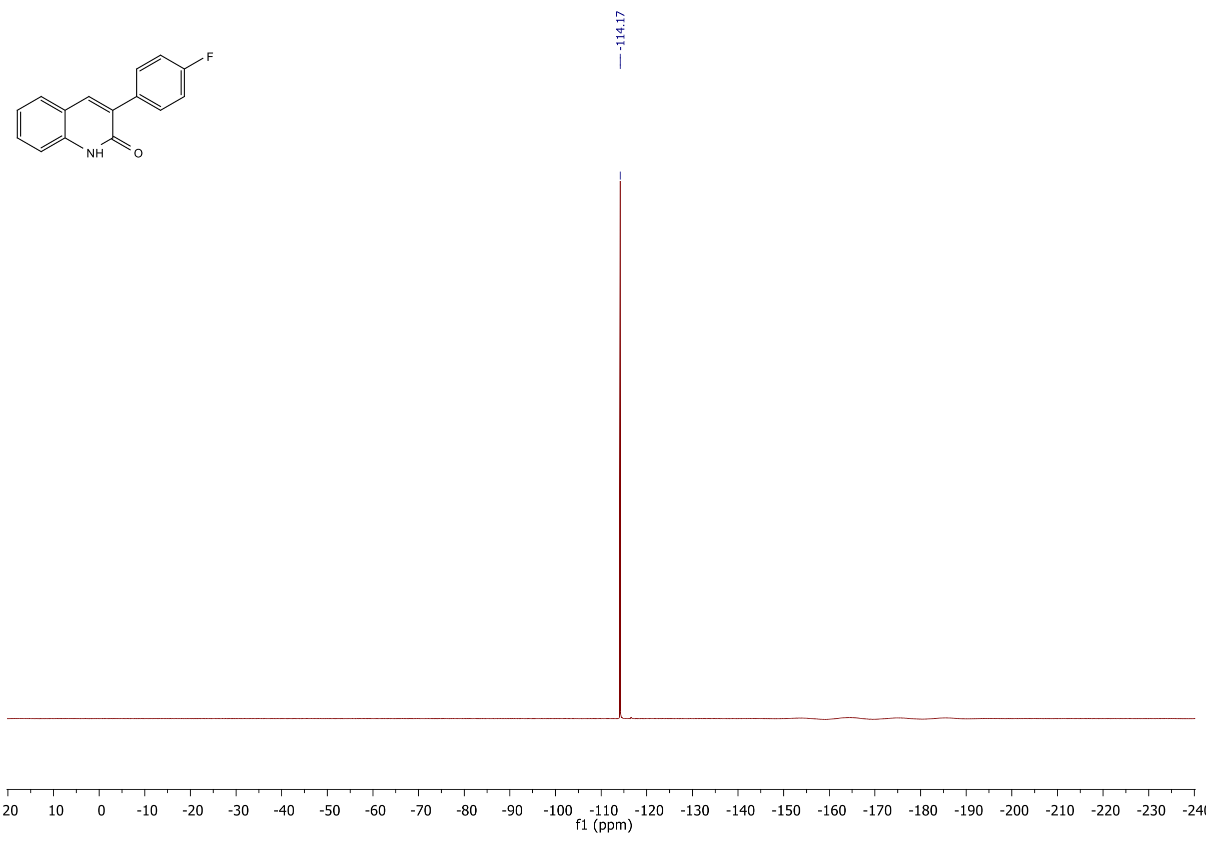


Figure S65: ^{19}F-NMR (500 MHz) in DMSO-d$_6$ of 2j.

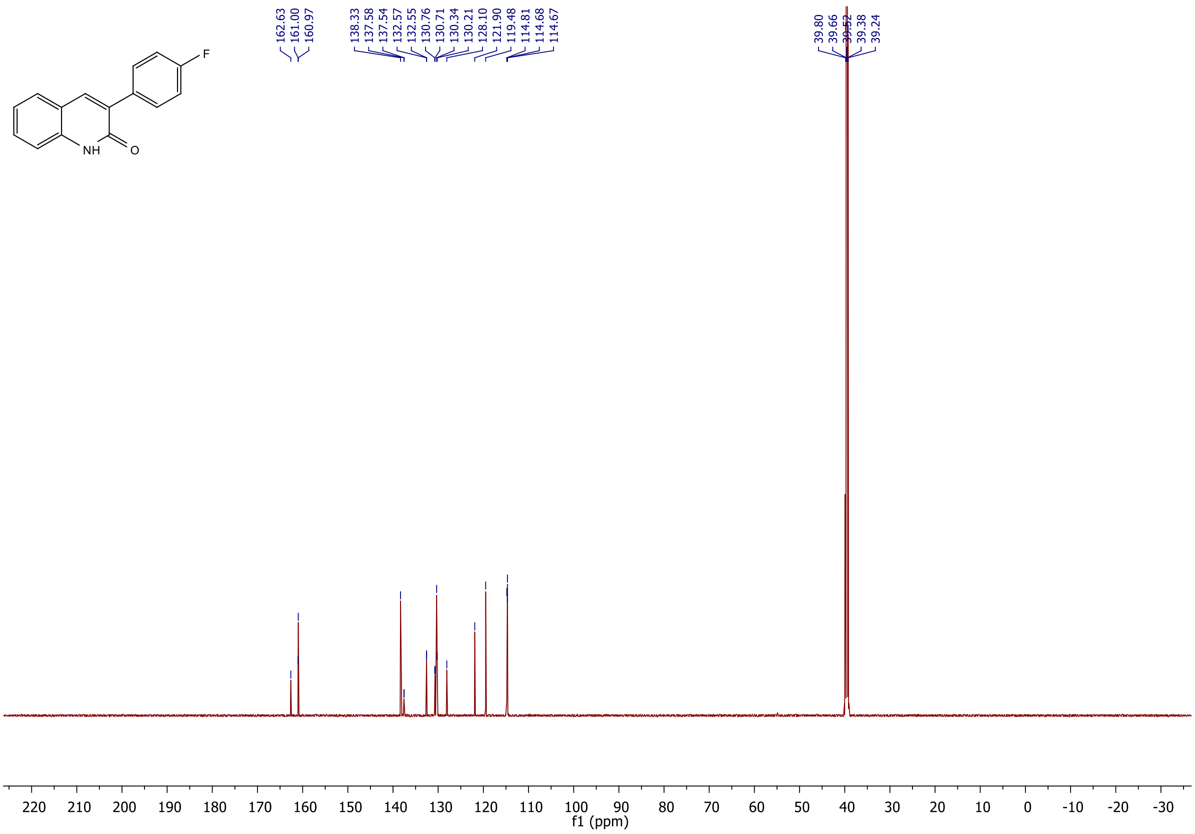


Figure S66: ^{13}C{^{1}H} NMR (125 MHz) in DMSO-d$_6$ of 2j.

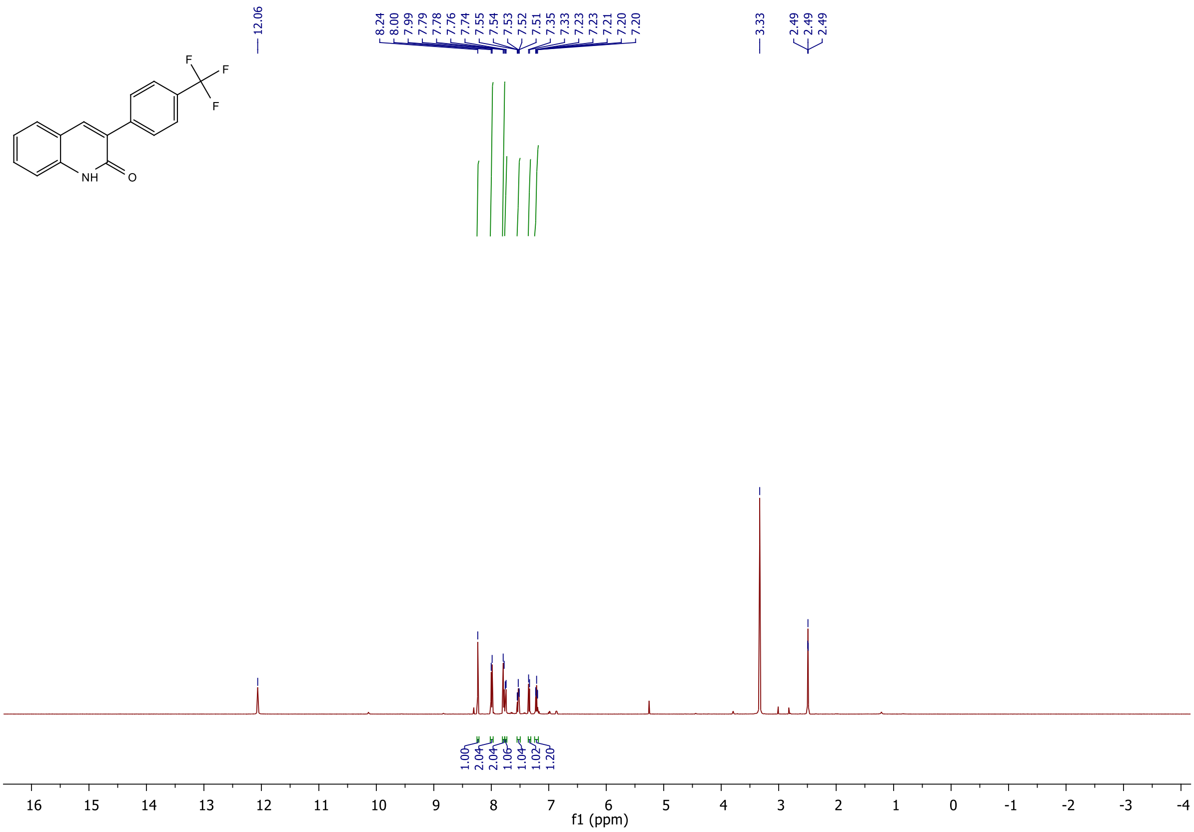


Figure S67: [1]H-NMR (500 MHz) in DMSO-d_6 of 2k.

