

Liquid Electron Ionization-Mass Spectrometry as a Novel Strategy for integrating Normal-Phase Liquid Chromatography with Low and High-Resolution Mass Spectrometry

Nicole Marittimo^a, Genny Grasselli^a, Adriana Arigò^a, Giorgio Famiglini^a, Marco Agostini^b, Caterina Renzoni^b, Pierangela Palma^{a,c}, Achille Capiello^{a,c,*}

^a University of Urbino Carlo Bo, Department of Pure and Applied Sciences, Piazza Rinascimento 6, 61029 Urbino, Italy

^b Laboratorio di Tossicologia, A.S.T. AV1, Via Lombroso 15, 61122 Pesaro, Italy

^c Vancouver Island University, Department of Chemistry, B360-R306, 900 Fifth St., Nanaimo, BC, Canada V9R 5S5

*Corresponding author: Achille Capiello, University of Urbino Carlo Bo, Department of Pure and Applied Sciences, Piazza Rinascimento 6, 61029 Urbino, Italy. Phone: +390722303344. E-mail address: achille.capiello@uniurb.it

Table of Contents

Figure S1 a-b. Low-resolution spectra of cannabinoids.

Figure S2 a-c. Low-resolution spectra of phthalates.

Figure S3 a-d. Low-resolution spectra of phenols.

Figure S4 a-b. High-resolution spectra of cannabinoids.

Figure S5 a-c. High-resolution spectra of phthalates.

Figure S6 a-d. High-resolution spectra of phenols.

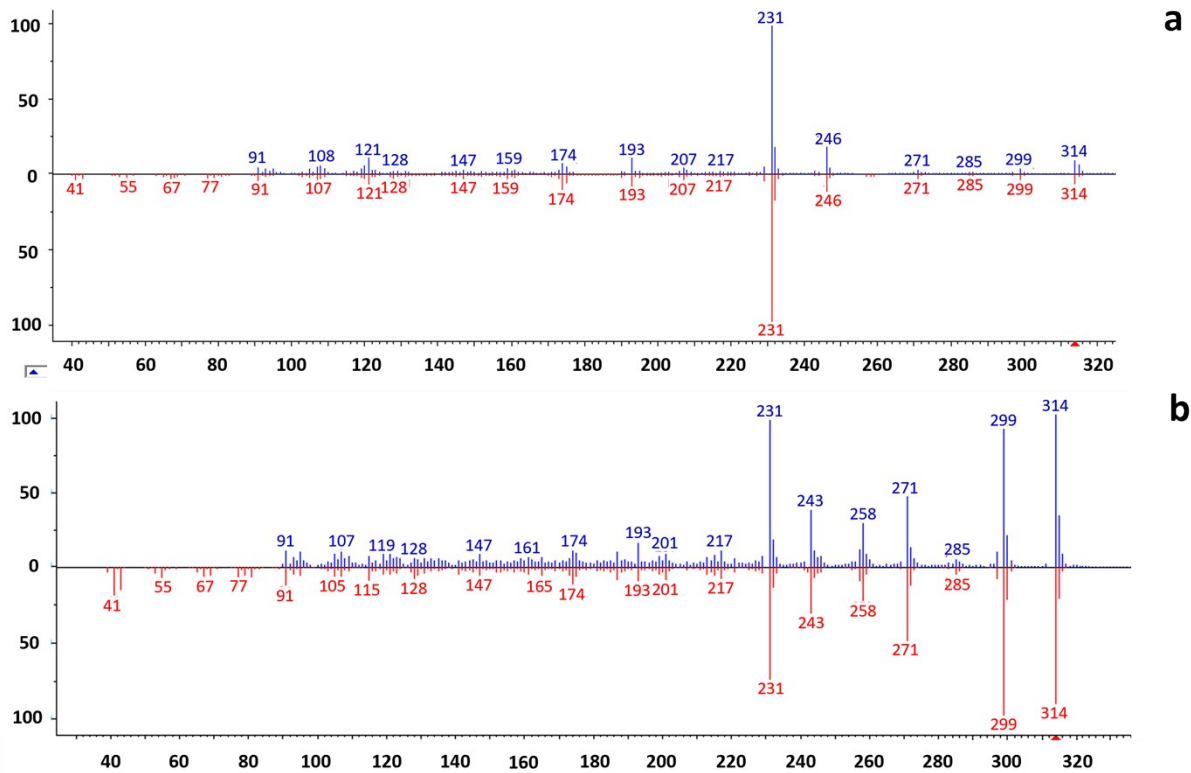


Figure S1 a-b. Low-resolution experiments. Comparison between the recorded and the NIST library reference spectra of a) CBD and b) THC. Top: experimental spectrum; Bottom: NIST reference spectrum. THC was identified with a matching factor of 790, and reverse match of 850; CBD with a matching factor of 820, and reverse match of 910.

