Supplementary Information for

Directionality and additivity effects of molecular acidity and aromaticity for substituted benzoic acids under external electric fields

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Table S1. Fitted pK_a values with the additivity effect for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x-axis in comparison with the calculated p*K*a values using the (MEP) descriptor from the acidic oxygen. Also shown in the last few rows are statistical analysis results, including correlation coefficient R^2, mean squared error (MSE), root mean square error (RMSE), and mean absolute error (MAE) between the calculated and fitted pK_a values.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	0.483	0.134	-0.357	0.943	0.780	0.780
-225	0.659	0.347	-0.151	1.138	0.995	0.993
-200	0.834	0.557	0.053	1.331	1.208	1.204
-175	1.007	0.764	0.255	1.521	1.417	1.411
-150	1.180	0.969	0.456	1.710	1.624	1.617
-125	1.351	1.172	0.655	1.897	1.828	1.820
-100	1.521	1.373	0.854	2.082	2.030	2.021
-75	1.690	1.572	1.052	2.265	2.230	2.220
-50	1.859	1.770	1.249	2.447	2.428	2.418
-25	2.027	1.966	1.445	2.628	2.624	2.614
0	2.194	2.162	1.642	2.807	2.819	2.809
25	2.361	2.356	1.838	2.986	3.012	3.003
50	2.528	2.550	2.034	3.163	3.204	3.196
75	2.694	2.743	2.230	3.340	3.395	3.387
100	2.860	2.936	2.426	3.516	3.585	3.578
125	3.026	3.128	2.623	3.691	3.774	3.769
150	3.192	3.319	2.820	3.866	3.962	3.959
175	3.358	3.511	3.018	4.040	4.150	4.148
200	3.524	3.702	3.217	4.215	4.337	4.338
225	3.691	3.893	3.416	4.389	4.523	4.527
250	3.858	4.083	3.618	4.564	4.709	4.717
R^2				1.000	1.000	1.000
MSE				0.368	0.421	1.322
RMSE				0.606	0.649	1.150
MAE				0.602	0.649	1.149

Table S2. Fitted pK_a values with the additivity effect for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along y-axis in comparison with the calculated p*K*a values using the (MEP) descriptor from the acidic oxygen. Also shown in the last few rows are statistical analysis results, including correlation coefficient R^2, mean squared error (MSE), root mean square error (RMSE), and mean absolute error (MAE) between the calculated and fitted pK_a values.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-1.071	-0.832	-1.703	-0.131	0.073	-0.027
-225	-0.703	-0.501	-1.333	0.198	0.374	0.286
-200	-0.348	-0.180	-0.973	0.516	0.667	0.589
-175	-0.004	0.133	-0.624	0.824	0.952	0.885
-150	0.330	0.439	-0.283	1.124	1.232	1.173
-125	0.655	0.739	0.051	1.417	1.506	1.456
-100	0.973	1.033	0.378	1.704	1.775	1.733
-75	1.285	1.321	0.700	1.985	2.040	2.007
-50	1.592	1.605	1.017	2.262	2.302	2.276
-25	1.895	1.885	1.331	2.536	2.562	2.544
0	2.194	2.162	1.642	2.807	2.819	2.809
25	2.492	2.436	1.951	3.077	3.074	3.074
50	2.788	2.707	2.259	3.346	3.329	3.338
75	3.085	2.977	2.569	3.616	3.584	3.603
100	3.384	3.247	2.880	3.887	3.839	3.870
125	3.687	3.516	3.195	4.161	4.096	4.140
150	3.995	3.786	3.515	4.440	4.355	4.415
175	4.311	4.058	3.843	4.725	4.617	4.695
200	4.639	4.333	4.181	5.019	4.883	4.982
225	4.981	4.611	4.534	5.323	5.154	5.278
250	5.341	4.893	4.903	5.640	5.430	5.586
R^2				1.000	1.000	1.000
MSE				0.416	0.476	1.465
RMSE				0.645	0.690	1.211
MAE				0.618	0.681	1.175

Table S3. Fitted pK_a values with the additivity effect for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along x-axis in comparison with the calculated p*K*a values using the (MEP) descriptor from the leaving protons. Also shown in the last few rows are statistical analysis results, including correlation coefficient R^2, mean squared error (MSE), root mean square error (RMSE), and mean absolute error (MAE) between the calculated and fitted pK_a values.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	1.927	1.759	1.633	2.083	2.033	2.043
-225	2.167	2.003	1.871	2.330	2.283	2.292
-200	2.397	2.237	2.099	2.566	2.522	2.531
-175	2.618	2.463	2.320	2.791	2.751	2.760
-150	2.830	2.679	2.532	3.008	2.971	2.980
-125	3.033	2.888	2.737	3.215	3.181	3.191
-100	3.229	3.089	2.935	3.414	3.384	3.393
-75	3.418	3.282	3.126	3.605	3.578	3.587
-50	3.600	3.469	3.312	3.788	3.766	3.774
-25	3.776	3.650	3.491	3.965	3.946	3.955
0	3.946	3.824	3.666	4.135	4.119	4.128
25	4.110	3.993	3.835	4.298	4.286	4.295
50	4.269	4.156	4.000	4.456	4.447	4.456
75	4.423	4.315	4.160	4.608	4.602	4.611
100	4.573	4.468	4.316	4.754	4.752	4.761
125	4.718	4.617	4.469	4.896	4.897	4.906
150	4.860	4.762	4.618	5.033	5.036	5.045
175	4.998	4.903	4.764	5.165	5.172	5.181
200	5.133	5.040	4.907	5.294	5.303	5.312
225	5.265	5.174	5.047	5.419	5.430	5.439
250	5.395	5.305	5.186	5.540	5.553	5.562
R^2				1.000	1.000	1.000
MSE				0.031	0.080	0.192
RMSE				0.176	0.283	0.438
MAE				0.175	0.283	0.437

Table S4. Fitted pK_a values with the additivity effect for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along y-axis in comparison with the calculated p*K*a values using the (MEP) descriptor from the leaving protons. Also shown in the last few rows are statistical analysis results, including correlation coefficient R^2, mean squared error (MSE), root mean square error (RMSE), and mean absolute error (MAE) between the calculated and fitted pK_a values.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	-0.503	-0.576	-0.796	-0.256	-0.252	-0.246
-225	-0.037	-0.111	-0.328	0.208	0.210	0.216
-200	0.423	0.347	0.133	0.665	0.664	0.669
-175	0.876	0.798	0.587	1.113	1.111	1.116
-150	1.324	1.242	1.036	1.556	1.552	1.557
-125	1.767	1.681	1.481	1.995	1.988	1.994
-100	2.207	2.116	1.922	2.428	2.419	2.426
-75	2.644	2.547	2.360	2.858	2.848	2.854
-50	3.079	2.975	2.797	3.286	3.273	3.281
-25	3.512	3.400	3.231	3.711	3.697	3.705
0	3.946	3.824	3.666	4.135	4.119	4.128
25	4.379	4.247	4.100	4.558	4.540	4.550
50	4.814	4.669	4.536	4.981	4.962	4.973
75	5.252	5.092	4.974	5.405	5.384	5.396
100	5.692	5.516	5.414	5.830	5.807	5.821
125	6.137	5.941	5.859	6.258	6.232	6.248
150	6.587	6.368	6.309	6.689	6.661	6.678
175	7.045	6.799	6.766	7.124	7.092	7.112
200	7.510	7.234	7.231	7.564	7.529	7.551
225	7.985	7.674	7.705	8.010	7.971	7.995
250	8.470	8.119	8.190	8.463	8.418	8.446
R^2				1.000	1.000	1.000
MSE				0.033	0.091	0.203
RMSE				0.182	0.301	0.451
MAE				0.166	0.301	0.443

Table S5. Calculated and fitted pK_a values using MEP results of the leaving protons for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x axis. Also shown are statistical analysis results for calculated and fitted pK_a values from MEP values on leaving protons.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	1.411	1.002	0.560	1.840	1.638	1.665
-225	1.600	1.240	0.779	2.055	1.881	1.900
-200	1.782	1.467	0.990	2.262	2.114	2.127
-175	1.958	1.686	1.195	2.462	2.338	2.345
-150	2.129	1.896	1.395	2.653	2.553	2.555
-125	2.294	2.099	1.589	2.838	2.759	2.758
-100	2.455	2.296	1.779	3.017	2.958	2.954
-75	2.611	2.486	1.965	3.190	3.150	3.144
-50	2.764	2.671	2.147	3.358	3.336	3.328
-25	2.914	2.852	2.327	3.520	3.516	3.507
0	3.061	3.028	2.504	3.679	3.690	3.681
25	3.205	3.199	2.678	3.833	3.859	3.850
50	3.347	3.367	2.851	3.983	4.023	4.016
75	3.487	3.532	3.022	4.130	4.183	4.177
100	3.625	3.693	3.191	4.273	4.338	4.334
125	3.761	3.851	3.360	4.414	4.489	4.488
150	3.896	4.007	3.527	4.551	4.636	4.639
175	4.031	4.159	3.693	4.687	4.779	4.787
200	4.164	4.308	3.859	4.820	4.919	4.932
225	4.297	4.455	4.024	4.951	5.055	5.075
250	4.430	4.599	4.188	5.081	5.189	5.216
R^2				1.000	1.000	0.999
MSE				0.352	0.414	1.292
RMSE				0.594	0.644	1.137
MAE				0.589	0.643	1.136

