Intramolecular Hydrogen Bonds in Normal and Sterically Compressed *o*-Hydroxy Aromatic Aldehydes. Isotope Effects on chemical shifts and Hydrogen Bond Strength.

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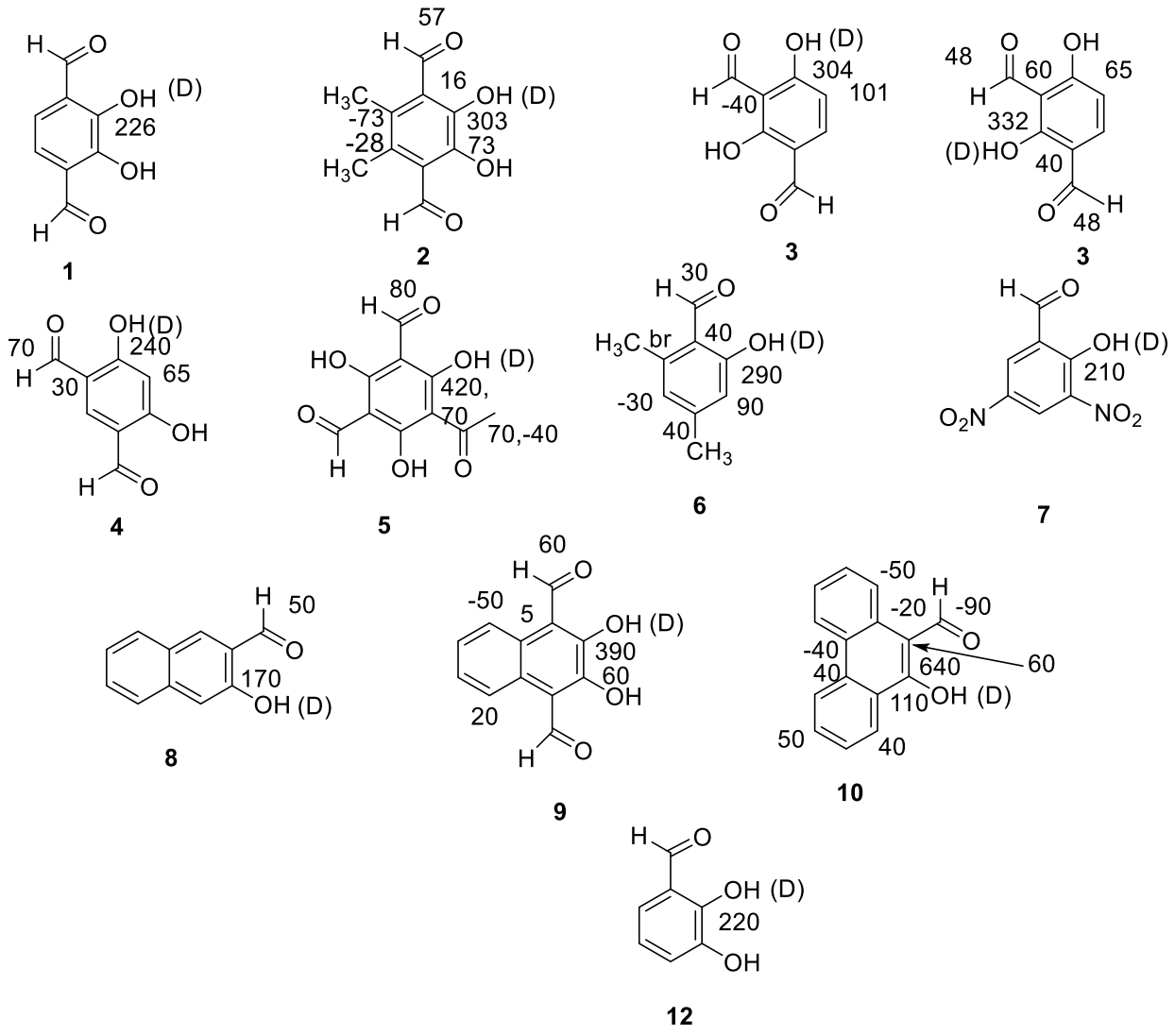

Scheme S1. Deuterium isotope effects on ^{13}C chemical shifts. Carbons not having a number attached did not show an isotope effect. For **5** the second set of isotope effects are due to deuteriation at the other OH group.