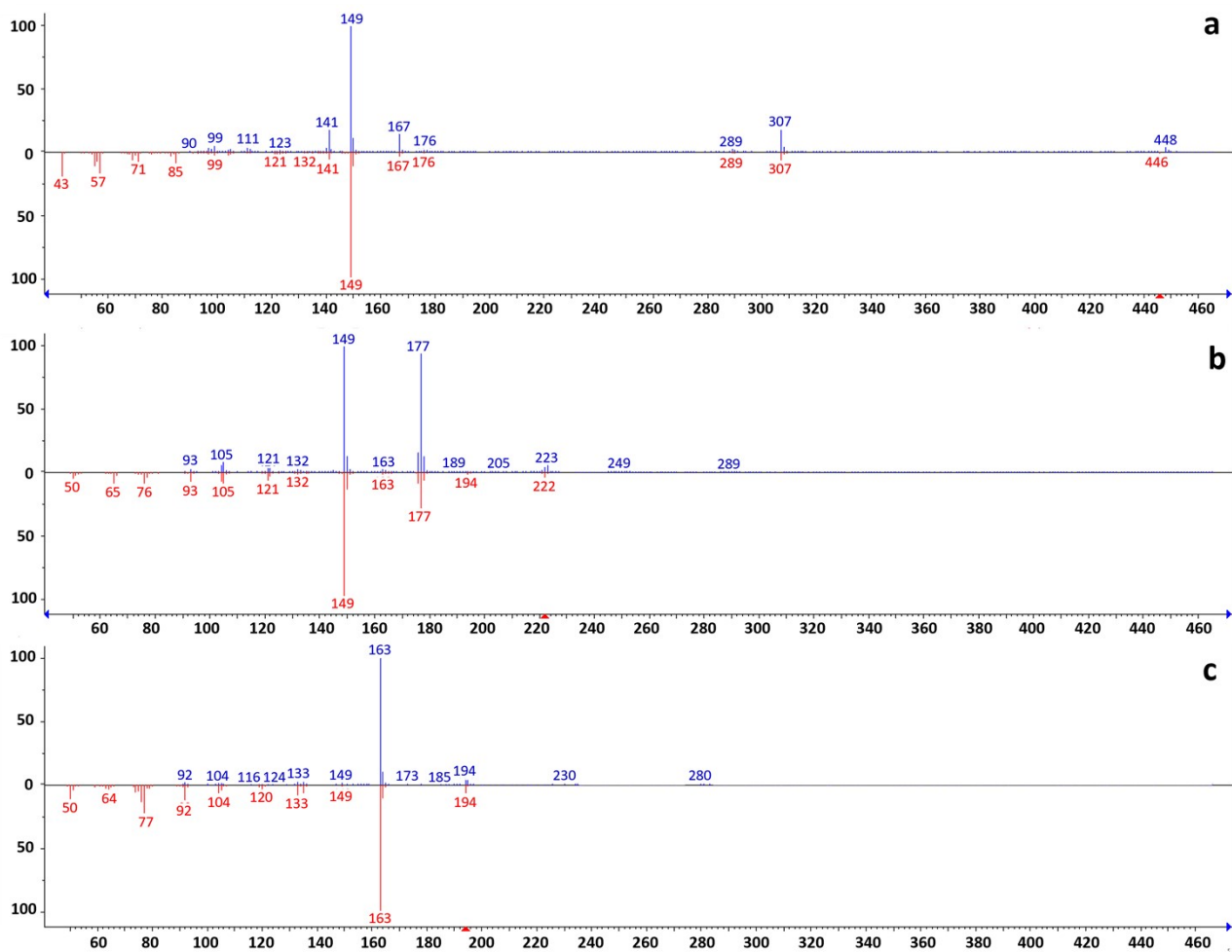


Figure S2 a-c. Low-resolution experiments. Comparison between the recorded and the NIST library reference spectra of a) diisodecyl phthalate; b) diethyl phthalate; c) dimethyl phthalate. Top: experimental spectrum; Bottom: NIST reference spectrum. Diisodecyl phthalate was identified with a matching factor of 771, and reverse match of 856; diethyl phthalate with a matching factor of 881, and reverse match of 891; dimethyl phthalate with a matching factor of 721, and reverse match of 840.