Table S6. Calculated and fitted pK_a values using MEP results of the leaving protons for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along y axis. Also shown are statistical analysis results for calculated and fitted pK_a values from MEP values on leaving protons.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-2.056	-1.827	-2.704	-1.114	-0.912	-1.014
-225	-1.500	-1.307	-2.143	-0.597	-0.424	-0.513
-200	-0.958	-0.797	-1.595	-0.092	0.056	-0.022
-175	-0.428	-0.297	-1.058	0.403	0.528	0.460
-150	0.091	0.195	-0.531	0.888	0.993	0.935
-125	0.601	0.680	-0.011	1.366	1.453	1.403
-100	1.104	1.159	0.501	1.837	1.907	1.866
-75	1.600	1.633	1.008	2.303	2.357	2.324
-50	2.091	2.102	1.510	2.765	2.804	2.779
-25	2.577	2.566	2.008	3.223	3.248	3.231
0	3.061	3.028	2.504	3.679	3.690	3.681
25	3.542	3.486	2.997	4.133	4.130	4.130
50	4.023	3.942	3.490	4.586	4.569	4.579
75	4.505	4.397	3.984	5.041	5.008	5.028
100	4.989	4.851	4.480	5.497	5.448	5.480
125	5.476	5.304	4.979	5.956	5.889	5.934
150	5.970	5.759	5.484	6.420	6.332	6.392
175	6.473	6.216	5.997	6.890	6.777	6.856
200	6.986	6.674	6.520	7.369	7.227	7.327
225	7.515	7.137	7.056	7.858	7.681	7.807
250	8.062	7.603	7.611	8.360	8.141	8.298
R^2				1.000	1.000	1.000
MSE				0.420	0.484	1.488
RMSE				0.648	0.695	1.220
MAE				0.621	0.686	1.184

Table S7. Calculated and fitted NICS(0) values for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along x-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	-10.496	-10.969	-12.744	-10.016	-11.421	-12.748
-225	-10.539	-10.985	-12.753	-10.082	-11.422	-12.745
-200	-10.581	-11.001	-12.762	-10.146	-11.425	-12.745
-175	-10.621	-11.015	-12.769	-10.206	-11.429	-12.746
-150	-10.659	-11.028	-12.776	-10.265	-11.435	-12.748
-125	-10.697	-11.040	-12.783	-10.322	-11.440	-12.751
-100	-10.734	-11.050	-12.789	-10.377	-11.445	-12.755
-75	-10.770	-11.059	-12.795	-10.431	-11.451	-12.758
-50	-10.805	-11.067	-12.800	-10.483	-11.456	-12.762
-25	-10.841	-11.073	-12.804	-10.535	-11.461	-12.766
0	-10.876	-11.077	-12.809	-10.586	-11.465	-12.770
25	-10.910	-11.080	-12.813	-10.636	-11.469	-12.774
50	-10.945	-11.081	-12.816	-10.686	-11.473	-12.778
75	-10.981	-11.081	-12.819	-10.736	-11.476	-12.783
100	-11.016	-11.079	-12.822	-10.786	-11.480	-12.788
125	-11.052	-11.076	-12.825	-10.837	-11.484	-12.794
150	-11.090	-11.072	-12.828	-10.889	-11.487	-12.800
175	-11.128	-11.067	-12.830	-10.942	-11.492	-12.808
200	-11.167	-11.060	-12.832	-10.997	-11.497	-12.817
225	-11.208	-11.054	-12.834	-11.054	-11.505	-12.829
250	-11.251	-11.047	-12.836	-11.115	-11.516	-12.845
R^2				1.000	0.490	0.762
MSE				0.098	0.171	0.001
RMSE				0.314	0.414	0.029
MAE				0.297	0.413	0.026

Table S8. Calculated and fitted NICS(0) values for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-7.849	-7.821	-8.169	-8.008	-7.655	-8.357
-225	-7.919	-7.912	-8.265	-8.049	-7.718	-8.410
-200	-7.978	-7.989	-8.345	-8.085	-7.780	-8.463
-175	-8.028	-8.054	-8.412	-8.114	-7.833	-8.507
-150	-8.069	-8.108	-8.467	-8.143	-7.877	-8.547
-125	-8.103	-8.153	-8.511	-8.163	-7.913	-8.577
-100	-8.131	-8.189	-8.547	-8.180	-7.943	-8.600
-75	-8.154	-8.217	-8.574	-8.194	-7.966	-8.618
-50	-8.172	-8.238	-8.594	-8.205	-7.983	-8.631
-25	-8.185	-8.251	-8.606	-8.213	-7.995	-8.640
0	-8.195	-8.258	-8.612	-8.219	-8.001	-8.645
25	-8.201	-8.258	-8.611	-8.224	-8.001	-8.646
50	-8.204	-8.251	-8.604	-8.226	-7.996	-8.642
75	-8.204	-8.237	-8.590	-8.226	-7.986	-8.635
100	-8.200	-8.216	-8.568	-8.224	-7.970	-8.623
125	-8.194	-8.187	-8.539	-8.219	-7.947	-8.607
150	-8.184	-8.149	-8.502	-8.234	-7.940	-8.607
175	-8.171	-8.102	-8.454	-8.224	-7.904	-8.579
200	-8.153	-8.044	-8.395	-8.210	-7.860	-8.545
225	-8.132	-7.974	-8.323	-8.165	-7.806	-8.476
250	-8.105	-7.890	-8.235	-8.142	-7.743	-8.423
R^2				0.979	0.983	0.971
MSE				0.004	0.051	0.010
RMSE				0.065	0.225	0.102
MAE				0.054	0.223	0.088

Table S9. Calculated and fitted NICS(1) values for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along x-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	-9.874	-9.900	-10.237	-9.628	-10.101	-10.015
-225	-9.907	-9.926	-10.253	-9.674	-10.116	-10.027
-200	-9.939	-9.949	-10.268	-9.717	-10.130	-10.039
-175	-9.968	-9.969	-10.281	-9.757	-10.143	-10.050
-150	-9.996	-9.987	-10.292	-9.795	-10.155	-10.060
-125	-10.022	-10.002	-10.301	-9.831	-10.165	-10.069
-100	-10.046	-10.014	-10.308	-9.865	-10.174	-10.076
-75	-10.069	-10.023	-10.314	-9.896	-10.180	-10.081
-50	-10.090	-10.030	-10.318	-9.926	-10.185	-10.085
-25	-10.111	-10.034	-10.321	-9.954	-10.189	-10.088
0	-10.130	-10.035	-10.321	-9.981	-10.190	-10.089
25	-10.147	-10.034	-10.321	-10.006	-10.190	-10.089
50	-10.164	-10.030	-10.319	-10.029	-10.188	-10.087
75	-10.180	-10.024	-10.315	-10.052	-10.184	-10.084
100	-10.195	-10.014	-10.309	-10.073	-10.179	-10.079
125	-10.210	-10.003	-10.302	-10.093	-10.171	-10.072
150	-10.223	-9.988	-10.293	-10.112	-10.162	-10.065
175	-10.236	-9.971	-10.283	-10.131	-10.152	-10.056
200	-10.248	-9.950	-10.270	-10.149	-10.140	-10.046
225	-10.259	-9.928	-10.256	-10.167	-10.127	-10.035
250	-10.270	-9.902	-10.240	-10.185	-10.113	-10.024
R^2				1.000	0.985	0.992
MSE				0.026	0.030	0.052
RMSE				0.162	0.173	0.229
MAE				0.155	0.173	0.229

Table S10. Calculated and fitted NICS(1) values for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along y-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	-10.531	-10.162	-10.782	-10.294	-10.316	-10.502
-225	-10.502	-10.169	-10.743	-10.294	-10.336	-10.498
-200	-10.472	-10.170	-10.703	-10.276	-10.335	-10.466
-175	-10.441	-10.167	-10.663	-10.253	-10.329	-10.431
-150	-10.407	-10.159	-10.622	-10.227	-10.319	-10.392
-125	-10.370	-10.148	-10.579	-10.197	-10.306	-10.351
-100	-10.331	-10.132	-10.533	-10.164	-10.289	-10.306
-75	-10.287	-10.113	-10.485	-10.125	-10.269	-10.258
-50	-10.240	-10.090	-10.434	-10.083	-10.246	-10.206
-25	-10.187	-10.065	-10.379	-10.034	-10.220	-10.150
0	-10.130	-10.035	-10.321	-9.981	-10.190	-10.089
25	-10.066	-10.002	-10.259	-9.920	-10.158	-10.024
50	-9.994	-9.965	-10.191	-9.853	-10.121	-9.953
75	-9.914	-9.924	-10.117	-9.778	-10.081	-9.875
100	-9.824	-9.877	-10.036	-9.692	-10.036	-9.790
125	-9.721	-9.825	-9.944	-9.595	-9.985	-9.696
150	-9.604	-9.766	-9.842	-9.484	-9.928	-9.590
175	-9.469	-9.699	-9.725	-9.357	-9.862	-9.472
200	-9.312	-9.622	-9.591	-9.211	-9.787	-9.338
225	-9.129	-9.532	-9.435	-9.042	-9.699	-9.185
250	-8.916	-9.427	-9.252	-8.844	-9.594	-9.007
R^2				0.999	1.000	0.999
MSE				0.023	0.026	0.058
RMSE				0.155	0.160	0.241
MAE				0.150	0.160	0.241

