

SUPPLEMENTARY INFORMATION

High desolvation temperature facilitates in ESI-source H/D exchange at non-labile sites of hydroxybenzoic acids and aromatic amino acids

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In-ESI source labeling

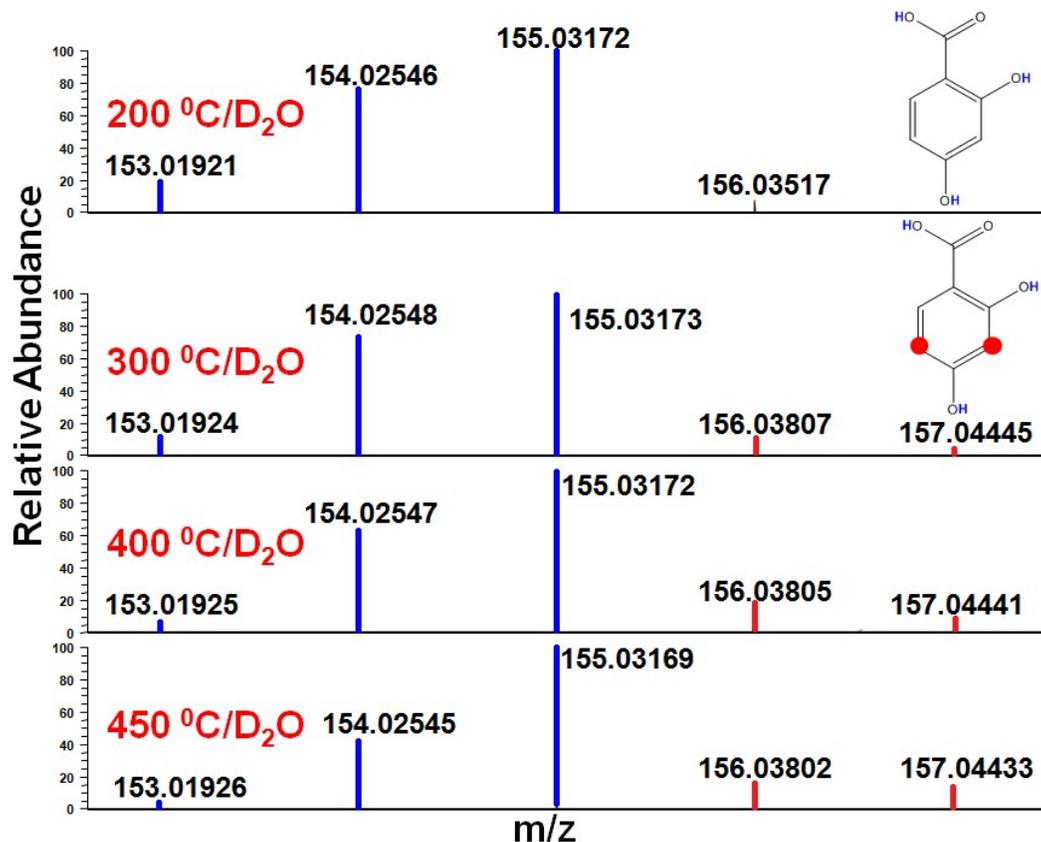


Fig. S1. In-ESI source H/D exchange series of DHB-2,4 at different temperatures of desolvation capillary: 200 °C (blue lines), 300, 400 and 450 °C (additional peaks are colored in red). Red dots in the structural formulas designate the feasible sites of deuteriation in accordance with keto-enol tautomerism and mesomeric substituent effects in the aromatic ring.

