

## SUPPORTING INFORMATION

**Manuscript Title:** Development of Potent and Selective Inhibitors of Aldo-Keto Reductase 1C3 (type 5 17 $\beta$ -hydroxysteroid dehydrogenase) Based on *N*-Phenyl-Aminobenzoates and their Structure Activity Relationships.

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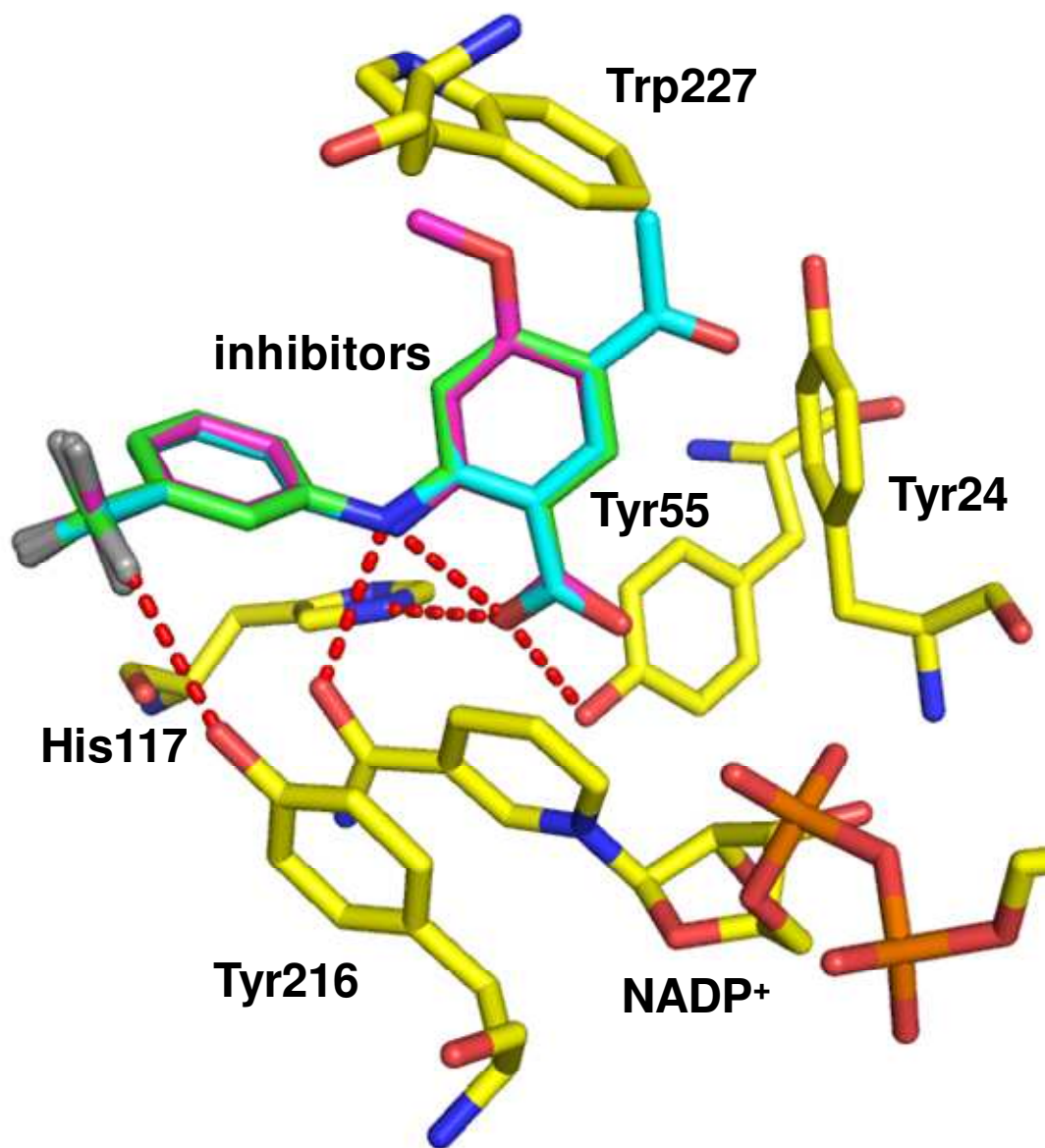
	<i>ortho</i> -substituted analogs	
	$pK_a$ (- <b>COOH</b> )	$pK_a$ (Ar-NH- Ar)
<b>4b</b>	4.32	-0.08
<b>4c</b>	4.20	-4.84
<b>4d</b>	4.26	-1.38
<b>4e</b>	4.24	-1.55
<b>4f</b>	4.30	-0.08

	<i>meta</i> -substituted analogs	
	$pK_a$ (- <b>COOH</b> )	$pK_a$ (Ar-NH- Ar)
<b>4a</b>	4.25	-1.35
<b>4g</b>	4.20	-2.13
<b>4h</b>	4.26	-1.08
<b>4i</b>	4.26	-1.10
<b>4j</b>	4.30	-0.38
<b>4k</b>	4.33	0.09

	<i>para</i> -substituted analogs	
	$pK_a$ (- <b>COOH</b> )	$pK_a$ (Ar-NH- Ar)
<b>4m</b>	4.20	-3.57
<b>4n</b>	4.26	-2.32
<b>4o</b>	4.24	-2.13
<b>4p</b>	4.26	-0.55
<b>4q</b>	4.26	-0.69
<b>4r</b>	4.30	0.70
<b>4s</b>	4.33	0.31
<b>4t</b>	4.33	0.34

**Table S1.  $pK_a$  values of class 4 analogs with single substitution on the B-ring.**

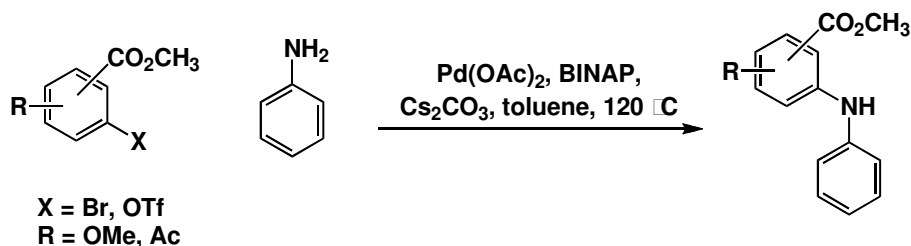
\*  $pK_a$  values were calculated using Accelrys Accord for excel software



**Figure S1.** Predicted binding conformations of **2a** (Class 2, 4-methoxy-2-phenylamino benzoate magenta) and **3a** (Class 3, 5-acetyl-3-phenylamino benzoate, cyan) compounds modeled based on the crystal structure of FLU (Class 1, green) in AKR1C3 (PDB 1S2C). The compounds are capable of maintaining the same hydrogen bonding network as FLU. Introduction of the 5-acetyl group on the A-ring shows possible clashing with Trp227 and Tyr24. Carbon atoms in AKR1C3 are colored in yellow and the non-carbon atoms are color coded as described in **Figure 4**. Hydrogen bonds are shown as red dashes. The figure was generated with PyMol (Delano Scientific).

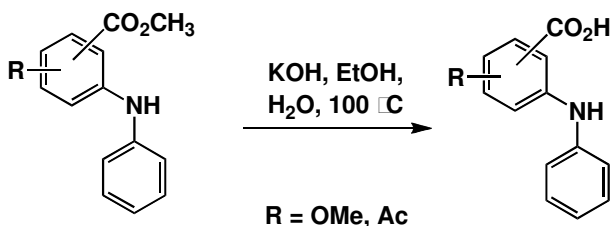
## Synthesis and Physicochemical Characterization

### General Procedure 1



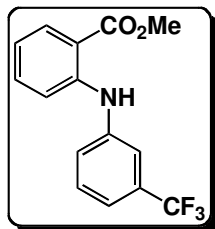
To a solution of bromide (or triflate) (1 equiv) in toluene (0.1 M) was added aniline (1.2 equiv),  $\text{Cs}_2\text{CO}_3$  (1.4 equiv) BINAP (0.08 equiv), and  $\text{Pd}(\text{OAc})_2$  (0.05 equiv) at room temperature. The reaction mixture was allowed to stir at 120 °C for 4-48 h. Once the reaction appeared to be complete by consumption of the bromide (or triflate) by TLC analysis, the mixture was allowed to cool to room temperature, diluted with EtOAc, washed with 2M aq HCl (2x), brine, and dried over sodium sulfate. The solution was concentrated, loaded on silica gel, and purified by silica gel chromatography.

### General Procedure 2



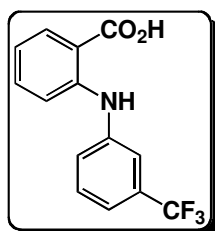
To a solution of the methyl ester (1 equiv) in EtOH (0.2 M) was added KOH (2 equiv per ester) in water (0.2 M) at room temperature. The reaction mixture was allowed to stir at 100 °C for 1-6 h. Once the reaction appeared complete by TLC analysis, EtOH was evaporated from the reaction mixture, the resultant solution was cooled to 0 °C and acidified to pH 2 w 2M aq HCl. The resultant precipitated product was collected by vacuum filtration and washed with water.

## Class 1 Compounds



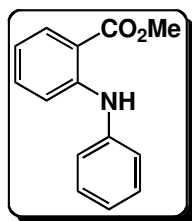
### **N-(3-trifluoromethylphenyl)anthranilic acid methyl ester**

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **1a** as a yellow oil (71% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ = 9.60 (s, 1H), 8.01 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.50 (s, 1H), 7.35-7.47 (m, 3H), 7.27-7.34 (m, 2H), 6.83 (t, *J* = 7.1 Hz, 1H), 3.93 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 169.1, 147.0, 141.9, 134.5, 132.0, 130.1, 124.8, 119.8, 118.6, 118.3, 114.6, 113.3, 52.1.



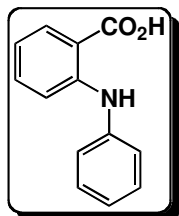
### **N-(3-trifluoromethylphenyl)anthranilic acid (FLU, **1a**)**

Reaction of the methyl ester of **1a** according to general procedure **2** provided **1a** as a white solid (55% yield). <sup>1</sup>H NMR (DMSO, 500 MHz): δ = 13.14 (bs, 1H), 9.66 (s, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.40-7.60 (m, 4H), 7.25-7.36 (m, 2H), 6.89 (t, *J* = 7.5 Hz, 1H). <sup>13</sup>C NMR (DMSO, 125 MHz): δ = 169.5, 145.4, 142.0, 134.1, 131.9, 130.5, 123.7, 118.9, 118.5, 116.3, 114.9, 114.5. HRMS (ES) Calcd. for C<sub>14</sub>H<sub>10</sub>F<sub>3</sub>NO<sub>2</sub>: 280.0585 (M-H<sup>-</sup>), found 280.0590 (M-H<sup>-</sup>).



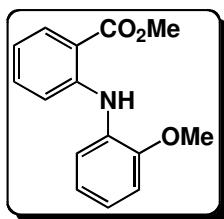
### **N-Phenylanthranilic acid methyl ester**

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with aniline according to general procedure **1** provided the methyl ester of **1b** as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.48$  (s, 1H), 7.97 (d,  $J = 8.0$  Hz, 1H), 7.22-7.40 (m, 6H), 7.10 (t,  $J = 7.3$  Hz, 1H), 6.74 (t,  $J = 7.5$  Hz, 1H), 3.91 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 169.1$ , 148.2, 141.0, 134.3, 131.8, 129.6, 123.8, 122.8, 117.3, 114.3, 112.2, 51.9.



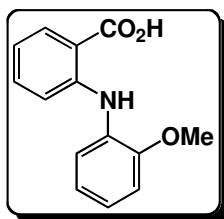
### N-Phenylanthranilic acid (**1b**)

Reaction of the methyl ester of **1b** according to general procedure **2** provided **1b** as a white solid (57% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 13.03$  (bs, 1H), 9.63 (bs, 1H), 7.91 (d,  $J = 7.9$  Hz, 1H), 7.30-7.45 (m, 3H), 7.17-7.27 (m, 3H), 7.07 (t,  $J = 7.3$  Hz, 1H), 6.78 (t,  $J = 7.5$  Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 169.9$ , 147.0, 140.5, 134.1, 131.8, 129.4, 123.0, 121.3, 117.4, 113.7, 112.6. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{11}\text{NO}_2$ : 212.0712 (M-H), found 212.0709 (M-H).



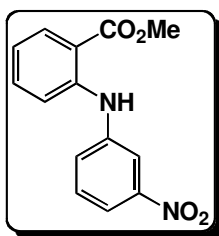
### N-(2-methoxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with *o*-anisidine according to general procedure **1** provided the methyl ester of **1c** as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.44$  (s, 1H), 7.97 (d,  $J = 8.0$  Hz, 1H), 7.44 (d,  $J = 7.8$  Hz, 1H), 7.30-7.36 (m, 2H), 7.05 (m, 1H), 6.92-7.00 (m, 2H), 6.75 (m, 1H), 3.92 (s, 3H), 3.90 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 169.0$ , 151.8, 147.5, 134.1, 131.9, 130.4, 123.5, 120.9, 120.7, 117.4, 114.6, 113.0, 111.6, 56.0, 52.0.



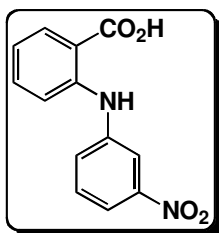
### N-(2-methoxyphenyl)anthranilic acid (**1c**)

Reaction of the methyl ester of 1c according to general procedure 2 provided 1c as a white solid (53% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.93 (bs, 1H), 9.57 (s, 1H), 7.90 (m, 1H), 7.31-7.42 (m, 2H), 7.19 (d,  $J$  = 8.4 Hz, 1H), 7.00-7.11 (m, 2H), 6.94 (m, 1H), 6.76 (m, 1H), 3.82 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.2, 150.5, 146.3, 133.6, 131.3, 128.9, 122.9, 120.1, 119.8, 116.7, 113.1, 112.4, 111.4, 55.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 242.0817 (M-H $^-$ ), found 242.0812 (M-H $^-$ ).



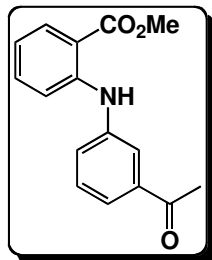
### N-(3-Nitrophenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3-nitroaniline according to general procedure 1 provided the methyl ester of 1d as a yellow oil (98% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.71 (s, 1H), 8.11 (t,  $J$  = 2.1 Hz, 1H), 8.03 (dd,  $J$  = 8.0, 1.6 Hz, 1H), 7.87 (m, 1H), 7.40-7.57 (m, 3H), 7.35 (d,  $J$  = 8.4 Hz, 1H), 6.89 (t,  $J$  = 7.6 Hz, 1H), 3.93 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.0, 149.5, 146.1, 142.9, 134.6, 132.1, 130.3, 126.8, 119.4, 117.4, 115.1, 114.9, 113.9, 52.3.



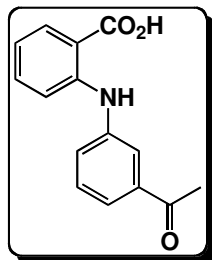
### N-(3-Nitrophenyl)anthranilic acid (1d)

Reaction of the methyl ester of 1d according to general procedure 2 provided 1d as a yellow solid (77% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 13.19 (bs, 1H), 9.72 (s, 1H), 8.00 (t,  $J$  = 2.2 Hz, 1H), 7.95 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.80 (ddd,  $J$  = 8.0, 2.2, 1.0 Hz, 1H), 7.65 (ddd,  $J$  = 8.1, 2.2, 1.0 Hz, 1H), 7.56 (t,  $J$  = 8.1 Hz, 1H), 7.48 (m, 1H), 7.38 (d,  $J$  = 7.5 Hz, 1H), 6.95 (t,  $J$  = 7.0 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 169.4, 148.7, 144.7, 142.8, 134.0, 131.9, 130.6, 125.7, 119.6, 116.2, 115.7, 115.4, 113.2. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H $^-$ ), found 257.0563 (M-H $^-$ ).



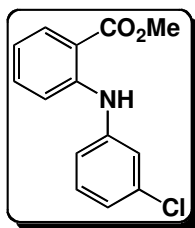
### N-(3-acetylphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3'-aminoacetophenone according to general procedure **1** provided the methyl ester of **1e** as a yellow oil (90% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.58 (s, 1H), 7.99 (d,  $J$  = 8.0 Hz, 1H), 7.84 (s, 1H), 7.65 (dd,  $J$  = 6.8, 1.7 Hz, 1H), 7.23-7.49 (m, 4H), 6.80 (t,  $J$  = 7.5 Hz, 1H), 3.92 (s, 3H), 2.60 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 198.0, 169.1, 147.4, 141.7, 138.7, 134.4, 132.0, 129.8, 126.5, 123.4, 121.6, 118.1, 114.3, 112.8, 52.1, 26.9.



### N-(3-acetylphenyl)anthranilic acid (**1e**)

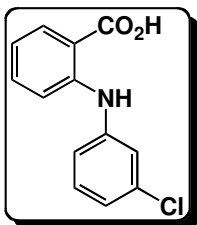
Reaction of the methyl ester of **1e** according to general procedure **2** provided **1e** as a yellow solid (83% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.70 (s, 1H), 7.93 (d,  $J$  = 7.8 Hz, 1H), 7.77 (s, 1H), 7.63 (d,  $J$  = 6.6 Hz, 1H), 7.37-7.57 (m, 3H), 7.27 (d,  $J$  = 8.4 Hz, 1H), 6.84 (t,  $J$  = 7.3 Hz, 1H), 2.58 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 197.7, 169.8, 146.3, 141.2, 138.1, 134.2, 131.9, 129.8, 125.4, 122.6, 120.0, 118.2, 114.2, 113.5, 26.8. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_3$ : 254.0817 (M-H<sup>-</sup>), found 254.0817 (M-H<sup>-</sup>).



### N-(3-chlorophenyl)anthranilic acid methyl ester

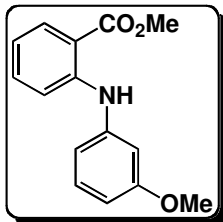


Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3-chloroaniline according to general procedure 1 provided the methyl ester of 1f as a yellow oil (92% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.51 (s, 1H), 7.99 (dd,  $J$  = 8.0, 1.6 Hz, 1H), 7.37 (m, 1H), 7.23-7.33 (m, 3H), 7.12 (d,  $J$  = 8.0 Hz, 1H), 7.04 (d,  $J$  = 7.9 Hz, 1H), 6.81 (t,  $J$  = 7.5 Hz, 1H), 3.92 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.0, 147.1, 142.6, 135.1, 134.4, 131.9, 130.5, 123.3, 121.7, 120.0, 118.3, 114.7, 113.0, 52.1.



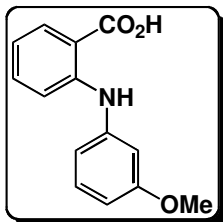
#### N-(3-chlorophenyl)anthranilic acid (1f)

Reaction of the methyl ester of 1f according to general procedure 2 provided 1f as a white solid (85% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.61 (bs, 1H), 7.92 (d,  $J$  = 7.8 Hz, 1H), 7.44 (t,  $J$  = 7.7 Hz, 1H), 7.25-7.37 (m, 3H), 7.19 (d,  $J$  = 8.1 Hz, 1H), 7.05 (d,  $J$  = 7.9 Hz, 1H), 6.86 (t,  $J$  = 7.5 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.6, 145.6, 142.6, 134.1, 133.8, 131.8, 130.9, 122.1, 119.8, 118.8, 118.6, 114.9, 114.1. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H), found 246.0322 (M-H).



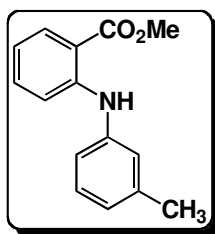
#### N-(3-methoxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with m-anisidine according to general procedure 1 provided the methyl ester of 1g as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.48 (s, 1H), 7.98 (d,  $J$  = 8.2 Hz, 1H), 7.31-7.37 (m, 2H), 7.25 (m, 1H), 6.86 (d,  $J$  = 7.9 Hz, 1H), 6.82 (s, 1H), 6.76 (m, 1H), 6.66 (dd,  $J$  = 8.2, 2.3 Hz, 1H), 3.92 (s, 3H), 3.82 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.1, 160.9, 147.9, 142.3, 134.3, 131.8, 130.2, 117.5, 114.8, 114.7, 112.4, 109.3, 108.1, 55.5, 52.0.



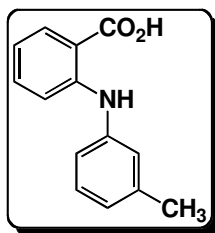
#### N-(3-methoxyphenyl)anthranilic acid (1g)

Reaction of the methyl ester of 1g according to general procedure 2 provided **1g** as a white solid (85% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 9.59$  (s, 1H), 7.90 (dd,  $J = 7.9$ , 1.3 Hz, 1H), 7.39 (m, 1H), 7.27-7.30 (m, 2H), 6.75-6.84 (m, 3H), 6.64 (dd,  $J = 8.2$ , 2.4 Hz, 1H), 3.75 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 169.8$ , 160.3, 146.7, 141.8, 134.1, 131.8, 130.1, 117.5, 114.2, 113.3, 112.9, 108.7, 106.7, 55.0. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H<sup>-</sup>), found 246.0322 (M-H<sup>-</sup>).



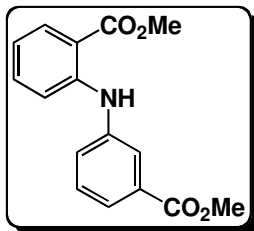
#### N-(3-methylphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with *m*-toluidine according to general procedure 1 provided the methyl ester of 1h as a yellow oil (69% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.44$  (s, 1H), 7.98 (dd,  $J = 8.0$ , 1.6 Hz, 1H), 7.22-7.36 (m, 3H), 7.09 (s, 2H), 6.93 (d,  $J = 7.5$  Hz, 1H), 6.74 (m, 1H), 3.92 (s, 3H), 2.37 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 169.1$ , 148.3, 140.9, 139.5, 134.3, 131.8, 129.4, 124.6, 123.5, 119.8, 117.1, 114.4, 112.1, 51.9, 21.6.



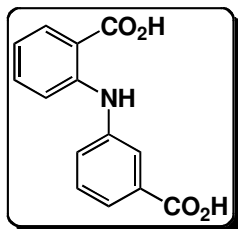
#### N-(3-methylphenyl)anthranilic acid (1h)

Reaction of the methyl ester of 1h according to general procedure 2 provided **1h** as a white solid (77% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 13.01$  (bs, 1H), 9.59 (s, 1H), 7.89 (d,  $J = 7.8$  Hz, 1H), 7.38 (m, 1H), 7.15-7.30 (m, 2H), 7.00-7.10 (m, 2H), 6.88 (m, 1H), 6.76 (m, 1H), 2.29 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 169.9$ , 147.1, 140.4, 138.9, 134.1, 131.8, 129.2, 123.8, 121.9, 118.4, 117.2, 113.8, 112.4, 20.9. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_2$ : 226.0868 (M-H<sup>-</sup>), found 226.0861 (M-H<sup>-</sup>).



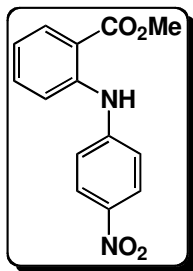
#### N-(3-methylcarboxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with methyl 3-aminobenzoate according to general procedure **1** provided the methyl ester of **1i** as a yellow oil (75% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.55 (s, 1H), 7.98 (d,  $J$  = 8.0 Hz, 1H), 7.93 (s, 1H), 7.73 (d,  $J$  = 7.3 Hz, 1H), 7.32-7.45 (m, 3H), 7.26 (m, 1H), 6.78 (t,  $J$  = 7.5 Hz, 1H), 3.91 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.1, 167.0, 147.5, 141.4, 134.4, 131.9, 131.7, 129.6, 126.5, 124.5, 123.0, 118.0, 114.3, 112.8, 52.3, 52.0.



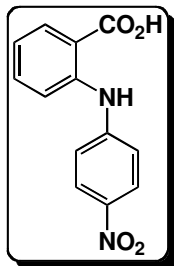
#### N-(3-carboxyphenyl)anthranilic acid (**1i**)

Reaction of the methyl ester of **1i** according to general procedure **2** provided **1i** as a white solid (83% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 9.70 (bs, 1H), 7.91 (d,  $J$  = 7.9 Hz, 1H), 7.74 (s, 1H), 7.60 (s, 1H), 7.40-7.53 (m, 3H), 7.24 (d,  $J$  = 8.4 Hz, 1H), 6.84 (t,  $J$  = 7.5 Hz, 1H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 170.0, 167.3, 146.4, 141.4, 134.4, 132.2, 132.1, 130.1, 125.2, 123.7, 121.0, 118.5, 114.5, 113.9. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{11}\text{NO}_4$ : 256.0610 (M-H<sup>-</sup>), found 256.0607 (M-H<sup>-</sup>).



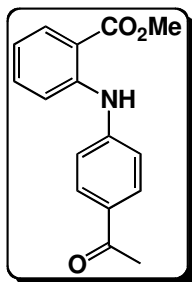
#### N-(4-nitrophenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 4-nitroaniline according to general procedure **1** provided the methyl ester of **1j** as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.87 (s, 1H), 8.18 (d,  $J$  = 9.0 Hz, 2H), 8.04 (d,  $J$  = 8.0 Hz, 1H), 7.45-7.56 (m, 2H), 7.25 (d,  $J$  = 9.0 Hz, 2H), 6.99 (t,  $J$  = 7.5 Hz, 1H), 3.94 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.8, 148.0, 144.3, 141.7, 134.3, 132.1, 126.0, 120.9, 117.7, 117.0, 115.7, 52.4.



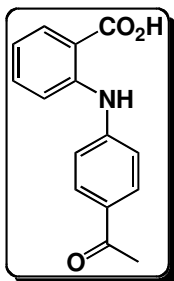
#### N-(4-nitrophenyl)anthranilic acid (1j)

Reaction of the methyl ester of 1j according to general procedure 2 provided **1j** as an orange solid (62% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.83 (bs, 1H), 8.12 (d,  $J$  = 8.1 Hz, 2H), 7.96 (d,  $J$  = 7.8 Hz, 1H), 7.50-7.60 (m, 2H), 7.26 (d,  $J$  = 8.1 Hz, 2H), 7.11 (t,  $J$  = 7.4 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 168.8, 148.9, 142.1, 139.6, 133.8, 131.8, 125.8, 121.9, 119.3, 118.8, 116.0. HRMS (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H<sup>-</sup>), found 257.0568 (M-H<sup>-</sup>).



#### N-(4-acetylphenyl)anthranilic acid methyl ester

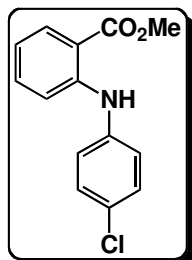
Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 4'-aminoacetophenone according to general procedure 1 provided the methyl ester of 1k as a yellow oil (87% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.73 (s, 1H), 8.00 (d,  $J$  = 8.0 Hz, 1H), 7.92 (d,  $J$  = 8.7 Hz, 2H), 7.48 (d,  $J$  = 8.5 Hz, 1H), 7.41 (m, 1H), 7.25 (d,  $J$  = 8.6 Hz, 2H), 6.88 (t,  $J$  = 7.6 Hz, 1H), 3.92 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 196.7, 168.9, 146.1, 145.4, 134.2, 132.0, 131.2, 130.4, 119.5, 118.7, 116.1, 114.4, 52.2, 26.5.



#### N-(4-acetylphenyl)anthranilic acid (1k)

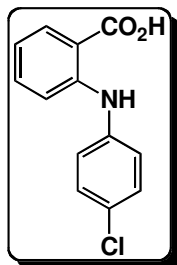
Reaction of the methyl ester of 1k according to general procedure 2 provided **1k** as a white solid (79% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.81 (s, 1H), 7.94 (d,  $J$  = 7.2

Hz, 1H), 7.89 (d,  $J = 7.5$  Hz, 2H), 7.48 (s, 2H), 7.27 (d,  $J = 7.6$  Hz, 2H), 6.96 (s, 1H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 195.9, 169.5, 145.9, 144.1, 134.0, 131.9, 130.2, 130.1, 119.9, 117.5, 116.6, 115.7, 26.3$ . HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_3$ : 254.0817 (M-H $^-$ ), found 254.0821 (M-H $^-$ ).



