

SUPPLEMENTARY MATERIAL

Diversity of cyanobacteria and cyanotoxins in Hartbeespoort Dam, South Africa

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Appendix A. Supplementary Data File (74 pp.)

Page S2 LC-MS Chromatograms of extracts of Hartbeespoort Dam and *M. aeruginosa* AB2011/53

Page S4 MS² spectra of microcystins. NB weaker peaks display some spurious peaks due to reduced signal-to-noise, and for some very weak peaks, suitable MS² spectra were not obtained.

Figure S1a. Chromatograms of Hartbeespoort Dam extract

LC-MS of Hartbeespoort Dam

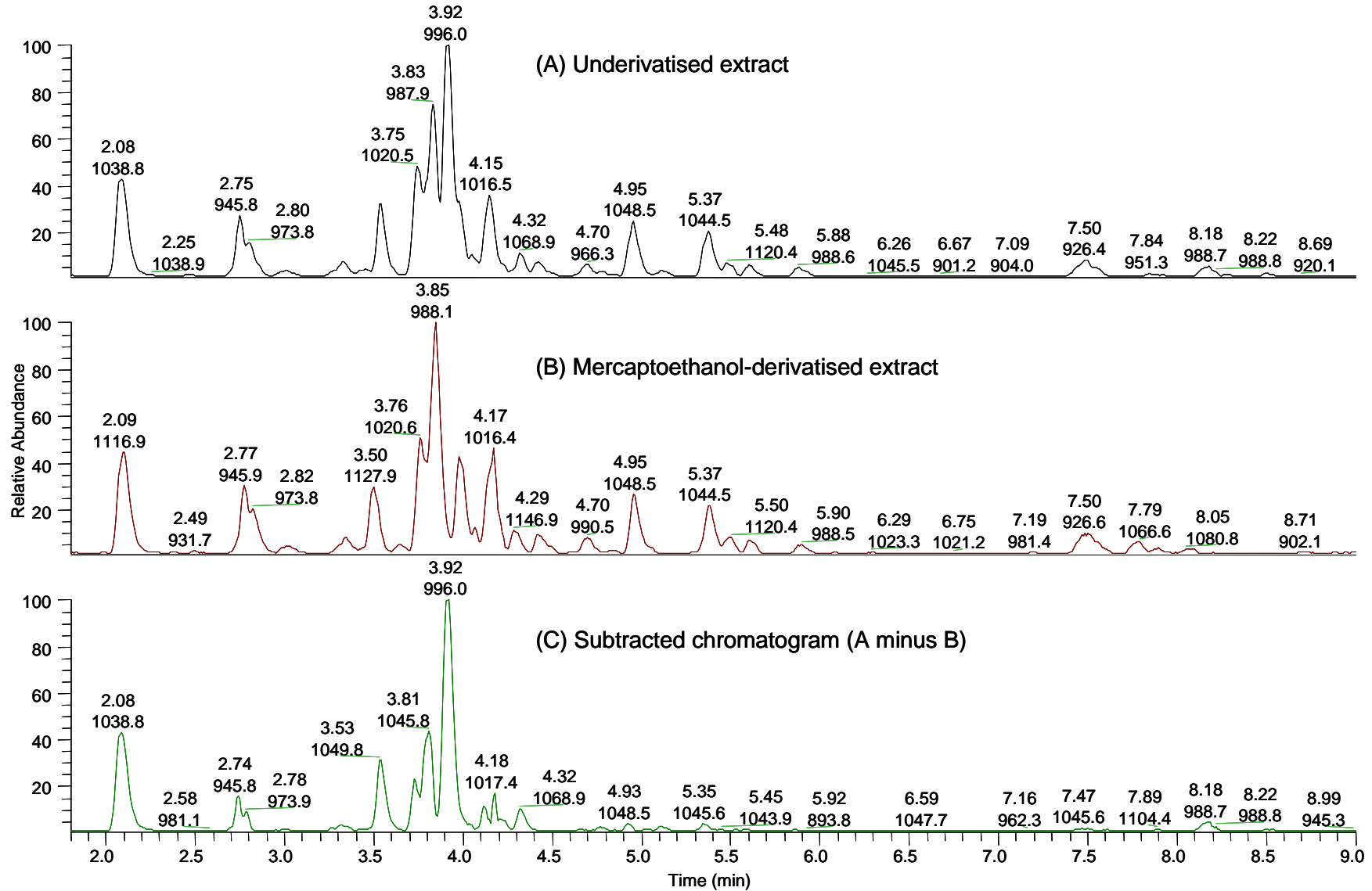


Figure S1b. Chromatograms of Hartbeespoort Dam extract

LC-MS of AB2011/53 (1.8-5.5 min)

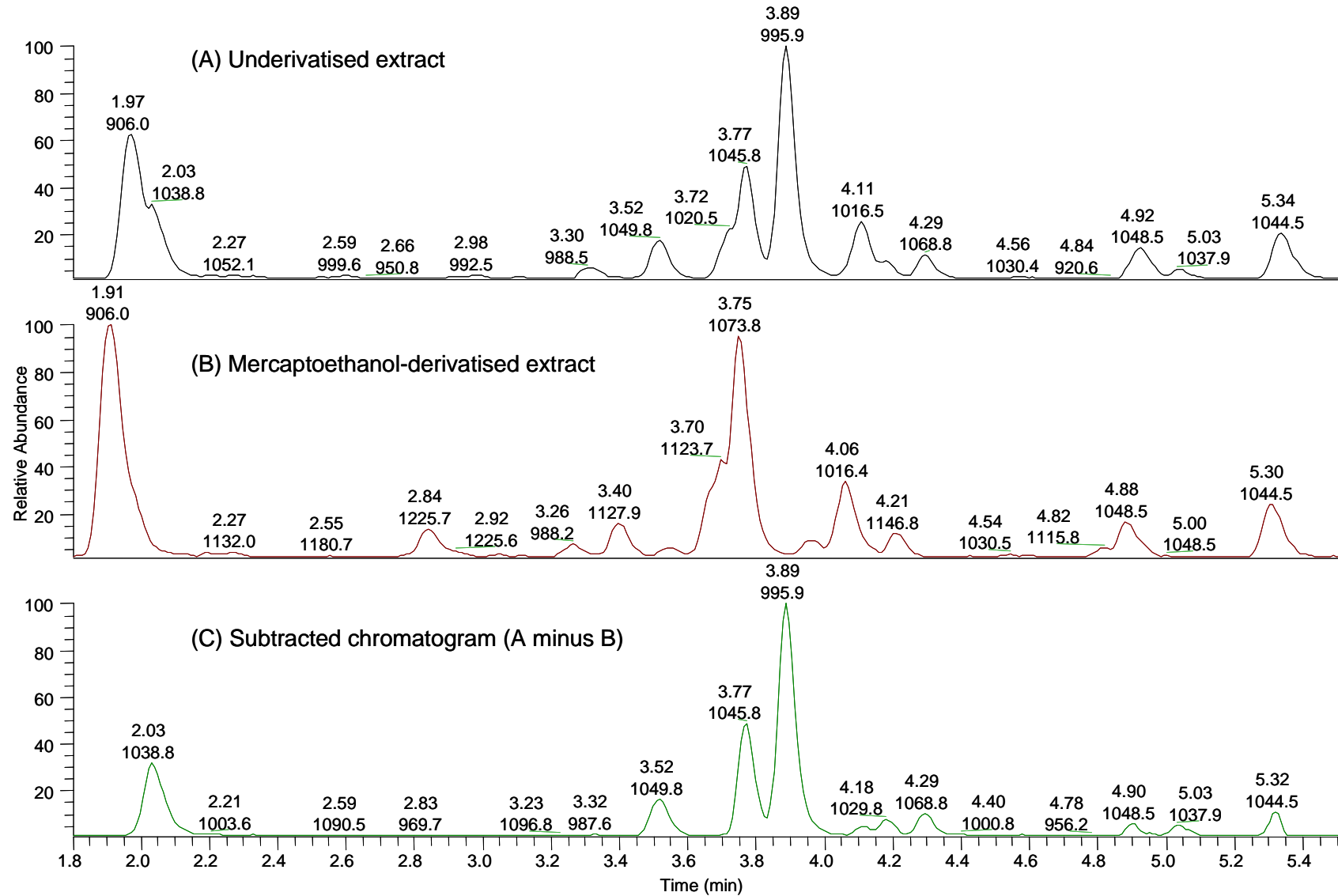


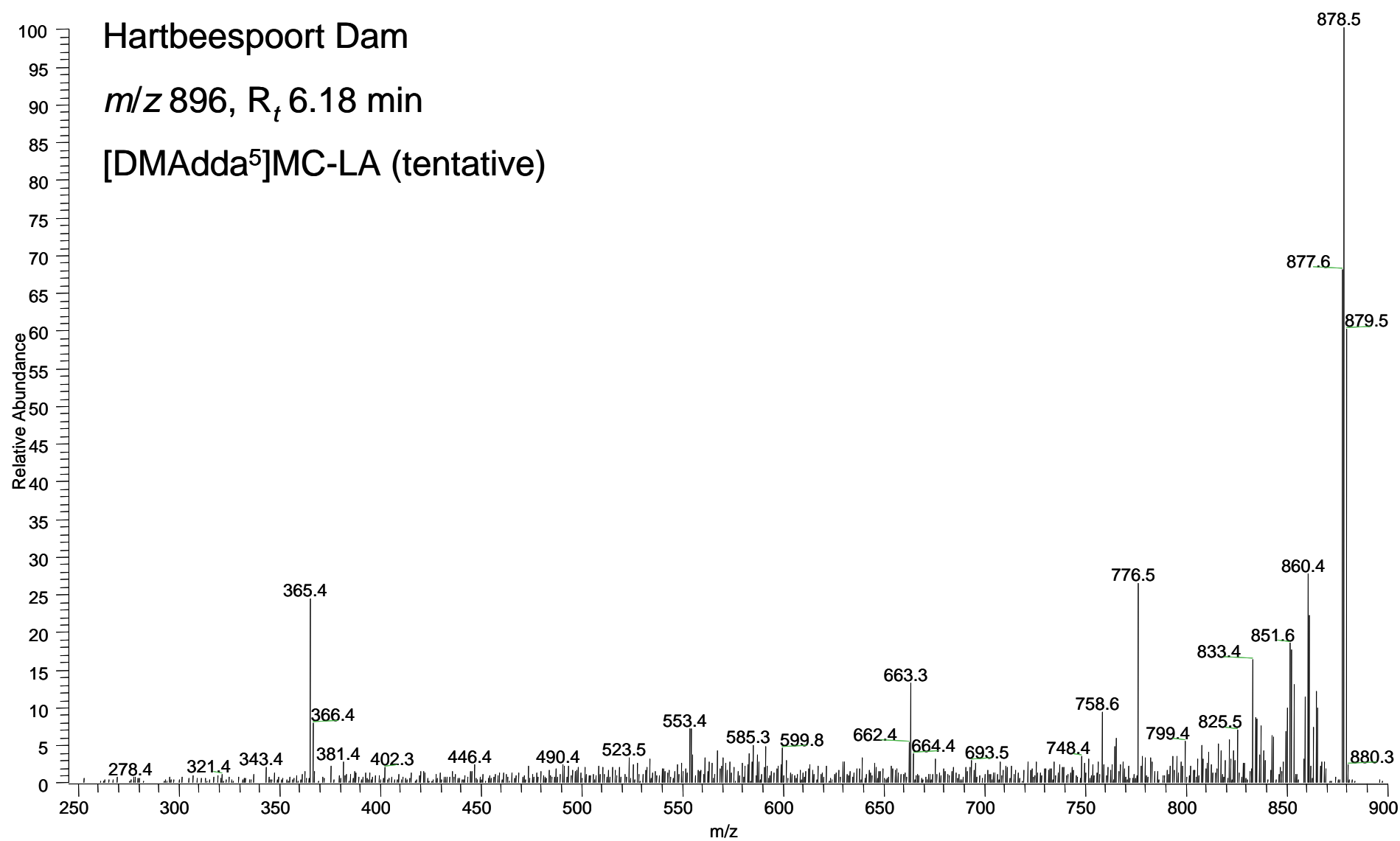
Figure S2a. MS² spectrum of tentative [DMAdda⁵]MC-LA

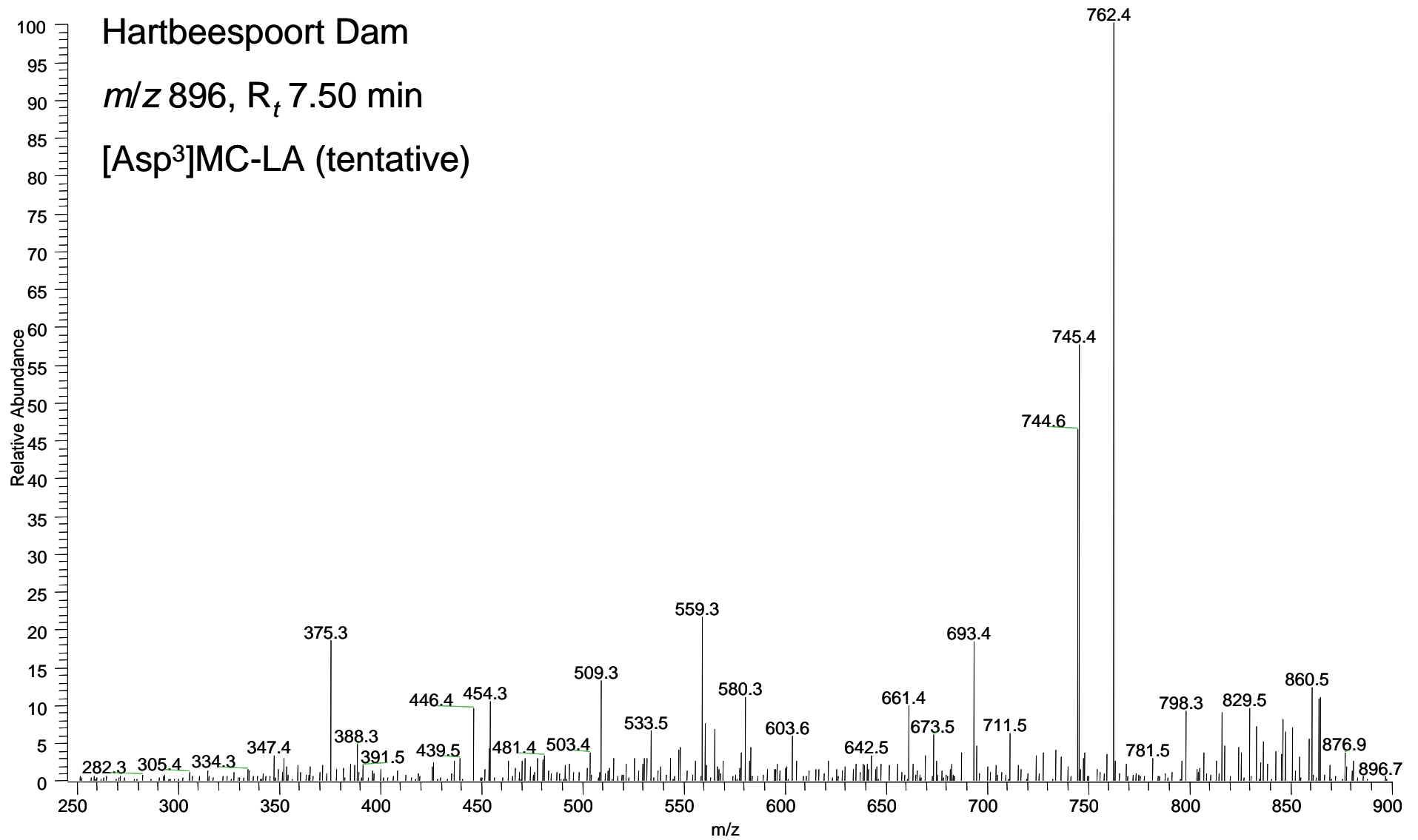
Figure S2b. MS² spectrum of tentative [Asp³]MC-LA

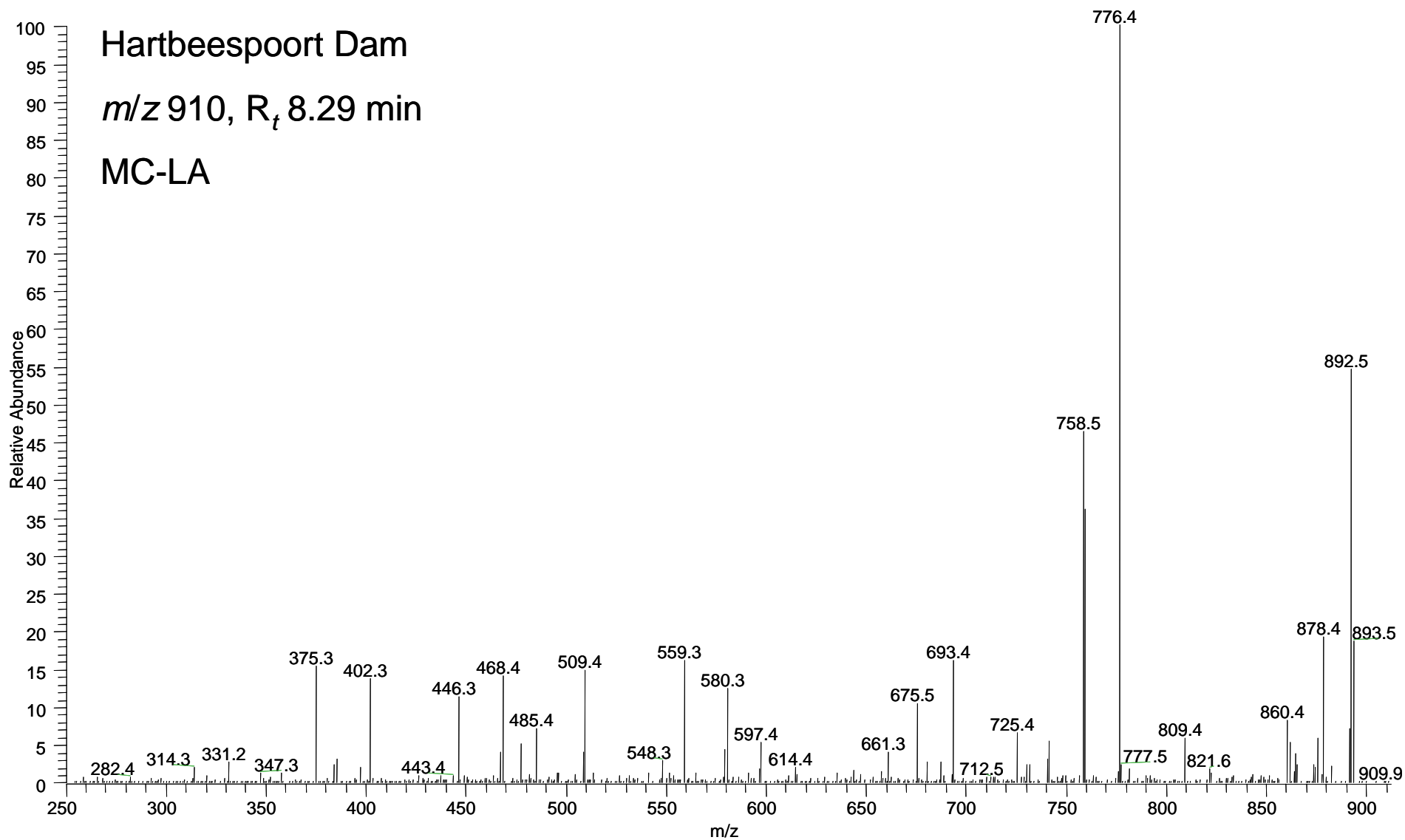
Figure S2c. MS² spectrum of tentative MC-LA

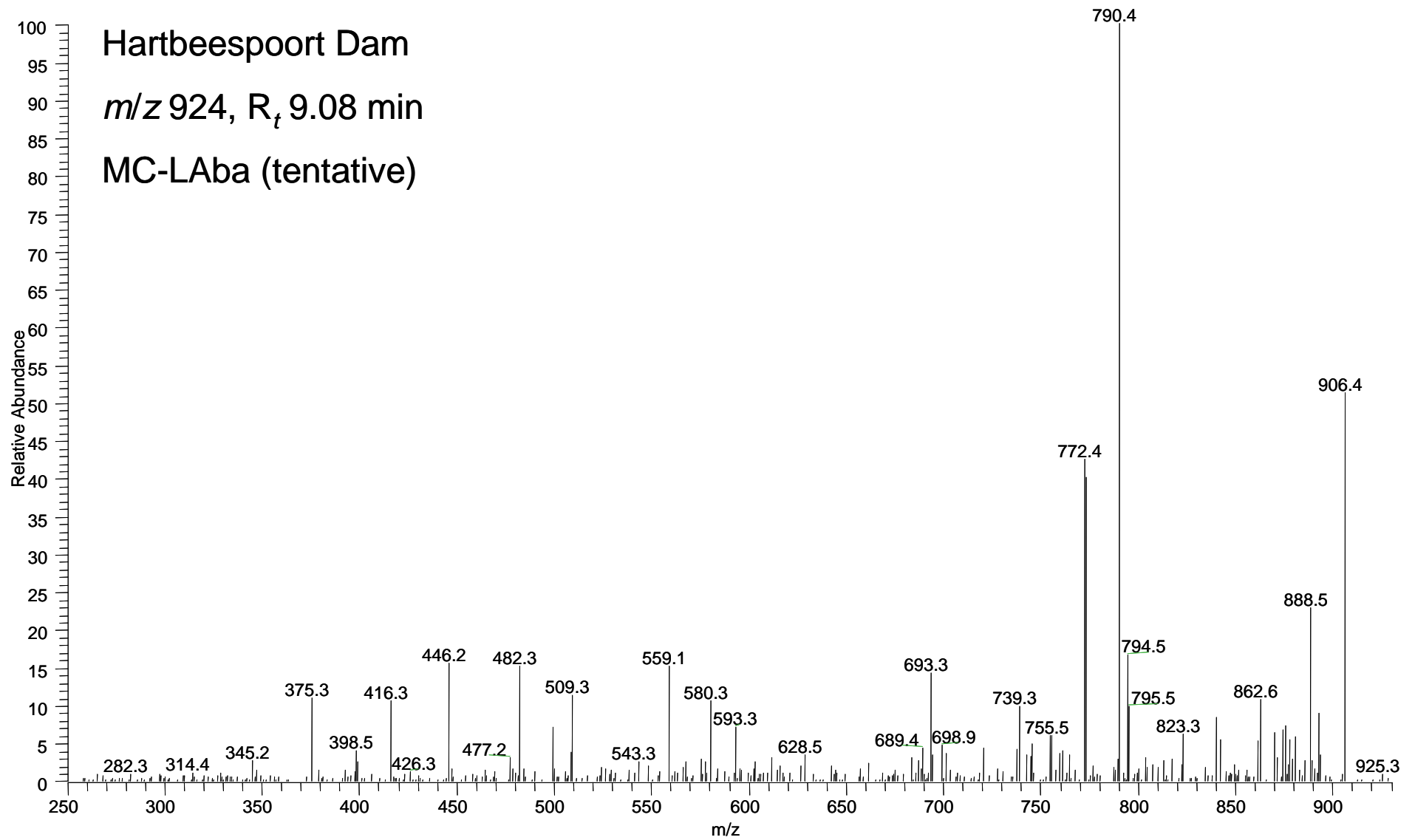
Figure S2d. MS² spectrum of tentative MC-LAba

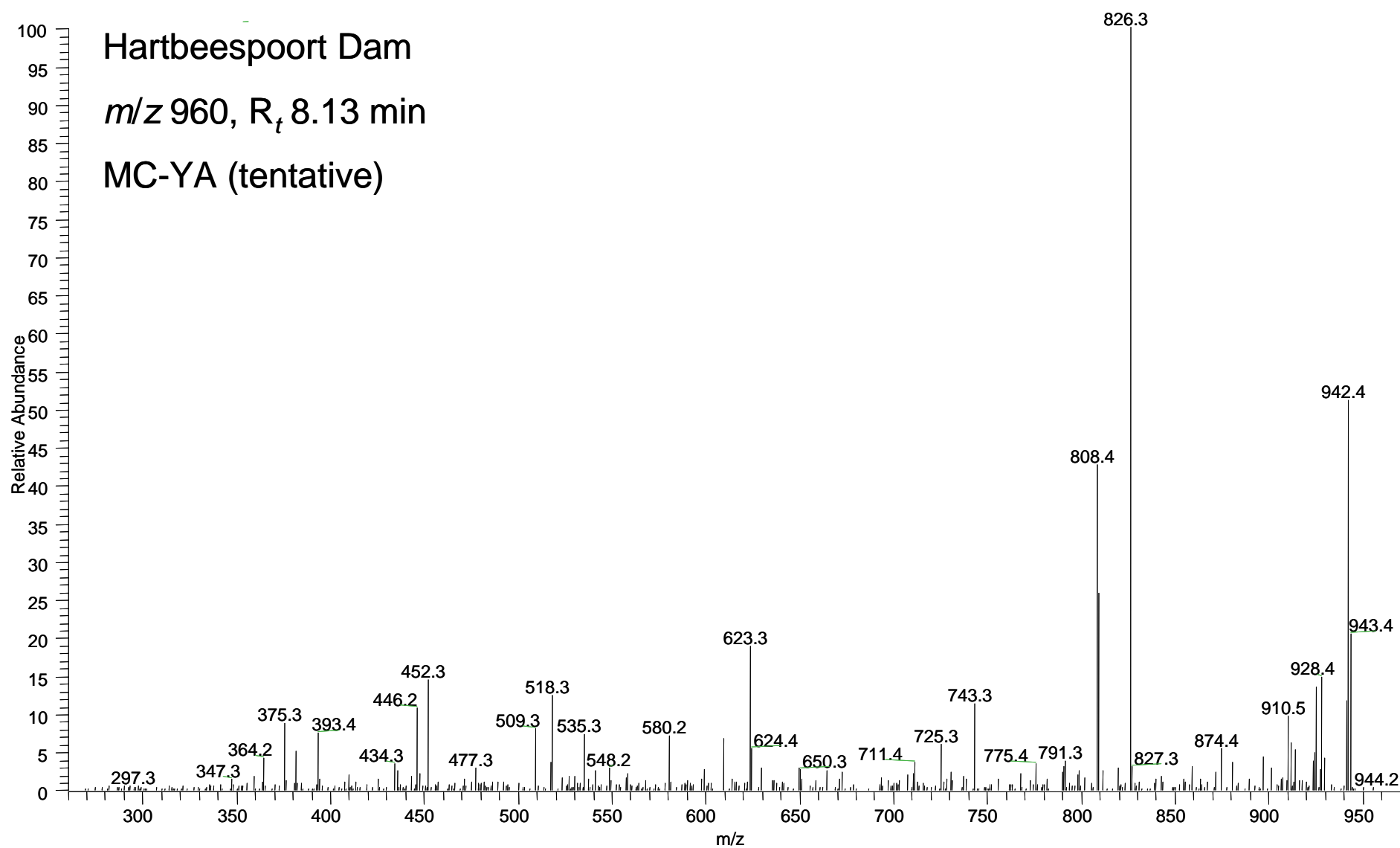
Figure S2e. MS² spectrum of tentative MC-YA from Hartbeespoort Dam

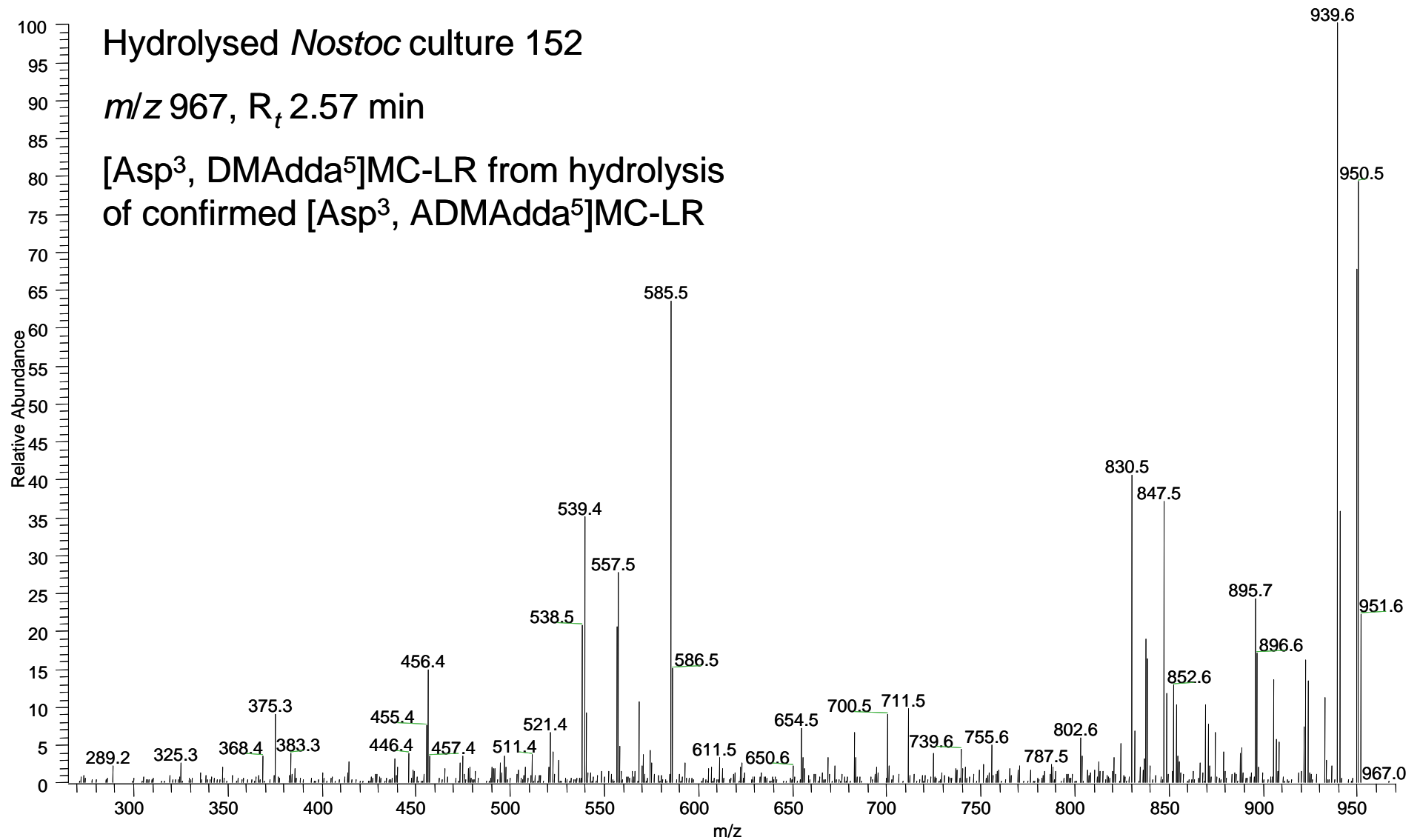
Figure S2f. MS² spectrum of [Asp³, DMAdda⁵]MC-L R standard from *Nostoc* 152

