

# Supplementary Materials: Cleaving Ergot Alkaloids by Hydrazinolysis—a Promising Approach for a Sum Parameter Screening Method

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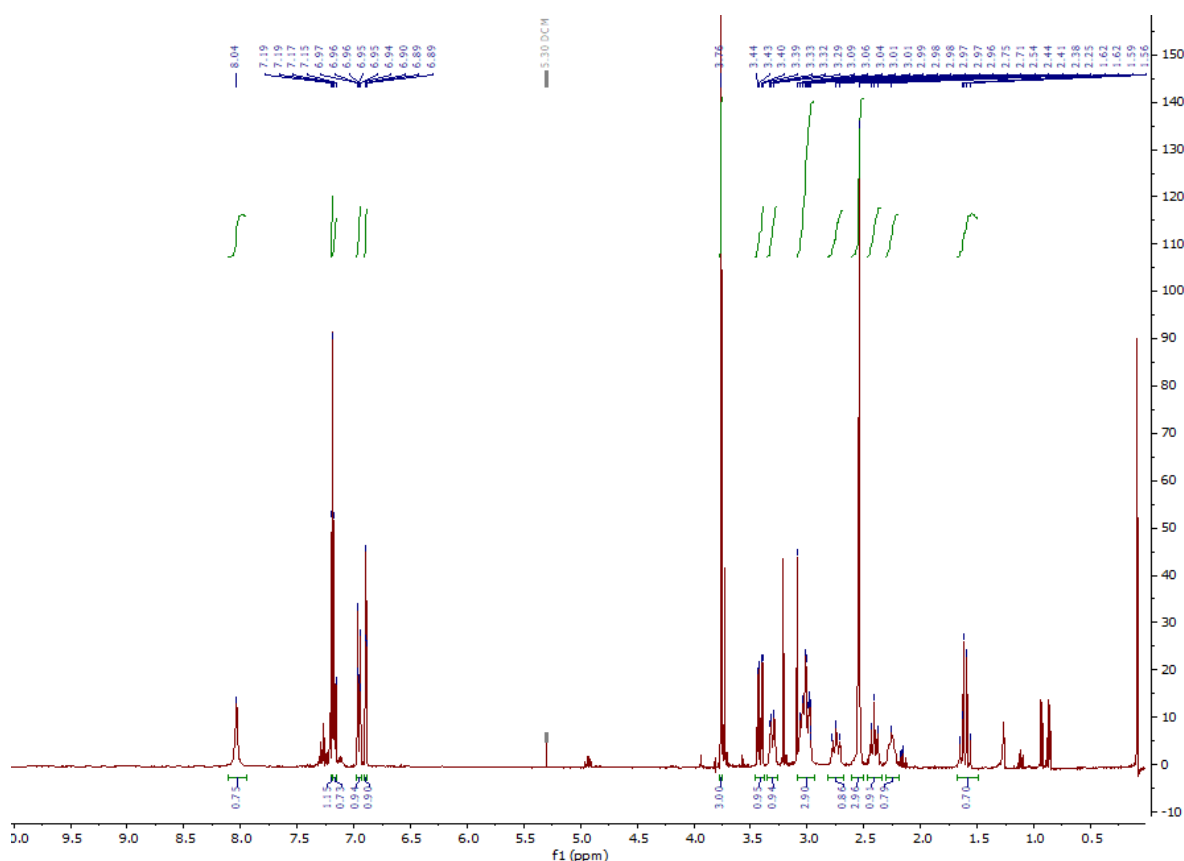


Figure S1. <sup>1</sup>H-NMR of dihydrolysergic acid methylester (I).

