

Unusual behavior of benzofuroxans under ESI MS conditions in negative ion mode

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ESI mass spectra of benzofuroxans

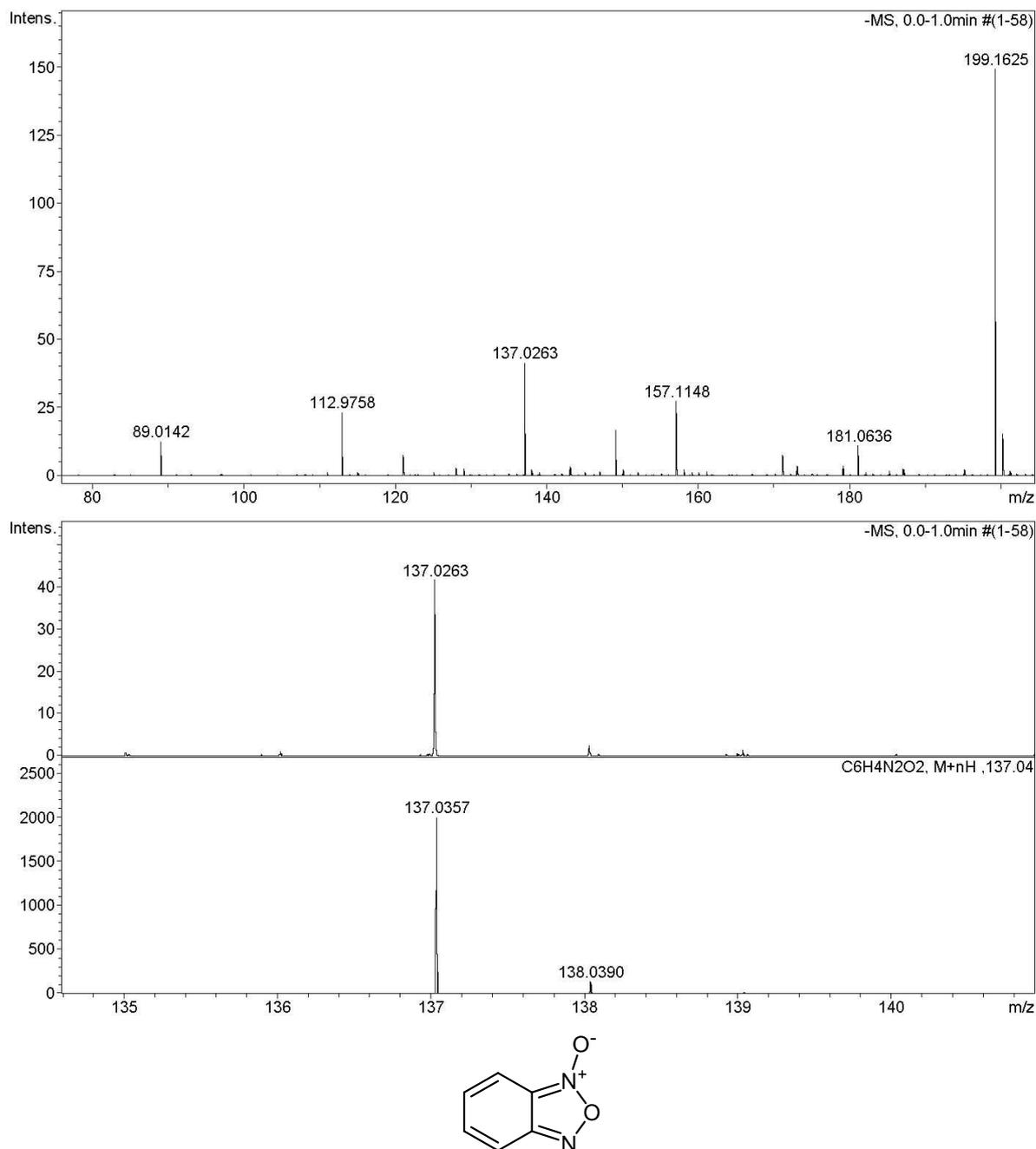


Figure S1 ESI (-) mass spectrum of benzofuroxan. ESI (-): $[M+H]^-$ m/z 137.0355 (corrected by internal calibration).