Table S11. Calculated and fitted NICS(1) values for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-9.567	-9.704	-9.558	-9.739	-9.782	-9.792
-225	-9.649	-9.777	-9.644	-9.799	-9.828	-9.847
-200	-9.719	-9.838	-9.716	-9.852	-9.878	-9.905
-175	-9.779	-9.889	-9.776	-9.897	-9.919	-9.953
-150	-9.830	-9.931	-9.825	-9.936	-9.954	-9.994
-125	-9.873	-9.966	-9.865	-9.970	-9.982	-10.027
-100	-9.909	-9.993	-9.897	-9.998	-10.005	-10.052
-75	-9.939	-10.013	-9.920	-10.022	-10.021	-10.071
-50	-9.964	-10.027	-9.937	-10.041	-10.033	-10.085
-25	-9.983	-10.035	-9.946	-10.055	-10.040	-10.092
0	-9.998	-10.037	-9.948	-10.066	-10.042	-10.094
25	-10.009	-10.033	-9.943	-10.072	-10.039	-10.090
50	-10.015	-10.023	-9.931	-10.075	-10.031	-10.080
75	-10.017	-10.008	-9.913	-10.073	-10.019	-10.065
100	-10.015	-9.985	-9.886	-10.067	-10.001	-10.044
125	-10.008	-9.956	-9.852	-10.057	-9.977	-10.016
150	-9.998	-9.919	-9.810	-10.055	-9.960	-9.994
175	-9.982	-9.875	-9.757	-10.036	-9.924	-9.953
200	-9.962	-9.821	-9.694	-10.011	-9.880	-9.903
225	-9.937	-9.756	-9.619	-9.983	-9.828	-9.845
250	-9.906	-9.680	-9.529	-9.947	-9.766	-9.775
R^2				0.981	0.996	0.998
MSE				0.008	0.002	0.032
RMSE				0.088	0.040	0.179
MAE				0.081	0.031	0.177

Table S12. Calculated and fitted NICS(1) values for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along y-axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-10.039	-9.977	-10.133	-9.890	-9.943	-9.877
-225	-10.071	-10.013	-10.143	-9.975	-9.994	-9.982
-200	-10.093	-10.042	-10.147	-10.036	-10.021	-10.043
-175	-10.108	-10.065	-10.145	-10.079	-10.049	-10.092
-150	-10.114	-10.080	-10.135	-10.100	-10.059	-10.117
-125	-10.114	-10.090	-10.121	-10.118	-10.072	-10.140
-100	-10.106	-10.092	-10.100	-10.127	-10.078	-10.151
-75	-10.090	-10.088	-10.072	-10.126	-10.078	-10.152
-50	-10.068	-10.078	-10.038	-10.115	-10.072	-10.142
-25	-10.037	-10.060	-9.997	-10.095	-10.060	-10.123
0	-9.998	-10.037	-9.948	-10.066	-10.042	-10.094
25	-9.951	-10.008	-9.891	-10.026	-10.018	-10.054
50	-9.893	-9.972	-9.826	-9.976	-9.988	-10.004
75	-9.828	-9.930	-9.750	-9.912	-9.951	-9.941
100	-9.746	-9.881	-9.663	-9.847	-9.919	-9.877
125	-9.648	-9.824	-9.562	-9.751	-9.866	-9.783
150	-9.530	-9.757	-9.444	-9.633	-9.804	-9.669
175	-9.388	-9.680	-9.305	-9.489	-9.731	-9.530
200	-9.217	-9.592	-9.142	-9.312	-9.659	-9.376
225	-9.010	-9.490	-8.949	-9.094	-9.558	-9.169
250	-8.755	-9.371	-8.719	-8.831	-9.439	-8.920
R^2				0.973	0.994	0.914
MSE				0.006	0.001	0.028
RMSE				0.079	0.035	0.169
MAE				0.071	0.028	0.152

Table S13. Calculated and fitted pK_a values using MEP results of the acidic oxygen applying this sum rule in Eqs. (10) and (11) for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along x axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	1.085	0.930	0.779	0.897	0.620	0.287
-225	1.295	1.141	0.990	1.124	0.857	0.540
-200	1.501	1.351	1.198	1.348	1.091	0.789
-175	1.706	1.558	1.404	1.570	1.321	1.036
-150	1.907	1.762	1.608	1.788	1.550	1.280
-125	2.106	1.965	1.810	2.004	1.775	1.522
-100	2.304	2.165	2.010	2.218	1.999	1.761
-75	2.499	2.364	2.209	2.430	2.220	1.999
-50	2.692	2.561	2.406	2.639	2.440	2.234
-25	2.884	2.757	2.601	2.847	2.658	2.468
0	3.074	2.951	2.796	3.053	2.874	2.699
25	3.262	3.144	2.989	3.257	3.088	2.930
50	3.450	3.335	3.182	3.459	3.301	3.159
75	3.636	3.526	3.373	3.661	3.513	3.387
100	3.821	3.715	3.564	3.861	3.723	3.613
125	4.005	3.904	3.754	4.061	3.933	3.840
150	4.189	4.092	3.944	4.259	4.142	4.065
175	4.373	4.280	4.134	4.457	4.350	4.290
200	4.556	4.467	4.324	4.655	4.558	4.514
225	4.739	4.654	4.514	4.852	4.765	4.739
250	4.923	4.842	4.704	5.050	4.973	4.965
R^2				1.000	1.000	1.000
MSE				0.010	0.024	0.062
RMSE				0.099	0.156	0.249
MAE				0.084	0.128	0.208

Table S14. Calculated and fitted pK_a values using MEP results of the acidic oxygen applying this sum rule in Eqs. (10) and (11) for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along y axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	0.481	0.412	0.193	0.264	0.062	-0.357
-225	0.759	0.688	0.473	0.561	0.364	-0.037
-200	1.032	0.959	0.746	0.855	0.663	0.286
-175	1.299	1.222	1.014	1.143	0.954	0.601
-150	1.560	1.480	1.277	1.426	1.240	0.911
-125	1.818	1.733	1.536	1.704	1.521	1.217
-100	2.073	1.982	1.791	1.978	1.798	1.518
-75	2.325	2.228	2.045	2.249	2.071	1.816
-50	2.576	2.471	2.296	2.518	2.341	2.112
-25	2.825	2.712	2.546	2.786	2.608	2.406
0	3.074	2.951	2.796	3.053	2.874	2.699
25	3.323	3.189	3.046	3.319	3.138	2.993
50	3.573	3.427	3.297	3.587	3.403	3.287
75	3.826	3.665	3.551	3.856	3.668	3.583
100	4.082	3.904	3.807	4.129	3.934	3.882
125	4.343	4.145	4.068	4.405	4.202	4.185
150	4.609	4.388	4.334	4.686	4.473	4.494
175	4.881	4.635	4.607	4.973	4.748	4.809
200	5.162	4.886	4.888	5.268	5.027	5.132
225	5.453	5.142	5.179	5.571	5.313	5.464
250	5.754	5.404	5.481	5.884	5.606	5.806
R^2				1.000	1.000	1.000
MSE				0.012	0.033	0.081
RMSE				0.111	0.182	0.285
MAE				0.094	0.153	0.240

Table S15. Calculated and fitted pK_a values using MEP results of the acidic oxygen applying this sum rule in Eqs. (10) and (11) for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	0.483	0.134	-0.357	0.273	0.240	-0.743
-225	0.659	0.347	-0.151	0.470	0.467	-0.502
-200	0.834	0.557	0.053	0.666	0.691	-0.264
-175	1.007	0.764	0.255	0.860	0.911	-0.028
-150	1.180	0.969	0.456	1.052	1.129	0.206
-125	1.351	1.172	0.655	1.243	1.344	0.439
-100	1.521	1.373	0.854	1.434	1.557	0.671
-75	1.690	1.572	1.052	1.623	1.769	0.901
-50	1.859	1.770	1.249	1.811	1.978	1.131
-25	2.027	1.966	1.445	1.999	2.186	1.360
0	2.194	2.162	1.642	2.186	2.392	1.588
25	2.361	2.356	1.838	2.373	2.598	1.817
50	2.528	2.550	2.034	2.559	2.802	2.045
75	2.694	2.743	2.230	2.745	3.006	2.274
100	2.860	2.936	2.426	2.931	3.208	2.503
125	3.026	3.128	2.623	3.118	3.410	2.733
150	3.192	3.319	2.820	3.304	3.611	2.963
175	3.358	3.511	3.018	3.491	3.812	3.194
200	3.524	3.702	3.217	3.678	4.013	3.427
225	3.691	3.893	3.416	3.867	4.213	3.661
250	3.858	4.083	3.618	4.057	4.413	3.897
R^2				1.000	1.000	1.000
MSE				0.015	0.056	0.043
RMSE				0.122	0.236	0.207
MAE				0.106	0.226	0.177

