ALKALOIDS FROM *Arundo donax* L. X. MASS SPECTROMETRIC FRAGMENTATION OF ARUNDAMINE AND ARUNDANINE

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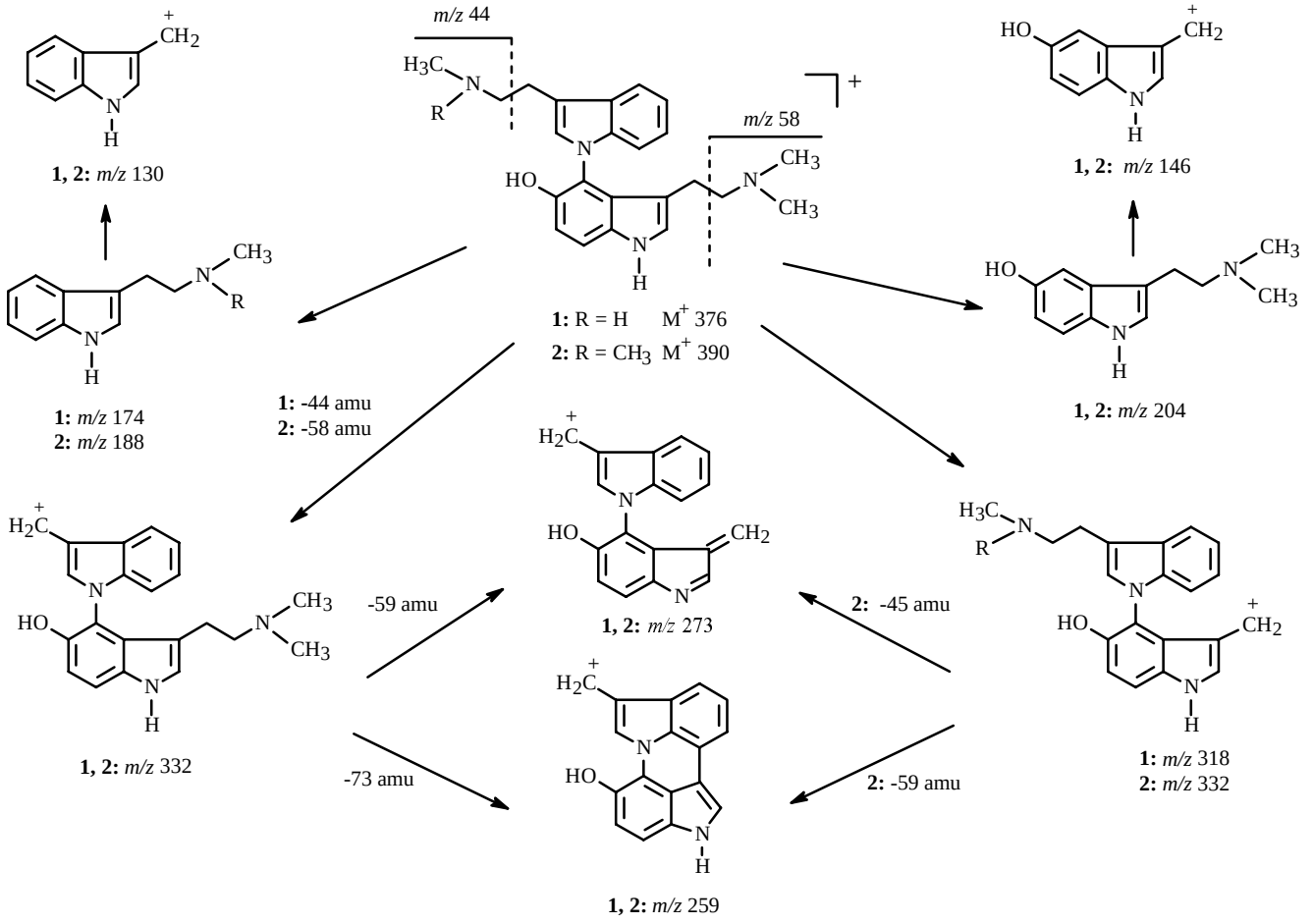
The isolation from roots of *Arundo donax* L. (cane reed) of two dimeric indole bases has been reported [1]. The structure of 3-*N*-dimethylaminoethyl-5-hydroxy-4-(3′-*N*′-methylaminoethylindol-1′-yl)indole was established for arundamine (**1**) based on IR, UV, mass, and NMR spectra in addition to an x-ray structure analysis [2]. The second dimeric alkaloid from this plant, arundanine (**2**) is the N-methyl derivative of arundamine [3]. The mass-spectrometric fragmentation of these compounds was studied in light of the structures established for them (Scheme 1).



Scheme 1. Mass-spectrometric fragmentation of arundamine and arundanine.

The molecular ion in the mass spectrum of arundamine appears as a weak peak at 376 amu whereas the peak for $[M]^+$ of arundanine with *m*/*z* 390 is strong.

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The compounds differ in molecular weight by 14 amu. Therefore, the fragmentation of these compounds is observed to be completely parallel. Thus, elimination from the side chains of a C_2H_6N fragment (44 amu) produces strong peaks with *m*/*z* 332 (arundamine) and 346 (arundanine). Loss of a C_3H_8N fragment (58 amu) in turn leads to ions with *m*/*z* 318 (**1**) and 332 (**2**), respectively. Loss of the side chains in both instances gives rise to peaks with *m*/*z* 273 and 259. Elimination of fragments of 28 amu converts them to ions with *m*/*z* 245 and 231, respectively.

It should be noted that one of the fragmentation pathways of $[M]^+$ is formation of fragments of certain monomers with *m*/*z* 174 (dipterin), 188 (N-methyltryptamine), and 204 (bufotenine) [4, 5]. The molecular ions of these monomers then decompose along the fragmentation pathway of indole derivatives to produce ions with *m*/*z* 146, 131, 130, etc.

Ions with *m*/*z* 44, 58, and 73 form from fragments of the side chains.

The proposed fragmentation pattern seems to us to be the most probable one.

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