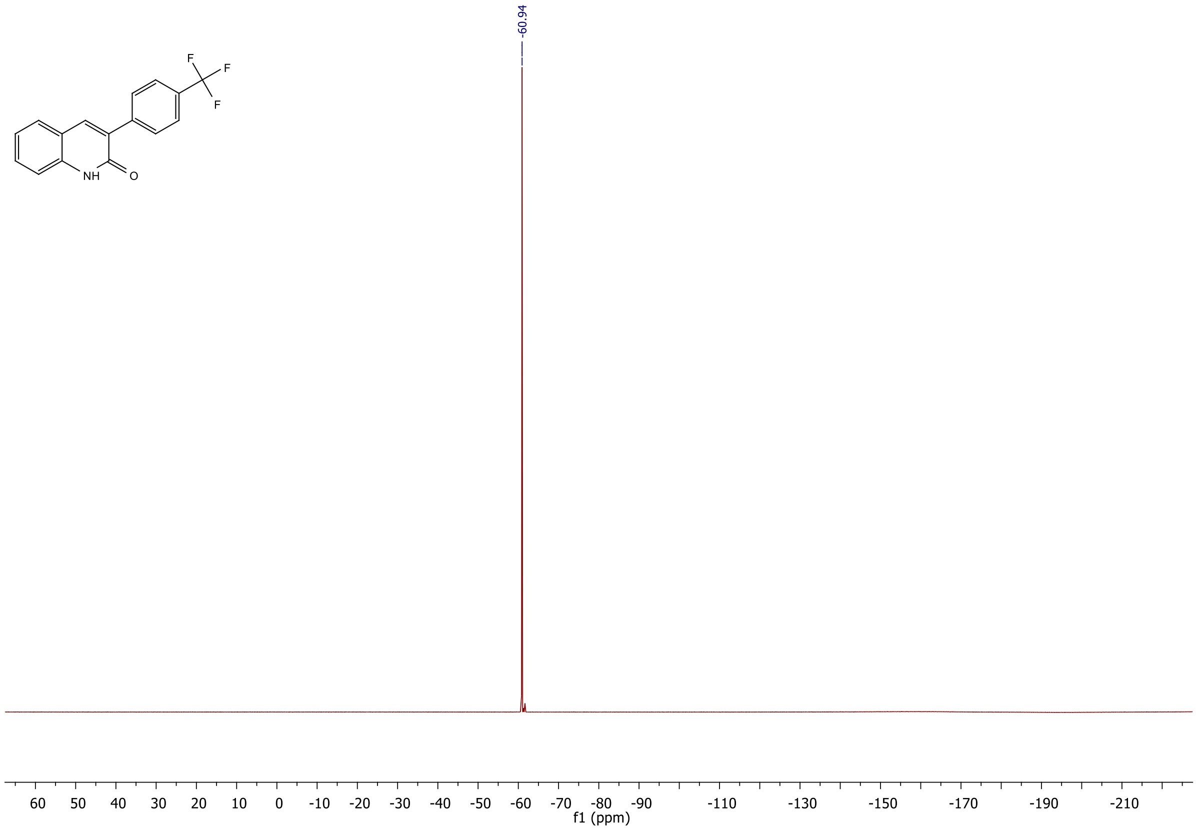


Figure S68: [19]F-NMR (500 MHz) in DMSO-d_6 of 2k.

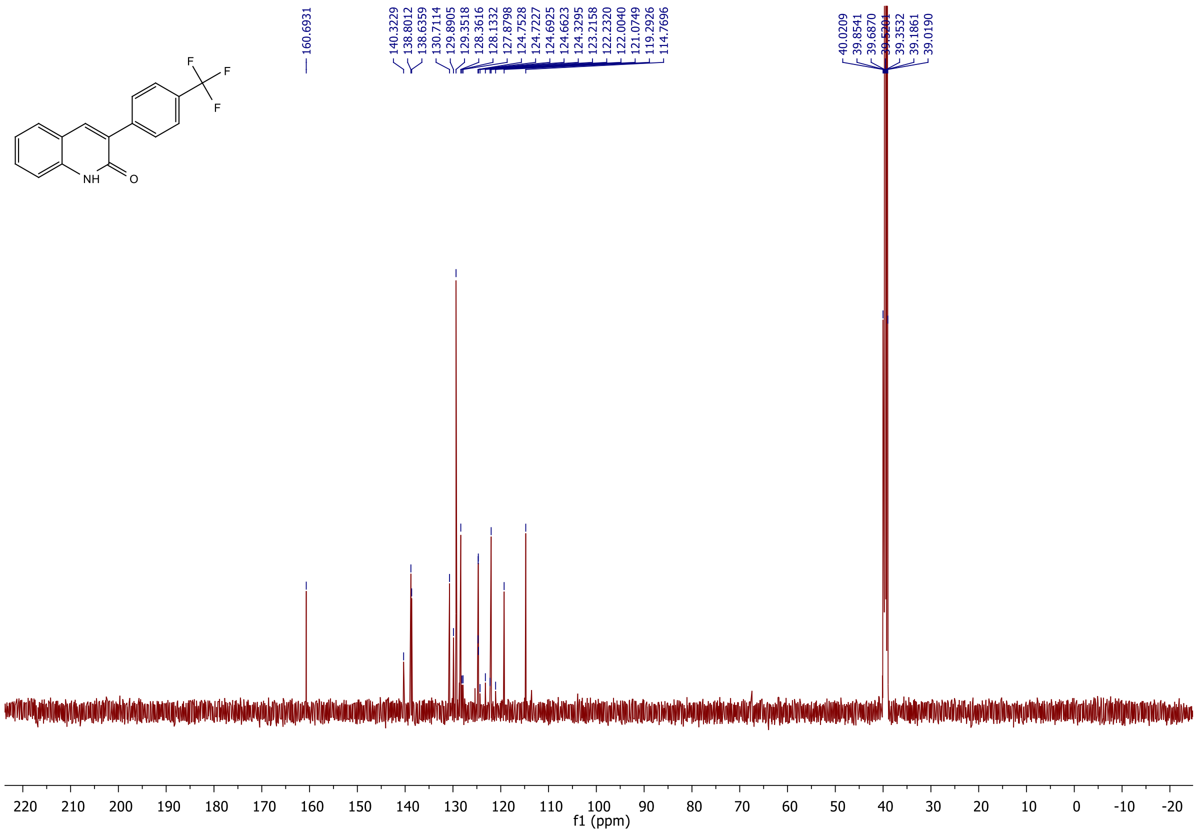


Figure S69: $^{13}C\{^{1}H\}$ NMR (125 MHz) in DMSO-d$_6$ of 2k.

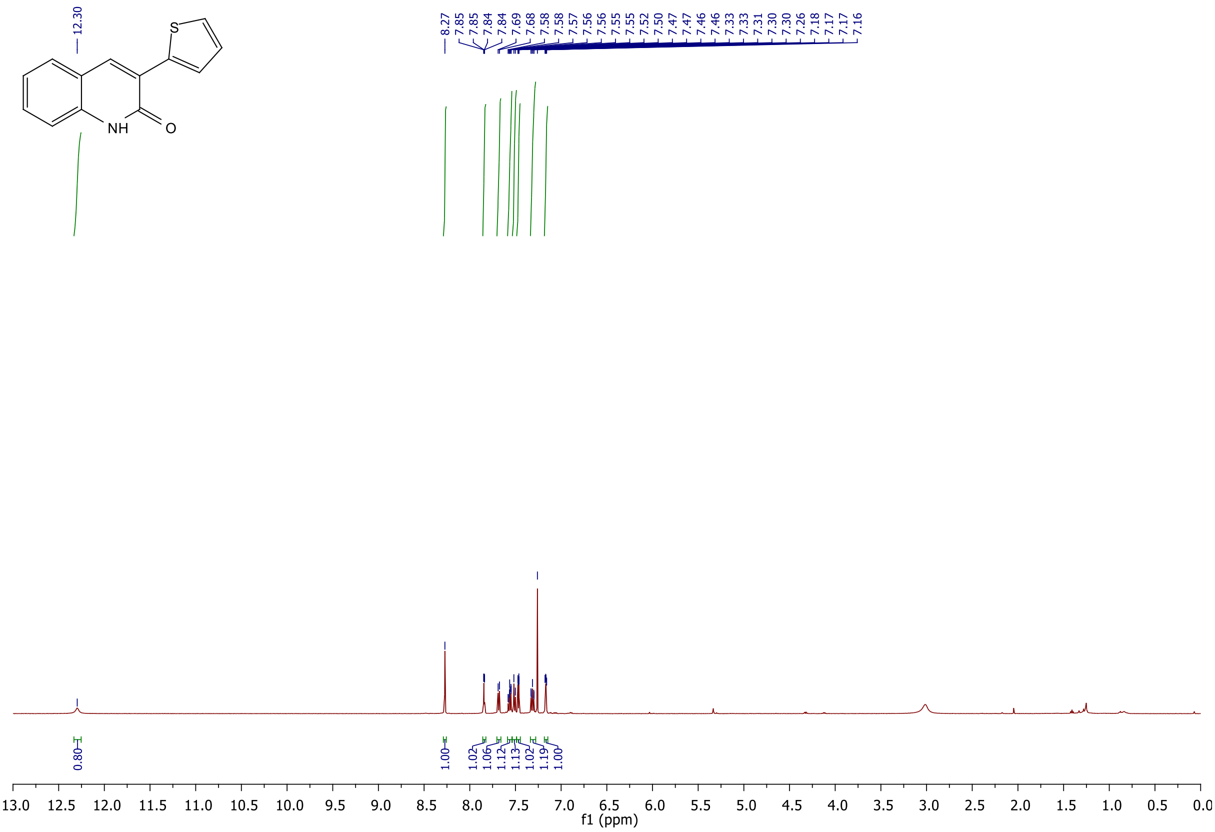


Figure S70: ^{1}H-NMR (125 MHz) in $CDCl_3$ of 2l.

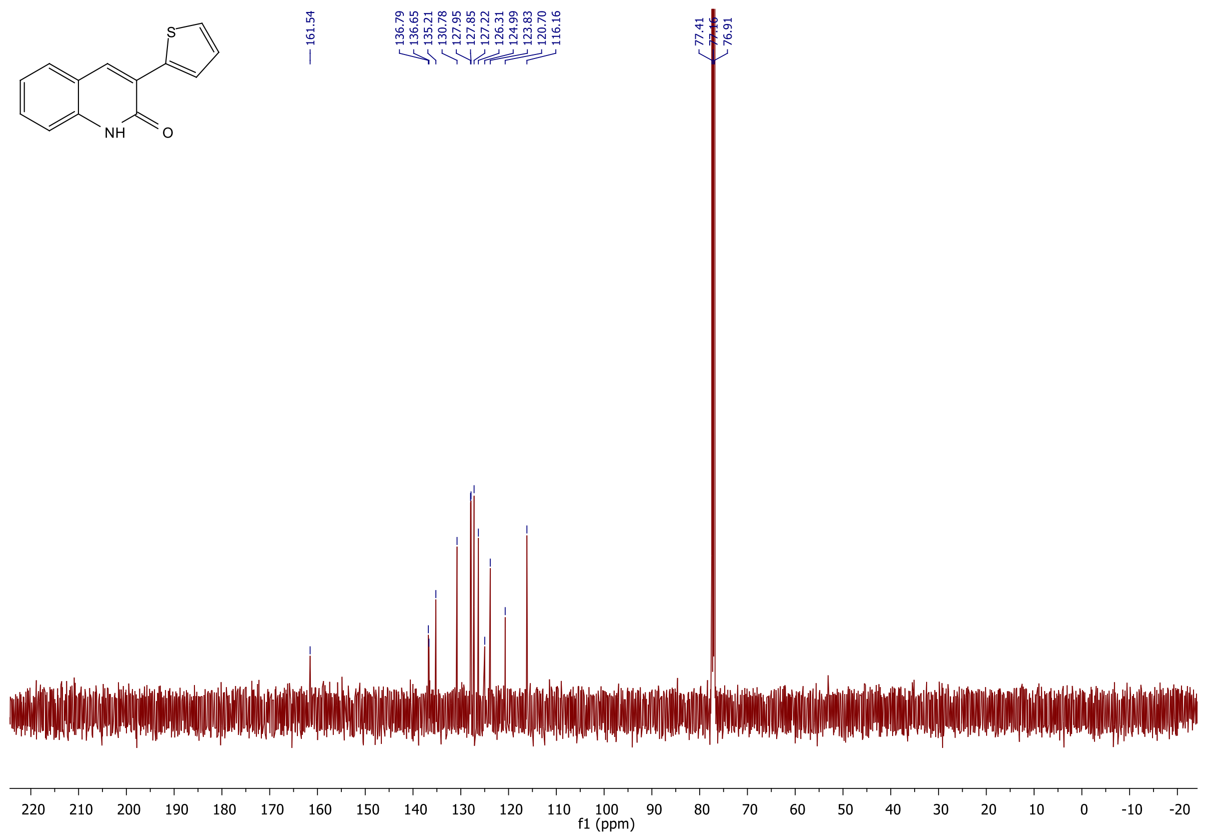


Figure S71: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 2l.