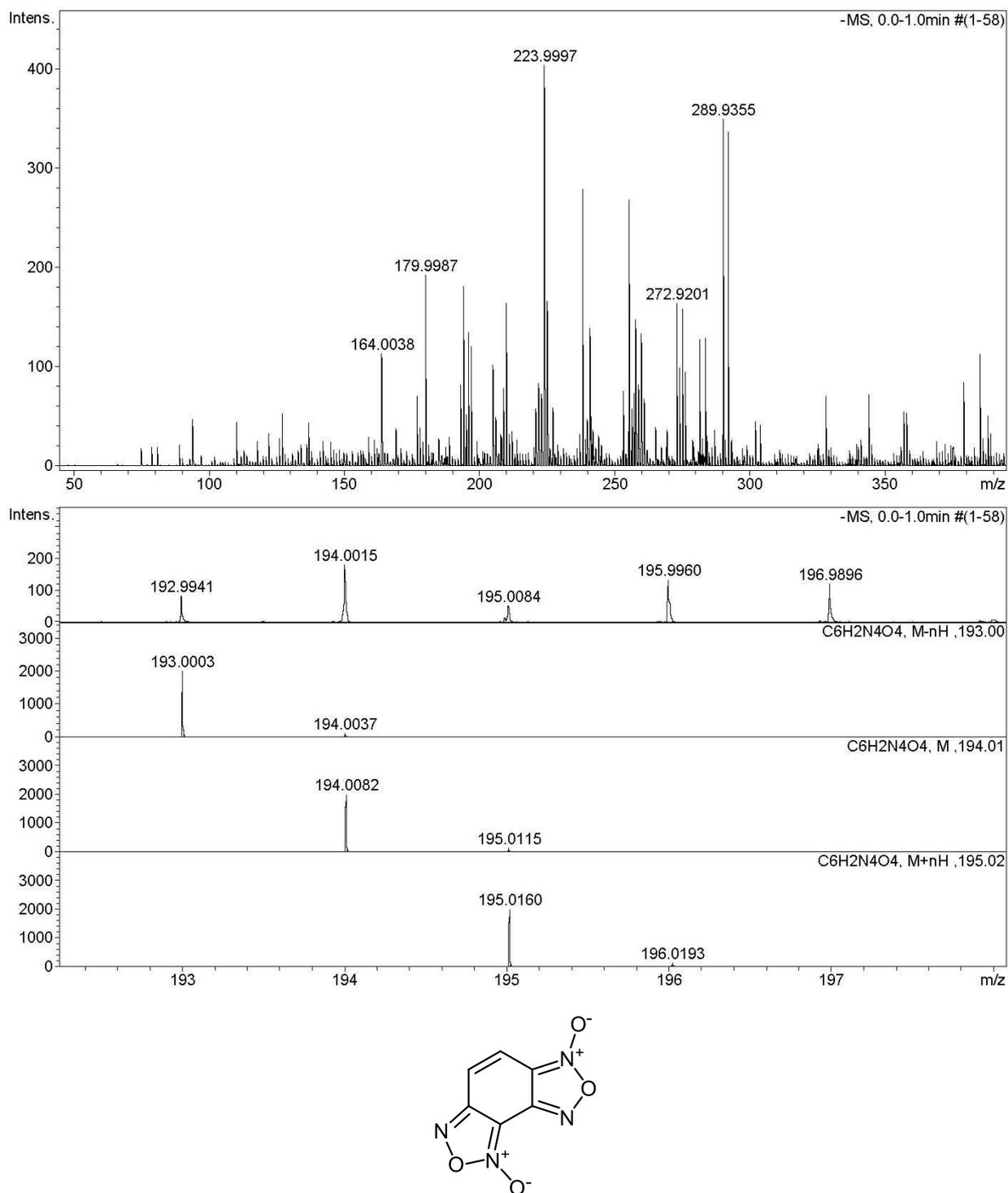
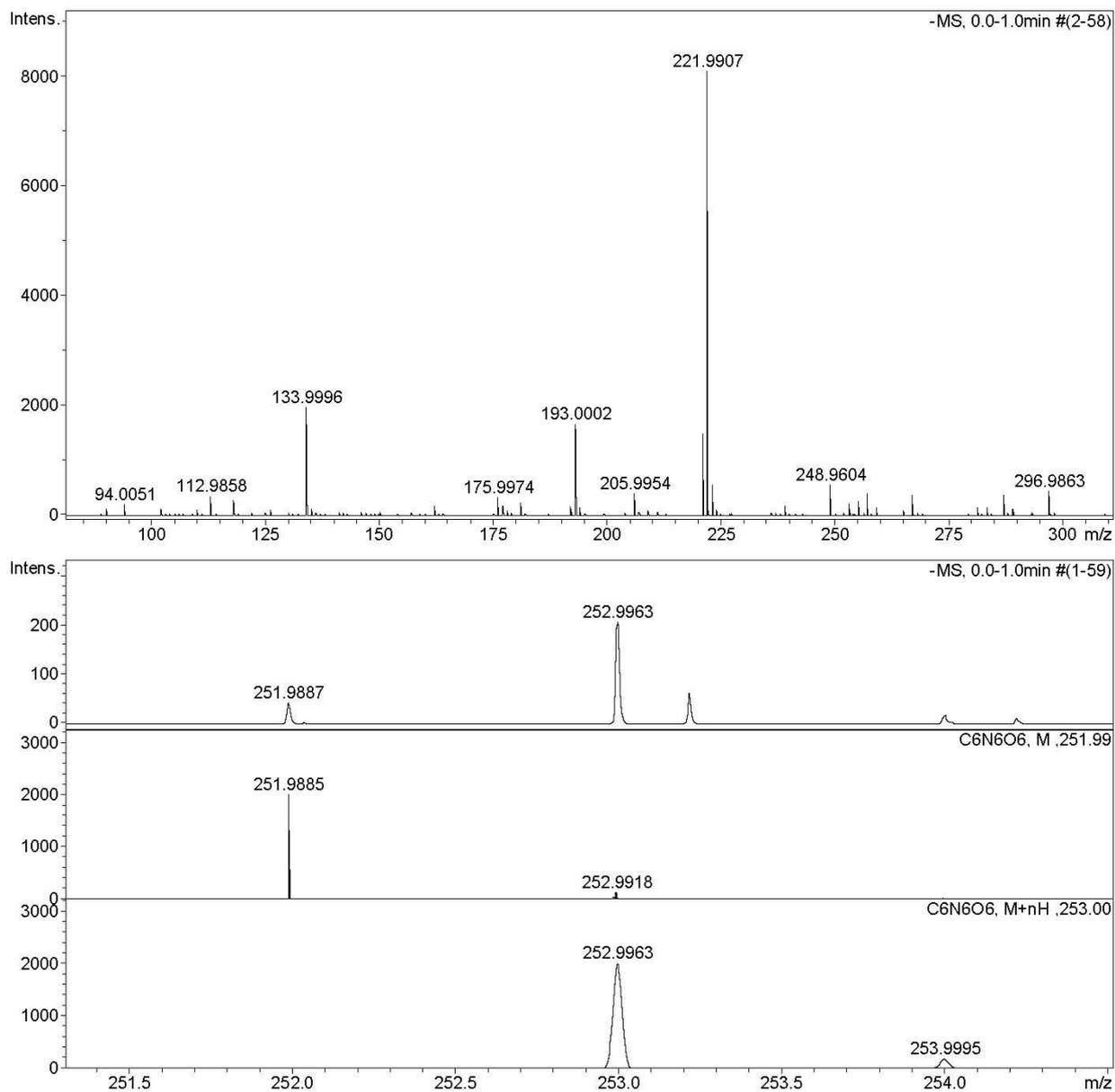
