Supplementary Materials: Linear Response Function of Bond-Order

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1. Linear Response Function of Bond-Order

Now we move on to the definition of linear response function of bond-order. As for the bond-order, we employ the Mayer bond order [1], the most standard definition of the bond-order in the field of ab initio quantum chemistry, which is defined as,

$$\mathbf{B}^{\mathrm{IJ}} \equiv \sum_{\mu}^{\mathrm{I}} \sum_{\nu}^{\mathrm{J}} \mathbf{Q}_{\mu\nu} \mathbf{Q}_{\nu\mu} . \tag{1}$$

The two summations of basis sets' indices, μ and ν, run over the I-th atom and the J-th atom, respectively and the matrix, **Q,** is the product of the density matrix (**P**) and the overlap matrix (**S**),

$$\mathbf{Q}_{\mu\nu} \equiv \sum_{\eta} \mathbf{P}_{\mu\eta} \mathbf{S}_{\eta\nu} . \tag{2}$$

From Equation (3), we have an expression for the linear response function of the **Q** matrix as

$$\frac{\delta \mathbf{Q}_{\mu\nu}}{\delta \mathrm{v}(\mathbf{r})} = \sum_{\sigma}^{\alpha,\beta} \sum_{ij} \frac{\psi_j^{\sigma}(\mathbf{r}) \psi_i^{\sigma}(\mathbf{r})}{\varepsilon_i^{\sigma} - \varepsilon_j^{\sigma}} \sum_{\eta} (C_{j\mu}^{\sigma} C_{i\eta}^{\sigma} + C_{i\mu}^{\sigma} C_{j\eta}^{\sigma}) \mathbf{S}_{\eta\nu} . \tag{3}$$

Finally, the linear response function of the bond-order can then be defined as

$$\delta \mathbf{B}^{\mathrm{IJ}} / \delta \mathrm{v}(\mathbf{r}) \equiv \sum_{\mu}^{\mathrm{I}} \sum_{\nu}^{\mathrm{J}} \left(\frac{\delta \mathbf{Q}_{\mu\nu}}{\delta \mathrm{v}(\mathbf{r})} \mathbf{Q}_{\nu\mu} + \mathbf{Q}_{\mu\nu} \frac{\delta \mathbf{Q}_{\nu\mu}}{\delta \mathrm{v}(\mathbf{r})} \right) . \tag{4}$$

It is convenient to consider perturbations that are applied to atomic sites. For this purpose, we define the LRF-BO for the local perturbation, $\delta \mathrm{v}(\xi)$, that is applied to a specific atomic orbital ϕ_{ξ} via the following relation,

$$\sum_{\xi} \frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\xi)} \equiv \int d\mathbf{r} \frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\mathbf{r})} \tag{5}$$

and we then have an expression of LRF-BO for the perturbation to an L-th atom,

$$\frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\mathrm{L})} \equiv \sum_{\xi}^{\mathrm{L}} \frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\xi)} . \tag{6}$$

Here, the summation, $\sum_{\xi}$, at the left side of Equation (8) runs over all AOs, and that at the right side of Equation (9), $\sum_{\xi}^{\mathrm{L}}$ is limited to the AOs that belong to the L-th atom. This is the scheme we employed in reference [2], which is the first implementation of the LRF-BO. The LRF-BO based on AO perturbations (Equation (8)) suits the linear combination of AOs (LCAO) formalism: for instance, we easily see the LRF-BO for the case that the perturbation is applied to a π orbital at a specific carbon atom in a π-conjugated system. However, when we would like to see the effects due to a nucleophilic or electrophilic attack to a specific atom, it is unclear whether the perturbation, $\delta \mathrm{v}(\xi)$, is attractive or repulsive since atomic orbitals except 1s orbitals have different (positive and negative) phases' parts in their distributions. To avoid such ambiguity, we here define $\delta \mathbf{B}^{\mathrm{IJ}} / \delta \mathrm{v}(\mathrm{L})$ using a numerical integration

$$\frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\mathrm{L})} \equiv \int^{\mathrm{L}} d\mathbf{r} \frac{\delta \mathbf{B}^{\mathrm{IJ}}}{\delta \mathrm{v}(\mathbf{r})}, \tag{7}$$

where the domain of integration for the L-th atom at the left side is defined as the Wigner-Seitz cell. The Wigner-Seitz cell for molecular systems is constructed in a similar manner to that of solid

systems: the region for a specific atom in the molecule can be defined as a region encircled by all perpendicular bisectors with neighboring atoms (See Figure S1).

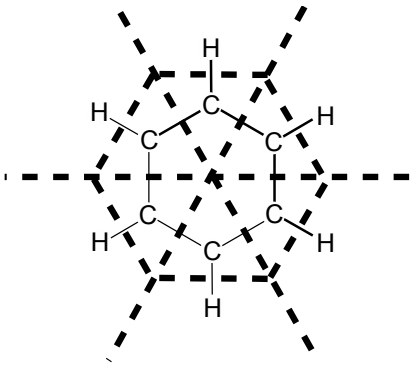


Figure S1. An example of Wigner-Seitz cells for molecular systems (C_6H_6). The region for each atom is defined as the region encircled by dashed spaced lines. For the terminal atoms (in this case, 6 hydrogens), the regions spread to infinity.

2. Computational Results

2.1. Inductive and Resonance Effects of Organic Molecules

The responses on all carbons ($\delta\rho(2)$~ $\delta\rho(7)$) for hexan-1-ol and hexa-1,3,5-trien-1-ol are plotted in Figure 6a (to be complete, we present all the LRF-D values in Tables S1–S3 in supplementary materials for hexan-1-ol, hexa-1,3,5-trien-1-ol, and π contributions of hexa-1,3,5- trien-1-ol, respectively). We can see from this figure that the response of hexan-1-ol decreases monotonically and rapidly from the nearest site to the farthest site, being consistent with the picture of the inductive effect of the saturated system. This contrasts with the response on the conjugated chain of hexa-1,3,5-trien-1-ol, which also decays from $\delta\rho(2)$ to $\delta\rho(7)$ but with the oscillating behavior. To analyze the behavior of the LRF-D values further, we divided the LRF-D values into σ and π contributions according to the method Fias et al. used [3]. The results are shown in Figure 6b. This figure shows that the σ contribution of the LRF-D of hexa-1,3,5-trien-1-ol is similar to that of hexan-1-ol. In particular, we found that the plus value of $\delta\rho(2)/\delta v(1)$ of hexa-1,3,5-trien-1-ol is a result of the inductive effect mainly from the σ contribution. On the other hand, being maximum at $\{\delta\rho(n)/\delta v(1)\}_{n=3,5,7}$ of the π contribution obviously corresponds to the resonance picture of the π conjugated network (see Figure 6a below), implying that LRF-D becomes an indicator of density fluctuations that are results from inductive and resonance effects of organic molecules. These results are similar to those of reference [3], indicating that our numerical treatment is valid for our purposes.

We then evaluated the LRF-BO values of all chemical bonds on the main chain for the perturbation, $\delta v(1)$. Figure 7a shows the LRF-BO values for the chemical bonds of the main chains of the hexan-1-ol and hexa-1,3,5-trien-1-ol (all calculated LRF-BO values are presented in Tables S4–S6 in supplementary materials for hexan-1-ol, hexa-1,3,5-trien-1-ol, and π contributions of hexa-1,3,5- trien-1-ol, respectively). It is found from Figure 7a that the fluctuation of bond-orders of the hexan-1-ol molecule is nearly localized in the bond between O(1) and C(2). In contrast, the profile of the LRF-BO values of hexa-1,3,5-trien-1-ol, in which points are indicated as squares, exhibits a oscillating behavior. As in the case of LRF-D values, we divide the LRF-BO values of the hexa-1,3,5-trien-1-ol into σ and π contributions, which are shown in Figure 7b. We can see from this figure that the σ contribution indicated by the X points shows the behavior similar to that of the hexan-1-ol molecule shown in Figure 7a, while the π contribution indicated by the triangular points is obviously a main cause of the oscillating behavior of the total LRF-BO values.

2.2. Acid Dissociation Reaction of Substituted Benzoic Acids

For completeness, we also examined the correlation between the Hammett constants and the LRF-BO values for the perturbation on each atom in benzoic acids and presented the resulting coefficients of determination in Figure S2a,b for meta- and para- substituted benzoic acids respectively, in the supplementary materials. Also, we listed all LRF-BO values of meta and para substituted benzoic acids in Tables S7 and S8 respectively. Surprisingly, in some of the cases that the virtual perturbation is applied to atoms in the phenyl part, we obtained large coefficients of determination values. Nevertheless, from Tables S7 and S8, the magnitudes of the LRF-BO values are found to be considerably small for such cases. This implies that although the bond-order between O and H in the carboxylate is remarkably sensitive to the perturbation at O(14) and H(15) in the carboxylate part, the description of substitution effects are affected by the perturbation not only of the O(14) and H(15) part, but also of the phenyl part because the induced and resonance effects work through the phenyl part. We also checked the bais set dependence of the results for 6-31G, 6-31G**, 6-31++G**, 6-311G, and 6-311++G**. See Tables S9–S18, and Figures S3–S6. A noteworthy point is that the use of diffuse functions (Figures S5 and S7) deteriorates the correlation between Hammett constants and LRF-BO values. This is due to a well-known fact that the Mulliken type of population analyses often fails when the diffuse function is used [4,5].

Table S1. All linear response function of density (LRF-D) values of hexan-1-ol at the B3LYP/6-311G** level. The numbering of the atoms listed is the same as presented in Figure 5a in the text.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**
1	−3.67	1.152	0.12	0.061	0.013	0.003	0.001	0.001	0.000	0.000	0.001	0.001	0.002	0.002	0.02	0.02	0.027	0.027	0.341	0.341	1.537
2	1.152	−4.865	0.879	0.101	0.05	0.015	0.003	0.002	0.000	0.000	0.001	0.001	0.011	0.011	0.033	0.033	0.173	0.173	0.991	0.991	0.242
3	0.12	0.879	−4.998	0.896	0.095	0.05	0.013	0.006	0.002	0.002	0.011	0.011	0.036	0.036	0.179	0.179	1.023	1.023	0.179	0.179	0.079
4	0.061	0.101	0.896	−5.062	0.896	0.095	0.048	0.025	0.011	0.011	0.037	0.037	0.176	0.176	1.023	1.023	0.176	0.176	0.035	0.035	0.027
5	0.013	0.05	0.095	0.896	−5.069	0.898	0.085	0.09	0.038	0.038	0.181	0.181	1.021	1.021	0.179	0.179	0.037	0.037	0.012	0.012	0.006
6	0.003	0.015	0.05	0.095	0.898	−5.056	0.851	0.219	0.197	0.197	1.038	1.038	0.176	0.176	0.038	0.038	0.011	0.011	0.001	0.001	0.002
7	0.001	0.003	0.013	0.048	0.085	0.851	−4.498	1.025	1.009	1.009	0.181	0.181	0.034	0.034	0.011	0.011	0.001	0.001	0.000	0.000	0.001
8	0.001	0.002	0.006	0.025	0.09	0.219	1.025	−1.987	0.288	0.288	−0.003	−0.003	0.021	0.021	0.002	0.002	0.001	0.001	0.000	0.000	0.000
9	0.000	0.000	0.002	0.011	0.038	0.197	1.009	0.288	−1.98	0.295	0.002	0.153	−0.001	−0.026	0.002	0.009	0.000	0.000	0.000	0.000	0.000
10	0.000	0.000	0.002	0.011	0.038	0.197	1.009	0.288	0.295	−1.98	0.153	0.002	−0.026	−0.001	0.009	0.002	0.000	0.000	0.000	0.000	0.000
11	0.001	0.001	0.011	0.037	0.181	1.038	0.181	−0.003	0.002	0.153	−2.003	0.27	0.149	0.003	−0.03	−0.001	0.002	0.009	0.000	0.000	0.000
12	0.001	0.001	0.011	0.037	0.181	1.038	0.181	−0.003	0.153	0.002	0.27	−2.003	0.003	0.149	−0.001	−0.03	0.009	0.002	0.000	0.000	0.000
13	0.002	0.011	0.036	0.176	1.021	0.176	0.034	0.021	−0.001	−0.026	0.149	0.003	−2.002	0.27	0.146	0.003	−0.001	−0.03	0.009	0.002	0.001
14	0.002	0.011	0.036	0.176	1.021	0.176	0.034	0.021	−0.026	−0.001	0.003	0.149	0.27	−2.002	0.003	0.146	−0.03	−0.001	0.002	0.009	0.001
15	0.02	0.033	0.179	1.023	0.179	0.038	0.011	0.002	0.002	0.009	−0.03	−0.001	0.146	0.003	−2.004	0.272	0.003	0.145	−0.031	0.000	0.003
16	0.02	0.033	0.179	1.023	0.179	0.038	0.011	0.002	0.009	0.002	−0.001	−0.03	0.003	0.146	0.272	−2.004	0.145	0.003	0.000	−0.031	0.003
17	0.027	0.173	1.023	0.176	0.037	0.011	0.001	0.001	0.000	0.000	0.002	0.009	−0.001	−0.03	0.003	0.145	−2.01	0.266	0.001	0.145	0.021
18	0.027	0.173	1.023	0.176	0.037	0.011	0.001	0.001	0.000	0.000	0.009	0.002	−0.03	−0.001	0.145	0.003	0.266	−2.01	0.145	0.001	0.021
19	0.341	0.991	0.179	0.035	0.012	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.009	0.002	−0.031	0.000	0.001	0.145	−1.962	0.27	0.008
20	0.341	0.991	0.179	0.035	0.012	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.009	0.000	−0.031	0.145	0.001	0.27	−1.962	0.008
21	1.537	0.242	0.079	0.027	0.006	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.003	0.003	0.021	0.021	0.008	0.008	−1.959

Table S2. All LRF−D values of hexa-1,3,5-trien-1-ol at the B3LYP/6-311G** level. The numbering of the atoms listed is the same as presented in Figure 5b in the text.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
1	−4.242	0.831	0.799	0.081	0.367	0.035	0.190	0.040	0.034	0.003	0.056	0.017	0.155	0.239	1.397
2	0.831	−7.088	2.847	0.135	1.013	0.086	0.502	0.103	0.089	0.008	0.153	0.029	0.569	0.521	0.203
3	0.799	2.847	−6.548	0.821	0.203	0.070	0.083	0.021	0.016	0.012	0.071	0.206	0.645	0.613	0.142
4	0.081	0.135	0.821	−7.012	2.865	0.221	1.021	0.217	0.183	0.050	0.554	0.597	0.191	0.053	0.024
5	0.367	1.013	0.203	2.865	−7.035	0.786	0.069	0.075	0.057	0.199	0.582	0.557	0.046	0.169	0.048
6	0.035	0.086	0.070	0.221	0.786	−6.595	3.063	0.684	0.685	0.668	0.190	0.076	0.013	0.013	0.005
7	0.190	0.502	0.083	1.021	0.069	3.063	−6.829	0.521	0.517	0.574	0.026	0.150	0.007	0.082	0.024
8	0.040	0.103	0.021	0.217	0.075	0.684	0.521	−1.990	0.154	0.104	0.018	0.031	0.002	0.016	0.005
9	0.034	0.089	0.016	0.183	0.057	0.685	0.517	0.154	−1.993	0.238	−0.033	0.032	0.002	0.015	0.004
10	0.003	0.008	0.012	0.050	0.199	0.668	0.574	0.104	0.238	−1.972	0.143	−0.041	0.009	0.002	0.000
11	0.056	0.153	0.071	0.554	0.582	0.190	0.026	0.018	−0.033	0.143	−1.994	0.228	−0.031	0.029	0.008
12	0.017	0.029	0.206	0.597	0.557	0.076	0.150	0.031	0.032	−0.041	0.228	−1.983	0.139	−0.040	0.003
13	0.155	0.569	0.645	0.191	0.046	0.013	0.007	0.002	0.002	0.009	−0.031	0.139	−2.015	0.223	0.044
14	0.239	0.521	0.613	0.053	0.169	0.013	0.082	0.016	0.015	0.002	0.029	−0.040	0.223	−1.915	−0.021
15	1.397	0.203	0.142	0.024	0.048	0.005	0.024	0.005	0.004	0.000	0.008	0.003	0.044	−0.021	−1.886