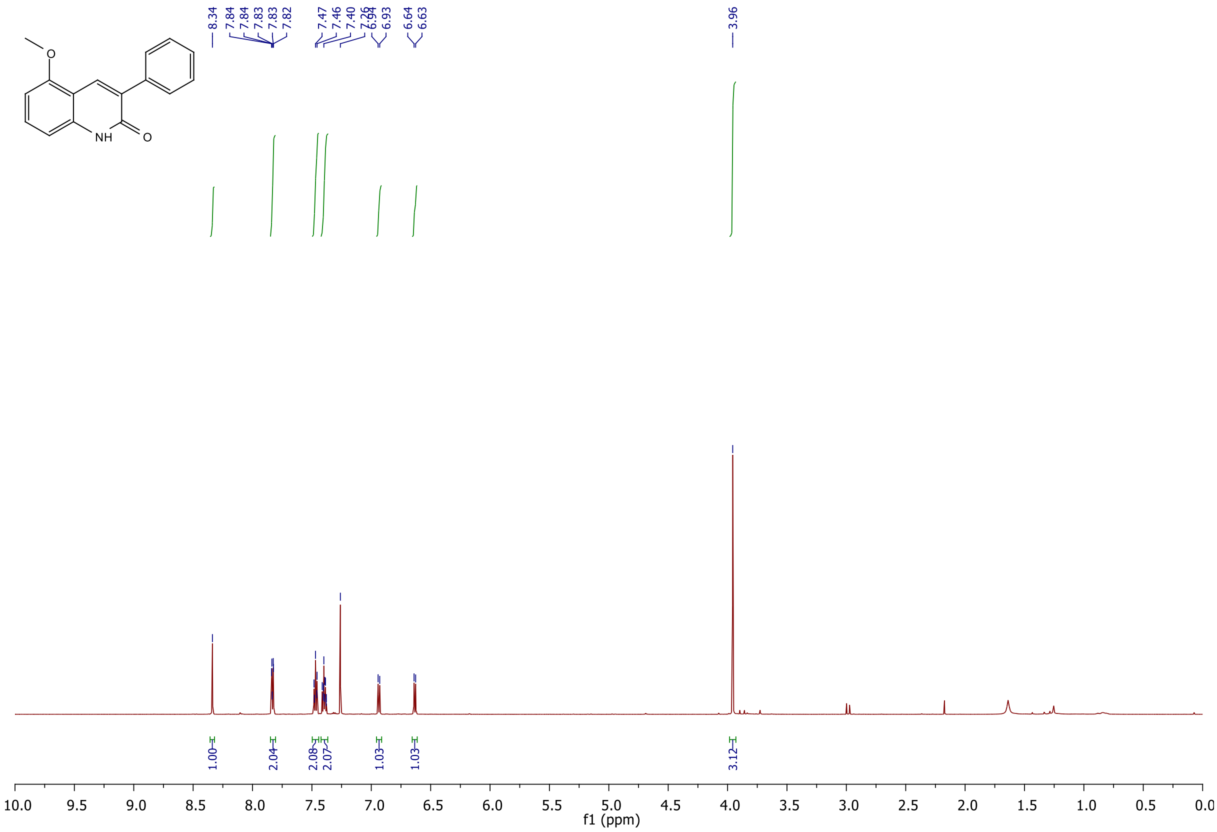


Figure S72: ^1H-NMR (125 MHz) in $CDCl_3$ of 2m.

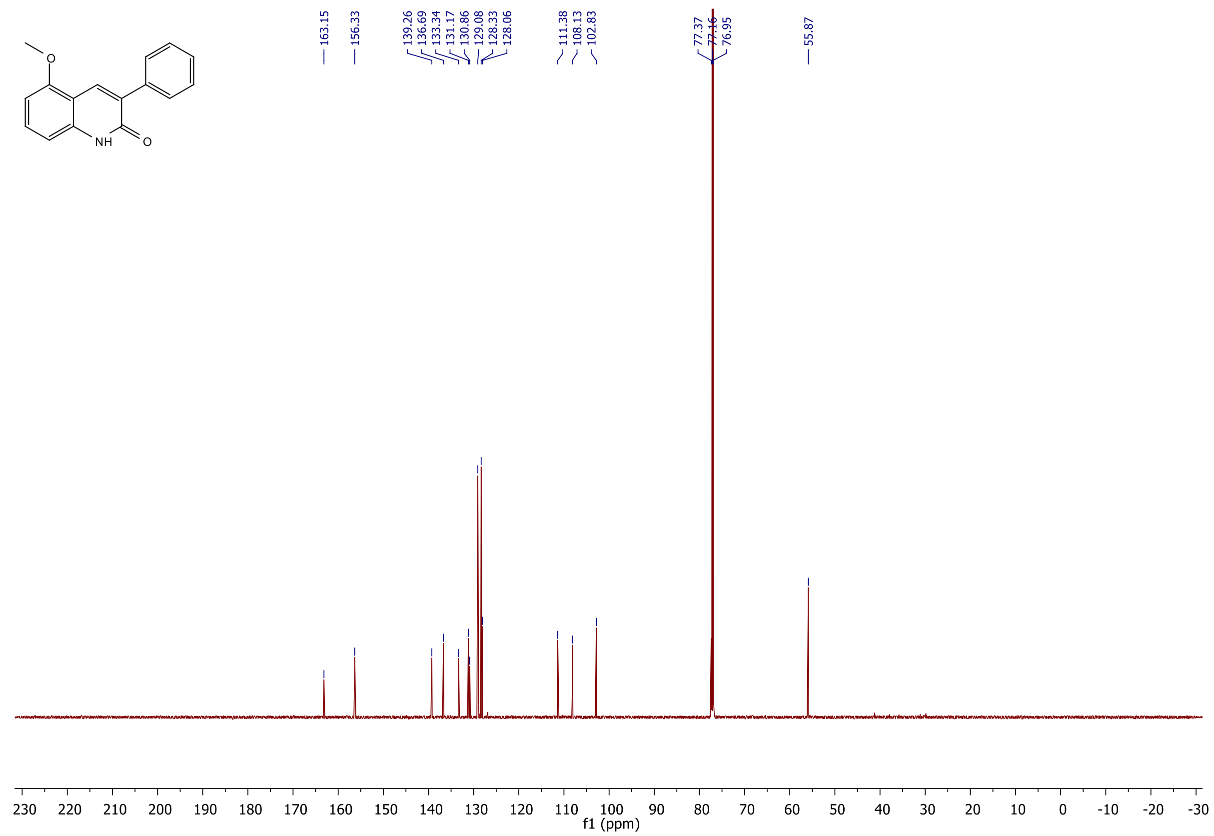


Figure S73: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 2m.

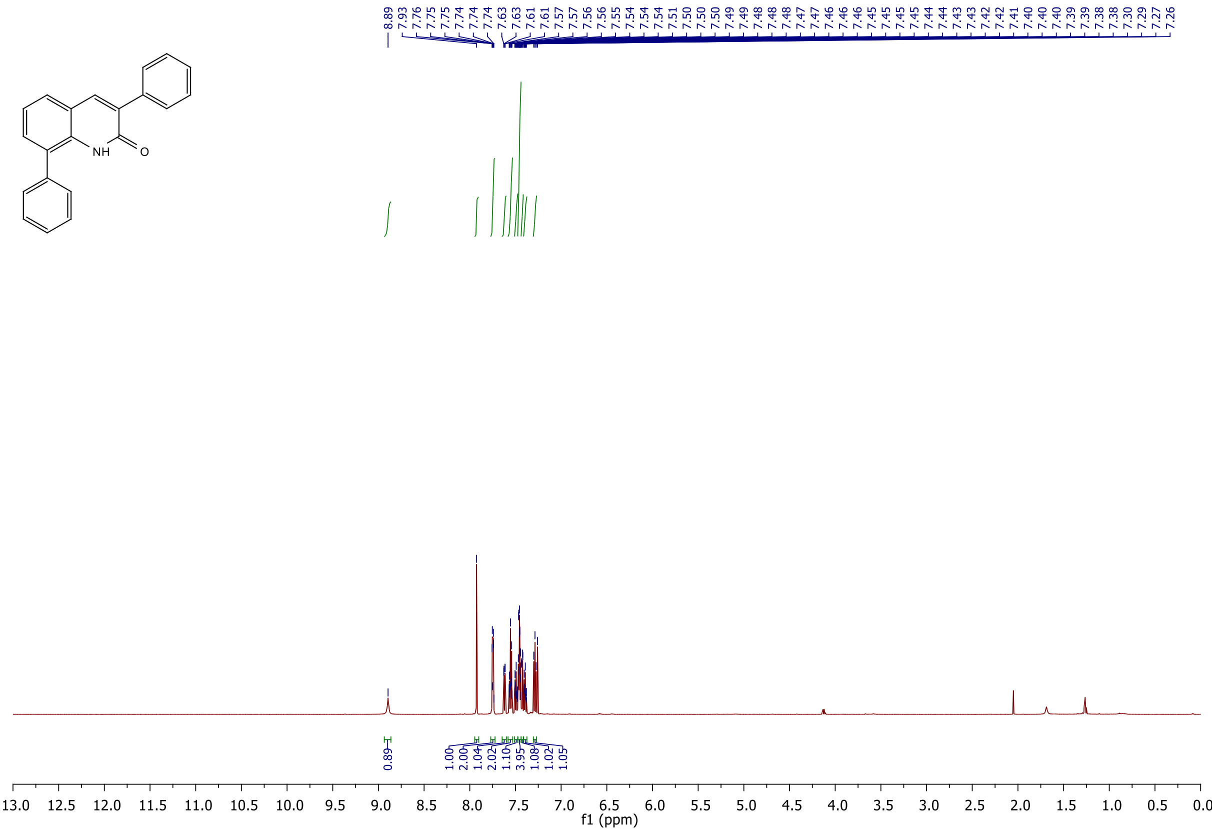


Figure S74: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 2n.