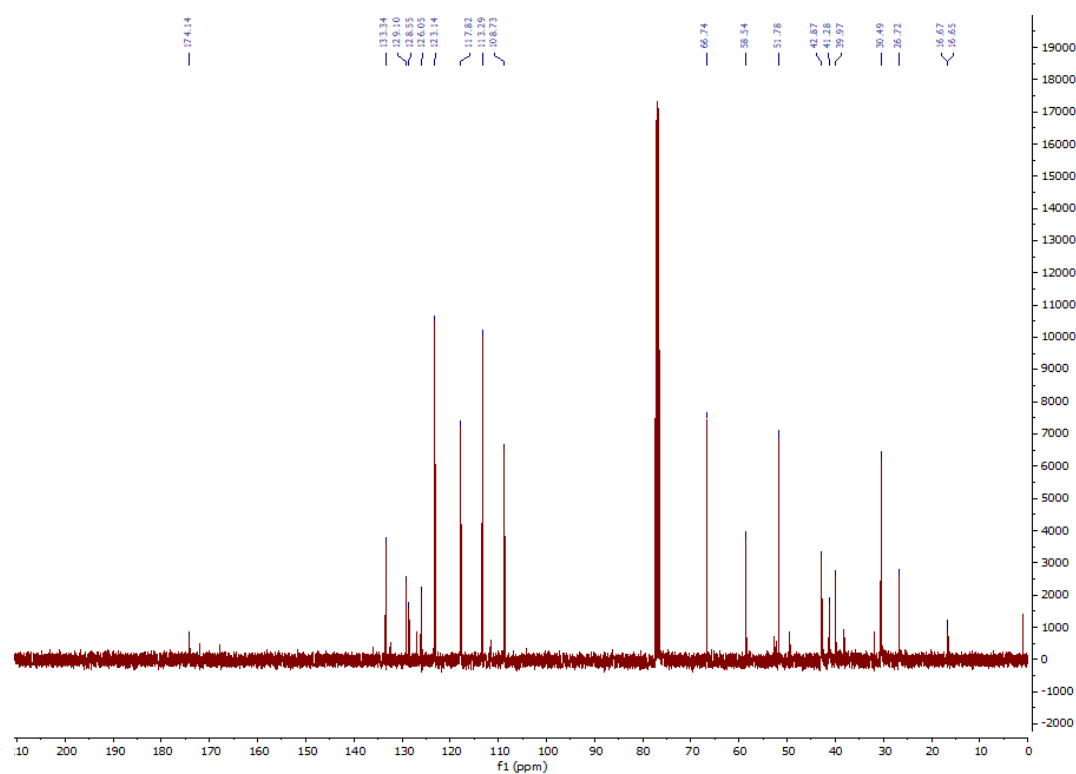


Figure S2.  $^{13}\text{C}$ -NMR of dihydrolysergic acid methylester (I).

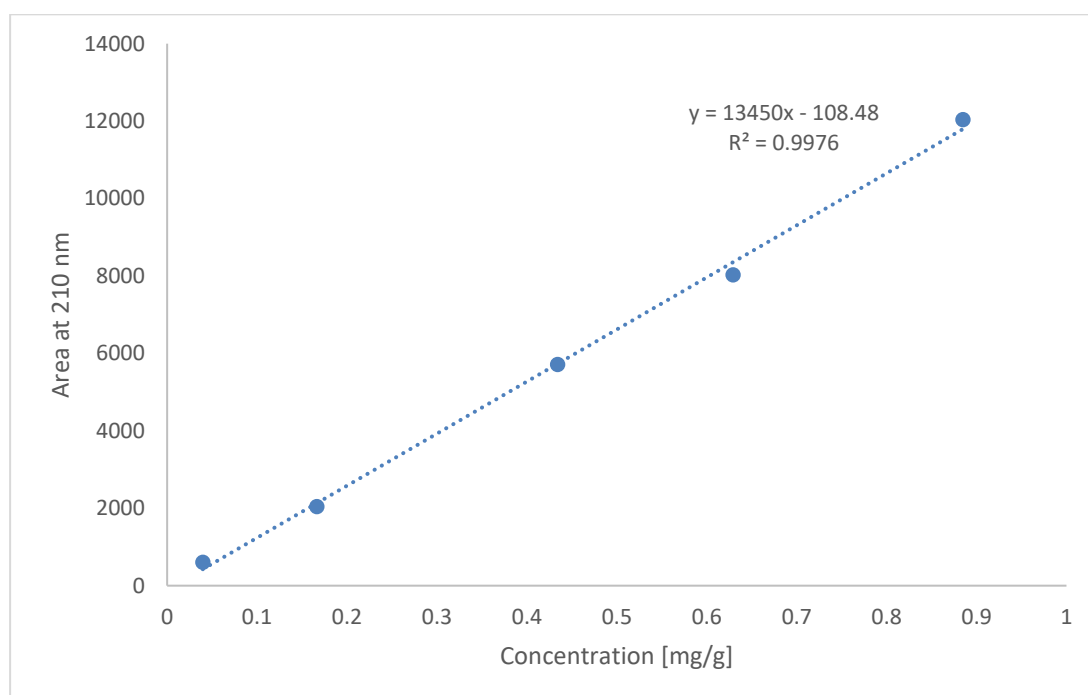


Figure S3. Exemplary calibration curve for the yield determination of I.