Table S3. π contributions of LRF-D values of hexa-1,3,5-trien-1-ol at the B3LYP/6-311G** level. The numbering of the atoms listed is the same as presented in Figure 5b in the text.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
1	−1.45	−0.108	0.698	0.032	0.358	0.034	0.19	0.04	0.034	0.004	0.054	−0.002	0.128	−0.062	0.054
2	−0.108	−3.86	2.188	0.018	0.984	0.078	0.5	0.102	0.088	0.008	0.142	−0.008	0.402	−0.512	−0.02
3	0.698	2.188	−3.272	−0.02	0.1	0.026	0.076	0.018	0.014	0.002	0.02	0.036	−0.43	0.46	0.084
4	0.032	0.018	−0.02	−3.676	2.188	0.114	0.994	0.202	0.174	0.006	0.398	−0.47	0.028	0.006	0.004
5	0.358	0.984	0.1	2.188	−3.698	−0.06	−0.024	−0.004	0.002	0.028	−0.484	0.404	0.004	0.158	0.044
6	0.034	0.078	0.026	0.114	−0.06	−3.268	2.43	0.49	0.512	−0.416	0.024	0.018	0.004	0.012	0.004
7	0.19	0.5	0.076	0.994	−0.024	2.43	−3.756	−0.54	−0.528	0.418	−0.012	0.14	0.006	0.082	0.024
8	0.04	0.102	0.018	0.202	−0.004	0.49	−0.54	−0.282	−0.152	0.08	−0.002	0.028	0.002	0.016	0.004
9	0.034	0.088	0.014	0.174	0.002	0.512	−0.528	−0.152	−0.28	0.096	−0.004	0.02	0.002	0.014	0.004
10	0.004	0.008	0.002	0.006	0.028	−0.416	0.418	0.08	0.096	−0.24	0.016	−0.004	0.000	0.002	0.000
11	0.054	0.142	0.02	0.398	−0.484	0.024	−0.012	−0.002	−0.004	0.016	−0.272	0.092	0.000	0.02	0.006
12	−0.002	−0.008	0.036	−0.47	0.404	0.018	0.14	0.028	0.02	−0.004	0.092	−0.262	0.018	−0.006	0.000
13	0.128	0.402	−0.43	0.028	0.004	0.004	0.006	0.002	0.002	0.000	0.000	0.018	−0.272	0.098	0.016
14	−0.062	−0.512	0.46	0.006	0.158	0.012	0.082	0.016	0.014	0.002	0.02	−0.006	0.098	−0.268	−0.018
15	0.054	−0.02	0.084	0.004	0.044	0.004	0.024	0.004	0.004	0.000	0.006	0.000	0.016	−0.018	−0.208

Table S4. The LRF-BO values, $\left\{\delta B^{IJ}/\delta v(K)\right\}$, of hexan-1-ol at the B3LYP/6-311G** level. The numbering of the atoms is the same as presented in Figure 5a in the text.

IJ of δB^{IJ}		The Site Which the Perturbation Is Applied to (K of $\delta v(K)$)																				
I	J	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	2	2.440	−1.186	−0.135	−0.049	−0.017	−0.004	−0.001	0.000	0.000	0.000	−0.001	−0.001	−0.003	−0.003	−0.024	−0.024	−0.006	−0.006	−0.632	−0.632	0.283	0.023
2	3	−0.057	0.064	0.029	0.052	−0.008	−0.006	−0.002	0.001	−0.001	−0.001	0.002	0.002	−0.009	−0.009	0.086	0.086	−0.103	−0.103	0.013	0.013	−0.048	0.023
3	4	−0.061	0.055	−0.058	0.089	0.042	−0.006	−0.006	−0.015	0.003	0.003	−0.009	−0.009	0.098	0.098	−0.107	−0.107	−0.118	−0.118	0.116	0.116	−0.002	0.030
4	5	0.002	−0.006	0.040	0.068	−0.002	0.041	−0.009	−0.044	−0.022	−0.022	0.104	0.104	−0.105	−0.105	−0.106	−0.106	0.100	0.100	−0.007	−0.007	-0.019	0.030
5	6	−0.004	−0.008	−0.008	0.029	0.043	0.060	0.065	−0.176	0.089	0.089	−0.027	−0.027	−0.145	−0.145	0.089	0.089	−0.009	−0.009	0.004	0.004	−0.004	0.237
6	7	0.000	−0.003	−0.008	−0.012	−0.012	0.037	−0.067	0.169	0.019	0.019	−0.147	−0.147	0.086	0.086	−0.011	−0.011	0.001	0.001	0.000	0.000	−0.001	0.237
1	21	1.400	0.144	0.037	0.011	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.003	0.011	0.011	0.062	0.062	−1.748	0.003
2	19	−0.224	0.438	0.029	0.002	0.001	0.000	0.000	0.000	0.000	0.000	−0.001	0.000	0.002	0.001	0.014	0.000	0.051	0.003	−0.380	0.056	0.007	0.001
2	20	−0.224	0.438	0.029	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.000	−0.001	0.001	0.002	0.000	0.014	0.003	0.051	0.056	−0.380	0.007	0.001
3	17	−0.003	0.043	0.564	0.036	0.004	0.002	0.000	0.001	0.000	0.000	0.001	0.001	0.000	0.006	0.029	0.005	−0.762	0.067	0.029	−0.011	−0.013	0.004
3	18	−0.003	0.043	0.564	0.036	0.004	0.002	0.000	0.001	0.000	0.000	0.001	0.001	0.006	0.000	0.005	0.029	0.067	−0.762	−0.011	0.029	−0.013	0.004
4	16	−0.006	0.003	0.031	0.479	0.029	0.001	0.001	0.004	0.000	0.002	0.000	0.004	0.026	−0.007	0.040	−0.634	0.000	0.023	0.001	0.003	0.001	0.003
7	8	0.000	0.000	0.000	−0.001	0.017	0.050	0.440	−0.702	0.034	0.034	0.055	0.055	0.007	0.007	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.755
7	9	0.000	0.000	0.000	0.002	0.005	0.043	0.455	0.041	−0.649	0.051	0.047	−0.013	0.004	0.012	0.002	0.002	−0.001	0.000	0.000	0.000	0.000	0.113
7	10	0.000	0.000	0.000	0.002	0.005	0.043	0.455	0.041	0.051	−0.649	−0.013	0.047	0.012	0.004	0.002	0.002	0.000	−0.001	0.000	0.000	0.000	0.014
4	15	−0.006	0.003	0.031	0.479	0.029	0.001	0.001	0.004	0.002	0.000	0.004	0.000	−0.007	0.026	−0.634	0.040	0.023	0.000	0.003	0.001	0.001	0.013
5	13	0.001	0.001	0.003	0.030	0.490	0.029	0.002	−0.004	0.000	0.002	0.003	0.020	−0.644	0.039	−0.003	0.029	0.000	0.001	0.000	0.002	0.001	0.002
5	14	0.001	0.001	0.003	0.030	0.490	0.029	0.002	−0.004	0.002	0.000	0.020	0.003	0.039	−0.644	0.029	−0.003	0.001	0.000	0.002	0.000	0.001	0.002
6	11	0.000	0.000	0.002	0.003	0.031	0.486	0.029	0.022	0.005	0.015	−0.669	0.035	−0.005	0.033	0.009	0.001	0.002	0.001	−0.001	0.000	0.000	0.001
6	12	0.000	0.000	0.002	0.003	0.031	0.486	0.029	0.022	0.015	0.005	0.035	−0.669	0.033	−0.005	0.001	0.009	0.001	0.002	0.000	−0.001	0.000	0.002

Table S5. LRF-BO values, $\left\{\delta B^{IJ}/\delta v(K)\right\}$, of hexa-1,3,5-trien-1-ol at the B3LYP/6-311G** level. The numbering of the atoms is the same as presented in Figure 5b in the text.

IJ of δB^{IJ}		The Site Which the Perturbation Is Applied to (K of $\delta v(K)$)														
I	J	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2	3.285	−0.589	−1.381	−0.070	−0.550	−0.047	−0.281	−0.056	−0.050	−0.004	−0.081	−0.014	−0.237	−0.219	0.293
2	3	−1.072	−0.396	0.612	0.285	0.388	0.060	0.232	0.065	0.049	0.010	0.022	0.122	0.013	0.041	−0.432
3	4	0.121	0.456	0.091	−0.171	−0.164	−0.078	−0.142	−0.031	−0.010	−0.083	0.000	−0.027	−0.042	0.088	−0.008
4	5	−0.165	−0.245	−0.003	−0.013	0.365	0.347	0.131	0.056	−0.043	0.097	−0.179	−0.230	−0.004	−0.078	−0.034
5	6	0.064	0.107	0.020	0.324	−0.145	−0.023	0.140	−0.298	−0.131	−0.063	−0.098	0.128	−0.060	0.024	0.010
6	7	−0.057	−0.090	−0.048	−0.187	0.046	0.030	0.446	0.160	−0.002	−0.287	0.046	−0.038	−0.003	−0.010	−0.006
1	15	1.397	0.169	0.062	0.010	0.019	0.002	0.010	0.002	0.002	0.000	0.003	0.003	0.020	0.075	−1.774
2	14	−0.098	0.371	0.030	−0.008	0.022	0.002	0.010	0.002	0.002	0.002	0.004	−0.035	−0.036	−0.494	0.227
3	13	0.060	0.126	0.437	0.022	0.002	0.003	0.000	0.000	0.001	−0.003	0.022	−0.031	−0.590	−0.030	−0.017
4	12	−0.004	−0.001	0.004	0.346	0.063	0.000	0.021	0.004	−0.005	−0.007	−0.032	−0.394	−0.034	0.039	0.000
5	11	0.006	0.021	0.001	0.066	0.350	0.005	0.001	−0.009	0.053	−0.038	−0.412	−0.026	−0.017	−0.003	0.002
6	10	0.000	−0.001	0.002	0.000	−0.009	0.327	0.053	0.106	0.013	−0.472	−0.029	0.007	0.001	0.001	0.000
7	8	0.004	0.012	0.003	0.025	0.016	0.108	0.328	−0.766	0.130	0.115	0.009	0.012	0.002	0.002	0.001
7	9	0.004	0.010	0.002	0.023	−0.006	0.064	0.379	0.181	−0.629	−0.022	−0.021	0.010	0.003	0.001	0.000

Table S6. π contributions of LRF-BO values, $\left\{\delta B^{IJ}/\delta v(K)\right\}$, of hexa-1,3,5-trien-1-ol at the B3LYP/6-311G** level. The numbering of the atom pair listed is the same as presented in Figure 5b in the text.

IJ of δB^{IJ}		The Site Which the Perturbation Is Applied to (K of $\delta v(K)$)														
I	J	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2	1.605	0.639	−1.275	−0.041	−0.544	−0.045	−0.280	−0.057	−0.050	−0.005	−0.076	0.010	−0.292	0.208	0.203
2	3	−1.079	−0.610	0.585	0.199	0.401	0.067	0.233	0.059	0.047	−0.001	0.134	−0.046	0.095	0.016	−0.101
3	4	0.197	0.328	0.031	−0.112	−0.225	−0.054	−0.131	−0.037	−0.027	0.013	−0.161	0.097	0.135	−0.073	0.018
4	5	−0.169	−0.229	−0.131	−0.236	0.207	0.205	0.168	0.087	0.119	−0.044	0.092	0.026	−0.131	0.055	−0.020
5	6	0.059	0.109	0.031	0.258	−0.126	−0.202	−0.039	−0.084	−0.147	0.074	0.092	−0.064	0.018	0.013	0.007
6	7	−0.059	−0.090	−0.044	−0.175	0.013	−0.197	0.263	0.184	0.239	−0.078	−0.087	0.059	−0.011	−0.010	−0.007
1	15	0.177	0.016	0.034	0.002	0.018	0.002	0.009	0.002	0.002	0.000	0.003	0.000	0.006	−0.004	−0.266
2	14	−0.006	−0.034	0.058	0.000	0.020	0.001	0.010	0.002	0.002	0.000	0.003	0.000	0.009	−0.066	0.000
3	13	0.015	0.056	−0.019	0.007	−0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.001	−0.068	0.009	0.002
4	12	−0.001	−0.004	0.006	−0.026	0.052	0.002	0.017	0.003	0.003	0.000	0.008	−0.061	0.000	0.000	0.000
5	11	0.007	0.018	0.002	0.052	−0.026	0.006	−0.004	−0.001	0.000	0.001	−0.065	0.008	0.001	0.003	0.001
6	10	0.000	−0.001	0.000	−0.002	0.006	−0.020	0.054	0.009	0.009	−0.056	0.001	0.000	0.000	0.000	0.000
7	8	0.004	0.011	0.002	0.022	−0.001	0.062	−0.037	−0.074	−0.003	0.008	0.000	0.003	0.000	0.002	0.001
7	9	0.004	0.010	0.002	0.020	0.000	0.062	−0.036	−0.003	−0.072	0.009	0.000	0.003	0.000	0.002	0.000