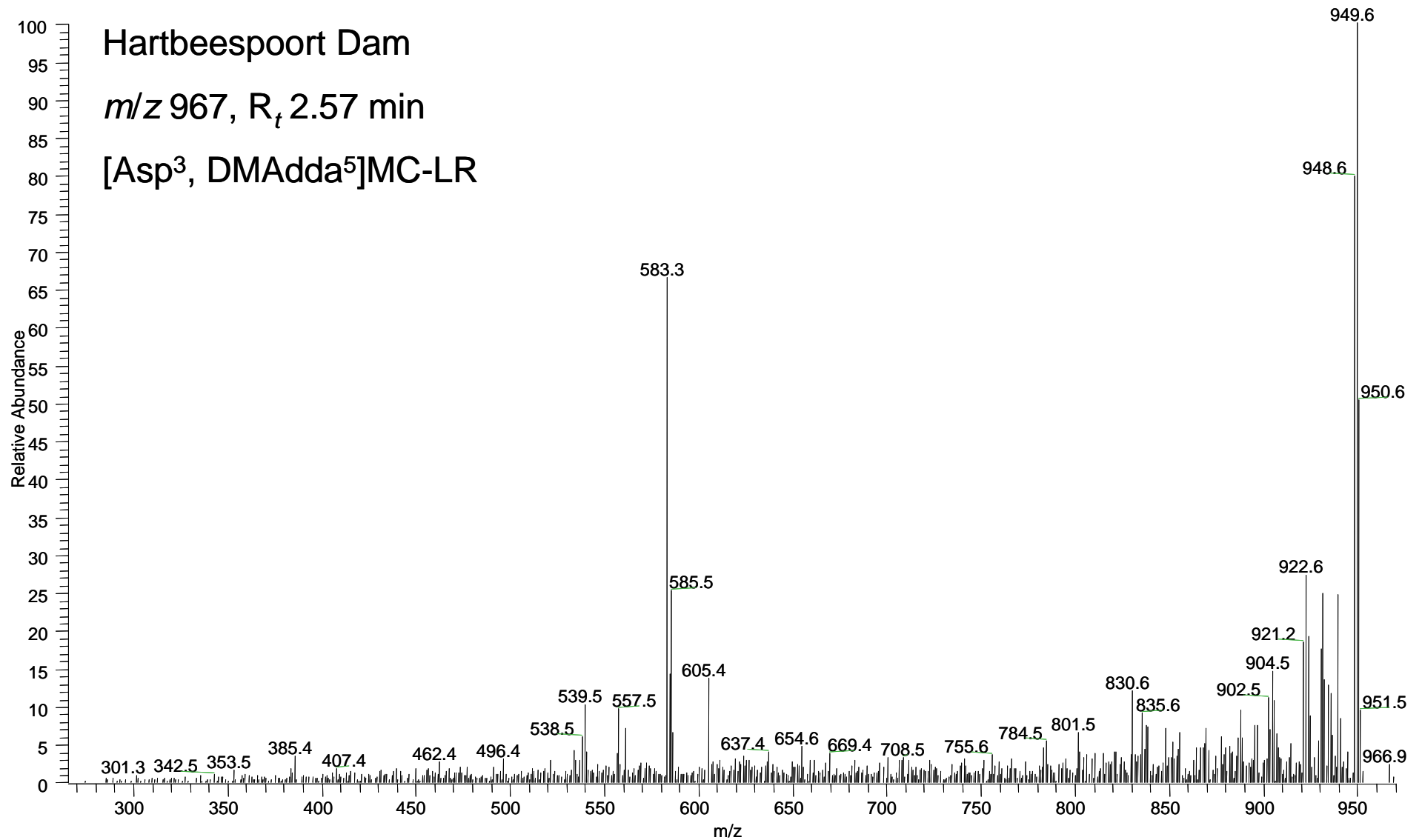
Figure S2g. MS² spectrum of confirmed [Asp³, DMAdda⁵]MC-LR standard from Hartbeespoort Dam

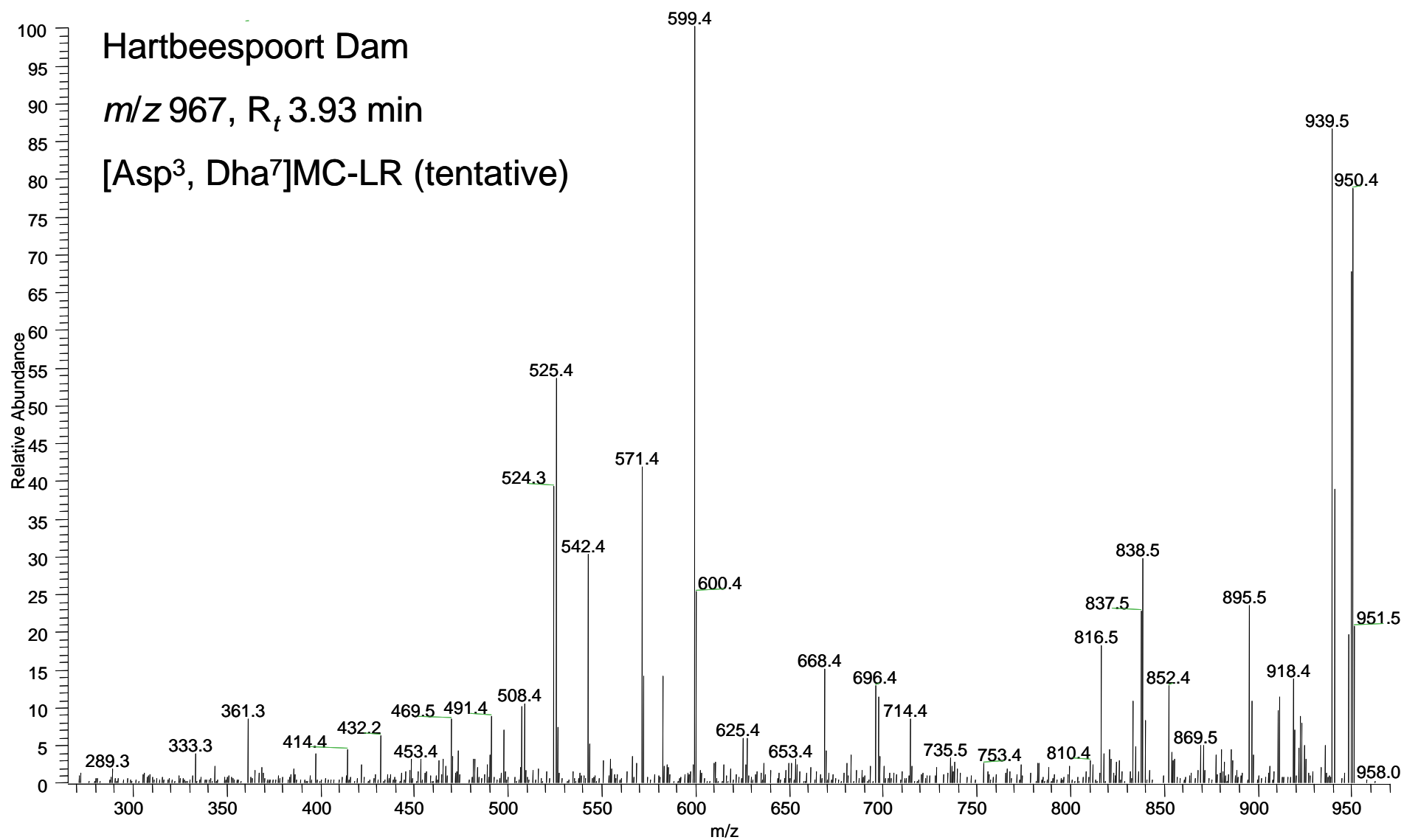
Figure S2h. MS² spectrum of tentative [Asp³, Dha⁷]MC-LR standard from Hartbeespoort Dam

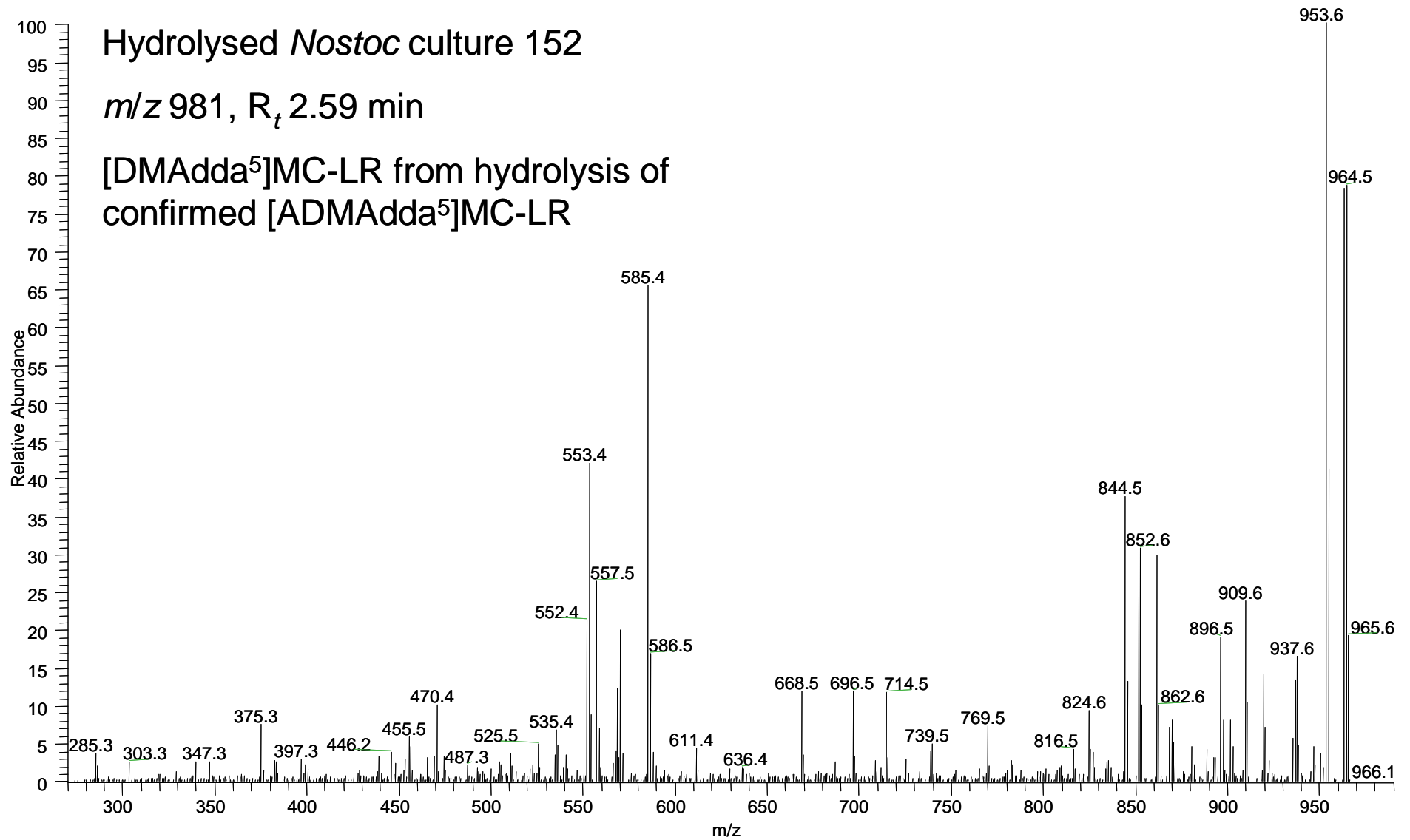
Figure S2i. MS² spectrum of [DMAdda⁵]MC-LR standard from *Nostoc* 152

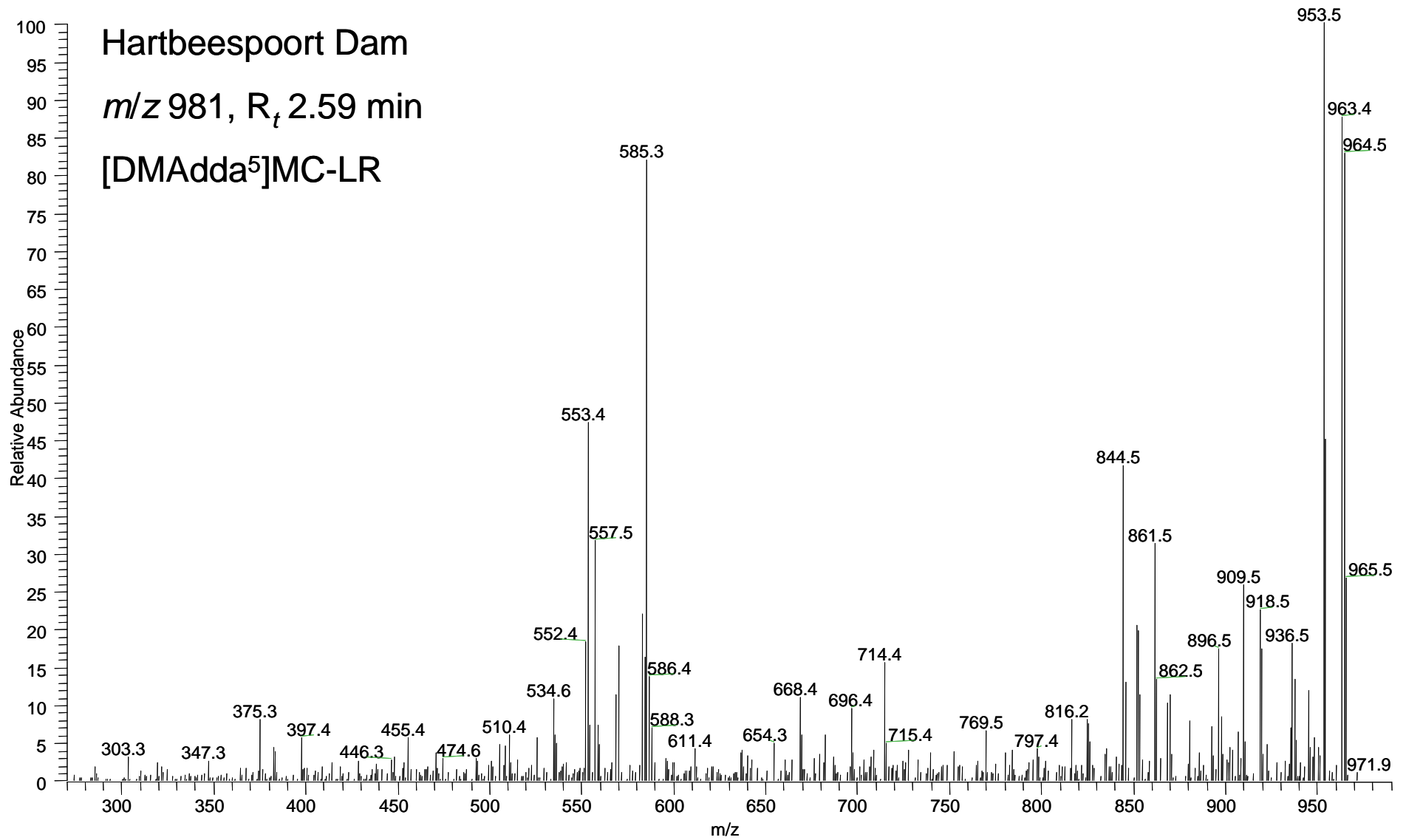
Figure S2j. MS² spectrum of confirmed [DMAdda⁵]MC-LR standard from Hartbeespoort Dam

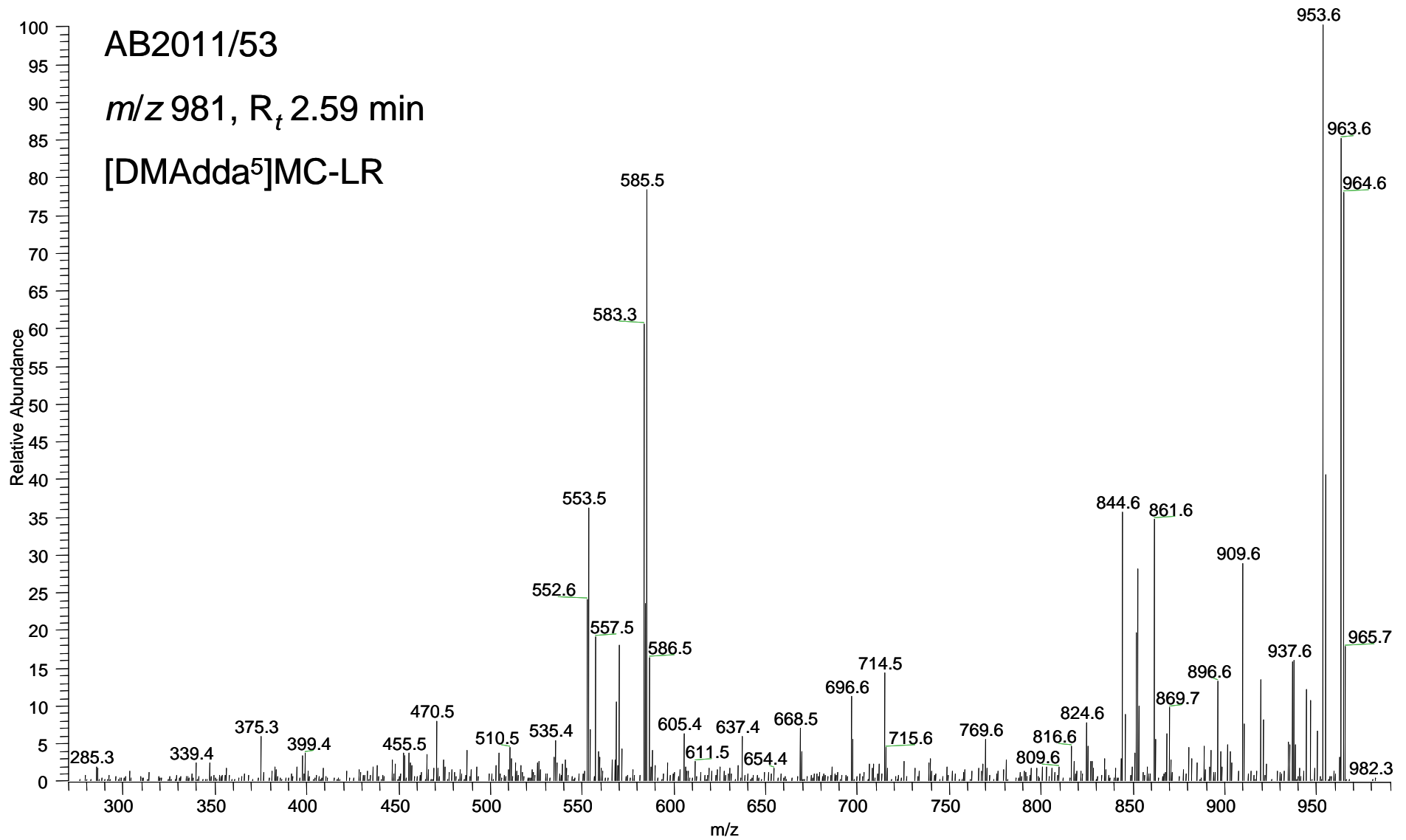
Figure S2k. MS² spectrum of confirmed [DMAdda⁵]MC-LR standard from *M. aeruginosa* AB2011/53

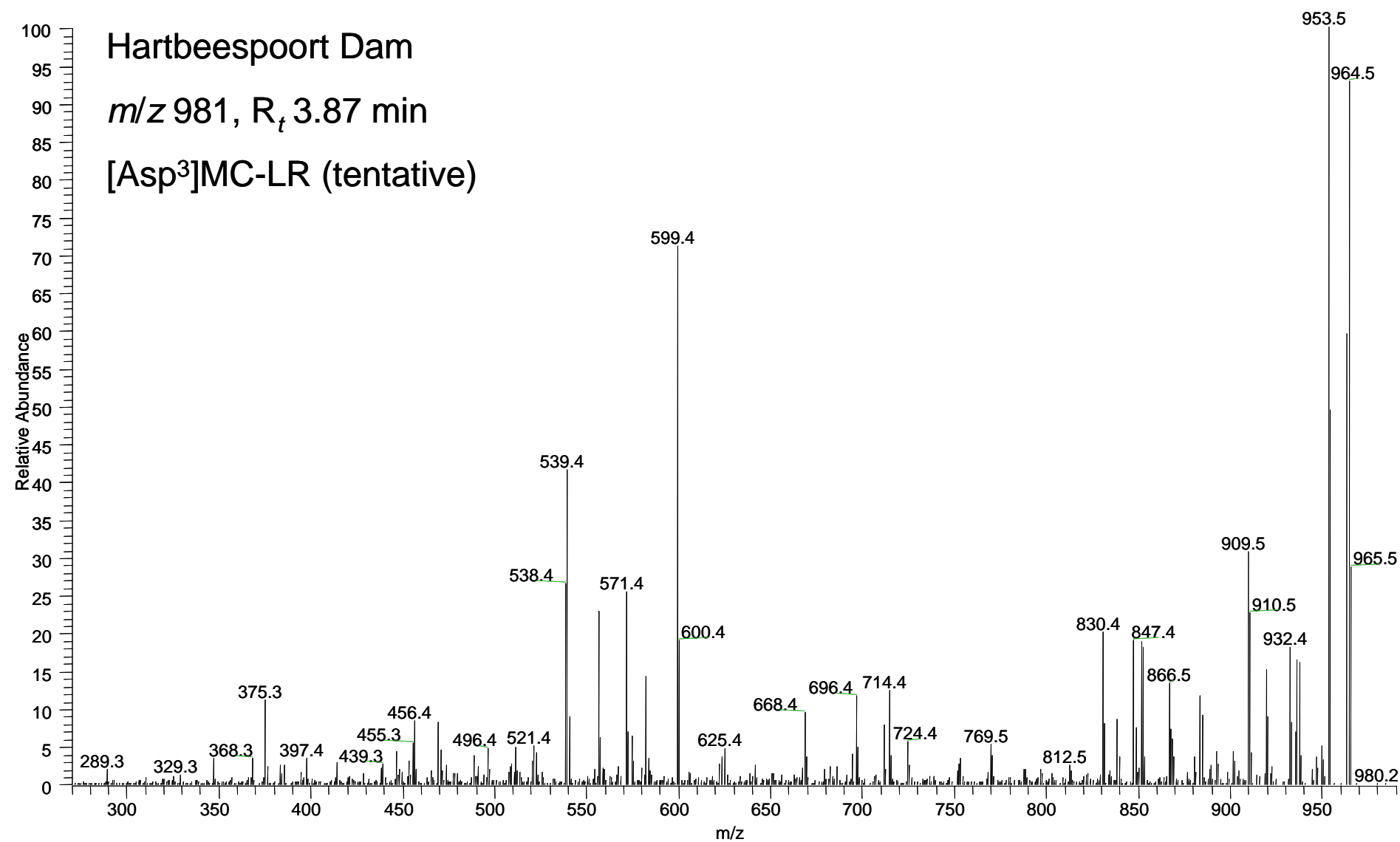
Figure S21. MS² spectrum of tentative [Asp³]MC-LR from Hartbeespoort Dam

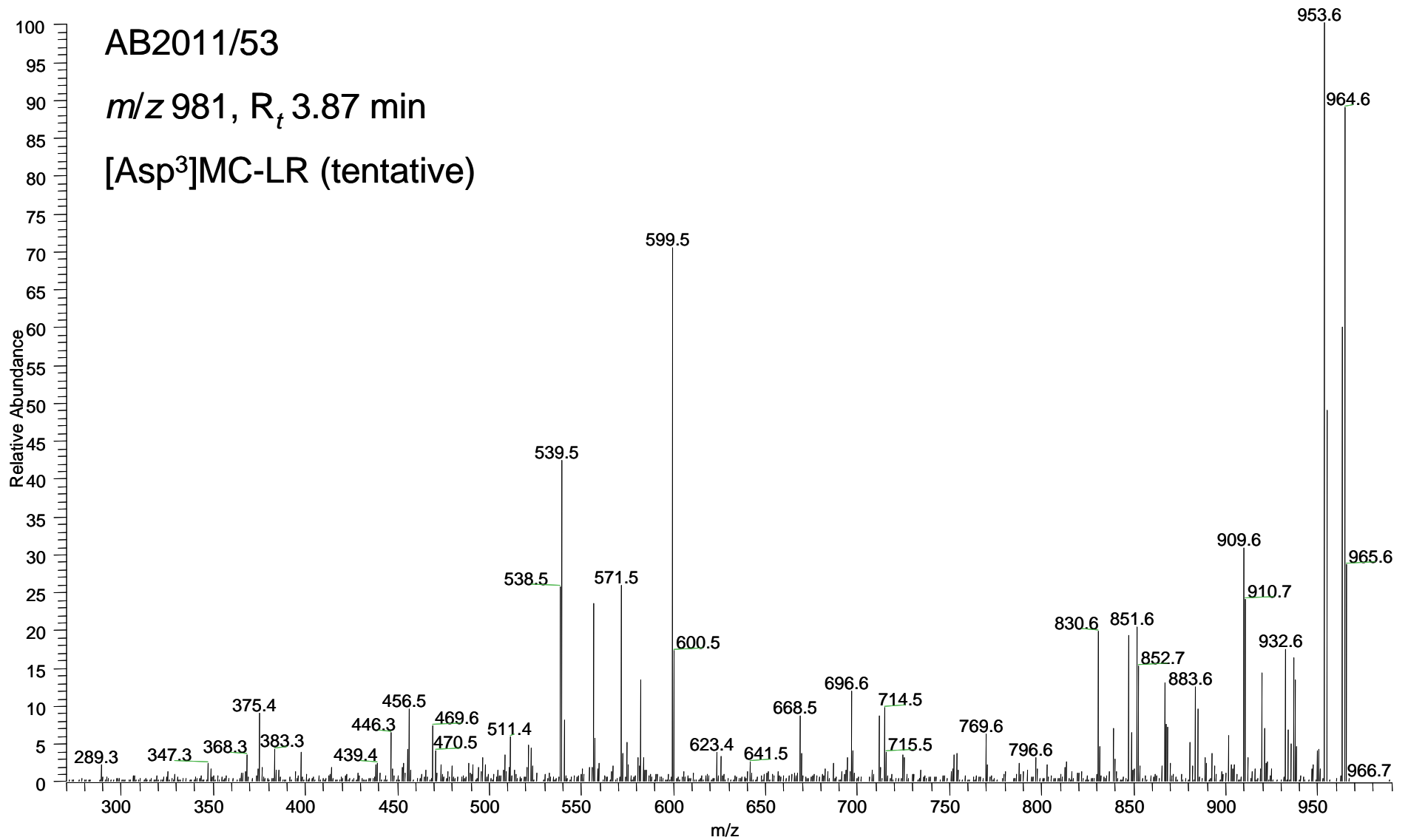
Figure S2m. MS² spectrum of tentative [Asp³]MC-LR from *M. aeruginosa* AB2011/53