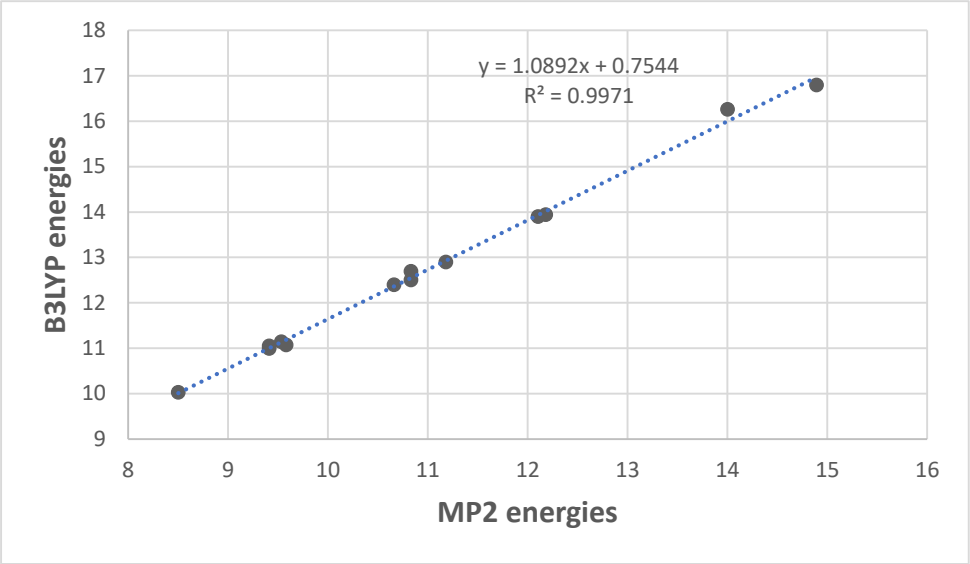

Figure S2. Plot of hydrogen bond energies in Kcal/mole, B3LYP vs. MP2

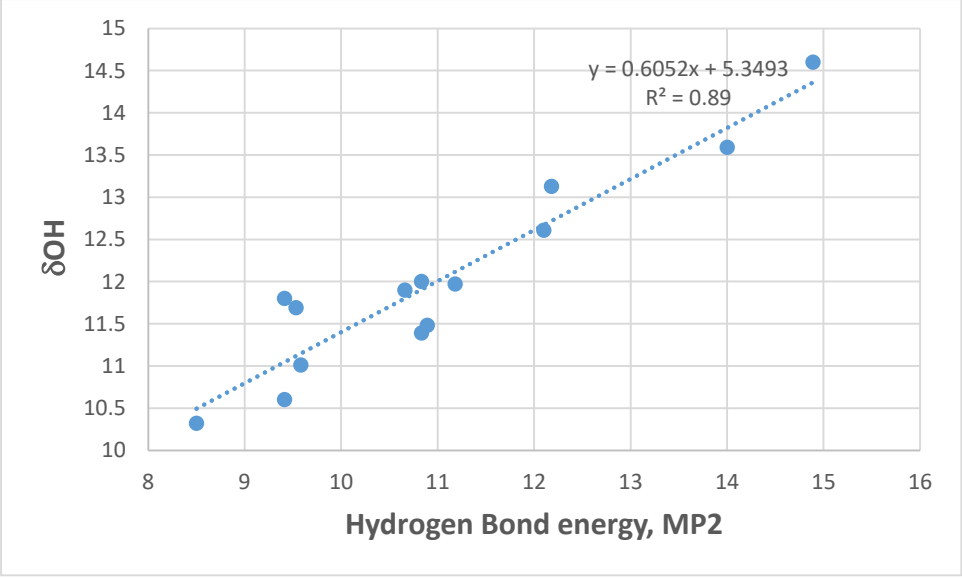

Fig. S3. Observed OH chemical shifts in ppm vs. hydrogen **bond** energies in Kcal/mole (MP2). Data for **13**-**17** and **21** and **22** are from Ref. 1. The one for 1-hydroxy-3,6-dimethoxy-2-naphthaldehyde (**23**) is from Ref. 2.

Table 1S . Calculated hydrogen bond energies hb and out method. Energies in kcal/mole

Compound	Calc. H-bond energy MP2	Calc. H-bond energy B3LYP
4	9.41	11.05
6	10.83	12.69
8	8.5	10.03
10	14.89	16.8
13	9.58	11.07
14	10.28	11.95
15	9.5	10.99
16	10.18	11.9
17	9.53	11.14
18	10.66	12.4
19	11.01	12.9
20	11.79	13.63
21	11.18	12.9
22	12.18	13.94
23	12.1	13.9

[1] Hansen, P.E Isotope Effects on Nuclear Shielding. Intra-molecular Hydrogen- bonded Ketones,Aldehydes and Esters. *Magn.Reson.Chem.* **1993**, *31*, 23-37.

[2] Pittelkow, M.; Boas, U. Jessing, M.; Jensen, K. J.; Christensen**,** J. B. Role of the peri-effect in synthesis and reactivity of highly substituted naphthaldehydes: a novel backbone amide linker for solid-phase synthesis. *Org.Biol.Mol.Chem*. **2005**, *3*, 508-51.