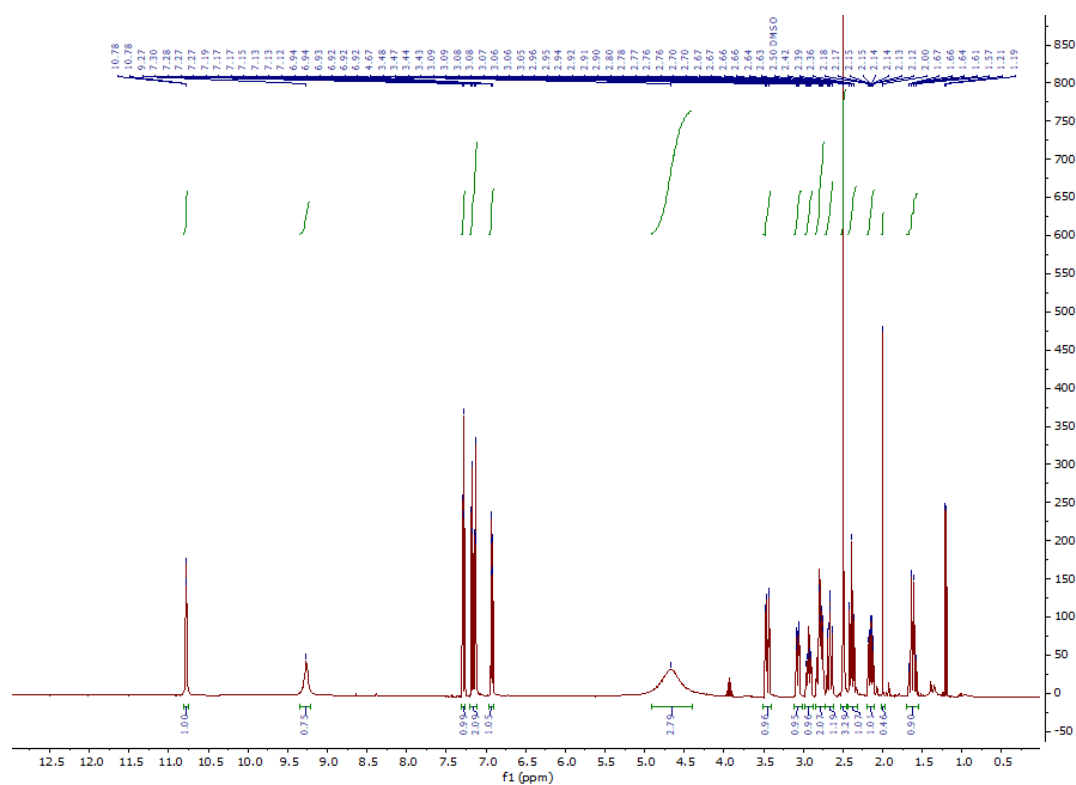


Figure S4.  $^1\text{H}$ -NMR of dihydrolysergic acid hydrazide (IV).