Table S16. Calculated and fitted pK_a values using MEP results of the acidic oxygen applying this sum rule in Eqs. (10) and (11) for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along y axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	-1.071	-0.832	-1.703	-1.326	-0.638	-2.226
-225	-0.703	-0.501	-1.333	-0.931	-0.307	-1.807
-200	-0.348	-0.180	-0.973	-0.546	0.017	-1.393
-175	-0.004	0.133	-0.624	-0.175	0.333	-0.992
-150	0.330	0.439	-0.283	0.185	0.642	-0.602
-125	0.655	0.739	0.051	0.535	0.945	-0.221
-100	0.973	1.033	0.378	0.877	1.243	0.151
-75	1.285	1.321	0.700	1.212	1.536	0.518
-50	1.592	1.605	1.017	1.541	1.824	0.879
-25	1.895	1.885	1.331	1.865	2.110	1.235
0	2.194	2.162	1.642	2.186	2.392	1.588
25	2.492	2.436	1.951	2.504	2.673	1.939
50	2.788	2.707	2.259	2.822	2.952	2.290
75	3.085	2.977	2.569	3.140	3.230	2.642
100	3.384	3.247	2.880	3.460	3.508	2.996
125	3.687	3.516	3.195	3.784	3.787	3.355
150	3.995	3.786	3.515	4.115	4.068	3.721
175	4.311	4.058	3.843	4.455	4.352	4.096
200	4.639	4.333	4.181	4.807	4.639	4.485
225	4.981	4.611	4.534	5.176	4.931	4.891
250	5.341	4.893	4.903	5.564	5.228	5.317
R^2				1.000	1.000	1.000
MSE				0.020	0.061	0.078
RMSE				0.140	0.246	0.280
MAE				0.119	0.243	0.238

Table S17. Calculated and fitted NICS(0) values using the additivity effect for doubly and triply substituted benzoic acid derivatives with no external electric field. The fitted values were obtained using Eqs. (10) and (11) with $a_{m1}=a_{m2}=0.9$ and $a_p=1.0$. Also shown are statistical analysis results in the bottom row of the table.

Molecule	Calculated	Molecule	Calculated	Molecule	Calculated	Fitted	Molecule	Calculated	Fitted
H	-7.137	4-NH_2	-6.622	3,5-Cl	-8.184	-8.271	3-NH_2-5-CN	-7.806	-7.776
3-F	-9.179	4-NMe_2	-8.969	3,5-Me	-6.922	-6.948	3-NH_2-5-F	-8.976	-9.157
3-Br	-7.497	4-NO_2	-8.461	3,5-NH_2	-7.097	-7.398	3-NH_2-5-Me	-7.050	-7.182
3-Cl	-7.760	4-OEt	-7.769	3,5-NMe_2	-7.548	-7.772	3-NH_2-5-NMe_2	-7.324	-7.574
3-Me	-7.041	4-OH	-7.820	3,5-NO_2	-9.743	-9.466	3-NH_2-5-NO_2	-8.558	-8.458
3-NH_2	-7.301	4-OMe	-7.830	3,5-OEt	-9.225	-9.119	3-NH_2-5-OEt	-8.150	-8.317
3-NMe_2	-7.521	5-F	-9.217	3,5-OH	-9.218	-9.386	3-NH_2-5-OMe	-8.135	-8.364
3-NO_2	-8.422	5-Br	-7.469	3-Cl-5-CN	-8.191	-8.188	3-NMe_2-5-Cl	-7.975	-8.056
3-OEt	-8.193	5-Cl	-7.775	3-Cl-5-NO_2	-8.958	-8.871	3-NMe_2-5-CN	-8.050	-7.973
3-OH	-8.370	5-Me	-7.023	3-F-5-Cl	-9.709	-9.548	3-NMe_2-5-F	-9.243	-9.355
3-CN	-7.699	5-NH_2	-7.263	3-F-5-CN	-9.652	-9.466	3-NMe_2-5-Me	-7.368	-7.380
3-OMe	-9.787	5-NMe_2	-7.459	3-F-5-NO_2	-10.452	-10.148	3-NMe_2-5-NO_2	-8.715	-8.656
4-F	-8.832	5-NO_2	-8.441	3-Me-5-Cl	-7.623	-7.624	3-NO_2-5-CN	-8.994	-8.784
4-CN	-7.769	5-OEt	-8.284	3-Me-5-CN	-7.621	-7.541	3-OEt-5-Cl	-8.755	-8.661
4-Br	-7.230	5-OH	-8.404	3-Me-5-F	-8.981	-8.923	3-OEt-5-CN	-8.812	-8.578
4-Cl	-7.497	5-OMe	-8.337	3-Me-5-NO_2	-8.370	-8.224	3-OEt-5-F	-10.147	-9.959
4-Me	-6.863	5-CN	-7.683	3-NH_2-5-Cl	-7.682	-7.859	3-OEt-5-Me	-8.014	-7.984

Continued

Molecule	Calculated	Fitted	Molecule	Calculated	Fitted	Molecule	Calculated	Fitted	Molecule	Calculated	Fitted
3-OEt-5-NMe_2	-8.321	-8.377	4-Cl-5-NMe_2	-8.025	-7.787	4-F-5-OMe	-10.014	-9.911	4-OEt-5-Cl	-8.542	-8.343
3-OEt-5-NO_2	-9.629	-9.260	4-Cl-5-NO_2	-8.928	-8.670	4-Me-5-Cl	-7.550	-7.437	4-OEt-5-CN	-8.036	-8.260
3-OH-5-Cl	-8.752	-8.820	4-Cl-5-OEt	-8.575	-8.529	4-Me-5-CN	-7.277	-7.354	4-OEt-5-F	-9.975	-9.641
3-OH-5-CN	-8.861	-8.738	4-Cl-5-OH	-8.662	-8.637	4-Me-5-F	-8.949	-8.735	4-OEt-5-Me	-7.908	-7.666
3-OH-5-F	-10.163	-10.119	4-Cl-5-OMe	-8.569	-8.577	4-Me-5-NH_2	-7.410	-6.976	4-OH-5-Cl	-8.414	-8.394
3-OH-5-Me	-8.069	-8.144	4-CN-5-Cl	-8.018	-8.342	4-Me-5-NMe_2	-7.530	-7.153	4-OH-5-CN	-8.102	-8.311
3-OH-5-NH_2	-8.107	-8.360	4-CN-5-F	-9.465	-9.641	4-Me-5-NO_2	-8.425	-8.036	4-OH-5-F	-10.047	-9.692
3-OH-5-NMe_2	-8.302	-8.536	4-CN-5-Me	-7.520	-7.666	4-Me-5-OEt	-8.113	-7.895	4-OH-5-Me	-7.750	-7.718
3-OH-5-NO_2	-9.598	-9.420	4-CN-5-NMe_2	-7.741	-8.058	4-Me-5-OH	-8.197	-8.003	4-OH-5-OEt	-9.236	-8.853
3-OH-5-OEt	-9.183	-9.279	4-CN-5-NO_2	-9.038	-8.942	4-Me-5-OMe	-8.134	-7.943	4-OH-5-OMe	-9.223	-8.900
3-OH-5-OMe	-9.160	-9.326	4-CN-5-OEt	-8.496	-8.801	4-NH_2-5-Cl	-7.443	-7.196	4-OMe-5-Cl	-8.624	-8.403
4,5-Cl	-7.825	-8.071	4-CN-5-OMe	-8.525	-8.848	4-NH_2-5-F	-9.156	-8.494	4-OMe-5-CN	-8.075	-8.321
4,5-Me	-6.876	-6.760	4-F-5-Cl	-9.252	-9.405	4-NH_2-5-Me	-6.898	-6.519	4-OMe-5-F	-10.205	-9.702
4,5-OEt	-9.462	-8.801	4-F-5-CN	-9.052	-9.322	4-NO_2-5-Cl	-9.151	-9.034	4-OMe-5-Me	-7.846	-7.727
4,5-OH	-9.513	-8.960	4-F-5-Me	-8.686	-8.729	4-NO_2-5-CN	-9.039	-8.951	4-OMe-5-NMe_2	-8.597	-8.119
4,5-OMe	-9.488	-8.909	4-F-5-NH_2	-9.378	-8.945	4-NO_2-5-F	-10.462	-10.333	4-OMe-5-NO_2	-9.376	-9.003
4-Cl-5-CN	-7.712	-7.988	4-F-5-NMe_2	-9.428	-9.121	4-NO_2-5-Me	-8.585	-8.358	4-OMe-5-OH	-9.476	-8.970
4-Cl-5-F	-9.318	-9.369	4-F-5-NO_2	-10.091	-10.004	4-NO_2-5-NMe_2	-9.148	-8.750	3,4,5-Me	-6.747	-6.674
4-Cl-5-Me	-7.434	-7.394	4-F-5-OEt	-10.029	-9.864	4-NO_2-5-OEt	-9.746	-9.493	3,5-Cl-4-OH	-8.837	-8.954
4-Cl-5-NH_2	-7.848	-7.610	4-F-5-OH	-10.191	-9.971	4-NO_2-5-OMe	-9.758	-9.540	3,5-NO_2-4-Cl	-10.495	-9.826
R^2		0.933	MSE		0.065	RMSE		0.255	MAE		0.207