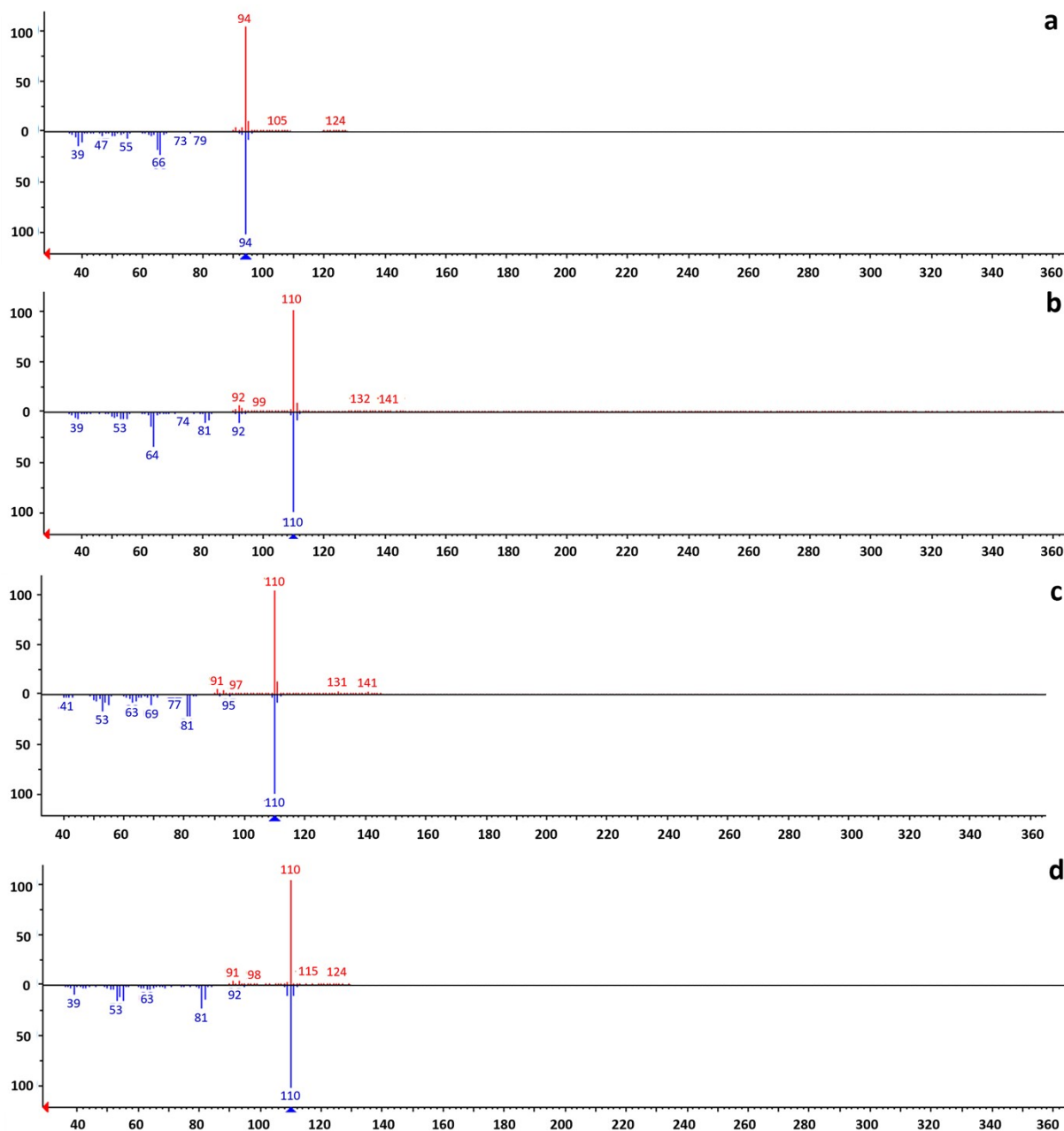


Figure S3 a-d. Low-resolution experiments. Comparison between the recorded and the NIST library reference spectra of a) phenol; b) catechol; c) resorcinol; d) hydroquinone. Top: experimental spectrum; Bottom: NIST reference spectrum. Phenol was identified with a matching factor of 700, and reverse match of 980; catechol with a matching factor of 850, and reverse match of 