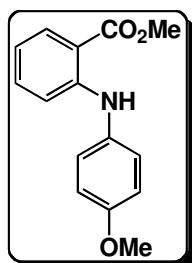
#### N-(4-chlorophenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 4-chloroaniline according to general procedure 1 provided the methyl ester of 11 as a yellow oil (96% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500MHz):  $\delta = 9.46$  (s, 1H), 7.98 (d,  $J = 8.0$  Hz, 1H), 7.15-7.37 (m, 6H), 6.77 (t,  $J = 7.6$  Hz, 1H), 3.92 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 169.1, 147.7, 139.7, 134.4, 131.9, 129.6, 128.6, 123.8, 117.8, 114.2, 112.5, 52.0$ .



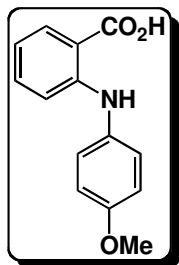
#### N-(4-chlorophenyl)anthranilic acid (11)

Reaction of the methyl ester of 11 according to general procedure 2 provided 11 as a yellow solid (39% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 9.59$  (bs, 1H), 7.91 (d,  $J = 7.8$  Hz, 1H), 7.15-7.45 (m, 6H), 6.82 (t,  $J = 7.6$  Hz, 1H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.8, 146.3, 139.7, 134.1, 131.8, 129.2, 126.3, 122.5, 118.0, 114.1, 113.3$ . HRMS (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H $^-$ ), found 246.0322 (M-H $^-$ ).



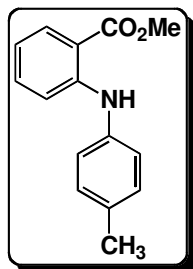
#### N-(4-methoxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with *p*-anisidine according to general procedure **1** provided the methyl ester of **1m** as a yellow oil (80% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500 MHz): δ = 9.28 (s, 1H), 7.95 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.27 (m, 1H), 7.16-7.22 (m, 2H), 6.99 (d, *J* = 8.5 Hz, 1H), 6.90-6.95 (m, 2H), 6.67 (t, *J* = 7.5 Hz, 1H), 3.91 (s, 3H), 3.83 (s, 3H). **<sup>13</sup>C NMR** (CDCl<sub>3</sub>, 125 MHz): δ = 169.2, 157.0, 149.8, 134.4, 133.7, 131.8, 126.2, 116.4, 114.9, 113.6, 111.1, 55.7, 51.9.



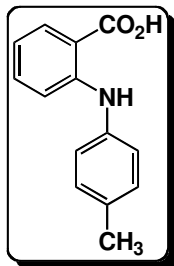
#### **N-(4-methoxyphenyl)anthranilic acid (1m)**

Reaction of the methyl ester of **1m** according to general procedure **2** provided **1m** as a yellow solid (53% yield). **<sup>1</sup>H NMR** (DMSO, 500 MHz): δ = 12.87 (bs, 1H), 9.41 (s, 1H), 7.86 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.35 (m, 1H), 7.17 (d, *J* = 8.9 Hz, 2H), 6.90-7.00 (m, 3H), 6.68 (t, *J* = 7.5 Hz, 1H), 3.76 (s, 3H). **<sup>13</sup>C NMR** (DMSO, 125 MHz): δ = 170.0, 156.1, 148.8, 134.1, 132.9, 131.7, 125.0, 116.2, 114.7, 112.8, 111.2, 55.2. **HRMS** (ES) Calcd. for C<sub>14</sub>H<sub>13</sub>NO<sub>3</sub>: 242.0817 (M-H), found 242.0828 (M-H).



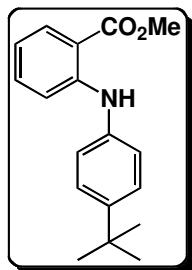
#### **N-(4-methylphenyl)anthranilic acid methyl ester**

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with *p*-toluidine according to general procedure **1** provided the methyl ester of **1n** as a yellow oil (99% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500 MHz): δ = 9.40 (s, 1H), 7.97 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.29 (m, 1H), 7.14-7.21 (m, 5H), 6.71 (t, *J* = 7.5 Hz, 1H), 3.92 (s, 3H), 2.37 (s, 3H). **<sup>13</sup>C NMR** (CDCl<sub>3</sub>, 125 MHz): δ = 169.2, 148.9, 138.2, 134.3, 133.7, 131.8, 130.1, 123.5, 116.8, 113.9, 111.6, 51.9, 21.1.



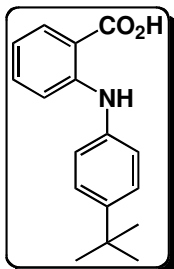
#### N-(4-methylphenyl)anthranilic acid (**1n**)

Reaction of the methyl ester of **1n** according to general procedure **2** provided **1n** as a white solid (70% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.00 (bs, 1H), 9.55 (s, 1H), 7.88 (d,  $J$  = 7.9 Hz, 1H), 7.34 (m, 1H), 7.05-7.25 (m, 5H), 6.72 (m, 1H), 2.28 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 170.0, 147.7, 137.7, 134.2, 132.6, 131.9, 130.0, 122.2, 116.9, 113.3, 111.9, 20.4. HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_2$ : 228.10245 ( $\text{M}+\text{H}^+$ ), found 228.10000 ( $\text{M}+\text{H}^+$ ).



#### N-(4-*tert*-butylphenyl)anthranilic acid methyl ester

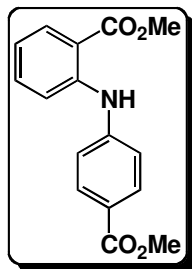
Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 4-*tert*-butylaniline according to general procedure **1** provided the methyl ester of **1o** as a yellow oil (90% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.42 (s, 1H), 7.97 (dd,  $J$  = 8.0, 1.7 Hz, 1H), 7.38 (d,  $J$  = 8.6 Hz, 2H), 7.31 (m, 1H), 7.17-7.25 (m, 3H), 6.71 (t,  $J$  = 7.5 Hz, 1H), 3.92 (s, 3H), 1.36 (s, 9H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.2, 148.7, 147.0, 138.3, 134.3, 131.8, 126.4, 122.9, 116.9, 114.2, 111.8, 51.9, 34.6, 31.7.



#### N-(4-*tert*-butylphenyl)anthranilic acid (**1o**)

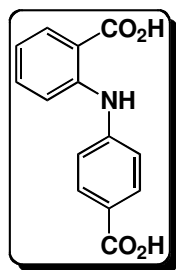
Reaction of the methyl ester of **1o** according to general procedure **2** provided **1o** as a white solid (37% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.97 (bs, 1H), 9.56 (s, 1H), 7.89 (d,  $J$  = 7.9 Hz, 1H), 7.33-7.42 (m, 3H), 7.12-7.23 (m, 3H), 6.74 (t,  $J$  = 7.5 Hz, 1H),

1.29 (s, 9H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta$  = 169.9, 147.5, 145.7, 137.7, 134.1, 131.8, 126.1, 121.5, 116.9, 113.4, 112.0, 34.0, 31.1. HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{19}\text{NO}_2$ : 268.1338 (M-H), found 268.1338 (M-H).



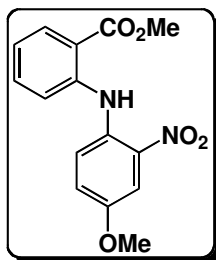
### N-(4-methylcarboxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with methyl 4-aminobenzoate according to general procedure 1 provided the methyl ester of 1p as a white solid (90% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.69 (s, 1H), 7.97-8.03 (m, 3H), 7.36-7.50 (m, 2H), 7.25 (d,  $J$  = 8.6 Hz, 1H), 6.87 (t,  $J$  = 7.6 Hz, 1H), 3.92 (s, 3H), 3.91 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 166.9, 145.9, 145.8, 134.2, 132.0, 131.5, 123.8, 119.3, 119.0, 115.9, 114.3, 52.2, 52.0.



### N-(4-carboxyphenyl)anthranilic acid (1p)

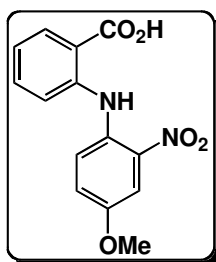
Reaction of the methyl ester of 1p according to general procedure 2 provided 1p as a white solid (75% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta$  = 9.79 (bs, 1H), 7.93 (d,  $J$  = 7.7 Hz, 1H), 7.86 (d,  $J$  = 8.5 Hz, 2H), 7.42-7.49 (m, 2H), 7.25 (d,  $J$  = 8.6 Hz, 2H), 6.93 (t,  $J$  = 7.2 Hz, 1H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta$  = 169.8, 167.2, 145.7, 144.6, 134.2, 132.1, 131.3, 123.5, 119.8, 118.0, 116.4, 115.6. HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{11}\text{NO}_4$ : 256.0610 (M-H), found 256.0614 (M-H).





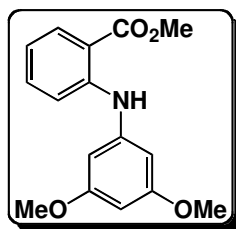
### N-(2-nitro-4-methoxyphenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 4-methoxy-2-nitroaniline according to general procedure 1 provided the methyl ester of 1q as an orange oil (77% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.89 (s, 1H), 8.02 (dd,  $J$  = 7.9, 1.5 Hz, 1H), 7.62 (d,  $J$  = 3.0 Hz, 1H), 7.55 (d,  $J$  = 9.2 Hz, 1H), 7.35-7.42 (m, 2H), 7.11 (dd,  $J$  = 9.2, 3.0 Hz, 1H), 6.96 (t,  $J$  = 7.3 Hz, 1H), 3.97 (s, 3H), 3.86 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.0, 153.6, 143.9, 138.9, 133.8, 132.7, 132.3, 123.7, 121.9, 120.8, 117.5, 108.6, 56.2, 52.4.



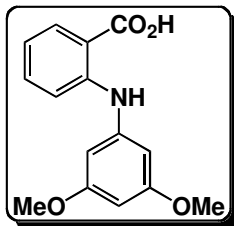
### N-(2-nitro-4-methoxyphenyl)anthranilic acid (1q)

Reaction of the methyl ester of 1q according to general procedure 2 provided 1q as an orange solid (81% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.25 (bs, 1H), 10.76 (s, 1H), 7.94 (d,  $J$  = 7.9 Hz, 1H), 7.58-7.63 (m, 2H), 7.45 (m, 1H), 7.28-7.34 (m, 2H), 6.97 (t,  $J$  = 7.4 Hz, 1H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 153.4, 139.1, 133.7, 130.9, 123.2, 122.8, 120.1, 116.5, 108.5, 55.9. HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5$ : 287.0668 (M-H), found 287.0674 (M-H).



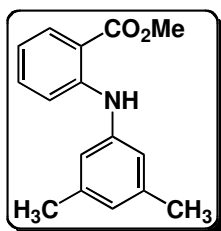
### N-(3,5-bis-(methoxy)phenyl)anthranilic acid methyl ester

Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3,5-dimethoxyaniline according to general procedure 1 provided the methyl ester of 1r as a yellow oil (87% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.44 (s, 1H), 7.97 (d,  $J$  = 9.6 Hz, 1H), 7.30-7.42 (m, 2H), 6.76 (t,  $J$  = 7.4 Hz, 1H), 6.43 (d,  $J$  = 2.2 Hz, 2H), 6.22 (t,  $J$  = 2.2 Hz, 1H), 3.91 (s, 3H), 3.79 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.1, 161.8, 147.7, 143.0, 134.3, 131.8, 117.7, 115.2, 112.6, 100.5, 96.0, 55.6, 52.0.



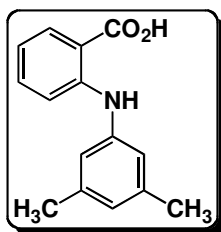
### N-(3,5-bis-(methoxy)phenyl)anthranilic acid (1r)

Reaction of the methyl ester of 1r according to general procedure 2 provided 1r as a yellow solid (45% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.03 (bs, 1H), 9.55 (s, 1H), 7.89 (d,  $J$  = 7.9 Hz, 1H), 7.41 (t,  $J$  = 7.7 Hz, 1H), 7.32 (d,  $J$  = 8.4 Hz, 1H), 6.80 (t,  $J$  = 7.5 Hz, 1H), 6.39 (s, 2H), 6.22 (s, 1H), 3.73 (s, 6H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.7, 161.1, 146.5, 142.4, 134.0, 131.8, 117.7, 114.7, 113.1, 99.0, 95.2, 55.1. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_4$ : 272.0923 (M-H $^-$ ), found 272.0919 (M-H $^-$ ).



### N-(3,5-bis-(methyl)phenyl)anthranilic acid methyl ester

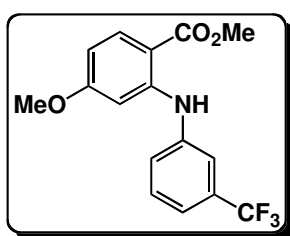
Reaction of methyl 2-(trifluoromethanesulfonyloxy)benzoate with 3,5-dimethylaniline according to general procedure 1 provided the methyl ester of 1s as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.41 (s, 1H), 7.97 (d,  $J$  = 8.0 Hz, 1H), 7.24-7.36 (m, 2H), 6.90 (s, 2H), 6.77 (s, 1H), 6.73 (m, 1H), 3.92 (s, 3H), 2.33 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.1, 148.4, 140.8, 139.2, 134.3, 131.8, 125.6, 120.5, 117.0, 114.5, 112.0, 51.9, 21.5.



### N-(3,5-bis-(methyl)phenyl)anthranilic acid (1s)

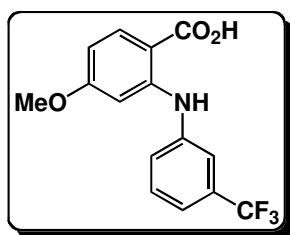
Reaction of the methyl ester of 1s according to general procedure 2 provided 1s as a white solid (52% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.03 (bs, 1H), 9.57 (s, 1H), 7.89 (d,  $J$  = 7.9 Hz, 1H), 7.38 (m, 1H), 7.22 (d,  $J$  = 8.5 Hz, 1H), 6.84 (s, 2H), 6.75 (m, 1H), 6.70 (s, 1H), 2.24 (s, 6H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 170.0, 147.2, 140.3, 138.6, 134.2, 131.8, 124.8, 119.1, 117.1, 113.9, 112.3, 20.9. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_2$ : 242.1181 (M+H $^+$ ), found 242.1184 (M+H $^+$ ).

## Class 2 Compounds



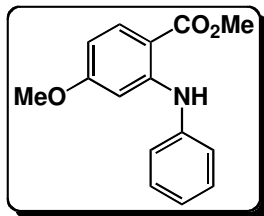
### **4-methoxy-2-(3-(trifluoromethyl)phenylamino)benzoic acid methyl ester**

Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **2a** as a yellow oil (98% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.77 (s, 1H), 7.94 (d,  $J$  = 8.9 Hz, 1H), 7.54 (s, 1H), 7.41-7.49 (m, 2H), 7.32 (d,  $J$  = 6.8 Hz, 1H), 6.74 (d,  $J$  = 2.4 Hz, 1H), 6.38 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.89 (s, 3H), 3.77 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.8, 164.6, 149.0, 141.7, 133.8, 132.2, 130.1, 125.2, 123.1, 120.0, 118.6, 106.3, 105.7, 98.2, 55.5, 51.8.



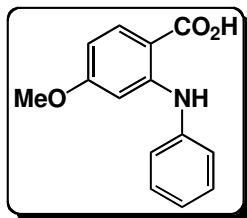
### **4-methoxy-2-(3-(trifluoromethyl)phenylamino)benzoic acid (2a)**

Reaction of the methyl ester of **2a** according to general procedure **2** provided **2a** as a white solid (85% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.85 (bs, 1H), 9.89 (s, 1H), 7.89 (s, 1H), 7.57 (s, 3H), 7.37 (s, 1H), 6.73 (s, 1H), 6.47 (s, 1H), 3.74 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.4, 163.8, 147.6, 141.6, 133.9, 130.6, 124.3, 118.9, 116.9, 106.8, 105.6, 98.4, 55.2. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{F}_3\text{NO}_3$ : 310.0691 (M-H $^-$ ), found 310.0681 (M-H $^-$ ).



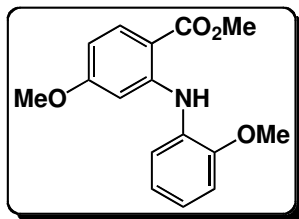
#### 4-methoxy-2-(phenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with aniline according to general procedure **1** provided the methyl ester of **2b** as a yellow oil (67% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.62 (s, 1H), 7.92 (d,  $J$  = 8.9 Hz, 1H), 7.25-7.40 (m, 4H), 7.11 (m, 1H), 6.72 (d,  $J$  = 2.5 Hz, 1H), 6.31 (dd,  $J$  = 8.9, 2.5 Hz, 1H), 3.89 (s, 3H), 3.75 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 164.6, 150.2, 140.8, 133.7, 129.6, 123.9, 123.1, 105.5, 104.7, 97.8, 55.4, 51.9.



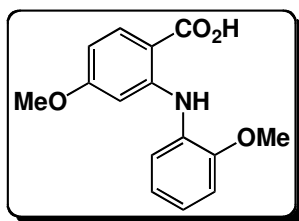
#### 4-methoxy-2-(phenylamino)benzoic acid (**2b**)

Reaction of the methyl ester of **2b** according to general procedure **2** provided **2b** as a white solid (51% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.70 (bs, 1H), 9.80 (s, 1H), 7.85 (d,  $J$  = 8.8 Hz, 1H), 7.23-7.42 (m, 4H), 7.09 (t,  $J$  = 7.3 Hz, 1H), 6.66 (d,  $J$  = 2.3 Hz, 1H), 6.38 (dd,  $J$  = 8.8, 2.3 Hz, 1H), 3.72 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.7, 163.9, 148.9, 140.2, 133.8, 129.5, 123.3, 121.7, 105.5, 104.4, 97.3, 55.1. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 242.0817 (M-H), found 242.0807 (M-H).



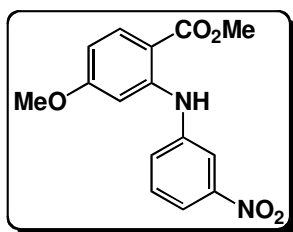
#### 4-methoxy-2-(2-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with *o*-anisidine according to general procedure **1** provided the methyl ester of **2c** as a yellow oil (89% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.59 (s, 1H), 7.93 (d,  $J$  = 8.9 Hz, 1H), 7.47 (dd,  $J$  = 7.8, 1.5 Hz, 1H), 7.06 (m, 1H), 6.92-6.99 (m, 2H), 6.86 (d,  $J$  = 2.4 Hz, 1H), 6.32 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.77 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.6, 164.4, 151.8, 149.4, 133.6, 130.1, 123.6, 121.1, 120.6, 111.4, 106.2, 104.5, 98.0, 55.9, 55.3, 51.6.



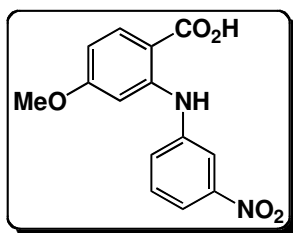
#### 4-methoxy-2-(2-methoxyphenylamino)benzoic acid (2c)

Reaction of the methyl ester of 2c according to general procedure 2 provided 2c as a white solid (88% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.61 (bs, 1H), 9.74 (s, 1H), 7.85 (d,  $J$  = 8.9 Hz, 1H), 7.43 (d,  $J$  = 6.7 Hz, 1H), 7.02-7.11 (m, 2H), 6.95 (m, 1H), 6.63 (d,  $J$  = 2.4 Hz, 1H), 6.36 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.82 (s, 3H), 3.71 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.5, 163.8, 151.0, 148.7, 133.8, 129.1, 123.6, 120.7, 120.6, 111.9, 105.8, 104.2, 97.2, 55.6, 55.1. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_4$ : 272.0923 (M-H), found 272.0962 (M-H).



#### 4-methoxy-2-(3-nitrophenylamino)benzoic acid methyl ester

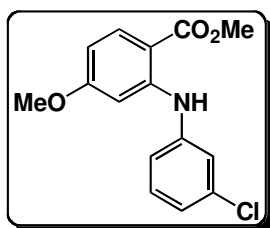
Reaction of methyl 4-methoxy-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with 3-nitroaniline according to general procedure 1 provided the methyl ester of 2d as a yellow oil (93% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.87 (s, 1H), 8.16 (s, 1H), 7.96 (d,  $J$  = 8.9 Hz, 1H), 7.88 (d,  $J$  = 8.0 Hz, 1H), 7.53 (d,  $J$  = 8.0 Hz, 1H), 7.48 (t,  $J$  = 8.0 Hz, 1H), 6.80 (d,  $J$  = 2.4 Hz, 1H), 6.43 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.90 (s, 3H), 3.80 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.8, 164.7, 149.5, 148.1, 142.6, 134.0, 130.3, 127.2, 117.6, 115.5, 106.9, 106.1, 98.9, 55.6, 51.9.



#### 4-methoxy-2-(3-nitrophenylamino)benzoic acid (2d)

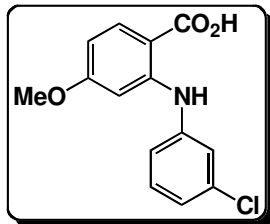
Reaction of the methyl ester of 2d according to general procedure 2 provided 2d as a yellow solid (79% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.91 (bs, 1H), 9.95 (s, 1H), 8.05 (s, 1H), 7.90 (d,  $J$  = 8.8 Hz, 1H), 7.82 (d,  $J$  = 8.1 Hz, 1H), 7.71 (d,  $J$  = 8.1 Hz, 1H),

7.59 (t,  $J = 8.1$  Hz, 1H), 6.81 (d,  $J = 2.0$  Hz, 1H), 6.52 (dd,  $J = 8.8, 2.0$  Hz, 1H), 3.76 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.3, 163.8, 148.7, 147.0, 142.3, 134.0, 130.7, 126.4, 116.7, 113.9, 107.4, 106.0, 99.2, 55.3$ . HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_5$ : 287.0668 (M-H $^-$ ), found 287.0656 (M-H $^-$ ).



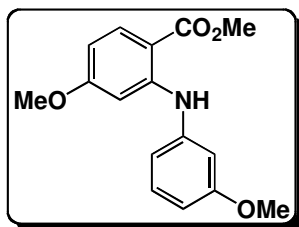
#### 4-methoxy-2-(3-chlorophenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3-chloroaniline according to general procedure 1 provided the methyl ester of 2e as a yellow oil (67% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.66$  (s, 1H), 7.93 (d,  $J = 9.0$  Hz, 1H), 7.24-7.31 (m, 2H), 7.15 (m, 1H), 7.06 (m, 1H), 6.75 (d,  $J = 2.4$  Hz, 1H), 6.36 (dd,  $J = 9.0, 2.4$  Hz, 1H), 3.88 (s, 3H), 3.78 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.8, 164.6, 149.1, 142.4, 135.1, 133.8, 130.5, 123.6, 122.2, 120.4, 106.1, 105.2, 98.4, 55.5, 51.8$ .



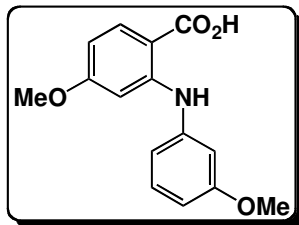
#### 4-methoxy-2-(3-chlorophenylamino)benzoic acid (2e)

Reaction of the methyl ester of 2e according to general procedure 2 provided 2e as a white solid (82% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.84$  (bs, 1H), 9.82 (s, 1H), 7.87 (d,  $J = 8.9$  Hz, 1H), 7.22-7.39 (m, 3H), 7.09 (d,  $J = 7.9$  Hz, 1H), 6.71 (d,  $J = 2.2$  Hz, 1H), 6.45 (dd,  $J = 8.9, 2.3$  Hz, 1H), 3.75 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.5, 163.8, 147.8, 142.3, 133.9, 133.8, 131.0, 122.5, 120.4, 119.3, 106.5, 105.2, 98.5, 55.2$ . HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{ClNO}_3$ : 276.0427 (M-H $^-$ ), found 276.0420 (M-H $^-$ ).



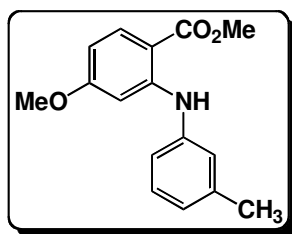
#### 4-methoxy-2-(3-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[(trifluoromethyl)sulfonyl]oxy]benzoate with *m*-anisidine according to general procedure **1** provided the methyl ester of **2f** as a colorless oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.63 (s, 1H), 7.92 (d,  $J$  = 8.9 Hz, 1H), 7.26 (m, 1H), 6.88 (m, 1H), 6.83 (t,  $J$  = 2.2 Hz, 1H), 6.79 (d,  $J$  = 2.5 Hz, 1H), 6.67 (dd,  $J$  = 8.2, 2.3 Hz, 1H), 6.32 (dd,  $J$  = 8.9, 2.5 Hz, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.76 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 164.6, 160.8, 149.9, 142.1, 133.7, 130.2, 115.0, 109.5, 108.3, 105.6, 104.9, 98.1, 55.5, 55.4, 51.7.



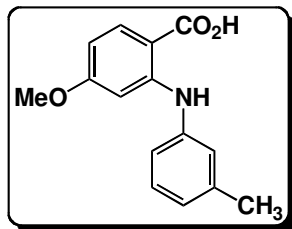
#### 4-methoxy-2-(3-methoxyphenylamino)benzoic acid (**2f**)

Reaction of the methyl ester of **2f** according to general procedure **2** provided **2f** as a white solid (77% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.72 (bs, 1H), 9.79 (s, 1H), 7.85 (d,  $J$  = 8.9 Hz, 1H), 7.26 (t,  $J$  = 8.1 Hz, 1H), 6.86 (m, 1H), 6.82 (t,  $J$  = 2.2 Hz, 1H), 6.72 (d,  $J$  = 2.4 Hz, 1H), 6.66 (ddd,  $J$  = 8.3, 2.4, 0.8 Hz, 1H), 6.38 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.7, 163.9, 160.3, 148.8, 141.6, 133.8, 130.3, 113.6, 109.1, 106.9, 105.6, 104.7, 97.7, 55.2, 55.1. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_4$ : 272.0923 (M-H<sup>-</sup>), found 272.0916 (M-H<sup>-</sup>).



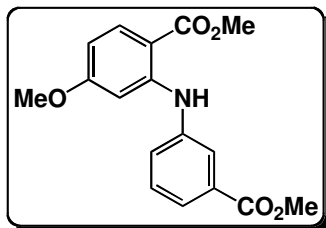
#### 4-methoxy-2-(3-methylphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[(trifluoromethyl)sulfonyl]oxy]benzoate with *m*-toluidine according to general procedure **1** provided the methyl ester of **2g** as a yellow oil (91% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.59 (s, 1H), 7.92 (d,  $J$  = 8.9 Hz, 1H), 7.25 (m, 1H), 7.08-7.13 (m, 2H), 6.94 (d,  $J$  = 7.5 Hz, 1H), 6.73 (d,  $J$  = 2.4 Hz, 1H), 6.31 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.89 (s, 3H), 3.76 (s, 3H), 2.37 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.8, 164.5, 150.2, 140.6, 139.4, 133.6, 129.3, 124.7, 123.7, 119.8, 105.3, 104.5, 97.7, 55.3, 51.6, 21.6.