Table S7. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-311G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	0.00270	0.04773	0.37158	−0.44517	0.00774	0.00141	0.00027	0.00080	0.00076	0.00282	0.00823	0.00020	0.00052
C_6H_5	0.00291	0.04775	0.37033	−0.44465	0.00772	0.00140	0.00030	0.00079	0.00078	0.00283	0.00870	0.00018	0.00049
Br	0.00356	0.04798	0.37153	−0.44643	0.00791	0.00142	0.00029	0.00078	0.00076	0.00283	0.00835	0.00017	0.00050
Cl	0.00360	0.04796	0.37162	−0.44650	0.00791	0.00141	0.00028	0.00078	0.00076	0.00283	0.00830	0.00017	0.00051
CN	0.00443	0.04816	0.37188	−0.44798	0.00800	0.00138	0.00029	0.00078	0.00079	0.00289	0.00826	0.00016	0.00053
$COCH_3$	0.00390	0.04831	0.36953	−0.44478	0.00795	0.00129	0.00026	0.00077	0.00080	0.00293	0.00789	0.00015	0.00052
$COOC_2H_5$	0.00376	0.04818	0.36973	−0.44476	0.00791	0.00131	0.00027	0.00081	0.00081	0.00294	0.00795	0.00015	0.00052
COOH	0.00391	0.04820	0.37010	−0.44535	0.00795	0.00132	0.00027	0.00081	0.00080	0.00295	0.00796	0.00015	0.00052
$C(CH_3)_3$	0.00252	0.04759	0.36945	−0.44387	0.00764	0.00143	0.00029	0.00077	0.00078	0.00279	0.00941	0.00016	0.00049
CH_3CH_3	0.00259	0.04770	0.37046	−0.44429	0.00772	0.00142	0.00029	0.00080	0.00078	0.00283	0.00860	0.00018	0.00049
F	0.00334	0.04791	0.37173	−0.44614	0.00793	0.00150	0.00031	0.00079	0.00075	0.00280	0.00801	0.00018	0.00047
I	0.00358	0.04796	0.37144	−0.44644	0.00789	0.00141	0.00029	0.00077	0.00076	0.00283	0.00850	0.00016	0.00050
IO_2	0.00457	0.04820	0.37179	−0.44794	0.00806	0.00137	0.00026	0.00078	0.00078	0.00291	0.00812	0.00016	0.00054
CH_3	0.00257	0.04768	0.37058	−0.44427	0.00768	0.00140	0.00028	0.00081	0.00078	0.00283	0.00855	0.00019	0.00050
$O(CH_2)_3CH_3$	0.00269	0.04784	0.37011	−0.44376	0.00779	0.00157	0.00032	0.00073	0.00075	0.00273	0.00815	0.00015	0.00043
$O(CH_3)_4CH_3$	0.00268	0.04784	0.37011	−0.44374	0.00779	0.00157	0.00032	0.00073	0.00075	0.00273	0.00814	0.00015	0.00043
$O(CH_2)_2CH_3$	0.00270	0.04784	0.37013	−0.44379	0.00779	0.00157	0.00032	0.00073	0.00075	0.00273	0.00815	0.00015	0.00043
NH_2	0.00228	0.04754	0.37053	−0.44394	0.00766	0.00154	0.00032	0.00072	0.00075	0.00271	0.00881	0.00016	0.00043
$NHCOCH_3$	0.00269	0.04752	0.37157	−0.44586	0.00775	0.00154	0.00031	0.00077	0.00076	0.00277	0.00909	0.00015	0.00043
NO_2	0.00456	0.04829	0.37131	−0.44761	0.00816	0.00140	0.00030	0.00081	0.00081	0.00296	0.00798	0.00014	0.00047
OC_6H_5	0.00302	0.04785	0.37067	−0.44469	0.00782	0.00149	0.00032	0.00078	0.00076	0.00280	0.00809	0.00017	0.00046
OCH_2CH_3	0.00241	0.04763	0.36996	−0.44415	0.00768	0.00141	0.00030	0.00079	0.00077	0.00281	0.00928	0.00017	0.00048
OH	0.00254	0.04752	0.37153	−0.44539	0.00773	0.00156	0.00033	0.00078	0.00075	0.00275	0.00883	0.00018	0.00044
$OCH(CH_3)_2$	0.00229	0.04751	0.36979	−0.44404	0.00765	0.00143	0.00030	0.00079	0.00076	0.00278	0.00961	0.00017	0.00047
OCH_3	0.00244	0.04760	0.37020	−0.44438	0.00769	0.00143	0.00030	0.00079	0.00076	0.00281	0.00928	0.00017	0.00047
SH	0.00323	0.04788	0.37097	−0.44552	0.00780	0.00141	0.00027	0.00073	0.00074	0.00277	0.00864	0.00018	0.00050
$Si(CH_3)_3$	0.00256	0.04768	0.36984	−0.44389	0.00767	0.00135	0.00026	0.00078	0.00078	0.00285	0.00898	0.00017	0.00053
SCH_3	0.00318	0.04791	0.37103	−0.44541	0.00785	0.00136	0.00028	0.00079	0.00077	0.00284	0.00834	0.00018	0.00051
$SOCH_3$	0.00341	0.04770	0.37231	−0.44716	0.00788	0.00149	0.00029	0.00078	0.00077	0.00283	0.00859	0.00017	0.00051
SO_2CH_3	0.00432	0.04819	0.37123	−0.44712	0.00804	0.00133	0.00027	0.00079	0.00078	0.00292	0.00816	0.00016	0.00054
SO_2NH_2	0.00413	0.04816	0.37100	−0.44668	0.00801	0.00133	0.00026	0.00079	0.00078	0.00291	0.00821	0.00016	0.00053
CF_3	0.00405	0.04809	0.37129	−0.44696	0.00795	0.00136	0.00027	0.00080	0.00079	0.00291	0.00836	0.00017	0.00052
$OCOCH_3$	0.00361	0.04789	0.37190	−0.44685	0.00793	0.00144	0.00030	0.00078	0.00076	0.00282	0.00831	0.00018	0.00047
$SCOCH_3$	0.00368	0.04801	0.37175	−0.44688	0.00794	0.00136	0.00028	0.00077	0.00076	0.00284	0.00840	0.00018	0.00052

Table S8. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-311G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	0.00270	0.04773	0.37158	−0.44517	0.00774	0.00141	0.00027	0.00080	0.00076	0.00282	0.00823	0.0002	0.00047	0.00052
C_6H_5	0.00272	0.04768	0.37153	−0.44526	0.00773	0.00140	0.00026	0.00083	0.00077	0.00287	0.00818	−0.00006	0.00041	0.00051
Br	0.00323	0.04783	0.37248	−0.44692	0.00789	0.00138	0.00025	0.00082	0.00079	0.00287	0.00817	−0.00010	0.00045	0.00055
Cl	0.00321	0.04781	0.37252	−0.44695	0.00788	0.00139	0.00025	0.00082	0.00080	0.00287	0.00818	−0.00010	0.00045	0.00054
CN	0.00424	0.04811	0.37281	−0.44851	0.00796	0.00136	0.00028	0.00076	0.00072	0.00285	0.00815	−0.00007	0.00044	0.00053
$COCH_3$	0.00354	0.04792	0.37178	−0.44653	0.00784	0.00142	0.00028	0.00080	0.00069	0.00282	0.00831	−0.00004	0.00036	0.00050
$CO_2C_2H_5$	0.00352	0.04791	0.37152	−0.44610	0.00781	0.00139	0.00030	0.00080	0.00072	0.00285	0.00815	−0.00003	0.00039	0.00050
COOH	0.00374	0.04797	0.37177	−0.44663	0.00786	0.00138	0.00030	0.00078	0.00071	0.00286	0.00814	−0.00003	0.00039	0.00050
$C(CH_3)_3$	0.00248	0.04762	0.37120	−0.44456	0.00776	0.00139	0.00026	0.00087	0.00080	0.00293	0.00816	−0.00004	0.00038	0.00052
CH_2CH_3	0.00245	0.04765	0.37143	−0.44483	0.00774	0.00143	0.00026	0.00087	0.00080	0.00288	0.00820	−0.00006	0.00043	0.00051
F	0.00282	0.04773	0.37258	−0.44667	0.00789	0.00142	0.00026	0.00080	0.00084	0.00289	0.00824	−0.00008	0.00044	0.00057
I	0.00328	0.04785	0.37243	−0.44692	0.00788	0.00138	0.00025	0.00083	0.00078	0.00286	0.00816	−0.00010	0.00045	0.00055
IO_2	0.00422	0.04814	0.37280	−0.44846	0.00802	0.00136	0.00028	0.00078	0.00075	0.00285	0.00821	−0.00004	0.00042	0.00055
$CH(CH_3)_2$	0.00248	0.04766	0.37133	−0.44471	0.00774	0.00140	0.00025	0.00086	0.00079	0.00290	0.00821	−0.00004	0.00042	0.00052
CH_3	0.00244	0.04764	0.37149	−0.44481	0.00772	0.00142	0.00026	0.00088	0.00080	0.00287	0.00817	−0.00007	0.00044	0.00052
SCN	0.00335	0.04781	0.37255	−0.44732	0.00784	0.00139	0.00025	0.00077	0.00077	0.00287	0.00819	−0.00008	0.00043	0.00056
$N(CH_3)_2$	0.00097	0.04709	0.37123	−0.44340	0.00770	0.00141	0.00025	0.00075	0.00098	0.00296	0.00832	−0.00005	0.00043	0.00048
NH_2	0.00128	0.04719	0.37189	−0.44429	0.00771	0.00140	0.00025	0.00083	0.00096	0.00293	0.00829	−0.00007	0.00046	0.00053
$NHCOCH_3$	0.00236	0.04768	0.37112	−0.44477	0.00777	0.00140	0.00024	0.00078	0.00085	0.00291	0.00818	−0.00005	0.00042	0.00053
$NHCH_3$	0.00104	0.04707	0.37181	−0.44395	0.00769	0.00135	0.00025	0.00080	0.00099	0.00300	0.00826	−0.00006	0.00045	0.00053
NO_2	0.00437	0.04816	0.37280	−0.44870	0.00805	0.00138	0.00031	0.00073	0.00071	0.00286	0.00817	−0.00003	0.00034	0.00055
OC_6H_5	0.00209	0.04748	0.37193	−0.44509	0.00777	0.00138	0.00025	0.00082	0.00089	0.00297	0.00818	−0.00007	0.00042	0.00056
$O(CH_2)_3CH_3$	0.00176	0.04740	0.37144	−0.44451	0.00777	0.00151	0.00027	0.00082	0.00089	0.00286	0.00841	−0.00006	0.00042	0.00050
$OCOCH_3$	0.00269	0.04763	0.37218	−0.44597	0.00783	0.00142	0.00027	0.00083	0.00081	0.00291	0.00820	−0.00007	0.00040	0.00055
OCH_2CH_3	0.00179	0.04741	0.37148	−0.44460	0.00778	0.00151	0.00027	0.00082	0.00089	0.00286	0.00841	−0.00006	0.00042	0.00050
OH	0.00202	0.04748	0.37198	−0.44513	0.00776	0.00138	0.00024	0.00080	0.00091	0.00295	0.00819	−0.00008	0.00045	0.00057
$OCH(CH_3)_2$	0.00182	0.04740	0.37176	−0.44464	0.00776	0.00136	0.00025	0.00081	0.00092	0.00301	0.00814	−0.00007	0.00041	0.00056
OCH_3	0.00196	0.04744	0.37184	−0.44486	0.00776	0.00135	0.00025	0.00080	0.00092	0.00301	0.00814	−0.00007	0.00043	0.00056
$O(CH_3)_4CH_3$	0.00177	0.04740	0.37143	−0.44449	0.00777	0.00151	0.00027	0.00082	0.00089	0.00286	0.00841	−0.00006	0.00042	0.00050
$O(CH_2)_2CH_3$	0.00178	0.04740	0.37147	−0.44455	0.00777	0.00151	0.00027	0.00082	0.00089	0.00286	0.00841	−0.00006	0.00042	0.00050
$SCH(CH_3)_2$	0.00231	0.04750	0.37168	−0.44522	0.00773	0.00142	0.00023	0.00084	0.00082	0.00285	0.00833	−0.00006	0.00045	0.00050
SC_2H_5	0.00234	0.04752	0.37177	−0.44520	0.00774	0.00133	0.00022	0.00083	0.00085	0.00295	0.00814	−0.00007	0.00043	0.00052
SH	0.00264	0.04762	0.37205	−0.44583	0.00776	0.00136	0.00022	0.00083	0.00082	0.00288	0.00817	−0.00009	0.00044	0.00054

Table S8. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_2CH_3)_3$	0.00274	0.04775	0.37103	−0.44469	0.00774	0.00142	0.00026	0.00089	0.00076	0.00285	0.00822	−0.00006	0.00043	0.00047
$Si(CH_3)_3$	0.00271	0.04772	0.37118	−0.44474	0.00773	0.00138	0.00026	0.00089	0.00076	0.00286	0.00819	−0.00007	0.00045	0.00049
SCH_3	0.00226	0.04751	0.37165	−0.44520	0.00774	0.00145	0.00024	0.00083	0.00082	0.00283	0.00834	−0.00006	0.00045	0.00050
SO_2CH_3	0.00411	0.04809	0.37256	−0.44801	0.00798	0.00138	0.00029	0.00078	0.00073	0.00284	0.00820	−0.00004	0.00040	0.00052
SO_2NH_2	0.00392	0.04804	0.37237	−0.44758	0.00795	0.00138	0.00028	0.00080	0.00073	0.00285	0.00819	−0.00005	0.00041	0.00052
$SOCH_3$	0.00338	0.04785	0.37262	−0.44713	0.00788	0.00137	0.00025	0.00083	0.00075	0.00286	0.00830	−0.00005	0.00037	0.00051
CF_3	0.00388	0.04803	0.37235	−0.44752	0.00794	0.00139	0.00029	0.00079	0.00074	0.00286	0.00816	−0.00004	0.00041	0.00052
$SCOCH_3$	0.00311	0.04784	0.37163	−0.44579	0.00779	0.00138	0.00026	0.00081	0.00076	0.00284	0.00816	−0.00009	0.00045	0.00052

Table S9. All LRF-BO values, $\left\{\delta \mathrm{B}^{\mathrm{O\text{-}H}}/\delta \mathrm{v(L)}\right\}_{\mathrm{L}}^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-31G level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	−0.00541	0.02780	0.29570	−0.33833	0.00156	0.00023	0.00010	0.00073	0.00254	0.00961	0.00552	0.00003	0.00029
C_6H_5	−0.00541	0.02780	0.29556	−0.33863	0.00152	0.00023	0.00009	0.00073	0.00256	0.00969	0.00593	0.00002	0.00028
Br	−0.00473	0.02799	0.29715	−0.34110	0.00158	0.00027	0.00010	0.00074	0.00257	0.00991	0.00555	0.00003	0.00030
Cl	−0.00465	0.02802	0.29741	−0.34159	0.00159	0.00028	0.00010	0.00075	0.00258	0.00996	0.00557	0.00003	0.00031
CN	−0.00427	0.02817	0.29821	−0.34309	0.00152	0.00022	0.00009	0.00075	0.00262	0.01012	0.00564	0.00002	0.00030
$COCH_3$	−0.00473	0.02818	0.29654	−0.34055	0.00145	0.00020	0.00009	0.00075	0.00267	0.01004	0.00539	0.00002	0.00029
$COOC_2H_5$	−0.00482	0.02811	0.29640	−0.34024	0.00147	0.00021	0.00009	0.00075	0.00266	0.00998	0.00546	0.00001	0.00029
COOH	−0.00465	0.02815	0.29689	−0.34106	0.00148	0.00022	0.00009	0.00075	0.00266	0.01004	0.00547	0.00001	0.00029
$C(CH_3)_3$	−0.00566	0.02768	0.29502	−0.33798	0.00155	0.00023	0.00010	0.00073	0.00254	0.00958	0.00628	0.00002	0.00029
CH_3CH_3	−0.00559	0.02776	0.29523	−0.33788	0.00154	0.00023	0.00010	0.00073	0.00255	0.00961	0.00580	0.00003	0.00029
F	−0.00479	0.02797	0.29715	−0.34101	0.00160	0.00026	0.00010	0.00074	0.00257	0.00994	0.00546	0.00003	0.00030
I	−0.00484	0.02797	0.29683	−0.34070	0.00158	0.00027	0.00010	0.00074	0.00256	0.00985	0.00568	0.00003	0.00031
IO_2	−0.00402	0.02819	0.29854	−0.34368	0.00157	0.00027	0.00009	0.00075	0.00263	0.01016	0.00546	0.00003	0.00031
CH_3	−0.00560	0.02777	0.29525	−0.33784	0.00154	0.00023	0.00010	0.00073	0.00254	0.00961	0.00577	0.00003	0.00029
$O(CH_2)_3CH_3$	−0.00551	0.02786	0.29528	−0.33798	0.00154	0.00023	0.00010	0.00073	0.00257	0.00974	0.00551	0.00002	0.00029
$O(CH_3)_4CH_3$	−0.00551	0.02786	0.29526	−0.33796	0.00154	0.00023	0.00010	0.00073	0.00257	0.00974	0.00551	0.00002	0.00029
$O(CH_2)_2CH_3$	−0.00550	0.02786	0.29529	−0.33801	0.00154	0.00023	0.00010	0.00073	0.00257	0.00974	0.00551	0.00002	0.00029
NH_2	−0.00601	0.02757	0.29458	−0.33671	0.00159	0.00024	0.00009	0.00073	0.00249	0.00951	0.00601	0.00003	0.00028
$NHCOCH_3$	−0.00540	0.02770	0.29604	−0.33933	0.00161	0.00024	0.00009	0.00073	0.00253	0.00966	0.00619	0.00002	0.00028
NO_2	−0.00399	0.02828	0.29880	−0.34430	0.00153	0.00024	0.00009	0.00076	0.00268	0.01035	0.00553	0.00002	0.00030
OC_6H_5	−0.00521	0.02791	0.29597	−0.33911	0.00155	0.00023	0.00009	0.00074	0.00257	0.00983	0.00548	0.00002	0.00029
OCH_2CH_3	−0.00562	0.02761	0.29536	−0.33841	0.00161	0.00027	0.00010	0.00074	0.00251	0.00961	0.00630	0.00003	0.00029
OH	−0.00535	0.02768	0.29612	−0.33931	0.00164	0.00027	0.00010	0.00073	0.00251	0.00967	0.00599	0.00003	0.00029
$OCH(CH_3)_2$	−0.00567	0.02756	0.29523	−0.33830	0.00162	0.00027	0.00010	0.00074	0.00249	0.00959	0.00646	0.00003	0.00029
OCH_3	−0.00558	0.02762	0.29558	−0.33866	0.00162	0.00027	0.00010	0.00074	0.00250	0.00963	0.00628	0.00003	0.00029
SH	−0.00509	0.02782	0.29666	−0.34027	0.00163	0.00027	0.00010	0.00074	0.00252	0.00976	0.00592	0.00003	0.00030
$Si(CH_3)_3$	−0.00559	0.02773	0.29518	−0.33790	0.00154	0.00024	0.00010	0.00073	0.00255	0.00958	0.00595	0.00003	0.00029
SCH_3	−0.00507	0.02792	0.29637	−0.33977	0.00155	0.00025	0.00010	0.00074	0.00257	0.00979	0.00561	0.00003	0.00030
$SOCH_3$	−0.00471	0.02787	0.29760	−0.34174	0.00164	0.00029	0.00010	0.00074	0.00257	0.00986	0.00580	0.00003	0.00030
SO_2CH_3	−0.00401	0.02823	0.29863	−0.34383	0.00155	0.00027	0.00009	0.00076	0.00266	0.01022	0.00540	0.00002	0.00031
SO_2NH_2	−0.00402	0.02824	0.29858	−0.34383	0.00156	0.00027	0.00009	0.00076	0.00265	0.01023	0.00543	0.00002	0.00031
CF_3	−0.00433	0.02814	0.29794	−0.34281	0.00153	0.00023	0.00009	0.00075	0.00263	0.01011	0.00572	0.00002	0.00030
$OCOCH_3$	−0.00463	0.02799	0.29759	−0.34182	0.00157	0.00024	0.00010	0.00074	0.00258	0.01000	0.00564	0.00003	0.00029
$SCOCH_3$	−0.00462	0.02805	0.29751	−0.34174	0.00156	0.00025	0.00010	0.00074	0.00259	0.00996	0.00561	0.00003	0.00030