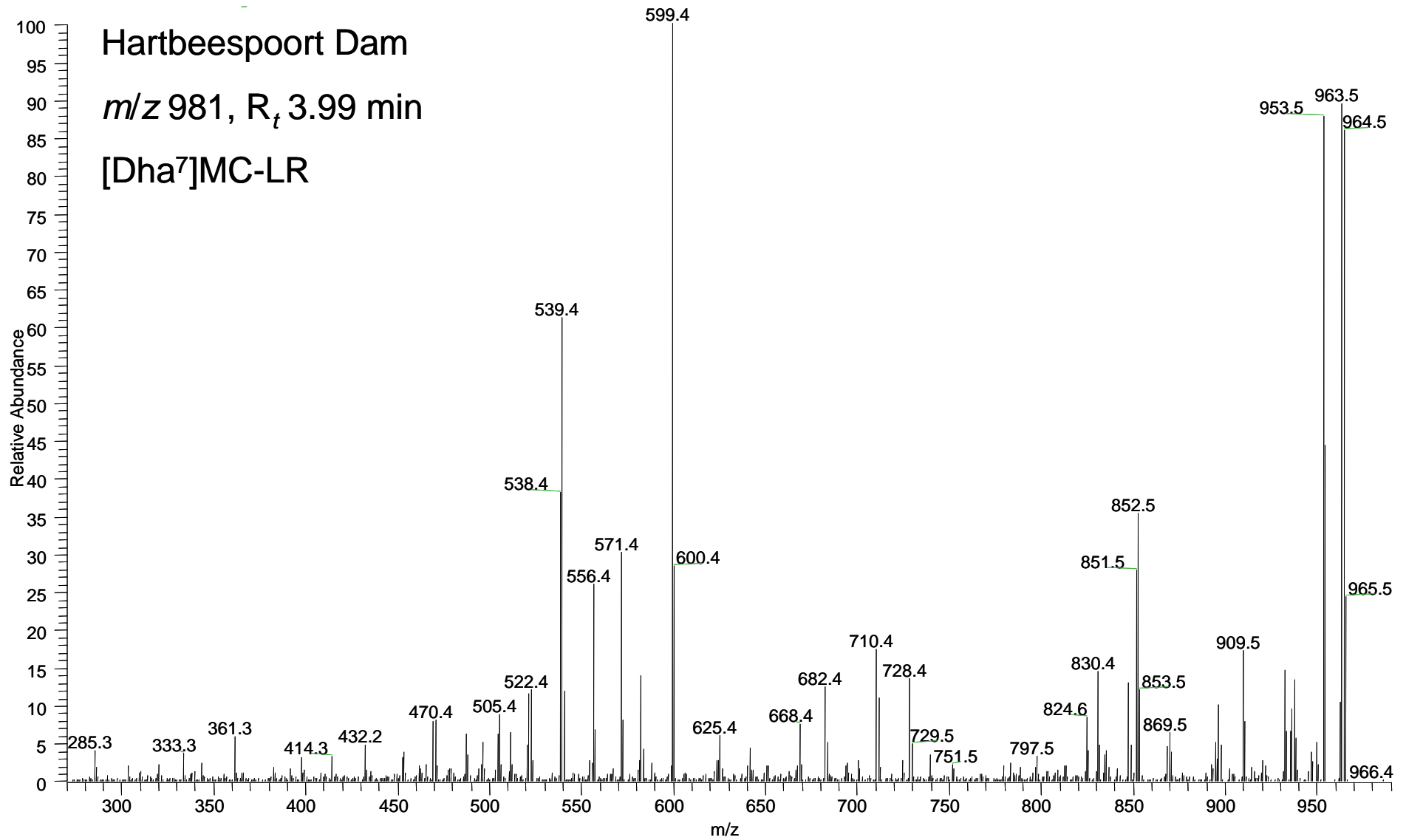
Figure S2n. MS² spectrum of confirmed [Dha⁷]MC-LR from Hartbeespoort Dam

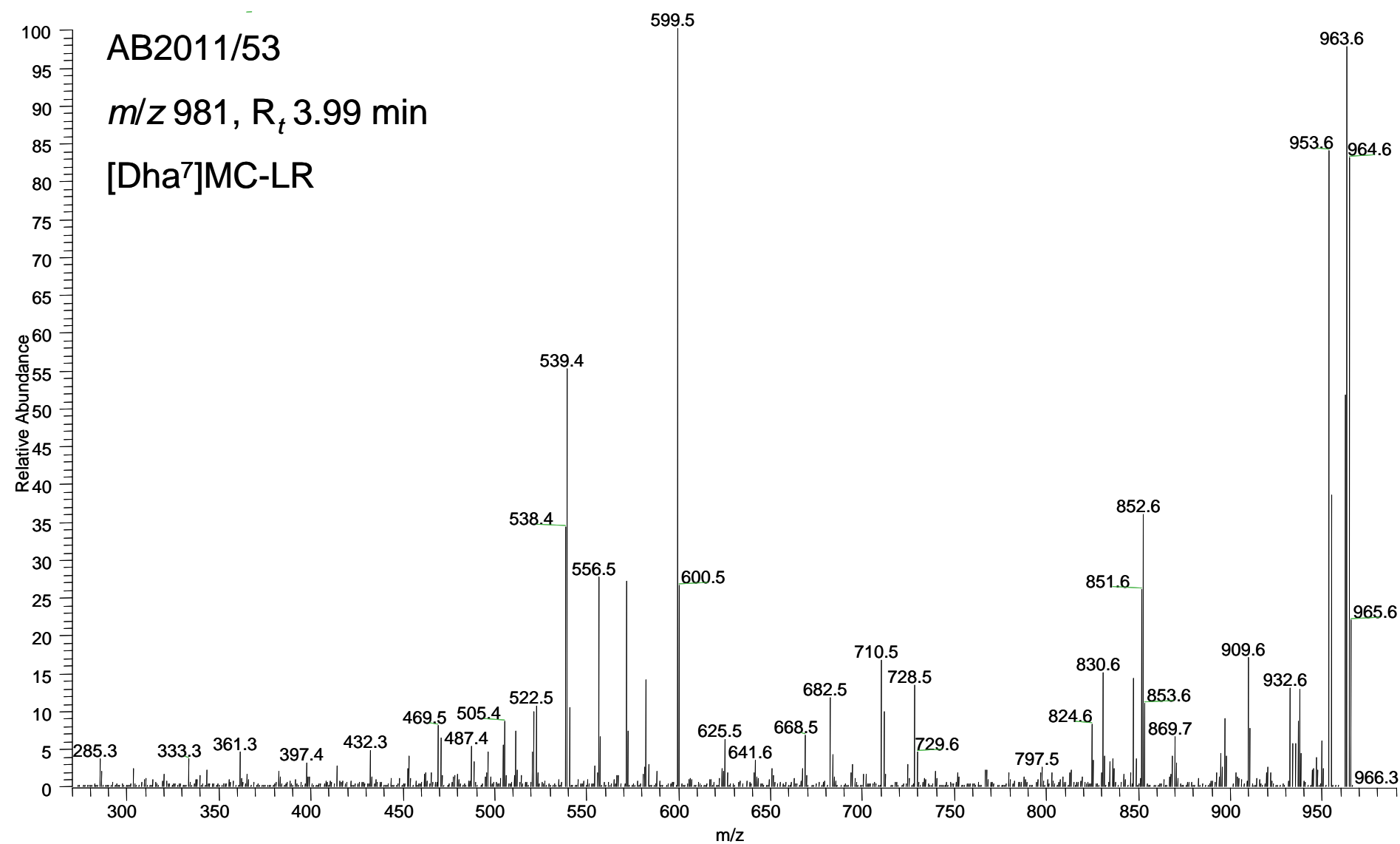
Figure S2o. MS² spectrum of confirmed [Dha⁷]MC-LR from *M. aeruginosa* AB2011/53

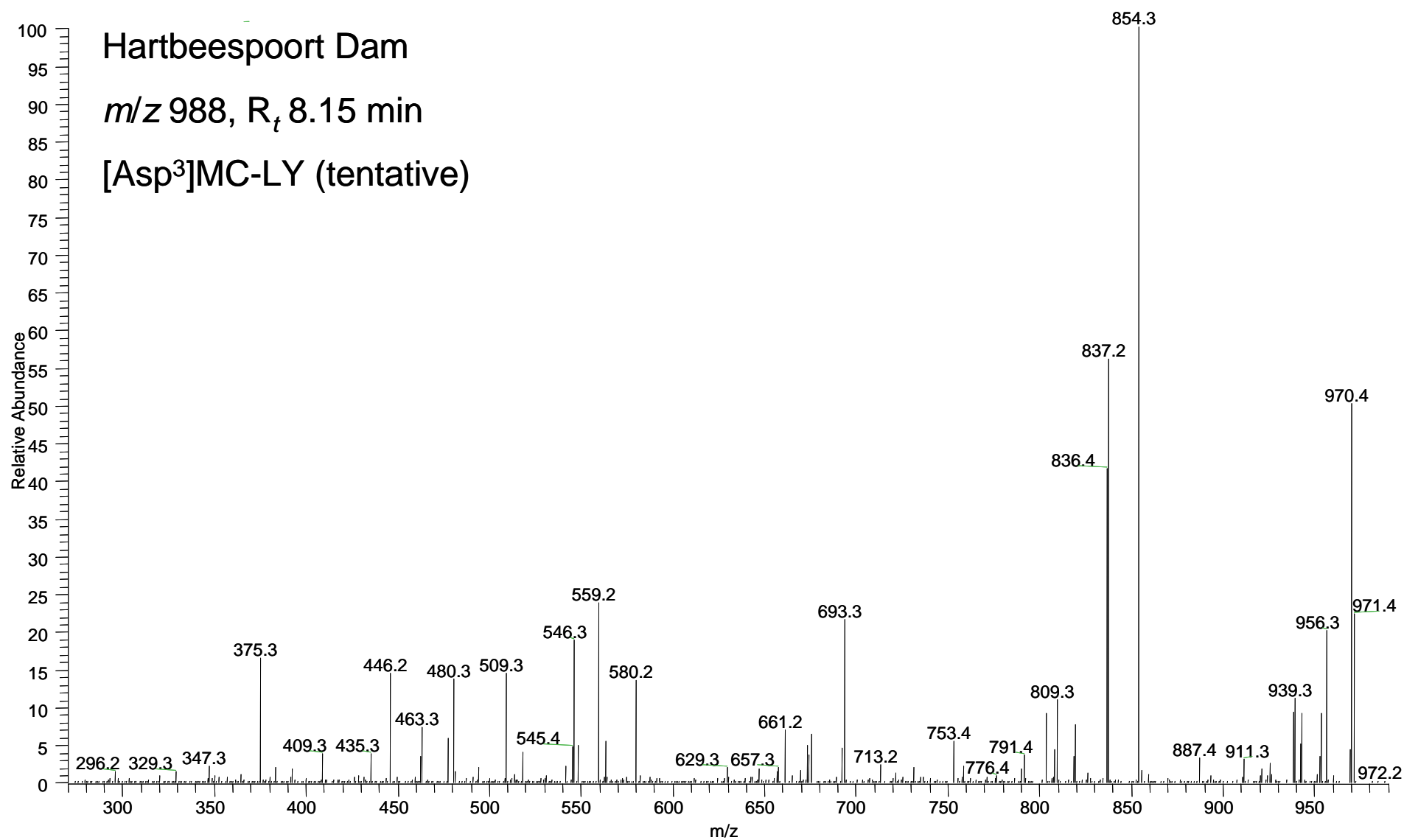
Figure S2p. MS² spectrum of confirmed [Asp³]MC-LY from Hartbeespoort Dam

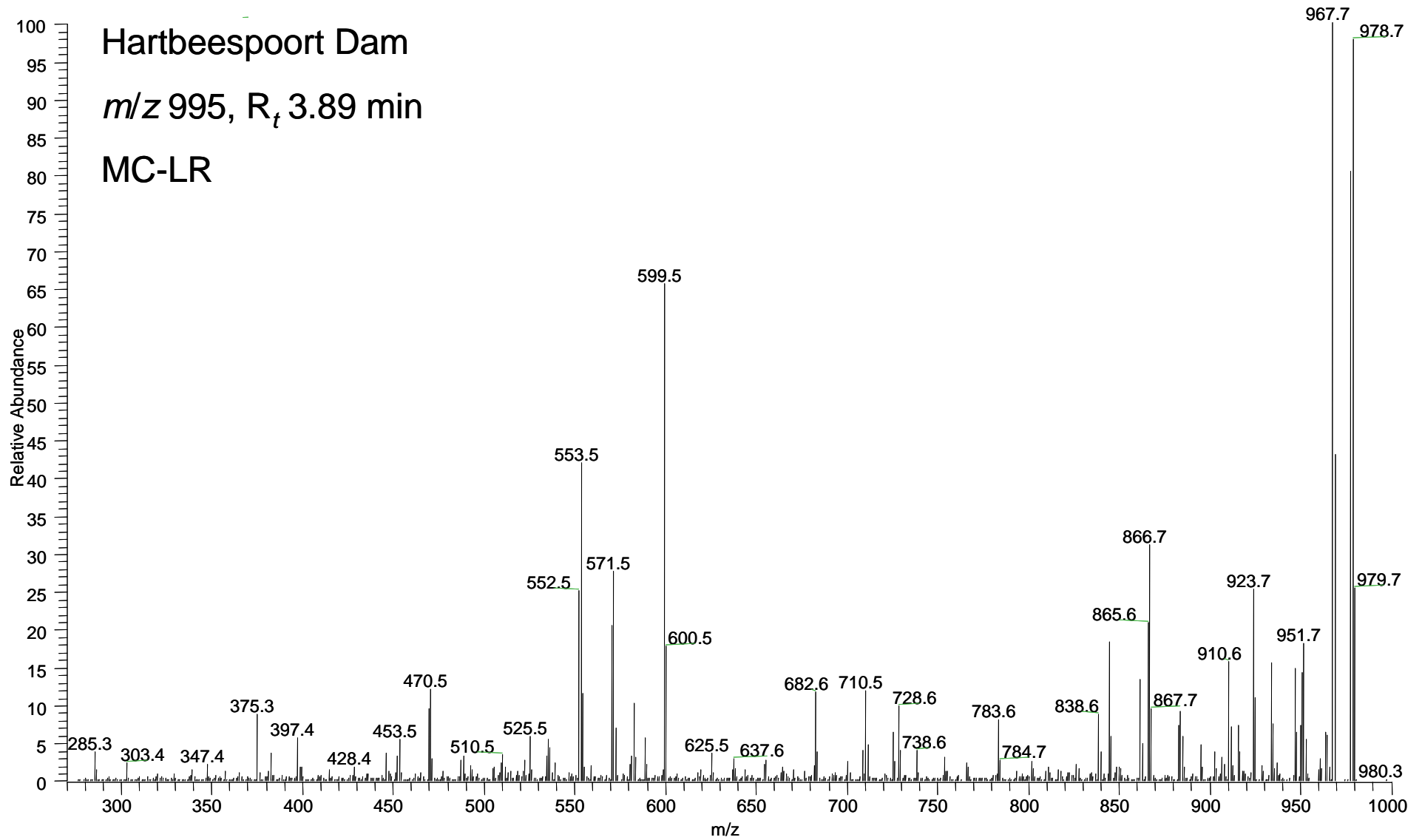
Figure S2q. MS² spectrum of confirmed MC-LR from Hartbeespoort Dam

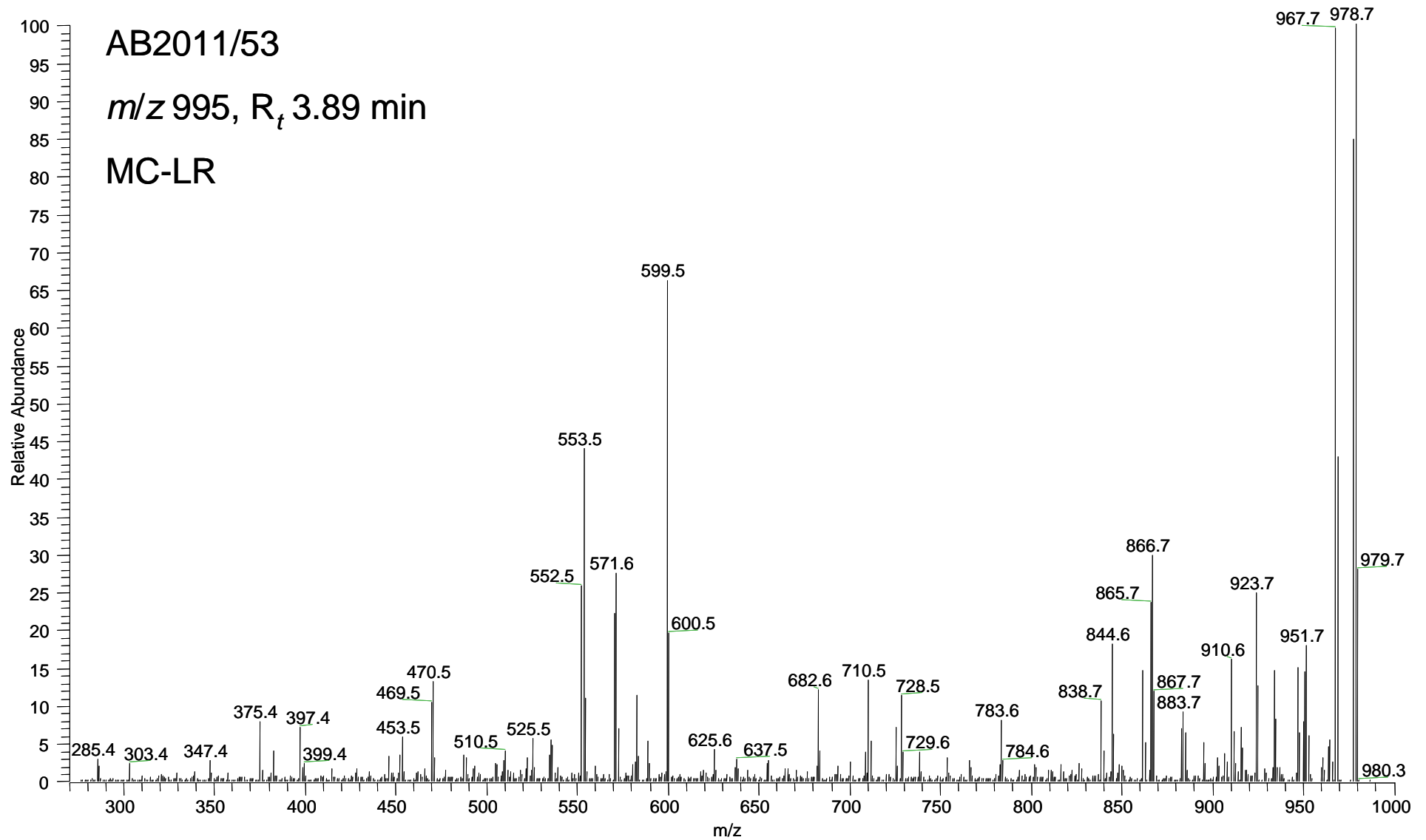
Figure S2r. MS² spectrum of confirmed MC-LR from *M. aeruginosa* AB2011/53

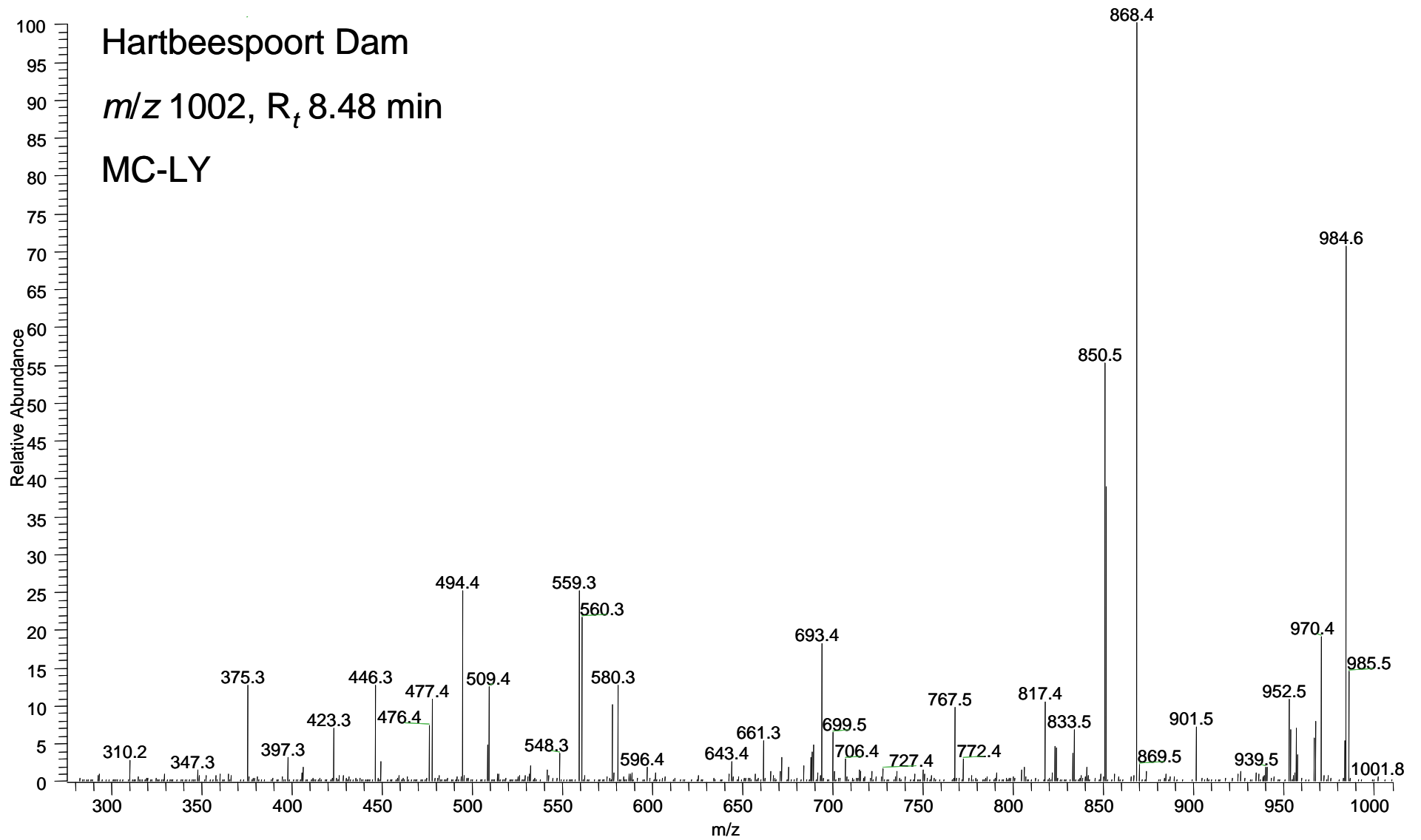
Figure S2s. MS² spectrum of confirmed MC-LY from Hartbeespoort Dam

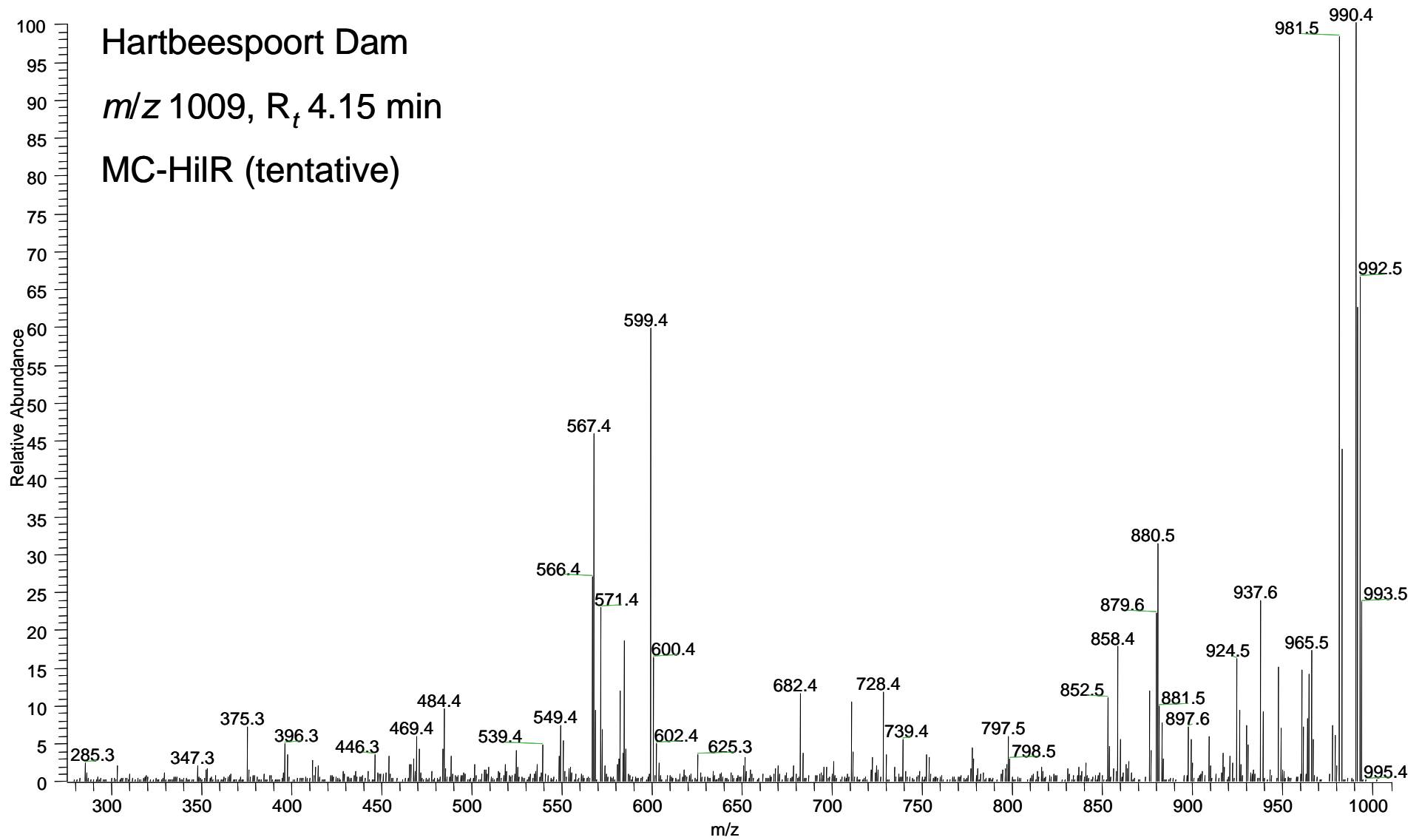
Figure S2t. MS² spectrum of tentative MC-HilR from Hartbeespoort Dam

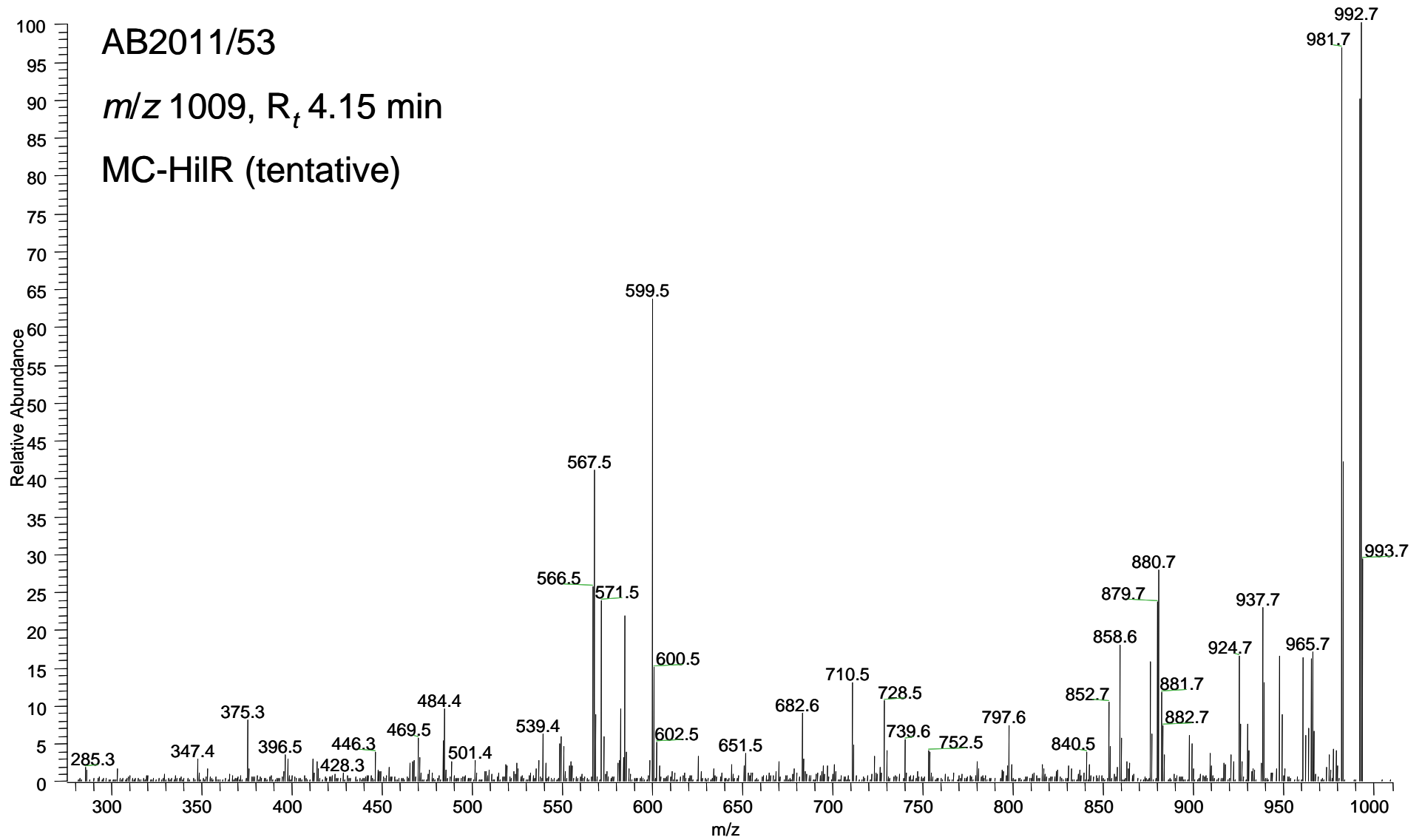
Figure S2u. MS² spectrum of tentative MC-HiIR from *M. aeruginosa* AB2011/53