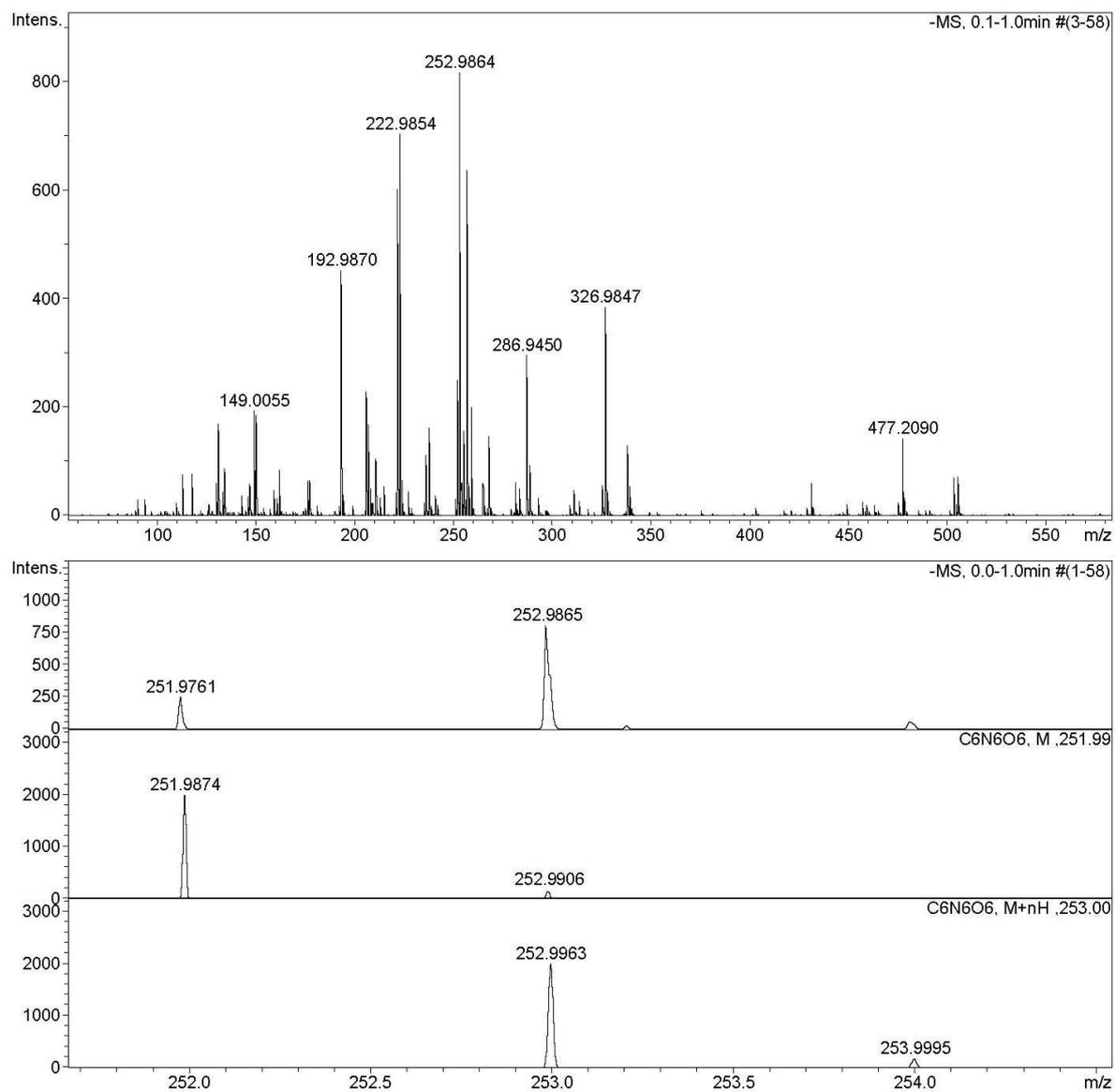