Table S10. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-31G level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	−0.00541	0.02780	0.29570	−0.33833	0.00156	0.00023	0.00010	0.00073	0.00254	0.00961	0.00552	0.00003	0.00029	−0.00038
C_6H_5	−0.00546	0.02784	0.29540	−0.33801	0.00158	0.00023	0.00009	0.00072	0.00256	0.00960	0.00553	0.00000	0.00027	−0.00037
Br	−0.00489	0.02796	0.29689	−0.34047	0.00157	0.00023	0.00011	0.00075	0.00258	0.00980	0.00549	−0.00001	0.00029	−0.00033
Cl	−0.00481	0.02799	0.29715	−0.34090	0.00157	0.00022	0.00011	0.00075	0.00259	0.00985	0.00549	−0.00001	0.00029	−0.00032
CN	−0.00442	0.02814	0.29817	−0.34270	0.00157	0.00022	0.00010	0.00074	0.00259	0.01009	0.00548	0.00000	0.00029	−0.00030
$COCH_3$	−0.00486	0.02797	0.29704	−0.34072	0.00157	0.00023	0.00010	0.00072	0.00257	0.00989	0.00556	0.00000	0.00027	−0.00033
$CO_2C_2H_5$	−0.00493	0.02797	0.29678	−0.34030	0.00156	0.00023	0.00010	0.00073	0.00257	0.00988	0.00547	0.00001	0.00027	−0.00034
COOH	−0.00475	0.02803	0.29728	−0.34112	0.00156	0.00023	0.00010	0.00073	0.00257	0.00996	0.00545	0.00001	0.00027	−0.00032
$C(CH_3)_3$	−0.00564	0.02778	0.29501	−0.33723	0.00157	0.00023	0.00009	0.00071	0.00255	0.00952	0.00550	0.00000	0.00026	−0.00038
CH_2CH_3	−0.00560	0.02778	0.29512	−0.33746	0.00158	0.00024	0.00009	0.00072	0.00256	0.00953	0.00552	0.00000	0.00028	−0.00039
F	−0.00500	0.02795	0.29668	−0.34018	0.00159	0.00023	0.00010	0.00074	0.00258	0.00978	0.00553	0.00000	0.00028	−0.00033
I	−0.00498	0.02795	0.29672	−0.34013	0.00156	0.00023	0.00010	0.00075	0.00258	0.00978	0.00546	−0.00001	0.00029	−0.00033
IO_2	−0.00430	0.02815	0.29866	−0.34332	0.00154	0.00022	0.00012	0.00076	0.00259	0.01013	0.00543	0.00001	0.00030	−0.00029
$CH(CH_3)_2$	−0.00561	0.02778	0.29513	−0.33742	0.00157	0.00023	0.00009	0.00072	0.00255	0.00953	0.00553	0.00000	0.00028	−0.00038
CH_3	−0.00559	0.02778	0.29514	−0.33748	0.00157	0.00024	0.00009	0.00072	0.00256	0.00953	0.00551	−0.00001	0.00028	−0.00038
SCN	−0.00468	0.02808	0.29739	−0.34150	0.00160	0.00023	0.00010	0.00073	0.00260	0.00993	0.00554	−0.00001	0.00029	−0.00031
$N(CH_3)_2$	−0.00648	0.02764	0.29286	−0.33396	0.00163	0.00024	0.00008	0.00069	0.00258	0.00918	0.00569	−0.00001	0.00025	−0.00044
NH_2	−0.00632	0.02766	0.29329	−0.33461	0.00164	0.00024	0.00009	0.00070	0.00258	0.00922	0.00566	−0.00001	0.00028	−0.00043
$NHCOCH_3$	−0.00553	0.02792	0.29500	−0.33763	0.00157	0.00022	0.00009	0.00072	0.00260	0.00958	0.00552	0.00000	0.00028	−0.00037
$NHCH_3$	−0.00643	0.02762	0.29306	−0.33418	0.00164	0.00024	0.00009	0.00070	0.00257	0.00918	0.00566	−0.00001	0.00026	−0.00044
NO_2	−0.00413	0.02823	0.29899	−0.34406	0.00157	0.00022	0.00011	0.00074	0.00260	0.01027	0.00545	0.00001	0.00026	−0.00027
OC_6H_5	−0.00556	0.02783	0.29515	−0.33762	0.00160	0.00023	0.00009	0.00072	0.00257	0.00954	0.00553	0.00000	0.00027	−0.00037
$O(CH_2)_3CH_3$	−0.00579	0.02777	0.29462	−0.33669	0.00160	0.00024	0.00009	0.00072	0.00257	0.00945	0.00552	0.00000	0.00026	−0.00038
$OCOCH_3$	−0.00527	0.02786	0.29594	−0.33886	0.00160	0.00024	0.00010	0.00073	0.00256	0.00968	0.00552	0.00000	0.00025	−0.00035
OCH_2CH_3	−0.00577	0.02777	0.29465	−0.33676	0.00160	0.00024	0.00009	0.00072	0.00257	0.00945	0.00553	0.00000	0.00027	−0.00038
OH	−0.00556	0.02784	0.29521	−0.33771	0.00160	0.00023	0.00010	0.00072	0.00258	0.00953	0.00553	−0.00001	0.00028	−0.00037
$OCH(CH_3)_2$	−0.00581	0.02777	0.29449	−0.33651	0.00160	0.00024	0.00009	0.00071	0.00257	0.00943	0.00552	0.00000	0.00026	−0.00039
OCH_3	−0.00574	0.02778	0.29474	−0.33709	0.00162	0.00023	0.00009	0.00071	0.00258	0.00947	0.00569	0.00000	0.00027	−0.00039
$O(CH_3)_4CH_3$	−0.00580	0.02777	0.29460	−0.33666	0.00160	0.00024	0.00009	0.00072	0.00256	0.00945	0.00552	0.00000	0.00026	−0.00038
$O(CH_2)_2CH_3$	−0.00577	0.02777	0.29460	−0.33669	0.00160	0.00024	0.00009	0.00072	0.00257	0.00944	0.00552	0.00000	0.00027	−0.00038
$SCH(CH_3)_2$	−0.00529	0.02784	0.29588	−0.33875	0.00157	0.00023	0.00010	0.00074	0.00257	0.00964	0.00554	0.00000	0.00029	−0.00036
SC_2H_5	−0.00548	0.02784	0.29530	−0.33786	0.00157	0.00023	0.00010	0.00073	0.00257	0.00955	0.00549	0.00000	0.00028	−0.00037
SH	−0.00519	0.02791	0.29607	−0.33915	0.00157	0.00023	0.00010	0.00074	0.00259	0.00966	0.00550	−0.00001	0.00029	−0.00035

Table S10. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_2CH_3)_3$	−0.00551	0.02780	0.29537	−0.33784	0.00155	0.00023	0.00009	0.00073	0.00255	0.00959	0.00551	0.00000	0.00029	−0.00038
$Si(CH_3)_3$	−0.00552	0.02779	0.29537	−0.33781	0.00155	0.00023	0.00010	0.00073	0.00255	0.00958	0.00550	0.00000	0.00029	−0.00038
SCH_3	−0.00542	0.02785	0.29545	−0.33811	0.00157	0.00023	0.00010	0.00073	0.00257	0.00958	0.00549	0.00000	0.00028	−0.00037
SO_2CH_3	−0.00426	0.02814	0.29875	−0.34353	0.00156	0.00022	0.00012	0.00076	0.00259	0.01016	0.00547	0.00001	0.00029	−0.00028
SO_2NH_2	−0.00426	0.02814	0.29872	−0.34352	0.00156	0.00022	0.00012	0.00076	0.00260	0.01017	0.00547	0.00001	0.00029	−0.00028
$SOCH_3$	−0.00482	0.02794	0.29738	−0.34105	0.00157	0.00022	0.00011	0.00074	0.00256	0.00987	0.00557	0.00001	0.00028	−0.00033
CF_3	−0.00445	0.02810	0.29811	−0.34254	0.00157	0.00023	0.00011	0.00074	0.00259	0.01007	0.00547	0.00000	0.00028	−0.00030
$SCOCH_3$	−0.00514	0.02788	0.29629	−0.33940	0.00157	0.00023	0.00010	0.00074	0.00257	0.00972	0.00550	−0.00001	0.00029	−0.00035

Table S11. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-31G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	−0.00650	0.03376	0.28371	−0.32881	0.00165	0.00026	0.00042	0.00069	0.00235	0.00719	0.00551	0.00010	0.00030
C_6H_5	−0.00646	0.03377	0.28338	−0.32907	0.00165	0.00027	0.00041	0.00069	0.00236	0.00726	0.00597	0.00009	0.00029
Br	−0.00550	0.03405	0.28387	−0.33077	0.00167	0.00029	0.00041	0.00070	0.00238	0.00749	0.00562	0.00009	0.00031
Cl	−0.00549	0.03405	0.28395	−0.33081	0.00167	0.00029	0.00041	0.00070	0.00238	0.00749	0.00558	0.00009	0.00031
CN	−0.00465	0.03430	0.28422	−0.33250	0.00164	0.00026	0.00040	0.00071	0.00244	0.00770	0.00565	0.00008	0.00030
$COCH_3$	−0.00543	0.03429	0.28339	−0.33041	0.00156	0.00025	0.00040	0.00071	0.00246	0.00758	0.00541	0.00008	0.00029
$COOC_2H_5$	−0.00560	0.03419	0.28340	−0.33018	0.00158	0.00026	0.00041	0.00071	0.00246	0.00754	0.00546	0.00007	0.00029
COOH	−0.00537	0.03424	0.28356	−0.33070	0.00159	0.00026	0.00041	0.00071	0.00247	0.00760	0.00546	0.00007	0.00029
$C(CH_3)_3$	−0.00687	0.03361	0.28308	−0.32853	0.00169	0.00027	0.00041	0.00069	0.00232	0.00716	0.00642	0.00008	0.00029
CH_3CH_3	−0.00674	0.03369	0.28339	−0.32847	0.00166	0.00027	0.00042	0.00069	0.00235	0.00718	0.00584	0.00009	0.00029
F	−0.00576	0.03394	0.28396	−0.33026	0.00171	0.00030	0.00042	0.00069	0.00236	0.00746	0.00540	0.00009	0.00030
I	−0.00557	0.03402	0.28377	−0.33055	0.00167	0.00028	0.00041	0.00070	0.00237	0.00743	0.00572	0.00009	0.00031
IO_2	−0.00446	0.03433	0.28411	−0.33246	0.00164	0.00027	0.00040	0.00071	0.00246	0.00772	0.00545	0.00009	0.00031
CH_3	−0.00676	0.03370	0.28339	−0.32841	0.00165	0.00027	0.00042	0.00069	0.00235	0.00718	0.00581	0.00009	0.00029
$O(CH_2)_3CH_3$	−0.00663	0.03381	0.28324	−0.32836	0.00173	0.00028	0.00038	0.00068	0.00231	0.00727	0.00556	0.00007	0.00028
$O(CH_3)_4CH_3$	−0.00663	0.03381	0.28324	−0.32836	0.00172	0.00028	0.00038	0.00068	0.00231	0.00727	0.00555	0.00007	0.00028
$O(CH_2)_2CH_3$	−0.00662	0.03381	0.28325	−0.32839	0.00173	0.00028	0.00038	0.00068	0.00231	0.00727	0.00556	0.00008	0.00028
NH_2	−0.00710	0.03353	0.28323	−0.32784	0.00174	0.00029	0.00039	0.00068	0.00228	0.00710	0.00598	0.00009	0.00029
$NHCOCH_3$	−0.00658	0.03360	0.28377	−0.32944	0.00175	0.00029	0.00041	0.00068	0.00232	0.00724	0.00621	0.00008	0.00028
NO_2	−0.00440	0.03441	0.28414	−0.33291	0.00165	0.00028	0.00041	0.00072	0.00249	0.00789	0.00552	0.00007	0.00030
OC_6H_5	−0.00619	0.03389	0.28354	−0.32927	0.00169	0.00028	0.00040	0.00069	0.00235	0.00736	0.00550	0.00008	0.00029
OCH_2CH_3	−0.00661	0.03383	0.28328	−0.32844	0.00172	0.00028	0.00038	0.00068	0.00231	0.00728	0.00555	0.00008	0.00029
OH	−0.00658	0.03357	0.28370	−0.32909	0.00176	0.00031	0.00042	0.00068	0.00231	0.00722	0.00597	0.00009	0.00029
$OCH(CH_3)_2$	−0.00699	0.03345	0.28306	−0.32841	0.00172	0.00030	0.00042	0.00069	0.00230	0.00714	0.00660	0.00009	0.00029
OCH_3	−0.00683	0.03353	0.28322	−0.32864	0.00172	0.00030	0.00042	0.00069	0.00232	0.00718	0.00639	0.00009	0.00029
SH	−0.00598	0.03394	0.28355	−0.32980	0.00167	0.00027	0.00040	0.00069	0.00234	0.00734	0.00580	0.00009	0.00030
$Si(CH_3)_3$	−0.00680	0.03369	0.28324	−0.32842	0.00164	0.00026	0.00042	0.00070	0.00236	0.00715	0.00607	0.00009	0.00029
SCH_3	−0.00658	0.03363	0.28349	−0.32928	0.00170	0.00029	0.00042	0.00069	0.00232	0.00720	0.00640	0.00009	0.00030
$SOCH_3$	−0.00568	0.03387	0.28421	−0.33092	0.00172	0.00029	0.00041	0.00070	0.00237	0.00743	0.00583	0.00009	0.00030
SO_2CH_3	−0.00478	0.03431	0.28400	−0.33203	0.00161	0.00027	0.00041	0.00071	0.00246	0.00769	0.00553	0.00008	0.00030
SO_2NH_2	−0.00499	0.03426	0.28387	−0.33162	0.00161	0.00028	0.00041	0.00071	0.00245	0.00765	0.00556	0.00008	0.00030
CF_3	−0.00522	0.03414	0.28386	−0.33134	0.00164	0.00027	0.00041	0.00070	0.00243	0.00758	0.00575	0.00008	0.00029
$OCOCH_3$	−0.00536	0.03401	0.28412	−0.33115	0.00168	0.00028	0.00041	0.00069	0.00238	0.00754	0.00558	0.00009	0.00030
$SCOCH_3$	−0.00532	0.03413	0.28409	−0.33125	0.00162	0.00027	0.00041	0.00070	0.00239	0.00753	0.00561	0.00009	0.00031