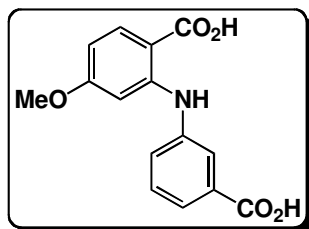
#### 4-methoxy-2-(3-methylphenylamino)benzoic acid (2g)

Reaction of the methyl ester of 2g according to general procedure 2 provided 2g as a white solid (91% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.67 (bs, 1H), 9.76 (s, 1H), 7.85 (d,  $J$  = 8.9 Hz, 1H), 7.34 (t,  $J$  = 7.6 Hz, 1H), 7.05-7.10 (m, 2H), 6.90 (d,  $J$  = 7.8 Hz, 1H), 6.66 (d,  $J$  = 2.4 Hz, 1H), 6.36 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.71 (s, 3H), 2.30 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.6, 163.8, 149.0, 140.1, 138.9, 133.8, 129.2, 124.0, 122.3, 118.6, 105.4, 104.3, 97.4, 55.1, 20.9. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_3$ : 256.0974 (M-H<sup>-</sup>), found 256.0978 (M-H<sup>-</sup>).



#### 4-methoxy-2-(3-methylcarboxyphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with methyl 3-aminobenzoate according to general procedure 1 provided the methyl ester of 2h as a white solid (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.71 (s, 1H), 7.96 (s, 1H), 7.93 (d,  $J$  = 9.0 Hz, 1H), 7.76 (d,  $J$  = 7.4 Hz, 1H), 7.38-7.48 (m, 2H), 6.72 (d,  $J$  = 2.4 Hz, 1H), 6.35 (dd,  $J$  = 9.0, 2.4 Hz, 1H), 3.92 (s, 3H), 3.88 (s, 3H), 3.76 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.8, 166.9, 164.6, 149.4, 141.2, 133.7, 131.6, 129.6, 126.8, 124.7, 123.3, 105.8, 105.2, 97.9, 55.4, 52.3, 51.7.

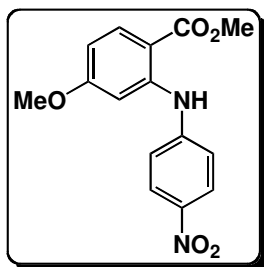


#### 4-methoxy-2-(3-carboxyphenylamino)benzoic acid (2h)

Reaction of the methyl ester of 2h according to general procedure 2 provided 2h as a white solid (79% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.64 (bs, 2H), 9.87 (s, 1H),

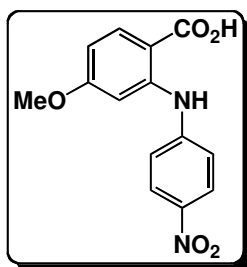


7.88 (d,  $J = 8.9$  Hz, 1H), 7.80 (s, 1H), 7.63 (d,  $J = 7.0$  Hz, 1H), 7.40-7.55 (m, 2H), 6.70 (s, 1H), 6.44 (dd,  $J = 8.8, 1.8$  Hz, 1H), 3.74 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.5, 167.0, 163.8, 148.2, 140.8, 133.9, 132.0, 129.8, 125.3, 123.7, 121.2, 106.2, 104.9, 98.0, 55.2$ . HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_5$ : 286.0715 (M-H<sup>-</sup>), found 286.0737 (M-H<sup>-</sup>).



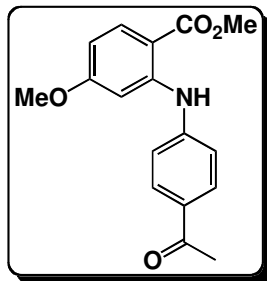
#### 4-methoxy-2-(4-nitrophenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-nitroaniline according to general procedure **1** provided the methyl ester of **2i** as an orange oil (62% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 10.05$  (s, 1H), 8.20 (d,  $J = 9.1$  Hz, 2H), 8.00 (d,  $J = 8.9$  Hz, 1H), 7.29 (d,  $J = 9.1$  Hz, 2H), 6.98 (d,  $J = 2.4$  Hz, 1H), 6.51 (dd,  $J = 8.9, 2.4$  Hz, 1H), 3.91 (s, 3H), 3.85 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.7, 164.5, 147.8, 146.3, 141.8, 134.0, 126.0, 118.2, 108.4, 107.0, 101.3, 55.7, 52.1$ .



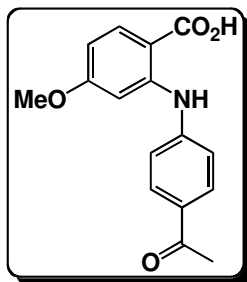
#### 4-methoxy-2-(4-nitrophenylamino)benzoic acid (**2i**)

Reaction of the methyl ester of **2i** according to general procedure **2** provided **2i** as an orange solid (91% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 13.01$  (bs, 1H), 10.10 (s, 1H), 8.15 (d,  $J = 9.1$  Hz, 2H), 7.93 (d,  $J = 8.9$  Hz, 1H), 7.37 (d,  $J = 9.1$  Hz, 2H), 6.98 (s, 1H), 6.65 (d,  $J = 8.9$  Hz, 1H), 3.82 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 168.9, 163.5, 148.2, 144.7, 140.1, 133.8, 125.8, 117.0, 107.9, 102.5, 55.5$ . HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5$ : 287.0668 (M-H<sup>-</sup>), found 287.0658 (M-H<sup>-</sup>).



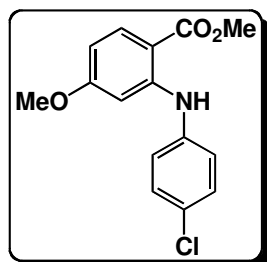
#### 4-methoxy-2-(4-acetylphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4'-aminoacetophenone according to general procedure 1 provided the methyl ester of 2j as a yellow oil (97% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.89 (s, 1H), 7.90-7.98 (m, 3H), 7.26-7.30 (m, 2H), 6.94 (s, 1H), 6.42 (d,  $J$  = 8.9 Hz, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 196.8, 168.7, 164.5, 147.5, 145.9, 133.8, 131.4, 130.4, 119.2, 107.3, 106.2, 99.9, 55.6, 51.9, 26.5.



#### 4-methoxy-2-(4-acetylphenylamino)benzoic acid (2j)

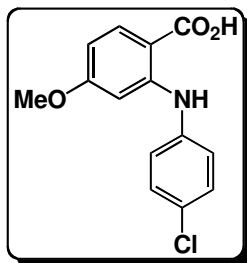
Reaction of the methyl ester of 2j according to general procedure 2 provided 2j as a white solid (99% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.05 (bs, 1H), 7.88-7.94 (m, 3H), 7.33 (d,  $J$  = 8.7 Hz, 2H), 6.90 (d,  $J$  = 2.4 Hz, 1H), 6.52 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.78 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 196.1, 169.4, 163.7, 146.4, 145.5, 133.9, 130.4, 130.3, 118.2, 107.7, 106.4, 99.9, 55.4, 26.3. **HRMS** (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_4$ : 284.0923 (M-H), found 284.0920 (M-H).



#### 4-methoxy-2-(4-chlorophenylamino)benzoic acid methyl ester

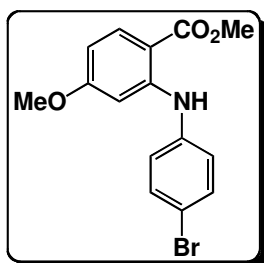
Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-chloroaniline according to general procedure 1 provided the methyl ester of 2k as a

yellow oil (62% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.59 (s, 1H), 7.92 (d,  $J$  = 8.9 Hz, 1H), 7.31 (d,  $J$  = 8.8 Hz, 2H), 7.20 (d,  $J$  = 8.8 Hz, 2H), 6.64 (d,  $J$  = 2.5 Hz, 1H), 6.33 (dd,  $J$  = 8.9, 2.5 Hz, 1H), 3.88 (s, 3H), 3.76 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 164.6, 149.8, 139.5, 133.8, 129.7, 128.9, 124.2, 105.7, 104.9, 97.9, 55.5, 51.8.



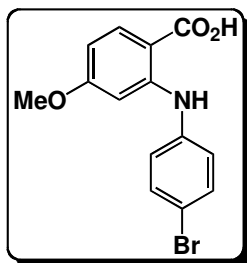
#### 4-methoxy-2-(4-chlorophenylamino)benzoic acid (2k)

Reaction of the methyl ester of 2k according to general procedure 2 provided 2k as a white solid (42% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 12.78 (bs, 1H), 9.80 (s, 1H), 7.86 (d,  $J$  = 8.9 Hz, 1H), 7.38 (d,  $J$  = 8.5 Hz, 2H), 7.30 (d,  $J$  = 8.5 Hz, 2H), 6.64 (d,  $J$  = 2.2 Hz, 1H), 6.41 (dd,  $J$  = 8.9, 2.0 Hz, 1H), 3.73 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 169.6, 163.9, 148.4, 139.4, 133.8, 129.3, 126.6, 123.0, 106.0, 104.9, 97.7, 55.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{ClNO}_3$ : 276.0427 (M-H $^-$ ), found 276.0423 (M-H $^-$ ).



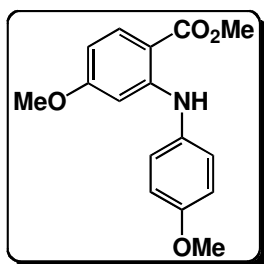
#### 4-methoxy-2-(4-bromophenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with 4-bromoaniline according to general procedure 1 provided the methyl ester of 2l as a green oil (46% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.58 (s, 1H), 7.92 (d,  $J$  = 8.9 Hz, 1H), 7.45 (d,  $J$  = 8.6 Hz, 2H), 7.15 (d,  $J$  = 8.6 Hz, 2H), 6.66 (d,  $J$  = 2.4 Hz, 1H), 6.34 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.86 (s, 3H), 3.76 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 164.6, 149.6, 140.0, 133.8, 132.6, 124.4, 116.3, 105.8, 105.0, 98.0, 55.5, 51.8.



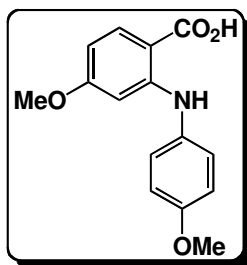
#### 4-methoxy-2-(4-bromophenylamino)benzoic acid (2l)

Reaction of the methyl ester of 2l according to general procedure 2 provided 2l as a brown solid (73% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 12.80 (bs, 1H), 9.79 (s, 1H), 7.85 (d,  $J$  = 8.8 Hz, 1H), 7.50 (d,  $J$  = 8.7 Hz, 2H), 7.25 (d,  $J$  = 8.7 Hz, 2H), 6.66 (d,  $J$  = 2.3 Hz, 1H), 6.41 (dd,  $J$  = 8.8, 2.4 Hz, 1H), 3.74 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 169.6, 163.9, 148.2, 139.9, 133.9, 132.3, 123.2, 114.4, 106.0, 105.1, 97.8, 55.2. HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{BrNO}_3$ : 319.9922 (M-H), found 319.9924 (M-H).



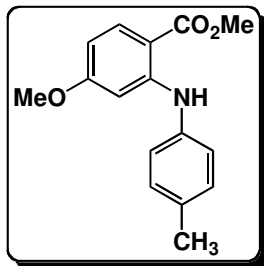
#### 4-methoxy-2-(4-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with *p*-anisidine according to general procedure 1 provided the methyl ester of 2m as a yellow oil (96% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.39 (s, 1H), 7.89 (d,  $J$  = 8.9 Hz, 1H), 7.19 (d,  $J$  = 8.9 Hz, 2H), 6.92 (d,  $J$  = 8.6 Hz, 2H), 6.43 (d,  $J$  = 2.4 Hz, 1H), 6.25 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.88 (s, 3H), 3.83 (s, 3H), 3.71 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 169.0, 164.7, 157.0, 151.8, 133.6, 133.5, 126.4, 114.9, 104.6, 104.0, 97.0, 55.7, 55.4, 51.6.



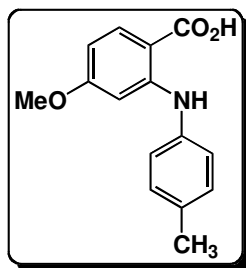
#### 4-methoxy-2-(4-methoxyphenylamino)benzoic acid (2m)

Reaction of the methyl ester of 2m according to general procedure 2 provided 2m as a white solid (89% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.59 (bs, 1H), 9.58 (s, 1H), 7.81 (d,  $J$  = 8.8 Hz, 1H), 7.20 (d,  $J$  = 8.6 Hz, 2H), 6.95 (d,  $J$  = 8.6 Hz, 2H), 6.37 (s, 1H), 6.29 (dd,  $J$  = 8.8, 2.1 Hz, 1H), 3.76 (s, 3H), 3.67 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.7, 164.0, 156.1, 150.7, 133.8, 132.7, 125.1, 114.8, 104.5, 103.5, 96.4, 55.2, 55.0. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_4$ : 272.0923 (M-H), found 272.0916 (M-H).



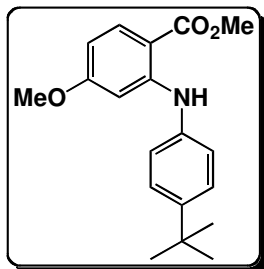
#### 4-methoxy-2-(4-methylphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with *p*-toluidine according to general procedure **1** provided the methyl ester of **2n** as a yellow oil (96% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.53$  (s, 1H), 7.91 (d,  $J = 8.9$  Hz, 1H), 7.18 (s, 4H), 6.63 (s, 1H), 6.28 (d,  $J = 8.9$  Hz, 1H), 3.88 (s, 3H), 3.74 (s, 3H), 2.36 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.9$ , 164.6, 150.9, 138.0, 133.9, 133.6, 130.2, 123.7, 105.0, 104.4, 97.3, 55.4, 51.6, 21.1.



#### 4-methoxy-2-(4-methylphenylamino)benzoic acid (**2n**)

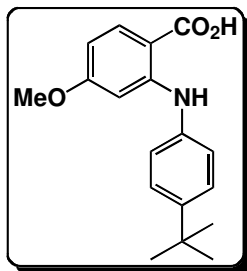
Reaction of the methyl ester of **2n** according to general procedure **2** provided **2n** as a white solid (80% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.63$  (bs, 1H), 9.70 (s, 1H), 7.83 (d,  $J = 8.9$  Hz, 1H), 7.13-7.21 (m, 4H), 6.56 (d,  $J = 2.4$  Hz, 1H), 6.30 (dd,  $J = 8.9$ , 2.4 Hz, 1H), 3.70 (s, 3H), 2.29 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 169.7$ , 163.9, 149.6, 137.5, 133.8, 132.7, 130.0, 122.4, 105.0, 104.1, 96.8, 55.1, 20.4. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_3$ : 280.0950 ( $\text{M}+\text{Na}^+$ ), found 280.0963 ( $\text{M}+\text{H}^+$ ).



#### 4-methoxy-2-(4-*tert*-butylphenylamino)benzoic acid methyl ester

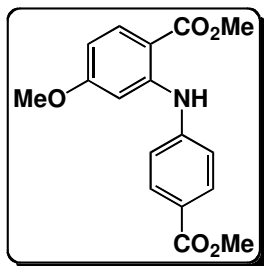
Reaction of methyl 4-methoxy-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-*tert*-butylaniline according to general procedure **1** provided the methyl ester of **2o** as a yellow oil (96% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.58$  (s, 1H), 7.93 (d,  $J = 9.0$  Hz, 1H),

7.39 (d,  $J = 8.6$  Hz, 2H), 7.22 (d,  $J = 8.4$  Hz, 2H), 6.71 (d,  $J = 2.4$  Hz, 1H), 6.30 (dd,  $J = 9.0, 2.4$  Hz, 1H), 3.89 (s, 3H), 3.77 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.9, 164.6, 150.6, 147.0, 138.0, 133.7, 126.4, 122.9, 105.2, 104.2, 97.6, 55.4, 51.6, 34.6, 31.6$ .



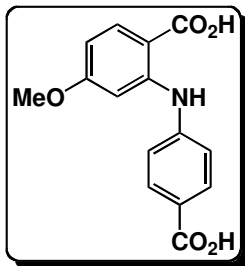
#### 4-methoxy-2-(4-*tert*-butylphenylamino)benzoic acid (**2o**)

Reaction of the methyl ester of **2o** according to general procedure **2** provided **2o** as a white solid (91% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.65$  (bs, 1H), 9.75 (s, 1H), 7.84 (d,  $J = 8.9$  Hz, 1H), 7.38 (d,  $J = 8.3$  Hz, 2H), 7.19 (d,  $J = 8.3$  Hz, 2H), 6.62 (s, 1H), 6.35 (d,  $J = 8.9$  Hz, 1H), 3.72 (s, 3H), 1.28 (s, 9H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.7, 163.9, 149.3, 145.8, 137.5, 133.8, 126.2, 121.5, 105.1, 104.0, 97.1, 55.1, 34.0, 31.2$ . HRMS (ES) Calcd. for  $\text{C}_{18}\text{H}_{21}\text{NO}_3$ : 298.1443 (M-H), found 298.1429 (M-H).



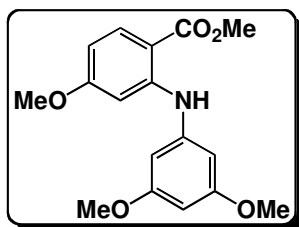
#### 4-methoxy-2-(4-methylcarboxyphenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with methyl 4-aminobenzoate according to general procedure **1** provided the methyl ester of **2p** as a white solid (99% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.86$  (s, 1H), 8.00 (d,  $J = 8.6$  Hz, 2H), 7.94 (d,  $J = 8.9$  Hz, 1H), 7.27 (d,  $J = 8.7$  Hz, 2H), 6.92 (d,  $J = 2.3$  Hz, 1H), 6.42 (dd,  $J = 8.9, 2.3$  Hz, 1H), 3.91 (s, 3H), 3.88 (s, 3H), 3.80 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.7, 166.9, 164.5, 147.8, 145.7, 133.8, 131.5, 123.9, 119.5, 107.1, 106.1, 99.6, 55.6, 52.1, 51.9$ .



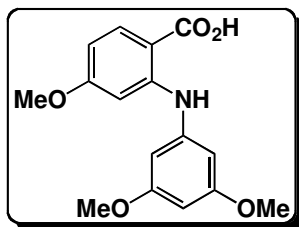
#### 4-methoxy-2-(4-carboxyphenylamino)benzoic acid (2p)

Reaction of the methyl ester of 2p according to general procedure **2** provided **2p** as a white solid (91% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.75 (bs, 2H), 10.02 (s, 1H), 7.86-7.94 (m, 3H), 7.33 (d,  $J$  = 8.5 Hz, 2H), 6.89 (d,  $J$  = 2.3 Hz, 1H), 6.51 (dd,  $J$  = 8.9, 2.4 Hz, 1H), 3.78 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 169.4, 166.9, 163.8, 146.7, 145.1, 133.9, 131.2, 123.7, 118.5, 107.4, 106.1, 99.6, 55.3. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_5$ : 286.0715 (M-H), found 286.0710 (M-H).



#### 4-methoxy-2-(3,5-bis(methoxy)phenylamino)benzoic acid methyl ester

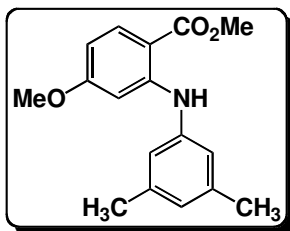
Reaction of methyl 4-methoxy-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with 3,5-dimethoxyaniline according to general procedure **1** provided the methyl ester of 2q as a yellow solid (88% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.62 (s, 1H), 7.91 (d,  $J$  = 9.0 Hz, 1H), 6.84 (d,  $J$  = 2.4 Hz, 1H), 6.45 (d,  $J$  = 2.2 Hz, 2H), 6.32 (dd,  $J$  = 9.0, 2.4 Hz, 1H), 6.23 (t,  $J$  = 2.2 Hz, 1H), 3.88 (s, 3H), 3.79 (s, 6H), 3.77 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 168.9, 164.6, 161.7, 149.7, 142.7, 133.6, 105.7, 105.1, 100.6, 98.5, 96.2, 55.6, 55.5, 51.7.



#### 4-methoxy-2-(3,5-bis(methoxy)phenylamino)benzoic acid (2q)

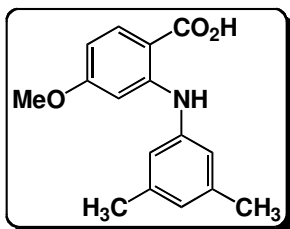
Reaction of the methyl ester of 2q according to general procedure **2** provided **2q** as a yellow solid (99% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.71 (bs, 1H), 9.76 (s, 1H),

7.84 (d,  $J = 8.9$  Hz, 1H), 6.77 (d,  $J = 2.4$  Hz, 1H), 6.42 (d,  $J = 2.0$  Hz, 2H), 6.38 (dd,  $J = 8.9, 2.1$  Hz, 1H), 6.23 (t,  $J = 2.0$  Hz, 1H), 3.73 (s, 9H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.5, 163.8, 161.2, 148.5, 142.2, 133.7, 105.8, 104.9, 99.3, 98.1, 95.6, 55.2, 55.1$ . HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{17}\text{NO}_5$ : 304.1185 ( $\text{M}+\text{H}^+$ ), found 304.1172 ( $\text{M}+\text{H}^+$ ).



#### 4-methoxy-2-(3,5-bis(methyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 4-methoxy-2-[[trifluoromethylsulfonyl]oxy]benzoate with 3,5-dimethylaniline according to general procedure 1 provided the methyl ester of 2r as a colorless oil (97% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.54$  (s, 1H), 7.92 (s, 1H), 6.91 (s, 2H), 6.71-6.82 (m, 2H), 6.30 (s, 1H), 3.87 (s, 3H), 3.75 (s, 3H), 2.32 (s, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 168.8, 164.5, 150.4, 140.7, 139.2, 133.6, 125.7, 120.7, 105.3, 104.4, 97.9, 55.4, 51.6, 21.5$ .

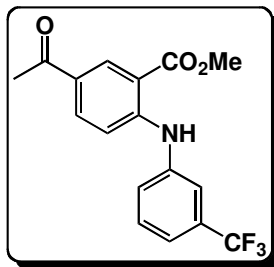


#### 4-methoxy-2-(3,5-bis(methyl)phenylamino)benzoic acid (2r)

Reaction of the methyl ester of 2r according to general procedure 2 provided 2r as a white solid (82% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.66$  (bs, 1H), 9.72 (s, 1H), 7.84 (d,  $J = 8.9$  Hz, 1H), 6.87 (s, 2H), 6.72 (s, 1H), 6.66 (d,  $J = 2.4$  Hz, 1H), 6.35 (dd,  $J = 8.9, 2.4$  Hz, 1H), 3.72 (s, 3H), 2.26 (s, 6H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 169.7, 163.8, 149.1, 140.1, 138.7, 133.8, 124.9, 119.3, 105.3, 104.1, 97.5, 55.1, 20.9$ . HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{17}\text{NO}_3$ : 272.1287 ( $\text{M}+\text{H}^+$ ), found 272.1281 ( $\text{M}+\text{H}^+$ ).

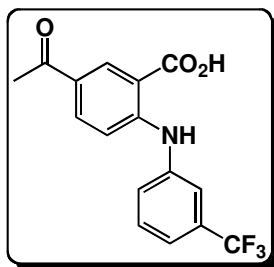


### Class 3 compounds



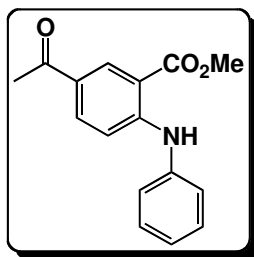
#### **5-acetyl-2-(3-(trifluoromethyl)phenylamino)benzoic acid methyl ester**

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3-aminobenzotrifluoride according to general procedure 1 provided the methyl ester of 3a as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 10.07$  (s, 1H), 8.64 (d,  $J = 2.2$  Hz, 1H), 7.96 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.40-7.56 (m, 4H), 7.18 (d,  $J = 8.9$  Hz, 1H), 3.96 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 195.7, 168.7, 150.9, 140.3, 134.4, 133.7, 130.4, 127.5, 126.6, 121.6, 120.2, 113.3, 111.6, 52.4, 26.2$ .



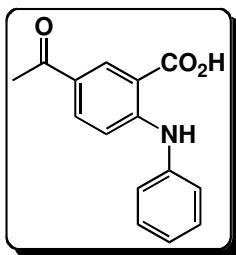
#### **5-acetyl-2-(3-(trifluoromethyl)phenylamino)benzoic acid (3a)**

Reaction of the methyl ester of 3a according to general procedure 2 provided 3a as a white solid (44% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 8.57$  (d,  $J = 2.3$  Hz, 1H), 7.91 (dd,  $J = 8.8, 2.3$  Hz, 1H), 7.57-7.63 (m, 2H), 7.55 (s, 1H), 7.41 (m, 1H), 7.25 (d,  $J = 8.8$  Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 195.3, 169.5, 149.3, 141.1, 133.0, 132.5, 130.6, 126.7, 124.8, 119.3, 117.4, 116.9, 112.6, 26.0$ . **HRMS** (ES) Calcd. for  $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NO}_3$ : 322.0691 (M-H), found 322.0694 (M-H).



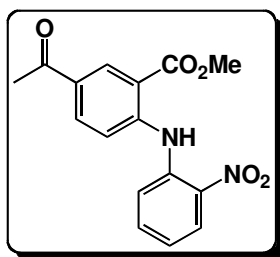
### 5-acetyl-2-(phenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with aniline according to general procedure 1 provided the methyl ester of 3b as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.97 (s, 1H), 8.62 (d,  $J$  = 2.2 Hz, 1H), 7.91 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.38-7.44 (m, 2H), 7.25-7.30 (m, 2H), 7.21 (m, 1H), 7.15 (d,  $J$  = 9.0 Hz, 1H), 3.96 (s, 3H), 2.51 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.9, 168.8, 152.0, 139.4, 134.2, 133.9, 129.8, 126.5, 125.5, 124.2, 113.3, 110.6, 52.3, 26.2.



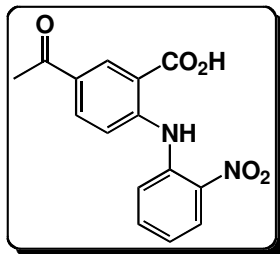
### 5-acetyl-2-(phenylamino)benzoic acid (3b)

Reaction of the methyl ester of 3b according to general procedure 2 provided 3b as a white solid (76% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 13.45 (bs, 1H), 10.12 (s, 1H), 8.51 (s, 1H), 7.93 (d,  $J$  = 6.9 Hz, 1H), 7.43 (t,  $J$  = 7.7 Hz, 2H), 7.31 (d,  $J$  = 7.9 Hz, 2H), 7.12-7.25 (m, 2H), 2.49 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 195.0, 169.6, 150.8, 139.0, 134.0, 133.2, 129.6, 126.0, 124.8, 123.1, 112.7, 111.1, 26.0. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_3$ : 254.0817 (M-H), found 254.0815 (M-H).



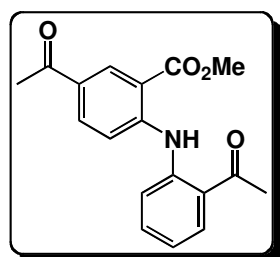
### 5-acetyl-2-(2-nitrophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 2-nitroaniline according to general procedure 1 provided the methyl ester of 3c as a yellow solid (82% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 11.41 (s, 1H), 8.63 (d,  $J$  = 2.1 Hz, 1H), 8.15 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 8.00 (dd,  $J$  = 8.8, 2.1 Hz, 1H), 7.66 (d,  $J$  = 8.4 Hz, 1H), 7.54 (m, 1H), 7.48 (d,  $J$  = 8.8 Hz, 1H), 7.11 (m, 1H), 4.00 (s, 3H), 2.58 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 167.5, 147.5, 139.7, 136.7, 134.7, 133.6, 133.5, 129.7, 126.7, 122.5, 121.2, 116.4, 115.8, 52.7, 26.4.



