

Crystallographic and NMR Investigation on Ergometrine and Methylegometrine, Two Alkaloids from *Claviceps purpurea*

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Supplementary data contents

S3	¹ H NMR of ergometrine maleate 6
S4	¹³ C NMR of ergometrine maleate 6
S5	COSY of ergometrine maleate 6
S6	HSQC of ergometrine maleate 6
S7	¹ H- ¹³ C HMBC of ergometrine maleate 6
S8	NOESY of ergometrine maleate 6
S9	¹ H- ¹⁵ N HMBC of ergometrine maleate 6
S10	¹ H NMR of methylergometrine maleate 7
S11	¹³ C NMR of methylergometrine maleate 7
S12	COSY of methylergometrine maleate 7
S13	HSQC of methylergometrine maleate 7
S14	¹ H- ¹³ C HMBC of methylergometrine maleate 7
S15	NOESY of methylergometrine maleate 7
S16	¹ H- ¹⁵ N HMBC of methylergometrine maleate 7
S17	¹ H NMR of ergometrine 4
S18	¹³ C NMR of ergometrine 4
S19	COSY of ergometrine 4
S20	HSQC of ergometrine 4
S21	¹ H- ¹³ C HMBC of ergometrine 4
S22	NOESY of ergometrine 4
S23	NOESY of ergometrine 4 (expansion of the 2.3 ÷ 3.6 ppm region)
S24	¹ H- ¹⁵ N HMBC of ergometrine 4
S25	¹ H NMR of methylergometrine 5
S26	¹³ C NMR of methylergometrine 5
S27	COSY of methylergometrine 5
S28	HSQC of methylergometrine 5
S29	¹ H- ¹³ C HMBC of methylergometrine 5
S30	NOESY of methylergometrine 5
S31	NOESY of methylergometrine 5 (expansion of the 2.3 ÷ 3.6 ppm region)
S32	¹ H- ¹⁵ N HMBC of methylergometrine 5



























