Table S12. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-31G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	−0.00650	0.03376	0.28371	−0.32881	0.00165	0.00026	0.00042	0.00069	0.00235	0.00719	0.00551	0.00010	0.00030	−0.00061
C_6H_5	−0.00661	0.03375	0.28369	−0.32873	0.00165	0.00026	0.00043	0.00068	0.00238	0.00720	0.00547	−0.00004	0.00027	−0.00060
Br	−0.00585	0.03395	0.28417	−0.33039	0.00165	0.00025	0.00043	0.00071	0.00240	0.00740	0.00545	−0.00005	0.00029	−0.00056
Cl	−0.00585	0.03394	0.28420	−0.33043	0.00165	0.00025	0.00043	0.00071	0.00240	0.00740	0.00547	−0.00005	0.00029	−0.00056
CN	−0.00485	0.03426	0.28455	−0.33234	0.00164	0.00026	0.00040	0.00067	0.00240	0.00763	0.00548	−0.00004	0.00029	−0.00053
$COCH_3$	−0.00566	0.03400	0.28405	−0.33049	0.00166	0.00027	0.00041	0.00065	0.00236	0.00742	0.00553	−0.00003	0.00026	−0.00057
$CO_2C_2H_5$	−0.00572	0.03400	0.28386	−0.33019	0.00166	0.00028	0.00042	0.00066	0.00238	0.00740	0.00548	−0.00003	0.00026	−0.00057
COOH	−0.00548	0.03407	0.28402	−0.33071	0.00165	0.00028	0.00042	0.00066	0.00238	0.00747	0.00546	−0.00003	0.00026	−0.00056
$C(CH_3)_3$	−0.00688	0.03371	0.28352	−0.32812	0.00167	0.00026	0.00044	0.00068	0.00237	0.00716	0.00546	−0.00003	0.00027	−0.00061
CH_2CH_3	−0.00685	0.03368	0.28361	−0.32826	0.00166	0.00026	0.00045	0.00070	0.00237	0.00716	0.00548	−0.00004	0.00028	−0.00061
F	−0.00629	0.03383	0.28404	−0.32970	0.00167	0.00025	0.00042	0.00072	0.00240	0.00734	0.00550	−0.00004	0.00029	−0.00057
I	−0.00590	0.03394	0.28420	−0.33029	0.00163	0.00025	0.00044	0.00071	0.00239	0.00737	0.00543	−0.00005	0.00030	−0.00056
IO_2	−0.00480	0.03424	0.28451	−0.33224	0.00163	0.00026	0.00043	0.00070	0.00239	0.00761	0.00549	−0.00002	0.00030	−0.00052
$CH(CH_3)_2$	−0.00686	0.03369	0.28363	−0.32822	0.00165	0.00026	0.00044	0.00069	0.00238	0.00715	0.00547	−0.00003	0.00028	−0.00061
CH_3	−0.00684	0.03369	0.28364	−0.32826	0.00166	0.00026	0.00045	0.00070	0.00237	0.00715	0.00546	−0.00004	0.00029	−0.00061
SCN	−0.00568	0.03399	0.28422	−0.33081	0.00166	0.00025	0.00040	0.00068	0.00240	0.00743	0.00548	−0.00004	0.00029	−0.00055
$N(CH_3)_2$	−0.00841	0.03324	0.28306	−0.32582	0.00167	0.00026	0.00038	0.00075	0.00240	0.00694	0.00554	−0.00004	0.00027	−0.00066
NH_2	−0.00799	0.03335	0.28337	−0.32666	0.00167	0.00026	0.00043	0.00075	0.00240	0.00700	0.00553	−0.00004	0.00029	−0.00065
$NHCOCH_3$	−0.00686	0.03377	0.28342	−0.32831	0.00164	0.00024	0.00041	0.00071	0.00241	0.00720	0.00546	−0.00003	0.00029	−0.00060
$NHCH_3$	−0.00828	0.03324	0.28324	−0.32611	0.00165	0.00026	0.00041	0.00076	0.00241	0.00695	0.00552	−0.00004	0.00028	−0.00065
NO_2	−0.00459	0.03435	0.28461	−0.33278	0.00165	0.00027	0.00039	0.00066	0.00240	0.00774	0.00544	−0.00002	0.00025	−0.00051
OC_6H_5	−0.00702	0.03362	0.28363	−0.32818	0.00166	0.00025	0.00042	0.00072	0.00241	0.00717	0.00546	−0.00004	0.00028	−0.00060
$O(CH_2)_3CH_3$	−0.00746	0.03352	0.28344	−0.32757	0.00171	0.00026	0.00042	0.00072	0.00238	0.00711	0.00562	−0.00003	0.00028	−0.00063
$OCOCH_3$	−0.00647	0.03375	0.28388	−0.32918	0.00167	0.00026	0.00043	0.00070	0.00239	0.00728	0.00548	−0.00004	0.00027	−0.00058
OCH_2CH_3	−0.00740	0.03353	0.28343	−0.32764	0.00171	0.00026	0.00042	0.00072	0.00238	0.00712	0.00562	−0.00003	0.00028	−0.00063
OH	−0.00712	0.03361	0.28365	−0.32812	0.00165	0.00025	0.00042	0.00075	0.00242	0.00716	0.00547	−0.00004	0.00029	−0.00060
$OCH(CH_3)_2$	−0.00744	0.03350	0.28344	−0.32739	0.00164	0.00025	0.00042	0.00074	0.00243	0.00709	0.00544	−0.00004	0.00028	−0.00061
OCH_3	−0.00726	0.03355	0.28352	−0.32771	0.00163	0.00025	0.00041	0.00074	0.00243	0.00712	0.00544	−0.00004	0.00028	−0.00060
$O(CH_3)_4CH_3$	−0.00746	0.03352	0.28344	−0.32754	0.00171	0.00026	0.00042	0.00072	0.00238	0.00710	0.00561	−0.00003	0.00028	−0.00063
$O(CH_2)_2CH_3$	−0.00744	0.03352	0.28344	−0.32758	0.00171	0.00026	0.00042	0.00072	0.00238	0.00711	0.00562	−0.00003	0.00028	−0.00063
$SCH(CH_3)_2$	−0.00689	0.03364	0.28369	−0.32849	0.00166	0.00025	0.00043	0.00071	0.00238	0.00715	0.00554	−0.00003	0.00029	−0.00061
SC_2H_5	−0.00696	0.03362	0.28364	−0.32838	0.00167	0.00025	0.00043	0.00071	0.00237	0.00715	0.00556	−0.00003	0.00029	−0.00061
SH	−0.00648	0.03377	0.28385	−0.32919	0.00164	0.00025	0.00044	0.00072	0.00240	0.00724	0.00546	−0.00005	0.00029	−0.00059

Table S12. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_2CH_3)_3$	−0.00659	0.03376	0.28358	−0.32855	0.00164	0.00026	0.00045	0.00068	0.00236	0.00718	0.00548	−0.00003	0.00029	−0.00060
$Si(CH_3)_3$	−0.00665	0.03375	0.28359	−0.32846	0.00165	0.00026	0.00046	0.00068	0.00235	0.00716	0.00547	−0.00003	0.00030	−0.00061
SCH_3	−0.00682	0.03367	0.28364	−0.32846	0.00162	0.00024	0.00043	0.00072	0.00241	0.00717	0.00545	−0.00004	0.00029	−0.00060
SO_2CH_3	−0.00496	0.03420	0.28438	−0.33191	0.00164	0.00027	0.00042	0.00069	0.00239	0.00758	0.00549	−0.00002	0.00028	−0.00053
SO_2NH_2	−0.00518	0.03415	0.28429	−0.33150	0.00164	0.00027	0.00043	0.00069	0.00239	0.00754	0.00548	−0.00003	0.00028	−0.00054
$SOCH_3$	−0.00579	0.03393	0.28423	−0.33045	0.00164	0.00026	0.00043	0.00069	0.00238	0.00738	0.00555	−0.00003	0.00027	−0.00057
CF_3	−0.00536	0.03411	0.28426	−0.33119	0.00165	0.00027	0.00042	0.00068	0.00239	0.00751	0.00548	−0.00003	0.00028	−0.00055
$SCOCH_3$	−0.00607	0.03391	0.28379	−0.32959	0.00163	0.00025	0.00043	0.00069	0.00238	0.00730	0.00545	−0.00004	0.00029	−0.00058

Table S13. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-31++G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	0.00431	0.03198	0.36323	−0.39894	−0.00021	0.00018	0.00040	0.00094	0.00221	0.00400	−0.00828	−0.00012	0.00037
C_6H_5	0.00629	0.03143	0.37215	−0.41081	0.00016	0.00039	0.00040	0.00094	0.00243	0.00488	−0.00870	0.00005	0.00042
Br	0.00513	0.03228	0.36400	−0.40109	−0.00003	0.00041	0.00047	0.00094	0.00220	0.00438	−0.00867	−0.00008	0.00039
Cl	0.00546	0.03210	0.36445	−0.40233	0.00001	0.00049	0.00048	0.00094	0.00218	0.00460	−0.00838	0.00006	0.00038
CN	0.00701	0.03204	0.36954	−0.40916	−0.00023	0.00022	0.00034	0.00090	0.00241	0.00496	−0.00874	0.00011	0.00042
$COCH_3$	0.00662	0.03241	0.37292	−0.40973	−0.00021	0.00024	0.00033	0.00099	0.00259	0.00565	−0.01197	−0.00001	0.00059
$COOC_2H_5$	0.00626	0.03251	0.37314	−0.40931	−0.00026	0.00025	0.00037	0.00097	0.00253	0.00519	−0.01153	−0.00009	0.00048
COOH	0.00687	0.03230	0.37140	−0.41078	−0.00043	0.00016	0.00036	0.00094	0.00249	0.00535	−0.00852	0.00004	0.00043
$C(CH_3)_3$	0.00405	0.03247	0.37229	−0.40648	0.00070	0.00043	0.00040	0.00094	0.00238	0.00415	−0.01141	−0.00022	0.00039
CH_3CH_3	0.00526	0.03232	0.36887	−0.40544	−0.00011	0.00030	0.00040	0.00089	0.00229	0.00402	−0.00886	−0.00002	0.00043
F	0.00500	0.03198	0.36257	−0.40046	0.00008	0.00029	0.00050	0.00097	0.00220	0.00486	−0.00823	−0.00003	0.00040
I	0.00524	0.03187	0.36407	−0.40164	0.00002	0.00046	0.00044	0.00095	0.00224	0.00450	−0.00863	0.00006	0.00043
IO_2	0.00689	0.03263	0.36959	−0.40826	−0.00037	0.00025	0.00037	0.00097	0.00242	0.00504	−0.00936	−0.00001	0.00045
CH_3	0.00518	0.03226	0.36807	−0.40527	−0.00020	0.00027	0.00040	0.00090	0.00232	0.00422	−0.00834	0.00005	0.00044
$O(CH_2)_3CH_3$	0.00404	0.03263	0.36323	−0.40068	−0.00020	0.00019	0.00037	0.00088	0.00218	0.00510	−0.00770	−0.00005	0.00035
$O(CH_3)_4CH_3$	0.00428	0.03269	0.36486	−0.40160	−0.00022	0.00022	0.00040	0.00095	0.00216	0.00506	−0.00847	−0.00005	0.00045
$O(CH_2)_2CH_3$	0.00400	0.03272	0.36254	−0.39962	−0.00019	0.00017	0.00034	0.00086	0.00216	0.00501	−0.00793	−0.00006	0.00033
NH_2	0.00409	0.03217	0.36340	−0.39959	0.00004	0.00029	0.00043	0.00093	0.00210	0.00431	−0.00835	−0.00013	0.00035
$NHCOCH_3$	0.00490	0.03210	0.37167	−0.40987	−0.00003	0.00025	0.00044	0.00097	0.00237	0.00496	−0.00825	−0.00001	0.00034
NO_2	0.00637	0.03274	0.36879	−0.40762	−0.00031	0.00013	0.00041	0.00096	0.00242	0.00554	−0.00881	−0.00008	0.00041
OC_6H_5	0.00502	0.03236	0.36550	−0.40278	−0.00033	0.00022	0.00042	0.00091	0.00223	0.00486	−0.00860	0.00007	0.00029
OCH_2CH_3	0.00553	0.03219	0.37411	−0.41149	−0.00001	0.00021	0.00043	0.00101	0.00242	0.00419	−0.00859	0.00001	0.00051
OH	0.00453	0.03187	0.36429	−0.40197	0.00029	0.00027	0.00048	0.00098	0.00219	0.00472	−0.00782	−0.00017	0.00033
$OCH(CH_3)_2$	0.00610	0.03206	0.37823	−0.41651	0.00040	0.00023	0.00042	0.00100	0.00248	0.00424	−0.00880	0.00000	0.00046
OCH_3	0.00467	0.03261	0.36397	−0.40011	−0.00031	0.00012	0.00029	0.00086	0.00207	0.00477	−0.00886	−0.00007	0.00035
SH	0.00536	0.03212	0.36695	−0.40418	−0.00006	0.00031	0.00036	0.00091	0.00218	0.00431	−0.00859	−0.00010	0.00042
$Si(CH_3)_3$	0.00568	0.03160	0.37935	−0.41585	0.00000	0.00051	0.00044	0.00105	0.00263	0.00388	−0.01033	0.00003	0.00054
SCH_3	0.00615	0.03138	0.37615	−0.41432	0.00041	0.00035	0.00037	0.00101	0.00245	0.00443	−0.00931	0.00010	0.00050
$SOCH_3$	0.00606	0.03216	0.37048	−0.40827	0.00030	0.00043	0.00039	0.00092	0.00222	0.00432	−0.00926	−0.00006	0.00043
SO_2CH_3	0.00726	0.03261	0.37320	−0.41237	−0.00025	0.00035	0.00036	0.00091	0.00241	0.00491	−0.00928	0.00004	0.00050
SO_2NH_2	0.00698	0.03242	0.37212	−0.41133	0.00000	0.00040	0.00039	0.00093	0.00238	0.00487	−0.00880	0.00001	0.00049
CF_3	0.00680	0.03222	0.37071	−0.41006	0.00005	0.00029	0.00036	0.00092	0.00233	0.00524	−0.00858	0.00004	0.00044
$OCOCH_3$	0.00601	0.03226	0.36869	−0.40635	−0.00034	0.00021	0.00039	0.00095	0.00228	0.00494	−0.00886	−0.00006	0.00039
$SCOCH_3$	0.00621	0.03225	0.37047	−0.40783	−0.00014	0.00043	0.00042	0.00092	0.00228	0.00436	−0.00964	−0.00006	0.00044