Figure S2 ESI (-) mass spectrum of benzodifuroxan. ESI (-): [M-H]⁻ m/z 193.0021, M⁻ m/z 194.0092, [M+H]⁻ m/z 195.0159 (corrected by internal calibration).

a



b



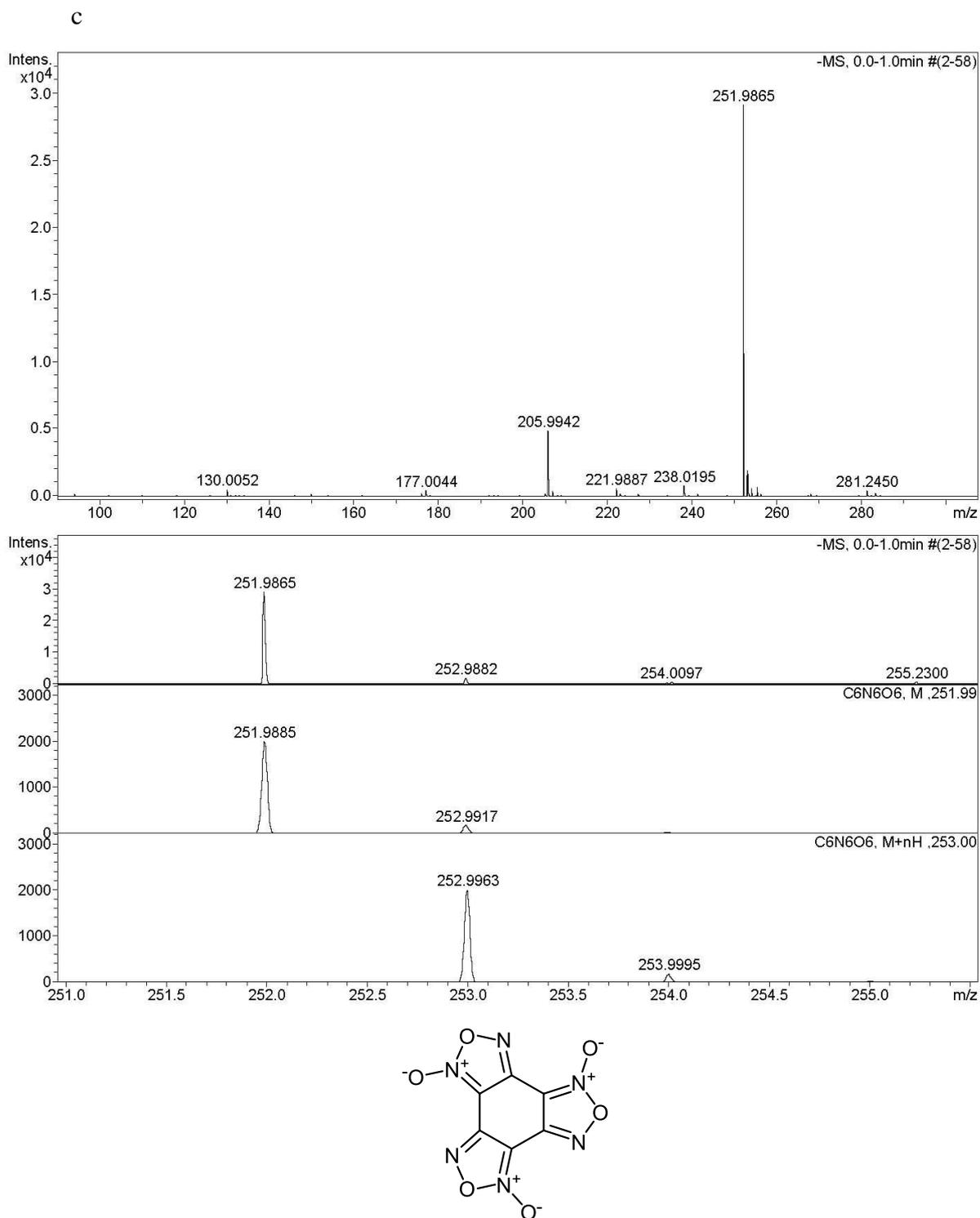


Figure S3 ESI(-) mass spectra (a, HCOONa added, b, no calibrant) and APCI(-) MS (c) of benzotrifuroxan in methanol. For digital data (a), see Table 1 in the main text.

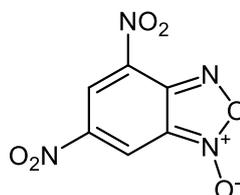
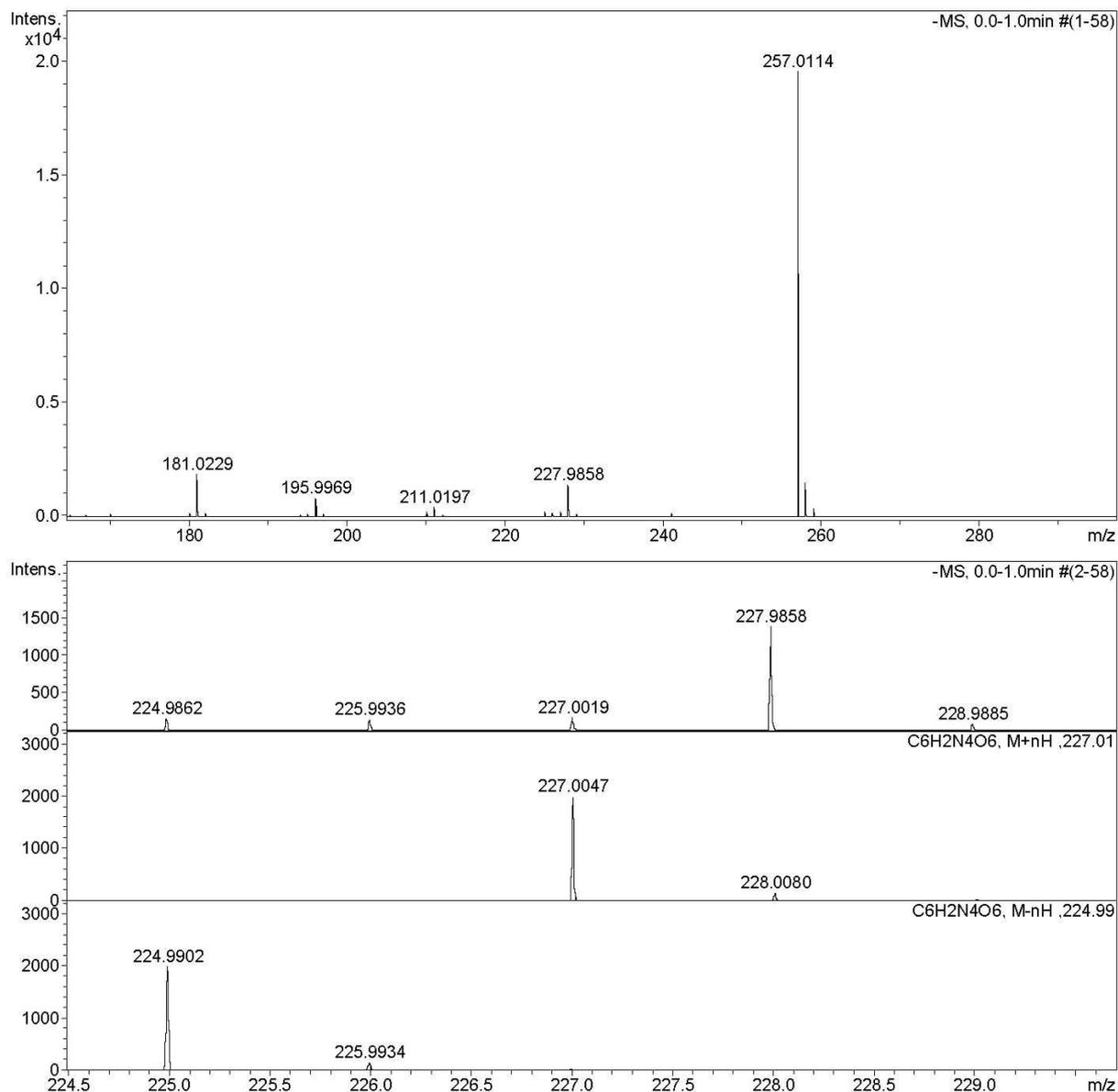


Figure S4 ESI (-) mass spectrum of 4,6-dinitrobenzofuroxan. ESI(-) $[M-H]^-$ m/z 224.9918, $[M-NO]^-$ m/z 196.0020 (increased *ca.* 100 times, corrected by internal calibration).