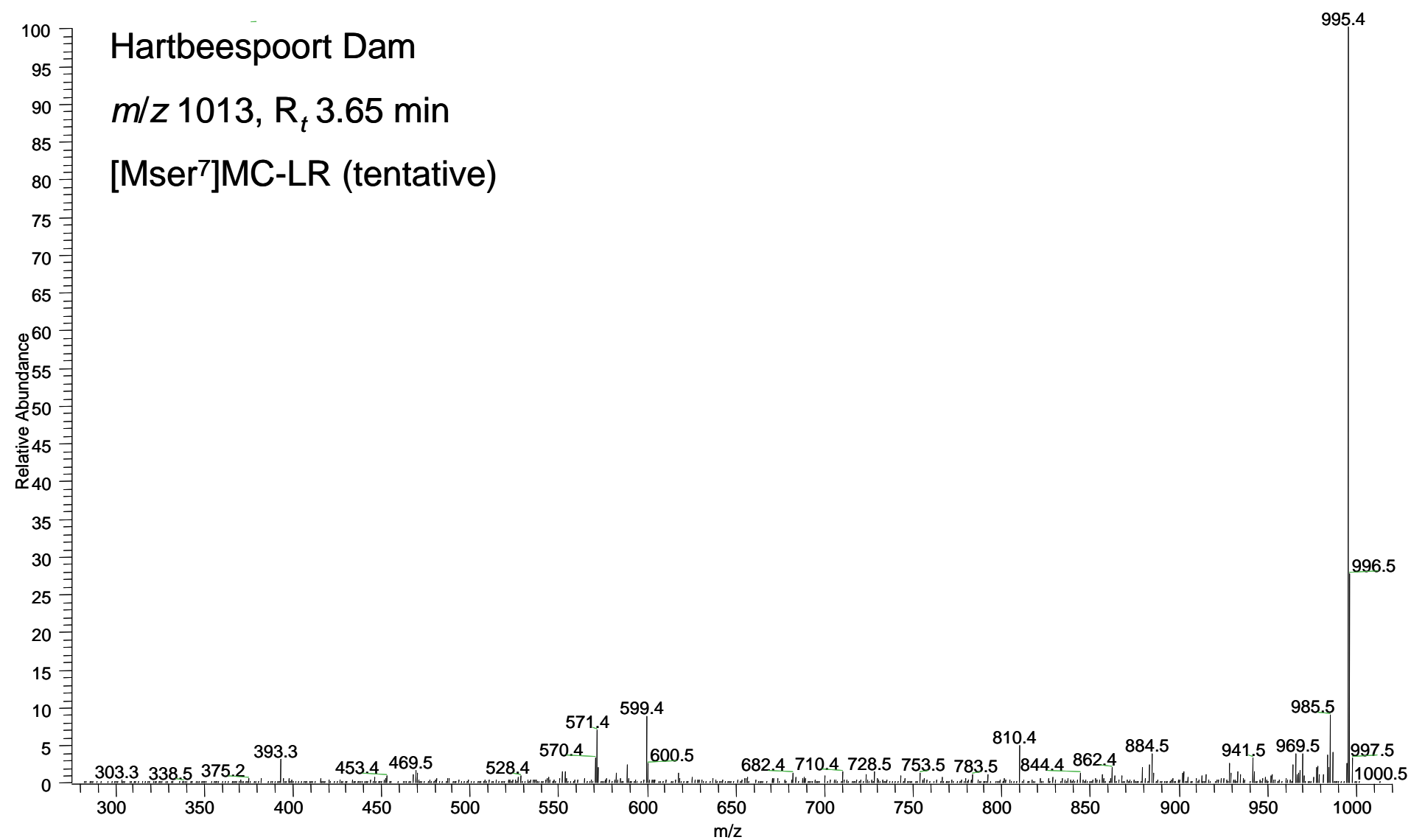
Figure S2v. MS² spectrum of tentative [Mser⁷]MC-LR from Hartbeespoort Dam

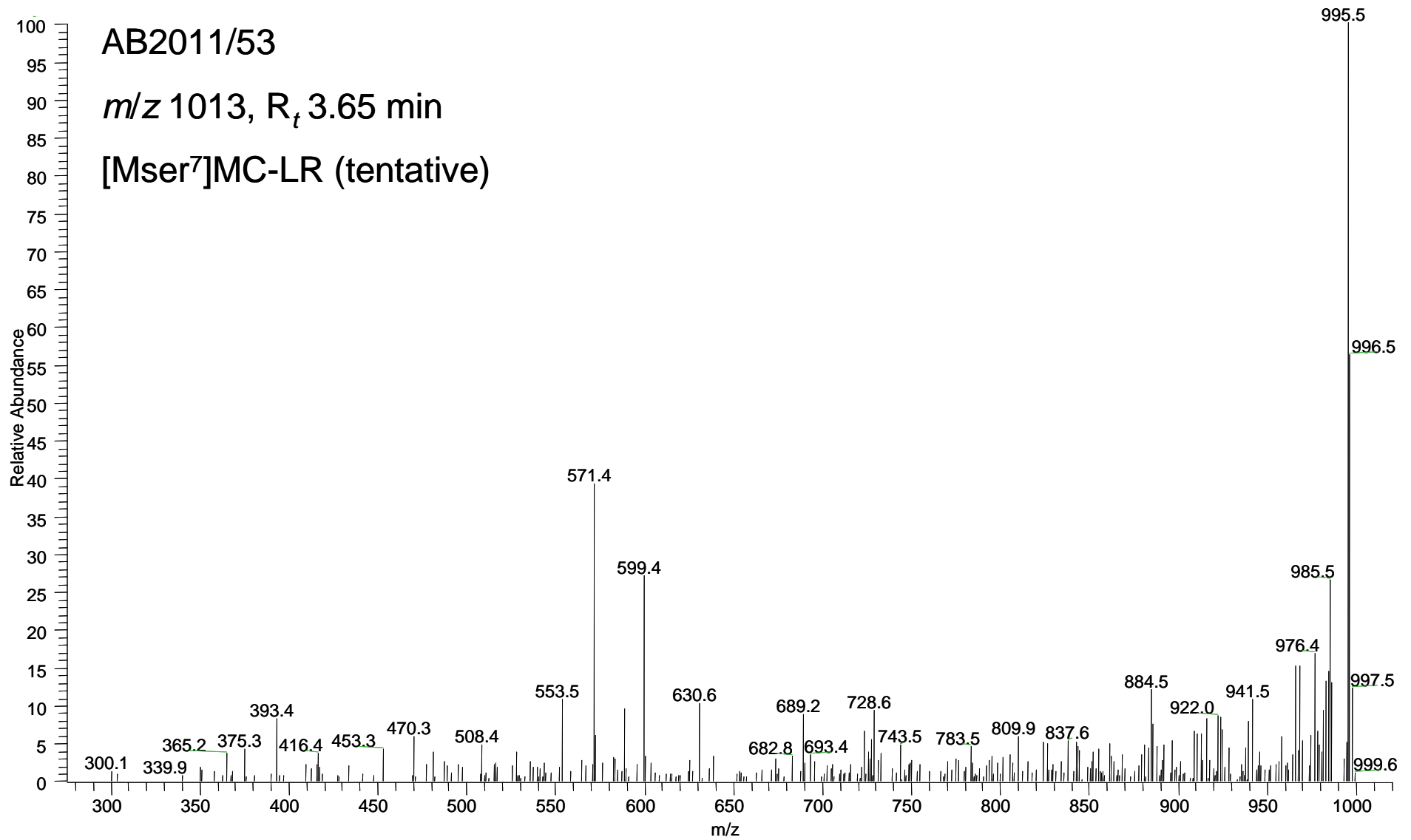
Figure S2w. MS² spectrum of tentative [Mser⁷]MC-LR from *M. aeruginosa* AB2011/53

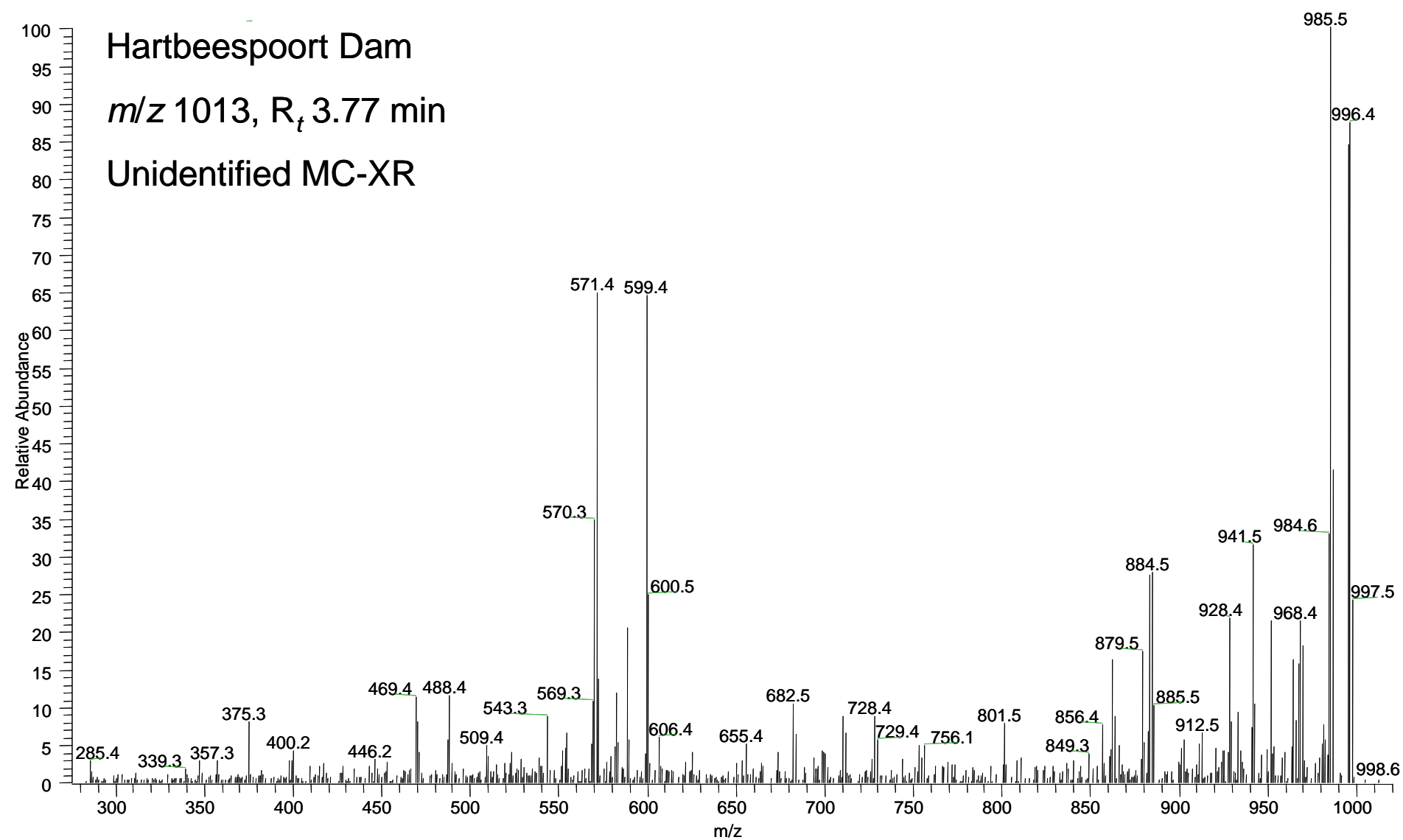
Figure S2x. MS² spectrum of unidentified MC-XR from Hartbeespoort Dam

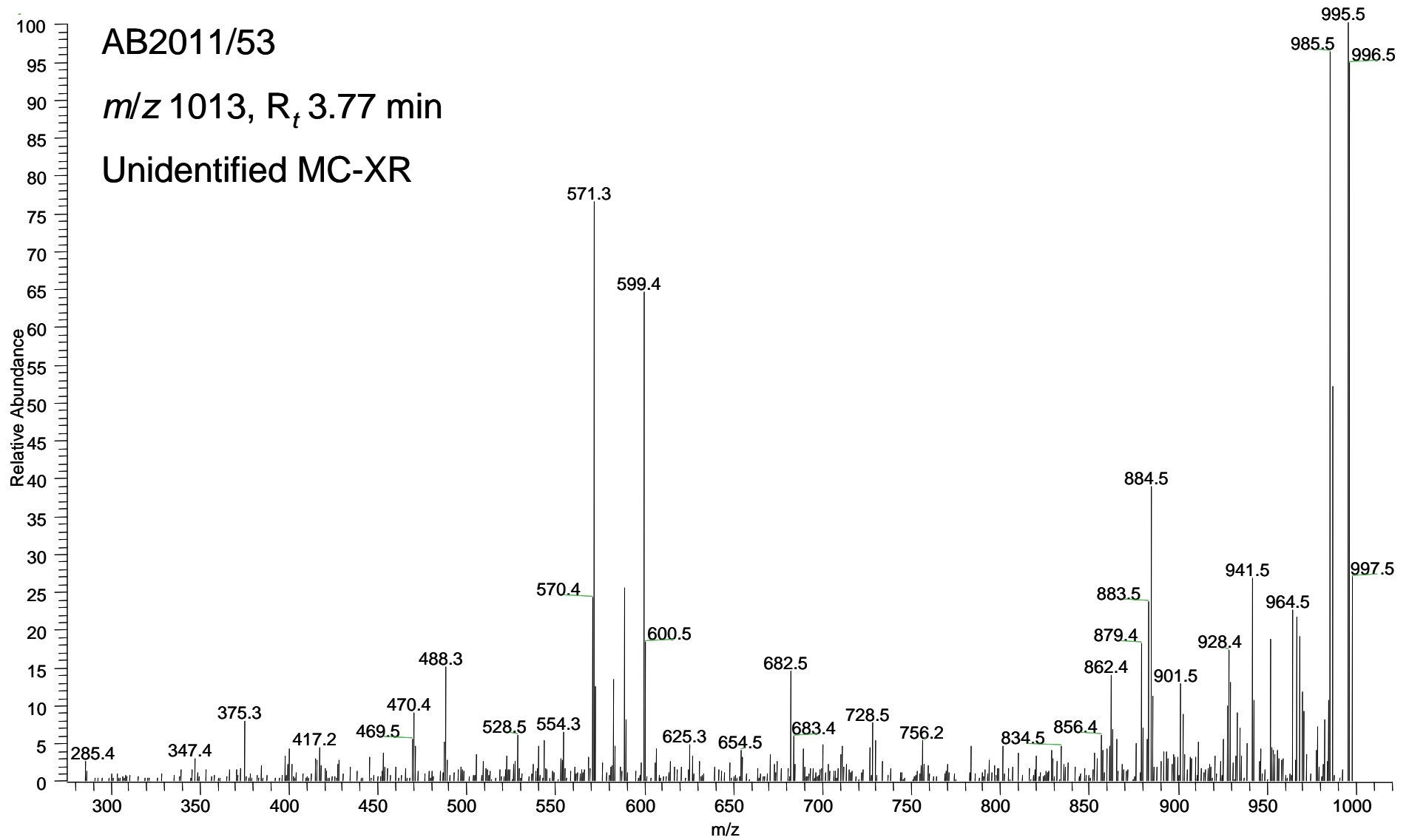
Figure S2y. MS² spectrum of unidentified MC-XR from *M. aeruginosa* AB2011/53

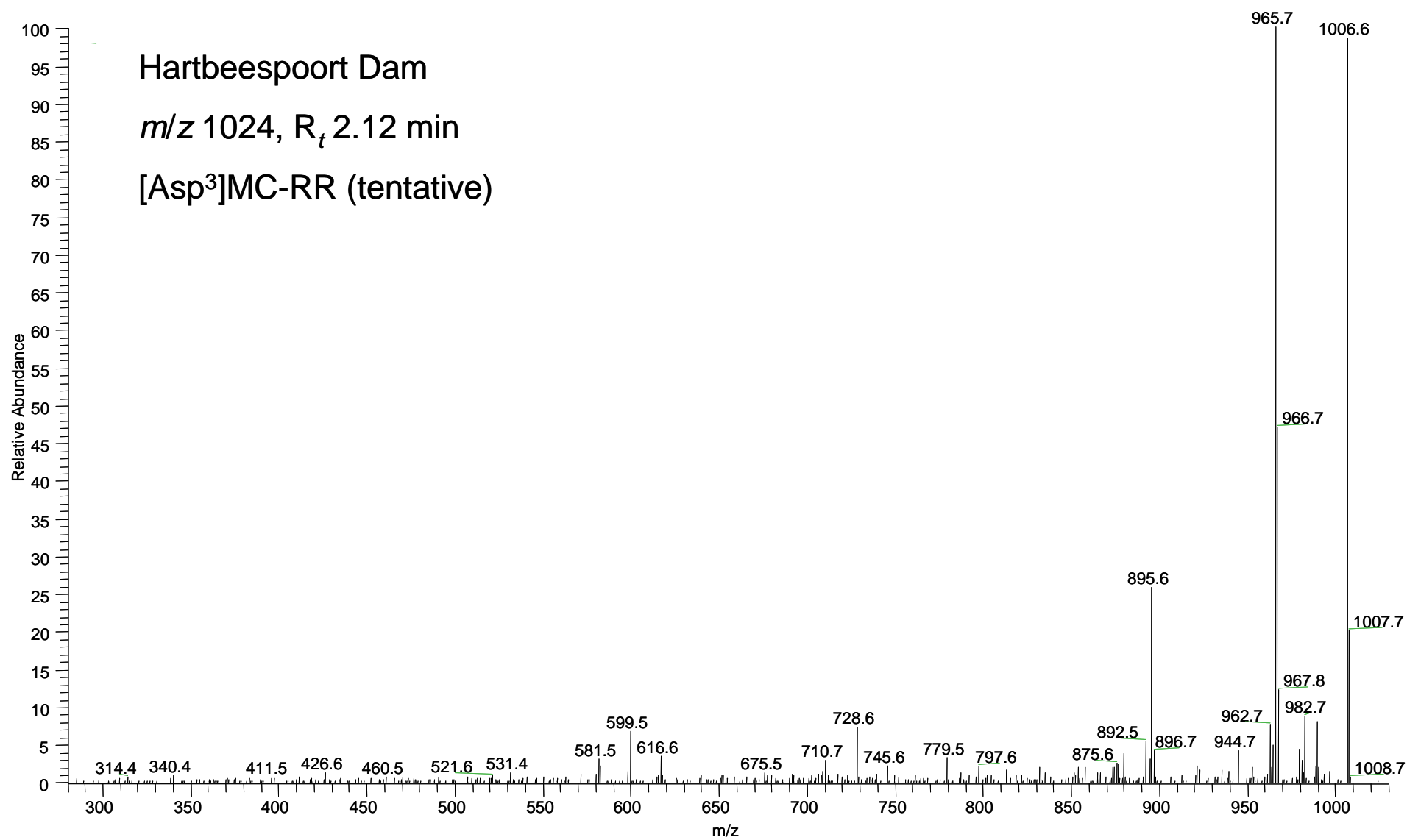
Figure S2z. MS² spectrum of tentative [Asp³]MC-RR from Hartbeespoort Dam

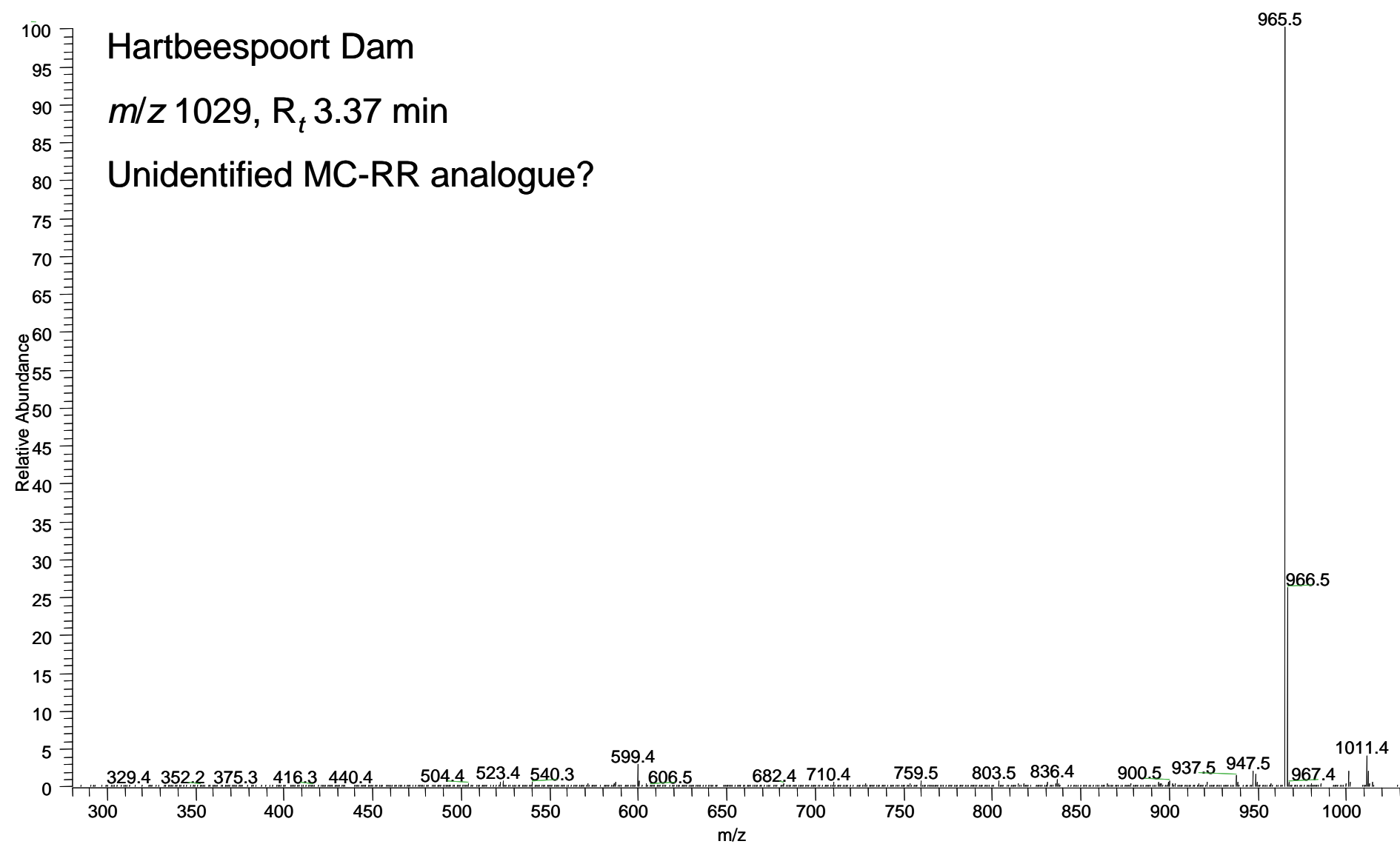
Figure S2aa. MS² spectrum of unidentified possible MC-RR analogue from Hartbeespoort Dam

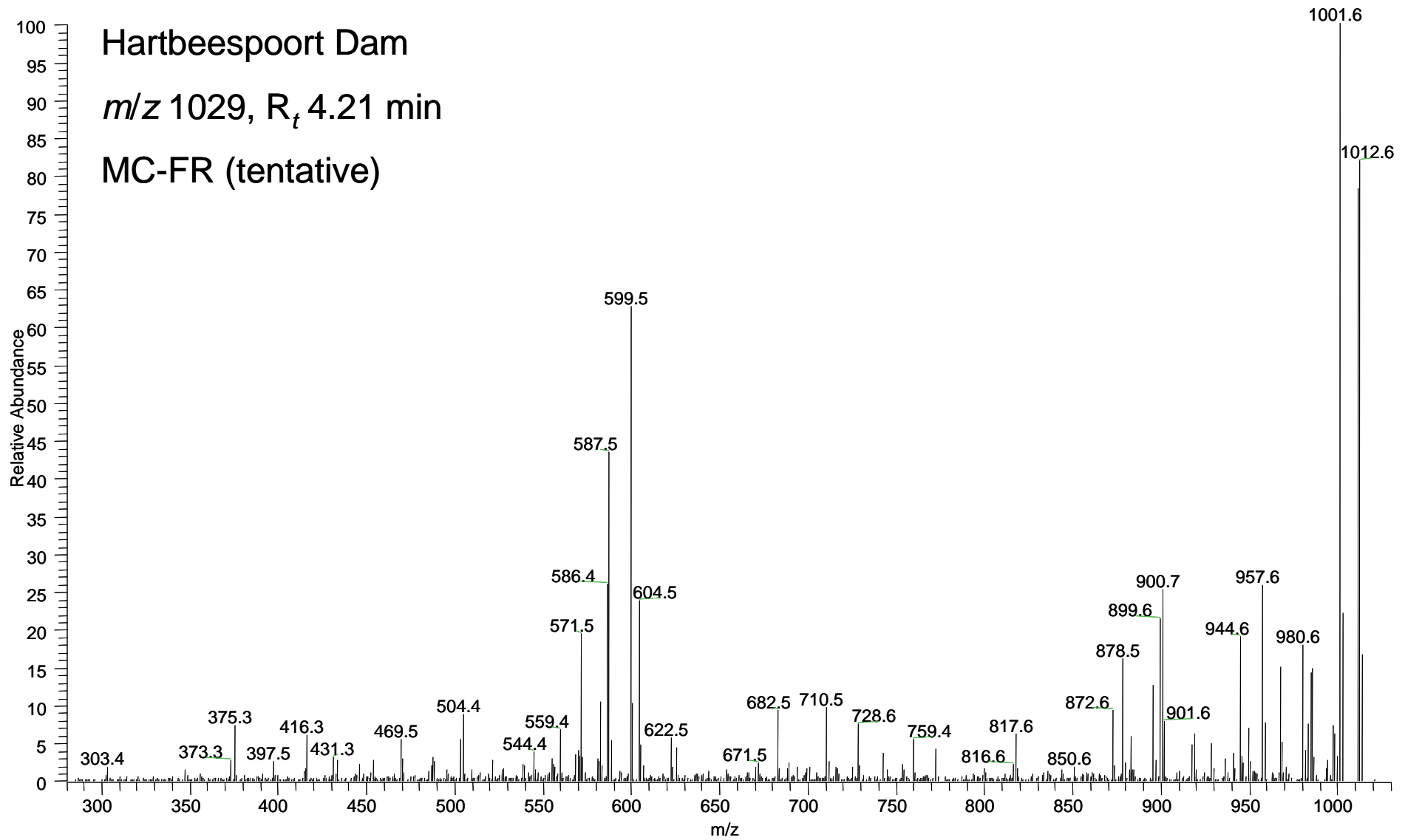
Figure S2ab. MS² spectrum of tentative MC-FR from Hartbeespoort Dam

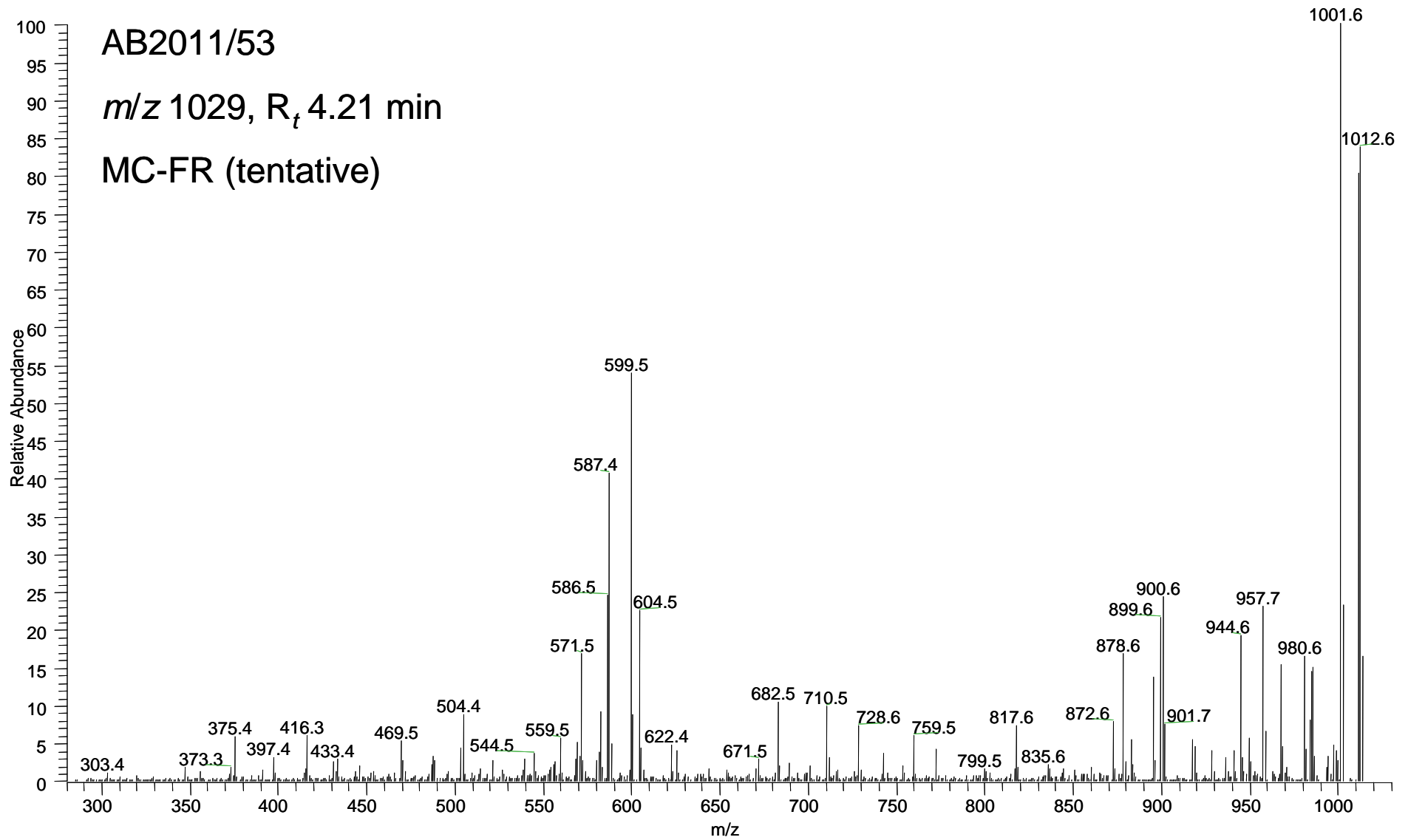
Figure S2ac. MS² spectrum of tentative MC-FR from *M. aeruginosa* AB2011/53