648; resorcinol with a matching factor of 636, and reverse match of 936; hydroquinone with a matching factor of 532, and reverse match of 888.

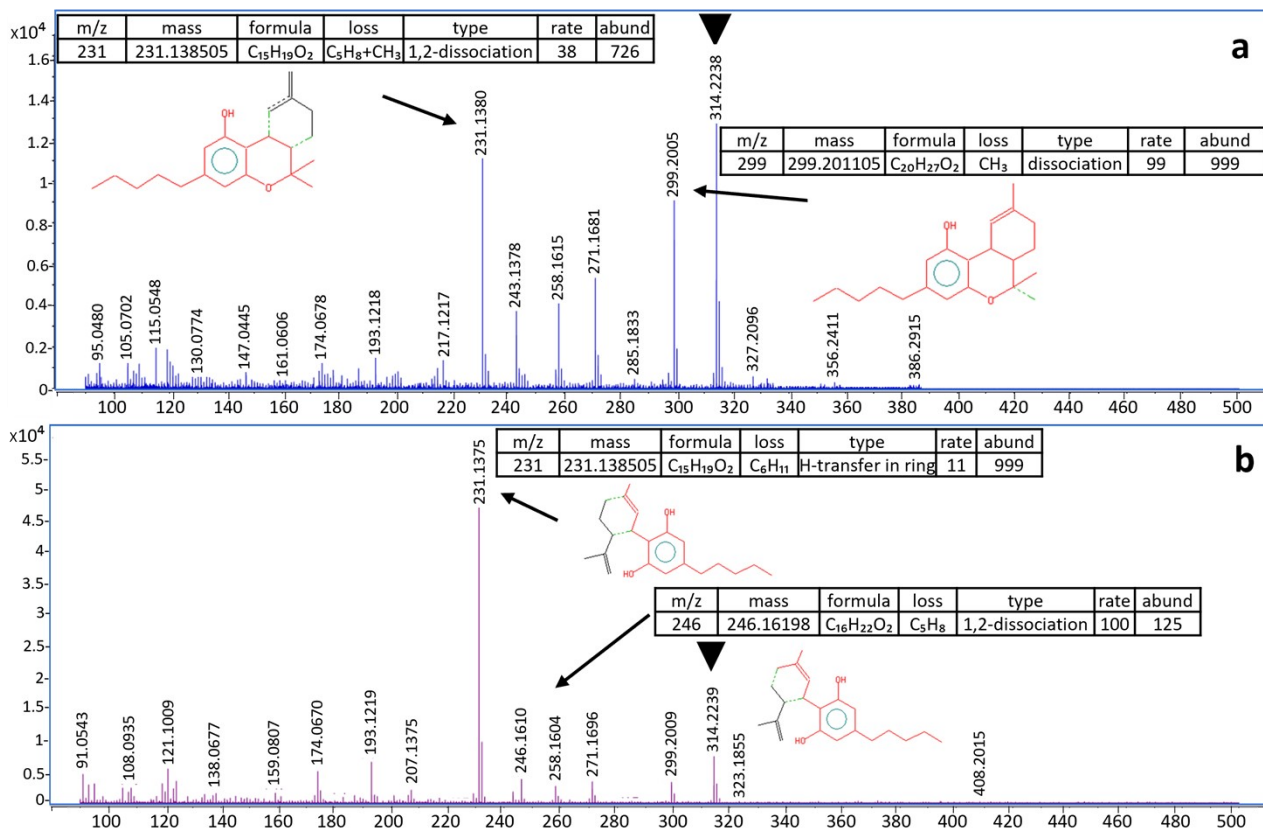


Figure S4 a-b. Recorded EI high-resolution full scan spectra of a) THC, b) CBD and assignment of the main fragments according to the MS Interpreter utility developed by NIST. Molecular ions are indicated by the black triangle.

