

## ***Electronic Supplementary Information***

### **Quantum Mechanical Based Approaches for Predicting $pK_a$ values of Carboxylic Acids: Evaluating the Performance of Different Strategies**

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**Table S1.** Error bars for pKa estimations with the different approaches, from asymmetric 95% confidence lower limits.

Scheme	B3LYP	BLYP	BH&HLYP	BMK	M05-2X	PBE	PBE0	PW91	TPSS
<b>PCM</b>									
A	1.14	1.71	1.92	1.10	0.98	1.37	1.38	1.63	1.07
D	1.81	1.27	1.23	1.02	1.71	1.57	1.28	1.70	1.70
E2	1.48	2.07	1.59	1.68	1.16	2.21	1.43	2.34	1.85
<b>SMD</b>									
A	1.08	0.94	1.71	0.76	0.83	0.87	1.30	0.88	1.43
D	1.14	1.13	1.01	0.96	1.18	1.34	0.76	1.16	1.07
E3	2.10	1.92	0.86	0.66	0.84	1.99	0.74	1.87	1.69
EN3	0.71	0.80	1.70	1.71	2.66	1.38	0.67	1.49	0.79
<b>FP</b>									
	0.25	0.19	0.29	0.22	0.24	0.17	0.18	0.21	0.19

**Table S2.** Error bars for pKa estimations with the different approaches, from asymmetric 95% confidence upper limits.

Scheme	B3LYP	BLYP	BH&HLYP	BMK	M05-2X	PBE	PBE0	PW91	TPSS
<b>PCM</b>									
A	0.66	0.99	1.11	0.64	0.56	0.79	0.79	0.94	0.61
D	1.05	0.73	0.71	0.59	0.99	0.90	0.74	0.98	0.98
E2	0.85	1.20	0.92	0.97	0.67	1.28	0.82	1.35	1.07
<b>SMD</b>									
A	0.62	0.54	0.99	0.44	0.48	0.50	0.75	0.51	0.83
D	0.66	0.65	0.58	0.56	0.68	0.77	0.44	0.67	0.62
E3	1.21	1.11	0.49	0.38	0.48	1.15	0.42	1.08	0.98
EN3	0.41	0.46	0.98	0.99	1.53	0.79	0.39	0.86	0.46
<b>FP</b>									
	0.15	0.11	0.17	0.12	0.14	0.10	0.11	0.12	0.11

**Table S3.** Uncertainties for the slope and the intercept of the linear fits used in the FP method.

	B3LYP	BLYP	BH&HLYP	BMK	M05-2X	PBE	PBE0	PW91	TPSS
<i>m</i>	0.04	0.03	0.04	0.04	0.05	0.04	0.04	0.04	0.04
<i>C<sub>0</sub></i>	9.8	8.6	9.9	11.6	13.9	11.3	12.2	11.9	11.2