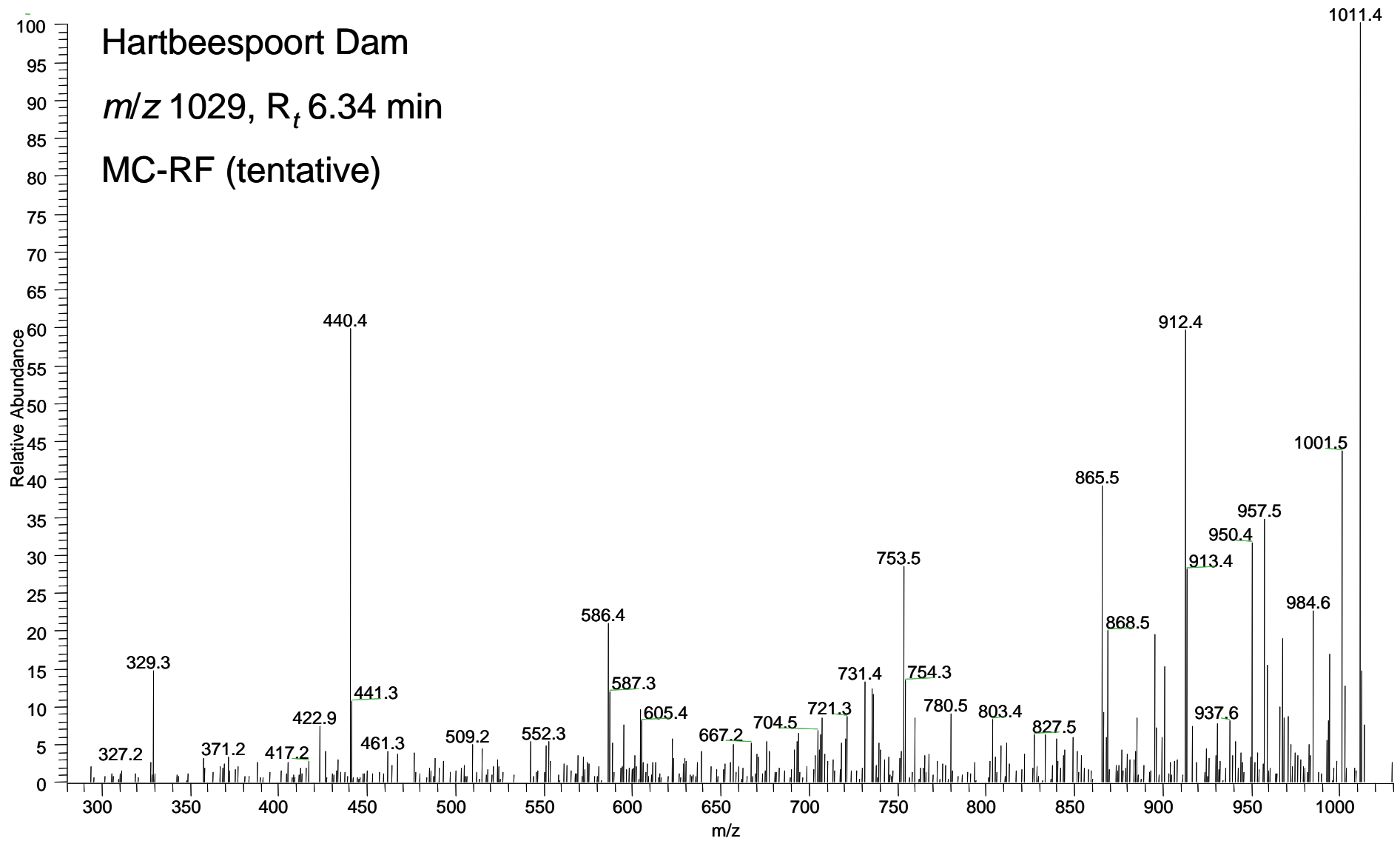
Figure S2ad. MS² spectrum of tentative MC-RF from Hartbeespoort Dam

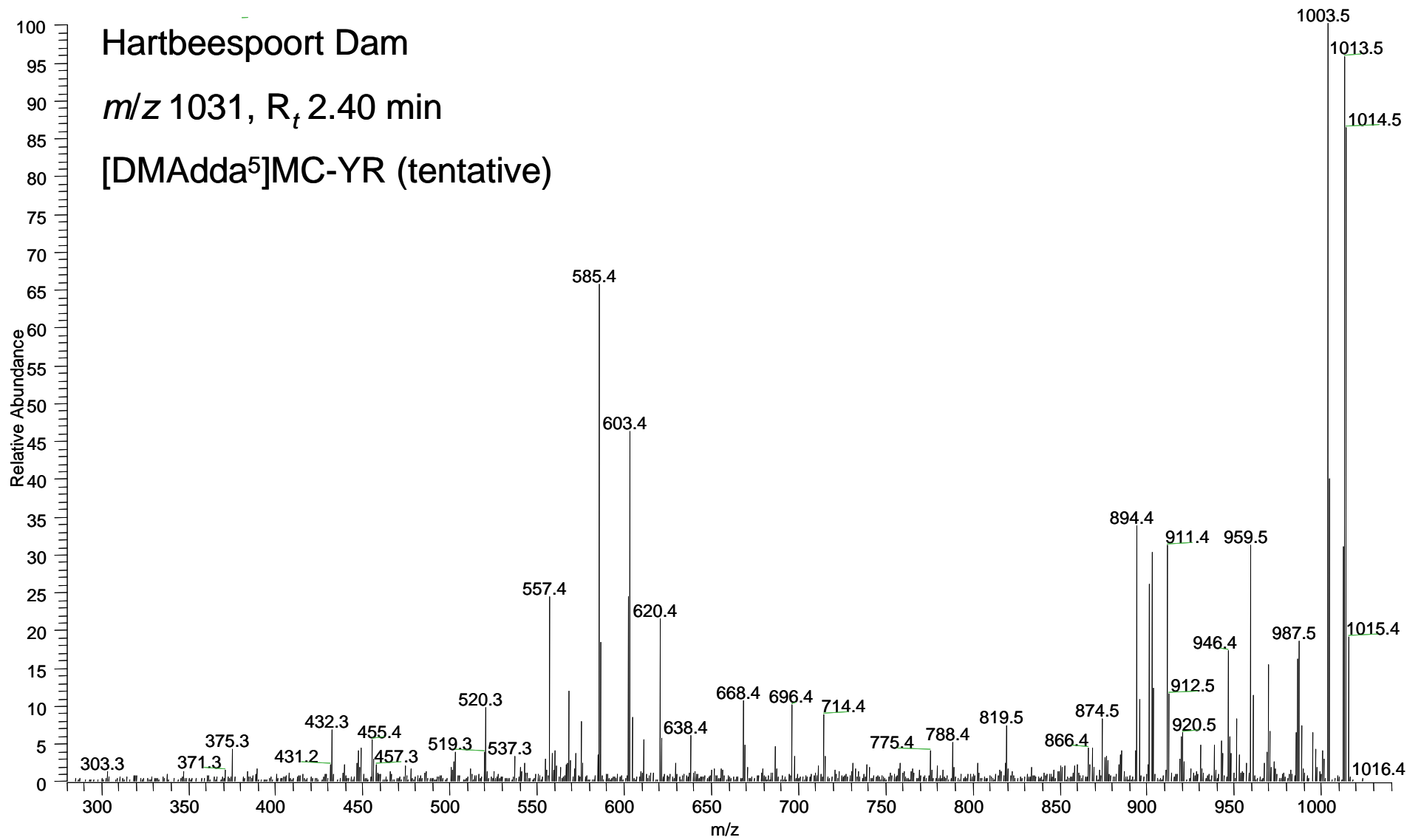
Figure S2ae. MS² spectrum of tentative [DMAdda⁵]MC-YR from Hartbeespoort Dam

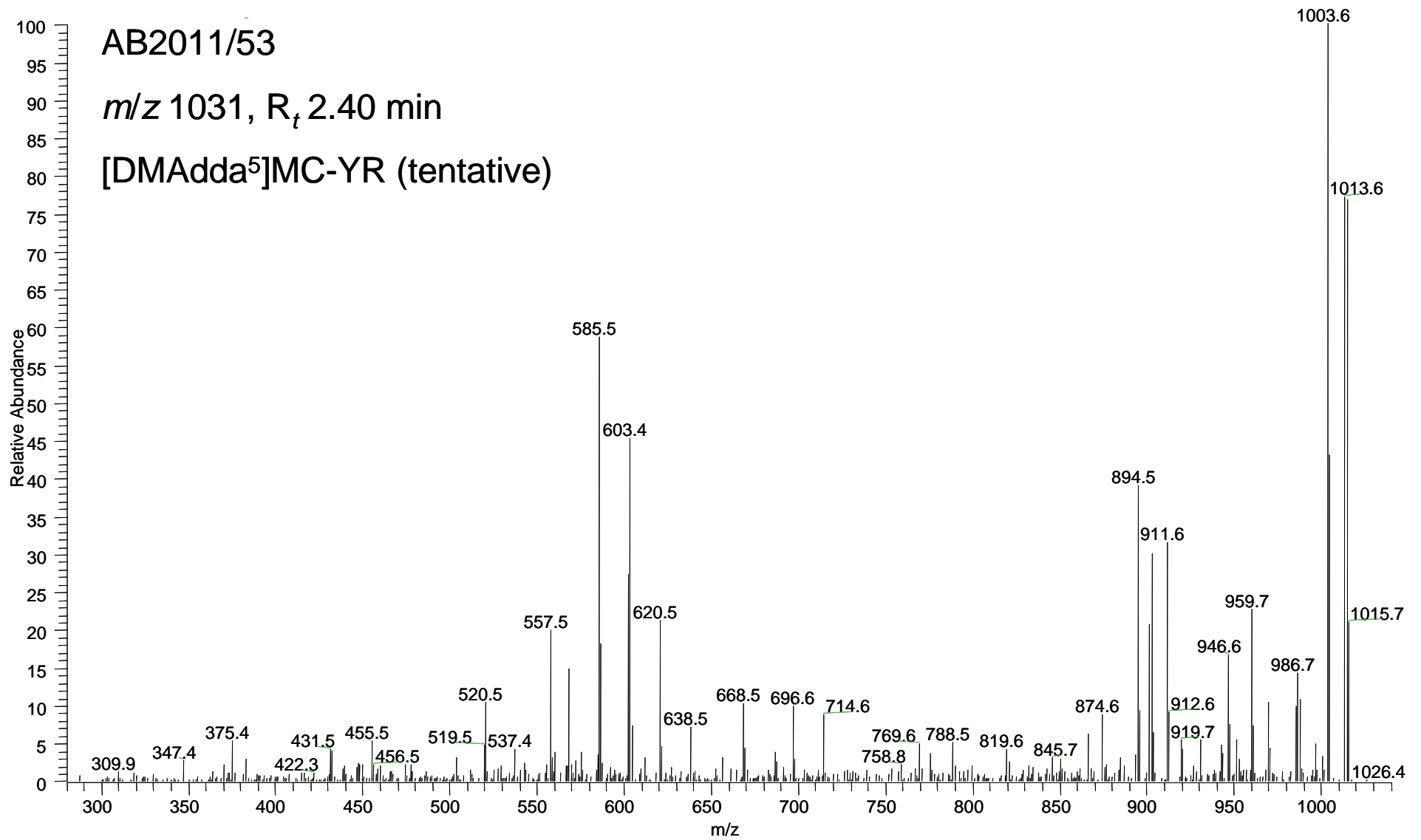
Figure S2af. MS² spectrum of tentative [DMAdda⁵]MC-YR from *M. aeruginosa* AB2011/53

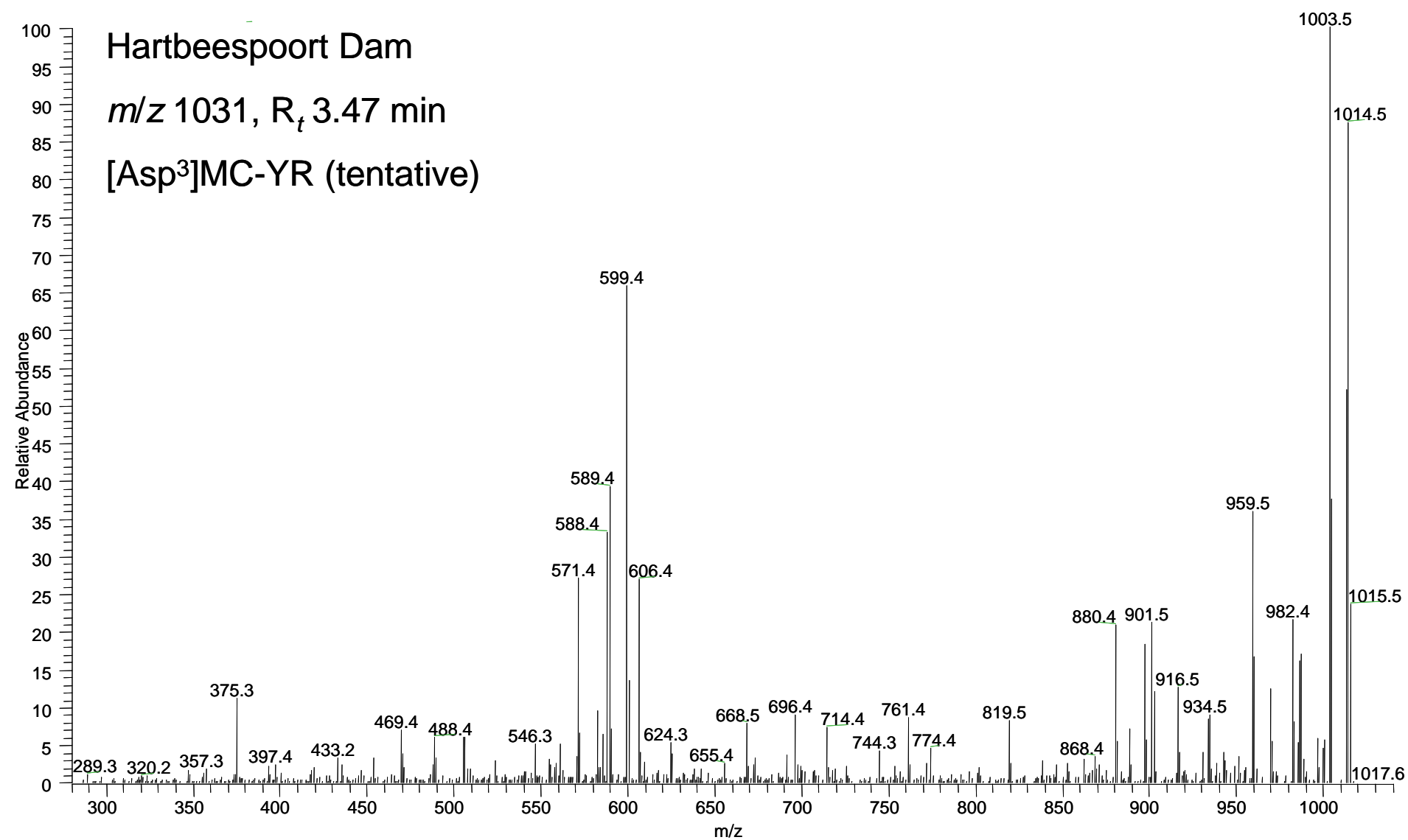
Figure S2ag. MS² spectrum of tentative [Asp³]MC-YR from Hartbeespoort Dam

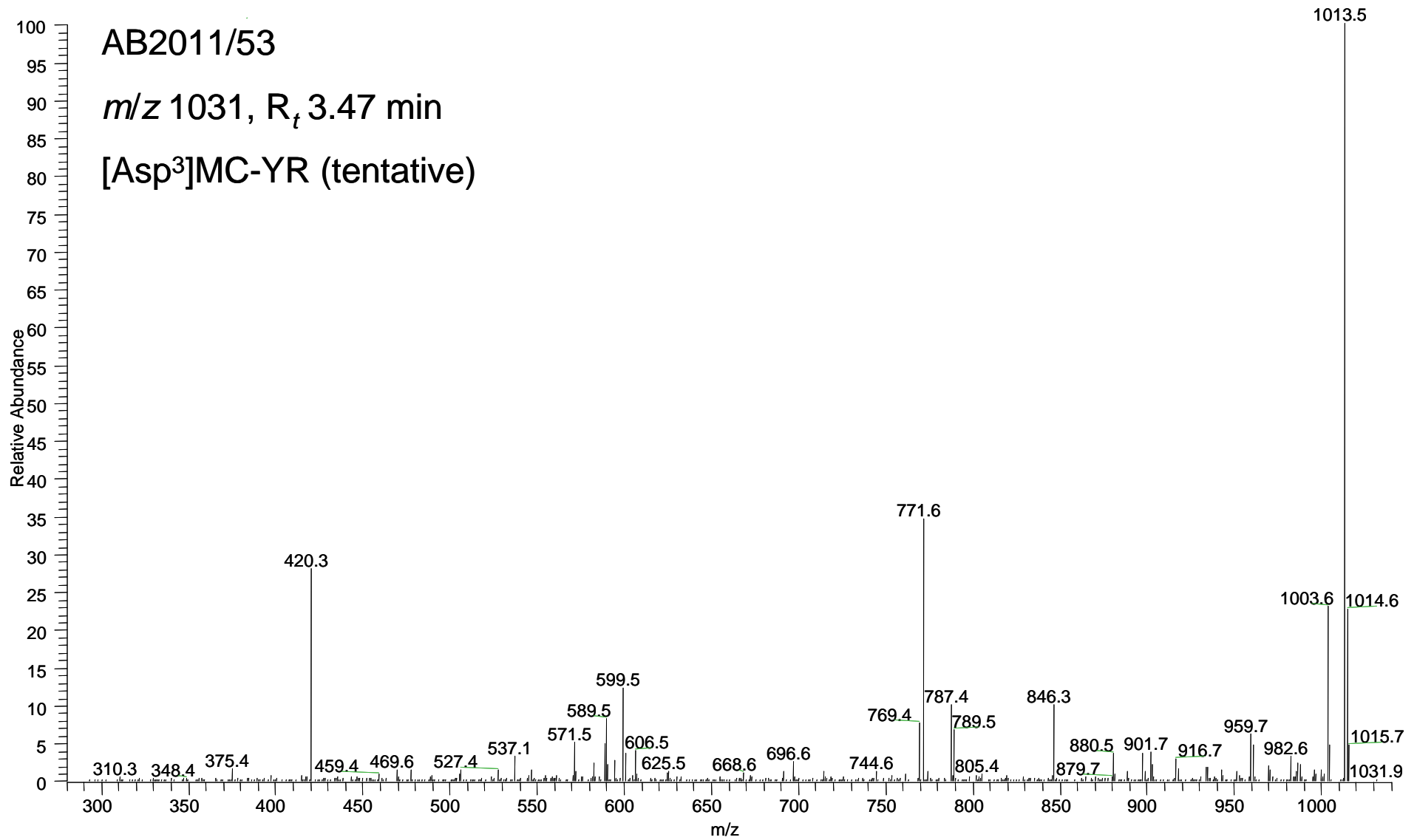
Figure S2ah. MS² spectrum of tentative [Asp³]MC-YR from *M. aeruginosa* AB2011/53

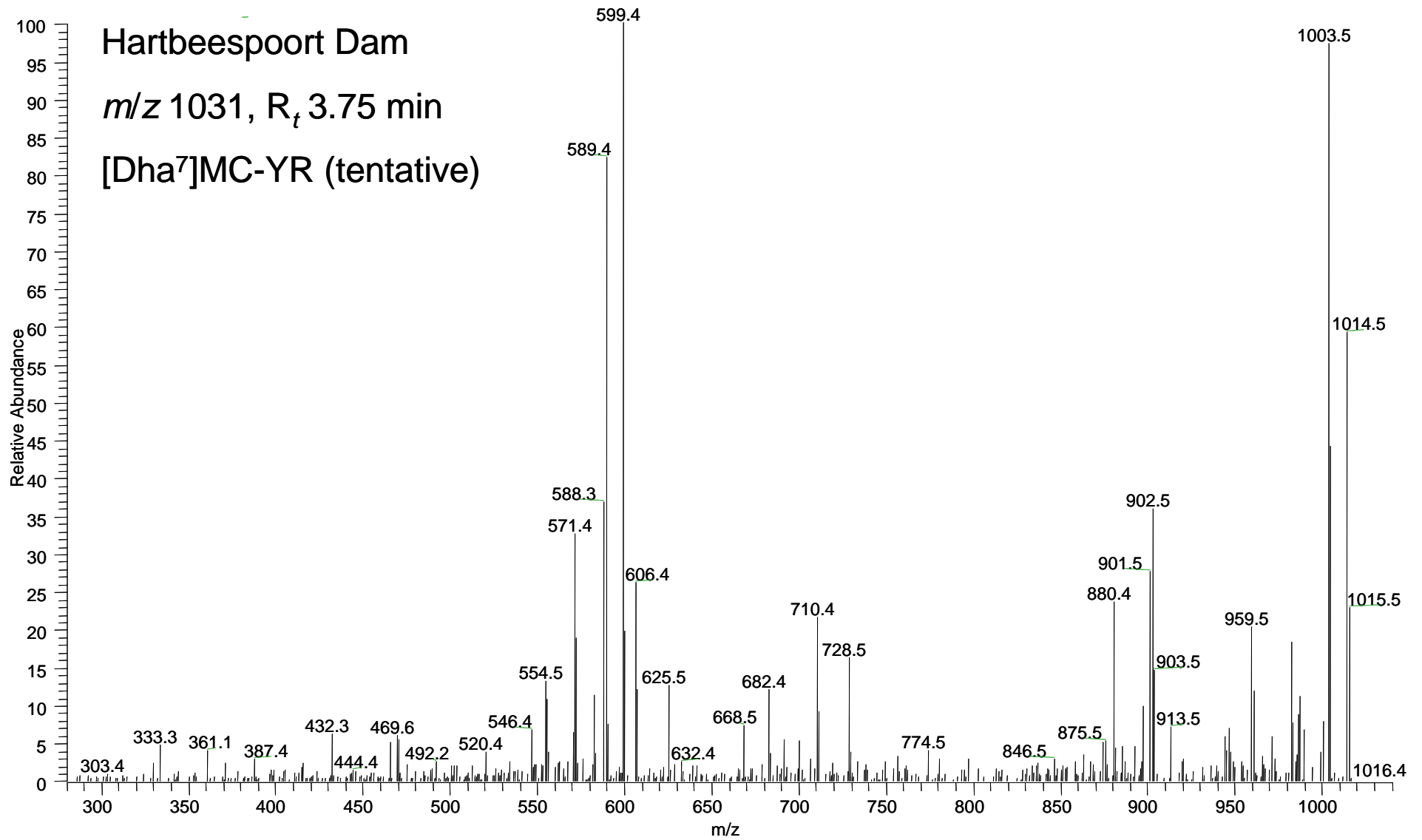
Figure S2ai. MS² spectrum of tentative [Dha⁷]MC-YR from Hartbeespoort Dam

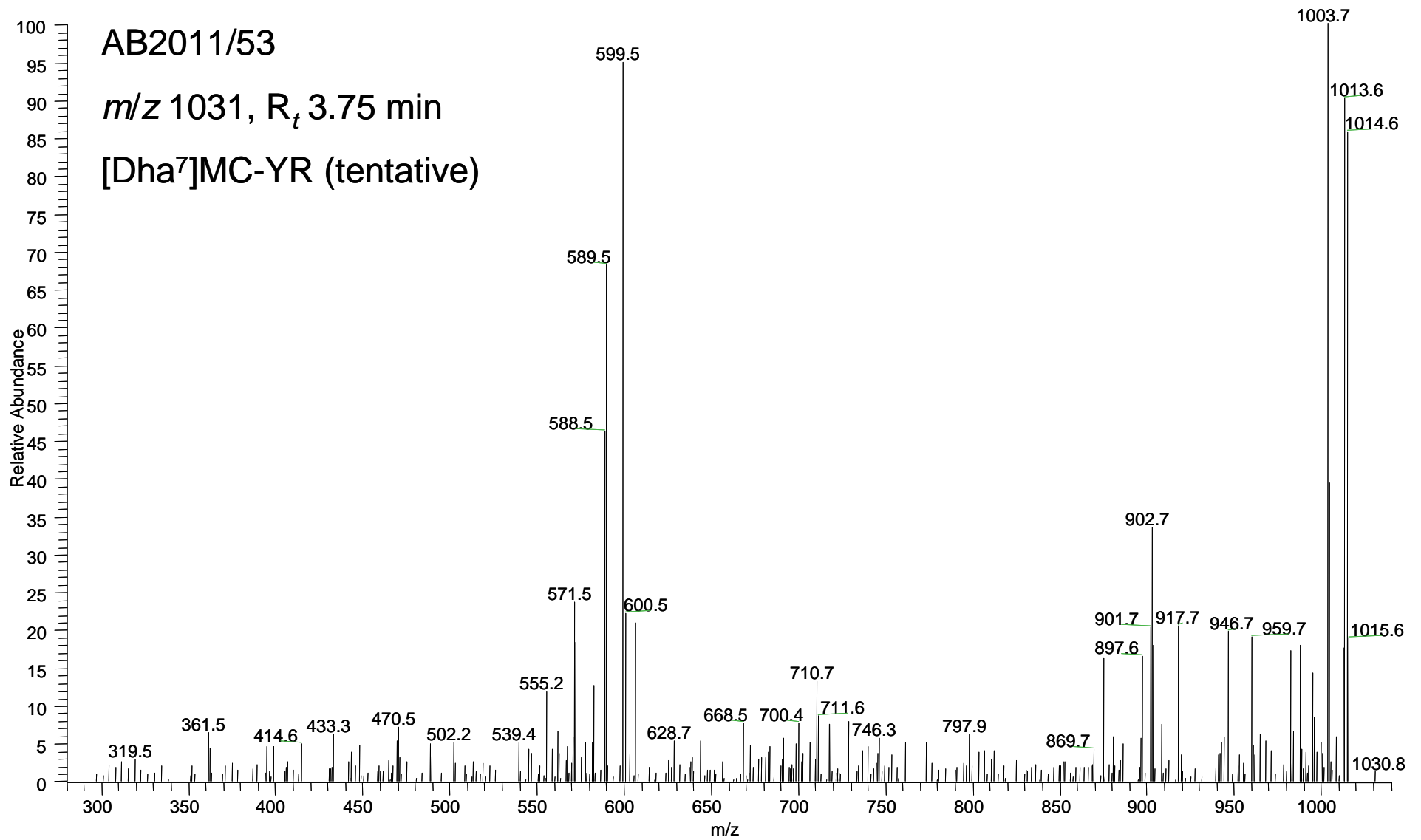
Figure S2aj. MS² spectrum of tentative [Dha⁷]MC-YR from *M. aeruginosa* AB2011/53

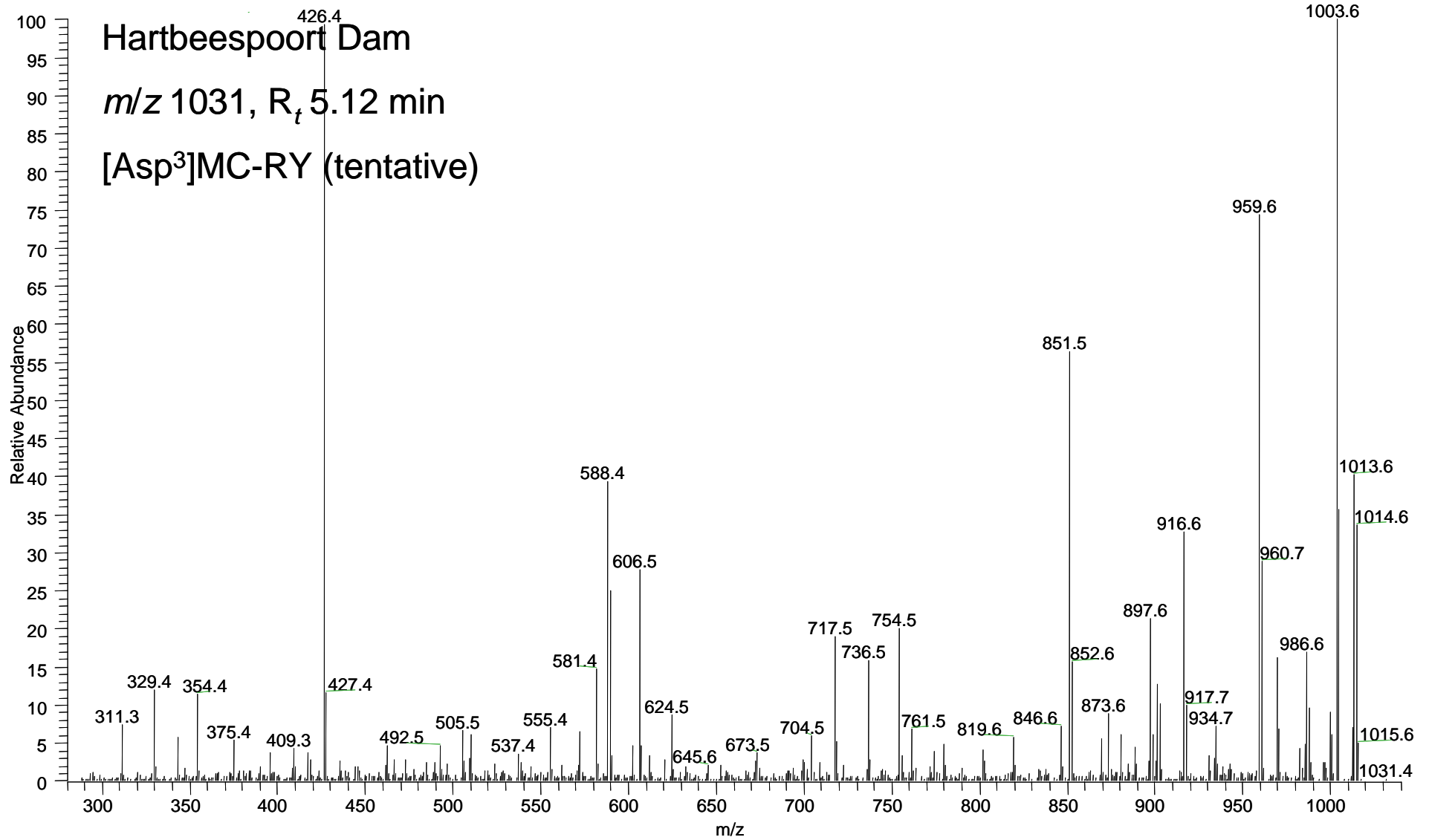
Figure S2ak. MS² spectrum of tentative [Asp³]MC-RY from Hartbeespoort Dam