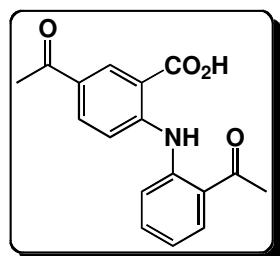
### 5-acetyl-2-(2-nitrophenylamino)benzoic acid (**3c**)

Reaction of the methyl ester of **3c** according to general procedure **2** provided **3c** as a green solid (89% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 11.36 (s, 1H), 8.53 (d,  $J$  = 2.2 Hz, 1H), 8.14 (dd,  $J$  = 8.4, 1.4 Hz, 1H), 8.02 (dd,  $J$  = 8.8, 2.2 Hz, 1H), 7.66-7.78 (m, 2H), 7.48 (d,  $J$  = 8.8 Hz, 1H), 7.25 (m, 1H), 2.54 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 195.6, 168.7, 147.2, 139.5, 135.7, 135.2, 133.6, 132.6, 128.9, 126.3, 123.0, 121.9, 116.2, 115.6, 26.3. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_5$ : 299.0668 (M-H<sup>-</sup>), found 299.0660 (M-H<sup>-</sup>).



### 5-acetyl-2-(2-acetylphenylamino)benzoic acid methyl ester

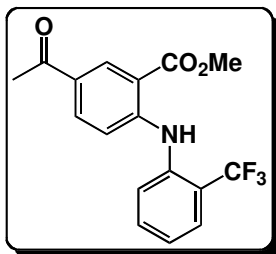
Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 2'-aminoacetophenone according to general procedure **1** provided the methyl ester of **3d** as a green solid (86% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 360 MHz):  $\delta$  = 11.87 (s, 1H), 8.61 (d,  $J$  = 2.1 Hz, 1H), 7.95 (dd,  $J$  = 8.9, 2.1 Hz, 1H), 7.86 (dd,  $J$  = 8.0, 1.4 Hz, 1H), 7.40-7.65 (m, 3H), 7.06 (t,  $J$  = 7.5 Hz, 1H), 4.00 (s, 3H), 2.65 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 90 MHz):  $\delta$  = 200.5, 196.0, 167.3, 148.6, 141.5, 133.7, 133.5, 131.9, 129.8, 128.6, 126.5, 121.8, 120.1, 116.3, 115.3, 52.5, 28.6, 26.4.



### 5-acetyl-2-(2-acetylphenylamino)benzoic acid (**3d**)

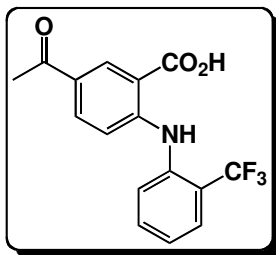
Reaction of the methyl ester of **3d** according to general procedure **2** provided **3d** as a yellow solid (82% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 11.48 (s, 1H), 8.50 (s, 1H), 7.90-8.05 (m, 2H), 7.50-7.62 (m, 2H), 7.43 (d,  $J$  = 9.2 Hz, 1H), 7.16 (m, 1H), 2.59 (s,

3H).  $^{13}\text{C}$  NMR (DMSO, 90 MHz):  $\delta = 200.3, 195.3, 168.1, 148.2, 140.1, 133.5, 133.3, 132.9, 131.9, 127.8, 126.9, 122.3, 120.5, 115.7, 115.1, 28.8, 26.2$ . HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{15}\text{NO}_4$ : 296.0923 (M-H $^-$ ), found 296.0910 (M-H $^-$ ).



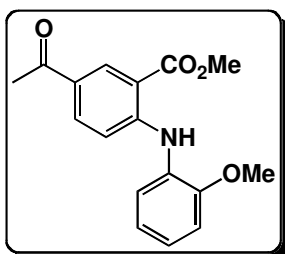
### 5-acetyl-2-(2-(trifluoromethyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 2-aminobenzotrifluoride according to general procedure 1 provided the methyl ester of 3e as a yellow solid (83% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 10.13$  (s, 1H), 8.64 (d,  $J = 2.2$  Hz, 1H), 7.92 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.73 (d,  $J = 7.9$  Hz, 1H), 7.50-7.60 (m, 2H), 7.31 (t,  $J = 7.5$  Hz, 1H), 7.03 (d,  $J = 8.9$  Hz, 1H), 3.97 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 195.9, 168.5, 151.4, 137.9, 134.1, 133.7, 132.9, 127.4, 126.3, 125.4, 113.7, 111.8, 52.4, 26.3$ .



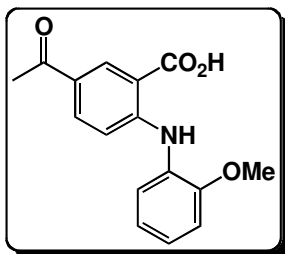
### 5-acetyl-2-(2-(trifluoromethyl)phenylamino)benzoic acid (3e)

Reaction of the methyl ester of 3e according to general procedure 2 provided 3e as a white solid (76% yield).  $^1\text{H}$  NMR (DMSO, 360 MHz):  $\delta = 10.40$  (s, 1H), 8.53 (d,  $J = 2.2$  Hz, 1H), 7.95 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.81 (d,  $J = 7.3$  Hz, 1H), 7.64-7.78 (m, 2H), 7.43 (t,  $J = 7.5$  Hz, 1H), 7.02 (d,  $J = 8.9$  Hz, 1H).  $^{13}\text{C}$  NMR (DMSO, 90 MHz):  $\delta = 195.2, 169.7, 150.6, 137.3, 134.1, 133.8, 133.0, 127.2, 126.9, 126.2, 125.5, 123.2, 113.2, 111.9, 26.1$ . HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NO}_3$ : 322.0691 (M-H $^-$ ), found 322.0700 (M-H $^-$ ).



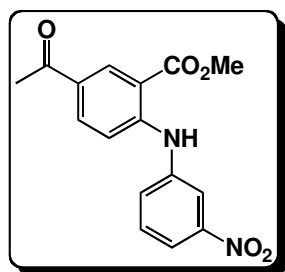
### 5-acetyl-2-(2-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with *o*-anisidine according to general procedure **1** provided the methyl ester of **3f** as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.91 (s, 1H), 8.62 (d,  $J$  = 2.2 Hz, 1H), 7.92 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.40 (d,  $J$  = 7.5 Hz, 1H), 7.13-7.20 (m, 2H), 6.95-7.02 (m, 2H), 3.96 (s, 3H), 3.88 (s, 3H), 2.55 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.9, 168.6, 152.7, 151.4, 133.9, 133.8, 128.3, 126.4, 125.6, 123.2, 120.7, 113.5, 111.7, 111.0, 55.9, 52.2, 26.2.



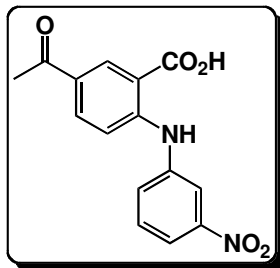
### 5-acetyl-2-(2-methoxyphenylamino)benzoic acid (**3f**)

Reaction of the methyl ester of **3f** according to general procedure **2** provided **3f** as a white solid (60% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.34 (bs, 1H), 10.04 (s, 1H), 8.50 (d,  $J$  = 2.2 Hz, 1H), 7.92 (dd,  $J$  = 8.9, 2.1 Hz, 1H), 7.40 (d,  $J$  = 7.8 Hz, 1H), 7.11-7.22 (m, 2H), 7.07 (d,  $J$  = 8.9 Hz, 1H), 7.00 (m, 1H), 3.82 (s, 3H), 2.48 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.0, 169.5, 151.9, 150.6, 133.9, 133.1, 127.6, 125.8, 125.5, 122.8, 120.6, 112.7, 112.1, 111.2, 55.7, 26.0. **HRMS** (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_4$ : 286.1079 ( $\text{M}+\text{H}^+$ ), found 286.1092 ( $\text{M}+\text{H}^+$ ).



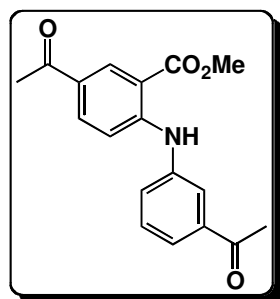
### 5-acetyl-2-(3-nitrophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3-nitroaniline according to general procedure **1** provided the methyl ester of **3g** as a yellow oil (94% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.15 (s, 1H), 8.63 (d,  $J$  = 2.1 Hz, 1H), 8.12 (s, 1H), 7.94-8.00 (m, 2H), 7.50-7.58 (m, 2H), 7.24 (m, 1H), 3.95 (s, 3H), 2.55 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.7, 168.7, 150.2, 149.5, 141.2, 134.5, 133.6, 130.6, 128.7, 128.2, 119.3, 117.4, 113.5, 112.2, 52.5, 26.3.



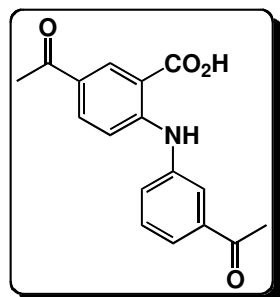
### 5-acetyl-2-(3-nitrophenylamino)benzoic acid (3g)

Reaction of the methyl ester of 3g according to general procedure 2 provided 3g as a yellow solid (86% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 10.25 (bs, 1H), 8.52 (d,  $J$  = 2.1 Hz, 1H), 8.11 (s, 1H), 7.92-8.02 (m, 2H), 7.77 (m, 1H), 7.65 (t,  $J$  = 8.1 Hz, 1H), 7.32 (d,  $J$  = 8.8 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 195.2, 169.2, 149.1, 148.6, 140.9, 133.9, 132.9, 130.8, 128.2, 127.4, 118.3, 116.1, 113.6, 113.2, 26.1. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_5$ : 299.0668 (M-H $^+$ ), found 299.0670 (M-H $^+$ ).



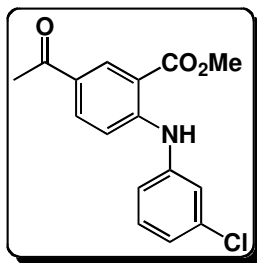
### 5-acetyl-2-(3-acetylphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3'-aminoacetophenone according to general procedure 1 provided the methyl ester of 3h as a yellow solid (97% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.05 (s, 1H), 8.62 (m, 1H), 7.92 (m, 1H), 7.85 (s, 1H), 7.75 (m, 1H), 7.42-7.52 (m, 2H), 7.15 (m, 1H), 3.95 (s, 3H), 2.61 (s, 3H), 2.54 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 197.6, 195.8, 168.7, 151.2, 140.0, 138.8, 134.3, 133.7, 130.0, 128.2, 127.1, 125.1, 123.2, 113.2, 111.1, 52.3, 26.9, 26.2.



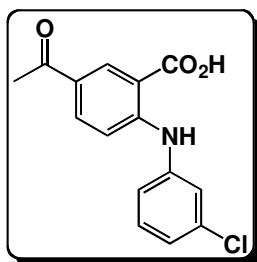
### 5-acetyl-2-(3-acetylphenylamino)benzoic acid (3h)

Reaction of the methyl ester of 3h according to general procedure 2 provided 3h as a yellow solid (84% yield). <sup>1</sup>H NMR (DMSO, 500 MHz): δ = 10.20 (s, 1H), 8.52 (d, *J* = 2.2 Hz, 1H), 7.95 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.84 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.53-7.61 (m, 2H), 7.20 (d, *J* = 8.9 Hz, 1H), 2.59 (s, 3H). <sup>13</sup>C NMR (DMSO, 125 MHz): δ = 197.6, 195.1, 169.5, 150.3, 139.6, 138.2, 134.1, 133.1, 130.0, 127.4, 126.5, 124.2, 122.2, 112.9, 111.8, 26.8, 26.1. HRMS (ES) Calcd. for C<sub>17</sub>H<sub>15</sub>NO<sub>4</sub>: 296.0923 (M-H<sup>-</sup>), found 296.0913 (M-H<sup>-</sup>).



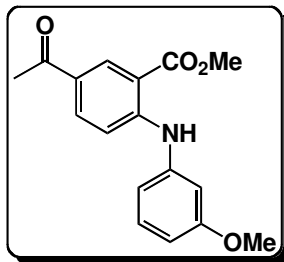
### 5-acetyl-2-(3-chlorophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3-chloroaniline according to general procedure 1 provided the methyl ester of 3i as an orange oil (41% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500MHz): δ = 9.98 (s, 1H), 8.63 (d, *J* = 2.1 Hz, 1H), 7.95 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.28 (s, 1H), 7.19 (d, *J* = 9.0 Hz, 1H), 7.13-7.18 (m, 2H), 3.96 (s, 3H), 2.56 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 195.9, 168.7, 151.1, 140.8, 135.4, 134.3, 133.7, 130.8, 127.2, 125.3, 123.7, 121.8, 113.5, 111.3, 52.4, 26.3.



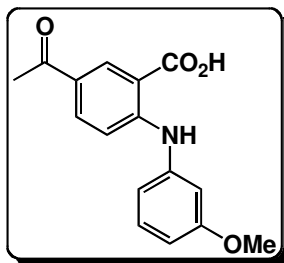
### 5-acetyl-2-(3-chlorophenylamino)benzoic acid (3i)

Reaction of the methyl ester of 3i according to general procedure 2 provided 3i as a white solid (64% yield). <sup>1</sup>H NMR (DMSO, 500 MHz): δ = 13.06 (bs, 1H), 8.55 (s, 1H), 7.78 (d, *J* = 6.7 Hz, 1H), 7.33 (t, *J* = 8.1 Hz, 1H), 7.10-7.27 (m, 4H), 7.01 (d, *J* = 8.7 Hz, 1H), 2.46 (s, 3H). <sup>13</sup>C NMR (DMSO, 125 MHz): δ = 195.5, 142.9, 133.7, 133.2, 131.0, 130.7, 126.3, 121.5, 119.1, 118.4, 111.9, 26.1. HRMS (ES) Calcd. for C<sub>15</sub>H<sub>12</sub>ClNO<sub>3</sub>: 288.0427 (M-H<sup>-</sup>), found 288.0427 (M-H<sup>-</sup>).



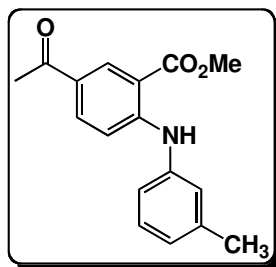
### 5-acetyl-2-(3-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with *m*-anisidine according to general procedure 1 provided the methyl ester of 3j as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.95 (s, 1H), 8.61 (d,  $J$  = 2.2 Hz, 1H), 7.91 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.29 (t,  $J$  = 8.1 Hz, 1H), 7.21 (d,  $J$  = 9.0 Hz, 1H), 6.86 (d,  $J$  = 7.9 Hz, 1H), 6.80 (t,  $J$  = 2.2 Hz, 1H), 6.75 (dd,  $J$  = 8.3, 2.3 Hz, 1H), 3.95 (s, 3H), 3.81 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 160.9, 151.7, 140.5, 134.1, 133.8, 130.5, 126.6, 116.2, 113.6, 110.9, 110.6, 109.7, 55.5, 52.2, 26.2.



### 5-acetyl-2-(3-methoxyphenylamino)benzoic acid (3j)

Reaction of the methyl ester of 3j according to general procedure 2 provided 3j as a white solid (25% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.89 (s, 1H), 8.56 (d,  $J$  = 2.2 Hz, 1H), 7.73 (dd,  $J$  = 8.7, 2.1 Hz, 1H), 7.17-7.27 (m, 2H), 6.77 (d,  $J$  = 8.0 Hz, 1H), 6.71 (s, 1H), 6.58 (d,  $J$  = 8.2 Hz, 1H), 3.75 (s, 3H), 2.44 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.4, 170.0, 160.2, 149.7, 142.4, 133.4, 130.5, 130.1, 125.5, 122.0, 112.6, 111.5, 107.9, 105.7, 55.0, 26.0. HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_4$ : 284.0923 (M-H $^-$ ), found 284.0925 (M-H $^-$ ).

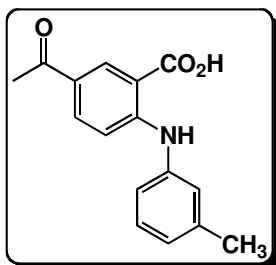


### 5-acetyl-2-(3-methylphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with *m*-toluidine according to general procedure 1 provided the methyl ester of 3k as a yellow oil (90%

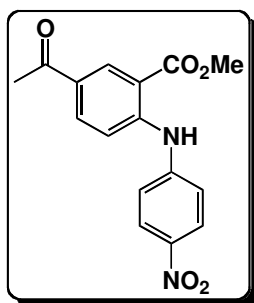


yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.93 (s, 1H), 8.61 (d,  $J$  = 2.2 Hz, 1H), 7.91 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.29 (m, 1H), 7.15 (d,  $J$  = 9.0 Hz, 1H), 7.06-7.10 (m, 2H), 7.02 (d,  $J$  = 7.5 Hz, 1H), 3.95 (s, 3H), 2.55 (s, 3H), 2.37 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 152.0, 139.7, 139.1, 134.1, 133.8, 129.5, 126.2, 126.1, 124.8, 121.1, 113.3, 110.3, 52.2, 26.2, 21.5.



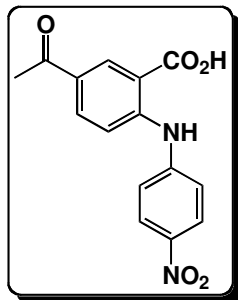
### 5-acetyl-2-(3-methylphenylamino)benzoic acid (3k)

Reaction of the methyl ester of 3k according to general procedure 2 provided 3k as a white solid (84% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.10 (s, 1H), 8.50 (d,  $J$  = 2.2 Hz, 1H), 7.92 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.30 (t,  $J$  = 7.6 Hz, 1H), 7.15 (d,  $J$  = 8.9 Hz, 1H), 7.08-7.13 (m, 2H), 7.01 (d,  $J$  = 7.6 Hz, 1H), 2.48 (s, 3H), 2.32 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 194.9, 169.6, 150.8, 139.1, 138.9, 133.9, 133.1, 129.4, 125.9, 125.4, 123.6, 120.0, 112.8, 111.1, 26.0, 20.9. HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_3$ : 268.0974 (M-H), found 268.0971 (M-H).



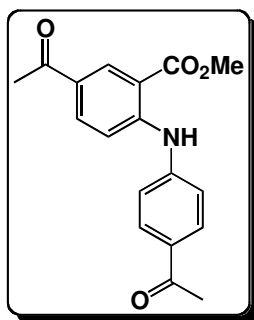
### 5-acetyl-2-(4-nitrophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[(trifluoromethyl)sulfonyl]oxy]benzoate with 4-nitroaniline according to general procedure 1 provided the methyl ester of 3l as an orange oil (73% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 10.35 (s, 1H), 8.67 (d,  $J$  = 2.1 Hz, 1H), 8.25 (d,  $J$  = 9.0 Hz, 2H), 8.05 (dd,  $J$  = 8.8, 2.2 Hz, 1H), 7.49 (d,  $J$  = 8.9 Hz, 1H), 7.35 (d,  $J$  = 9.0 Hz, 2H), 3.99 (s, 3H), 2.60 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.5, 148.6, 146.2, 134.3, 133.5, 129.1, 125.9, 120.2, 115.0, 113.6, 52.7, 26.4.



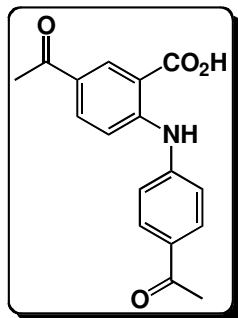
### 5-acetyl-2-(4-nitrophenylamino)benzoic acid (**3l**)

Reaction of the methyl ester of **3l** according to general procedure **2** provided **3l** as an orange solid (74% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.59 (s, 1H), 8.15 (d,  $J$  = 8.1 Hz, 2H), 7.85 (d,  $J$  = 8.6 Hz, 1H), 7.49 (d,  $J$  = 8.6 Hz, 1H), 7.31 (d,  $J$  = 9.0 Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 196.0, 148.2, 146.9, 139.5, 132.8, 130.3, 128.2, 126.0, 116.9, 114.1, 26.3. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_5$ : 299.0668 (M-H<sup>-</sup>), found 299.0658 (M-H<sup>-</sup>).



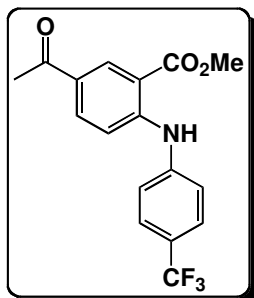
### 5-acetyl-2-(4-acetylphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with 4'-aminoacetophenone according to general procedure **1** provided the methyl ester of **3m** as a yellow solid (87% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.20 (s, 1H), 8.64 (s, 1H), 7.95-8.03 (m, 3H), 7.41 (d,  $J$  = 8.9 Hz, 1H), 7.32 (d,  $J$  = 8.5 Hz, 2H), 3.97 (s, 3H), 2.60 (s, 3H), 2.58 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 196.8, 195.8, 168.6, 149.7, 144.3, 134.2, 133.6, 133.0, 130.4, 128.0, 121.1, 114.4, 112.4, 52.5, 26.6, 26.3.



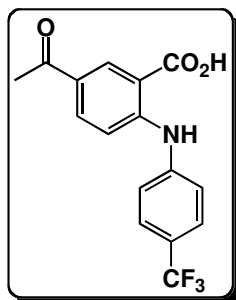
### 5-acetyl-2-(4-acetylphenylamino)benzoic acid (3m)

Reaction of the methyl ester of 3m according to general procedure 2 provided 3m as a white solid (84% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.32 (s, 1H), 8.52 (d,  $J$  = 2.1 Hz, 1H), 8.01 (dd,  $J$  = 8.8, 1.8 Hz, 1H), 7.96 (d,  $J$  = 8.4 Hz, 2H), 7.45 (d,  $J$  = 8.8 Hz, 1H), 7.40 (d,  $J$  = 8.4 Hz, 2H), 2.54 (s, 3H), 2.51 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 196.2, 195.3, 169.3, 148.6, 144.0, 133.9, 132.9, 131.8, 130.1, 127.5, 120.1, 114.4, 113.4, 26.4, 26.2. **HRMS** (ES) Calcd. for  $\text{C}_{17}\text{H}_{15}\text{NO}_4$ : 296.0923 (M-H<sup>-</sup>), found 296.0919 (M-H<sup>-</sup>).



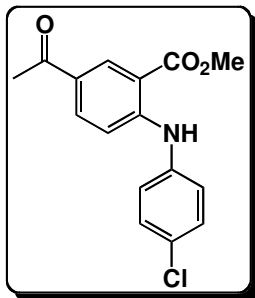
### 5-acetyl-2-(4-(trifluoromethyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-aminobenzotrifluoride according to general procedure 1 provided the methyl ester of 3n as a yellow solid (89% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.13 (s, 1H), 8.64 (d,  $J$  = 2.2 Hz, 1H), 7.97 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.63 (d,  $J$  = 8.4 Hz, 2H), 7.35 (d,  $J$  = 8.6 Hz, 2H), 7.31 (d,  $J$  = 8.9 Hz, 1H), 3.97 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 150.3, 142.9, 134.3, 133.7, 127.8, 127.0, 122.3, 113.8, 112.0, 52.5, 26.3.



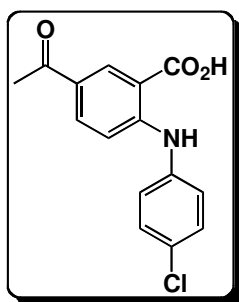
### 5-acetyl-2-(4-(trifluoromethyl)phenylamino)benzoic acid (3n)

Reaction of the methyl ester of 3n according to general procedure 2 provided 3n as a white solid (80% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 10.27 (s, 1H), 8.51 (d,  $J$  = 2.2 Hz, 1H), 7.99 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.70 (d,  $J$  = 8.5 Hz, 2H), 7.49 (d,  $J$  = 8.3 Hz, 2H), 7.39 (d,  $J$  = 8.9 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 195.3, 169.3, 148.9, 143.3, 134.0, 133.0, 127.4, 126.8, 126.7, 121.3, 114.1, 113.1, 26.2. **HRMS** (ES) Calcd. for  $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NO}_3$ : 322.0691 (M-H<sup>-</sup>), found 322.0677 (M-H<sup>-</sup>).



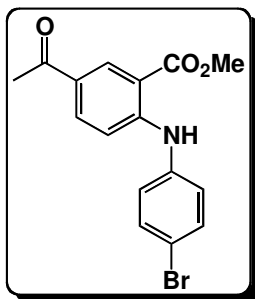
### 5-acetyl-2-(4-chlorophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-chloroaniline according to general procedure 1 provided the methyl ester of **3o** as a yellow oil (90% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.93 (s, 1H), 8.61 (d,  $J$  = 2.1 Hz, 1H), 7.92 (dd,  $J$  = 9.0, 1.8 Hz, 1H), 7.36 (d,  $J$  = 8.5 Hz, 2H), 7.20 (d,  $J$  = 8.5 Hz, 2H), 7.10 (d,  $J$  = 9.0 Hz, 1H), 3.95 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 151.6, 138.0, 134.3, 133.8, 130.6, 129.9, 126.9, 125.4, 113.2, 110.9, 52.3, 26.2.



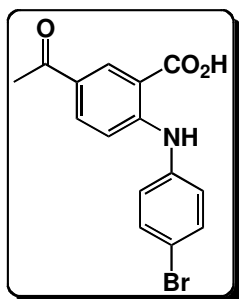
### 5-acetyl-2-(4-chlorophenylamino)benzoic acid (**3o**)

Reaction of the methyl ester of **3o** according to general procedure 2 provided **3o** as a white solid (84% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 13.48 (bs, 1H), 10.09 (s, 1H), 8.50 (s, 1H), 7.94 (d,  $J$  = 8.9 Hz, 1H), 7.45 (d,  $J$  = 8.7 Hz, 2H), 7.34 (d,  $J$  = 8.7 Hz, 2H), 7.15 (d,  $J$  = 8.9 Hz, 1H), 2.49 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 195.1, 169.5, 150.3, 138.1, 134.0, 133.1, 129.5, 128.3, 126.4, 124.6, 112.9, 111.7, 26.1. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{ClNO}_3$ : 288.0427 (M-H $^-$ ), found 288.0431 (M-H $^-$ ).



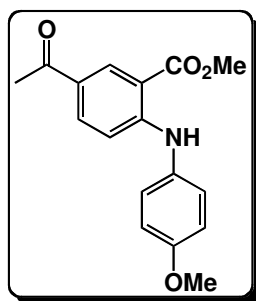
### 5-acetyl-2-(4-bromophenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-bromoaniline according to general procedure 1 provided the methyl ester of 3p as a yellow solid (80% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.89 (s, 1H), 8.59 (d,  $J$  = 2.2 Hz, 1H), 7.89 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.47 (d,  $J$  = 8.7 Hz, 2H), 7.06-7.14 (m, 3H), 3.93 (s, 3H), 2.52 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 151.4, 138.6, 134.3, 133.8, 132.9, 127.0, 125.6, 118.2, 113.3, 111.1, 52.3, 26.2.



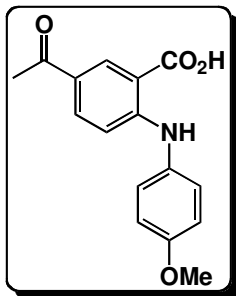
#### 5-acetyl-2-(4-bromophenylamino)benzoic acid (3p)

Reaction of the methyl ester of 3p according to general procedure 2 provided 3p as a white solid (72% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.08 (s, 1H), 8.50 (d,  $J$  = 2.2 Hz, 1H), 7.93 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.56 (d,  $J$  = 8.7 Hz, 2H), 7.28 (d,  $J$  = 8.7 Hz, 2H), 7.17 (d,  $J$  = 8.9 Hz, 1H), 2.48 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.1, 169.5, 150.2, 138.6, 134.0, 133.1, 132.4, 126.4, 124.9, 116.3, 113.0, 111.7, 26.1. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{12}\text{BrNO}_3$ : 331.9922 (M-H $^-$ ), found 331.9927 (M-H $^-$ ).