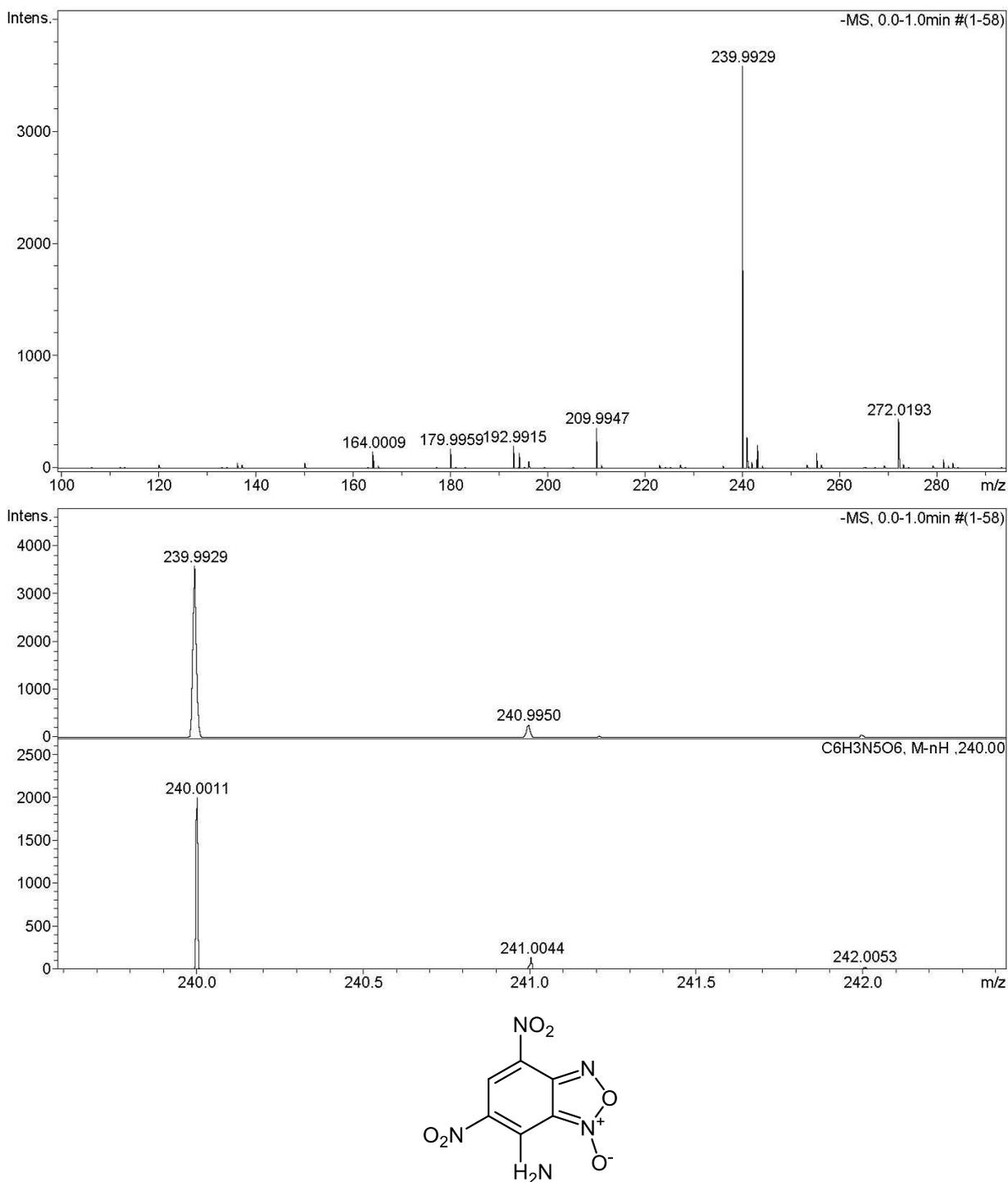


Figure S5 ESI (-)mass spectrum of 7-amino-4,6-dinitrobenzofuroxan. ESI (-): $[M-H]^-$ m/z 240.0012 $[M-H-NO]^-$ m/z 210.0031, $[M-HNO_2]^-$ m/z 194.0079, $[M-H-HNO_2]^-$ m/z 193.0003, $[M-H-NO-NO_2]^-$ m/z 164.0099, $[M-H-2NO-NO_2]^-$ m/z 134.0116 (corrected by internal calibration).