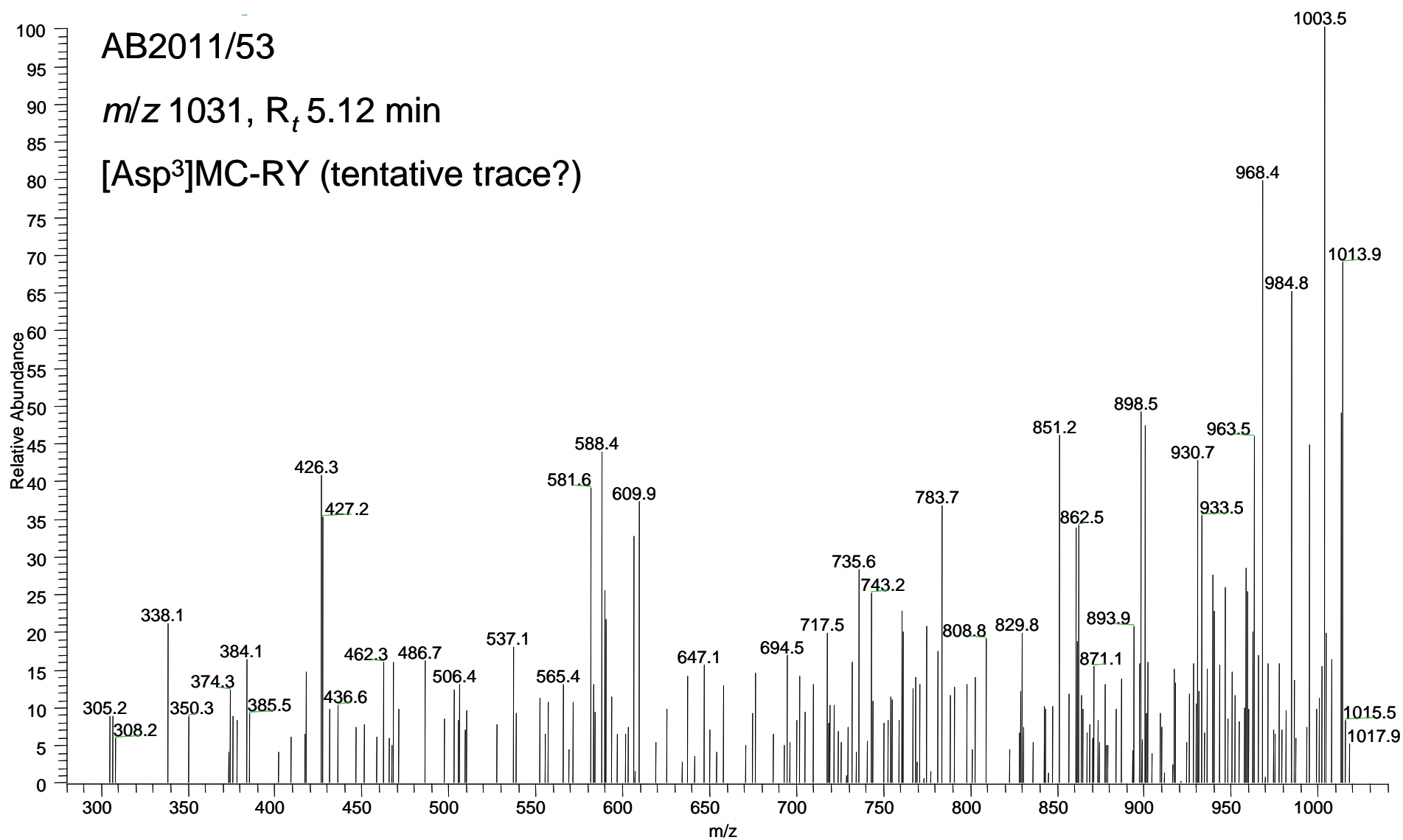
Figure S2a. MS² spectrum of tentative trace [Asp³]MC-RY from *M. aeruginosa* AB2011/53

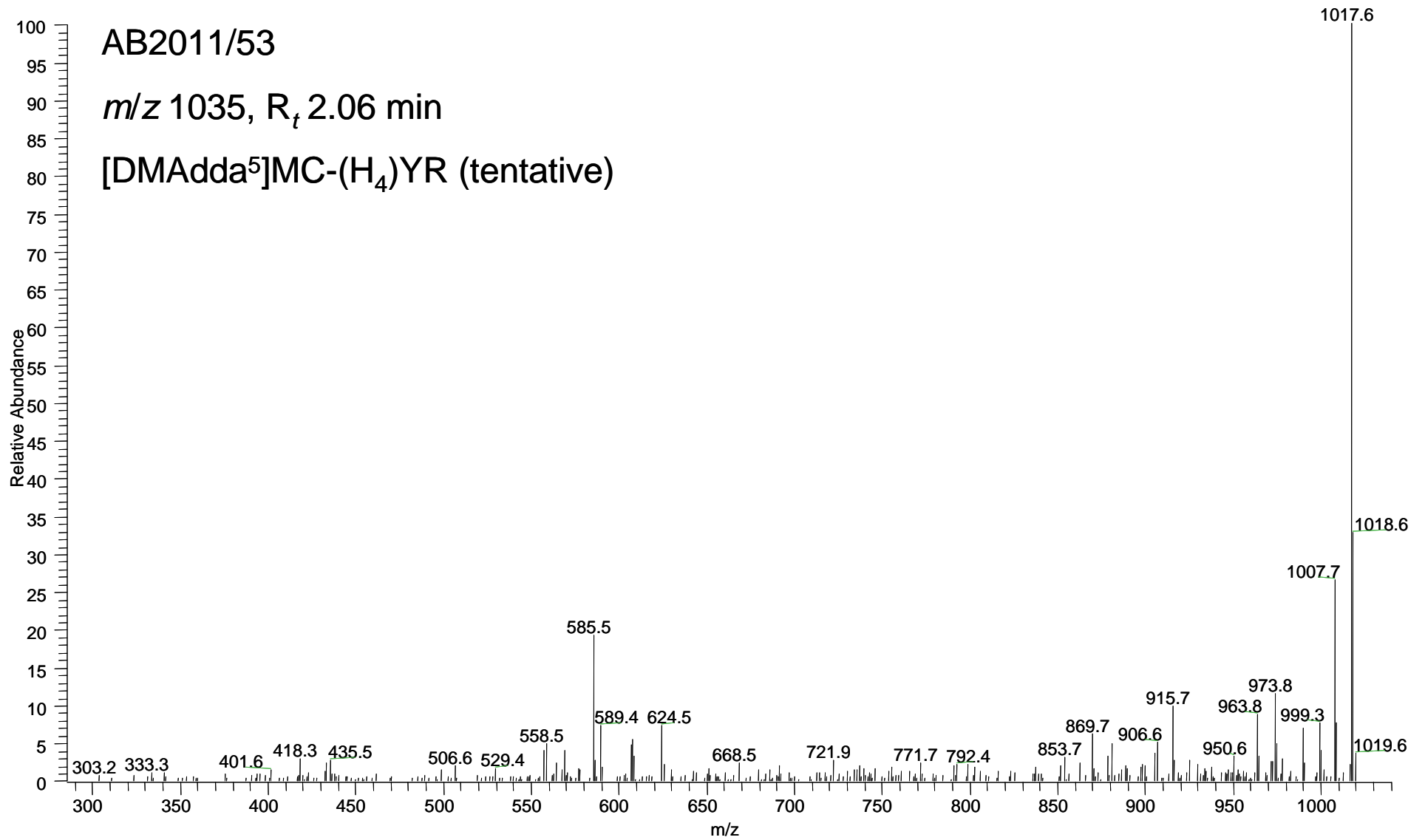
Figure S2am. MS² spectrum of tentative [DMAdda⁵]C-(H₄)YR from Hartbeespoort Dam

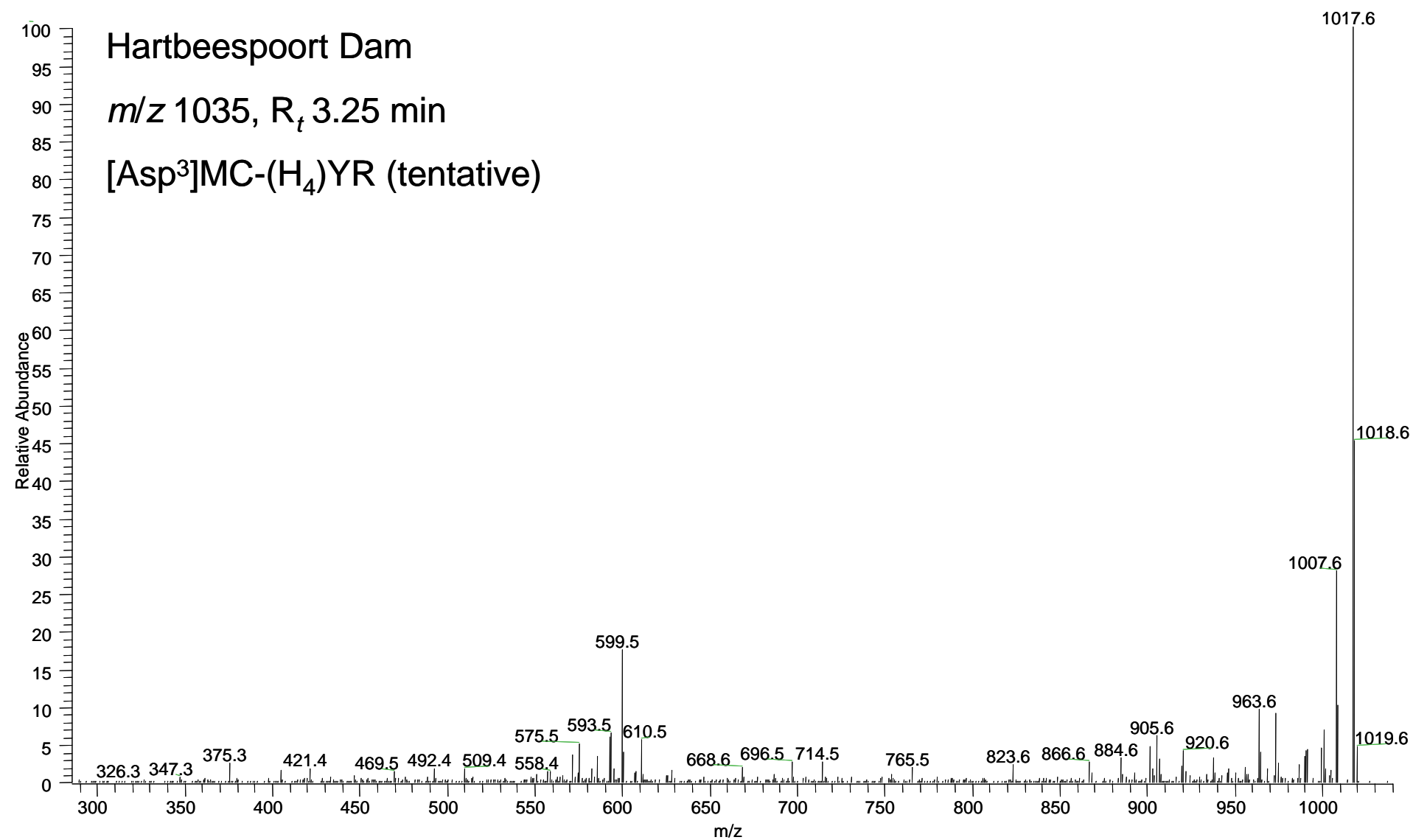
Figure S2an. MS² spectrum of tentative [Asp³]MC-(H₄)YR from Hartbeespoort Dam

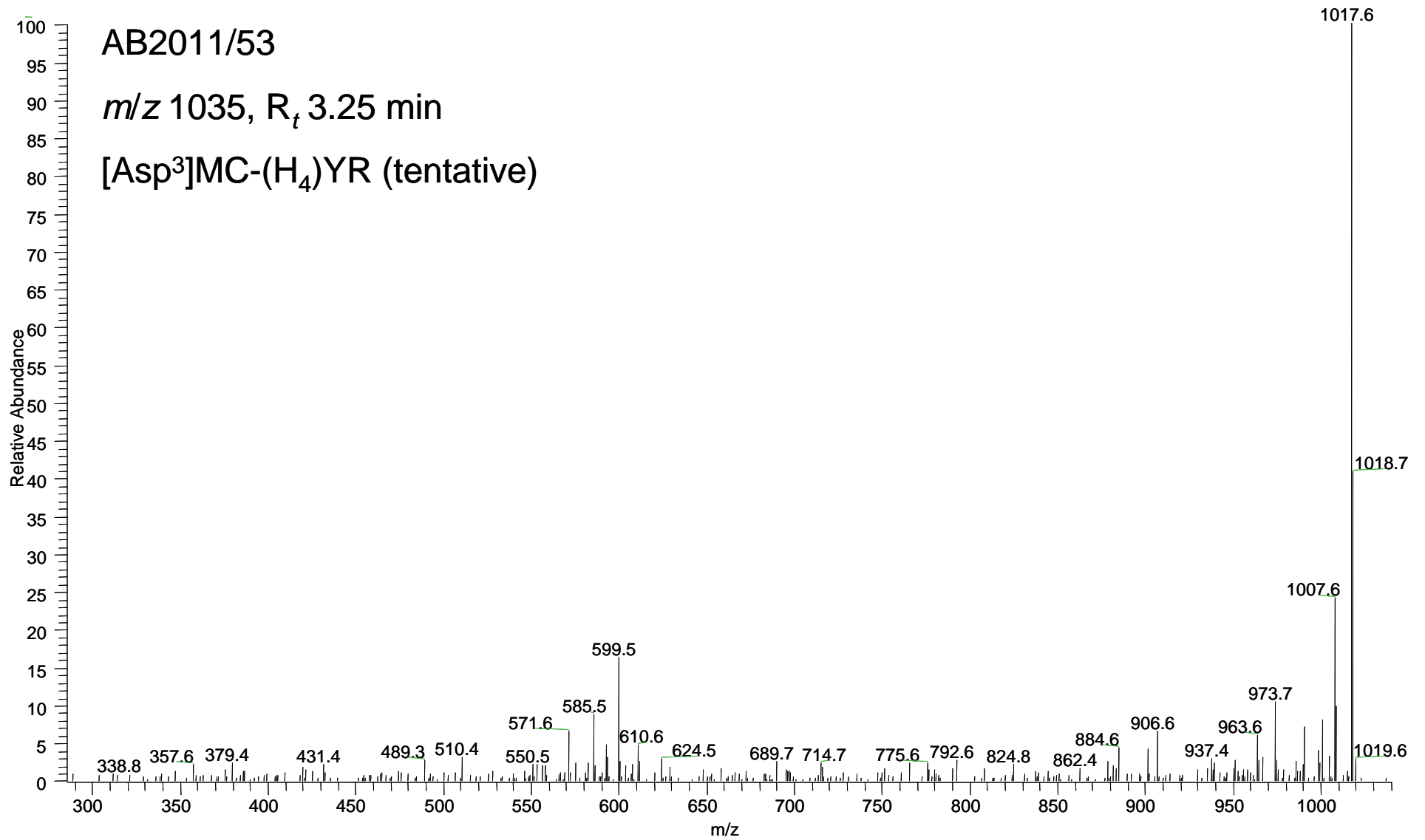
Figure S2ao. MS² spectrum of tentative [Asp³]MC-(H₄)YR from *M. aeruginosa* AB2011/53

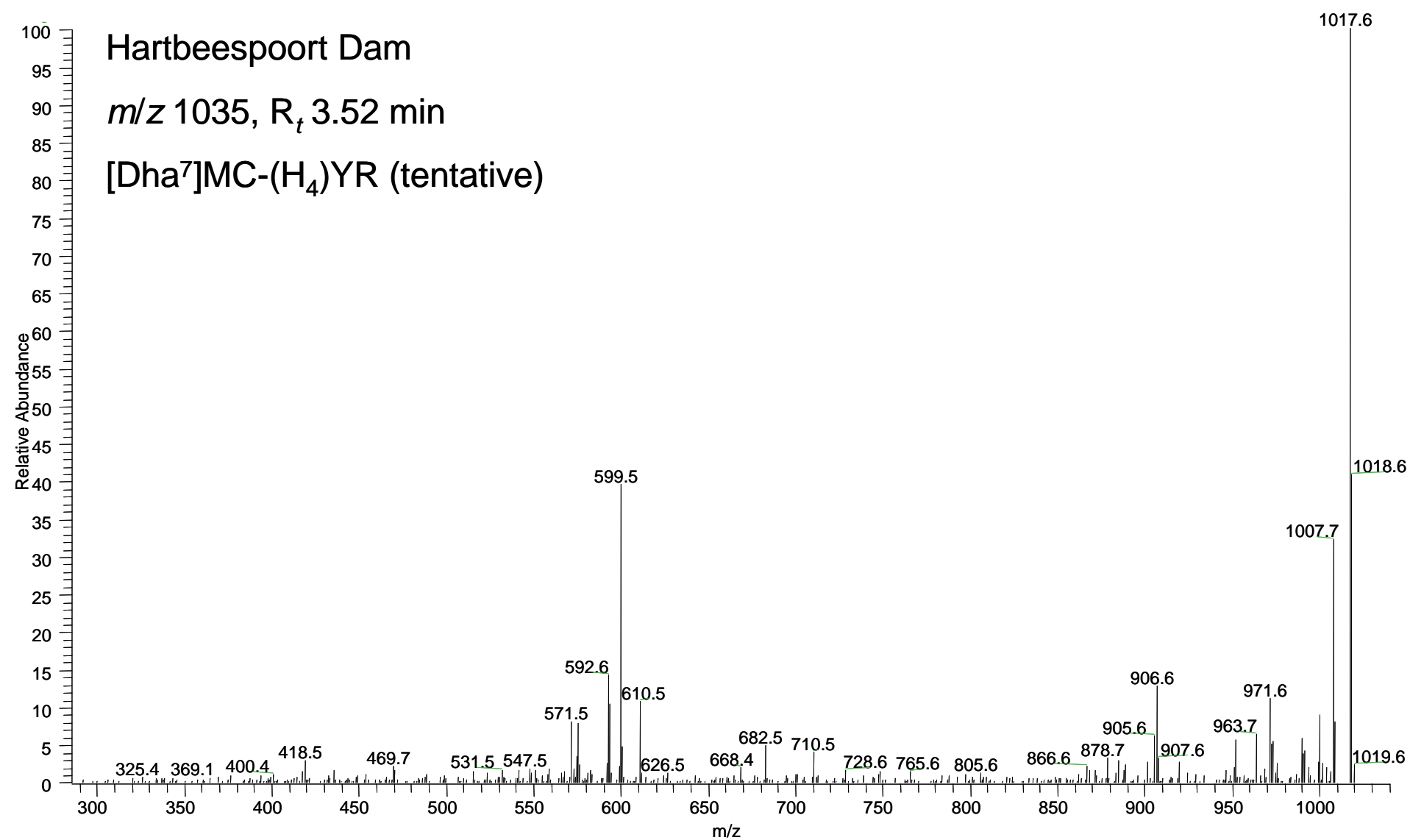
Figure S2ap. MS² spectrum of tentative [Dha⁷]MC-(H₄)YR from Hartbeespoort Dam

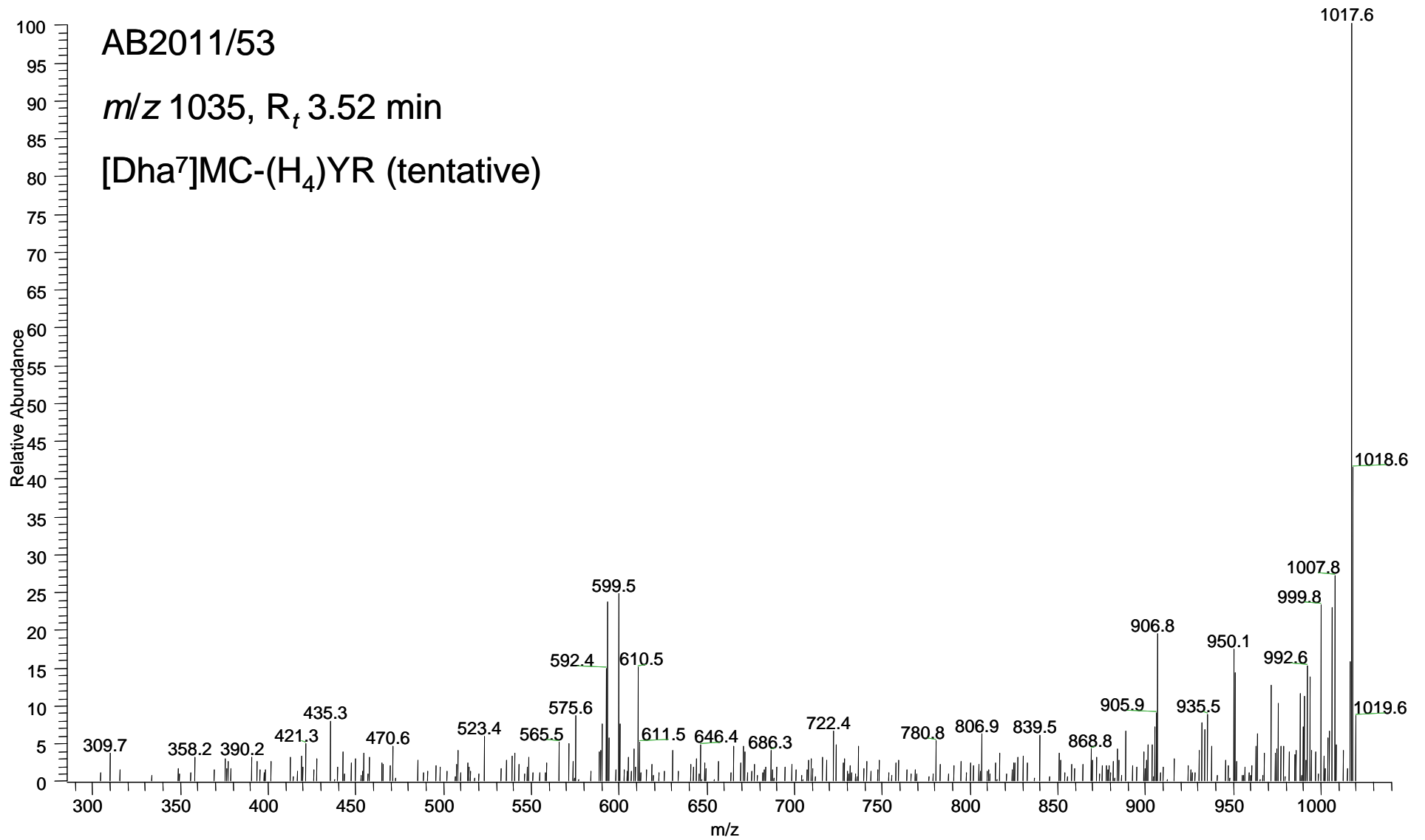
Figure S2aq. MS² spectrum of tentative [Dha⁷]MC-(H₄)YR from *M. aeruginosa* AB2011/53

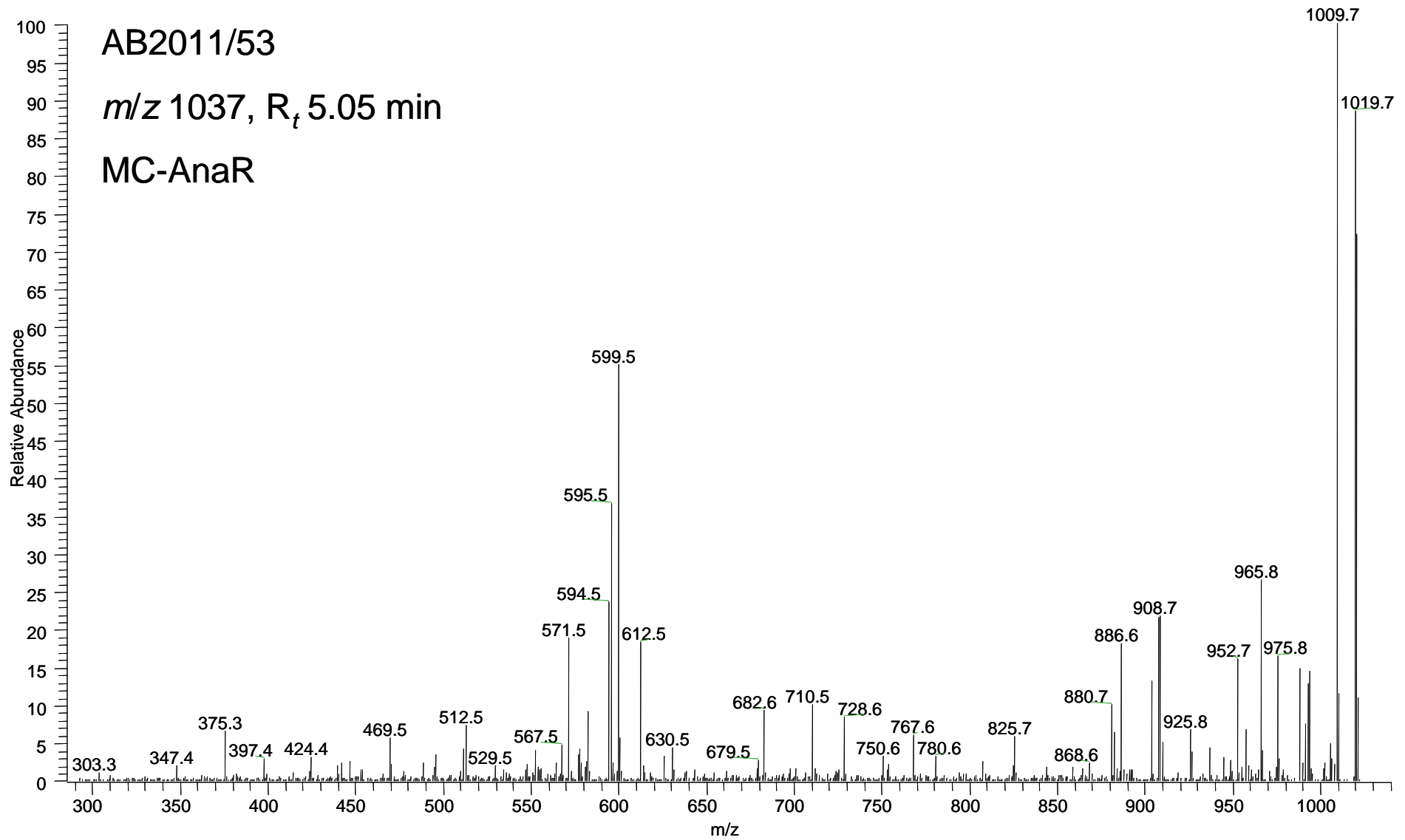
Figure S2ar. MS² spectrum of tentative MC-AnaR from *M. aeruginosa* AB2011/53