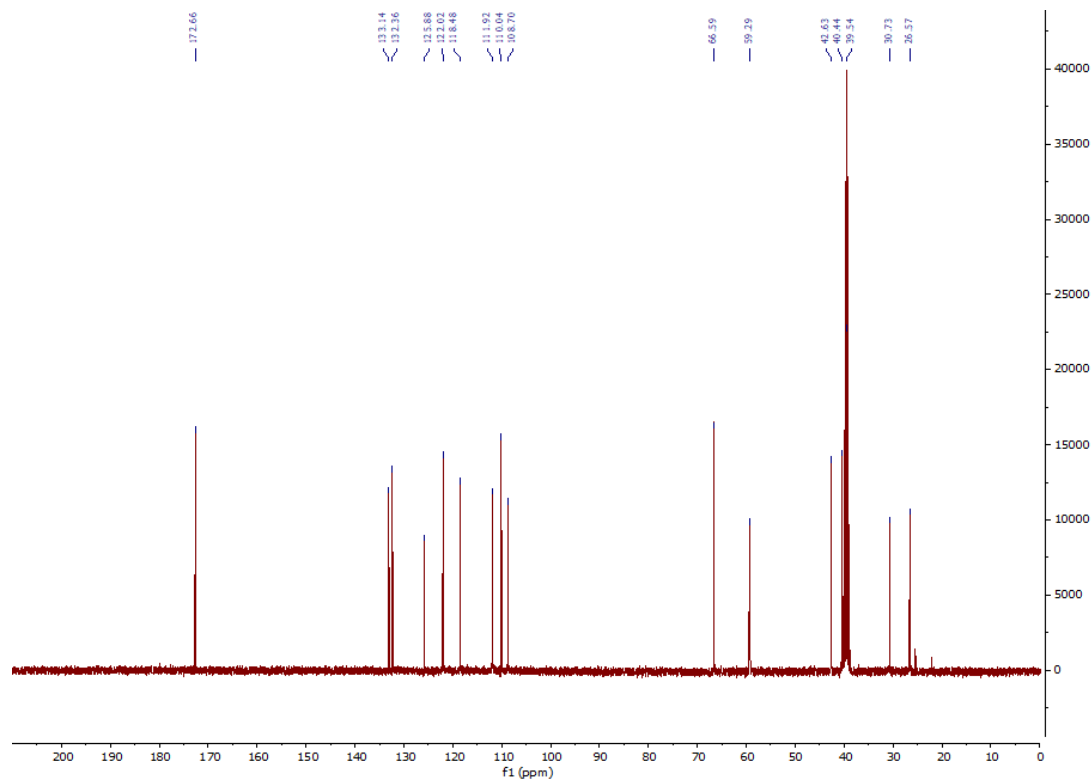
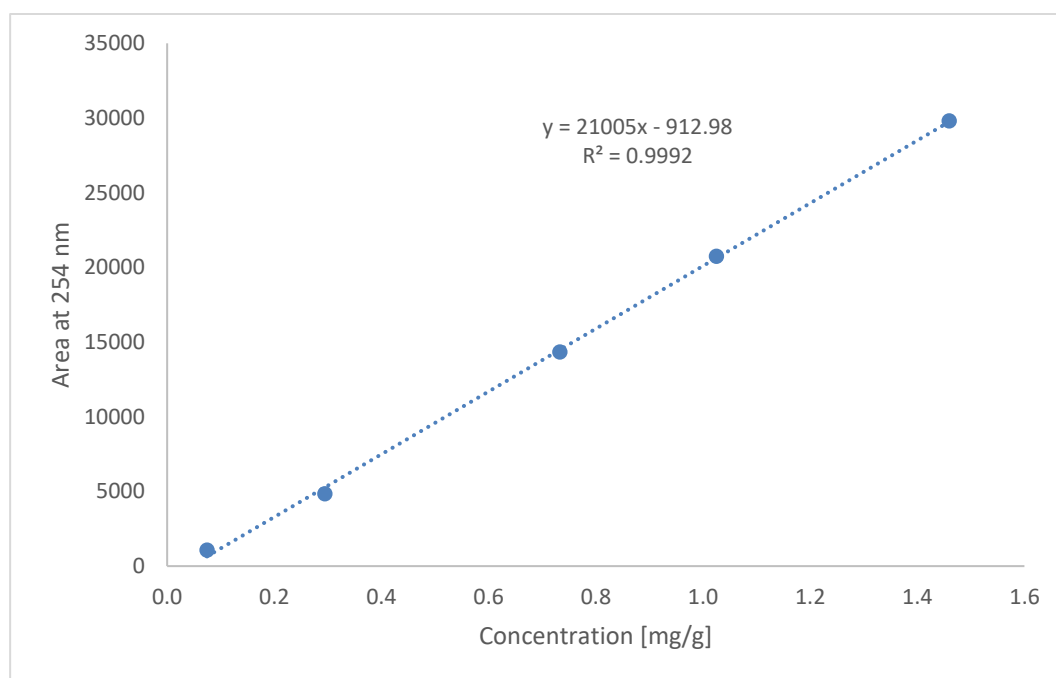
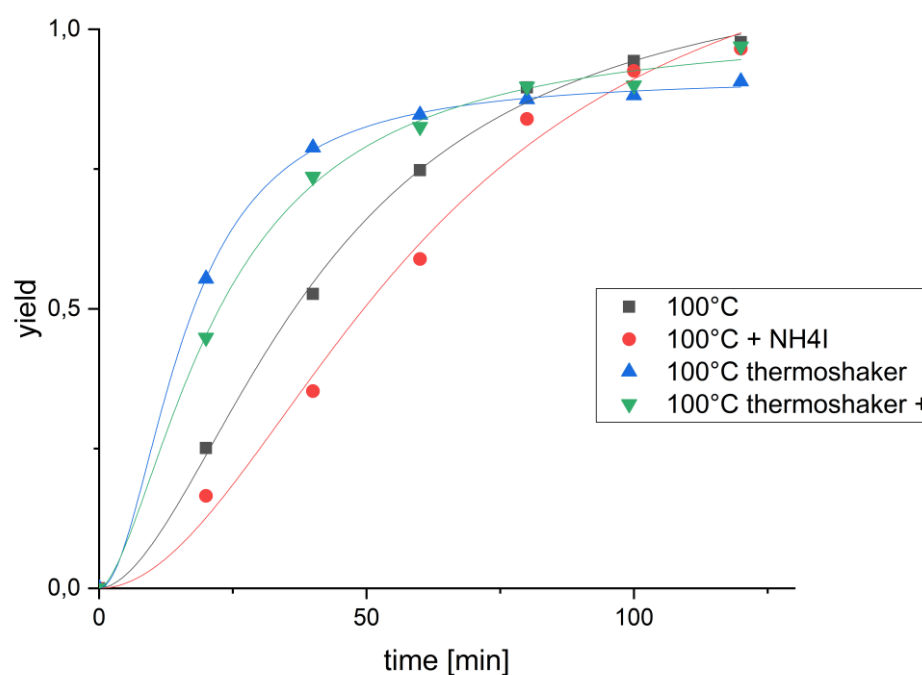