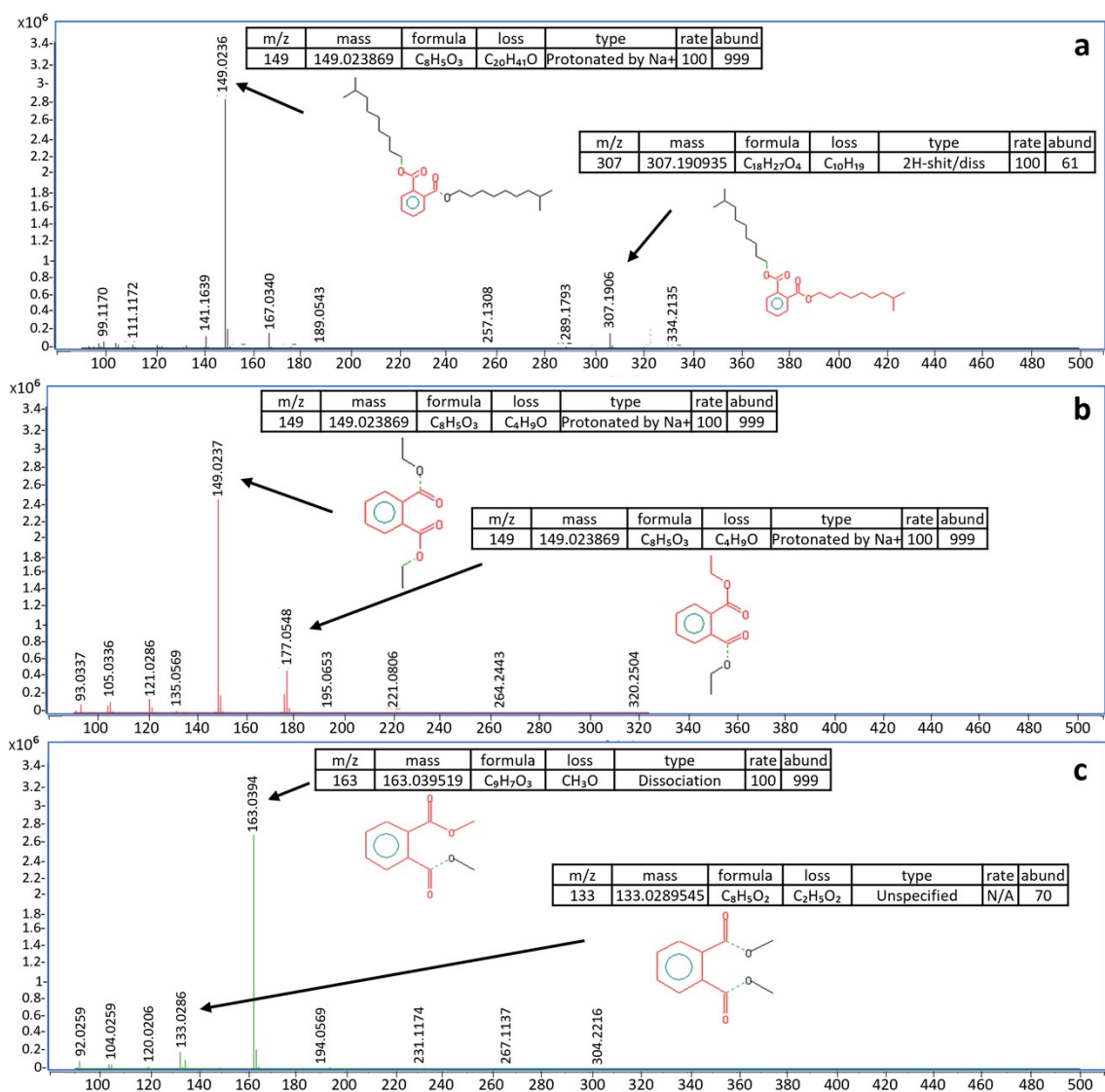


Figure S5 a-c. Recorded EI high-resolution full scan spectra of a) diisodecyl phthalate; b) diethyl phthalate; c) dimethyl phthalate and assignment of the main fragments according to the MS Interpreter utility developed by NIST.