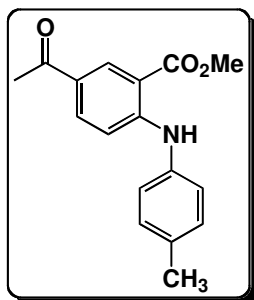
#### 5-acetyl-2-(4-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with *p*-anisidine according to general procedure 1 provided the methyl ester of 3q as a yellow oil (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 9.78 (s, 1H), 8.60 (d,  $J$  = 2.2 Hz, 1H), 7.87 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.18 (d,  $J$  = 9.0 Hz, 2H), 6.90-6.99 (m, 3H), 3.95 (s, 3H), 3.84 (s, 3H), 2.54 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.9, 168.8, 157.9, 153.2, 134.2, 133.9, 132.0, 126.9, 125.9, 115.1, 113.0, 109.8, 55.7, 52.2, 26.2.



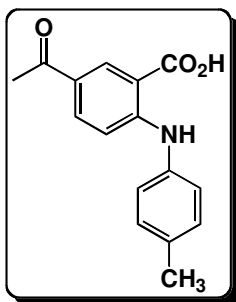
### 5-acetyl-2-(4-methoxyphenylamino)benzoic acid (3q)

Reaction of the methyl ester of 3q according to general procedure 2 provided 3q as a white solid (79% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.34 (bs, 1H), 9.93 (s, 1H), 8.48 (d,  $J$  = 2.2 Hz, 1H), 7.88 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.23 (d,  $J$  = 8.9 Hz, 2H), 7.00 (d,  $J$  = 8.9 Hz, 2H), 6.89 (d,  $J$  = 9.0 Hz, 1H), 3.78 (s, 3H), 2.46 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 194.9, 169.6, 156.9, 152.2, 134.0, 133.3, 131.4, 126.1, 125.3, 114.9, 112.3, 110.2, 55.3, 26.0. HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_4$ : 286.1079 ( $\text{M}+\text{H}^+$ ), found 286.1083 ( $\text{M}+\text{H}^+$ ).



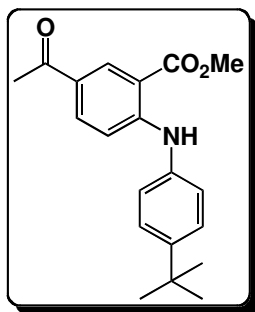
### 5-acetyl-2-(4-methylphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with *p*-toluidine according to general procedure 1 provided the methyl ester of 3r as a yellow oil (84% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.87 (s, 1H), 8.61 (d,  $J$  = 2.2 Hz, 1H), 7.88 (dd,  $J$  = 9.0, 2.2 Hz, 1H), 7.21 (d,  $J$  = 8.2 Hz, 2H), 7.15 (d,  $J$  = 8.2 Hz, 2H), 7.06 (d,  $J$  = 9.0 Hz, 1H), 3.95 (s, 3H), 2.54 (s, 3H), 2.38 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.8, 152.4, 136.6, 135.4, 134.1, 133.9, 130.4, 126.2, 124.6, 113.2, 110.2, 52.2, 26.2, 21.1.



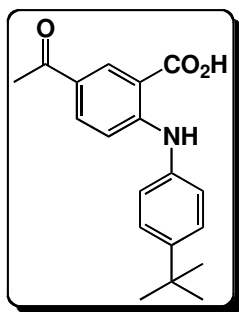
### 5-acetyl-2-(4-methylphenylamino)benzoic acid (3r)

Reaction of the methyl ester of 3r according to general procedure 2 provided 3r as a white solid (69% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.35 (bs, 1H), 10.03 (s, 1H), 8.49 (d,  $J$  = 2.0 Hz, 1H), 7.90 (dd,  $J$  = 8.9, 2.0 Hz, 1H), 7.23 (d,  $J$  = 8.3 Hz, 2H), 7.18 (d,  $J$  = 8.3 Hz, 2H), 7.05 (d,  $J$  = 8.9 Hz, 1H), 2.47 (s, 3H), 2.31 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 194.9, 169.6, 151.3, 136.2, 134.2, 133.9, 133.2, 130.0, 125.6, 123.6, 112.5, 110.7, 25.9, 20.4. **HRMS** (ES) Calcd. for  $\text{C}_{16}\text{H}_{15}\text{NO}_3$ : 268.0974 (M-H<sup>-</sup>), found 268.0987 (M-H<sup>-</sup>).



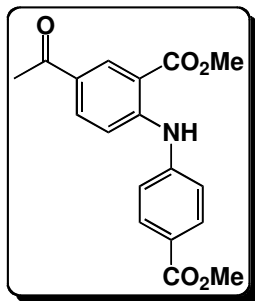
### 5-acetyl-2-(4-tert-butylphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with 4-tert-butylaniline according to general procedure 1 provided the methyl ester of 3s as a yellow oil (79% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.91 (s, 1H), 8.61 (s, 1H), 7.89 (d,  $J$  = 9.0 Hz, 1H), 7.41 (d,  $J$  = 8.2 Hz, 2H), 7.19 (d,  $J$  = 8.2 Hz, 2H), 7.12 (d,  $J$  = 9.0 Hz, 1H), 3.94 (s, 3H), 2.54 (s, 3H), 1.35 (s, 9H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.7, 152.2, 148.6, 136.5, 134.1, 133.8, 126.6, 126.1, 124.0, 113.2, 110.2, 52.1, 34.7, 31.5, 26.1.



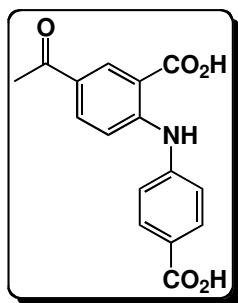
### 5-acetyl-2-(4-tert-butylphenylamino)benzoic acid (3s)

Reaction of the methyl ester of 3s according to general procedure 2 provided 3s as a white solid (71% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.40 (bs, 1H), 10.07 (s, 1H), 8.50 (s, 1H), 7.91 (d,  $J$  = 8.9 Hz, 1H), 7.43 (d,  $J$  = 7.8 Hz, 2H), 7.23 (d,  $J$  = 7.8 Hz, 2H), 7.11 (d,  $J$  = 8.9 Hz, 1H), 2.47 (s, 3H), 1.29 (s, 9H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 194.9, 169.6, 151.1, 147.3, 136.2, 133.9, 133.2, 126.3, 125.6, 123.0, 112.6, 110.7, 34.1, 31.1, 25.9. **HRMS** (ES) Calcd. for  $\text{C}_{19}\text{H}_{21}\text{NO}_3$ : 310.1443 (M-H<sup>-</sup>), found 310.1458 (M-H<sup>-</sup>).



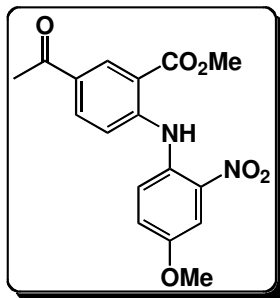
### 5-acetyl-2-(4-methylcarboxyphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with methyl 4-aminobenzoate according to general procedure **1** provided the methyl ester of **3t** as a yellow oil (64% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 10.18 (s, 1H), 8.64 (s, 1H), 8.05 (d,  $J$  = 8.6 Hz, 2H), 7.98 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.39 (d,  $J$  = 8.9 Hz, 1H), 7.30 (d,  $J$  = 8.6 Hz, 2H), 3.97 (s, 3H), 3.92 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 168.6, 166.7, 150.0, 144.1, 134.3, 133.6, 131.5, 127.9, 125.8, 121.3, 114.2, 112.2, 52.5, 52.3, 26.3.



### 5-acetyl-2-(4-carboxyphenylamino)benzoic acid (**3t**)

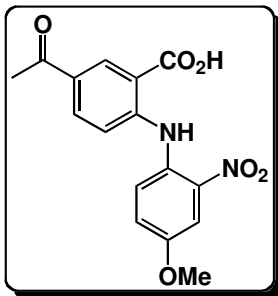
Reaction of the methyl ester of **3t** according to general procedure **2** provided **3t** as a white solid (83% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.34 (s, 1H), 8.52 (d,  $J$  = 2.2 Hz, 1H), 8.00 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.94 (d,  $J$  = 8.6 Hz, 2H), 7.43 (d,  $J$  = 8.9 Hz, 1H), 7.39 (d,  $J$  = 8.6 Hz, 2H), 2.51 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.3, 169.4, 166.8, 148.8, 143.7, 134.0, 133.0, 131.0, 127.4, 125.4, 120.3, 114.2, 113.2, 26.2. HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{13}\text{NO}_5$ : 298.0715 (M-H $^-$ ), found 298.0715 (M-H $^-$ ).





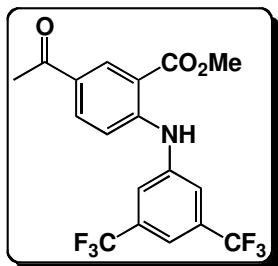
### 5-acetyl-2-(2-nitro-4-methoxyphenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 4-methoxy-2-nitroaniline according to general procedure **1** provided the methyl ester of **3u** as an orange oil (66% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 11.12 (s, 1H), 8.64 (s, 1H), 7.96 (d,  $J$  = 9.0 Hz, 1H), 7.61 (d,  $J$  = 2.6 Hz, 1H), 7.56 (d,  $J$  = 9.1 Hz, 1H), 7.28 (s, 1H), 7.17 (dd,  $J$  = 9.0, 2.6 Hz, 1H), 4.00 (s, 3H), 3.89 (s, 3H), 2.57 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.8, 167.8, 155.4, 148.9, 141.5, 133.8, 133.7, 129.4, 128.7, 124.5, 122.6, 115.0, 114.2, 109.2, 56.2, 52.6, 26.4.



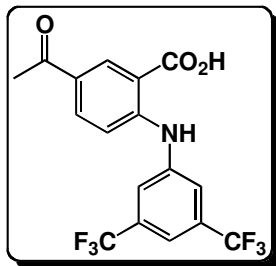
### 5-acetyl-2-(2-nitro-4-methoxyphenylamino)benzoic acid (**3u**)

Reaction of the methyl ester of **3u** according to general procedure **2** provided **3u** as an orange solid (96% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.94 (s, 1H), 8.51 (d,  $J$  = 2.1 Hz, 1H), 7.96 (dd,  $J$  = 8.9, 2.1 Hz, 1H), 7.66 (d,  $J$  = 9.1 Hz, 1H), 7.63 (d,  $J$  = 2.9 Hz, 1H), 7.36 (dd,  $J$  = 9.0, 2.9 Hz, 1H), 7.20 (d,  $J$  = 8.9 Hz, 1H), 3.86 (s, 3H), 2.51 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.3, 169.0, 155.2, 148.9, 141.9, 133.8, 132.8, 127.9, 127.6, 125.7, 122.2, 114.5, 113.7, 109.2, 56.0, 26.2. HRMS (ES) Calcd. for  $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_6$ : 329.0774 (M-H), found 329.0778 (M-H).



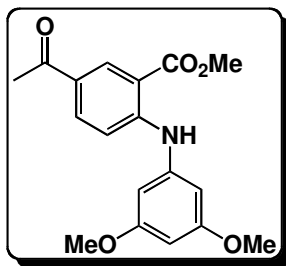
### 5-acetyl-2-(3,5-bis(trifluoromethyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with 3,5-bis(trifluoromethyl)aniline according to general procedure **1** provided the methyl ester of **3v** as a white solid (96% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.21 (s, 1H), 8.64 (d,  $J$  = 2.2 Hz, 1H), 8.00 (dd,  $J$  = 8.9, 2.2 Hz, 1H), 7.68 (s, 2H), 7.61 (s, 1H), 7.24 (s, 1H), 3.96 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.7, 168.7, 149.7, 141.6, 134.6, 133.6, 133.5, 133.3, 128.6, 124.3, 122.2, 113.5, 112.7, 52.6, 26.4.



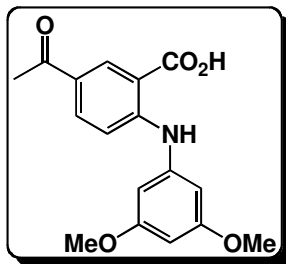
### 5-acetyl-2-(3,5-bis(trifluoromethyl)phenylamino)benzoic acid (3v)

Reaction of the methyl ester of 3v according to general procedure 2 provided 3v as a white solid (87% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.56 (d,  $J$  = 2.2 Hz, 1H), 7.94 (dd,  $J$  = 8.7, 2.2 Hz, 1H), 7.85 (s, 2H), 7.63 (s, 1H), 7.35 (d,  $J$  = 8.7 Hz, 1H), 2.51 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.6, 169.2, 148.1, 142.9, 132.8, 132.4, 131.6, 131.3, 127.9, 124.3, 122.1, 120.0, 113.5, 26.2. HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{11}\text{F}_6\text{NO}_3$ : 390.0565 (M-H<sup>-</sup>), found 390.0559 (M-H<sup>-</sup>).



### 5-acetyl-2-(3,5-bis(methoxy)phenylamino)benzoic acid methyl ester

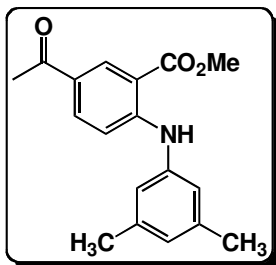
Reaction of methyl 5-acetyl-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with 3,5-dimethoxyaniline according to general procedure 1 provided the methyl ester of 3w as a white solid (89% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.92 (s, 1H), 8.61 (s, 1H), 7.92 (d,  $J$  = 9.0 Hz, 1H), 7.26 (m, 1H), 6.43 (s, 2H), 6.31 (m, 1H), 3.95 (s, 3H), 3.79 (s, 6H), 2.55 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 195.9, 168.7, 161.8, 151.6, 141.1, 134.2, 133.7, 126.6, 113.9, 110.8, 102.1, 97.5, 55.6, 52.3, 26.2.



### 5-acetyl-2-(3,5-bis(methoxy)phenylamino)benzoic acid (3w)

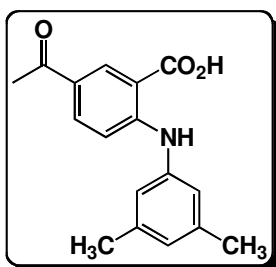
Reaction of the methyl ester of 3w according to general procedure 2 provided 3w as a yellow solid (98% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 10.05 (s, 1H), 8.49 (s, 1H), 7.94 (d,  $J$  = 8.3 Hz, 1H), 7.26 (d,  $J$  = 8.7 Hz, 1H), 6.46 (s, 2H), 6.32 (s, 1H), 3.74 (s, 6H),

2.48 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 195.2, 169.6, 161.3, 150.5, 140.9, 134.1, 133.2, 126.2, 113.5, 111.5, 100.9, 96.9, 55.4, 26.1$ . HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{17}\text{NO}_5$ : 314.1028 (M-H $^-$ ), found 314.1031 (M-H $^-$ ).



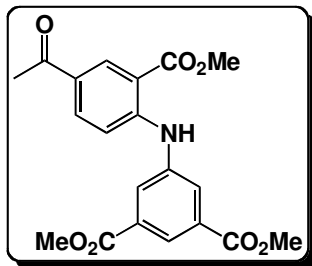
### 5-acetyl-2-(3,5-bis(methyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[[(trifluoromethyl)sulfonyl]oxy]benzoate with 3,5-dimethylaniline according to general procedure 1 provided the methyl ester of 3x as a yellow oil (87% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.87$  (s, 1H), 8.61 (d,  $J = 2.2$  Hz, 1H), 7.91 (dd,  $J = 9.0, 2.2$  Hz, 1H), 7.15 (d,  $J = 9.0$  Hz, 1H), 6.89 (s, 2H), 6.85 (s, 1H), 3.95 (s, 3H), 2.54 (s, 3H), 2.33 (s, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 195.8, 168.7, 152.2, 139.5, 139.2, 134.1, 133.8, 127.2, 126.3, 121.9, 113.5, 110.4, 52.2, 26.2, 21.5$ .



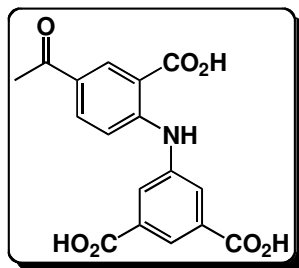
### 5-acetyl-2-(3,5-bis(methyl)phenylamino)benzoic acid (3x)

Reaction of the methyl ester of 3x according to general procedure 2 provided 3x as a white solid (83% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 13.40$  (bs, 1H), 10.04 (s, 1H), 8.49 (d,  $J = 2.2$  Hz, 1H), 7.93 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.16 (d,  $J = 8.9$  Hz, 1H), 6.92 (s, 2H), 6.84 (s, 1H), 2.48 (s, 3H), 2.28 (s, 6H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 194.9, 169.6, 150.9, 138.8, 138.7, 134.0, 133.1, 126.3, 125.7, 120.6, 112.9, 110.9, 25.9, 20.8$ . HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{17}\text{NO}_3$ : 284.1287 (M+H $^+$ ), found 284.1290 (M+H $^+$ ).



### 5-acetyl-2-(3,5-bis(methylcarboxy)phenylamino)benzoic acid methyl ester

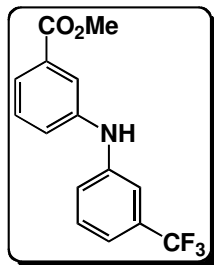
Reaction of methyl 5-acetyl-2-[[trifluoromethyl)sulfonyl]oxy]benzoate with dimethyl 5-aminoisophthalate according to general procedure **1** provided the methyl ester of **3y** as a white solid (89% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 360 MHz):  $\delta$  = 10.13 (s, 1H), 8.63 (d,  $J$  = 2.2 Hz, 1H), 8.45 (s, 1H), 8.11 (s, 2H), 7.96 (dd,  $J$  = 9.0, 1.9 Hz, 1H), 7.19 (d,  $J$  = 8.9 Hz, 1H), 3.96 (s, 3H), 3.95 (s, 6H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 90 MHz):  $\delta$  = 195.8, 168.7, 165.9, 150.6, 140.3, 134.5, 133.7, 132.3, 128.2, 127.6, 126.8, 113.2, 111.7, 52.8, 52.4, 26.3.



### 5-acetyl-2-(3,5-bis(carboxy)phenylamino)benzoic acid (**3y**)

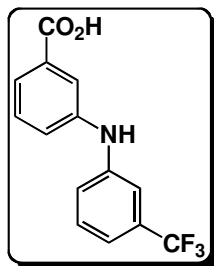
Reaction of the methyl ester of **3y** according to general procedure **2** provided **3y** as a yellow solid (77% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.40 (s, 3H), 10.20 (s, 1H), 8.51 (d,  $J$  = 2.2 Hz, 1H), 8.21 (d,  $J$  = 1.4 Hz, 1H), 7.98-8.08 (m, 3H), 7.25 (d,  $J$  = 8.9 Hz, 1H). **HRMS** (ES) Calcd. for  $\text{C}_{17}\text{H}_{13}\text{NO}_7$ : 342.0614 (M-H $^-$ ), found 342.0612 (M-H $^-$ ).

## Class 4 compounds



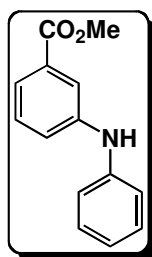
### **3-[(3-trifluoromethylphenyl)amino]benzoic acid methyl ester**

Reaction of methyl 3-bromobenzoate with 3-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **4a** as a yellow oil (55% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500 MHz): δ = 7.76 (t, *J* = 1.9 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.15-7.43 (m, 6H), 5.97 (s, 1H), 3.92 (s, 3H). **<sup>13</sup>C NMR** (CDCl<sub>3</sub>, 125 MHz): δ = 167.1, 143.6, 142.6, 131.9, 130.2, 129.8, 123.3, 122.8, 120.5, 119.7, 118.0, 114.3, 52.4.



### **3-[(3-trifluoromethylphenyl)amino]benzoic acid (**4a**)**

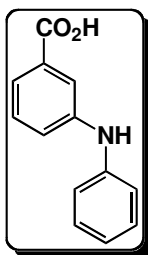
Reaction of the methyl ester of **4a** according to general procedure **2** provided **4a** as a white solid (65% yield). **<sup>1</sup>H NMR** (DMSO, 500 MHz): δ = 8.71 (s, 1H), 7.68 (t, *J* = 1.8 Hz, 1H), 7.44-7.51 (m, 2H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.33-7.37 (m, 2H), 7.30 (s, 1H), 7.15 (d, *J* = 7.7 Hz, 1H). **<sup>13</sup>C NMR** (DMSO, 125 MHz): δ = 167.2, 144.0, 142.5, 131.9, 130.4, 129.6, 121.6, 121.5, 120.0, 117.9, 115.9, 112.4. **HRMS** (ES) Calcd. for C<sub>14</sub>H<sub>10</sub>F<sub>3</sub>NO<sub>2</sub>: 280.0585 (M-H), found 280.0591 (M-H).



### **3-phenylamino benzoic acid methyl ester**

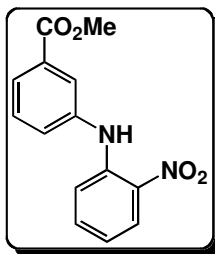
Reaction of methyl 3-bromobenzoate with aniline according to general procedure **1** provided the methyl ester of **4b** as a yellow oil (94% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500MHz):

$\delta = 7.73$  (s, 1H), 7.56 (d,  $J = 7.6$  Hz, 1H), 7.22-7.35 (m, 4H), 7.10 (d,  $J = 8.5$  Hz, 2H), 7.00 (t,  $J = 7.4$  Hz, 1H), 5.81 (s, 1H), 3.91 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.3, 143.9, 142.6, 131.6, 129.7, 129.6, 122.0, 121.9, 121.7, 118.7, 118.4, 52.3$ .



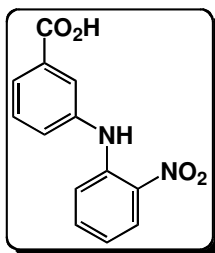
### 3-phenylamino benzoic acid (4b)

Reaction of the methyl ester of 4a according to general procedure 2 provided 4b as a white solid (74% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.79$  (bs, 1H), 8.33 (s, 1H), 7.65 (s, 1H), 7.24-7.38 (m, 5H), 7.10 (d,  $J = 8.5$  Hz, 2H), 6.88 (t,  $J = 7.3$  Hz, 1H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 167.4, 143.9, 142.7, 131.7, 129.3, 129.2, 120.4, 120.2, 120.1, 117.5, 116.5$ . HRMS (ES) Calcd. for  $\text{C}_{13}\text{H}_{11}\text{NO}_2$ : 212.0712 (M-H), found 212.0712 (M-H).



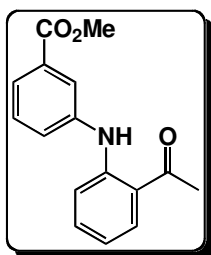
### 3-[(2-nitrophenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 2-nitroaniline according to general procedure 1 provided the methyl ester of 4c as a red oil (67% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 9.48$  (s, 1H), 8.20 (d,  $J = 8.6$  Hz, 1H), 7.95 (s, 1H), 7.88 (m, 1H), 7.44-7.54 (m, 2H), 7.40 (t,  $J = 7.8$  Hz, 1H), 7.22 (d,  $J = 8.6$  Hz, 1H), 6.82 (t,  $J = 7.8$  Hz, 1H), 3.93 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 166.5, 142.4, 139.4, 136.0, 133.9, 132.0, 130.0, 128.4, 126.9, 126.6, 125.0, 118.3, 116.1, 52.5$ .



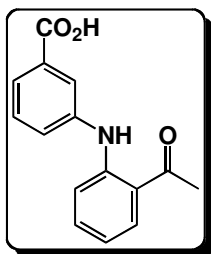
### 3-[(2-nitrophenyl)amino]benzoic acid (4c)

Reaction of the methyl ester of 4c according to general procedure 2 provided 4c as an orange solid (81% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.05 (bs, 1H), 9.35 (s, 1H), 8.11 (d,  $J$  = 8.5 Hz, 1H), 7.84 (s, 1H), 7.72 (d,  $J$  = 7.4 Hz, 1H), 7.49-7.57 (m, 3H), 7.23 (d,  $J$  = 8.6 Hz, 1H), 6.94 (t,  $J$  = 7.8 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 166.9, 141.0, 140.1, 135.9, 134.6, 132.1, 129.8, 127.2, 126.2, 125.0, 123.4, 118.8, 117.4. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H<sup>-</sup>), found 257.0560 (M-H<sup>-</sup>).



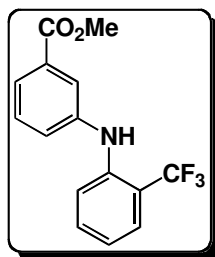
### 3-[(2-acetylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 2'-aminoacetophenone according to general procedure 1 provided the methyl ester of 4d as a yellow oil (89% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 10.60 (s, 1H), 7.92 (s, 1H), 7.80 (d,  $J$  = 8.0 Hz, 1H), 7.74 (d,  $J$  = 7.0 Hz, 1H), 7.35-7.45 (m, 2H), 7.31 (t,  $J$  = 7.6 Hz, 1H), 7.23 (d,  $J$  = 8.5 Hz, 1H), 6.76 (t,  $J$  = 7.5 Hz, 1H), 3.89 (s, 3H), 2.63 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 201.5, 166.9, 147.4, 141.0, 134.8, 132.7, 131.6, 129.6, 127.2, 124.9, 123.7, 119.7, 117.4, 114.4, 52.3, 28.3.



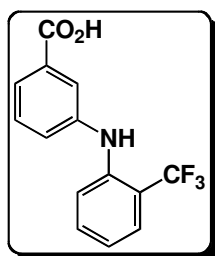
### 3-[(2-acetylphenyl)amino]benzoic acid (4d)

Reaction of the methyl ester of 4d according to general procedure 2 provided 4d as a yellow solid (75% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 10.40 (s, 1H), 7.95 (d,  $J$  = 8.0 Hz, 1H), 7.77 (s, 1H), 7.64 (m, 1H), 7.40-7.51 (m, 3H), 7.25 (d,  $J$  = 8.4 Hz, 1H), 6.86 (t,  $J$  = 7.5 Hz, 1H), 2.50 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 201.7, 167.1, 145.7, 140.7, 134.7, 133.0, 132.5, 129.8, 125.5, 123.9, 121.6, 120.2, 117.9, 114.3, 28.3. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_3$ : 254.0817 (M-H<sup>-</sup>), found 254.0819 (M-H<sup>-</sup>).



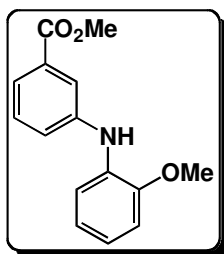
### 3-[(2-trifluoromethylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 2-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **4e** as a colorless oil (79% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.77 (s, 1H), 7.69 (d,  $J$  = 7.7 Hz, 1H), 7.60 (d,  $J$  = 7.5 Hz, 1H), 7.32-7.44 (m, 3H), 7.29 (d,  $J$  = 8.0 Hz, 1H), 7.01 (t,  $J$  = 7.6 Hz, 1H), 6.13 (s, 1H), 3.92 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.0, 142.4, 141.6, 133.0, 131.8, 129.7, 127.2, 127.1, 124.1, 123.7, 120.9, 120.6, 118.7, 52.4.



### 3-[(2-trifluoromethylphenyl)amino]benzoic acid (**4e**)

Reaction of the methyl ester of **4e** according to general procedure **2** provided **4e** as a white solid (81% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 7.73 (s, 1H), 7.69 (d,  $J$  = 7.9 Hz, 1H), 7.52-7.62 (m, 2H), 7.42 (d,  $J$  = 7.6 Hz, 1H), 7.38 (d,  $J$  = 8.1 Hz, 1H), 7.32 (t,  $J$  = 7.8 Hz, 1H), 7.16-7.25 (m, 2H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 167.4, 144.9, 141.2, 133.5, 131.8, 129.3, 127.0, 126.9, 123.7, 122.8, 121.3, 120.9, 117.6. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{10}\text{F}_3\text{NO}_2$ : 280.0585 (M-H $^-$ ), found 280.0584 (M-H $^-$ ).

