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## Electrospray Tandem Mass Spectrometry Of The Dimethylimidazolesulfonyl Derivatives Of Phenols, Polycyclic Aromatic Hydrocarbon Metabolites, And Estrogens

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A novel derivatization method employing 1,2-dimethylimidazole-4-sulfonyl chloride (DMIS) to improve the mass spectrometric response for phenolic compounds in electrospray ionization mass spectrometry (ESI-MS) is described. Several environmentally relevant compounds, including chlorophenols, alkylphenols, hydroxy-polycyclic aromatic hydrocarbons (OHPAHs), and steroidal estrogens, were selected to evaluate this technique. A facile derivatization procedure employing DMIS results in dimethylimidazole sulfonyl (DMIS) derivatives that are stable in aqueous solution. When analyzed by positive-ion electrospray ionization mass spectrometry, the DMIS derivatives showed intense  $[M+H]^+$  ions. Product-ion spectra of the  $[M+H]^+$  ions of simple phenols were dominated by ions representing the dimethylimidazole-sulfonyl and dimethylimidazole moieties, whereas product-ion spectra of the DMIS derivatives of OHPAHs with three or more fused aromatic rings showed prominent  $ArO^+$  ions, the relative intensity of which increased with the number of rings. The DMIS derivatives of the selected phenols showed excellent chromatographic properties, and could readily be analyzed by LC-MS/MS the multiple-reaction-monitoring mode. For example, 1-hydroxypyrene, a widely used biomarker for monitoring human exposure to polycyclic aromatic hydrocarbons, can be determined as its DMIS derivative by positive-ion LC-ESI-MS/MS in the selected-reaction-monitoring mode with high sensitivity ( $< 10$  pg on column). Similarly, the DMSI derivatives of 17 $\beta$ -estradiol, estrone, and 17 $\alpha$ -ethenylestradiol were analyzed with pg sensitivity. These results suggest a broad utility of the use of DMIS derivatization for the determination of trace levels of phenolic compounds by LC/ESI-MS/MS.