^2H NMR spectroscopy

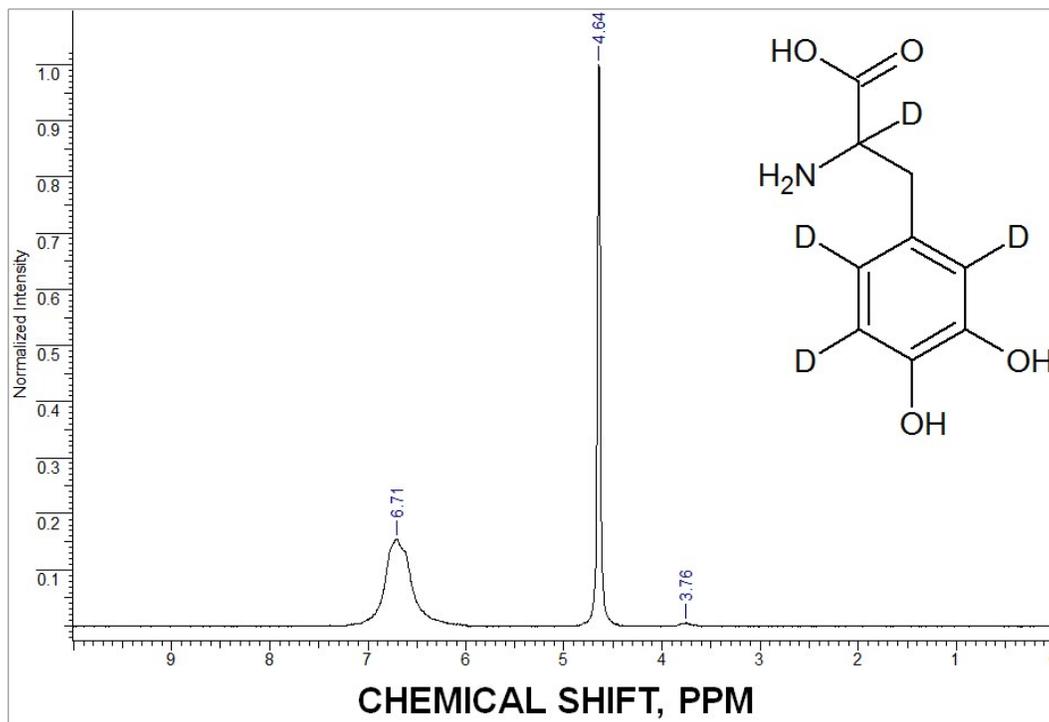


Fig. S2. ^2H NMR spectra of DOPA labeled under basic catalysis.