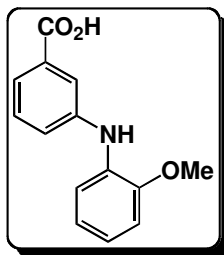


### 3-[(2-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with *o*-anisidine according to general procedure **1** provided the methyl ester of **4f** as a yellow oil (79% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.81 (s, 1H), 7.60 (m, 1H), 7.30-7.38 (m, 3H), 6.90-6.95 (m, 3H), 6.25 (s, 1H), 3.92

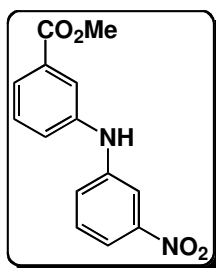


(s, 3H), 3.90 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.2, 148.7, 143.3, 132.3, 131.4, 129.4, 122.2, 122.0, 121.0, 120.9, 119.0, 115.5, 110.8, 55.7, 55.2$ .



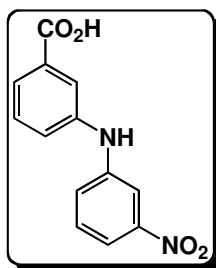
### 3-[(2-methoxyphenyl)amino]benzoic acid (4f)

Reaction of the methyl ester of 4f according to general procedure 2 provided 4f as a white solid (89% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.75$  (bs, 1H), 7.63 (s, 1H), 7.57 (s, 1H), 7.26-7.35 (m, 2H), 7.17-7.23 (m, 2H), 6.87-7.07 (m, 3H), 3.80 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 167.6, 150.6, 144.7, 131.4, 131.2, 129.0, 122.2, 120.6, 120.2, 119.7, 119.0, 116.3, 111.8, 55.4$ . HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 244.0974 ( $\text{M}+\text{H}^+$ ), found 244.0972 ( $\text{M}+\text{H}^+$ ).



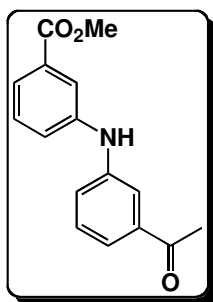
### 3-[(3-nitrophenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 3-nitroaniline according to general procedure 1 provided the methyl ester of 4g as an orange oil (89% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.86$  (t,  $J = 2.2$  Hz, 1H), 7.79 (t,  $J = 1.9$  Hz, 1H), 7.70-7.75 (m, 2H), 7.38-7.45 (m, 2H), 7.32-7.37 (m, 2H), 6.19 (s, 1H), 3.93 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.0, 149.6, 144.6, 141.8, 131.9, 130.4, 129.9, 124.1, 123.6, 122.5, 120.5, 115.6, 111.3, 52.5$ .



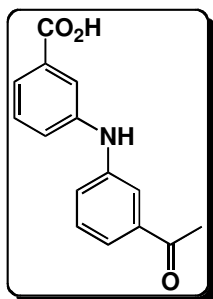
### 3-[(3-nitrophenyl)amino]benzoic acid (4g)

Reaction of the methyl ester of 4g according to general procedure 2 provided **4g** as an orange solid (91% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.97 (bs, 1H), 8.92 (s, 1H), 7.82 (s, 1H), 7.71 (s, 1H), 7.64 (m, 1H), 7.38-7.57 (m, 5H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.2, 148.8, 144.7, 142.1, 132.1, 130.6, 129.7, 122.2, 122.1, 122.0, 118.6, 113.9, 109.6. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H), found 257.0566 (M-H).



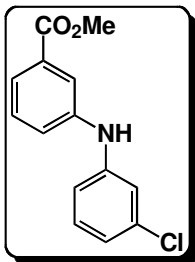
### 3-[(3-acetylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 3'-aminoacetophenone according to general procedure 1 provided the methyl ester of 4h as a yellow solid (55% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.75 (t,  $J$  = 1.8 Hz, 1H), 7.65 (t,  $J$  = 1.9 Hz, 1H), 7.62 (d,  $J$  = 7.6 Hz, 1H), 7.52 (d,  $J$  = 7.6 Hz, 1H), 7.27-7.39 (m, 4H), 6.16 (s, 1H), 3.91 (s, 3H), 2.58 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 198.3, 167.2, 143.4, 143.0, 138.6, 131.6, 129.8, 129.7, 122.7, 122.2, 121.6, 119.1, 117.4, 52.4, 26.9.



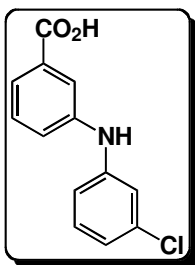
### 3-[(3-acetylphenyl)amino]benzoic acid (4h)

Reaction of the methyl ester of 4h according to general procedure 2 provided **4h** as a yellow solid (73% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.59 (s, 1H), 7.20-7.80 (m, 8H), 2.54 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 198.0, 167.5, 143.4, 143.3, 138.0, 131.9, 129.8, 129.6, 121.5, 121.1, 121.0, 120.5, 117.3, 115.8, 26.8. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{13}\text{NO}_3$ : 278.0793 (M+Na<sup>+</sup>), found 278.0791 (M+Na<sup>+</sup>).



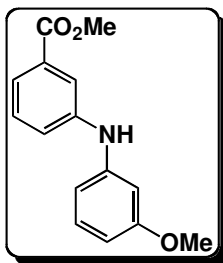
### 3-[(3-chlorophenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 3-chloroaniline according to general procedure **1** provided the methyl ester of **4i** as a yellow oil (90% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.73$  (t,  $J = 2.0$  Hz, 1H), 7.65 (dt,  $J = 7.6, 1.3$  Hz, 1H), 7.36 (t,  $J = 7.8$  Hz, 1H), 7.28 (ddd,  $J = 8.1, 2.4, 1.1$  Hz, 1H), 7.19 (t,  $J = 8.0$  Hz, 1H), 7.05 (t,  $J = 2.1$ , 1H), 6.90-6.96 (m, 2H), 5.90 (s, 1H), 3.92 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.1, 144.3, 142.7, 135.3, 131.7, 130.7, 129.7, 123.0, 122.7, 121.4, 119.6, 117.6, 115.8, 52.4$ .



### 3-[(3-chlorophenyl)amino]benzoic acid (**4i**)

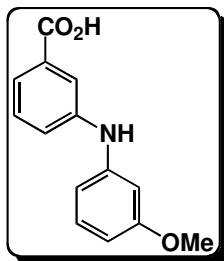
Reaction of the methyl ester of **4i** according to general procedure **2** provided **4i** as a white solid (83% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.90$  (bs, 1H), 8.58 (s, 1H), 7.66 (s, 1H), 7.46 (d,  $J = 7.5$  Hz, 1H), 7.38 (t,  $J = 7.8$  Hz, 1H), 7.32 (m, 1H), 7.26 (t,  $J = 8.0$  Hz, 1H), 7.01-7.07 (m, 2H), 6.87 (d,  $J = 7.9$  Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 167.3, 144.8, 142.7, 133.7, 131.8, 130.9, 129.6, 121.4, 121.3, 119.5, 117.8, 115.9, 114.9$ . **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H<sup>-</sup>), found 246.0315 (M-H<sup>-</sup>).



### 3-[(3-methoxyphenyl)amino]benzoic acid methyl ester

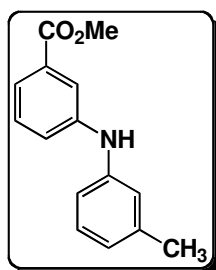
Reaction of methyl 3-bromobenzoate with *m*-anisidine according to general procedure **1** provided the methyl ester of **4j** as a yellow oil (97% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.74$  (t,  $J = 1.9$  Hz, 1H), 7.59 (dt,  $J = 7.5, 1.4$  Hz, 1H), 7.32 (t,  $J = 7.8$  Hz, 1H), 7.28

(m, 1H), 7.20 (t,  $J = 8.1$  Hz, 1H), 6.69 (ddd,  $J = 8.0, 2.1, 0.8$ , 1H), 6.65 (t,  $J = 2.3$  Hz, 1H), 6.54 (ddd,  $J = 8.2, 2.4, 0.8$  Hz, 1H), 5.88 (s, 1H), 3.91 (s, 3H), 3.79 (s, 3H).  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta = 167.3, 161.0, 144.0, 143.5, 131.5, 130.4, 129.5, 122.2, 122.1, 118.9, 110.9, 107.1, 104.2, 55.4, 52.3$ .



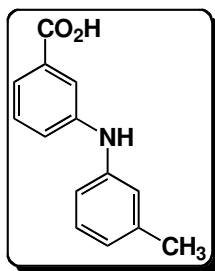
### 3-[(3-methoxyphenyl)amino]benzoic acid (4j)

Reaction of the methyl ester of 4j according to general procedure 2 provided 4j as a white solid (73% yield).  $^1\text{H}$  NMR (DMSO, 500 MHz):  $\delta = 12.83$  (bs, 1H), 8.37 (s, 1H), 7.66 (s, 1H), 7.27-7.40 (m, 3H), 7.17 (t,  $J = 8.1$  Hz, 1H), 6.68 (d,  $J = 8.0$  Hz, 1H), 6.63 (s, 1H), 6.46 (d,  $J = 8.2$  Hz, 1H), 3.72 (s, 3H).  $^{13}\text{C}$  NMR (DMSO, 125 MHz):  $\delta = 167.4, 160.2, 144.1, 143.7, 131.7, 130.0, 129.4, 120.7, 120.4, 116.9, 109.7, 105.8, 103.0, 54.9$ . HRMS (ES) Calcd. for C<sub>14</sub>H<sub>13</sub>NO<sub>3</sub>: 242.0817 (M-H<sup>-</sup>), found 242.0810 (M-H<sup>-</sup>).



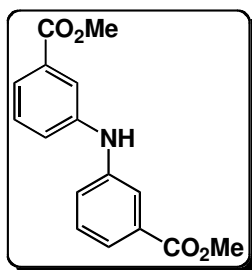
### 3-[(3-methylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with *m*-toluidine according to general procedure 1 provided the methyl ester of 4k as a yellow oil (88% yield).  $^1\text{H}$  NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta = 7.73$  (s, 1H), 7.59 (d,  $J = 7.6$  Hz, 1H), 7.33 (t,  $J = 7.8$  Hz, 1H), 7.26 (m, 1H), 7.21 (t,  $J = 7.7$  Hz, 1H), 6.90-6.97 (m, 2H), 6.83 (d,  $J = 7.5$  Hz, 1H), 5.85 (s, 1H), 3.92 (s, 3H), 2.34 (s, 3H).  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta = 167.3, 143.8, 142.4, 139.5, 131.4, 129.4, 122.7, 121.7, 121.5, 119.3, 118.3, 115.6, 52.2, 21.6$ .



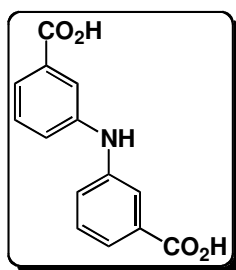
### 3-[(3-methylphenyl)amino]benzoic acid (4k)

Reaction of the methyl ester of 4k according to general procedure **2** provided **4k** as a white solid (34% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.24 (s, 1H), 7.63 (s, 1H), 7.20-7.40 (m, 3H), 7.14 (s, 1H), 6.86-6.96 (m, 2H), 6.69 (s, 1H), 2.25 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.5, 144.1, 142.7, 138.5, 131.7, 129.3, 129.1, 121.3, 120.2, 120.1, 118.3, 116.7, 114.7, 21.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_2$ : 228.1025 ( $\text{M}+\text{H}^+$ ), found 228.1017 ( $\text{M}+\text{H}^+$ ).



### 3-[(3-methylcarboxyphenyl)amino]benzoic acid methyl ester

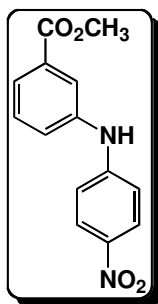
Reaction of methyl 3-bromobenzoate with methyl 3-aminobenzoate according to general procedure **1** provided the methyl ester of 4l as a white solid (68% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.73 (t,  $J$  = 1.7 Hz, 2H), 7.61 (dt,  $J$  = 7.4, 1.4 Hz, 2H), 7.33 (t,  $J$  = 7.8 Hz, 2H), 7.29 (ddd,  $J$  = 8.1, 2.3, 1.3 Hz, 2H), 6.20 (s, 1H), 3.91 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.1, 143.1, 131.5, 129.5, 122.5, 122.0, 119.0, 52.3.



### 3-[(3-carboxyphenyl)amino]benzoic acid (4l)

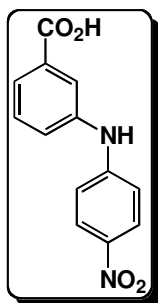
Reaction of the methyl ester of 4l according to general procedure **2** provided **4l** as a white solid (83% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.88 (bs, 2H), 8.60 (s, 1H), 7.67 (s, 2H), 7.31-7.46 (m, 6H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.3, 143.3, 131.8, 129.5,

120.9, 117.3. **HRMS** (ES) Calcd. for  $C_{14}H_{11}NO_4$ : 280.0586 (M-H), found 280.0581 (M-H).



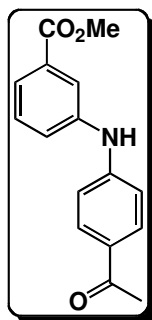
### 3-[(4-nitrophenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-nitroaniline according to general procedure **1** provided the methyl ester of **4m** as an orange solid (59% yield).  **$^1H$  NMR** ( $CDCl_3$ , 500MHz):  $\delta$  = 8.16 (d,  $J$  = 9.1 Hz, 2H), 7.89 (s, 1H), 7.83 (d,  $J$  = 7.6 Hz, 1H), 7.47 (t,  $J$  = 7.8 Hz, 1H), 7.41 (m, 1H), 6.98 (d,  $J$  = 9.1 Hz, 2H), 6.31 (s, 1H), 3.94 (s, 3H).  **$^{13}C$  NMR** ( $CDCl_3$ , 125 MHz):  $\delta$  = 166.7, 149.7, 140.7, 140.3, 132.2, 130.1, 126.5, 125.9, 125.7, 122.6, 114.4, 52.6.



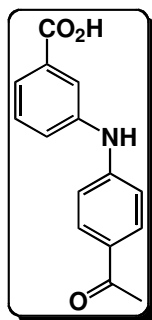
### 3-[(4-nitrophenyl)amino]benzoic acid (**4m**)

Reaction of the methyl ester of **4m** according to general procedure **2** provided **4m** as an orange solid (30% yield).  **$^1H$  NMR** (DMSO, 500 MHz):  $\delta$  = 13.00 (bs, 1H), 9.41 (s, 1H), 8.12 (d,  $J$  = 9.2 Hz, 2H), 7.78 (s, 1H), 7.64 (m, 1H), 7.46-7.54 (m, 2H), 7.10 (d,  $J$  = 9.2 Hz, 2H).  **$^{13}C$  NMR** (DMSO, 125 MHz):  $\delta$  = 166.9, 150.1, 140.6, 138.5, 132.1, 129.8, 126.1, 124.3, 123.8, 120.7, 113.8. **HRMS** (ES) Calcd. for  $C_{13}H_{10}N_2O_4$ : 257.0562 (M-H), found 257.0556 (M-H).



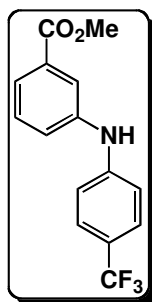
### 3-[(4-acetylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4'-aminoacetophenone according to general procedure **1** provided the methyl ester of **4n** as a white solid (84% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500MHz): δ = 7.89 (d, *J* = 8.7 Hz, 2H), 7.85 (s, 1H), 7.73 (m, 1H), 7.36-7.42 (m, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.31 (s, 1H), 3.92 (s, 3H), 2.55 (s, 3H). **<sup>13</sup>C NMR** (CDCl<sub>3</sub>, 125 MHz): δ = 196.7, 167.0, 147.9, 141.3, 131.8, 130.9, 129.9, 129.8, 124.6, 124.2, 121.2, 115.1, 52.5, 26.4.



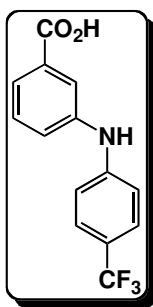
### 3-[(4-acetylphenyl)amino]benzoic acid (**4n**)

Reaction of the methyl ester of **4n** according to general procedure **2** provided **4n** as a yellow solid (43% yield). **<sup>1</sup>H NMR** (DMSO, 500 MHz): δ = 8.98 (s, 1H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.75 (s, 1H), 7.54 (m, 1H), 7.40-7.46 (m, 2H), 7.09 (d, *J* = 8.3 Hz, 2H), 2.47 (s, 3H). **<sup>13</sup>C NMR** (DMSO, 125 MHz): δ = 195.6, 167.2, 147.9, 141.8, 131.9, 130.5, 129.7, 128.3, 122.9, 122.4, 119.3, 114.5, 26.2. **HRMS** (ES) Calcd. for C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>: 278.0793 (M+Na<sup>+</sup>), found 278.0800 (M+Na<sup>+</sup>).



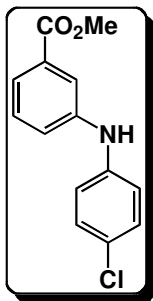
### 3-[(4-trifluoromethylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **4o** as a white solid (86% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.82 (s, 1H), 7.71 (d,  $J$  = 7.6 Hz, 1H), 7.50 (d,  $J$  = 8.4 Hz, 2H), 7.40 (t,  $J$  = 7.8 Hz, 1H), 7.33 (m, 1H), 7.08 (d,  $J$  = 8.5 Hz, 2H), 6.11 (bs, 1H), 3.93 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.0, 146.3, 141.9, 131.8, 129.8, 127.0, 123.9, 120.5, 116.1, 52.5.



### 3-[(4-trifluoromethylphenyl)amino]benzoic acid (**4o**)

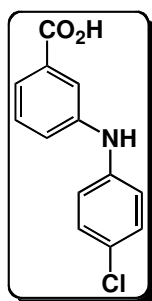
Reaction of the methyl ester of **4o** according to general procedure **2** provided **4o** as a white solid (90% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 12.91 (bs, 1H), 8.91 (s, 1H), 7.73 (s, 1H), 7.55 (d,  $J$  = 8.6 Hz, 2H), 7.52 (m, 1H), 7.40-7.43 (m, 2H), 7.18 (d,  $J$  = 8.6 Hz, 2H), 2.47 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 167.2, 146.9, 142.0, 132.0, 129.6, 126.6, 122.5, 122.2, 118.9, 115.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{10}\text{F}_3\text{NO}_2$ : 280.0585 (M-H<sup>-</sup>), found 280.0577 (M-H<sup>-</sup>).



### 3-[(4-chlorophenyl)amino]benzoic acid methyl ester

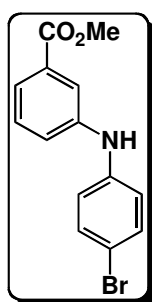
Reaction of methyl 3-bromobenzoate with 4-chloroaniline according to general procedure **1** provided the methyl ester of **4p** as a yellow oil (52% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.70 (s, 1H), 7.61 (d,  $J$  = 7.6 Hz, 1H), 7.33 (t,  $J$  = 7.9 Hz, 1H), 7.21-7.27 (m, 3H), 7.01 (d,  $J$  = 8.8 Hz, 2H), 5.78 (s, 1H), 3.91 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 143.4, 141.4, 131.7, 129.7, 126.7, 122.5, 122.0, 119.8, 118.7, 52.4.





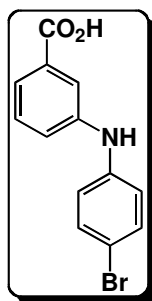
### 3-[(4-chlorophenyl)amino]benzoic acid (4p)

Reaction of the methyl ester of 4p according to general procedure **2** provided **4p** as a white solid (81% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.83 (bs, 1H), 8.47 (s, 1H), 7.63 (s, 1H), 7.41 (d,  $J$  = 7.7 Hz, 1H), 7.35 (t,  $J$  = 7.8 Hz, 1H), 7.26-7.30 (m, 3H), 7.08 (d,  $J$  = 8.8 Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.3, 143.3, 141.9, 131.8, 129.4, 129.0, 123.4, 120.7, 120.6, 118.5, 117.0. HRMS (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H<sup>-</sup>), found 246.0321 (M-H<sup>-</sup>).



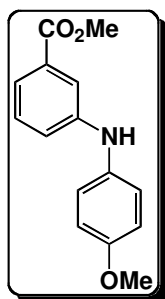
### 3-[(4-bromophenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-bromoaniline according to general procedure **1** provided the methyl ester of 4q as a green oil (46% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.71 (s, 1H), 7.61 (d,  $J$  = 7.7 Hz, 1H), 7.38 (d,  $J$  = 8.6 Hz, 2H), 7.34 (t,  $J$  = 7.9 Hz, 1H), 7.23 (d,  $J$  = 8.1 Hz, 1H), 6.96 (d,  $J$  = 8.7 Hz, 2H), 5.81 (s, 1H), 3.91 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 143.1, 141.9, 132.6, 131.7, 129.7, 122.6, 122.1, 119.9, 118.8, 113.8, 52.4.



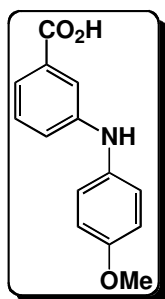
### 3-[(4-bromophenyl)amino]benzoic acid (4q)

Reaction of the methyl ester of 4q according to general procedure 2 provided 4q as a green solid (57% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.85 (bs, 1H), 8.48 (s, 1H), 7.64 (s, 1H), 7.37-7.45 (m, 3H), 7.35 (t,  $J$  = 7.8 Hz, 1H), 7.29 (d,  $J$  = 8.0 Hz, 1H), 7.03 (d,  $J$  = 8.9 Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.3, 143.2, 142.3, 131.9, 131.8, 129.4, 120.9, 120.8, 118.8, 117.2, 111.0. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{BrNO}_2$ : 289.9817 (M-H $^-$ ), found 289.9817 (M-H $^-$ ).



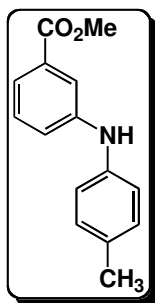
### 3-[(4-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with *p*-anisidine according to general procedure 1 provided the methyl ester of 4r as a yellow oil (93% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.57 (s, 1H), 7.50 (d,  $J$  = 7.6 Hz, 1H), 7.28 (m, 1H), 7.07-7.12 (m, 3H), 6.90 (d,  $J$  = 8.8 Hz, 2H), 5.62 (s, 1H), 3.90 (s, 3H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.5, 156.0, 145.8, 135.2, 131.5, 129.5, 123.1, 120.7, 119.7, 116.4, 115.0, 55.8, 52.2.



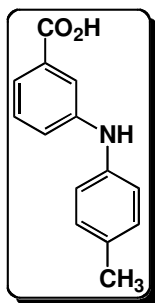
### 3-[(4-methoxyphenyl)amino]benzoic acid (4r)

Reaction of the methyl ester of 4r according to general procedure 2 provided 4r as a white solid (76% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.69 (bs, 1H), 8.01 (s, 1H), 7.49 (s, 1H), 7.22-7.30 (m, 2H), 7.05-7.11 (m, 3H), 6.90 (d,  $J$  = 8.8 Hz, 2H), 3.73 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.5, 154.4, 145.7, 135.3, 131.6, 129.2, 121.4, 118.8, 118.5, 114.7, 114.6, 55.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 242.0817 (M-H $^-$ ), found 242.0822 (M-H $^-$ ).



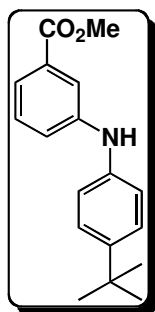
### 3-[(4-methylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with *p*-toluidine according to general procedure **1** provided the methyl ester of **4s** as a yellow oil (69% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.68 (s, 1H), 7.55 (d,  $J$  = 7.6 Hz, 1H), 7.29 (t,  $J$  = 7.7 Hz, 1H), 7.19 (m, 1H), 7.13 (d,  $J$  = 8.0 Hz, 2H), 7.03 (d,  $J$  = 8.3 Hz, 2H), 5.77 (s, 1H), 3.91 (s, 3H), 2.34 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.4, 144.6, 139.8, 131.9, 131.5, 130.2, 129.5, 121.3, 120.8, 119.7, 117.5, 52.2, 20.9.



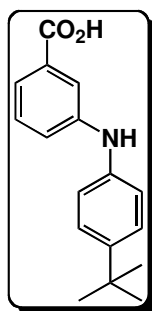
### 3-[(4-methylphenyl)amino]benzoic acid (**4s**)

Reaction of the methyl ester of **4s** according to general procedure **2** provided **4s** as a white solid (70% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta$  = 8.17 (s, 1H), 7.58 (s, 1H), 7.16-7.36 (m, 3H), 7.08 (d,  $J$  = 8.2 Hz, 2H), 7.00 (d,  $J$  = 8.0 Hz, 2H), 2.24 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):  $\delta$  = 167.5, 144.6, 140.0, 131.7, 129.6, 129.2, 119.5, 119.4, 118.4, 115.8, 20.5. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_2$ : 226.0868 (M-H), found 226.0861 (M-H).



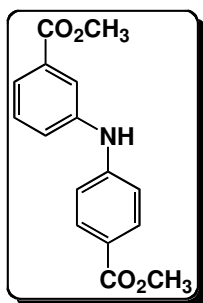
### 3-[(4-*tert*-butylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-*tert*-butylaniline according to general procedure **1** provided the methyl ester of 4t as a yellow oil (81% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.73$  (s, 1H), 7.57 (d,  $J = 7.6$  Hz, 1H), 7.21-7.42 (m, 4H), 7.06-7.13 (m, 2H), 5.85 (s, 1H), 3.92 (s, 3H), 1.36 (s, 9H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.4$ , 145.1, 144.3, 139.8, 131.4, 129.4, 126.4, 121.3, 120.9, 118.9, 117.7, 52.3, 34.4, 31.6.



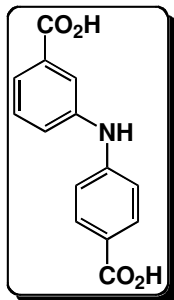
### 3-[(4-*tert*-butylphenyl)amino]benzoic acid (4t)

Reaction of the methyl ester of 4t according to general procedure **2** provided **4t** as a white solid (91% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 8.17$  (s, 1H), 7.62 (s, 1H), 6.95-7.40 (m, 7H), 1.26 (s, 9H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 168.0$ , 144.1, 142.7, 140.3, 128.9, 125.8, 119.8, 118.9, 117.5, 116.2, 116.1, 33.8, 31.3. **HRMS** (ES) Calcd. for  $\text{C}_{17}\text{H}_{19}\text{NO}_2$ : 268.1338 (M-H $^-$ ), found 268.1355 (M-H $^-$ ).



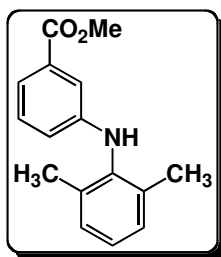
### 3-[(4-methylcarboxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with methyl 3-aminobenzoate according to general procedure **1** provided the methyl ester of 4u as a white solid (70% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta = 7.95$  (d,  $J = 8.8$  Hz, 2H), 7.83 (t,  $J = 1.9$  Hz, 1H), 7.72 (dt,  $J = 7.5$ , 1.4 Hz, 1H), 7.40 (t,  $J = 7.7$  Hz, 1H), 7.36 (m, 1H), 7.02 (d,  $J = 8.8$  Hz, 2H), 6.12 (s, 1H), 3.93 (s, 3H), 3.89 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.1$ , 167.0, 147.6, 141.6, 131.9, 131.8, 129.8, 124.3, 124.1, 122.2, 121.1, 115.4, 52.4, 52.0.