Table S18. Calculated and fitted Shannon entropy values applying this sum rule in Eqs. (10) and (11) for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along x axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	46.852	46.840	43.455	47.452	46.492	43.860
-225	46.799	46.789	43.407	47.399	46.441	43.812
-200	46.753	46.745	43.364	47.352	46.397	43.769
-175	46.713	46.707	43.328	47.312	46.360	43.733
-150	46.680	46.675	43.298	47.278	46.328	43.702
-125	46.652	46.649	43.273	47.250	46.302	43.677
-100	46.630	46.628	43.253	47.228	46.281	43.657
-75	46.614	46.613	43.239	47.211	46.267	43.643
-50	46.602	46.604	43.230	47.200	46.257	43.634
-25	46.597	46.600	43.227	47.194	46.253	43.631
0	46.596	46.602	43.228	47.194	46.255	43.632
25	46.601	46.608	43.235	47.198	46.262	43.639
50	46.611	46.621	43.247	47.209	46.274	43.652
75	46.627	46.639	43.265	47.224	46.292	43.669
100	46.648	46.662	43.288	47.245	46.315	43.692
125	46.674	46.691	43.316	47.271	46.345	43.721
150	46.706	46.727	43.350	47.303	46.379	43.755
175	46.743	46.768	43.390	47.341	46.420	43.795
200	46.787	46.815	43.436	47.385	46.468	43.841
225	46.837	46.869	43.489	47.435	46.522	43.893
250	46.894	46.930	43.548	47.491	46.583	43.953
R^2				1.000	1.000	1.000
MSE				0.358	0.120	0.164
RMSE				0.598	0.347	0.404
MAE				0.598	0.347	0.404

Table S19. Calculated and fitted Shannon entropy values applying this sum rule in Eqs. (10) and (11) for doubly and triply fluorine-substituted benzoic acid derivatives under external electric filed along y axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-F	3,5-F	3,4,5-F	Fitted 3,4-F	Fitted 3,5-F	Fitted 3,4,5-F
-250	46.852	46.840	43.455	47.452	46.492	43.860
-225	46.799	46.789	43.407	47.399	46.441	43.812
-200	46.753	46.745	43.364	47.352	46.397	43.769
-175	46.713	46.707	43.328	47.312	46.360	43.733
-150	46.680	46.675	43.298	47.278	46.328	43.702
-125	46.652	46.649	43.273	47.250	46.302	43.677
-100	46.630	46.628	43.253	47.228	46.281	43.657
-75	46.614	46.613	43.239	47.211	46.267	43.643
-50	46.602	46.604	43.230	47.200	46.257	43.634
-25	46.597	46.600	43.227	47.194	46.253	43.631
0	46.596	46.602	43.228	47.194	46.255	43.632
25	46.601	46.608	43.235	47.198	46.262	43.639
50	46.611	46.621	43.247	47.209	46.274	43.652
75	46.627	46.639	43.265	47.224	46.292	43.669
100	46.648	46.662	43.288	47.245	46.315	43.692
125	46.674	46.691	43.316	47.271	46.345	43.721
150	46.706	46.727	43.350	47.303	46.379	43.755
175	46.743	46.768	43.390	47.341	46.420	43.795
200	46.787	46.815	43.436	47.385	46.468	43.841
225	46.837	46.869	43.489	47.435	46.522	43.893
250	46.894	46.930	43.548	47.491	46.583	43.953
R^2				0.998	0.998	1.000
MSE				0.357	0.121	0.163
RMSE				0.597	0.348	0.403
MAE				0.597	0.348	0.403

Table S20. Calculated and fitted Shannon entropy values applying this sum rule in Eqs. (10) and (11) for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along x axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	65.917	65.985	72.124	64.655	63.236	69.470
-225	65.853	65.910	72.047	64.597	63.168	69.404
-200	65.798	65.846	71.981	64.547	63.109	69.346
-175	65.750	65.790	71.924	64.503	63.058	69.296
-150	65.711	65.744	71.876	64.467	63.016	69.254
-125	65.678	65.706	71.837	64.437	62.981	69.219
-100	65.653	65.676	71.806	64.414	62.954	69.192
-75	65.634	65.654	71.783	64.397	62.933	69.172
-50	65.622	65.639	71.767	64.386	62.920	69.158
-25	65.617	65.632	71.760	64.382	62.914	69.152
0	65.618	65.632	71.760	64.383	62.914	69.152
25	65.625	65.640	71.767	64.391	62.922	69.160
50	65.639	65.655	71.783	64.405	62.936	69.174
75	65.660	65.678	71.806	64.425	62.958	69.195
100	65.687	65.708	71.837	64.451	62.986	69.223
125	65.721	65.746	71.876	64.484	63.022	69.258
150	65.762	65.793	71.923	64.523	63.065	69.301
175	65.810	65.848	71.980	64.569	63.117	69.352
200	65.865	65.912	72.045	64.623	63.176	69.410
225	65.929	65.985	72.121	64.683	63.245	69.478
250	66.001	66.069	72.206	64.753	63.323	69.555
R^2				0.998	1.000	0.999
MSE				1.542	7.443	6.882
RMSE				1.242	2.728	2.623
MAE				1.242	2.728	2.623

Table S21. Calculated and fitted Shannon entropy values applying this sum rule in Eqs. (10) and (11) for doubly and triply cyano-substituted benzoic acid derivatives under external electric filed along y axis. Also shown are statistical analysis results in the bottom four rows of the table.

EF	3,4-CN	3,5-CN	3,4,5-CN	Fitted 3,4-CN	Fitted 3,5-CN	Fitted 3,4,5-CN
-250	65.917	65.985	72.124	64.655	63.236	69.470
-225	65.853	65.910	72.047	64.597	63.168	69.404
-200	65.798	65.846	71.981	64.547	63.109	69.346
-175	65.750	65.790	71.924	64.503	63.058	69.296
-150	65.711	65.744	71.876	64.467	63.016	69.254
-125	65.678	65.706	71.837	64.437	62.981	69.219
-100	65.653	65.676	71.806	64.414	62.954	69.192
-75	65.634	65.654	71.783	64.397	62.933	69.172
-50	65.622	65.639	71.767	64.386	62.920	69.158
-25	65.617	65.632	71.760	64.382	62.914	69.152
0	65.618	65.632	71.760	64.383	62.914	69.152
25	65.625	65.640	71.767	64.391	62.922	69.160
50	65.639	65.655	71.783	64.405	62.936	69.174
75	65.660	65.678	71.806	64.425	62.958	69.195
100	65.687	65.708	71.837	64.451	62.986	69.223
125	65.721	65.746	71.876	64.484	63.022	69.258
150	65.762	65.793	71.923	64.523	63.065	69.301
175	65.810	65.848	71.980	64.569	63.117	69.352
200	65.865	65.912	72.045	64.623	63.176	69.410
225	65.929	65.985	72.121	64.683	63.245	69.478
250	66.001	66.069	72.206	64.753	63.323	69.555
R^2				1.000	0.998	1.000
MSE				1.523	7.401	6.788
RMSE				1.234	2.720	2.605
MAE				1.234	2.720	2.605

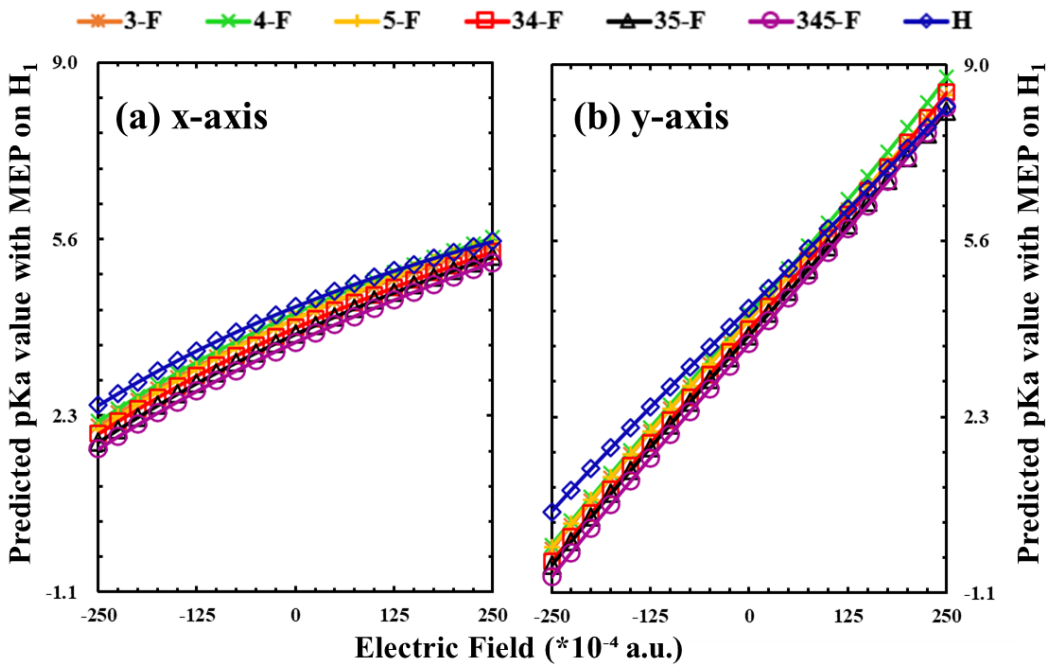

Figure S1. Profiles of calculated pK_a values using MEP from H_1 in Scheme 1 for fluorine-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis.