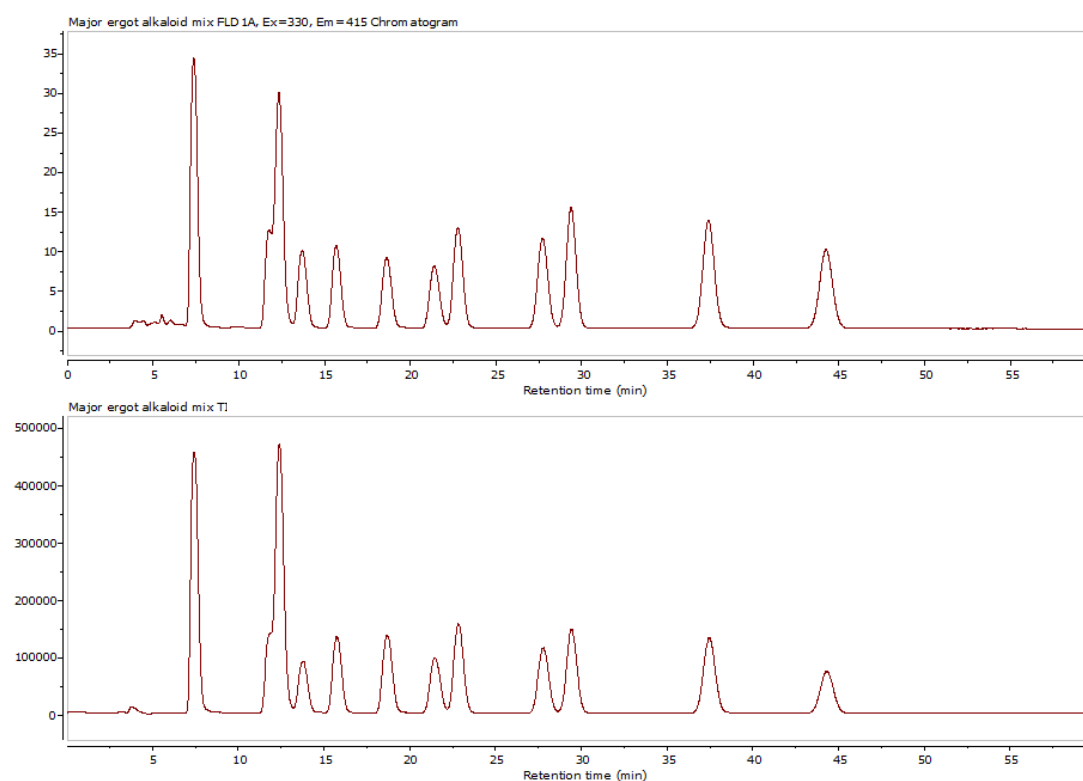
Figure S5.  $^{13}\text{C}$ -NMR of dihydrolysergic acid methylester (IV).