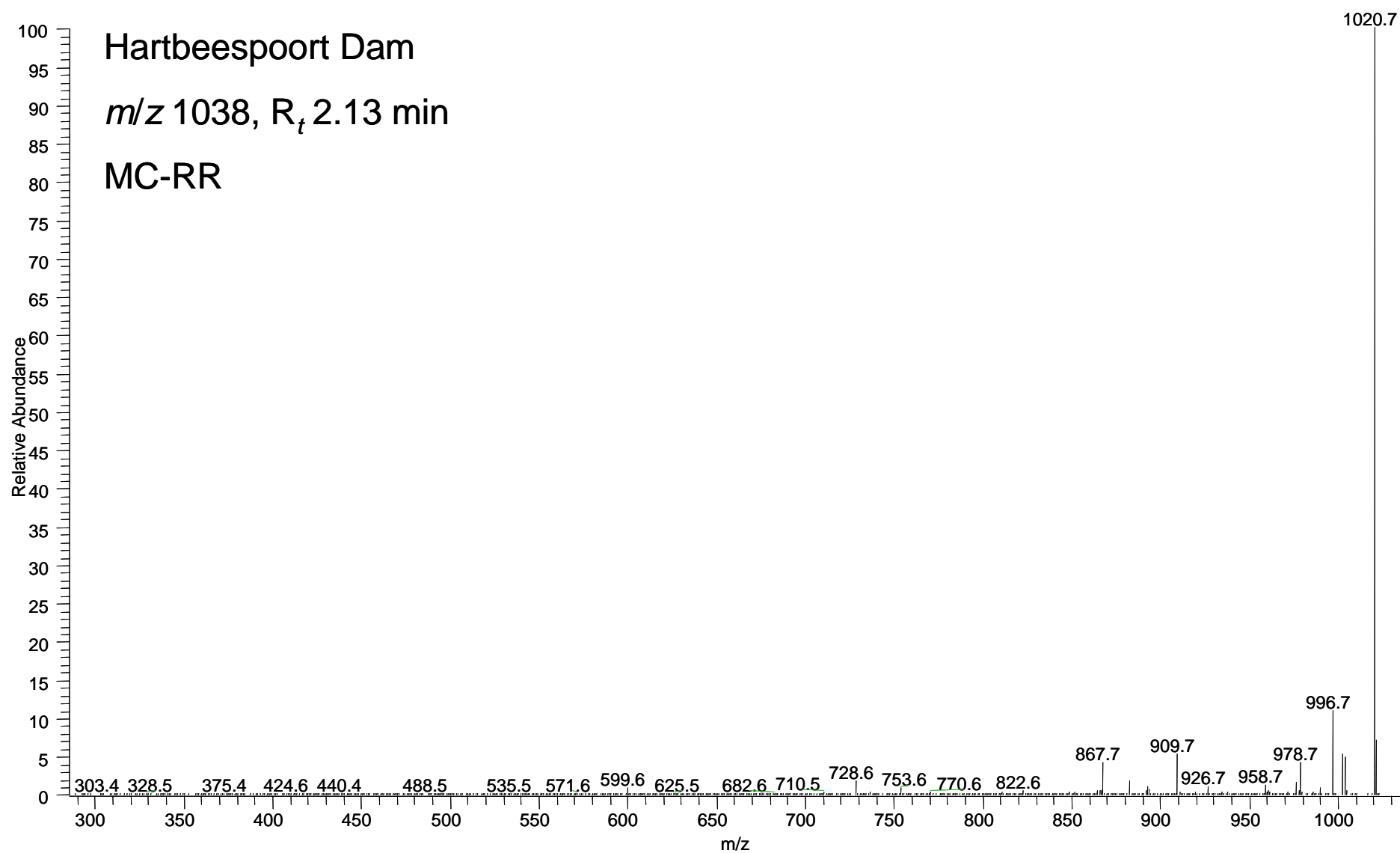
Figure S2as. MS² spectrum of confirmed MC-RR from Hartbeespoort Dam

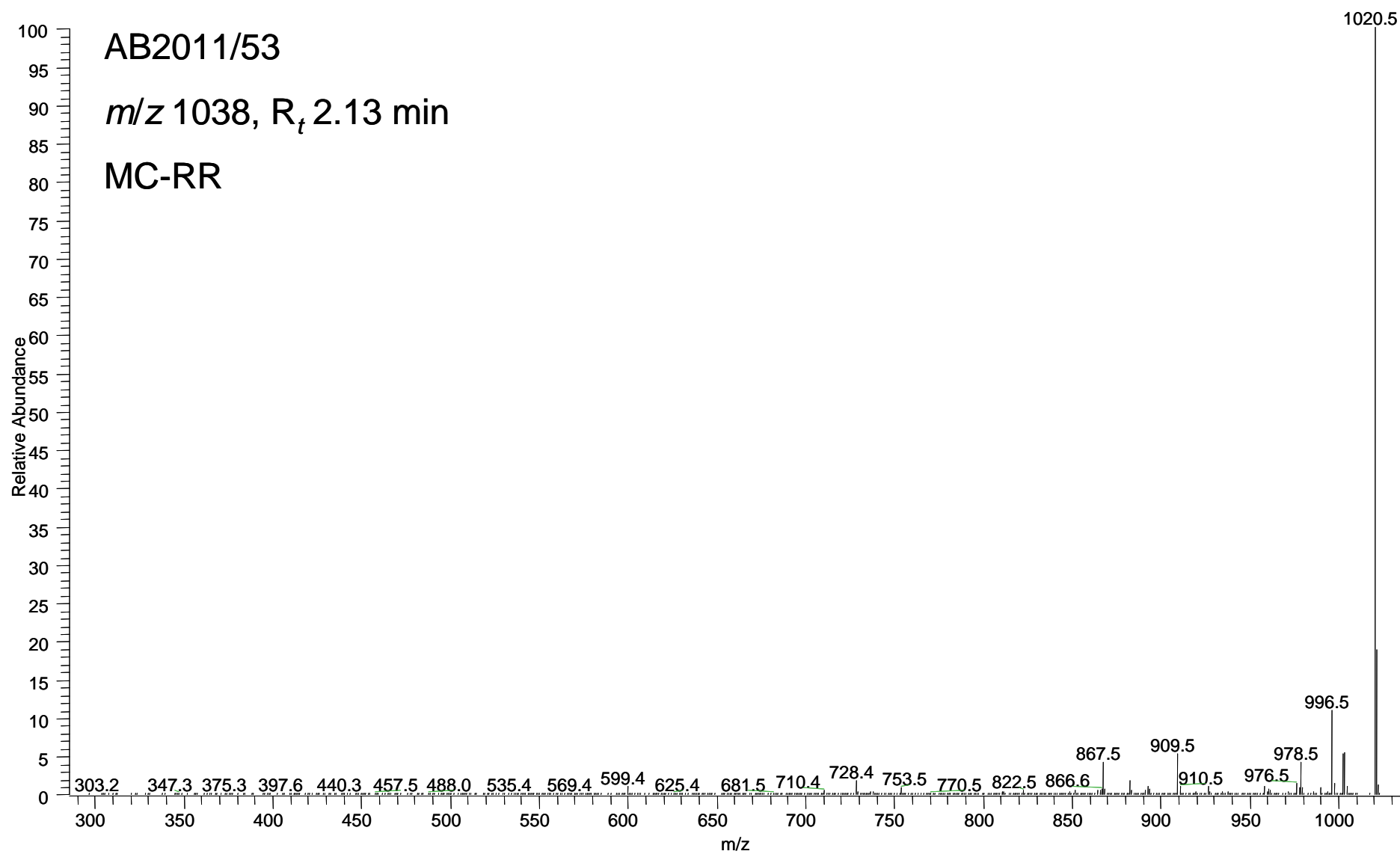
Figure S2at. MS² spectrum of confirmed MC-RR from *M. aeruginosa* AB2011/53

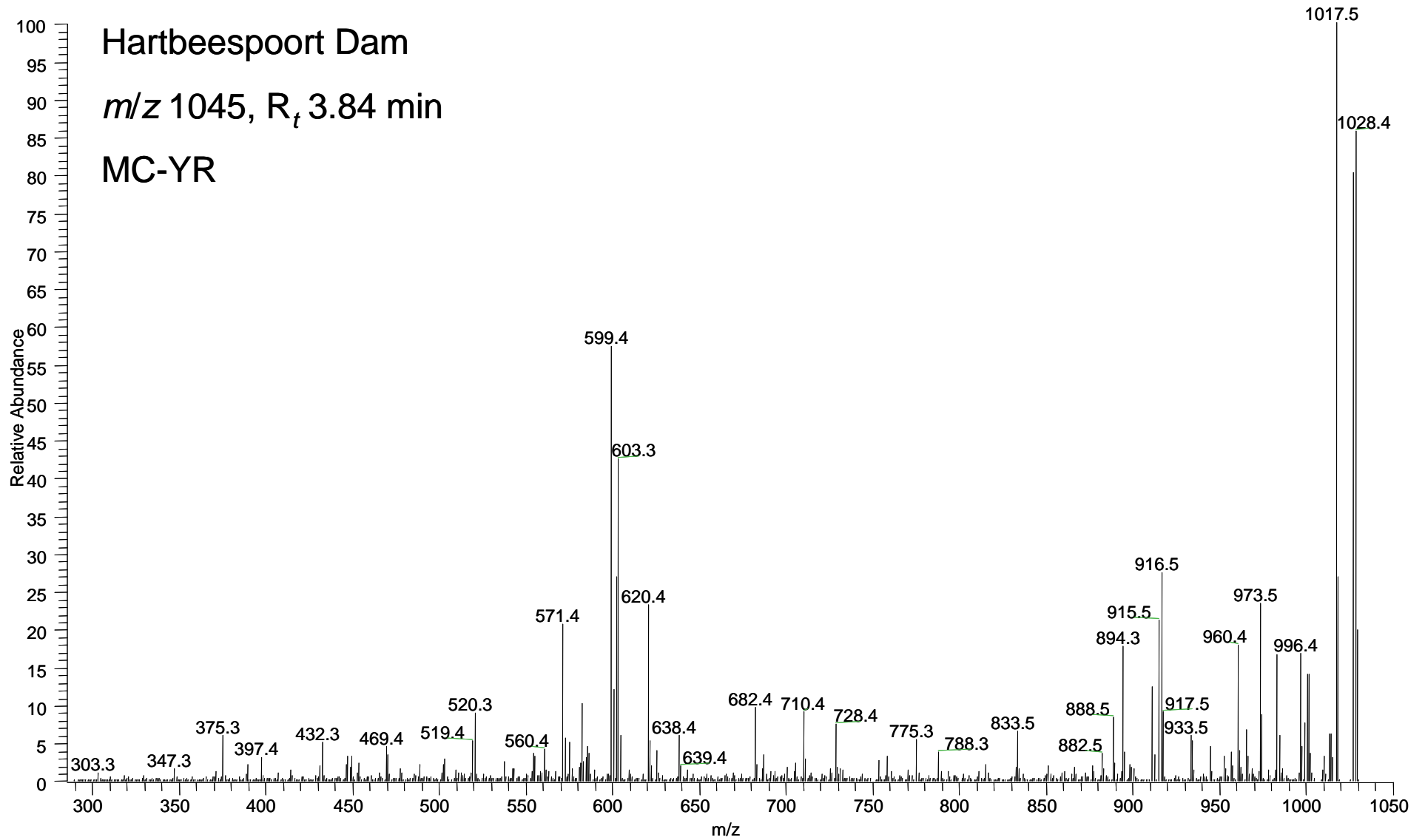
Figure S2au. MS² spectrum of confirmed MC-YR from Hartbeespoort Dam

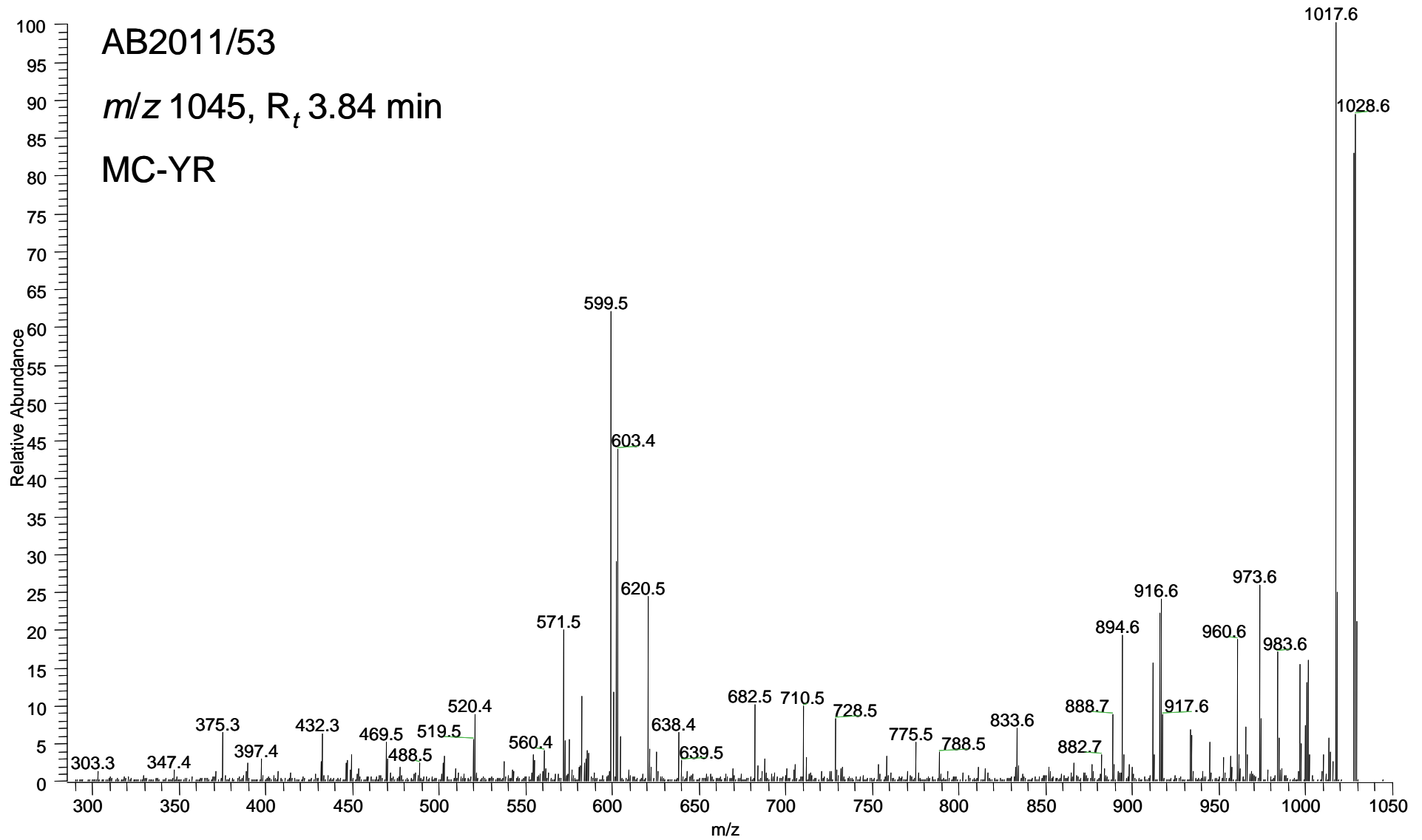
Figure S2av. MS² spectrum of confirmed MC-YR from *M. aeruginosa* AB2011/53

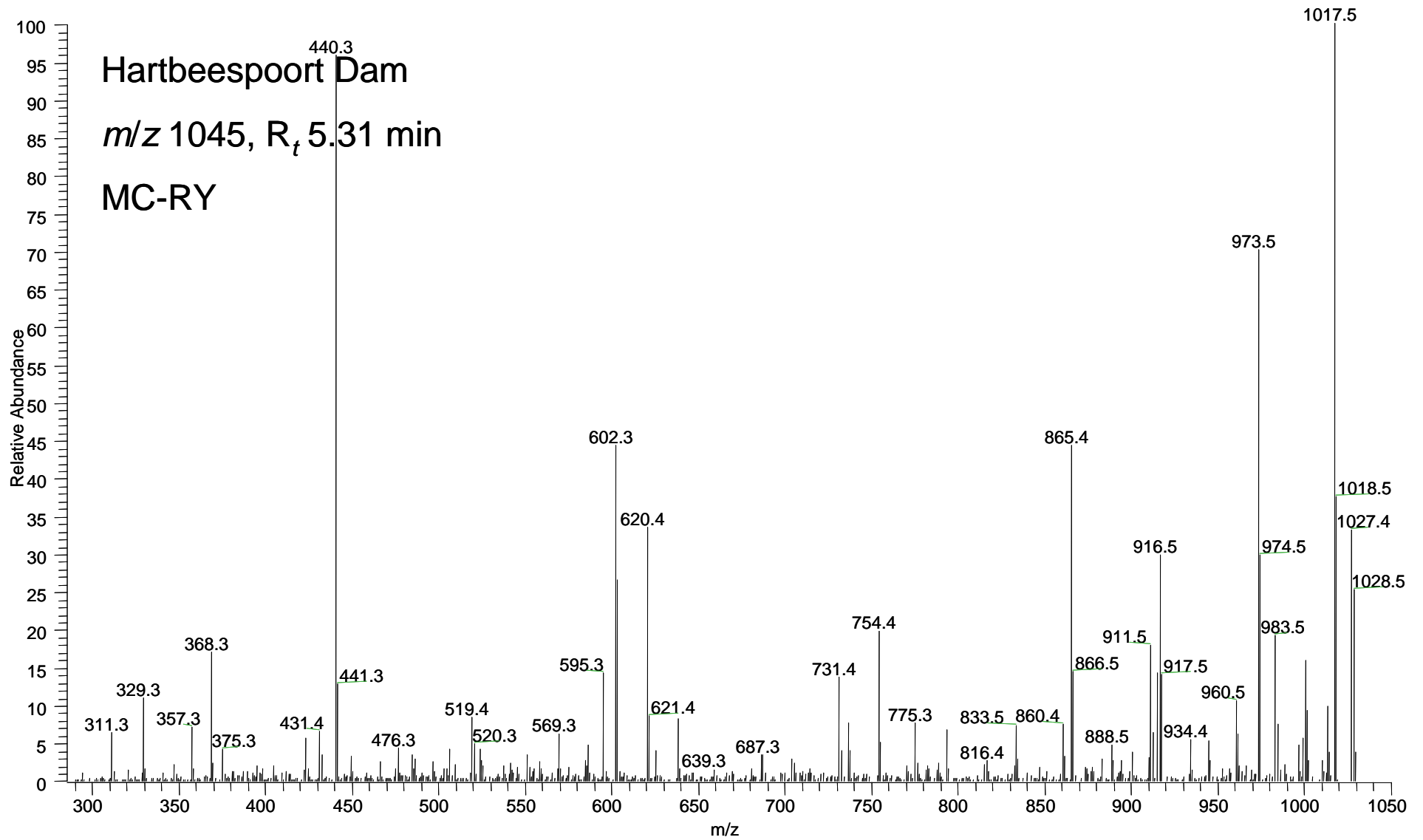
Figure S2aw. MS² spectrum of confirmed MC-YR from Hartbeespoort Dam

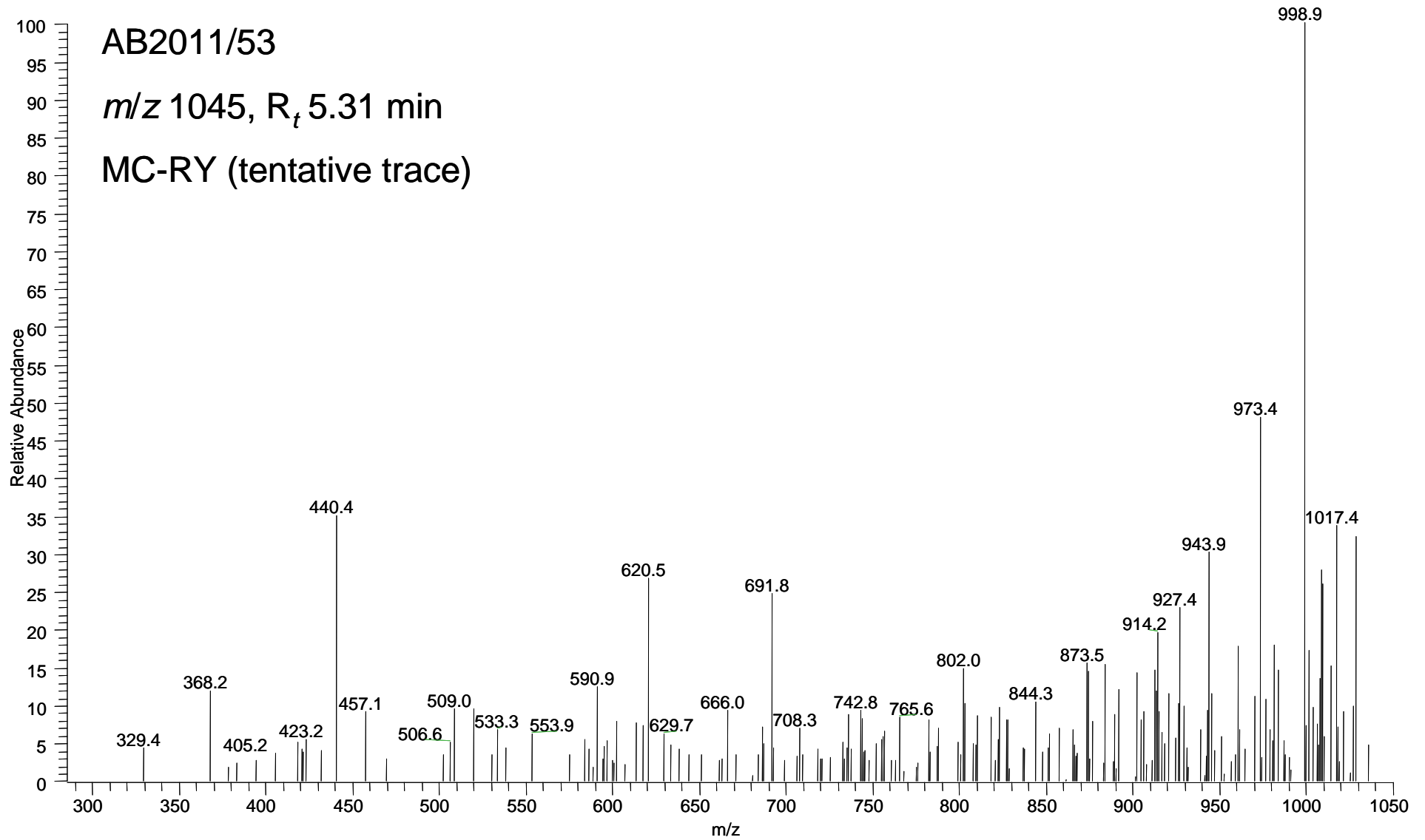
Figure S2ax. MS² spectrum of probable MC-RY from *M. aeruginosa* AB2011/53

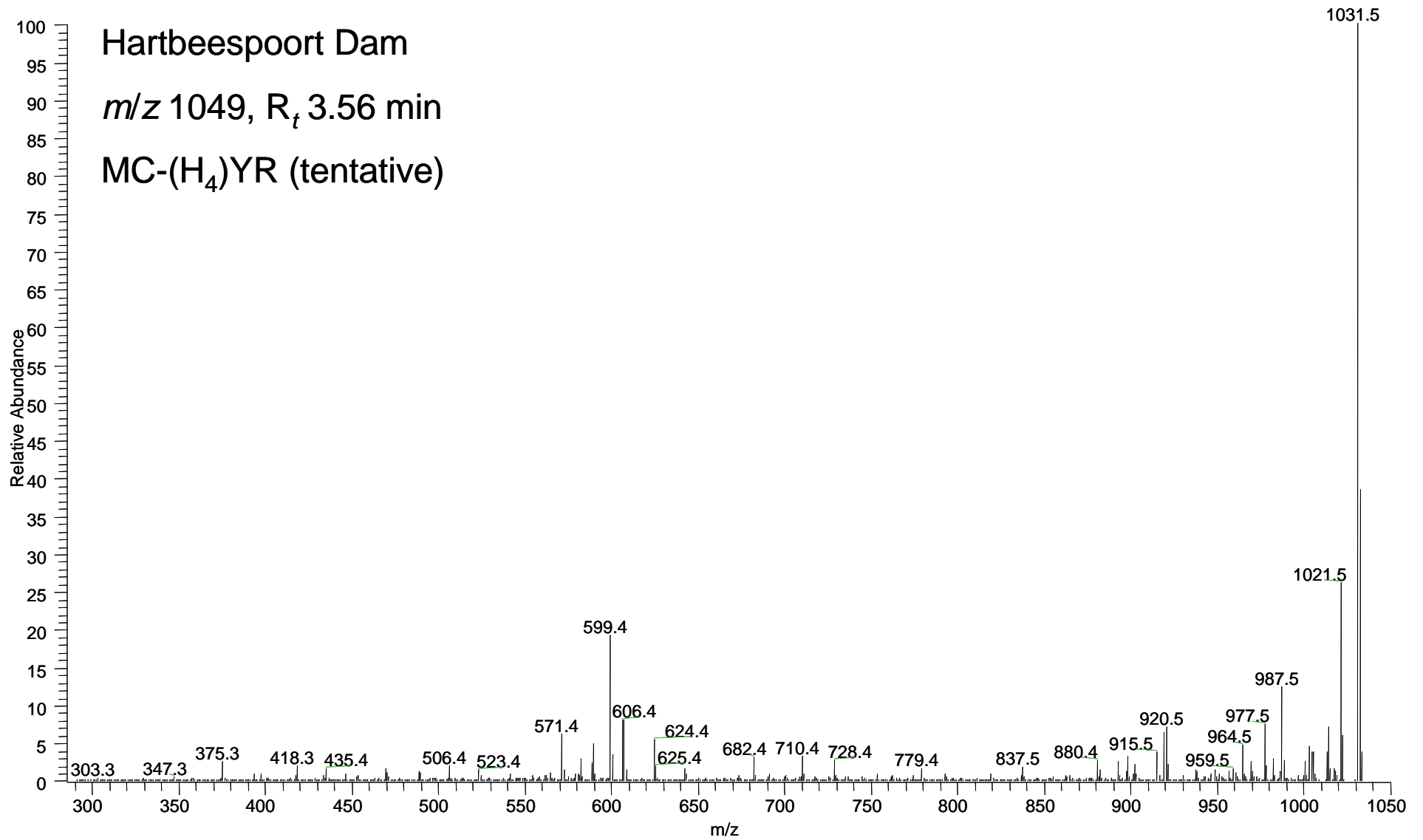
Figure S2ay. MS² spectrum of tentative MC-(H₄)YR from Hartbeespoort Dam

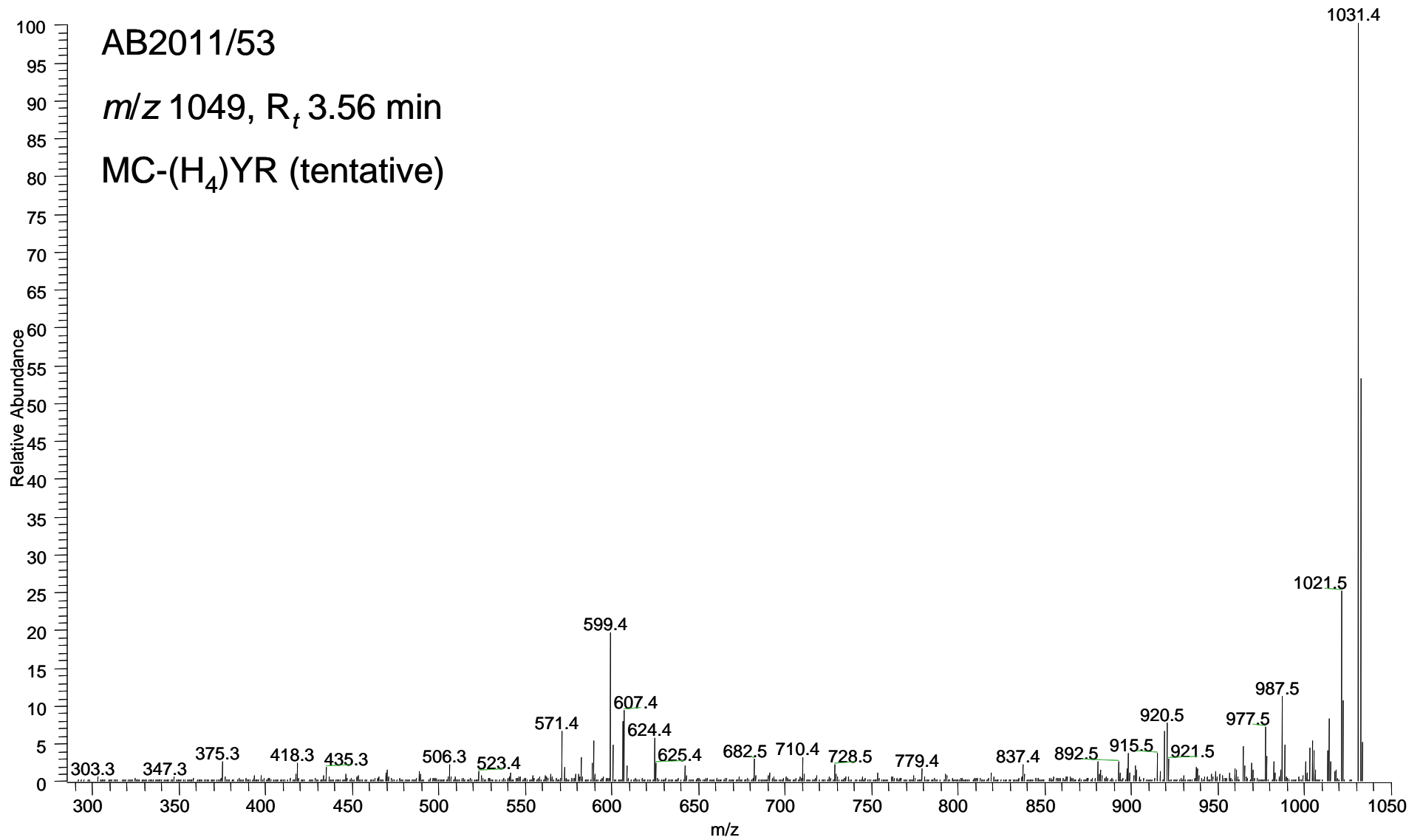
Figure S2az. MS² spectrum of tentative MC-(H₄)YR from *M. aeruginosa* AB2011/53