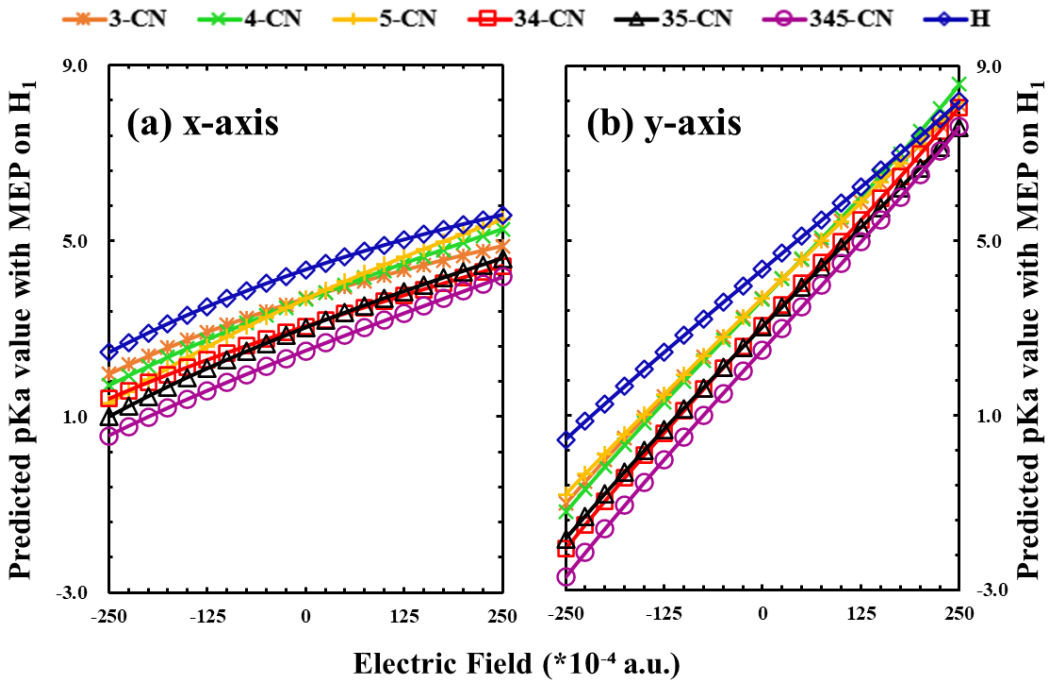

Figure S2. Profiles of calculated pK_a values using MEP from H_1 in Scheme 1 for cyano-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis.

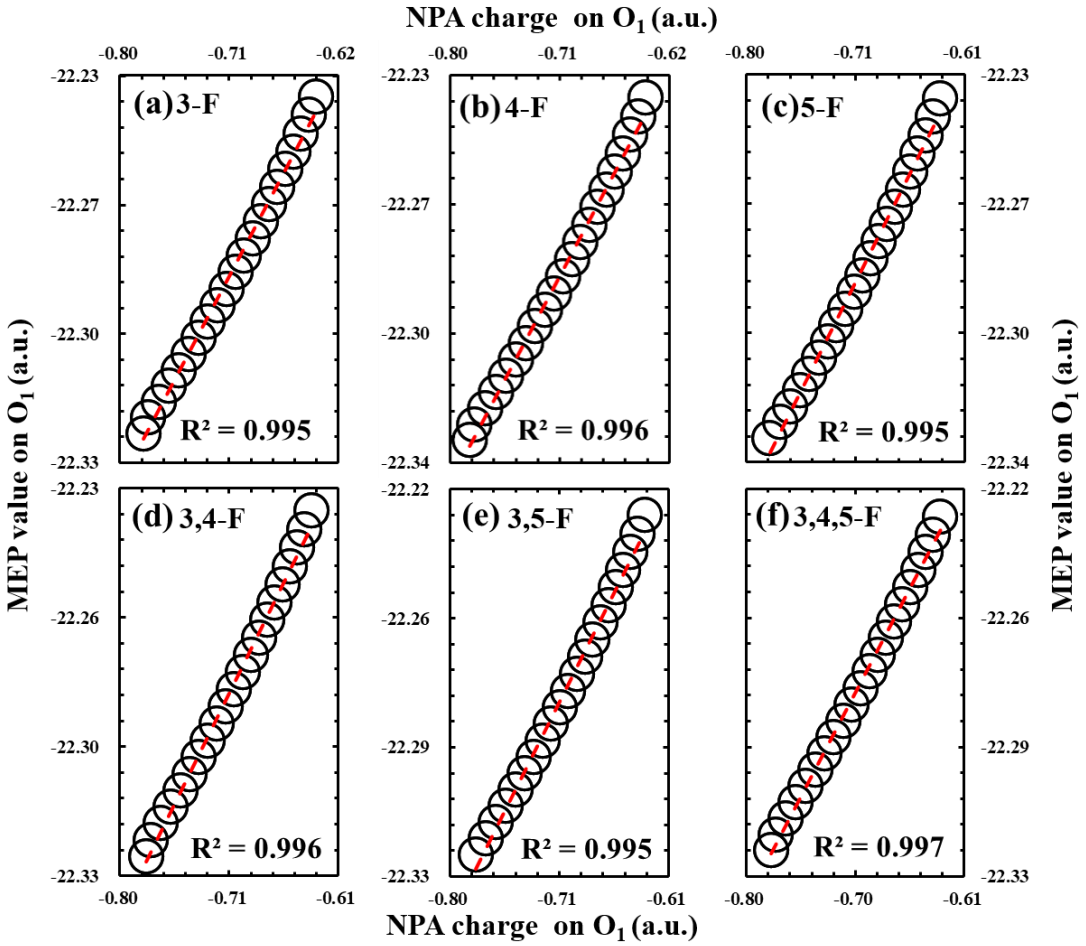

Figure S3. Strong linear correlations of MEP values with NPA partial charges on O_1 in Scheme 1 for fluorine-substituted benzoic acid derivatives for when the external electric field is applied to x-axis.

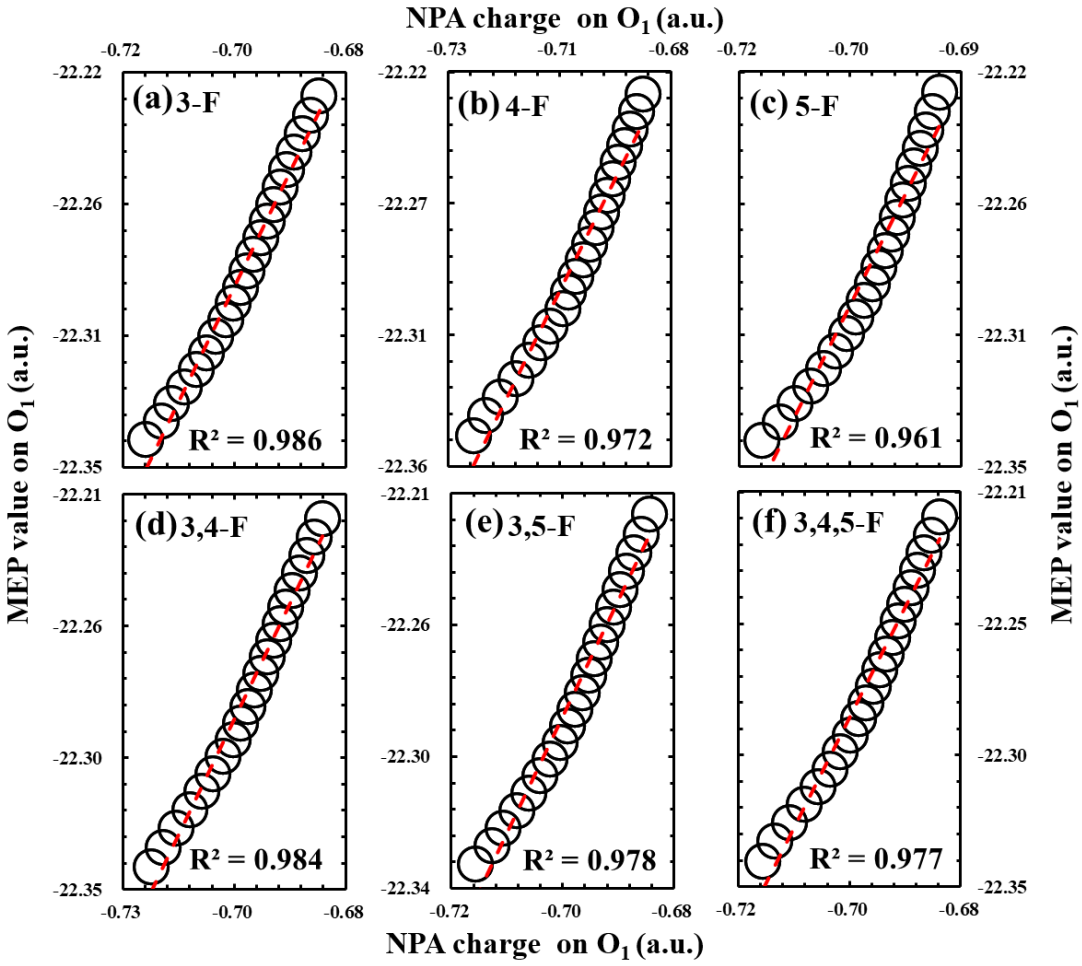

Figure S4. Strong linear correlations of MEP values with NPA partial charges on O_1 in Scheme 1 for fluorine-substituted benzoic acid derivatives for when the external electric field is applied to y-axis.