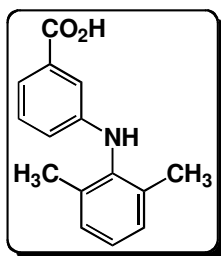
### 3-[(4-carboxyphenyl)amino]benzoic acid (**4u**)

Reaction of the methyl ester of **4u** according to general procedure **2** provided **4u** as a brown solid (68% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.62$  (bs, 2H), 8.88 (s, 1H), 7.82 (d,  $J = 8.6$  Hz, 2H), 7.73 (s, 1H), 7.52 (m, 1H), 7.39-7.45 (m, 2H), 7.09 (d,  $J = 8.6$  Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 167.2, 167.0, 147.5, 142.0, 131.9, 131.2, 129.6, 122.6, 122.1, 121.1, 119.1, 114.6$ . HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{11}\text{NO}_4$ : 256.0610 (M-H<sup>-</sup>), found 256.0612 (M-H<sup>-</sup>).



### 3-[(2,6-bis(methyl)phenyl)amino]benzoic acid methyl ester

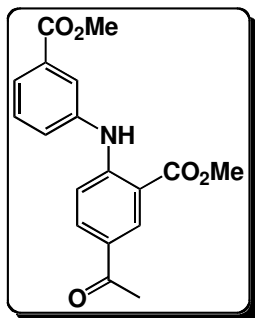
Reaction of methyl 3-bromobenzoate with 2,6-dimethylaniline according to general procedure **1** provided the methyl ester of **4v** as a colorless oil (78% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.44$  (d,  $J = 7.6$  Hz, 1H), 7.27 (s, 1H), 7.22 (t,  $J = 7.9$  Hz, 1H), 7.10-7.19 (m, 3H), 6.64 (d,  $J = 8.1$  Hz, 1H), 5.39 (s, 1H), 3.89 (s, 3H), 2.23 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.6, 146.6, 137.7, 136.2, 131.3, 129.4, 128.8, 126.3, 119.3, 117.4, 114.5, 52.1, 18.5$ .



### 3-[(2,6-bis(methyl)phenyl)amino]benzoic acid (**4v**)

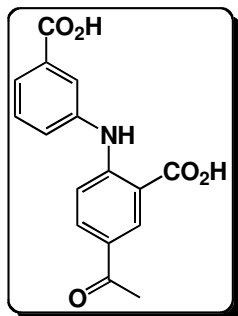
Reaction of the methyl ester of **4v** according to general procedure **2** provided **4v** as a white solid (80% yield).  $^1\text{H NMR}$  (DMSO, 360 MHz):  $\delta = 12.67$  (bs, 1H), 7.57 (s, 1H), 7.02-7.25 (m, 5H), 6.98 (s, 1H), 6.64 (s, 1H), 2.16 (s, 6H).  $^{13}\text{C NMR}$  (DMSO, 90 MHz):

$\delta = 167.7, 147.1, 138.0, 135.7, 131.5, 129.1, 128.4, 125.7, 117.5, 116.6, 112.8, 18.0$ .  
**HRMS** (ES) Calcd. for  $C_{15}H_{15}NO_2$ : 240.1025 (M-H<sup>-</sup>), found 240.1015 (M-H<sup>-</sup>).



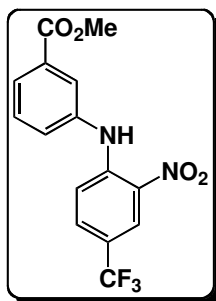
### 3-[(2-methylcarboxy-4-acetylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 5-acetyl-2-[[trifluoromethyl]sulfonyl]oxy]benzoate with methyl 3-aminobenzoate according to general procedure **1** provided the methyl ester of **4w** as a yellow oil (87% yield). **<sup>1</sup>H NMR** ( $CDCl_3$ , 500MHz):  $\delta = 10.03$  (s, 1H), 8.61 (d,  $J = 2.2$  Hz, 1H), 7.90-7.96 (m, 2H), 7.41-7.49 (m, 2H), 7.14 (d,  $J = 9.0$  Hz, 1H), 3.95 (s, 3H), 3.92 (s, 3H), 2.54 (s, 3H). **<sup>13</sup>C NMR** ( $CDCl_3$ , 125 MHz):  $\delta = 195.7, 168.6, 166.5, 151.2, 139.7, 134.2, 133.6, 131.8, 129.8, 128.0, 127.0, 126.1, 124.6, 113.1, 111.0, 52.4, 52.2, 26.2$ .



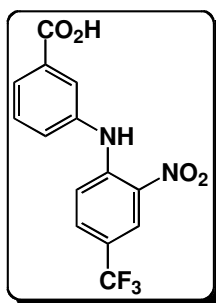
### 3-[(2-carboxy-4-acetylphenyl)amino]benzoic acid (**4w**)

Reaction of the methyl ester of **4w** according to general procedure **2** provided **4w** as a white solid (25% yield). **<sup>1</sup>H NMR** (DMSO, 500 MHz):  $\delta = 13.30$  (bs, 2H), 10.17 (s, 1H), 8.51 (d,  $J = 2.2$  Hz, 1H), 7.96 (dd,  $J = 8.9, 2.2$  Hz, 1H), 7.83 (s, 1H), 7.73 (d,  $J = 7.3$  Hz, 1H), 7.50-7.60 (m, 2H), 7.19 (d,  $J = 8.9$  Hz, 1H). **<sup>13</sup>C NMR** (DMSO, 125 MHz):  $\delta = 195.1, 169.5, 166.9, 150.3, 139.5, 134.1, 133.1, 132.2, 130.0, 127.1, 126.5, 125.2, 123.1, 113.0, 111.9, 26.1$ . **HRMS** (ES) Calcd. for  $C_{16}H_{13}NO_5$ : 300.0872 (M+H<sup>+</sup>), found 300.0866 (M+H<sup>+</sup>).



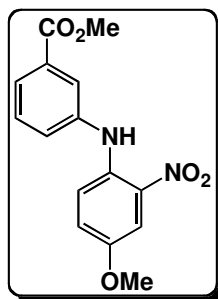
### 3-[(2-nitro-4-trifluoromethylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-amino-3-nitrobenzotrifluoride according to general procedure **1** provided the methyl ester of **4x** as a yellow solid (87% yield). **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 500 MHz): δ = 9.73 (s, 1H), 8.52 (s, 1H), 7.96-8.00 (m, 2H), 7.46-7.60 (m, 3H), 7.23 (d, *J* = 9.0 Hz, 1H), 3.94 (s, 3H). **<sup>13</sup>C NMR** (CDCl<sub>3</sub>, 125 MHz): δ = 166.3, 144.9, 138.1, 132.5, 132.4, 132.2, 130.4, 129.4, 127.9, 126.1, 125.0, 122.4, 120.0, 116.6, 52.7. **FTIR** (thin film) 3342, 3089, 2955, 1725, 1635, 1575, 1534, 1486, 1444, 1357, 1325, 1269, 1215, 1154, 1126, 1082, 992, 914, 888, 825, 774, 752, 695 cm<sup>-1</sup>. **HRMS** (ES) Calcd. for C<sub>15</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>: 339.0593 (M-H<sup>-</sup>), found 339.0597 (M-H<sup>-</sup>).



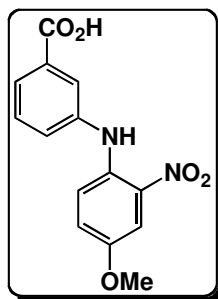
### 3-[(2-nitro-4-trifluoromethylphenyl)amino]benzoic acid (**4x**)

Reaction of the methyl ester of **4x** according to general procedure **2** provided **4x** as a yellow solid (90% yield). **<sup>1</sup>H NMR** (DMSO, 500 MHz): δ = 9.82 (s, 1H), 8.37 (s, 1H), 7.89 (s, 1H), 7.84 (m, 1H), 7.77 (dd, *J* = 9.0, 1.9 Hz, 1H), 7.55-7.64 (m, 2H), 7.23 (d, *J* = 9.0 Hz, 1H). **<sup>13</sup>C NMR** (DMSO, 125 MHz): δ = 166.8, 144.5, 138.9, 132.7, 132.5, 131.8, 131.7, 130.0, 129.3, 126.7, 125.6, 124.7, 124.1, 117.9. **HRMS** (ES) Calcd. for C<sub>14</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>: 325.0436 (M-H<sup>-</sup>), found 325.0434 (M-H<sup>-</sup>).



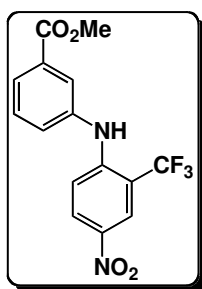
### 3-[(2-nitro-4-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 4-methoxy-2-nitroaniline according to general procedure **1** provided the methyl ester of **4y** as an orange oil (93% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 9.27 (s, 1H), 7.90 (s, 1H), 7.82 (m, 1H), 7.64 (m, 1H), 7.38-7.48 (m, 2H), 7.24 (m, 1H), 7.10 (m, 1H), 3.92 (s, 3H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 166.6, 151.9, 140.1, 137.0, 134.0, 131.9, 129.9, 127.4, 126.1, 125.8, 123.8, 118.2, 107.6, 56.1, 52.5.



### 3-[(2-nitro-4-methoxyphenyl)amino]benzoic acid (**4y**)

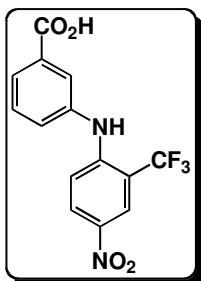
Reaction of the methyl ester of **4y** according to general procedure **2** provided **4y** as an orange solid (85% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.95 (bs, 1H), 8.93 (s, 1H), 7.71 (s, 1H), 7.56-7.61 (m, 2H), 7.34-7.46 (m, 2H), 7.22-7.34 (m, 2H), 3.81 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.0, 152.4, 141.7, 136.7, 134.0, 132.0, 129.6, 124.6, 124.3, 123.4, 121.2, 120.8, 108.0, 55.8. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5$ : 289.0824 ( $\text{M}+\text{H}^+$ ), found 289.0837 ( $\text{M}+\text{H}^+$ ).





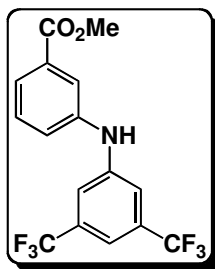
### 3-(4-nitro-2-(trifluoromethyl)phenylamino)benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 2-amino-5-nitrobenzotrifluoride according to general procedure **1** provided the methyl ester of **4z** as a yellow oil (56% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.50 (s, 1H), 8.20 (dd,  $J$  = 9.2, 2.3 Hz, 1H), 7.91-7.98 (m, 2H), 7.53 (t,  $J$  = 7.8 Hz, 1H), 7.45 (m, 1H), 7.13 (d,  $J$  = 9.3 Hz, 1H), 6.73 (s, 1H), 3.94 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 166.3, 148.0, 139.2, 138.8, 132.4, 130.4, 128.9, 128.4, 127.4, 125.1, 124.3, 114.7, 52.7. HRMS (ES) Calcd. for  $\text{C}_{15}\text{H}_{11}\text{F}_3\text{N}_2\text{O}_4$ : 339.0593 (M-H), found 339.0587 (M-H).



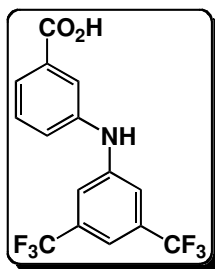
### 3-(4-nitro-2-(trifluoromethyl)phenylamino)benzoic acid **4z**

Reaction of the methyl ester of **4z** according to general procedure **2** provided **4z** as a brown solid (87% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.76 (s, 1H), 8.35 (d,  $J$  = 2.6 Hz, 1H), 8.22 (dd,  $J$  = 9.4, 2.6 Hz, 1H), 7.75-7.90 (m, 2H), 7.54-7.58 (m, 2H), 7.11 (d,  $J$  = 9.4 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 166.8, 148.3, 139.9, 137.7, 132.3, 129.9, 129.0, 128.6, 126.1, 125.1, 123.6, 116.0. HRMS (ESI) calcd. for  $\text{C}_{14}\text{H}_8\text{N}_2\text{O}_4\text{F}_3$  325.0436 (M-H<sup>-</sup>), found 325.0442 (M-H<sup>-</sup>).



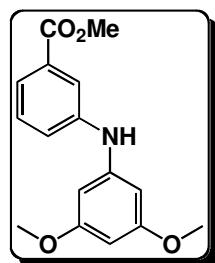
### 3-[(3,5-bis(trifluoromethyl)phenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 3,5-bis(trifluoromethyl)aniline according to general procedure **1** provided the methyl ester of **4zi** as a white solid (51% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.80 (s, 1H), 7.77 (d,  $J$  = 7.7 Hz, 1H), 7.45 (t,  $J$  = 7.8 Hz, 1H), 7.41 (s, 2H), 7.34-7.39 (m, 2H), 6.21 (bs, 1H), 3.94 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 166.9, 144.9, 141.1, 133.2, 132.9, 132.1, 130.1, 124.8, 124.1, 121.2, 116.0, 114.0, 52.6.



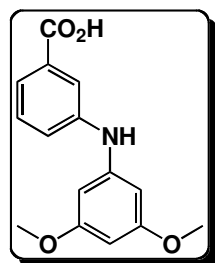
### 3-[(3,5-bis(trifluoromethyl)phenyl)amino]benzoic acid (**4zi**)

Reaction of the methyl ester of **4zi** according to general procedure **2** provided **4zi** as a brown solid (75% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.13 (s, 1H), 7.72 (s, 1H), 7.59 (d,  $J$  = 7.5 Hz, 1H), 7.52 (s, 2H), 7.47 (t,  $J$  = 7.7 Hz, 1H), 7.43 (m, 1H), 7.38 (s, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.0, 145.6, 141.2, 132.4, 131.2, 129.9, 124.4, 123.2, 122.9, 122.3, 119.5, 114.7. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_9\text{F}_6\text{NO}_2$ : 348.0459 (M-H<sup>-</sup>), found 348.0449 (M-H<sup>-</sup>).



### 3-[(3,5-bis(methoxy)phenyl)amino]benzoic acid methyl ester

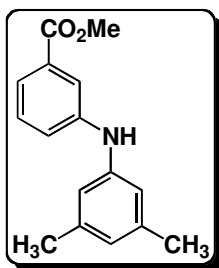
Reaction of methyl 3-bromobenzoate with 3,5-dimethoxyaniline according to general procedure **1** provided the methyl ester of **4zii** as a yellow oil (88% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.75 (s, 1H), 7.60 (d,  $J$  = 7.2 Hz, 1H), 7.28-7.35 (m, 2H), 6.25 (d,  $J$  = 2.1 Hz, 2H), 6.12 (t,  $J$  = 2.1 Hz, 1H), 5.83 (s, 1H), 3.91 (s, 3H), 3.77 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 161.9, 144.8, 143.3, 131.6, 129.5, 122.6, 122.4, 119.4, 96.7, 94.0, 55.5, 52.3.



### 3-[(3,5-bis(methoxy)phenyl)amino]benzoic acid (**4zii**)

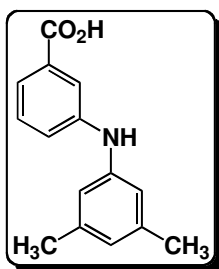
Reaction of the methyl ester of **4zii** according to general procedure **2** provided **4zii** as a white solid (90% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.83 (bs, 1H), 8.35 (s, 1H), 7.68 (s, 1H), 7.25-7.45 (m, 3H), 6.24 (s, 2H), 6.06 (s, 1H), 3.70 (s, 6H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.4, 161.2, 144.7, 143.5, 131.7, 129.4, 121.1, 120.6, 117.4,

95.5, 92.5, 55.0. **HRMS** (ES) Calcd. for C<sub>15</sub>H<sub>15</sub>NO<sub>4</sub>: 274.1079 (M+H<sup>+</sup>), found 274.1078 (M+H<sup>+</sup>).



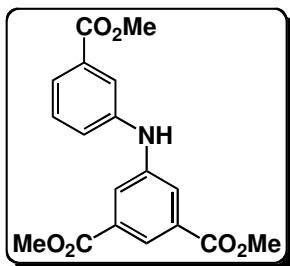
### 3-[(3,5-bis(methyl)phenyl)amino]benzoic acid methyl ester

Reaction of methyl 3-bromobenzoate with 3,5-dimethylaniline according to general procedure **1** provided the methyl ester of 4ziii as a yellow oil (79% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ = 7.68 (s, 1H), 7.55 (d, *J* = 6.5 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.24 (m, 1H), 6.72 (s, 2H), 6.64 (s, 1H), 5.75 (s, 1H), 3.90 (s, 3H), 2.28 (s, 6H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz): δ = 167.3, 144.1, 142.5, 139.3, 131.5, 129.4, 123.8, 121.7, 121.5, 118.5, 116.5, 52.2, 21.6.



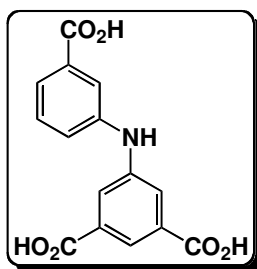
### 3-[(3,5-bis(methyl)phenyl)amino]benzoic acid (4ziii)

Reaction of the methyl ester of 4ziii according to general procedure **2** provided **4ziii** as a white solid (74% yield). <sup>1</sup>H NMR (DMSO, 500 MHz): δ = 12.74 (bs, 1H), 8.16 (s, 1H), 7.60 (s, 1H), 7.23-7.38 (m, 3H), 6.70 (s, 2H), 6.53 (s, 1H), 2.21 (s, 6H). <sup>13</sup>C NMR (DMSO, 125 MHz): δ = 167.4, 144.1, 142.6, 138.1, 131.6, 129.2, 122.3, 120.1, 119.9, 116.8, 115.4, 21.0. **HRMS** (ES) Calcd. for C<sub>15</sub>H<sub>15</sub>NO<sub>2</sub>: 240.1025 (M-H<sup>-</sup>), found 240.1035 (M-H<sup>-</sup>).



### 3-[(3,5-bis(methylcarboxy)phenyl)amino]benzoic acid methyl ester

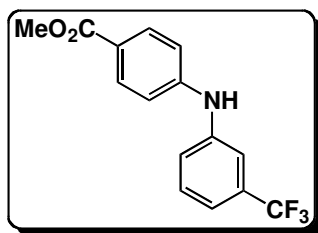
Reaction of methyl 3-bromobenzoate with dimethyl 5-aminoisophthalate according to general procedure 1 provided the methyl ester of 4ziv as a yellow solid (60% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 8.21 (s, 1H), 7.92 (d,  $J$  = 1.5 Hz, 2H), 7.75 (m, 1H), 7.66 (m, 1H), 7.33-7.40 (m, 2H), 6.42 (bs, 1H), 3.93 (s, 9H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.1, 166.5, 143.8, 142.4, 131.9, 131.8, 129.8, 123.3, 123.1, 122.6, 122.2, 120.1, 52.6, 52.4.



### 3-[(3,5-bis(methylcarboxy)phenyl)amino]benzoic acid (4ziv)

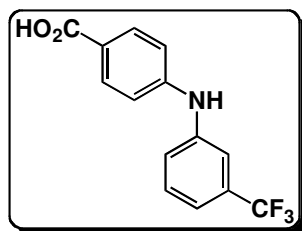
Reaction of the methyl ester of 4ziv according to general procedure 2 provided 4ziv as a yellow solid (50% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 13.06 (bs, 3H), 8.78 (s, 1H), 7.94 (s, 1H), 7.83 (s, 2H), 7.67 (s, 1H), 7.30-7.55 (m, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.2, 166.7, 144.0, 142.5, 132.3, 132.0, 129.7, 121.8, 121.7, 121.2, 120.3, 118.3. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{11}\text{NO}_6$ : 300.0508 (M-H $^-$ ), found 300.0511 (M-H $^-$ ).

## Class 5 compounds



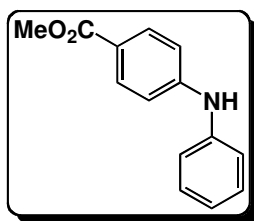
### 4-[(3-trifluoromethylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 3-aminobenzotrifluoride according to general procedure **1** provided the methyl ester of **5a** as a yellow oil (83% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.97 (d,  $J$  = 8.6 Hz, 2H), 7.43 (t,  $J$  = 7.9 Hz, 1H), 7.39 (s, 1H), 7.34 (d,  $J$  = 8.0 Hz, 1H), 7.28 (d,  $J$  = 7.9 Hz, 1H), 7.04 (d,  $J$  = 8.6 Hz, 2H), 6.26 (s, 1H), 3.90 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.1, 147.1, 142.0, 131.8, 130.3, 122.6, 119.3, 116.2, 115.7, 52.1.



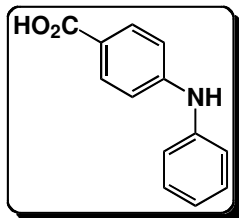
### 4-[(3-trifluoromethylphenyl)amino]benzoic acid (**5a**)

Reaction of the methyl ester of **5a** according to general procedure **2** provided **5a** as a white solid (75% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 12.45 (bs, 1H), 9.03 (s, 1H), 7.84 (d,  $J$  = 8.5 Hz, 2H), 7.45-7.59 (m, 2H), 7.39 (s, 1H), 7.24 (s, 1H), 7.12 (d,  $J$  = 8.5 Hz, 2H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 167.0, 146.8, 142.7, 131.2, 130.5, 121.8, 121.4, 117.2, 115.2, 114.1. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{10}\text{F}_3\text{NO}_2$ : 280.0585 (M-H), found 280.0584 (M-H).



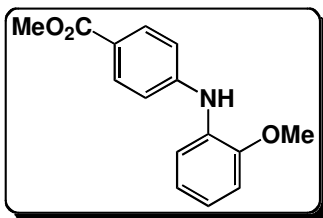
### 4-phenylamino benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with aniline according to general procedure **1** provided the methyl ester of **5b** as a yellow oil (84% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.92 (d,  $J$  = 8.8 Hz, 2H), 7.32-7.38 (m, 2H), 7.18 (d,  $J$  = 7.5 Hz, 2H), 7.09 (m, 1H), 6.99 (d,  $J$  = 8.8 Hz, 2H), 6.02 (s, 1H), 3.89 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 148.3, 141.1, 131.7, 129.7, 123.4, 121.5, 120.7, 114.9, 51.9.



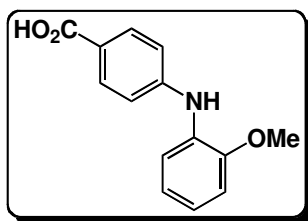
#### 4-phenylamino benzoic acid (**5b**)

Reaction of the methyl ester of **5b** according to general procedure **2** provided **5b** as a white solid (81% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.69 (s, 1H), 7.78 (d,  $J$  = 8.7 Hz, 2H), 7.31 (t,  $J$  = 7.9 Hz, 2H), 7.17 (d,  $J$  = 7.6 Hz, 2H), 7.05 (d,  $J$  = 8.7 Hz, 2H), 6.96 (t,  $J$  = 7.3 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.2, 148.0, 141.5, 131.1, 129.3, 121.6, 120.6, 119.1, 114.0. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{11}\text{NO}_2$ : 212.0712 (M-H<sup>-</sup>), found 212.0717 (M-H<sup>-</sup>).



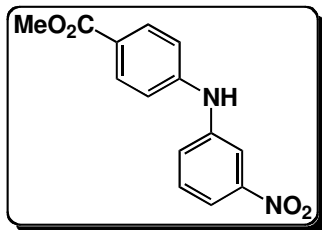
#### 4-[(2-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with *o*-anisidine according to general procedure **1** provided the methyl ester of **5c** as a colorless oil (76% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.94 (d,  $J$  = 8.7 Hz, 2H), 7.41 (d,  $J$  = 7.8 Hz, 1H), 7.08 (d,  $J$  = 8.7 Hz, 2H), 6.91-7.03 (m, 3H), 6.38 (s, 1H), 3.89 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 149.8, 147.8, 131.6, 130.8, 122.4, 121.5, 121.0, 118.0, 115.4, 111.2, 55.9, 51.9.



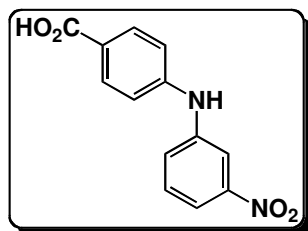
#### 4-[(2-methoxyphenyl)amino]benzoic acid (**5c**)

Reaction of the methyl ester of **5c** according to general procedure **2** provided **5c** as a brown solid (51% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.19 (bs, 1H), 8.03 (s, 1H), 7.72 (s, 2H), 7.27 (s, 1H), 7.06 (s, 2H), 6.88-6.96 (m, 3H), 3.80 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.2, 151.6, 149.1, 130.9, 129.7, 123.8, 121.6, 120.6, 119.6, 113.6, 112.0, 55.4. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 242.0817 (M-H<sup>-</sup>), found 242.0813 (M-H<sup>-</sup>).



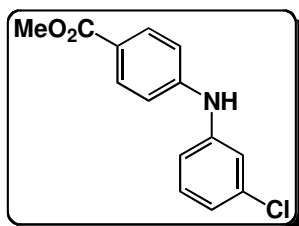
#### 4-[(3-nitrophenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 3-nitroaniline according to general procedure **1** provided the methyl ester of **5d** as a yellow solid (57% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.22 (s, 1H), 7.92 (t,  $J$  = 2.1 Hz, 1H), 7.88 (d,  $J$  = 8.8 Hz, 2H), 7.74 (m, 1H), 7.54-7.63 (m, 2H), 7.19 (d,  $J$  = 8.8 Hz, 2H), 3.81 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 165.9, 148.7, 146.8, 143.1, 131.1, 130.7, 123.9, 121.0, 115.6, 115.3, 111.7, 51.7.



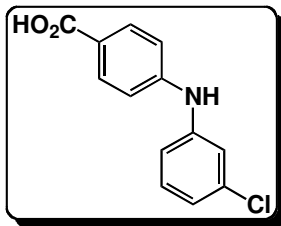
#### 4-[(3-nitrophenyl)amino]benzoic acid (**5d**)

Reaction of the methyl ester of **5d** according to general procedure **2** provided **5d** as a yellow solid (79% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 9.19 (s, 1H), 7.91 (s, 1H), 7.87 (d,  $J$  = 8.5 Hz, 2H), 7.72 (m, 1H), 7.50-7.63 (m, 2H), 7.18 (d,  $J$  = 8.5 Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.0, 148.7, 146.3, 143.4, 131.2, 130.7, 123.6, 122.5, 115.7, 115.1, 111.4. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H<sup>-</sup>), found 257.0567 (M-H<sup>-</sup>).



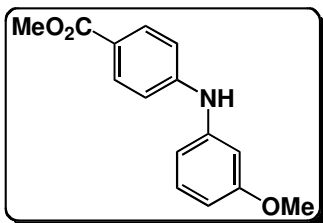
#### 4-[(3-chlorophenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 3-chloroaniline according to general procedure **1** provided the methyl ester of **5e** as a yellow oil (71% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta$  = 7.95 (d,  $J$  = 8.7 Hz, 2H), 7.24 (t,  $J$  = 8.1 Hz, 1H), 7.16 (s, 1H), 6.99-7.06 (m, 4H), 6.07 (s, 1H), 3.89 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.0, 147.2, 142.7, 135.4, 131.7, 130.7, 122.9, 122.4, 119.8, 117.9, 115.7, 52.0.



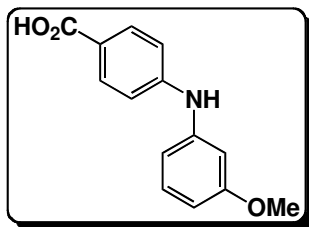
#### 4-[(3-chlorophenyl)amino]benzoic acid (**5e**)

Reaction of the methyl ester of **5e** according to general procedure **2** provided **5e** as a white solid (86% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 8.87 (s, 1H), 7.82 (d,  $J$  = 8.6 Hz, 2H), 7.31 (t,  $J$  = 8.0 Hz, 1H), 7.06-7.17 (m, 4H), 6.96 (d,  $J$  = 7.8 Hz, 1H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.0, 146.9, 143.5, 133.7, 131.1, 130.9, 121.7, 120.7, 117.6, 116.6, 115.1. **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{ClNO}_2$ : 246.0322 (M-H<sup>-</sup>), found 246.0330 (M-H<sup>-</sup>).