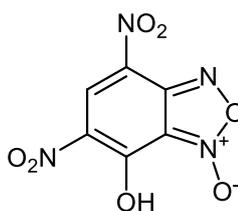
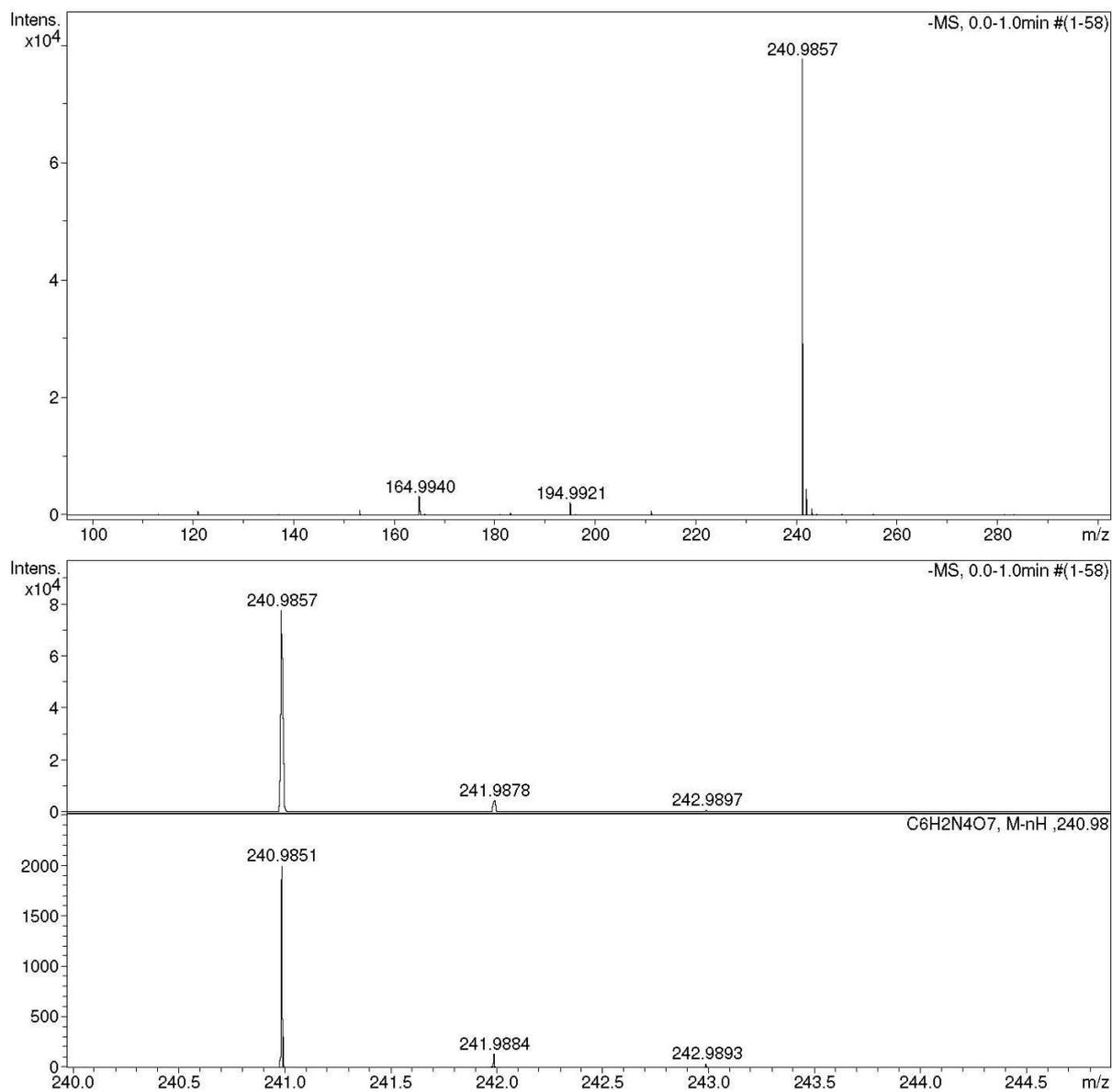


Figure S6 ESI (-) mass spectrum of 7-hydroxy-4,6-dinitrobenzofuroxan. ESI (-): [M-H]⁻ *m/z* 240.9857, [M-H-NO]⁻ *m/z* 210.9871, [M-HNO₂]⁻ *m/z* 194.9921, [M-H-NO-NO₂]⁻ *m/z* 164.9940 (corrected by internal calibration).