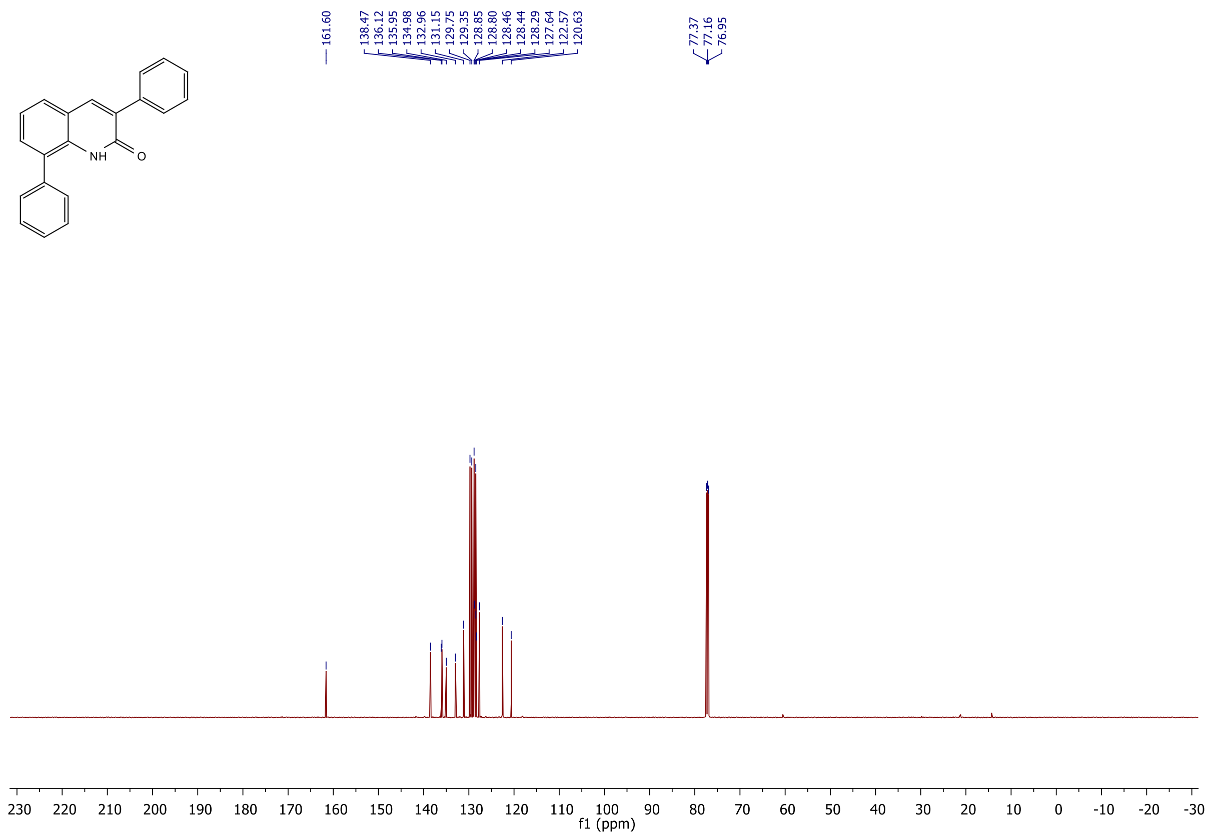


Figure S75: $^{13}C\{^1H\}$ NMR (125 MHz) in $CDCl_3$ of 2n.

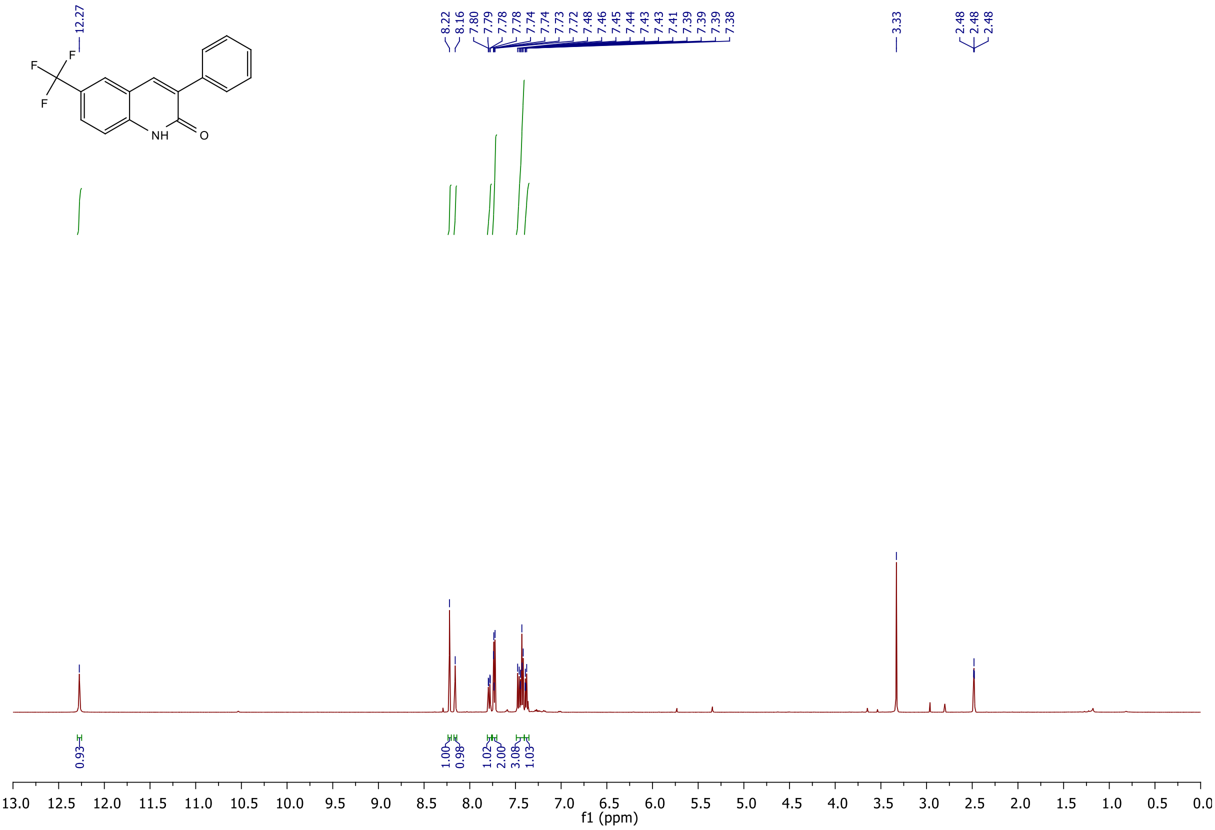


Figure S76: ^1H-NMR (500 MHz) in DMSO-d_6 of 2o.

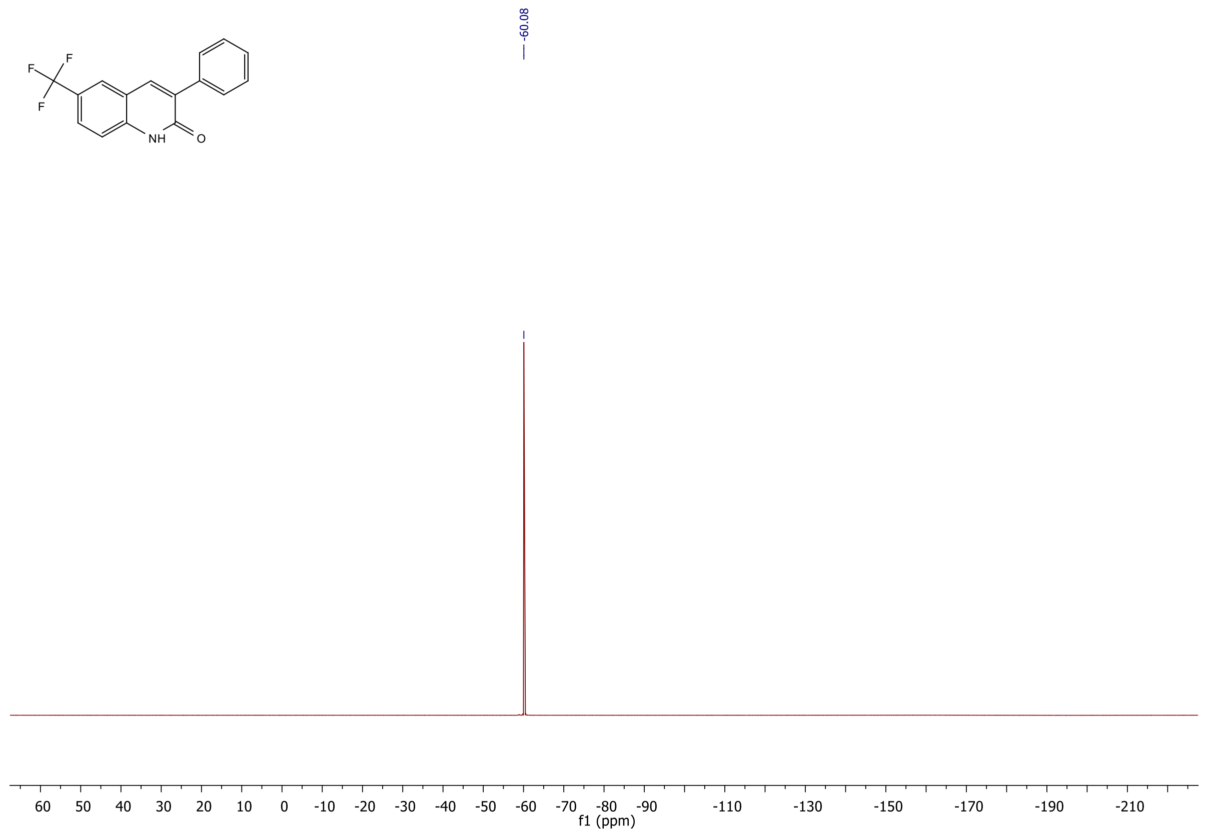


Figure S77: ^{19}F-NMR (500 MHz) in DMSO-d$_6$ of 2o.