#### 4-[(3-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with *m*-anisidine according to general procedure **1** provided the methyl ester of **5f** as a yellow oil (94% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.92 (d,  $J$  = 8.8 Hz, 2H), 7.24 (t,  $J$  = 8.1 Hz, 1H), 7.01 (d,  $J$  = 8.8 Hz, 2H), 6.76 (d,  $J$  = 7.9 Hz, 1H), 6.73 (t,  $J$  = 2.2 Hz, 1H), 6.61 (dd,  $J$  = 8.2, 2.4 Hz, 1H), 6.13 (s, 1H), 3.88 (s, 3H), 3.80 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 160.9, 148.0, 142.4, 131.6, 130.4, 121.5, 115.2, 112.8, 108.5, 106.2, 55.5, 51.9.

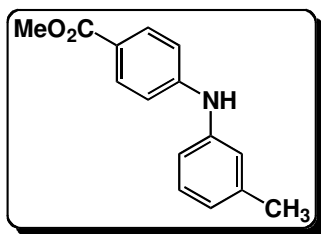


#### 4-[(3-methoxyphenyl)amino]benzoic acid (**5f**)

Reaction of the methyl ester of **5f** according to general procedure **2** provided **5f** as a white solid (75% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.31 (bs, 1H), 8.70 (s, 1H), 7.79 (d,  $J$  = 8.7 Hz, 2H), 7.21 (t,  $J$  = 8.1 Hz, 1H), 7.07 (d,  $J$  = 8.7 Hz, 2H), 6.76 (d,  $J$  = 8.0 Hz, 1H), 6.70 (t,  $J$  = 2.2 Hz, 1H), 6.55 (dd,  $J$  = 8.2, 2.4 Hz, 1H), 3.74 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.1, 160.2, 147.9, 142.8, 131.1, 130.1, 120.5, 114.4, 111.3,

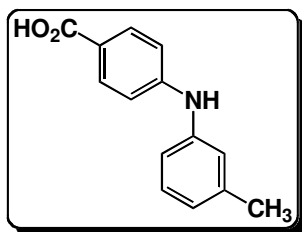


107.1, 104.6, 54.9. **HRMS** (ES) Calcd. for  $C_{14}H_{13}NO_3$ : 242.0817 (M-H), found 242.0818 (M-H).



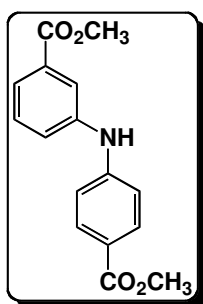
#### 4-[(3-methylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with *m*-toluidine according to general procedure **1** provided the methyl ester of **5g** as a yellow oil (96% yield).  $^1H$  NMR ( $CDCl_3$ , 500MHz):  $\delta$  = 7.92 (d,  $J$  = 8.8 Hz, 2H), 7.23 (m, 1H), 6.95-7.02 (m, 4H), 6.90 (d,  $J$  = 7.5 Hz, 1H), 6.02 (s, 1H), 3.89 (s, 3H), 2.36 (s, 3H).  $^{13}C$  NMR ( $CDCl_3$ , 125 MHz):  $\delta$  = 167.2, 148.5, 141.0, 139.7, 131.7, 129.5, 124.2, 121.4, 121.2, 117.8, 114.8, 51.9, 21.7.



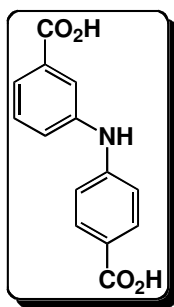
#### 4-[(3-methylphenyl)amino]benzoic acid (**5g**)

Reaction of the methyl ester of **5g** according to general procedure **2** provided **5g** as a white solid (57% yield).  $^1H$  NMR (DMSO, 500 MHz):  $\delta$  = 12.28 (bs, 1H), 8.62 (s, 1H), 7.77 (d,  $J$  = 8.6 Hz, 2H), 7.19 (t,  $J$  = 7.6 Hz, 1H), 7.03 (d,  $J$  = 8.6 Hz, 2H), 6.95-7.00 (m, 2H), 6.79 (d,  $J$  = 7.4 Hz, 1H), 2.28 (s, 3H).  $^{13}C$  NMR (DMSO, 125 MHz):  $\delta$  = 167.1, 148.3, 141.4, 138.5, 131.1, 129.1, 122.5, 120.2, 119.8, 116.3, 114.0, 21.1. **HRMS** (ES) Calcd. for  $C_{14}H_{13}NO_2$ : 228.1025 (M-H), found 228.1016 (M-H).



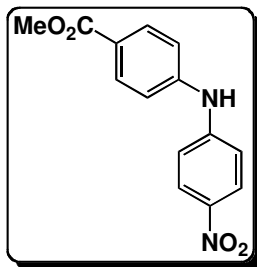
### 3-[(4-methylcarboxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with methyl 3-aminobenzoate according to general procedure **1** provided the methyl ester of **5h** as a white solid (70% yield). (REF)  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta = 7.95$  (d,  $J = 8.8$  Hz, 2H), 7.83 (t,  $J = 1.9$  Hz, 1H), 7.72 (dt,  $J = 7.5$ , 1.4 Hz, 1H), 7.40 (t,  $J = 7.7$  Hz, 1H), 7.36 (m, 1H), 7.02 (d,  $J = 8.8$  Hz, 2H), 6.12 (s, 1H), 3.93 (s, 3H), 3.89 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.1$ , 167.0, 147.6, 141.6, 131.9, 131.8, 129.8, 124.3, 124.1, 122.2, 121.1, 115.4, 52.4, 52.0.



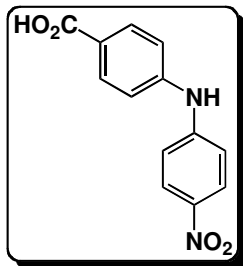
### 3-[(4-carboxyphenyl)amino]benzoic acid (**5h**)

Reaction of the methyl ester of **5o** according to general procedure **2** provided **5o** as a brown solid (68% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.62$  (bs, 2H), 8.88 (s, 1H), 7.82 (d,  $J = 8.6$  Hz, 2H), 7.73 (s, 1H), 7.52 (m, 1H), 7.39-7.45 (m, 2H), 7.09 (d,  $J = 8.6$  Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 167.2$ , 167.0, 147.5, 142.0, 131.9, 131.2, 129.6, 122.6, 122.1, 121.1, 119.1, 114.6. HRMS (ES) Calcd. for  $\text{C}_{14}\text{H}_{11}\text{NO}_4$ : 256.0610 (M-H $^-$ ), found 256.0612 (M-H $^-$ ).



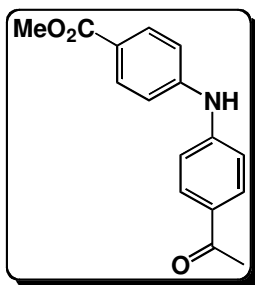
### 4-[(4-nitrophenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 4-nitroaniline according to general procedure **1** provided the methyl ester of **5i** as a yellow solid (99% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta = 8.18$  (d,  $J = 9.1$  Hz, 2H), 8.04 (d,  $J = 8.7$  Hz, 2H), 7.21 (d,  $J = 8.7$  Hz, 2H), 7.13 (d,  $J = 9.1$  Hz, 2H), 6.58 (s, 1H), 3.92 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 166.7$ , 148.2, 144.6, 131.7, 126.3, 125.0, 118.8, 116.0, 113.0, 52.3.



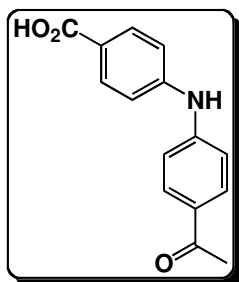
#### 4-[(4-nitrophenyl)amino]benzoic acid (**5i**)

Reaction of the methyl ester of **5i** according to general procedure **2** provided **5i** as an orange solid (68% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.65 (bs, 1H), 9.62 (s, 1H), 8.14 (d,  $J$  = 9.2 Hz, 2H), 7.91 (d,  $J$  = 8.6 Hz, 2H), 7.29 (d,  $J$  = 8.6 Hz, 2H), 7.21 (d,  $J$  = 9.2 Hz, 2H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 166.8, 149.0, 144.8, 139.2, 131.1, 125.9, 124.1, 118.1, 115.3. HRMS (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_4$ : 257.0562 (M-H), found 257.0558 (M-H).



#### 4-[(4-acetylphenyl)amino]benzoic acid methyl ester

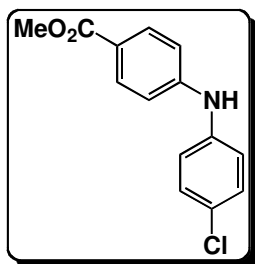
Reaction of methyl 4-bromobenzoate with 4'-aminoacetophenone according to general procedure **1** provided the methyl ester of **5j** as a yellow oil (80% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.98 (d,  $J$  = 7.5 Hz, 2H), 7.92 (d,  $J$  = 7.5 Hz, 2H), 7.11-7.18 (m, 4H), 6.71 (bs, 1H), 3.90 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 196.8, 166.9, 146.4, 145.9, 131.6, 130.7, 123.4, 117.3, 116.9, 52.1, 26.5.



#### 4-[(4-acetylphenyl)amino]benzoic acid (**5j**)

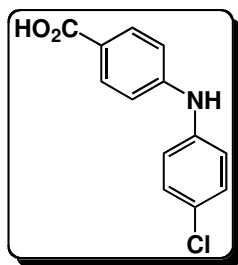
Reaction of the methyl ester of **5j** according to general procedure **2** provided **5j** as a white solid (52% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.50 (bs, 1H), 9.24 (s, 1H), 7.84-7.92 (m, 4H), 7.17-7.27 (m, 4H), 2.48 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 195.8,

167.1, 146.7, 146.1, 131.2, 130.3, 129.2, 122.6, 116.6, 116.0, 26.2. **HRMS** (ES) Calcd. for  $C_{15}H_{13}NO_3$ : 254.0817 (M-H), found 254.0826 (M-H).



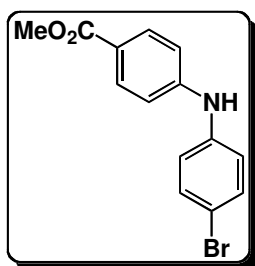
#### 4-[(4-chlorophenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 4-chloroaniline according to general procedure **1** provided the methyl ester of **5k** as a yellow solid (79% yield).  **$^1H$  NMR** ( $CDCl_3$ , 500MHz):  $\delta$  = 7.93 (d,  $J$  = 8.7 Hz, 2H), 7.29 (d,  $J$  = 8.7 Hz, 2H), 7.10 (d,  $J$  = 8.7 Hz, 2H), 6.97 (d,  $J$  = 8.7 Hz, 2H), 6.01 (s, 1H), 3.89 (s, 3H).  **$^{13}C$  NMR** ( $CDCl_3$ , 125 MHz):  $\delta$  = 167.1, 147.8, 139.8, 131.8, 129.8, 128.1, 121.9, 121.8, 115.0, 52.0.



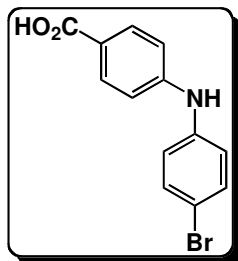
#### 4-[(4-chlorophenyl)amino]benzoic acid (**5k**)

Reaction of the methyl ester of **5k** according to general procedure **2** provided **5k** as a white solid (75% yield).  **$^1H$  NMR** (DMSO, 500 MHz):  $\delta$  = 12.35 (bs, 1H), 8.80 (s, 1H), 7.80 (d,  $J$  = 8.5 Hz, 2H), 7.32 (d,  $J$  = 8.7 Hz, 2H), 7.17 (d,  $J$  = 8.7 Hz, 2H), 7.05 (d,  $J$  = 8.5 Hz, 2H).  **$^{13}C$  NMR** (DMSO, 125 MHz):  $\delta$  = 167.1, 147.5, 140.6, 131.2, 129.1, 124.8, 120.9, 120.3, 114.5. **HRMS** (ES) Calcd. for  $C_{13}H_{10}ClNO_2$ : 246.0322 (M-H), found 246.0316 (M-H).



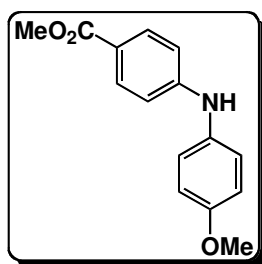
#### 4-[(4-bromophenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 4-bromoaniline according to general procedure **1** provided the methyl ester of **5l** as a green oil (22% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta = 7.93$  (d,  $J = 8.9$  Hz, 2H),  $7.43$  (d,  $J = 8.8$  Hz, 2H),  $7.05$  (d,  $J = 8.8$  Hz, 2H),  $6.98$  (d,  $J = 8.9$  Hz, 2H),  $6.06$  (s, 1H),  $3.89$  (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.1, 147.6, 140.3, 132.7, 131.7, 121.9, 115.4, 115.1, 52.0$ .



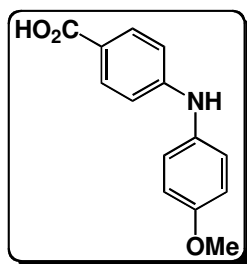
#### 4-[(4-bromophenyl)amino]benzoic acid (**5l**)

Reaction of the methyl ester of **5l** according to general procedure **2** provided **5l** as a green solid (58% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.35$  (bs, 1H),  $8.82$  (s, 1H),  $7.79$  (d,  $J = 8.6$  Hz, 2H),  $7.45$  (d,  $J = 8.7$  Hz, 2H),  $7.12$  (d,  $J = 8.7$  Hz, 2H),  $7.06$  (d,  $J = 8.6$  Hz, 2H). **HRMS** (ES) Calcd. for  $\text{C}_{13}\text{H}_{10}\text{BrNO}_2$ : 289.9817 (M-H $^-$ ), found 289.9831 (M-H $^-$ ).



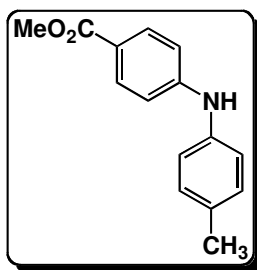
#### 4-[(4-methoxyphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with *p*-anisidine according to general procedure **1** provided the methyl ester of **5m** as a white solid (79% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta = 7.88$  (d,  $J = 8.8$  Hz, 2H),  $7.14$  (d,  $J = 8.9$  Hz, 2H),  $6.91$  (d,  $J = 8.9$  Hz, 2H),  $6.81$  (d,  $J = 8.8$  Hz, 2H),  $5.86$  (s, 1H),  $3.87$  (s, 3H),  $3.83$  (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.3, 156.8, 150.1, 133.7, 131.7, 124.7, 120.3, 115.0, 113.5, 55.8, 51.8$ .



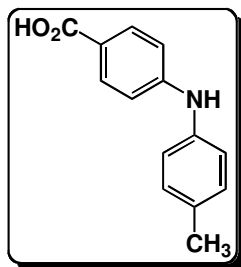
#### 4-[(4-methoxyphenyl)amino]benzoic acid (**5m**)

Reaction of the methyl ester of **5m** according to general procedure **2** provided **5m** as a white solid (82% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.17 (bs, 1H), 8.42 (s, 1H), 7.72 (d,  $J$  = 8.8 Hz, 2H), 7.12 (d,  $J$  = 8.9 Hz, 2H), 6.92 (d,  $J$  = 8.9 Hz, 2H), 6.86 (d,  $J$  = 8.8 Hz, 2H), 3.74 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.2, 155.1, 149.7, 134.0, 131.2, 122.7, 119.1, 114.6, 112.6, 55.2. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_3$ : 242.0817 (M-H $^-$ ), found 242.0823 (M-H $^-$ ).



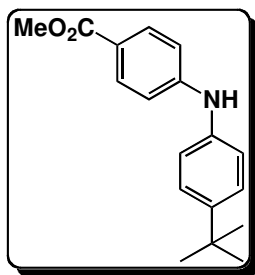
#### 4-[(4-methylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with *p*-toluidine according to general procedure **1** provided the methyl ester of **5n** as a yellow oil (40% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.98 (d,  $J$  = 8.7 Hz, 2H), 7.16 (d,  $J$  = 8.1 Hz, 2H), 7.09 (d,  $J$  = 8.3 Hz, 2H), 6.92 (d,  $J$  = 8.7 Hz, 2H), 5.96 (bs, 1H), 3.88 (s, 3H), 2.35 (s, 3H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 149.1, 138.3, 133.4, 131.7, 130.3, 121.6, 120.8, 114.2, 51.8, 21.0.



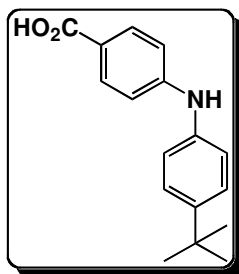
#### 4-[(4-methylphenyl)amino]benzoic acid (**5n**)

Reaction of the methyl ester of **5n** according to general procedure **2** provided **5n** as a white solid (88% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.20 (bs, 1H), 8.55 (s, 1H), 7.75 (d,  $J$  = 8.4 Hz, 2H), 7.13 (d,  $J$  = 8.0 Hz, 2H), 7.07 (d,  $J$  = 8.1 Hz, 2H), 6.97 (d,  $J$  = 8.5 Hz, 2H), 2.26 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.1, 148.7, 138.7, 131.1, 130.9, 129.7, 119.9, 119.7, 113.4, 20.3. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{13}\text{NO}_2$ : 226.0868 (M-H $^-$ ), found 226.0864 (M-H $^-$ ).



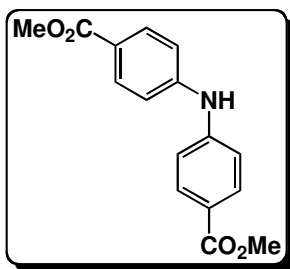
#### 4-[(4-*tert*-butylphenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 4-*tert*-butylaniline according to general procedure **1** provided the methyl ester of **5o** as a yellow oil (86% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500MHz):  $\delta = 7.91$  (d,  $J = 8.8$  Hz, 2H),  $7.37$  (d,  $J = 8.6$  Hz, 2H),  $7.12$  (d,  $J = 8.5$  Hz, 2H),  $6.96$  (d,  $J = 8.8$  Hz, 2H),  $6.00$  (s, 1H),  $3.88$  (s, 3H),  $1.35$  (s, 9H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta = 167.2$ ,  $148.9$ ,  $146.6$ ,  $138.3$ ,  $131.7$ ,  $126.5$ ,  $120.9$ ,  $114.4$ ,  $51.9$ ,  $34.6$ ,  $31.6$ .



#### 4-[(4-*tert*-butylphenyl)amino]benzoic acid (**5o**)

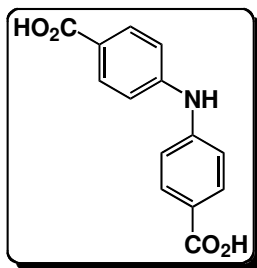
Reaction of the methyl ester of **5o** according to general procedure **2** provided **5o** as a white solid (87% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta = 12.23$  (bs, 1H),  $8.61$  (s, 1H),  $7.75$  (d,  $J = 8.7$  Hz, 2H),  $7.33$  (d,  $J = 8.6$  Hz, 2H),  $7.11$  (d,  $J = 8.5$  Hz, 2H),  $7.00$  (d,  $J = 8.7$  Hz, 2H),  $1.27$  (s, 9H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta = 167.1$ ,  $148.6$ ,  $144.3$ ,  $138.7$ ,  $131.1$ ,  $125.9$ ,  $119.8$ ,  $119.4$ ,  $113.5$ ,  $33.9$ ,  $31.2$ . HRMS (ES) Calcd. for  $\text{C}_{17}\text{H}_{19}\text{NO}_2$ : 268.1338 (M-H), found 268.1342 (M-H).



#### 4-[(4-methylcarboxyphenyl)amino]benzoic acid methyl ester

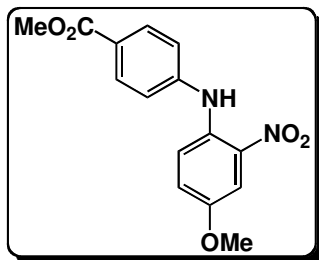
Reaction of methyl 4-bromobenzoate with methyl 4-aminobenzoate according to general procedure **1** provided the methyl ester of **5p** as a white solid (68% yield).  $^1\text{H NMR}$

(CDCl<sub>3</sub>, 500 MHz):  $\delta$  = 7.98 (d,  $J$  = 8.7 Hz, 4H), 7.14 (d,  $J$  = 8.7 Hz, 4H), 6.38 (bs, 1H), 3.90 (s, 6H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  = 166.9, 146.0, 131.7, 123.3, 117.1, 52.1.



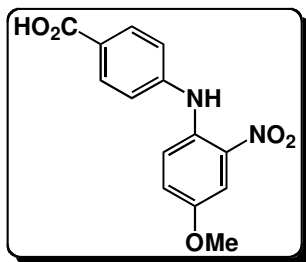
#### 4-[(4-carboxyphenyl)amino]benzoic acid (5p)

Reaction of the methyl ester of 5p according to general procedure 2 provided 5p as a white solid (87% yield). <sup>1</sup>H NMR (DMSO, 500 MHz):  $\delta$  = 12.48 (bs, 2H), 9.15 (s, 1H), 7.85 (d,  $J$  = 8.8 Hz, 4H), 7.20 (d,  $J$  = 8.8 Hz, 4H). <sup>13</sup>C NMR (DMSO, 125 MHz):  $\delta$  = 167.0, 146.3, 131.1, 122.3, 116.3. HRMS (ES) Calcd. for C<sub>14</sub>H<sub>11</sub>NO<sub>4</sub>: 256.0610 (M-H), found 256.0605 (M-H).



#### 4-[(2-nitro-4-methoxyphenyl)amino]benzoic acid methyl ester

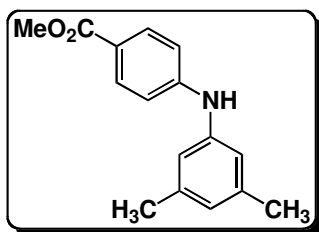
Reaction of methyl 4-bromobenzoate with 4-methoxy-2-nitroaniline according to general procedure 1 provided the methyl ester of 5q as an orange oil (65% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  = 9.18 (s, 1H), 8.03 (d,  $J$  = 8.7 Hz, 2H), 7.66 (d,  $J$  = 3.0 Hz, 1H), 7.46 (d,  $J$  = 9.3 Hz, 1H), 7.23 (d,  $J$  = 8.7 Hz, 2H), 7.15 (dd,  $J$  = 9.3, 3.0 Hz, 1H), 3.92 (s, 3H), 3.86 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  = 166.7, 152.9, 144.7, 135.8, 134.8, 131.6, 125.4, 125.2, 120.0, 119.8, 108.1, 56.2, 52.2.





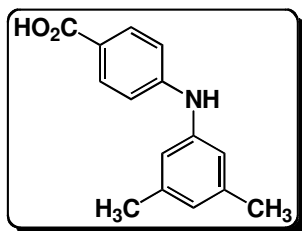
#### 4-[(2-nitro-4-methoxyphenyl)amino]benzoic acid (5q)

Reaction of the methyl ester of 5q according to general procedure 2 provided 5q as an orange solid (88% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.46 (bs, 1H), 8.88 (s, 1H), 7.81 (d,  $J$  = 8.7 Hz, 2H), 7.57 (d,  $J$  = 3.0 Hz, 1H), 7.47 (d,  $J$  = 9.1 Hz, 1H), 7.30 (dd,  $J$  = 9.1, 3.0 Hz, 1H), 7.07 (d,  $J$  = 8.7 Hz, 2H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 166.9, 154.0, 147.1, 140.1, 131.0, 130.6, 124.5, 122.9, 122.5, 116.4, 108.6, 55.9. **HRMS** (ES) Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_5$ : 287.0668 (M-H $^-$ ), found 287.0651 (M-H $^-$ ).



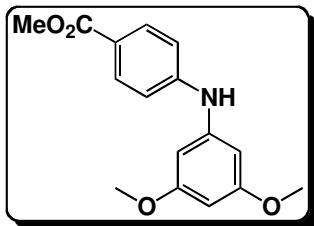
#### 4-[(3,5-bis(methyl)phenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 3,5-dimethylaniline according to general procedure 1 provided the methyl ester of 5r as a yellow oil (78% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.93 (d,  $J$  = 8.6 Hz, 2H), 6.98 (d,  $J$  = 8.6 Hz, 2H), 6.81 (s, 2H), 6.73 (s, 1H), 6.00 (s, 1H), 3.89 (s, 3H), 2.32 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.2, 148.6, 141.0, 139.4, 131.6, 125.2, 121.0, 118.5, 114.8, 51.8, 21.5.



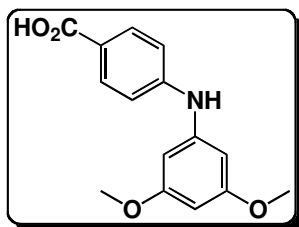
#### 4-[(3,5-bis(methyl)phenyl)amino]benzoic acid (5r)

Reaction of the methyl ester of 5r according to general procedure 2 provided 5r as a white solid (81% yield).  $^1\text{H NMR}$  (DMSO, 500 MHz):  $\delta$  = 12.22 (bs, 1H), 8.52 (s, 1H), 7.76 (d,  $J$  = 8.7 Hz, 2H), 7.02 (d,  $J$  = 8.7 Hz, 2H), 6.78 (s, 2H), 6.02 (s, 1H), 2.23 (s, 6H).  $^{13}\text{C NMR}$  (DMSO, 125 MHz):  $\delta$  = 167.0, 148.3, 141.3, 138.2, 131.0, 123.4, 120.0, 117.0, 114.0, 21.0. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_2$ : 240.1025 (M-H $^-$ ), found 240.1013 (M-H $^-$ ).



#### 4-[(3,5-bis(methoxy)phenyl)amino]benzoic acid methyl ester

Reaction of methyl 4-bromobenzoate with 3,5-dimethoxyaniline according to general procedure **1** provided the methyl ester of **5s** as a yellow oil (76% yield).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  = 7.93 (d,  $J$  = 8.7 Hz, 2H), 7.03 (d,  $J$  = 8.7 Hz, 2H), 6.33 (d,  $J$  = 2.1 Hz, 2H), 6.19 (t,  $J$  = 2.1 Hz, 1H), 6.05 (bs, 1H), 3.89 (s, 3H), 3.78 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  = 167.1, 161.9, 147.8, 143.1, 131.6, 121.7, 115.6, 98.5, 95.2, 55.6, 52.0.



#### 4-[(3,5-bis(methoxy)phenyl)amino]benzoic acid (**5s**)

Reaction of the methyl ester of **5s** according to general procedure **2** provided **5s** as a white solid (86% yield).  $^1\text{H NMR}$  ( $\text{DMSO}$ , 500 MHz):  $\delta$  = 12.30 (bs, 1H), 8.67 (s, 1H), 7.79 (d,  $J$  = 8.2 Hz, 2H), 7.08 (d,  $J$  = 8.2 Hz, 2H), 6.32 (s, 2H), 6.13 (s, 1H), 3.72 (s, 6H).  $^{13}\text{C NMR}$  ( $\text{DMSO}$ , 125 MHz):  $\delta$  = 167.1, 161.1, 147.7, 143.4, 131.1, 120.7, 114.8, 97.0, 93.7, 55.0. **HRMS** (ES) Calcd. for  $\text{C}_{15}\text{H}_{15}\text{NO}_4$ : 274.1079 ( $\text{M}+\text{H}^+$ ), found 274.1086 ( $\text{M}+\text{H}^+$ ).