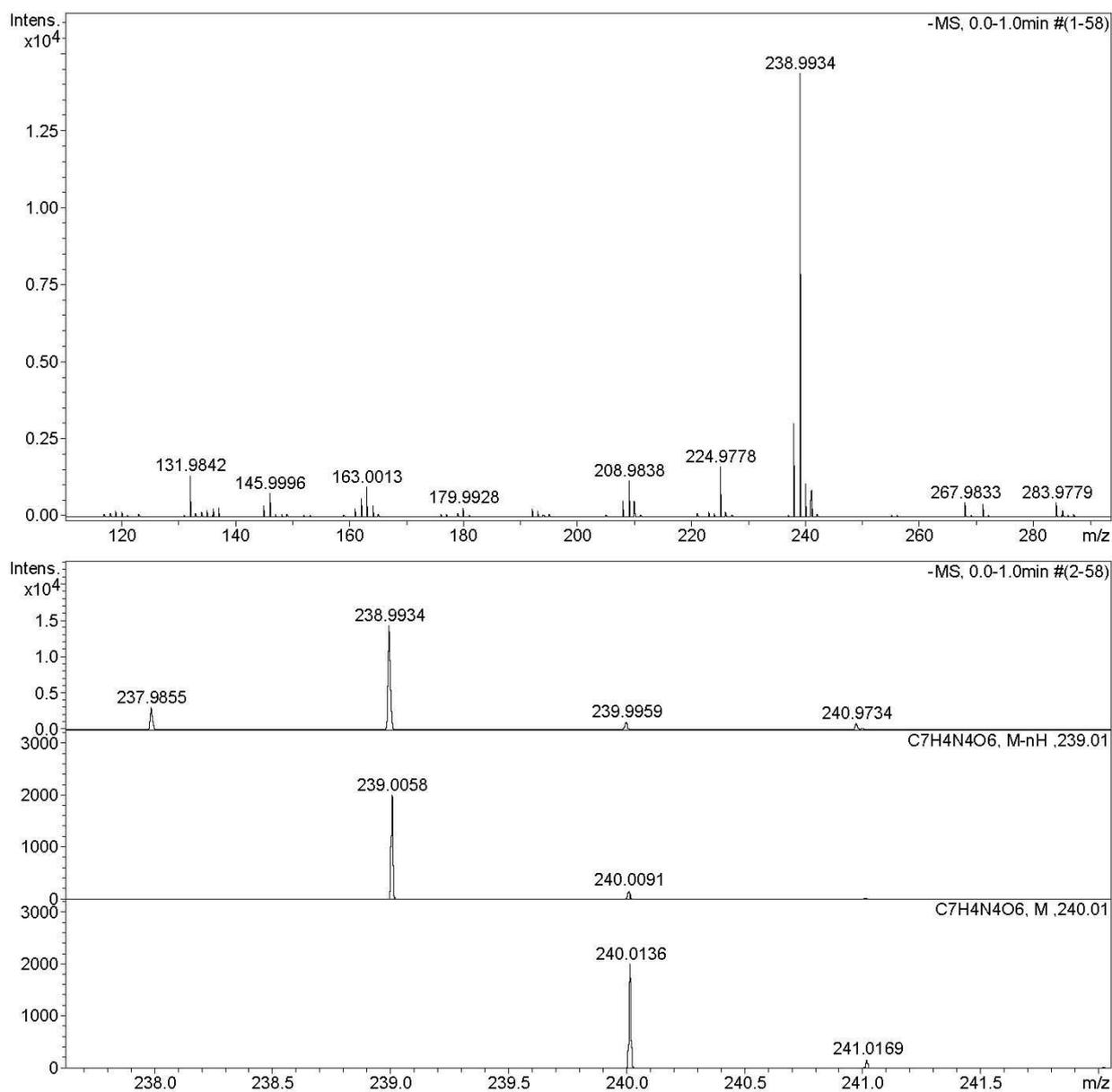
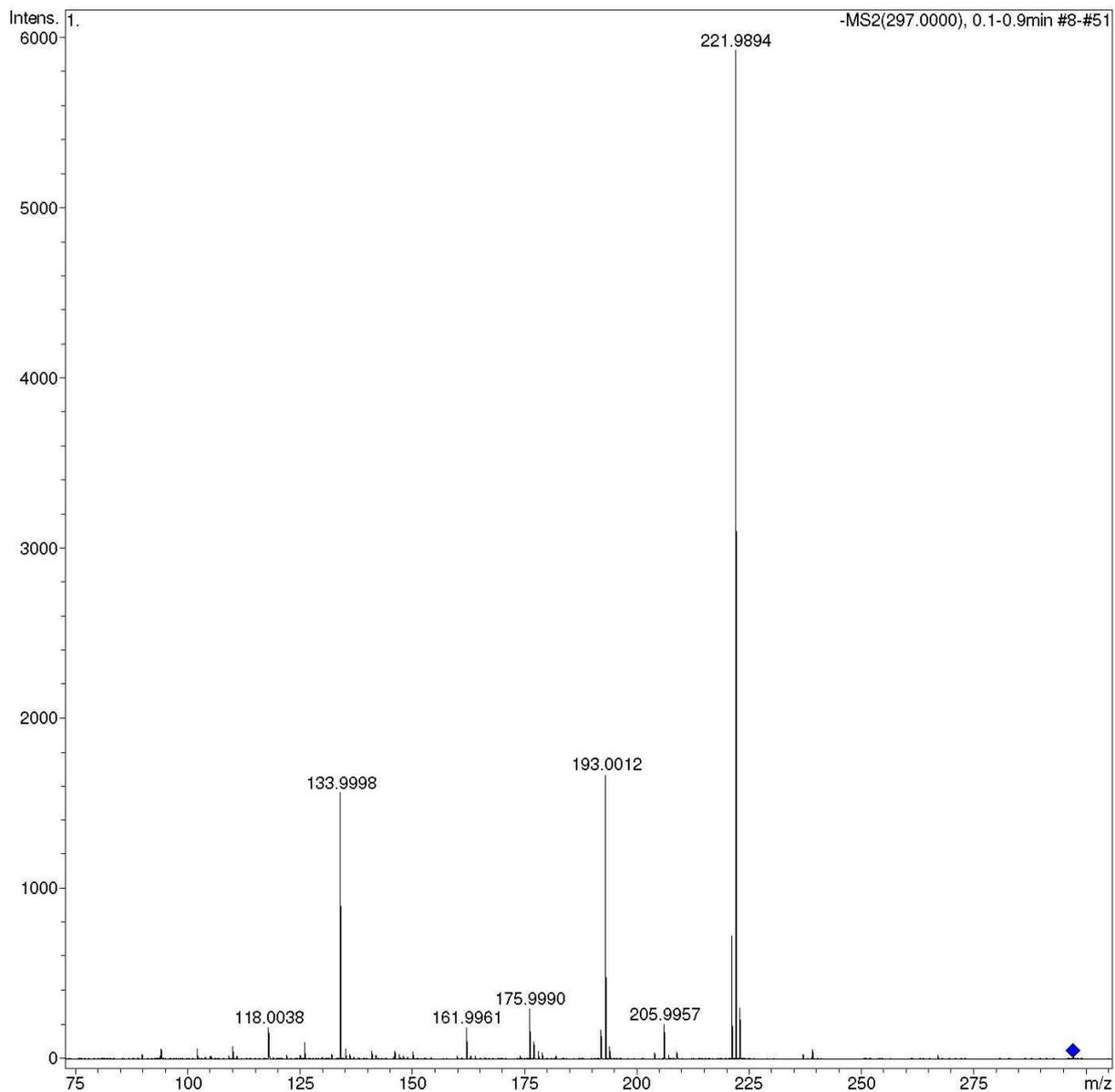
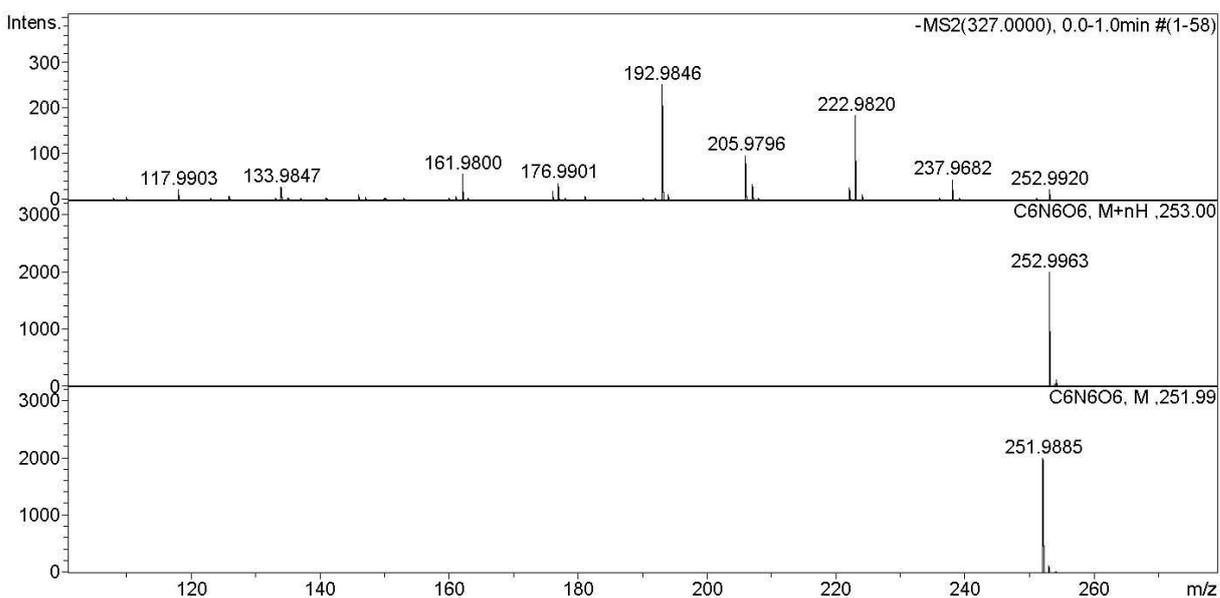


