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Database on the relationship between MS/MS fragmentation pattern and chemical structure of soyasaponin in soybean

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Profile analysis is a new technique using a small amount of soybean extract to elucidate the chemical structures of unknown soyasaponins without purification and NMR analysis. It consists of "genetic analysis" (polymorphism analysis of codominant, dominant, and recessive acting saponin biosynthetic genes) and "instrumental analysis" (TLC banding pattern, HPLC elution time, UV spectrum of HPLC peak, fragment pattern of MS and MS/MS and acid hydrolysis). Seed saponin compositions correspond exactly with the genetic polymorphisms, depending on combinations of at least 19 different saponin biosynthetic genes. For example, the *Sg-3* gene encodes UDP-glucosyltransferase which transfers a glucose residue at the third terminal position of the C-3 sugar chain of soyasaponin glycosides. The *Sg-6* gene controls Sg-6 saponin production which contains a specific soyasapogenol H, I, or J as the aglycone. The *sg-3* genotype soybeans produce no DDMP-ag (Glc-Gal-GlcUA-DDMP) but it accumulates minor soyasaponin DDMP-γg (Gal-GlcUA-DDMP). The *sg-6* line cannot produce Sg-6 saponins. The *sg-3/sg-6* double recessive line accumulates DDMP-γg but cannot produce either DDMP-ag or Sg-6 saponins. If both DDMP-ag and Sg-6 saponins were detected simultaneously, it should be *Sg-3/Sg-6* line. Neither DDMP-ag nor Sg-6 J-ag is detected in the *sg-3/Sg-6* line which should accumulate new Sg-6 saponin J-γg (Gal-GlcUA-soyasapogenol J). We have collected over 200 soyasaponin component profile database on the relationship between MS/MS fragmentation pattern and chemical structure. The chemical structures of new and unknown soyasaponins in mutant soybeans can be elucidated by the profile analysis.