Table 1
Calculated and literature pK_a values of select compounds.

	pK_a _MeCN COSMO-RS	pK_a _MeCN Experimental	pK_a _MeCN Correlation 1	pK_a _MeCN Correlation 2
CH_3OCO_2H	20.5	5.7[a]	18.5	18.0
$CH_3CH_2OCO_2H$	22.3		19.9	19.7
$CH_3CH_2CH_2OCO_2H$	22.2		19.8	19.6
$(CH_3)_2CHOCO_2H$	22.6		20.1	19.9
$CH_3(CH_2)_3OCO_2H$	22.2		19.8	19.6
$CH_3(CH_2)_4OCO_2H$	22.2		19.8	19.6
$CH_3(CH_2)_5OCO_2H$	22.2		19.8	19.6
CH_3CO_2H	27.0	23.51[b]	23.6	24.2
$C_6H_5CO_2H$	24.2	21.51[b]	21.4	21.6
3,5-Dinitrobenzoic acid	18.8	17.00 [28]	17.2	16.4
3-Nitrobenzoic acid	21.3	19.20 [28]	19.1	18.8
Chloroacetic acid	20.8	18.80 [28]	18.7	18.2
Dichloroacetic acid	16.8	13.20 [28]	15.5	14.4
Trichloroacetic acid	12.7	10.75 [28]	12.3	10.4
DBU		24.3 [27]		
TMG		23.3 [28]		
Ph-TMG		20.8 [27]		
NEt_3		18.8 [27]		
Hünig's	18.6[c]			

[a] In methanol (see text for details).
[b] Ref. [34].
[c] Estimated using the PCM model [29,30].