Table S14. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-31++G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	0.00431	0.03198	0.36323	−0.39894	−0.00021	0.00018	0.00040	0.00094	0.00221	0.00400	−0.00828	−0.00012	0.00037	−0.00063
C_6H_5	0.00538	0.03207	0.36478	−0.39964	0.00028	0.00025	0.00032	0.00083	0.00223	0.00465	−0.01149	0.00055	0.00031	−0.00051
Br	0.00489	0.03200	0.36393	−0.40150	−0.00033	0.00012	0.00037	0.00089	0.00221	0.00422	−0.00724	0.00033	0.00046	−0.00062
Cl	0.00525	0.03169	0.36552	−0.40378	−0.00027	0.00020	0.00039	0.00087	0.00227	0.00421	−0.00688	0.00049	0.00050	−0.00061
CN	0.00681	0.03201	0.36929	−0.40788	−0.00032	0.00018	0.00027	0.00080	0.00225	0.00458	−0.00824	0.00030	0.00042	−0.00062
$COCH_3$	0.00580	0.03169	0.36645	−0.40128	0.00054	0.00029	0.00034	0.00077	0.00217	0.00493	−0.01210	0.00043	0.00029	−0.00032
$CO_2C_2H_5$	0.00647	0.03179	0.36896	−0.40480	0.00036	0.00029	0.00035	0.00081	0.00226	0.00497	−0.01162	0.00034	0.00025	−0.00043
COOH	0.00647	0.03213	0.36705	−0.40360	0.00036	0.00031	0.00032	0.00084	0.00230	0.00528	−0.01156	0.00040	0.00022	−0.00057
$C(CH_3)_3$	0.00569	0.03227	0.36891	−0.40314	0.00018	0.00030	0.00041	0.00079	0.00214	0.00415	−0.01154	0.00032	0.00026	−0.00046
CH_2CH_3	0.00557	0.03156	0.36839	−0.40557	−0.00018	0.00025	0.00035	0.00090	0.00235	0.00413	−0.00764	0.00039	0.00029	−0.00074
F	0.00462	0.03186	0.36428	−0.40079	−0.00021	0.00015	0.00038	0.00089	0.00224	0.00425	−0.00812	0.00060	0.00037	−0.00061
I	0.00479	0.03187	0.36401	−0.40080	−0.00032	0.00010	0.00039	0.00092	0.00226	0.00412	−0.00790	0.00045	0.00052	−0.00061
IO_2	0.00640	0.03203	0.36801	−0.40662	−0.00020	0.00020	0.00038	0.00090	0.00233	0.00457	−0.00818	0.00045	0.00040	−0.00062
$CH(CH_3)_2$	0.00562	0.03184	0.36828	−0.40278	0.00032	0.00027	0.00041	0.00089	0.00229	0.00468	−0.01199	0.00047	0.00042	−0.00055
CH_3	0.00532	0.03171	0.36774	−0.40441	−0.00031	0.00019	0.00035	0.00088	0.00228	0.00404	−0.00783	0.00042	0.00030	−0.00072
SCN	0.00673	0.03152	0.37115	−0.41024	−0.00019	0.00028	0.00032	0.00085	0.00234	0.00444	−0.00759	0.00029	0.00036	−0.00073
$N(CH_3)_2$	0.00392	0.03157	0.36493	−0.39798	0.00044	0.00030	0.00035	0.00086	0.00212	0.00431	−0.01153	0.00037	0.00036	−0.00030
NH_2	0.00349	0.03178	0.36419	−0.39941	−0.00039	0.00016	0.00033	0.00093	0.00225	0.00371	−0.00757	0.00055	0.00032	−0.00070
$NHCOCH_3$	0.00480	0.03182	0.36682	−0.40114	0.00040	0.00025	0.00035	0.00084	0.00225	0.00464	−0.01167	0.00028	0.00052	−0.00037
$NHCH_3$	0.00466	0.03161	0.36763	−0.40496	−0.00029	0.00024	0.00033	0.00091	0.00230	0.00370	−0.00659	0.00051	0.00028	−0.00067
NO_2	0.00675	0.03194	0.36855	−0.40797	−0.00015	0.00023	0.00031	0.00079	0.00228	0.00488	−0.00799	0.00043	0.00029	−0.00064
OC_6H_5	0.00588	0.03168	0.36841	−0.40632	−0.00012	0.00030	0.00037	0.00083	0.00225	0.00413	−0.00750	0.00056	0.00040	−0.00048
$O(CH_2)_3CH_3$	0.00393	0.03159	0.36149	−0.39603	0.00024	0.00030	0.00036	0.00077	0.00210	0.00419	−0.00998	0.00062	0.00035	−0.00014
$OCOCH_3$	0.00607	0.03155	0.36884	−0.40672	−0.00023	0.00025	0.00034	0.00084	0.00223	0.00422	−0.00766	0.00039	0.00041	−0.00064
OCH_2CH_3	0.00425	0.03222	0.36420	−0.39961	−0.00037	0.00029	0.00030	0.00080	0.00213	0.00351	−0.00814	0.00032	0.00026	−0.00050
OH	0.00415	0.03199	0.36443	−0.40016	−0.00036	0.00017	0.00035	0.00091	0.00224	0.00392	−0.00803	0.00042	0.00027	−0.00071
$OCH(CH_3)_2$	0.00505	0.03189	0.36713	−0.40432	−0.00040	0.00027	0.00033	0.00083	0.00218	0.00360	−0.00711	0.00041	0.00039	−0.00043
OCH_3	0.00583	0.03147	0.36911	−0.40798	−0.00014	0.00029	0.00035	0.00088	0.00234	0.00415	−0.00677	0.00054	0.00022	−0.00066
$O(CH_3)_4CH_3$	0.00387	0.03174	0.36145	−0.39605	0.00016	0.00028	0.00034	0.00076	0.00207	0.00404	−0.00973	0.00060	0.00032	−0.00010
$O(CH_2)_2CH_3$	0.00395	0.03137	0.36123	−0.39579	0.00032	0.00031	0.00036	0.00079	0.00213	0.00432	−0.01010	0.00066	0.00036	−0.00020
$SCH(CH_3)_2$	0.00513	0.03147	0.36884	−0.40610	0.00004	0.00019	0.00035	0.00081	0.00224	0.00419	−0.00760	0.00027	0.00045	−0.00050
SC_2H_5	0.00509	0.03146	0.36951	−0.40638	0.00009	0.00017	0.00035	0.00084	0.00223	0.00431	−0.00816	0.00027	0.00060	−0.00050
SH	0.00493	0.03180	0.36569	−0.40271	−0.00042	0.00010	0.00032	0.00091	0.00227	0.00404	−0.00746	0.00031	0.00032	−0.00065

Table S14. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_2CH_3)_3$	0.00537	0.03257	0.36467	−0.39902	0.00030	0.00026	0.00035	0.00077	0.00211	0.00426	−0.01204	0.00039	0.00051	−0.00033
$Si(CH_3)_3$	0.00612	0.03110	0.37051	−0.40729	0.00001	0.00020	0.00035	0.00082	0.00228	0.00431	−0.00862	0.00045	0.00058	−0.00053
SCH_3	0.00495	0.03227	0.36510	−0.40162	−0.00029	0.00021	0.00034	0.00086	0.00212	0.00363	−0.00794	0.00007	0.00037	−0.00045
SO_2CH_3	0.00716	0.03164	0.37152	−0.41100	−0.00002	0.00026	0.00037	0.00086	0.00235	0.00477	−0.00780	0.00040	0.00030	−0.00062
SO_2NH_2	0.00672	0.03205	0.36701	−0.40411	0.00047	0.00028	0.00039	0.00089	0.00230	0.00533	−0.01154	0.00041	0.00021	−0.00058
$SOCH_3$	0.00647	0.03171	0.37045	−0.40919	−0.00018	0.00017	0.00038	0.00086	0.00228	0.00448	−0.00755	0.00045	0.00020	−0.00070
CF_3	0.00695	0.03165	0.37035	−0.41019	−0.00011	0.00030	0.00034	0.00087	0.00239	0.00481	−0.00737	0.00033	0.00028	−0.00066
$SCOCH_3$	0.00619	0.03145	0.36912	−0.40751	−0.00010	0.00018	0.00032	0.00085	0.00233	0.00446	−0.00756	0.00044	0.00040	−0.00063

Table S15. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_L^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-311G level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	−0.00325	0.03320	0.34799	−0.40180	0.00081	0.00019	0.00008	0.00071	0.00255	0.00986	0.00904	0.00004	0.00038
C_6H_5	−0.00292	0.03326	0.34793	−0.40237	0.00074	0.00017	0.00008	0.00072	0.00258	0.00985	0.00933	0.00003	0.00038
Br	−0.00275	0.03348	0.34976	−0.40462	0.00082	0.00021	0.00008	0.00072	0.00256	0.01009	0.00904	0.00003	0.00039
Cl	−0.00266	0.03349	0.35023	−0.40517	0.00084	0.00022	0.00009	0.00072	0.00257	0.01014	0.00893	0.00003	0.00039
CN	−0.00215	0.03366	0.35100	−0.40665	0.00078	0.00017	0.00009	0.00074	0.00262	0.01020	0.00888	0.00003	0.00038
$COCH_3$	−0.00248	0.03365	0.34895	−0.40367	0.00068	0.00015	0.00009	0.00073	0.00268	0.01016	0.00839	0.00001	0.00038
$COOC_2H_5$	−0.00248	0.03357	0.34884	−0.40349	0.00071	0.00016	0.00009	0.00073	0.00266	0.01009	0.00849	0.00002	0.00038
COOH	−0.00241	0.03361	0.34950	−0.40436	0.00072	0.00016	0.00009	0.00074	0.00266	0.01015	0.00852	0.00002	0.00038
$C(CH_3)_3$	−0.00317	0.03312	0.34726	−0.40190	0.00071	0.00017	0.00008	0.00071	0.00256	0.00978	0.01003	0.00002	0.00038
CH_3CH_3	−0.00315	0.03320	0.34758	−0.40159	0.00076	0.00018	0.00008	0.00071	0.00256	0.00982	0.00925	0.00003	0.00038
F	−0.00282	0.03347	0.35022	−0.40477	0.00088	0.00023	0.00010	0.00072	0.00257	0.01015	0.00861	0.00004	0.00038
I	−0.00280	0.03346	0.34943	−0.40432	0.00081	0.00020	0.00008	0.00072	0.00256	0.01006	0.00923	0.00003	0.00039
IO_2	−0.00221	0.03368	0.35173	−0.40758	0.00084	0.00021	0.00008	0.00073	0.00262	0.01029	0.00897	0.00003	0.00039
CH_3	−0.00319	0.03318	0.34754	−0.40145	0.00077	0.00018	0.00008	0.00071	0.00255	0.00980	0.00923	0.00003	0.00038
$O(CH_2)_3CH_3$	−0.00317	0.03328	0.34799	−0.40168	0.00079	0.00018	0.00010	0.00072	0.00258	0.00995	0.00865	0.00002	0.00037
$O(CH_3)_4CH_3$	−0.00318	0.03328	0.34799	−0.40167	0.00079	0.00018	0.00010	0.00072	0.00258	0.00995	0.00864	0.00002	0.00037
$O(CH_2)_2CH_3$	−0.00317	0.03329	0.34802	−0.40172	0.00079	0.00018	0.00010	0.00072	0.00258	0.00995	0.00865	0.00002	0.00037
NH_2	−0.00353	0.03301	0.34741	−0.40109	0.00078	0.00020	0.00009	0.00071	0.00253	0.00975	0.00954	0.00002	0.00038
$NHCOCH_3$	−0.00304	0.03319	0.34908	−0.40382	0.00082	0.00019	0.00008	0.00071	0.00255	0.00986	0.00976	0.00001	0.00037
NO_2	−0.00216	0.03382	0.35202	−0.40781	0.00079	0.00021	0.00010	0.00075	0.00268	0.01044	0.00850	0.00002	0.00038
OC_6H_5	−0.00300	0.03334	0.34872	−0.40265	0.00080	0.00019	0.00010	0.00072	0.00257	0.00999	0.00860	0.00003	0.00038
OCH_2CH_3	−0.00317	0.03330	0.34802	−0.40173	0.00079	0.00018	0.00010	0.00072	0.00258	0.00996	0.00864	0.00002	0.00037
OH	−0.00319	0.03316	0.34899	−0.40339	0.00088	0.00023	0.00009	0.00071	0.00251	0.00989	0.00950	0.00004	0.00038
$OCH(CH_3)_2$	−0.00329	0.03314	0.34759	−0.40238	0.00078	0.00021	0.00009	0.00071	0.00252	0.00982	0.01019	0.00003	0.00038
OCH_3	−0.00321	0.03323	0.34794	−0.40263	0.00081	0.00022	0.00009	0.00072	0.00253	0.00986	0.00985	0.00003	0.00038
SH	−0.00286	0.03343	0.34925	−0.40376	0.00079	0.00020	0.00008	0.00072	0.00257	0.01005	0.00896	0.00003	0.00039
$Si(CH_3)_3$	−0.00325	0.03316	0.34726	−0.40152	0.00073	0.00016	0.00007	0.00071	0.00256	0.00982	0.00965	0.00002	0.00038
SCH_3	−0.00294	0.03337	0.34880	−0.40317	0.00079	0.00020	0.00008	0.00072	0.00257	0.01001	0.00900	0.00003	0.00038
$SOCH_3$	−0.00265	0.03334	0.35064	−0.40570	0.00089	0.00024	0.00008	0.00072	0.00257	0.01006	0.00924	0.00003	0.00039
SO_2CH_3	−0.00211	0.03374	0.35150	−0.40708	0.00079	0.00021	0.00009	0.00074	0.00264	0.01035	0.00850	0.00002	0.00039
SO_2NH_2	−0.00212	0.03374	0.35148	−0.40712	0.00080	0.00021	0.00009	0.00074	0.00264	0.01035	0.00855	0.00002	0.00039
CF_3	−0.00218	0.03368	0.35088	−0.40660	0.00076	0.00017	0.00009	0.00074	0.00263	0.01023	0.00893	0.00003	0.00038
$OCOCH_3$	−0.00266	0.03345	0.35051	−0.40544	0.00083	0.00020	0.00009	0.00072	0.00257	0.01015	0.00893	0.00003	0.00038
$SCOCH_3$	−0.00266	0.03351	0.35008	−0.40510	0.00080	0.00020	0.00009	0.00072	0.00258	0.01014	0.00907	0.00003	0.00039