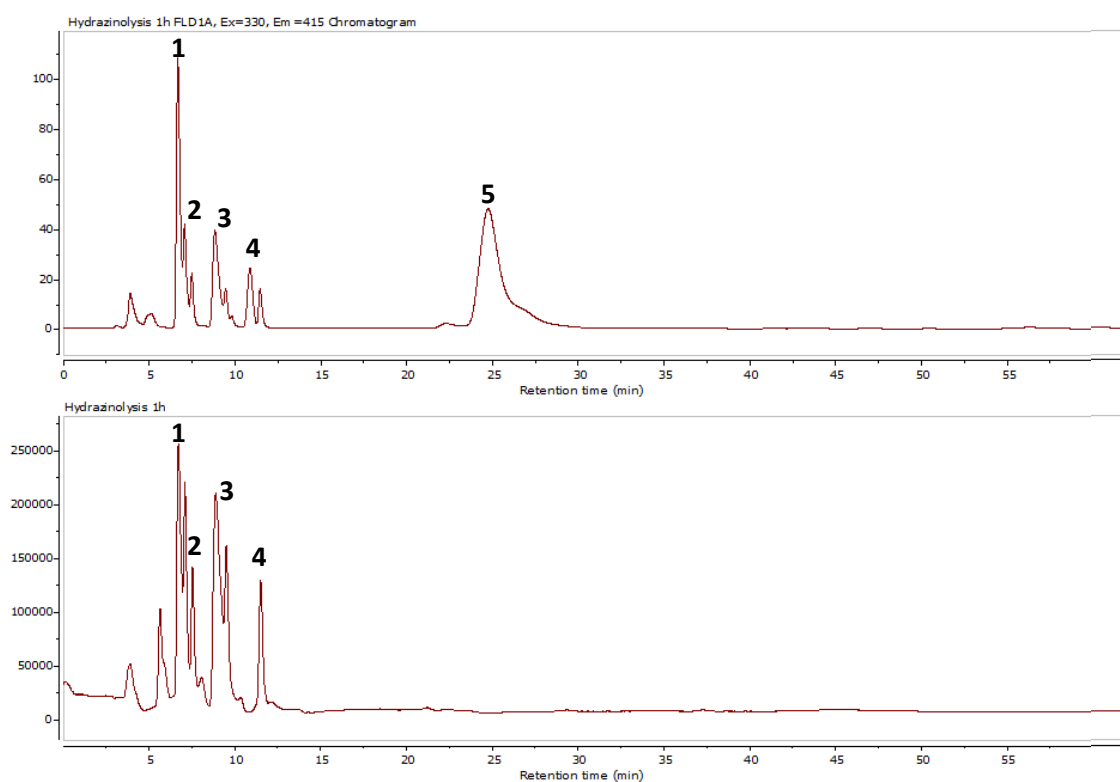
**Figure S6.** Exemplary calibration curve for the yield determination of IV.



**Figure S7:** Yields of IV measured by HPLC-UV (254 nm) against reaction time at 100°C. The reaction was conducted either in a Schlenk flask heated in an oil bath or in headspace vials heated and stirred in a thermoshaker.



**Figure S1:** HPLC-FLD (top) and -MS (bottom) (SIM masses of the major ergot alkaloids ( $m/z$  ( $M+H$ )<sup>+</sup> = 326.4; 576.7; 548.6; 582.7; 610.7; and 562.1) and lysergic acid hydrazide ( $m/z$  ( $M+H$ )<sup>+</sup> = 283.1)) of the ergot alkaloid mix solution before hydrazinolysis.



**Figure S9:** HPLC-FLD (top) and -MS (bottom) (SIM masses of the major ergot alkaloids ( $m/z$  ( $M+H$ )<sup>+</sup> = 326.4; 576.7; 548.6; 582.7; 610.7; and 562.1) and lysergic acid hydrazide ( $m/z$  ( $M+H$ )<sup>+</sup> = 283.1) of the ergot alkaloid mix solution after hydrazinolysis (same HPLC conditions as in S8). 1 and 3 are peaks of the two isomers of lysergic acid hydrazide. 2 is unreacted ergometrine and 4 unreacted ergometrinine. 5 is always present, when hydrazine hydrate is heated (also without ergot alkaloids).