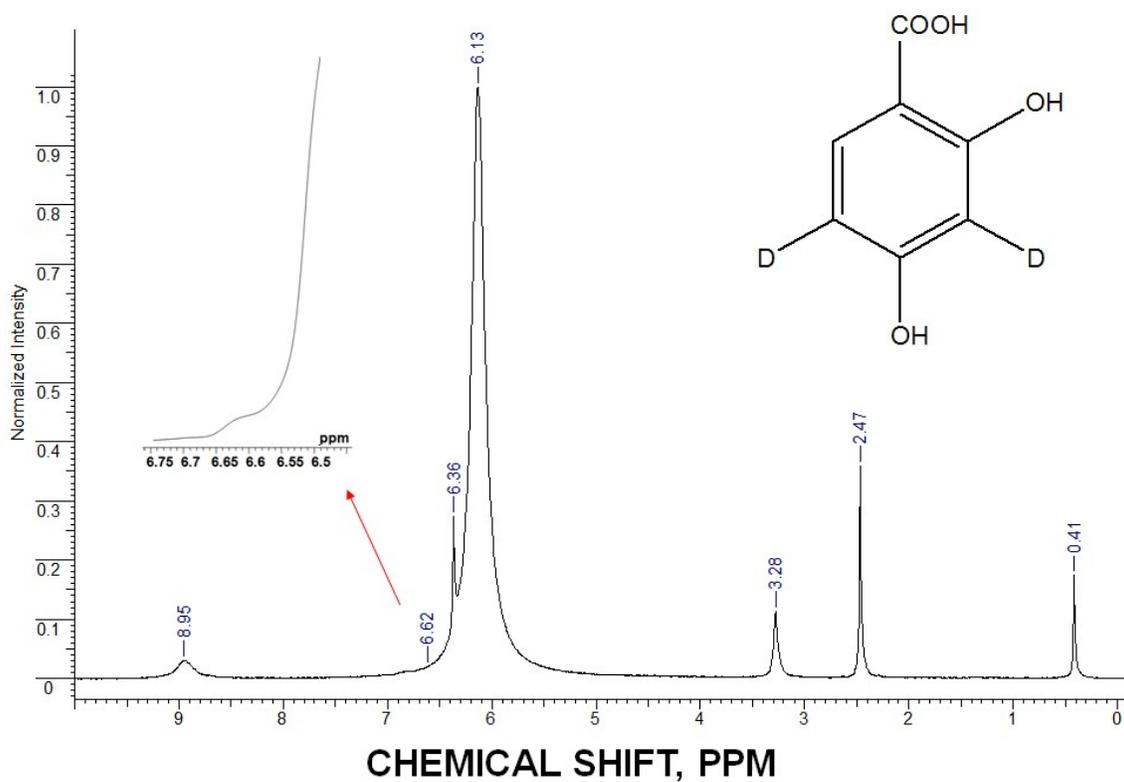


Fig. S3. ^2H NMR spectra of 2-4 dihydroxybenzoic acid labeled under basic catalysis. Spectrum includes signals of C_6D_{12} (0.44 ppm), CDCl_3 (6.36 ppm), which were used as external standards.