Table S16. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-311G level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	−0.00325	0.03320	0.34799	−0.40180	0.00081	0.00019	0.00008	0.00071	0.00255	0.00986	0.00904	0.00004	0.00038	0.00023
C_6H_5	−0.00309	0.03325	0.34774	−0.40170	0.00082	0.00018	0.00008	0.00070	0.00259	0.00985	0.00898	−0.00003	0.00034	0.00024
Br	−0.00286	0.03338	0.34941	−0.40395	0.00082	0.00018	0.00009	0.00073	0.00259	0.01003	0.00894	−0.00004	0.00037	0.00026
Cl	−0.00280	0.03341	0.34976	−0.40447	0.00083	0.00018	0.00009	0.00073	0.00260	0.01007	0.00896	−0.00003	0.00037	0.00027
CN	−0.00241	0.03360	0.35066	−0.40604	0.00081	0.00018	0.00010	0.00072	0.00261	0.01026	0.00889	−0.00003	0.00037	0.00026
$COCH_3$	−0.00274	0.03344	0.34953	−0.40434	0.00081	0.00017	0.00009	0.00071	0.00260	0.01011	0.00905	−0.00002	0.00033	0.00025
$CO_2C_2H_5$	−0.00276	0.03339	0.34916	−0.40369	0.00079	0.00018	0.00009	0.00072	0.00259	0.01007	0.00888	−0.00001	0.00033	0.00025
COOH	−0.00268	0.03346	0.34975	−0.40451	0.00080	0.00018	0.00009	0.00072	0.00260	0.01015	0.00885	−0.00001	0.00034	0.00025
$C(CH_3)_3$	−0.00330	0.03315	0.34734	−0.40092	0.00082	0.00018	0.00008	0.00071	0.00258	0.00978	0.00897	−0.00002	0.00032	0.00026
CH_2CH_3	−0.00326	0.03318	0.34743	−0.40113	0.00082	0.00019	0.00008	0.00071	0.00258	0.00979	0.00900	−0.00003	0.00036	0.00023
F	−0.00294	0.03336	0.34941	−0.40398	0.00084	0.00020	0.00009	0.00073	0.00259	0.01001	0.00903	−0.00002	0.00035	0.00027
I	−0.00289	0.03337	0.34926	−0.40370	0.00082	0.00018	0.00009	0.00073	0.00259	0.01001	0.00890	−0.00004	0.00038	0.00026
IO_2	−0.00245	0.03361	0.35136	−0.40675	0.00079	0.00018	0.00010	0.00074	0.00260	0.01031	0.00888	0.00000	0.00037	0.00027
$CH(CH_3)_2$	−0.00325	0.03319	0.34741	−0.40108	0.00081	0.00018	0.00007	0.00071	0.00258	0.00979	0.00902	−0.00002	0.00035	0.00024
CH_3	−0.00326	0.03318	0.34740	−0.40108	0.00082	0.00019	0.00008	0.00071	0.00257	0.00979	0.00900	−0.00003	0.00036	0.00024
SCN	−0.00269	0.03345	0.34989	−0.40485	0.00084	0.00019	0.00009	0.00072	0.00261	0.01010	0.00900	−0.00003	0.00036	0.00027
$N(CH_3)_2$	−0.00382	0.03298	0.34531	−0.39823	0.00088	0.00019	0.00008	0.00070	0.00263	0.00950	0.00921	−0.00003	0.00032	0.00023
NH_2	−0.00375	0.03299	0.34585	−0.39893	0.00089	0.00020	0.00008	0.00070	0.00263	0.00954	0.00922	−0.00002	0.00035	0.00023
$NHCOCH_3$	−0.00321	0.03332	0.34725	−0.40124	0.00083	0.00018	0.00008	0.00071	0.00263	0.00984	0.00897	−0.00001	0.00035	0.00026
$NHCH_3$	−0.00382	0.03293	0.34559	−0.39847	0.00088	0.00021	0.00008	0.00070	0.00262	0.00949	0.00920	−0.00002	0.00033	0.00024
NO_2	−0.00233	0.03367	0.35168	−0.40736	0.00082	0.00019	0.00009	0.00074	0.00263	0.01040	0.00887	0.00000	0.00031	0.00028
OC_6H_5	−0.00332	0.03318	0.34750	−0.40119	0.00085	0.00020	0.00008	0.00072	0.00260	0.00976	0.00900	−0.00001	0.00034	0.00027
$O(CH_2)_3CH_3$	−0.00340	0.03315	0.34708	−0.40084	0.00086	0.00019	0.00009	0.00071	0.00261	0.00972	0.00923	−0.00003	0.00033	0.00023
$OCOCH_3$	−0.00307	0.03323	0.34854	−0.40265	0.00085	0.00020	0.00009	0.00073	0.00260	0.00991	0.00899	−0.00001	0.00031	0.00027
OCH_2CH_3	−0.00343	0.03313	0.34718	−0.40068	0.00085	0.00020	0.00008	0.00072	0.00261	0.00972	0.00900	−0.00001	0.00034	0.00026
OH	−0.00327	0.03319	0.34777	−0.40173	0.00087	0.00020	0.00008	0.00071	0.00260	0.00978	0.00919	−0.00003	0.00034	0.00025
$OCH(CH_3)_2$	−0.00346	0.03312	0.34699	−0.40041	0.00085	0.00020	0.00008	0.00072	0.00260	0.00970	0.00899	−0.00001	0.00033	0.00026
OCH_3	−0.00336	0.03317	0.34724	−0.40107	0.00086	0.00019	0.00009	0.00071	0.00261	0.00974	0.00924	−0.00002	0.00033	0.00024
$O(CH_3)_4CH_3$	−0.00340	0.03315	0.34708	−0.40082	0.00087	0.00019	0.00009	0.00071	0.00261	0.00971	0.00922	−0.00003	0.00033	0.00023
$O(CH_2)_2CH_3$	−0.00342	0.03313	0.34714	−0.40062	0.00085	0.00020	0.00008	0.00072	0.00260	0.00972	0.00898	−0.00001	0.00034	0.00026
$SCH(CH_3)_2$	−0.00307	0.03328	0.34851	−0.40261	0.00081	0.00018	0.00008	0.00072	0.00257	0.00992	0.00898	−0.00004	0.00037	0.00024
SC_2H_5	−0.00304	0.03330	0.34865	−0.40279	0.00081	0.00018	0.00008	0.00072	0.00257	0.00995	0.00894	−0.00004	0.00037	0.00025
SH	−0.00307	0.03329	0.34844	−0.40259	0.00083	0.00018	0.00008	0.00071	0.00259	0.00989	0.00898	−0.00003	0.00036	0.00026
$Si(CH_2CH_3)_3$	−0.00323	0.03321	0.34761	−0.40135	0.00080	0.00018	0.00008	0.00071	0.00258	0.00984	0.00899	−0.00003	0.00037	0.00022

Table S16. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_3)_3$	−0.00324	0.03320	0.34762	−0.40132	0.00080	0.00018	0.00008	0.00071	0.00256	0.00983	0.00899	−0.00003	0.00037	0.00022
SCH_3	−0.00300	0.03332	0.34880	−0.40302	0.00081	0.00018	0.00008	0.00072	0.00258	0.00997	0.00895	−0.00004	0.00037	0.00025
SO_2CH_3	−0.00242	0.03360	0.35148	−0.40696	0.00080	0.00018	0.00011	0.00074	0.00261	0.01033	0.00893	0.00000	0.00035	0.00027
SO_2NH_2	−0.00242	0.03360	0.35144	−0.40695	0.00080	0.00018	0.00011	0.00074	0.00261	0.01034	0.00893	0.00000	0.00035	0.00027
$SOCH_3$	−0.00279	0.03338	0.35006	−0.40476	0.00081	0.00018	0.00010	0.00073	0.00258	0.01010	0.00909	−0.00001	0.00031	0.00024
CF_3	−0.00243	0.03358	0.35081	−0.40618	0.00081	0.00018	0.00010	0.00073	0.00260	0.01027	0.00888	−0.00002	0.00035	0.00026
$SCOCH_3$	−0.00300	0.03332	0.34864	−0.40285	0.00080	0.00018	0.00008	0.00072	0.00258	0.00997	0.00894	−0.00004	0.00037	0.00025

Table S17. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of meta-substituted benzoic acids at the B3LYP/6-311++G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(13)	H(15)
H	−0.01529	0.04904	0.26933	−0.29333	0.00125	0.00082	0.00124	0.00119	0.00205	0.00647	−0.02633	0.00013	0.00135
C_6H_5	−0.01409	0.04894	0.26206	−0.28745	0.00129	0.00080	0.00094	0.00128	0.00256	0.00909	−0.02908	0.00000	0.00134
Br	−0.01285	0.04901	0.26411	−0.29400	0.00123	0.00116	0.00124	0.00125	0.00228	0.00749	−0.02386	0.00030	0.00127
Cl	−0.01342	0.04947	0.26401	−0.29329	0.00148	0.00125	0.00126	0.00129	0.00225	0.00758	−0.02414	0.00039	0.00111
CN	−0.00989	0.04855	0.26424	−0.29498	0.00095	0.00076	0.00091	0.00118	0.00257	0.00871	−0.02647	0.00036	0.00129
$COCH_3$	−0.01172	0.04966	0.25613	−0.28735	0.00101	0.00070	0.00090	0.00141	0.00287	0.01019	−0.02741	0.00012	0.00132
$COOC_2H_5$	−0.01103	0.04868	0.26059	−0.28828	0.00045	0.00077	0.00096	0.00128	0.00280	0.00916	−0.02871	0.00001	0.00136
COOH	−0.01206	0.04904	0.26074	−0.28854	0.00086	0.00077	0.00098	0.00132	0.00276	0.00933	−0.02894	0.00004	0.00147
$C(CH_3)_3$	−0.01324	0.04806	0.25991	−0.28801	0.00174	0.00085	0.00095	0.00135	0.00265	0.00968	−0.02823	−0.00001	0.00112
CH_3CH_3	−0.01562	0.04885	0.25953	−0.28837	0.00149	0.00086	0.00111	0.00136	0.00253	0.00848	−0.02511	0.00041	0.00085
F	−0.01393	0.04915	0.26417	−0.29282	0.00145	0.00080	0.00122	0.00129	0.00224	0.00754	−0.02409	0.00034	0.00130
I	−0.01343	0.04953	0.26303	−0.29299	0.00118	0.00123	0.00116	0.00125	0.00224	0.00748	−0.02311	0.00048	0.00123
IO_2	−0.00972	0.04966	0.26565	−0.29888	0.00098	0.00093	0.00108	0.00138	0.00260	0.00845	−0.02472	0.00026	0.00125
CH_3	−0.01327	0.04847	0.26362	−0.29078	0.00127	0.00083	0.00107	0.00125	0.00245	0.00810	−0.02656	0.00022	0.00117
$O(CH_2)_3CH_3$	−0.01692	0.05037	0.25781	−0.28561	0.00155	0.00074	0.00106	0.00140	0.00243	0.00878	−0.02476	0.00020	0.00128
$O(CH_3)_4CH_3$	−0.01639	0.05034	0.25884	−0.28681	0.00142	0.00072	0.00103	0.00138	0.00244	0.00881	−0.02479	0.00015	0.00125
$O(CH_2)_2CH_3$	−0.01730	0.05037	0.25721	−0.28506	0.00163	0.00075	0.00109	0.00141	0.00241	0.00875	−0.02445	0.00026	0.00129
NH_2	−0.01739	0.04961	0.26150	−0.28926	0.00204	0.00098	0.00122	0.00136	0.00221	0.00775	−0.02329	0.00064	0.00080
$NHCOCH_3$	−0.01522	0.04917	0.25881	−0.28841	0.00199	0.00089	0.00112	0.00147	0.00269	0.00971	−0.02668	0.00026	0.00126
NO_2	−0.01036	0.04966	0.26406	−0.29799	0.00113	0.00064	0.00115	0.00139	0.00272	0.00901	−0.02285	0.00003	0.00113
OC_6H_5	−0.01481	0.04973	0.26029	−0.29001	0.00123	0.00068	0.00110	0.00132	0.00247	0.00840	−0.02355	0.00038	0.00080
OCH_2CH_3	−0.01545	0.04991	0.25804	−0.28815	0.00154	0.00069	0.00102	0.00130	0.00239	0.00862	−0.02256	0.00015	0.00081
OH	−0.01540	0.04863	0.26394	−0.29226	0.00201	0.00072	0.00124	0.00135	0.00222	0.00786	−0.02365	0.00018	0.00132
$OCH(CH_3)_2$	−0.01450	0.04907	0.25148	−0.28008	0.00122	0.00072	0.00108	0.00143	0.00260	0.00883	−0.02368	0.00044	0.00103
OCH_3	−0.01385	0.04812	0.26665	−0.29591	0.00145	0.00049	0.00109	0.00156	0.00272	0.00880	−0.02519	0.00021	0.00115
SH	−0.01191	0.04859	0.26772	−0.29624	0.00139	0.00085	0.00093	0.00124	0.00230	0.00800	−0.02564	0.00026	0.00123
$Si(CH_3)_3$	−0.01618	0.04873	0.26306	−0.28552	0.00147	0.00137	0.00133	0.00150	0.00242	0.00731	−0.02963	0.00060	0.00126
SCH_3	−0.01084	0.04670	0.27075	−0.29805	0.00102	0.00082	0.00093	0.00149	0.00279	0.00792	−0.02852	0.00043	0.00117
$SOCH_3$	−0.01341	0.04935	0.26280	−0.29498	0.00212	0.00093	0.00101	0.00138	0.00250	0.00923	−0.02471	0.00053	0.00090
SO_2CH_3	−0.01218	0.04968	0.26297	−0.29458	0.00128	0.00081	0.00095	0.00142	0.00279	0.01056	−0.02809	0.00023	0.00140
SO_2NH_2	−0.01342	0.04992	0.26098	−0.29334	0.00151	0.00086	0.00112	0.00151	0.00274	0.01013	−0.02567	0.00035	0.00132
CF_3	−0.01055	0.04912	0.26271	−0.29437	0.00118	0.00071	0.00100	0.00131	0.00261	0.00915	−0.02545	0.00019	0.00114
$OCOCH_3$	−0.01341	0.04978	0.26704	−0.29431	0.00143	0.00070	0.00102	0.00128	0.00239	0.00844	−0.02692	0.00045	0.00099
$SCOCH_3$	−0.01232	0.04890	0.26611	−0.29588	0.00151	0.00107	0.00109	0.00135	0.00254	0.00876	−0.02700	0.00049	0.00094

Table S18. All LRF-BO values, $\left\{\delta B^{O\text{-}H}/\delta v(L)\right\}_{L}^{All\ atoms}$, of para-substituted benzoic acids at the B3LYP/6-311++G** level. The numbering of the atoms listed in the top row is the same as presented in Figure 9 in the text.