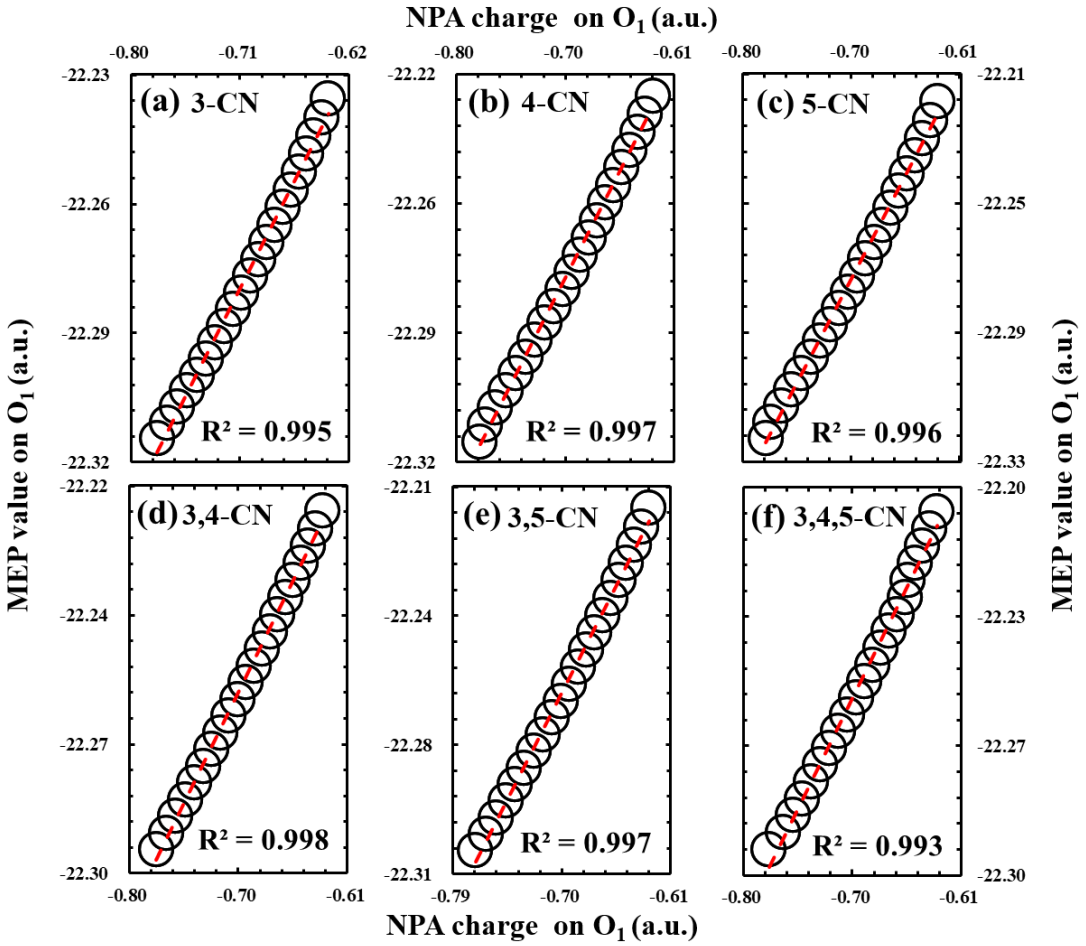

Figure S5. Strong linear correlations of MEP values with NPA partial charges on O_1 in Scheme 1 for cyano-substituted benzoic acid derivatives for when the external electric field is applied to x-axis.

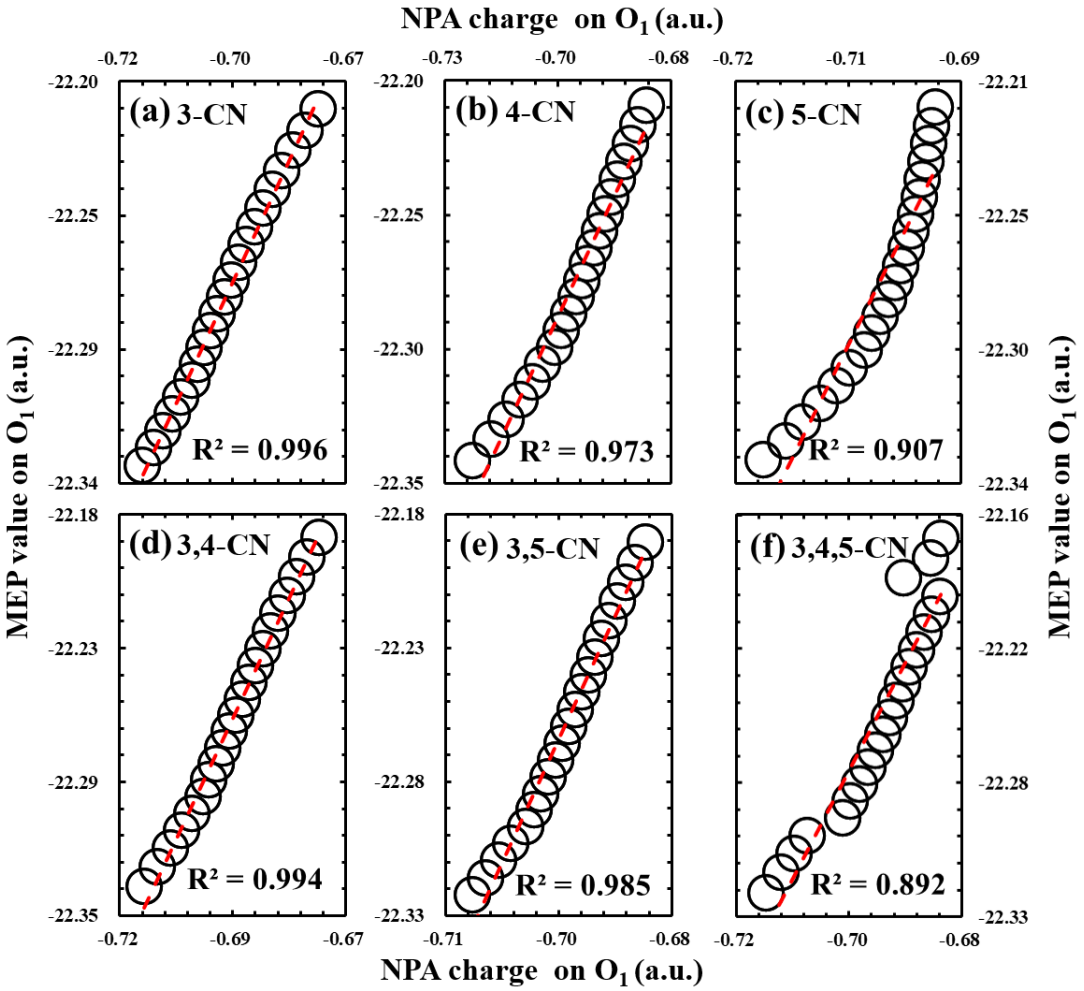

Figure S6. Strong linear correlations of MEP values with NPA partial charges on O_1 in Scheme 1 for cyano-substituted benzoic acid derivatives for when the external electric field is applied to y-axis.

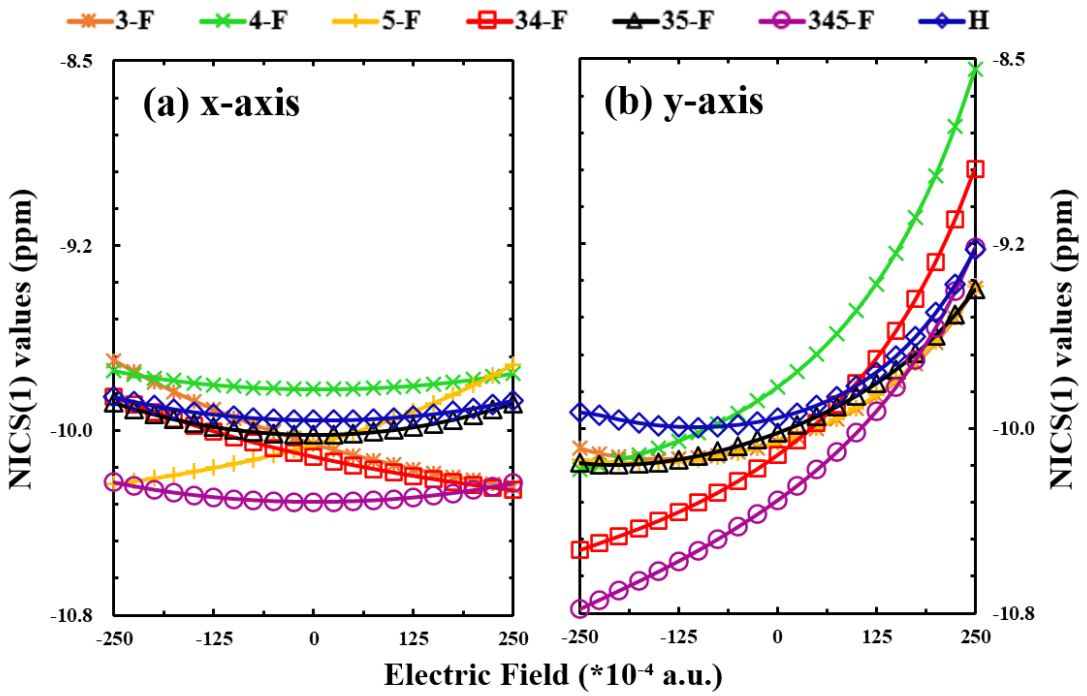

Figure S7. Profiles of the calculated aromaticity index, NICS(1), for singly, doubly, and triply fluorine-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis.