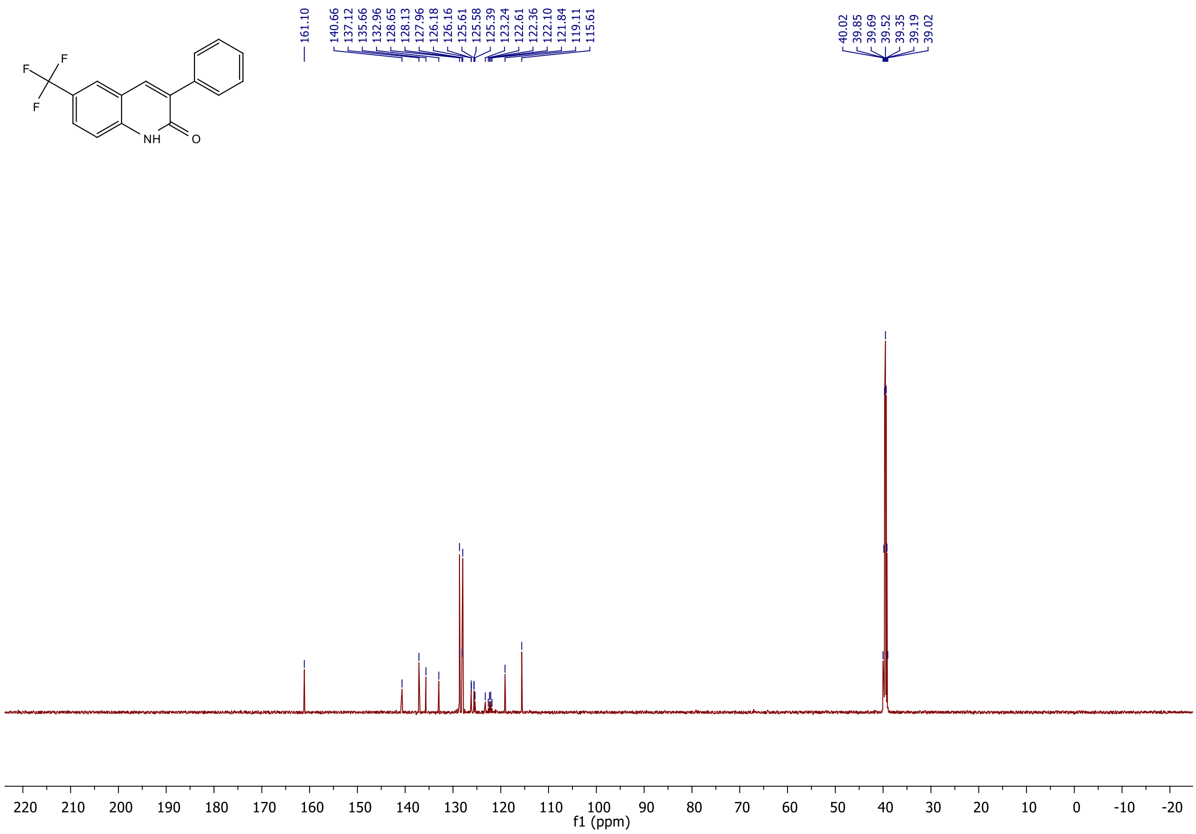


Figure S78: ^{13}C{^{1}H} NMR (125 MHz) in DMSO-d$_6$ of 2o.

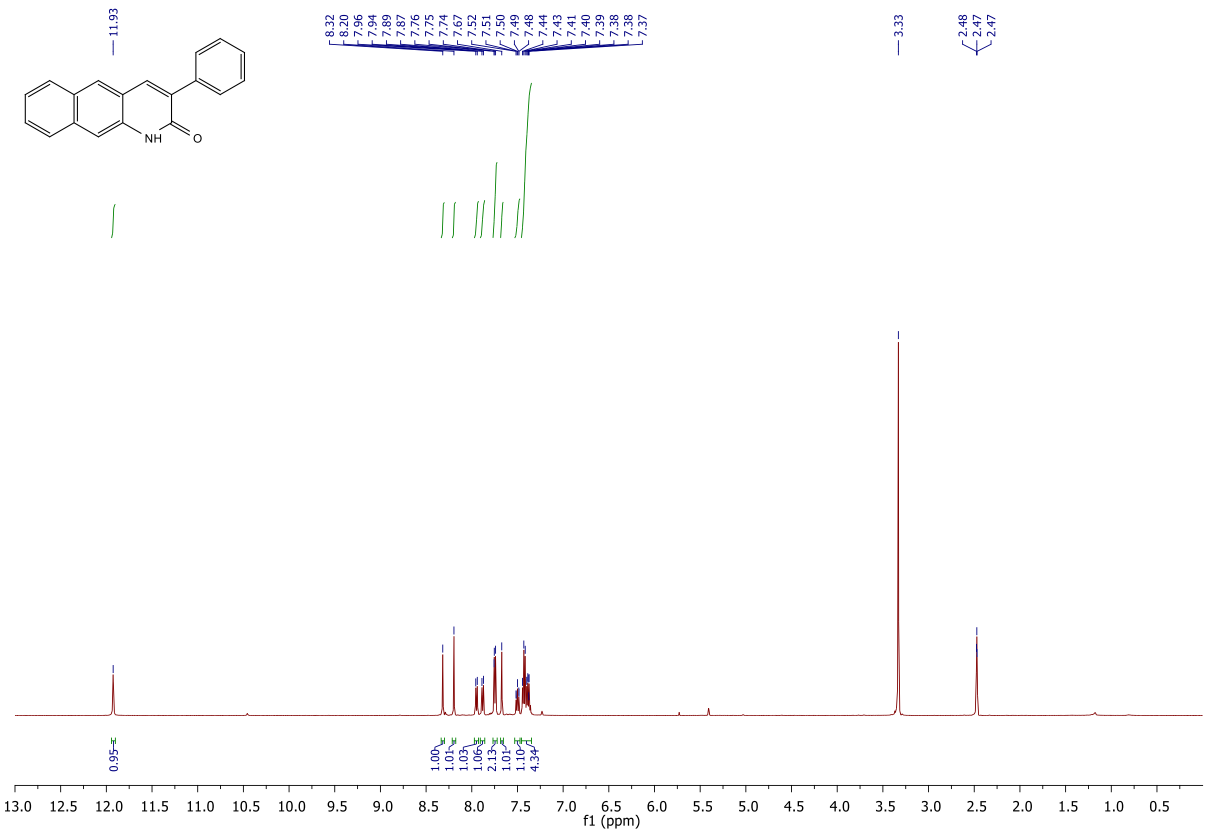


Figure S79: [1]H-NMR (500 MHz) in DMSO-d$_6$ of 2p.

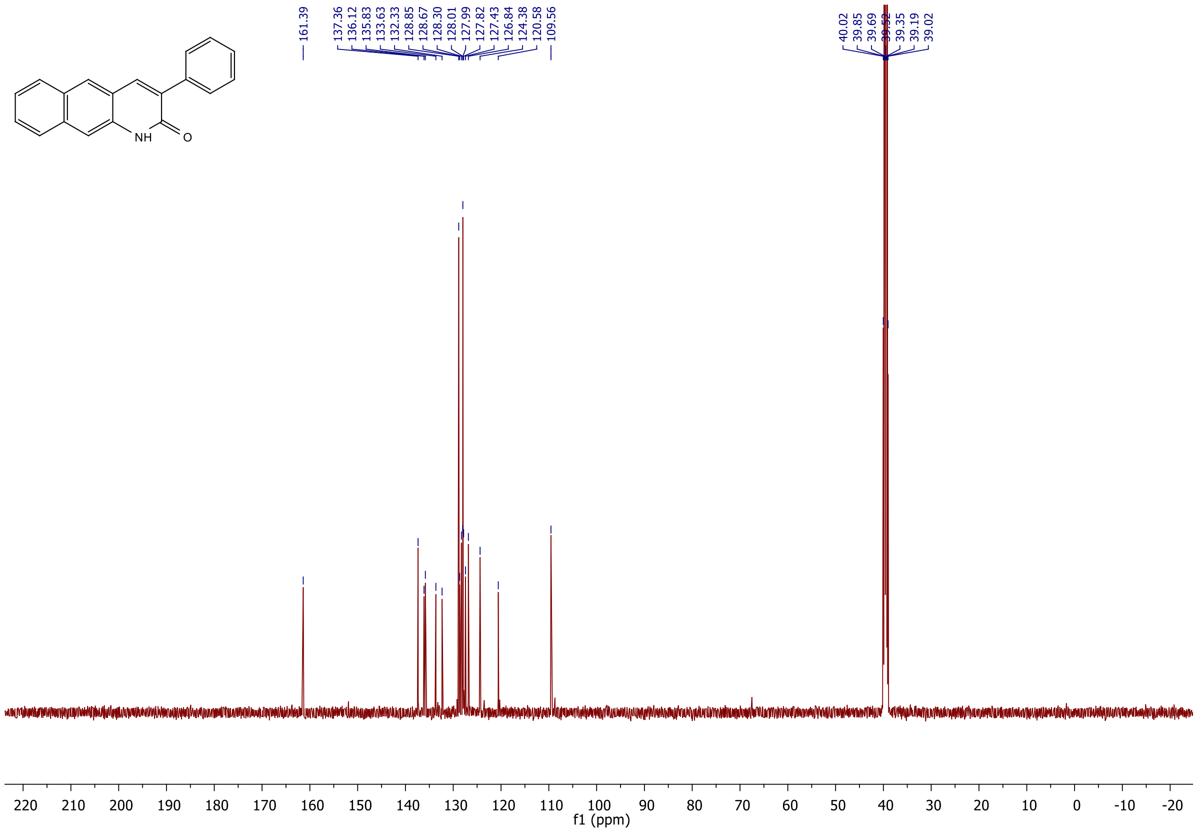


Figure S80: [13]C{[1]H} NMR (125 MHz) in DMSO-d$_6$ of 2p.

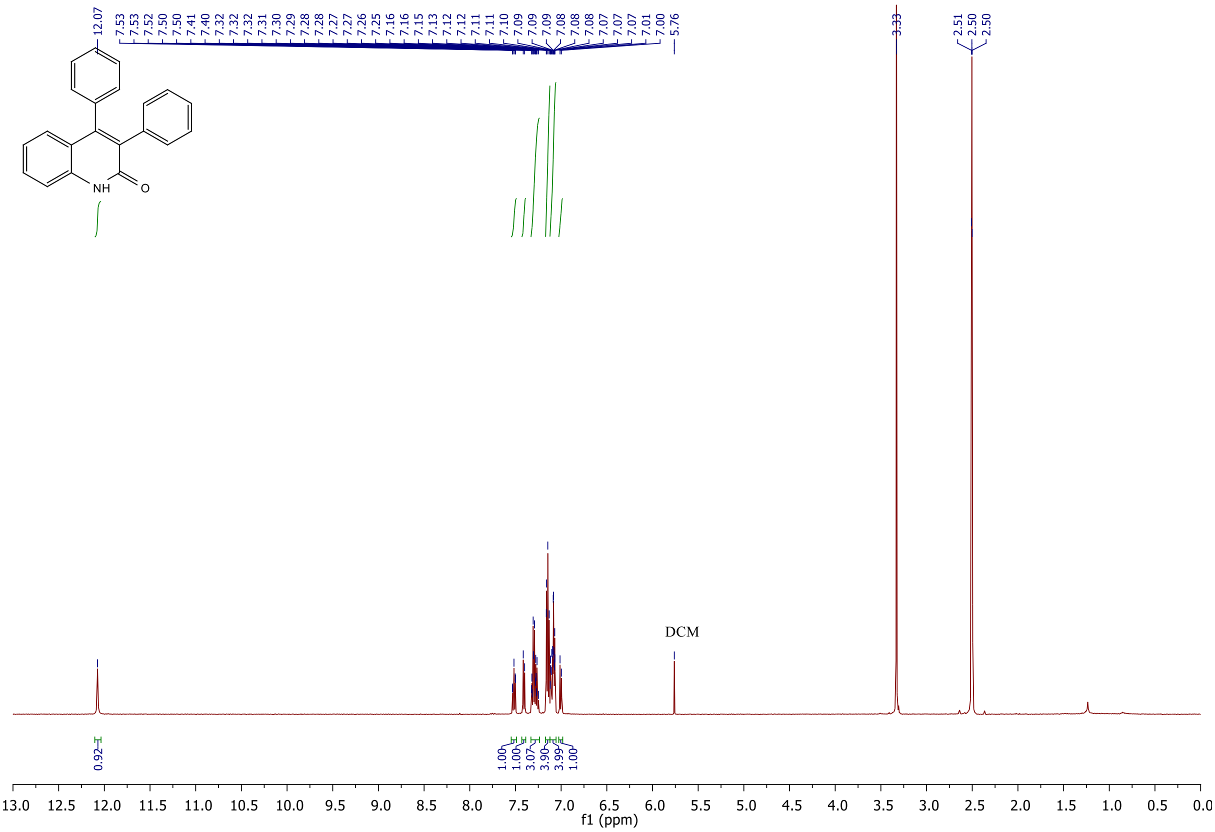


Figure S81: ^{1}H-NMR (500 MHz) in DMSO-d_6 of 2q.