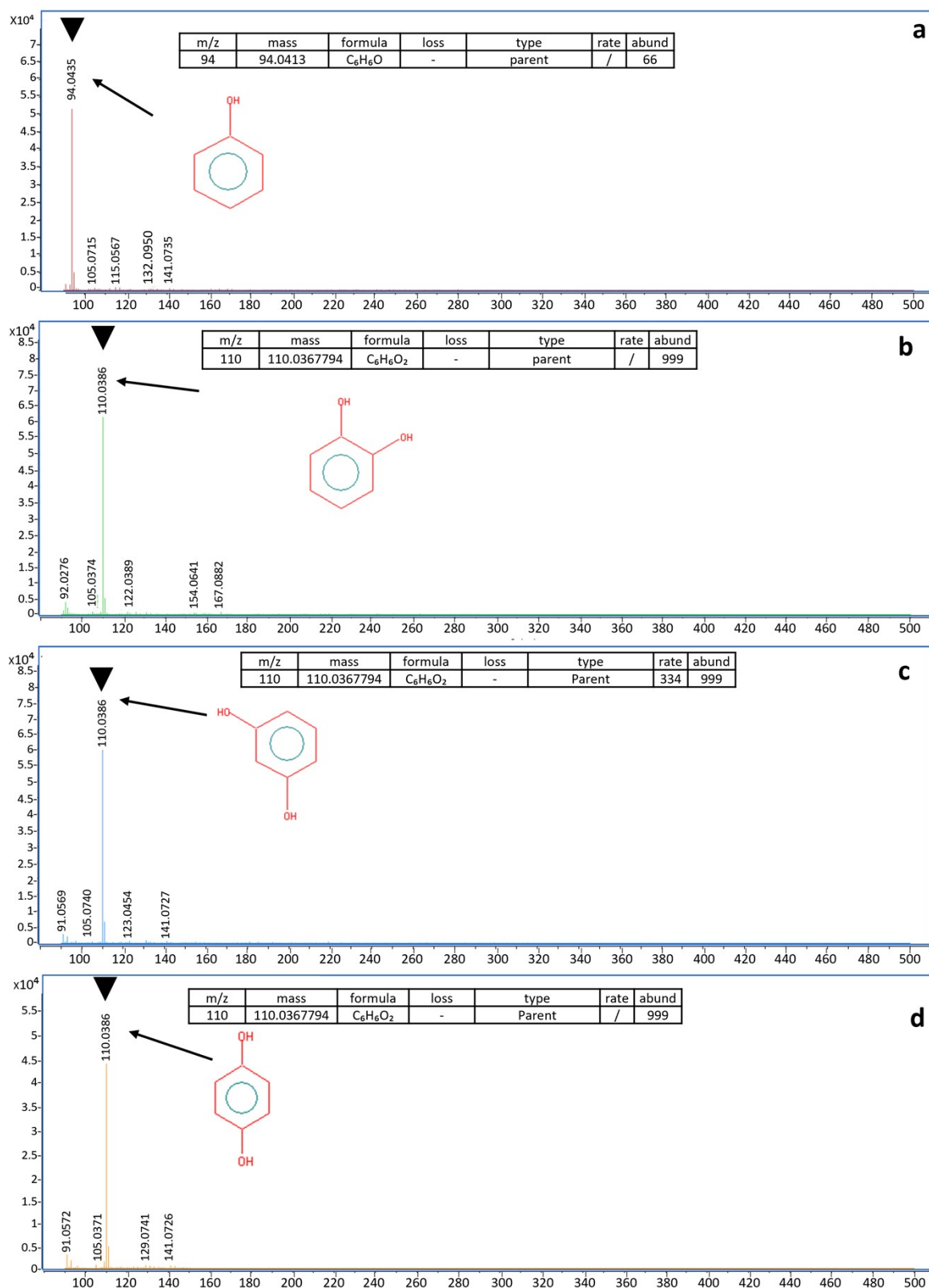


Figure S6 a-d. Recorded EI high-resolution full scan spectra of a) phenol; b) catechol; c) resorcinol; d) hydroquinone and assignment of the main fragments according to the MS Interpreter utility developed by NIST. Molecular ions are indicated by the black triangle.