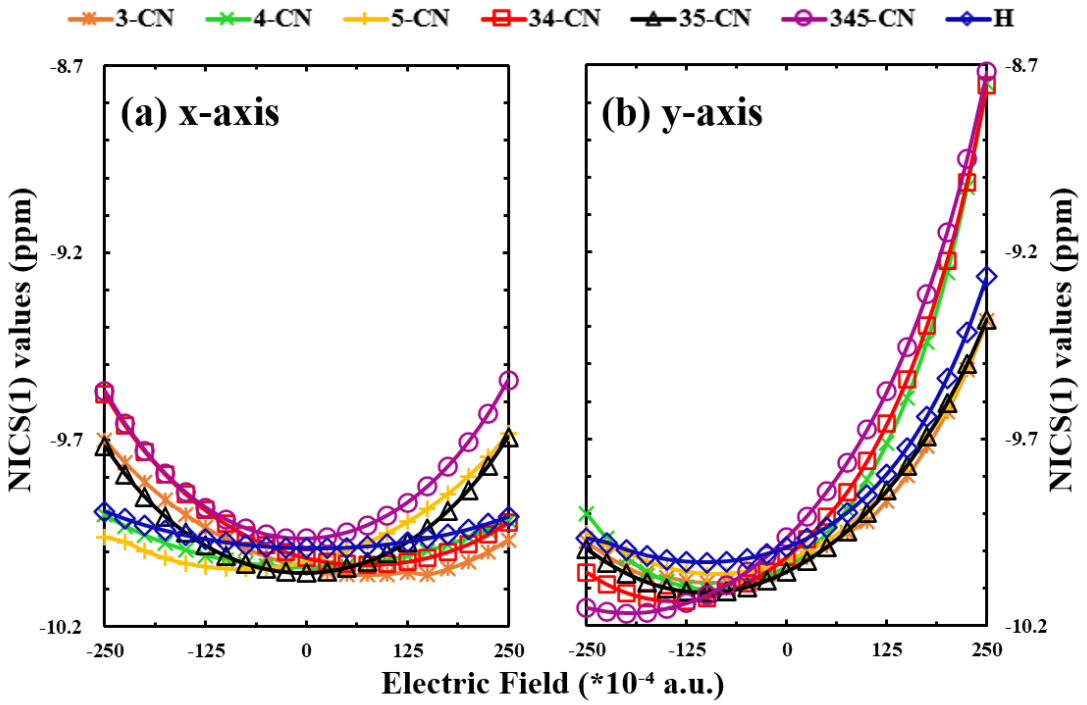

Figure S8. Profiles of the calculated aromaticity index, NICS(1), for singly, doubly, and triply cyano-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis.

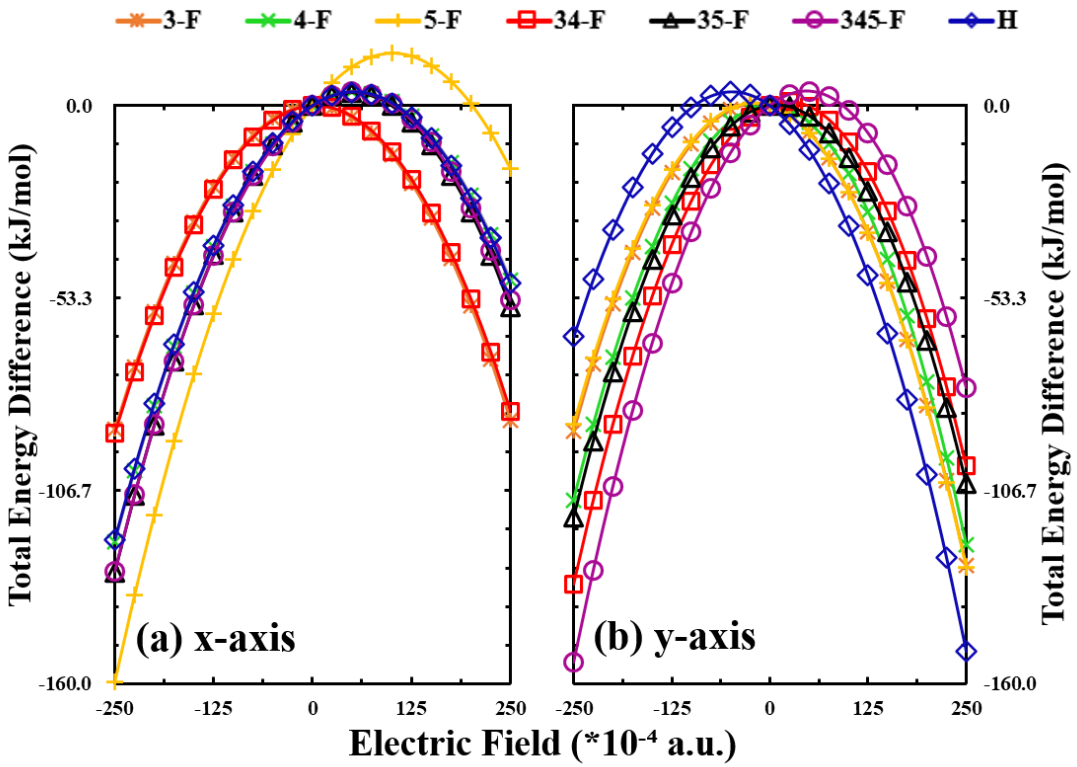

Figure S9. Profiles of the total energy change for singly, doubly, and triply fluorine-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis. The reference is the zero electric field.

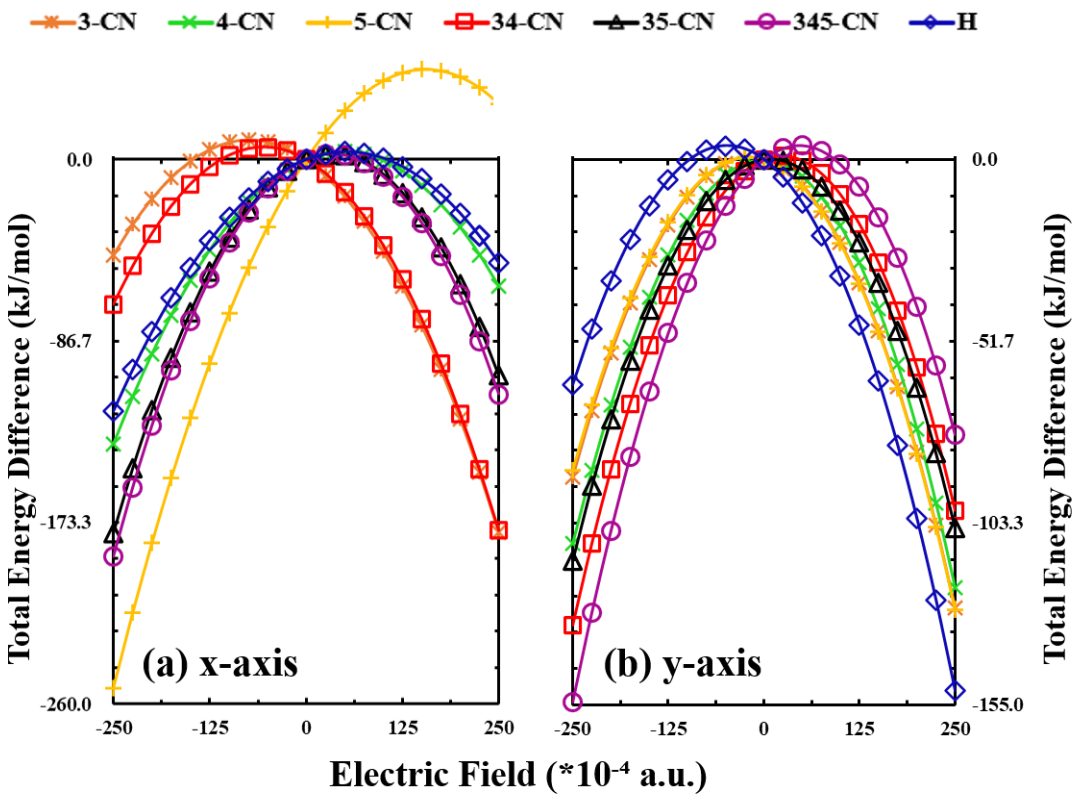

Figure S10. Profiles of the total energy change for singly, doubly, and triply cyano-substituted benzoic acid derivatives as a function of the strength of the applied external electric field along (a) x-axis; and (b) y-axis. The reference is the zero electric field.

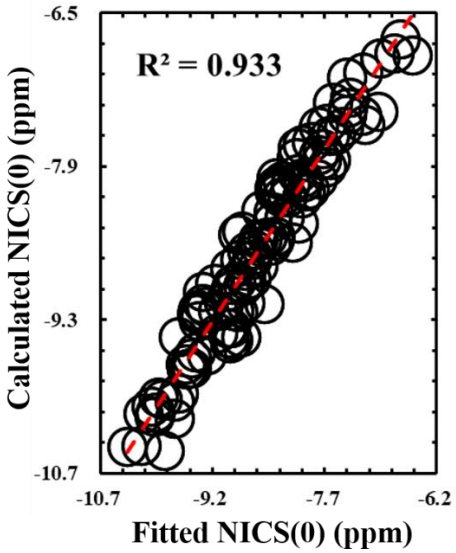

Figure S11. Strong linear correlations of calculated and fitted NICS(0) values for doubly and triply substituted benzoic acid derivatives with no external electric field applied. The fitted NICS(0) values were obtained using Eqs. (10) and (11) with $a_{m1}=a_{m2}=0.9$ and $a_p=1.0$.