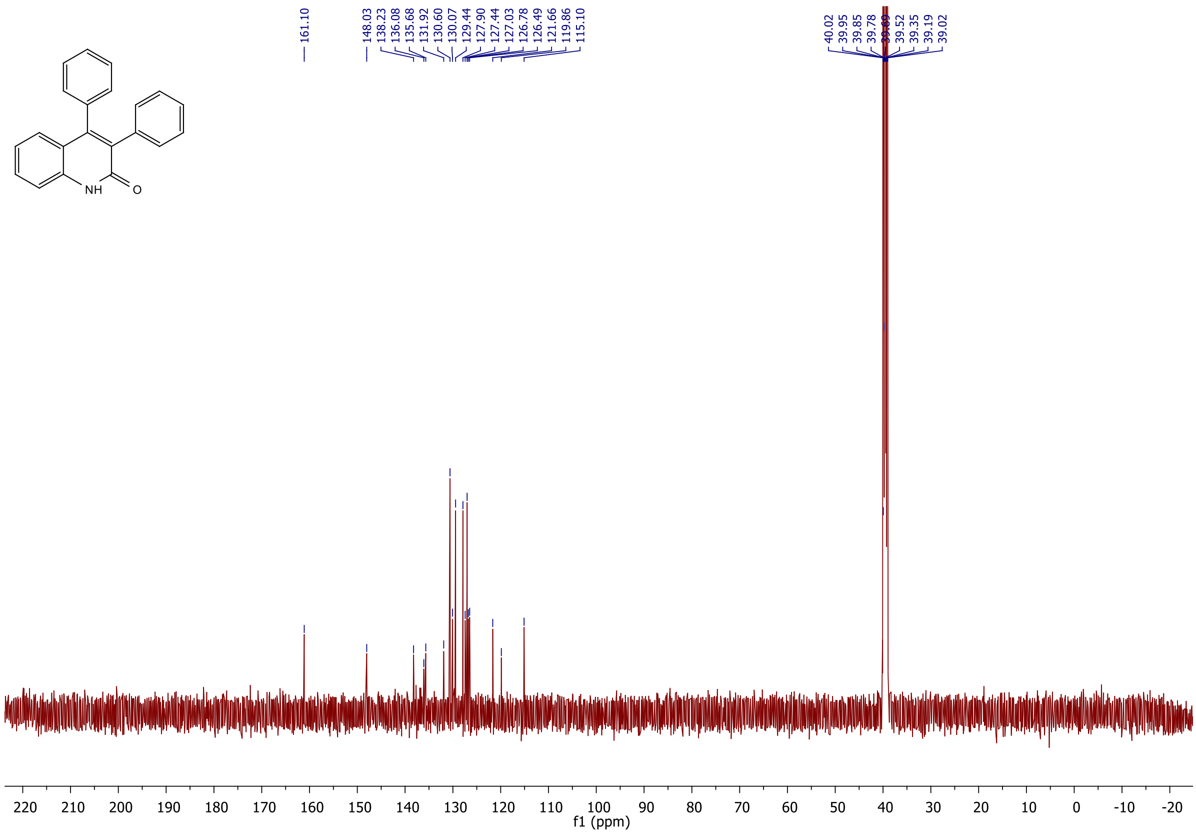


Figure S82: ^{13}C{^{1}H} NMR (125 MHz) in DMSO-d_6 of 2q.

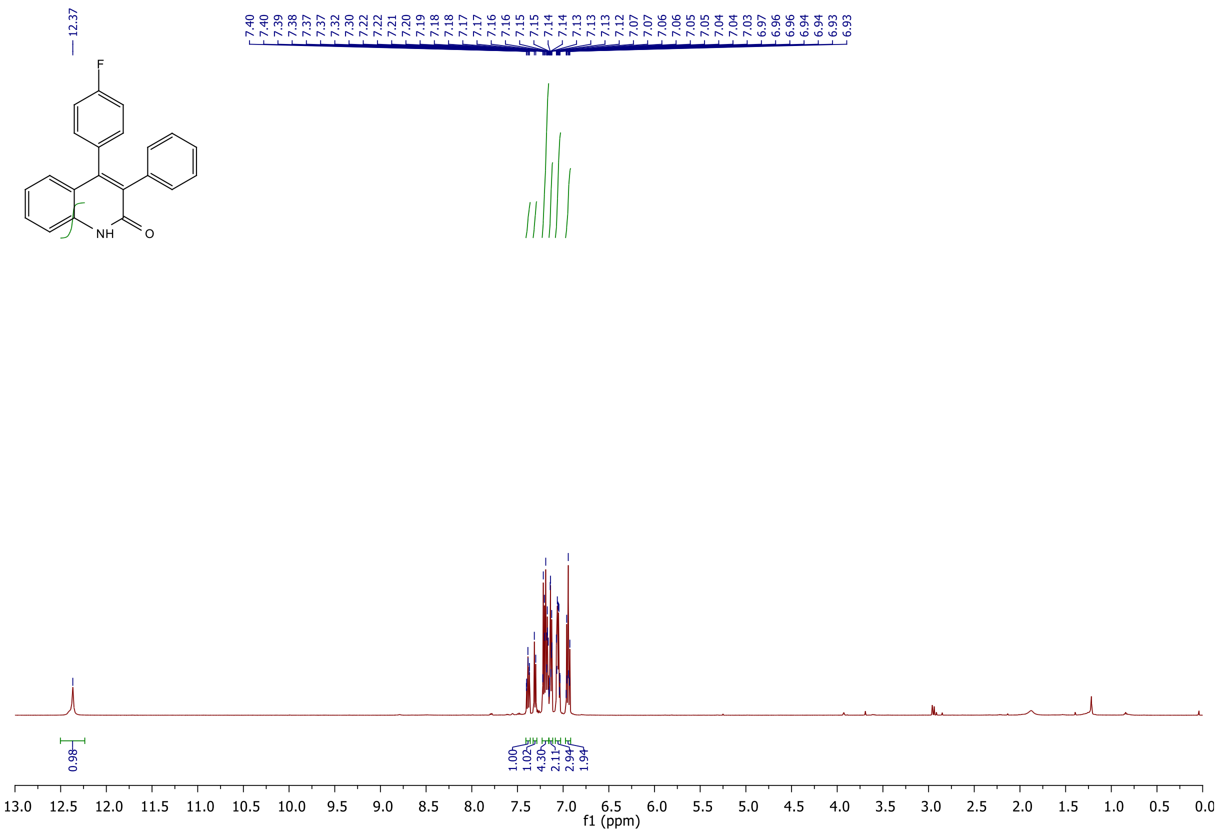


Figure S83: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2r.

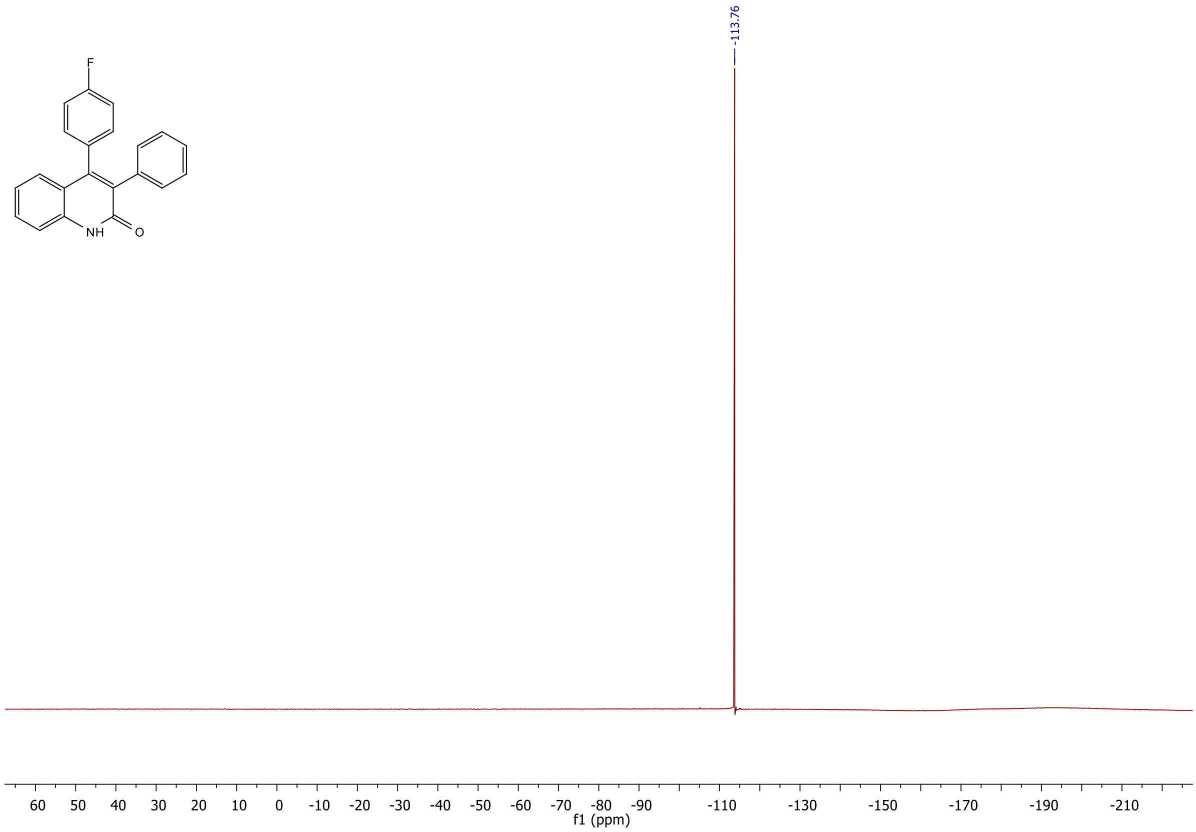


Figure S84: ^{19}F-NMR (500 MHz) in $CDCl_3$ of 2r.