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
H	−0.01529	0.04904	0.26933	−0.29333	0.00125	0.00082	0.00124	0.00119	0.00205	0.00647	−0.02633	0.00013	0.00135	0.00029
C_6H_5	−0.01398	0.04904	0.26368	−0.28555	0.00160	0.00078	0.00090	0.00104	0.00220	0.00799	−0.03089	0.00142	0.00088	0.00016
Br	−0.01485	0.04913	0.26772	−0.29428	0.00149	0.00082	0.00125	0.00117	0.00219	0.00688	−0.02479	0.00123	0.00120	0.00027
Cl	−0.01388	0.04859	0.26886	−0.29520	0.00123	0.00080	0.00105	0.00111	0.00220	0.00678	−0.02527	0.00158	0.00144	0.00022
CN	−0.01059	0.04887	0.26866	−0.29590	0.00118	0.00082	0.00084	0.00096	0.00221	0.00769	−0.02728	0.00109	0.00116	−0.00009
$COCH_3$	−0.01316	0.04907	0.26040	−0.28541	0.00203	0.00073	0.00090	0.00091	0.00219	0.00925	−0.03014	0.00103	0.00080	0.00034
$CO_2C_2H_5$	−0.01227	0.04887	0.26320	−0.28773	0.00183	0.00087	0.00090	0.00093	0.00228	0.00894	−0.03055	0.00118	0.00083	0.00026
COOH	−0.01243	0.04915	0.26190	−0.28735	0.00186	0.00086	0.00086	0.00096	0.00231	0.00902	−0.03017	0.00124	0.00086	0.00038
$C(CH_3)_3$	−0.01348	0.04878	0.26044	−0.28471	0.00200	0.00065	0.00095	0.00093	0.00225	0.00900	−0.02904	0.00102	0.00082	0.00003
CH_2CH_3	−0.01447	0.04819	0.26742	−0.29095	0.00169	0.00083	0.00103	0.00105	0.00226	0.00713	−0.02654	0.00131	0.00101	−0.00015
F	−0.01497	0.04885	0.26991	−0.29477	0.00124	0.00081	0.00120	0.00119	0.00218	0.00672	−0.02600	0.00175	0.00130	0.00030
I	−0.01444	0.04898	0.27013	−0.29540	0.00113	0.00077	0.00129	0.00115	0.00212	0.00661	−0.02602	0.00140	0.00153	0.00022
IO_2	−0.01111	0.04897	0.26898	−0.29853	0.00127	0.00078	0.00107	0.00108	0.00222	0.00747	−0.02511	0.00119	0.00123	0.00018
$CH(CH_3)_2$	−0.01426	0.04883	0.26534	−0.28636	0.00174	0.00086	0.00105	0.00109	0.00228	0.00843	−0.03190	0.00137	0.00112	0.00008
CH_3	−0.01454	0.04829	0.26953	−0.29206	0.00147	0.00083	0.00107	0.00104	0.00217	0.00691	−0.02744	0.00145	0.00095	−0.00005
SCN	−0.01330	0.04879	0.26070	−0.28534	0.00191	0.00082	0.00090	0.00104	0.00224	0.00883	−0.03033	0.00152	0.00102	0.00025
$N(CH_3)_2$	−0.01780	0.04884	0.26062	−0.28143	0.00216	0.00080	0.00097	0.00130	0.00229	0.00837	−0.02968	0.00091	0.00083	0.00034
NH_2	−0.01845	0.04886	0.26801	−0.28956	0.00158	0.00083	0.00120	0.00133	0.00221	0.00653	−0.02622	0.00150	0.00086	0.00035
$NHCOCH_3$	−0.01540	0.04906	0.26343	−0.28658	0.00190	0.00080	0.00102	0.00120	0.00234	0.00835	−0.02963	0.00098	0.00111	0.00034
$NHCH_3$	−0.01811	0.04876	0.26201	−0.28198	0.00191	0.00088	0.00110	0.00137	0.00232	0.00786	−0.03012	0.00156	0.00090	0.00043
NO_2	−0.01230	0.04964	0.26344	−0.29400	0.00185	0.00083	0.00111	0.00103	0.00224	0.00840	−0.02495	0.00099	0.00054	0.00032
OC_6H_5	−0.01534	0.04920	0.25724	−0.28122	0.00207	0.00074	0.00094	0.00108	0.00230	0.00832	−0.02848	0.00150	0.00088	0.00027
$O(CH_2)_3CH_3$	−0.01840	0.04891	0.26232	−0.28433	0.00197	0.00075	0.00098	0.00115	0.00233	0.00789	−0.02748	0.00129	0.00102	0.00031
$OCOCH_3$	−0.01429	0.04902	0.26765	−0.29132	0.00152	0.00085	0.00093	0.00100	0.00215	0.00705	−0.02715	0.00137	0.00102	0.00010
OCH_2CH_3	−0.01737	0.04845	0.25907	−0.27947	0.00189	0.00081	0.00100	0.00113	0.00225	0.00789	−0.02988	0.00169	0.00101	0.00056
OH	−0.01709	0.04871	0.26785	−0.29139	0.00166	0.00085	0.00118	0.00122	0.00223	0.00684	−0.02586	0.00148	0.00083	0.00037
$OCH(CH_3)_2$	−0.01683	0.04880	0.25753	−0.27912	0.00194	0.00076	0.00095	0.00111	0.00225	0.00798	−0.02912	0.00159	0.00093	0.00052
OCH_3	−0.01532	0.04885	0.26786	−0.29200	0.00175	0.00089	0.00095	0.00115	0.00239	0.00704	−0.02656	0.00140	0.00068	0.00007
$O(CH_3)_4CH_3$	−0.01610	0.04839	0.26182	−0.28352	0.00176	0.00074	0.00092	0.00110	0.00225	0.00755	−0.02881	0.00156	0.00098	0.00070
$O(CH_2)_2CH_3$	−0.01845	0.04896	0.26247	−0.28418	0.00199	0.00075	0.00101	0.00119	0.00232	0.00784	−0.02767	0.00129	0.00102	0.00033
$SCH(CH_3)_2$	−0.01577	0.04902	0.26260	−0.28464	0.00189	0.00076	0.00108	0.00122	0.00224	0.00851	−0.03108	0.00110	0.00126	0.00036
SC_2H_5	−0.01658	0.04937	0.26297	−0.28535	0.00204	0.00082	0.00112	0.00127	0.00223	0.00825	−0.03007	0.00097	0.00126	0.00029
SH	−0.01485	0.04862	0.27026	−0.29479	0.00148	0.00080	0.00122	0.00113	0.00218	0.00690	−0.02613	0.00122	0.00090	0.00023

Table S18. *Cont.*

	O(1)	C(2)	O(3)	H(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	H(11)	H(12)	H(14)	H(15)
$Si(CH_2CH_3)_3$	−0.01223	0.04894	0.25971	−0.28464	0.00181	0.00069	0.00096	0.00100	0.00226	0.00843	−0.02949	0.00112	0.00094	0.00002
$Si(CH_3)_3$	−0.01365	0.04930	0.26097	−0.28425	0.00184	0.00071	0.00098	0.00108	0.00220	0.00832	−0.03025	0.00100	0.00120	0.00012
SCH_3	−0.01556	0.04900	0.26090	−0.28234	0.00192	0.00085	0.00112	0.00114	0.00221	0.00830	−0.03143	0.00125	0.00094	0.00051
SO_2CH_3	−0.01101	0.04925	0.26167	−0.28973	0.00215	0.00088	0.00095	0.00100	0.00229	0.00975	−0.02965	0.00097	0.00078	0.00029
SO_2NH_2	−0.01161	0.04920	0.26196	−0.28966	0.00211	0.00084	0.00098	0.00104	0.00228	0.00929	−0.02912	0.00098	0.00077	0.00025
$SOCH_3$	−0.01256	0.04924	0.26236	−0.28736	0.00194	0.00076	0.00101	0.00104	0.00223	0.00909	−0.03113	0.00128	0.00070	0.00034
CF_3	−0.01196	0.04943	0.26008	−0.28663	0.00206	0.00084	0.00089	0.00099	0.00231	0.00957	−0.03053	0.00114	0.00082	0.00027
$SCOCH_3$	−0.01281	0.04865	0.27003	−0.29568	0.00147	0.00087	0.00105	0.00112	0.00226	0.00712	−0.02666	0.00105	0.00122	−0.00003

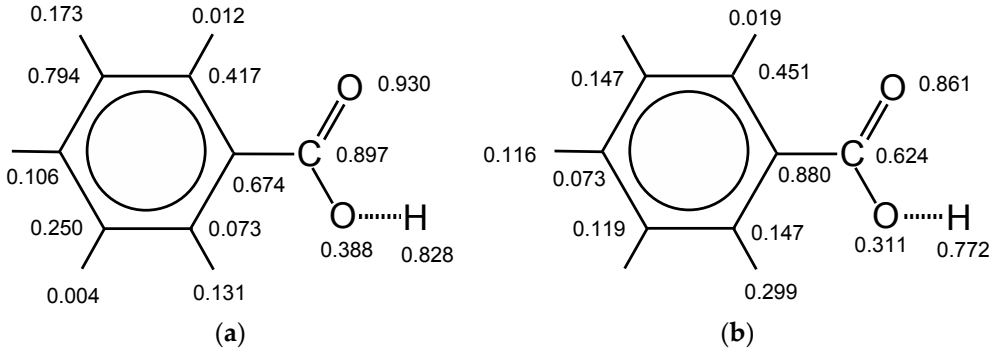


Figure S2. The coefficients of determination for the correlations between the Hammett constants and the LRF-BO values, $\delta B^{O\text{-}H}/\delta v(L)$ with the virtual perturbation on each atomic site. (**a**) Meta-substituted benzoic acids; (**b**) Para-substituted benzoic acids.

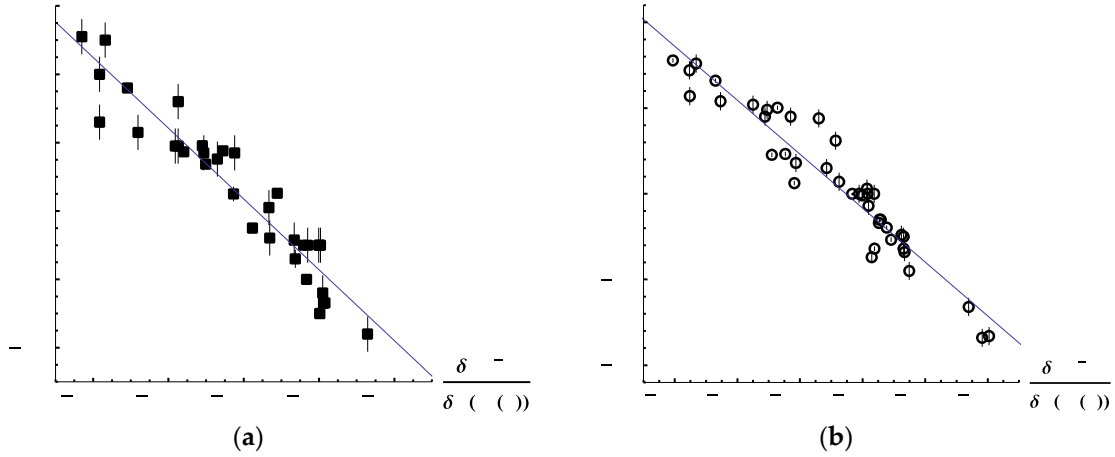


Figure S3. Correlation between Hammett constants and $\delta B^{O\text{-}H}/\delta v(H(4))$ values at the B3LYP/6-31G level. (**a**) Meta-substituted benzoic acids; (**b**) Para-substituted benzoic acids. The coefficients of determination (R^2) are (**a**) 0.906 and (**b**) 0.917, respectively.

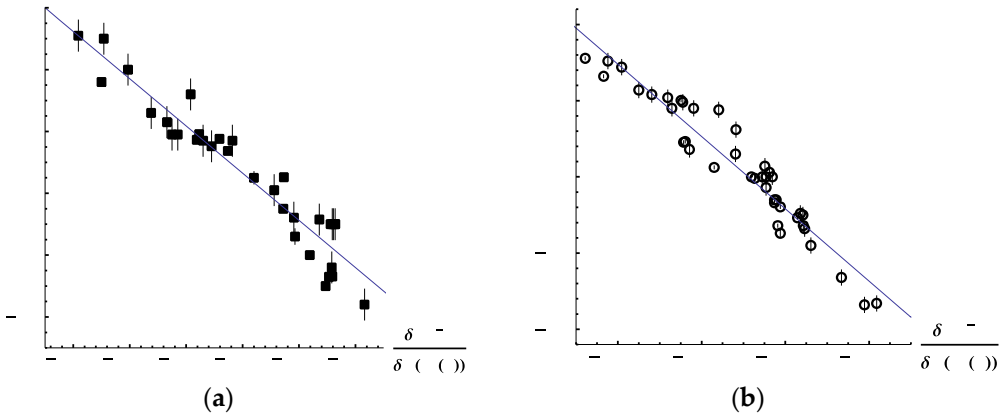
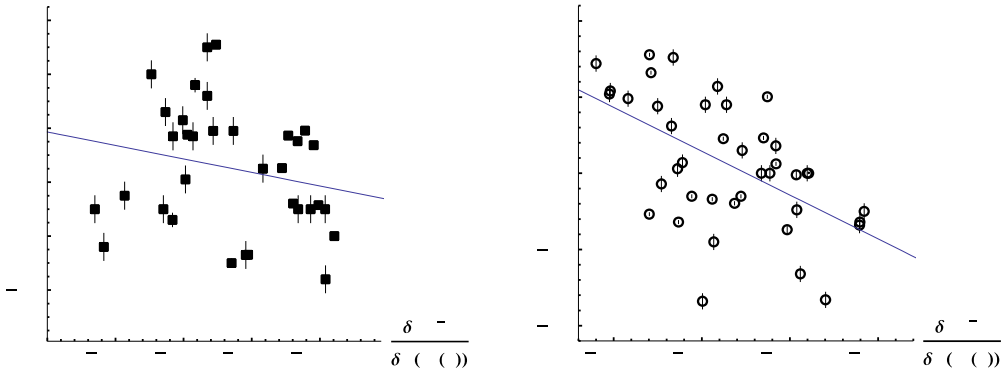
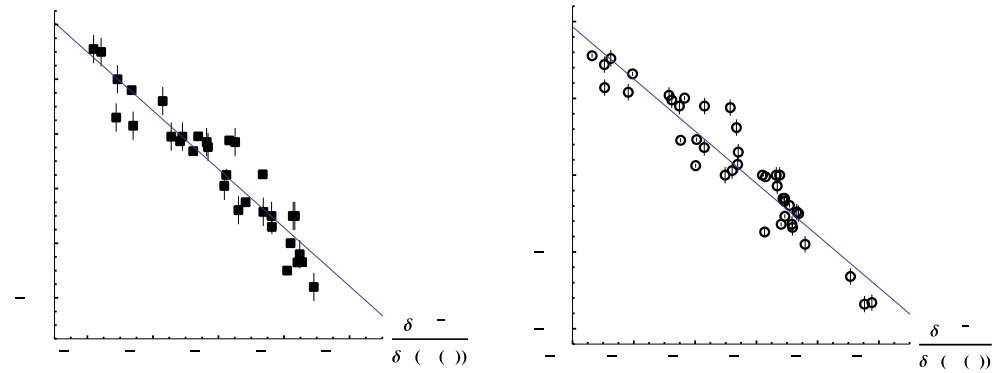


Figure S4. Correlation between Hammett constants and $\delta B^{O\text{-}H}/\delta v(H(4))$ values at the B3LYP/6-31G** level. (**a**) meta-substituted benzoic acids; (**b**) para-substituted benzoic acids. The coefficients of determination (R^2) are (**a**) 0.912 and (**b**) 0.923, respectively.



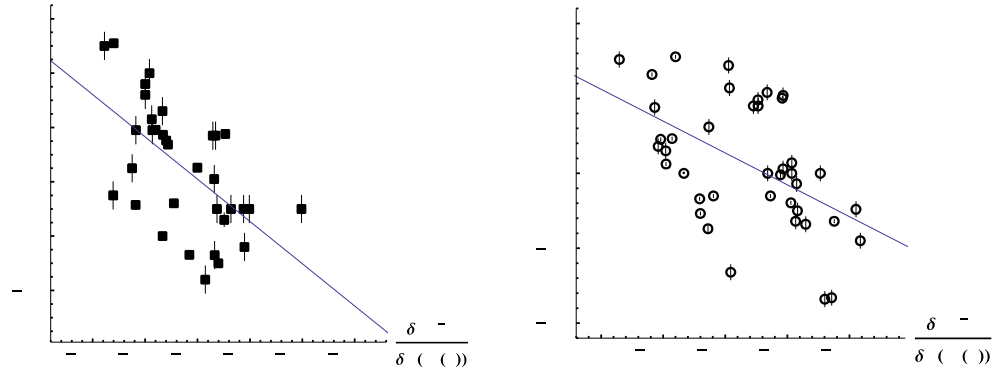
(**a**) (**b**)

Figure S5. Correlation between Hammett constants and $\delta B^{O\text{-}H}/\delta\nu(H(4))$ values at the B3LYP/6-31++G** level. (**a**) Meta-substituted benzoic acids; (**b**) Para-substituted benzoic acids. The coefficients of determination (R^2) are (**a**) 0.047 and (**b**) 0.309 respectively.



(**a**) (**b**)

Figure S6. Correlation between Hammett constants and $\delta B^{O\text{-}H}/\delta\nu(H(4))$ values at the B3LYP/6-311G level. (**a**) meta-substituted benzoic acids; (**b**) para-substituted benzoic acids. The coefficients of determination (R^2) are (**a**) 0.887 and (**b**) 0.895 respectively.



(**a**) (**b**)

Figure S7. Correlation between Hammett constants and $\delta B^{O\text{-}H}/\delta\nu(H(4))$ values at the B3LYP/6-311++G** level. (**a**) Meta-substituted benzoic acids; (**b**) Para-substituted benzoic acids. The coefficients of determination (R^2) are (**a**) 0.351 and (**b**) 0.268 respectively.

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