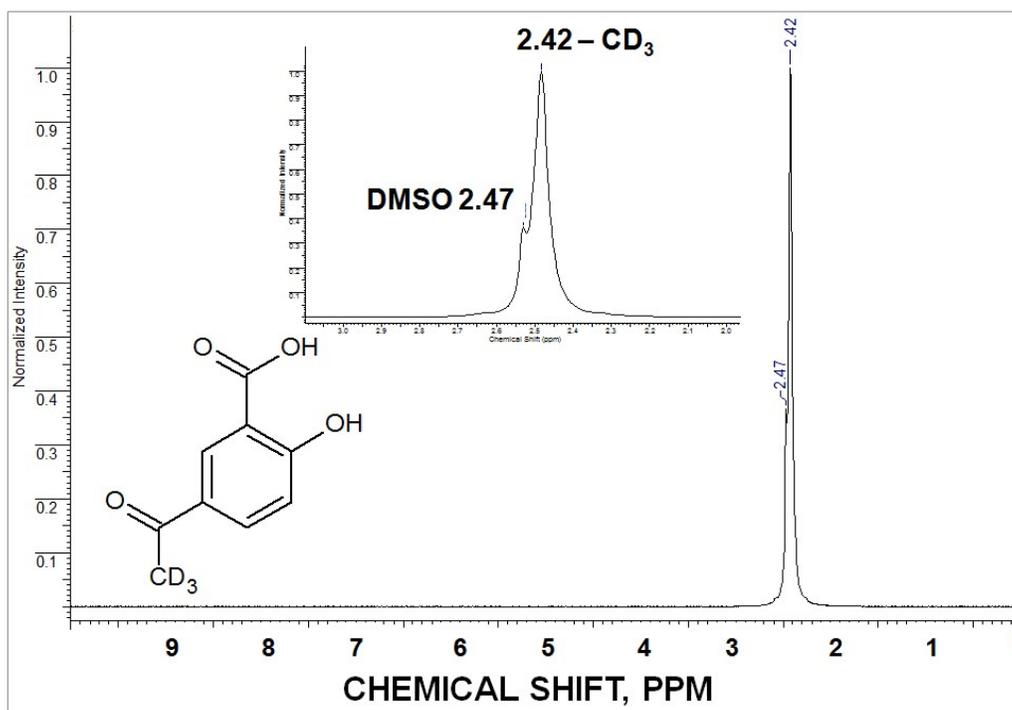


Fig. S4. ^2H NMR spectra of 5-acetylsalicylic acid

Mass-spectrometry of labeled compound

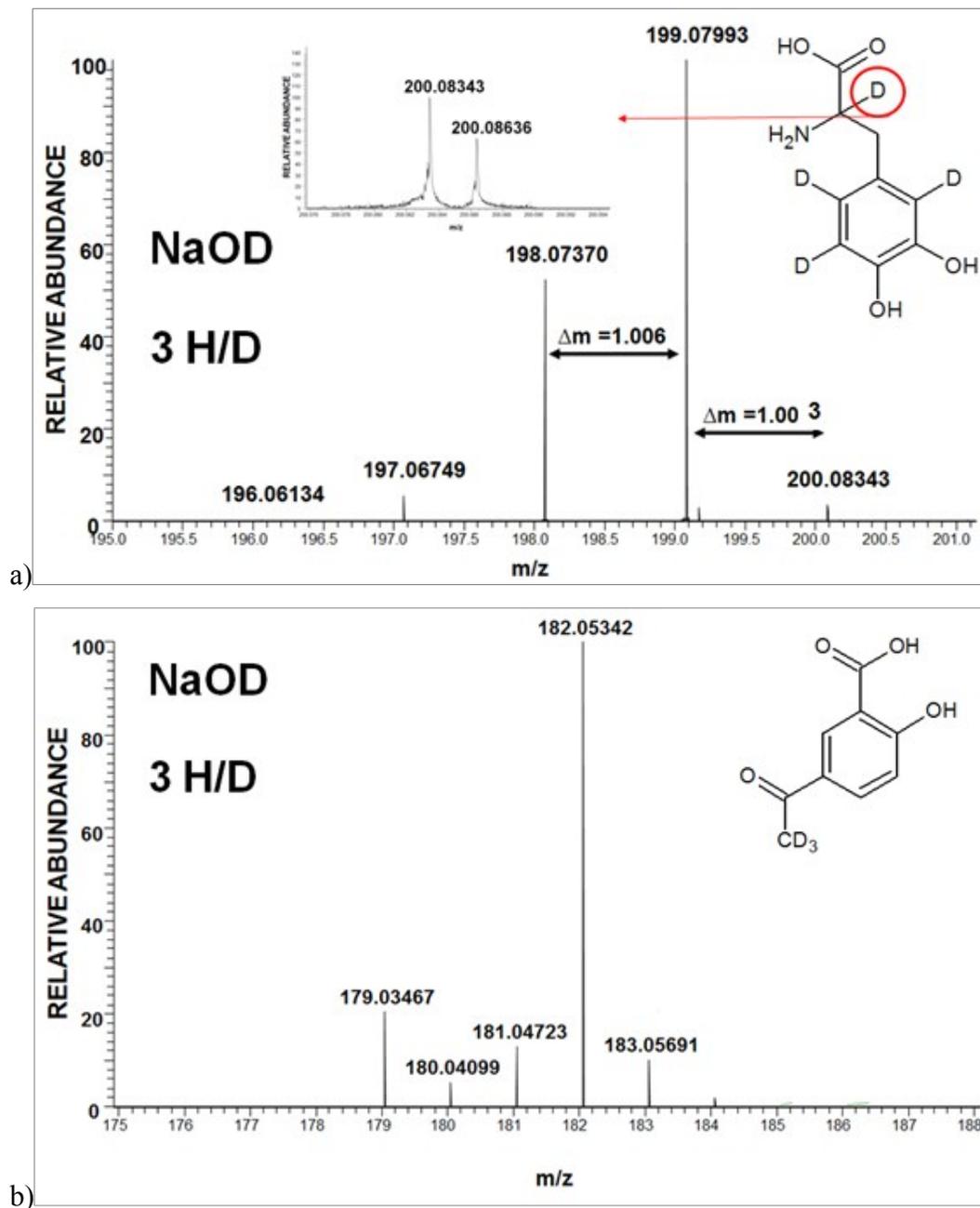


Fig. S5. Mass-spectra of a) DOPA b) 5-acetylsalicylic acid labeled under basic condition.