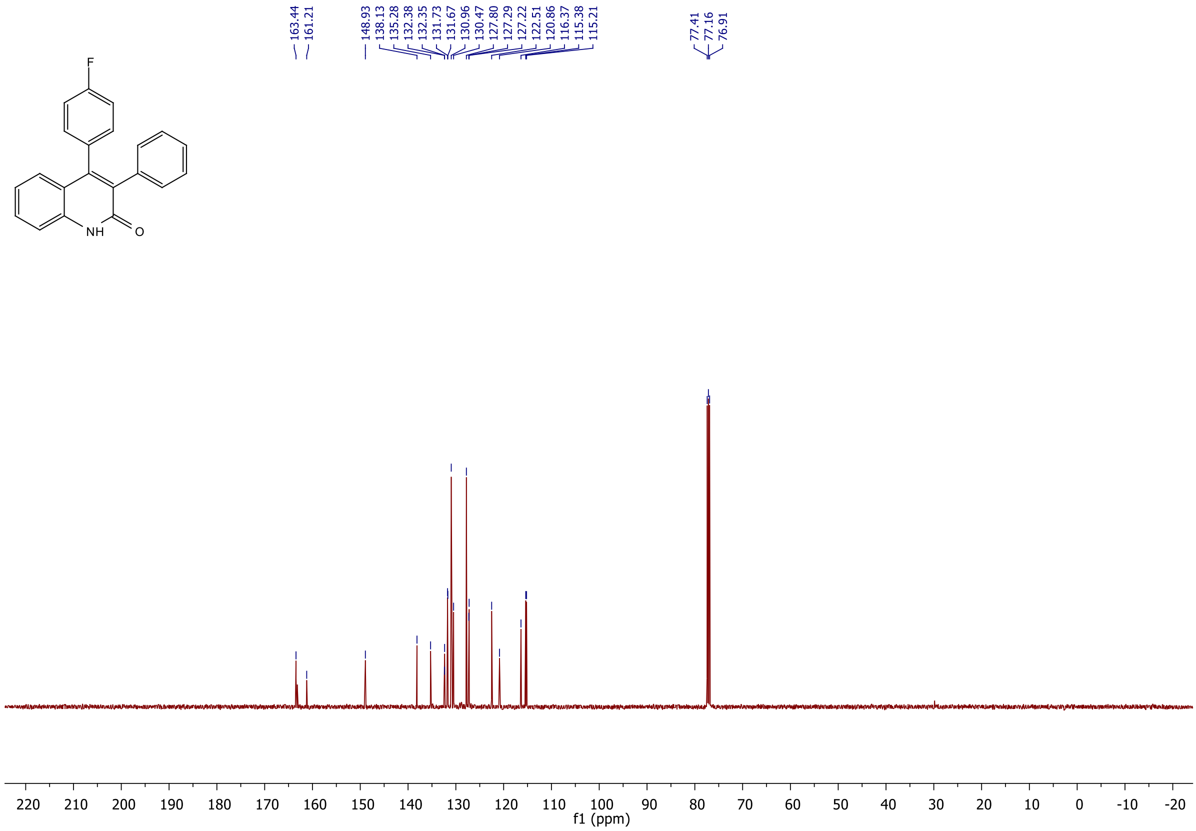


Figure S85: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2r.

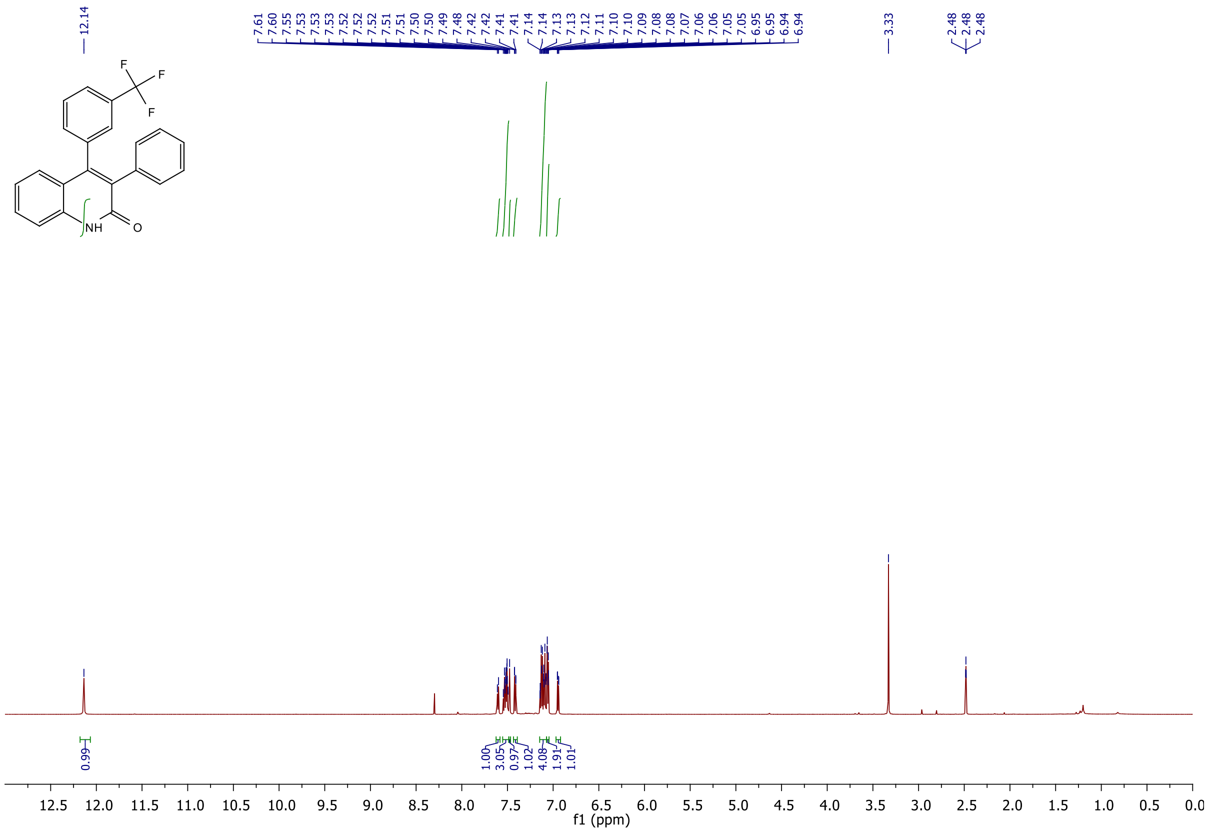


Figure S86: ^{1}H-NMR (500 MHz) in DMSO-d_6 of 2s.

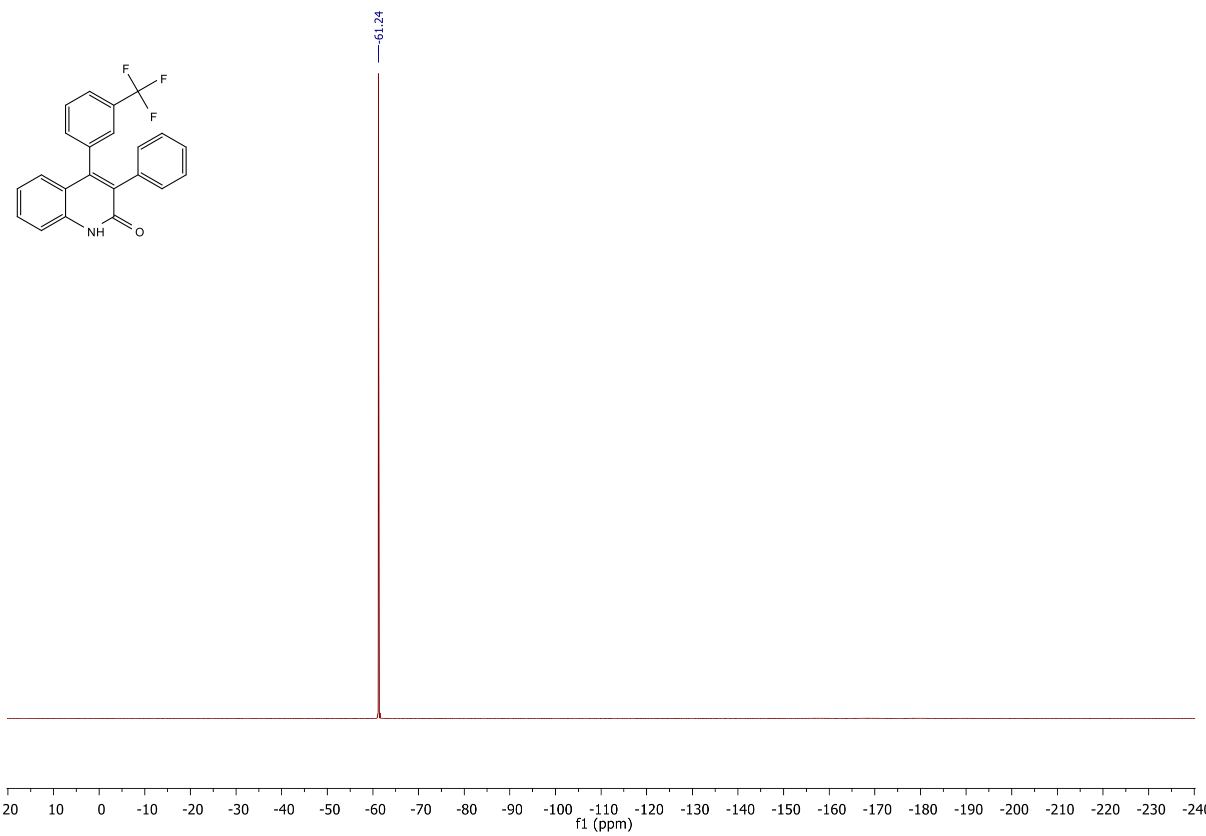


Figure S87: ^{19}F-NMR (500 MHz) in DMSO-d$_6$ of 2s.