Figure S7 ESI (-) (b) mass spectrum of 7-methyl-4,6-dinitrobenzofuroxan. ESI (-): $[M+HCO_2]^-$ m/z 284.9992 (weak), $[M-H]^-$ m/z 238.9946, $[M-H-NO]^-$ m/z 208.9849, $[M-NO]^-$ m/z 209.9914, $[M-HNO]^-$ m/z 207.9889, $[M-2H-NO_2]^-$ m/z 191.9937 (corrected by internal calibration).

a



b



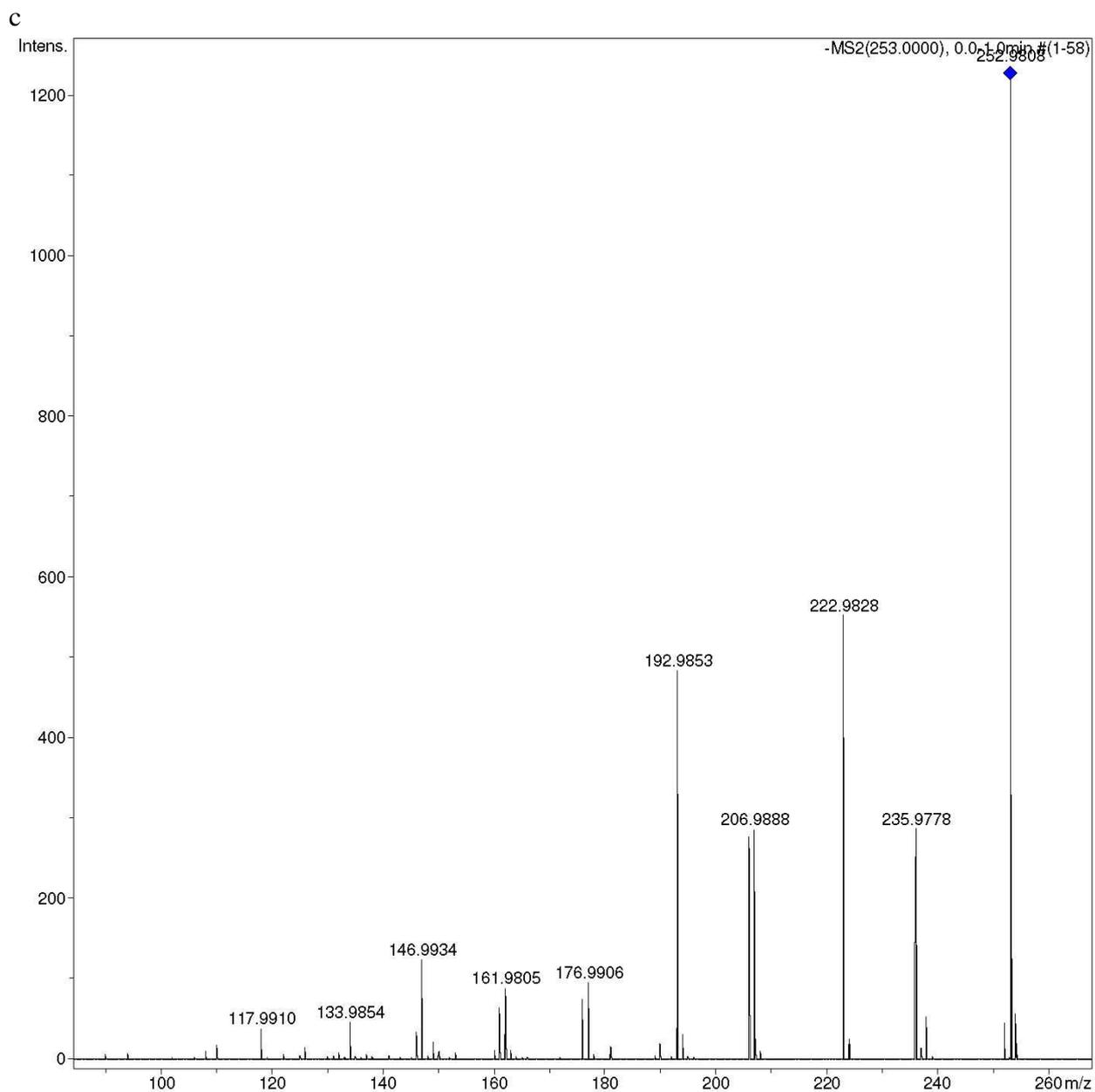


Figure S8 Negative ion mode ESI MS² spectra of selected ions of BTF **3** (collision cell activation energy 10 eV) (a) m/z 297, HCOOH added, (b) m/z 327, (c) m/z 253.