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Michely, JA, Helfer, AG, Brandt, SD, Meyer, MR and Maurer, HH

Metabolism of the new psychoactive substances N,N-diallyltryptamine (DALT) and 5-methoxy-DALT and their detectability in urine by GC-MS, LC-MS (n) , and LC-HR-MS-MS

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Analytical and Bioanalytical Chemistry

**Electronic Supplementary Material** 

Metabolism of the new psychoactive substances *N*,*N*-diallyltryptamine (DALT) and 5-methoxy-DALT and their detectability in urine by GC-MS, LC-MS<sup>n</sup>, and LC-HR-MS/MS

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**Fig. S1** LC-HR-MS/MS spectra of DALT and its phase I metabolites arranged according to their precursor values, proposed chemical structures, accurate masses, calculated elemental formulas, and mass error values in parts per million (ppm) rounded to two decimals











**Fig. S2** LC-HR-MS/MS spectra of 5-MeO-DALT and its phase I metabolites arranged according to their precursor values, proposed chemical structures, accurate masses, calculated elemental formulas, and mass error values in parts per million (ppm) rounded to two decimals



DALT-M (N-dealkyl-HO-aryl-glucuronide) isomer 1; RT 2.7



**Fig. S3** LC-HR-MS/MS spectra of DALT phase II metabolites arranged according to their precursor values, proposed chemical structures, accurate masses, calculated elemental formulas, and mass error values in parts per million (ppm) rounded to two decimals





5-MeO-DALT-M (N-dealkyl-HO-alkyl-glucuronide); RT 3.0





**Fig. S4** LC-HR-MS/MS spectra of 5-MeO-DALT phase II metabolites arranged according to their precursor values, proposed chemical structures, accurate masses, calculated elemental formulas, and mass error values in parts per million (ppm) rounded to two decimals