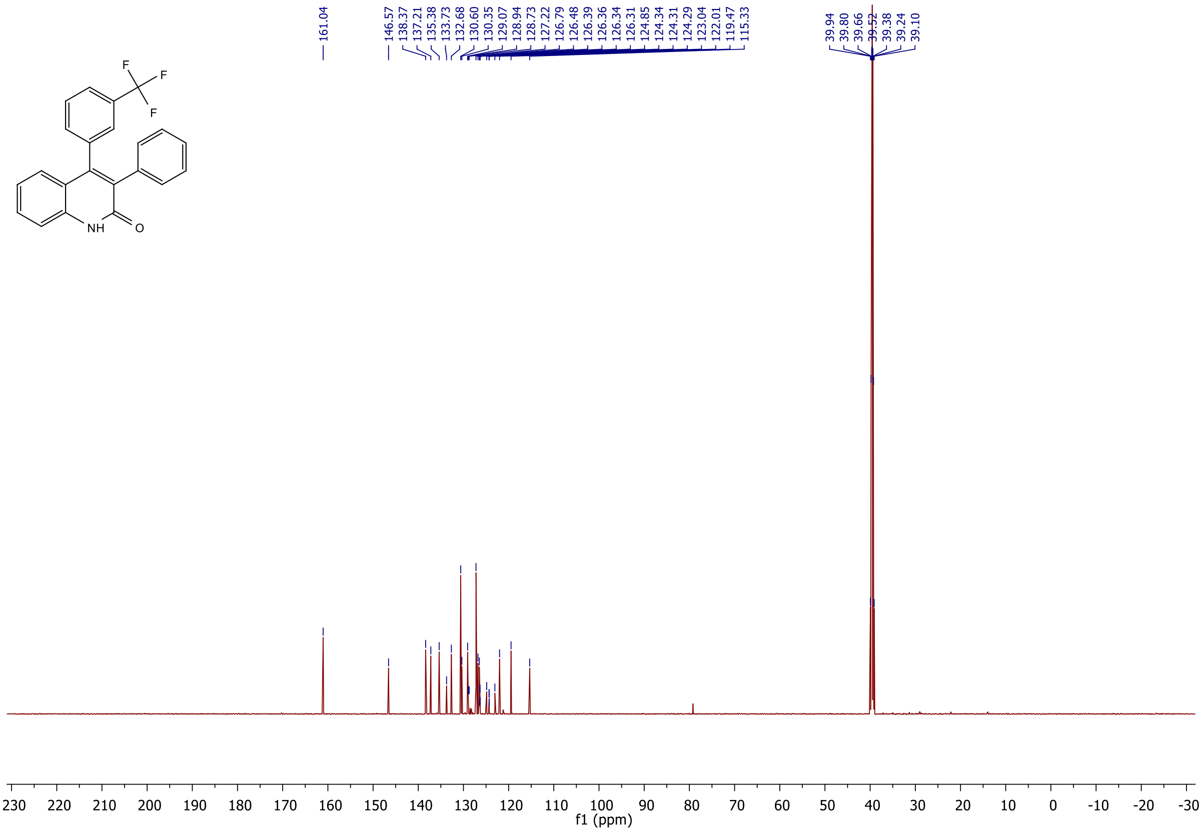


Figure S88: ^{13}C{^{1}H} NMR (125 MHz) in DMSO-d$_6$ of 2s.

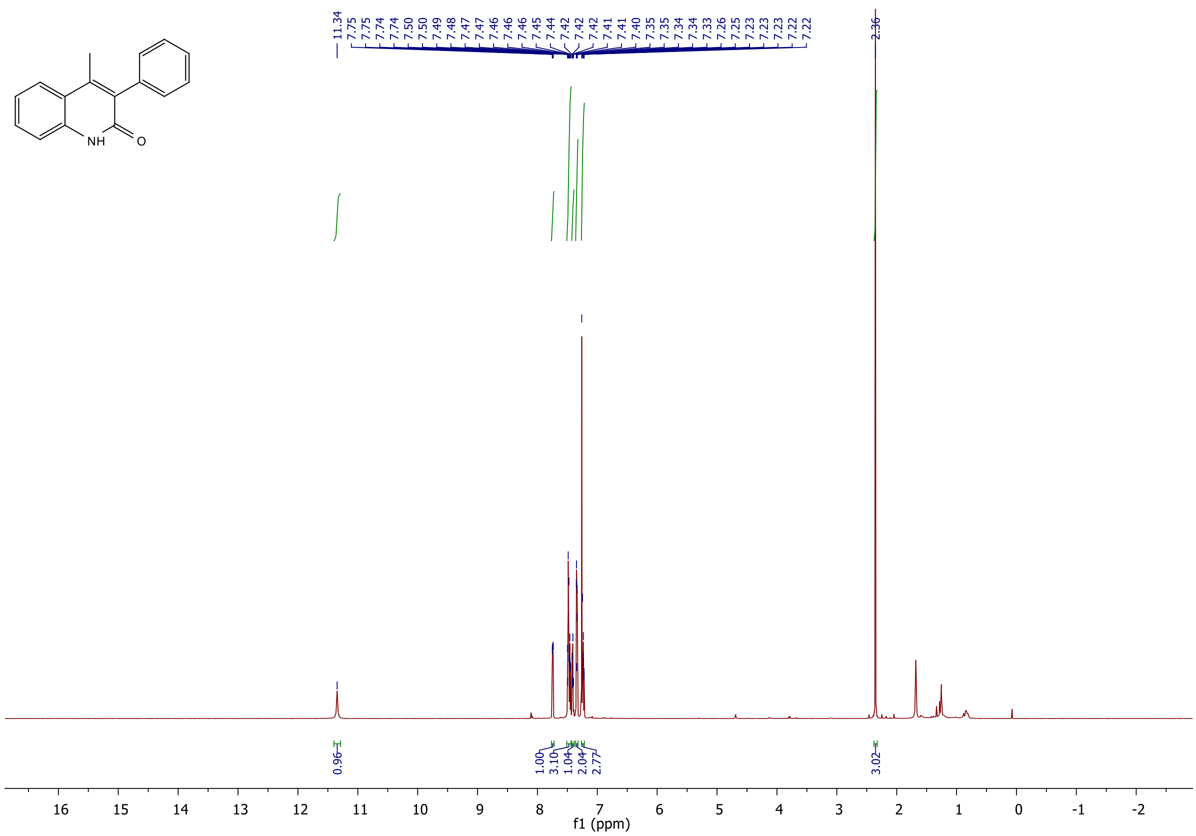


Figure S89: ^{1}H-NMR (500 MHz) in $CDCl_3$ of 2t.

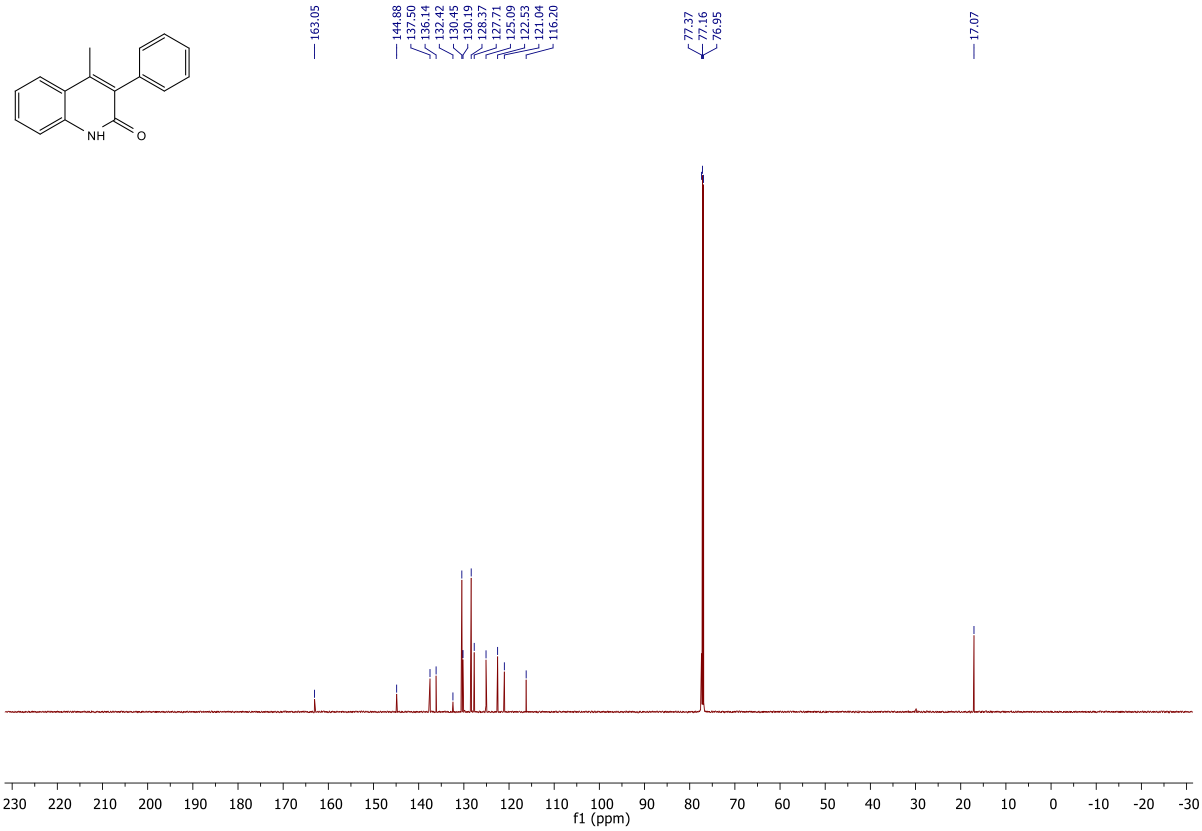
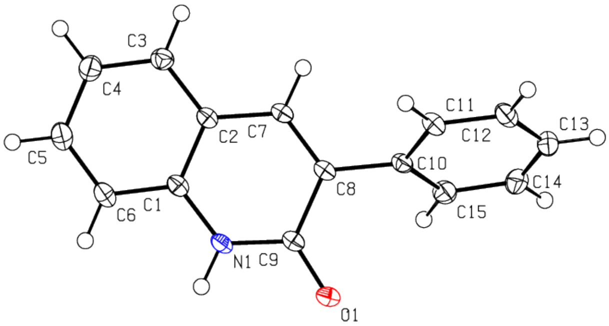


Figure S90: $^{13}C\{^{1}H\}$ NMR (125 MHz) in $CDCl_3$ of 2t.

Part 7: X-Ray data.

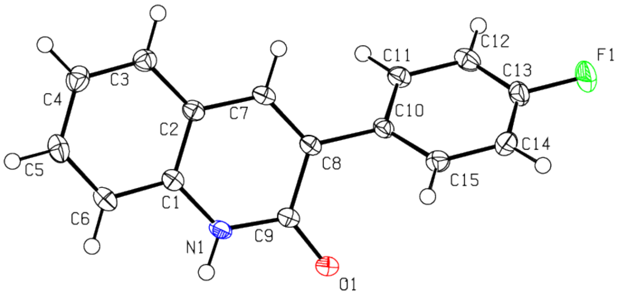
- **X-Ray data of compound 2a.**



Single crystals suitable for X-Ray crystallographic analysis were obtained by slow evaporation of a methanol solution of **2a**.

Crystal data	
Chemical formula	$C_{15}H_{11}NO$
M_r	221.25
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	17.8048 (14), 5.7547 (5), 21.5754 (16)
β (°)	105.736 (3)
V (Å^3)	2127.8 (3)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.18 × 0.09 × 0.08
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan *SADABS* 2016/2
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32875, 6340, 4220
R_{int}	0.057
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.895
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.164, 1.03
No. of reflections	6340
No. of parameters	158
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.27

- **X-Ray data of compound 2j.**



Single crystals suitable for X-Ray crystallographic analysis were obtained by slow evaporation of a methanol solution of **2j**.

Crystal data	
Chemical formula	$C_{15}H_{10}FNO$
M_r	239.24
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	170
a, *b*, *c* (Å)	17.5169 (8), 5.7876 (3), 22.1074 (11)
β (°)	102.879 (2)
V (Å^3)	2184.88 (19)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	0.25 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan *SADABS* 2016/2
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13357, 2714, 2322
R_{int}	0.029
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.116, 1.03
No. of reflections	2714
No. of parameters	167
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.26