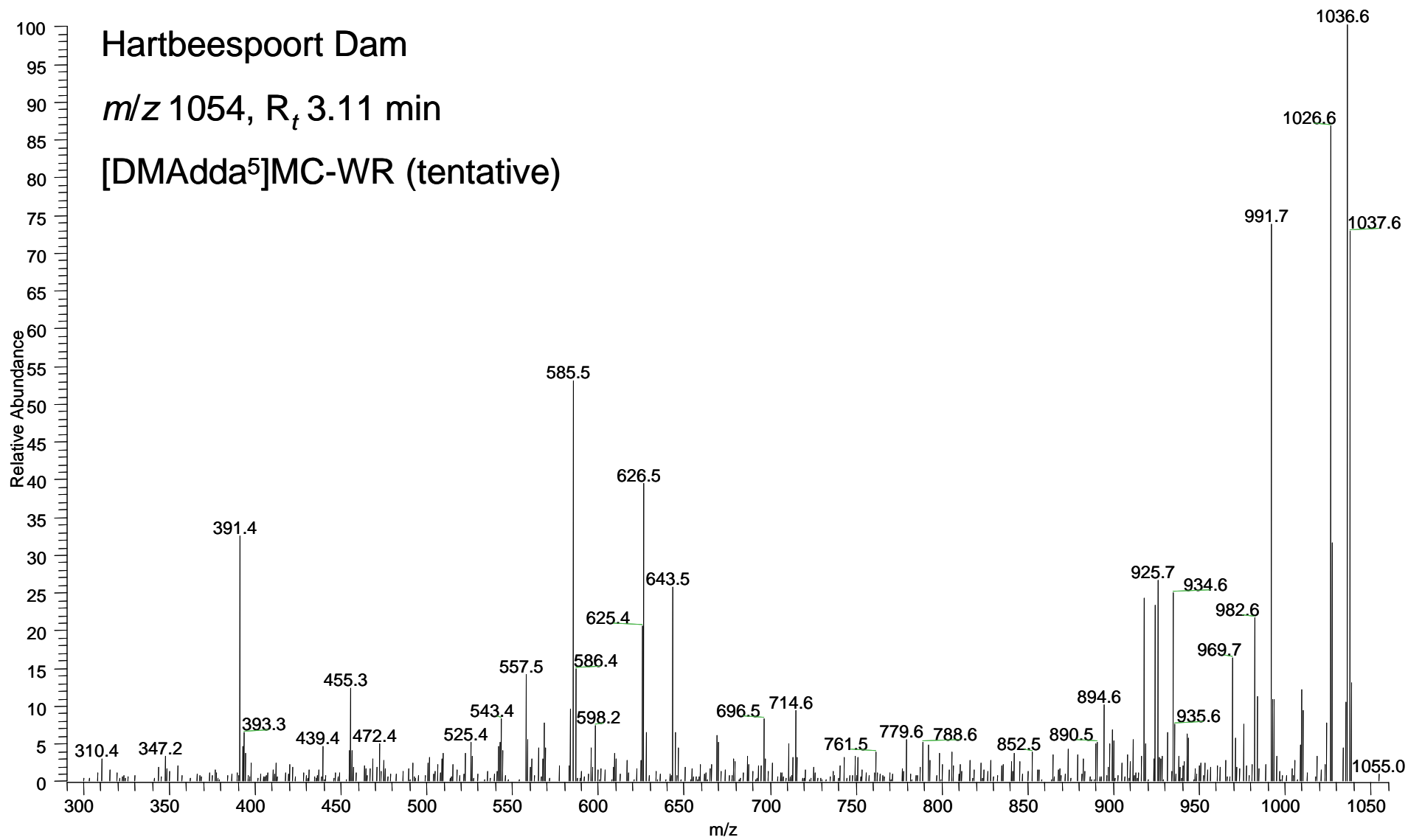
Figure S2ba. MS² spectrum of tentative [DMAdda⁵]MC-WR from Hartbeespoort Dam

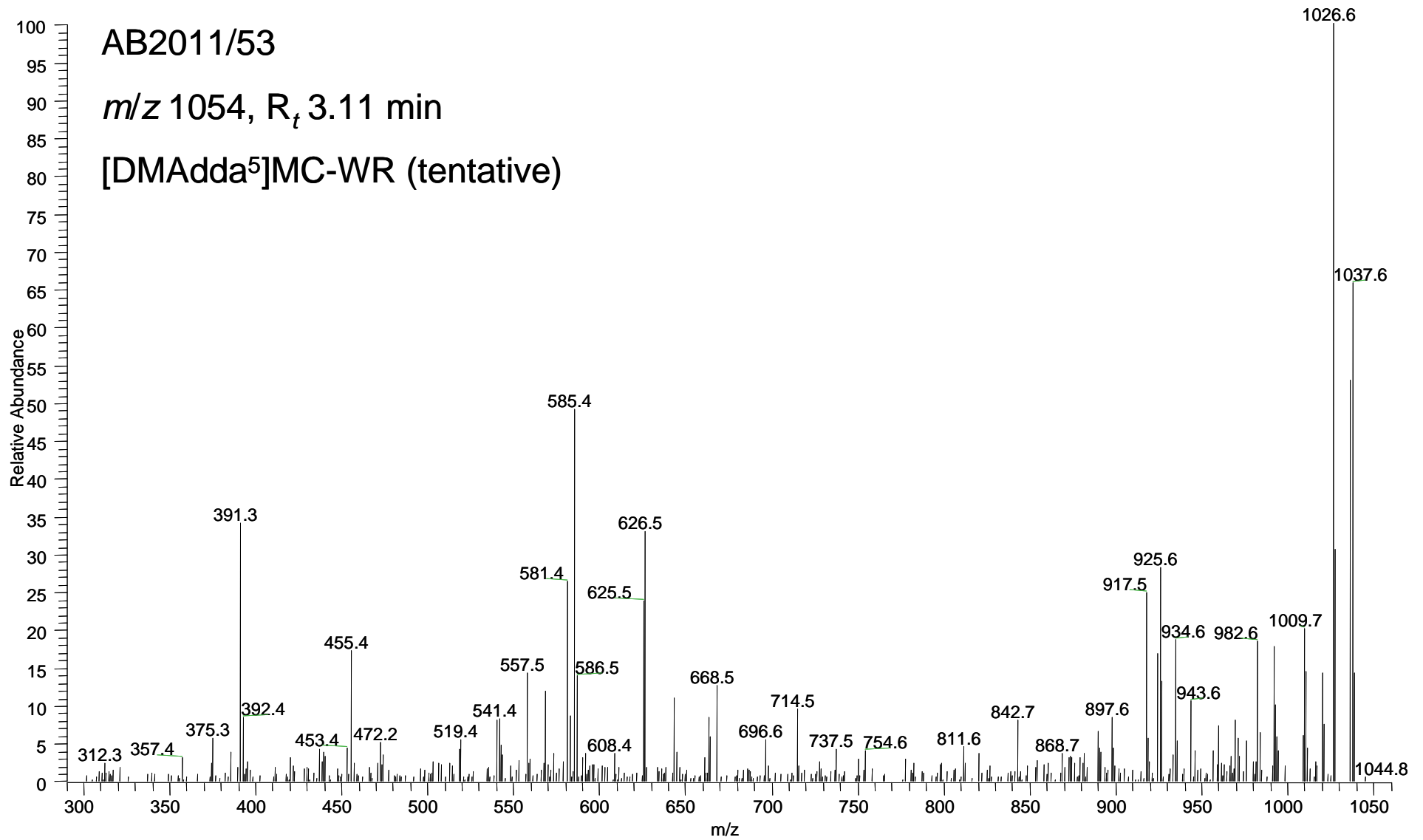
Figure S2bb. MS² spectrum of tentative [DMAdda⁵]MC-WR from *M. aeruginosa* AB2011/53

Figure S2bc. MS² spectrum of tentative [Asp³]MC-WR from Hartbeespoort Dam

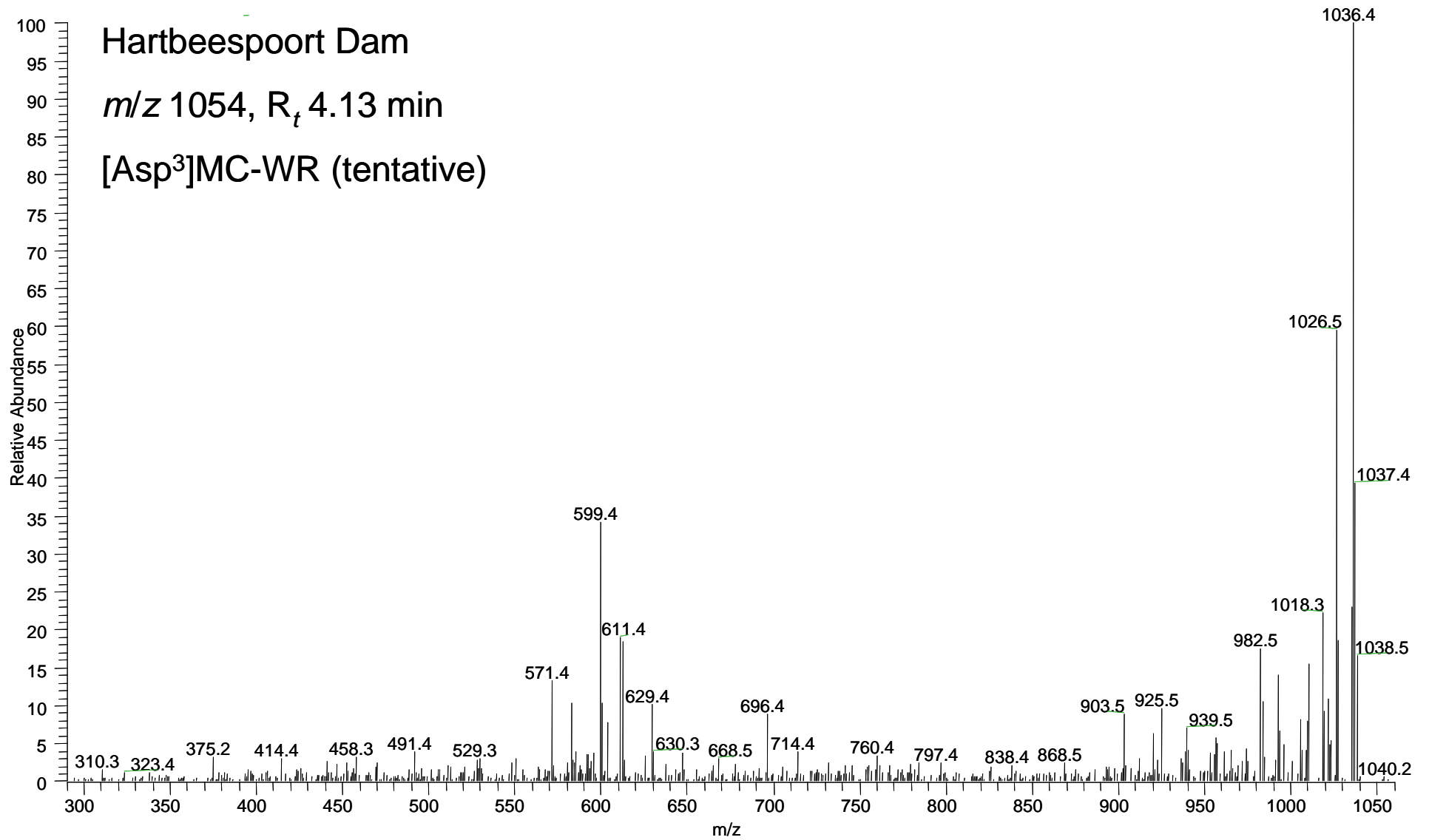


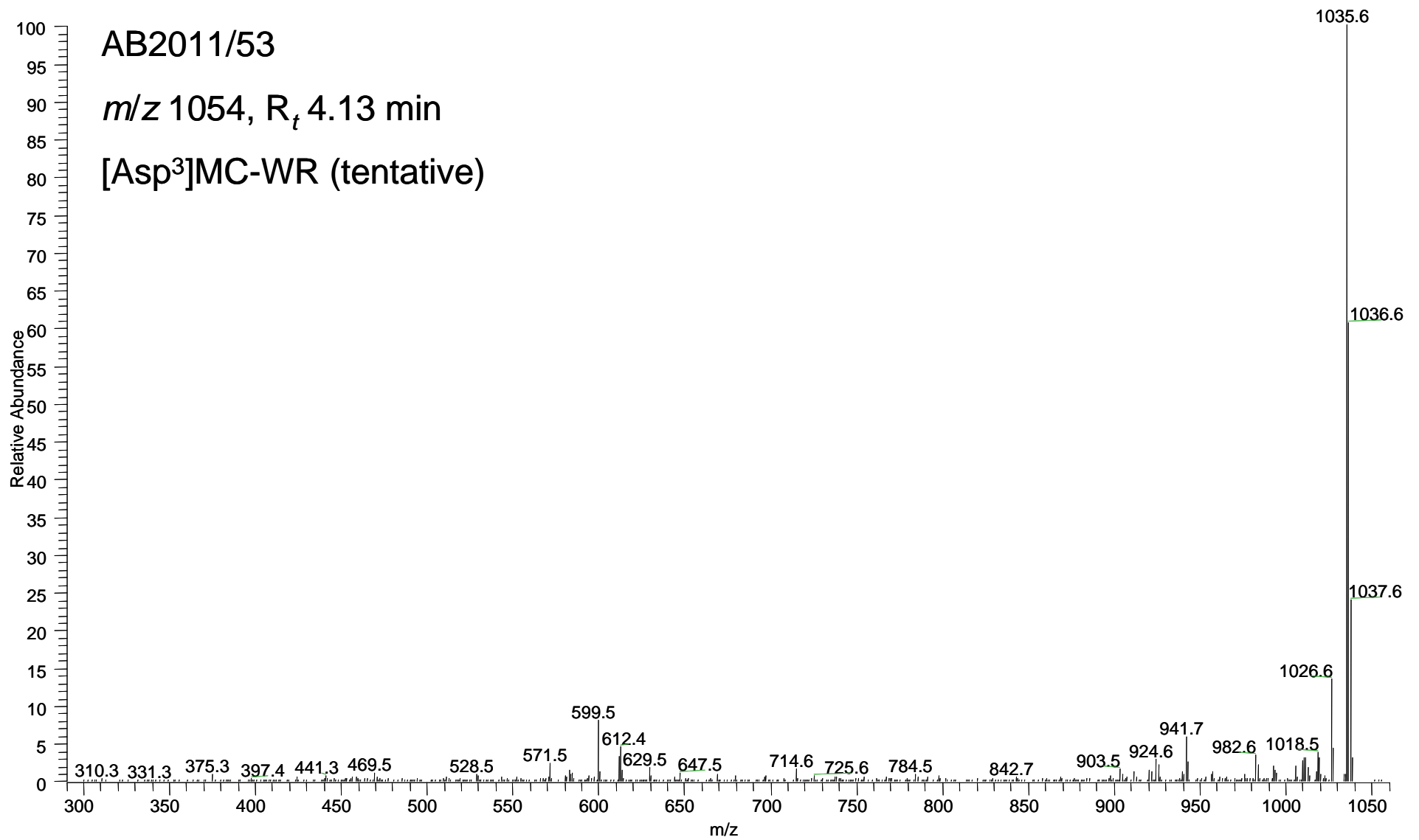
Figure S2bd. MS² spectrum of tentative [Asp³]MC-WR from *M. aeruginosa* AB2011/53

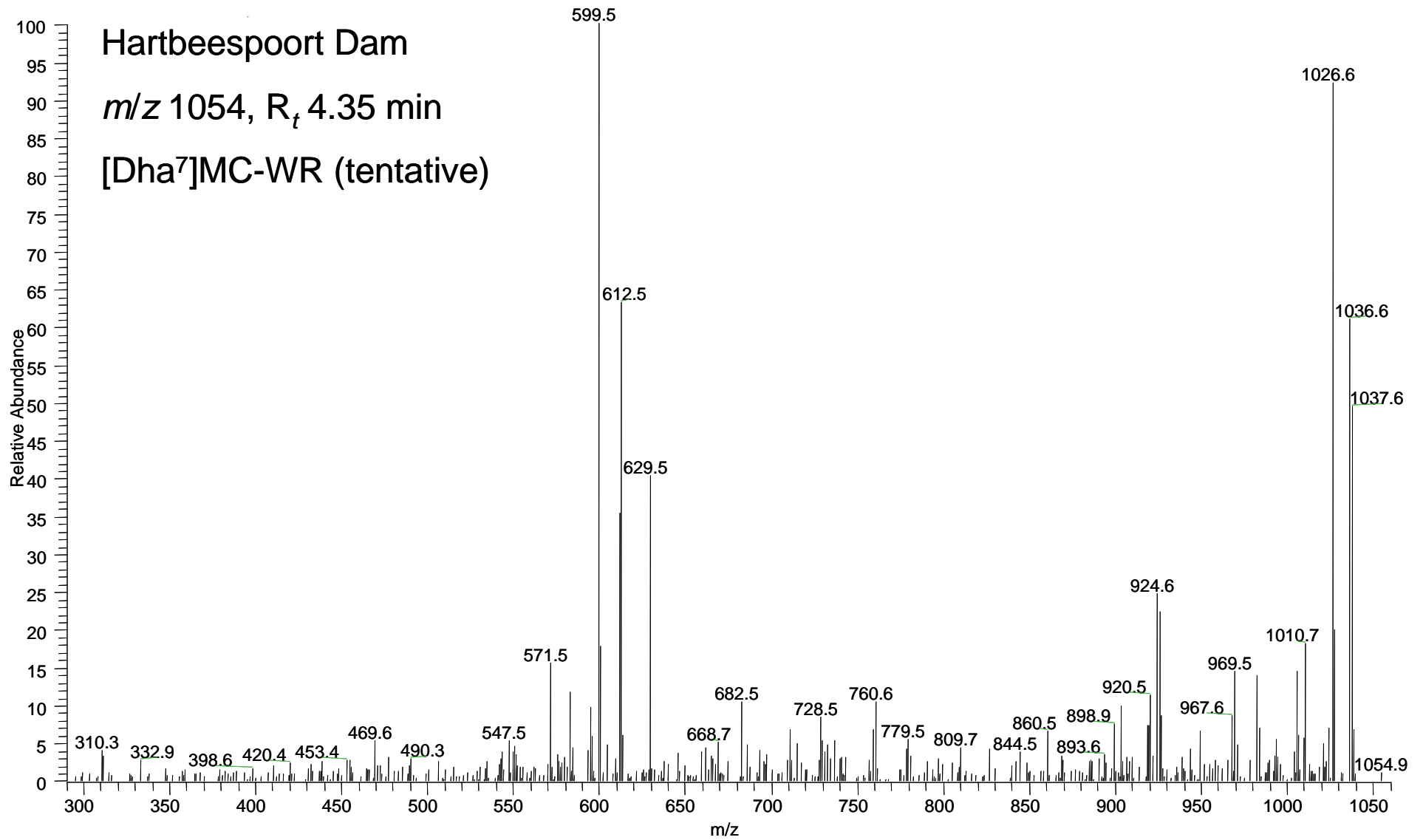
Figure S2be. MS² spectrum of tentative [Dha⁷]MC-WR from Hartbeespoort Dam

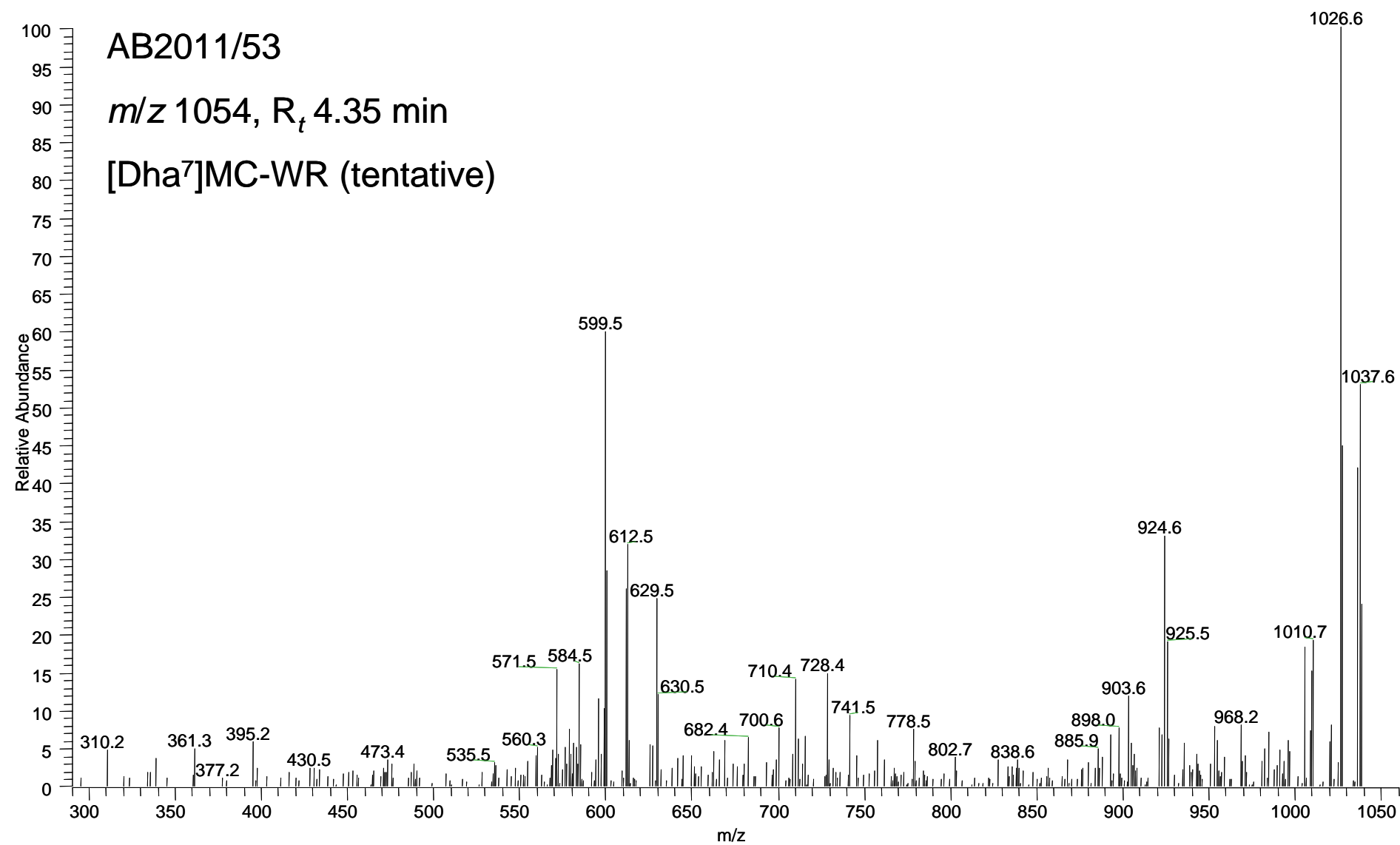
Figure S2bf. MS² spectrum of tentative [Dha⁷]MC-WR from *M. aeruginosa* AB2011/53

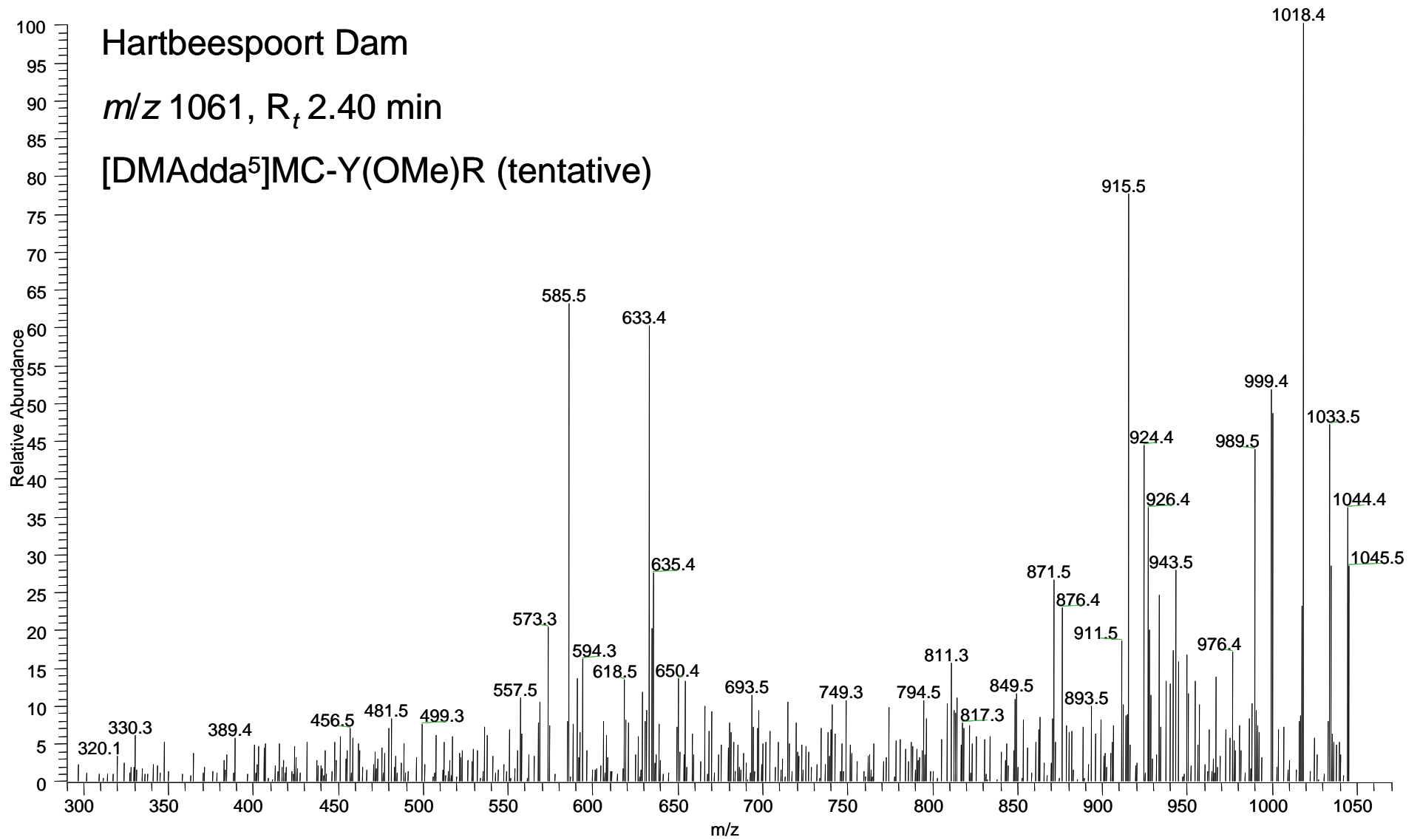
Figure S2bg. MS² spectrum of tentative [DMAdda⁵]MC-Y(OMe)R from Hartbeespoort Dam

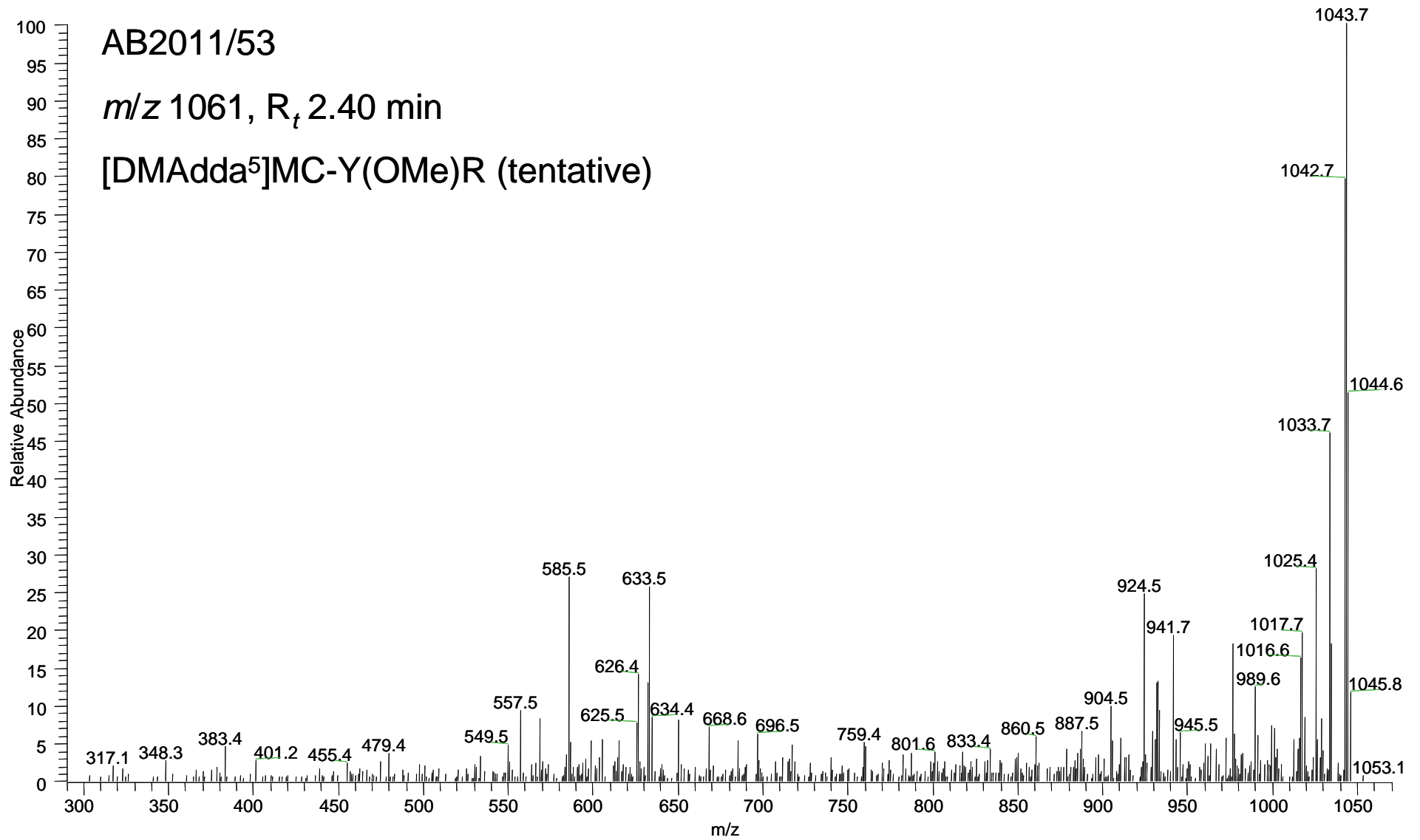
Figure S2bh. MS² spectrum of tentative [DMAdda⁵]MC-Y(OMe)R from *M. aeruginosa* AB2011/53

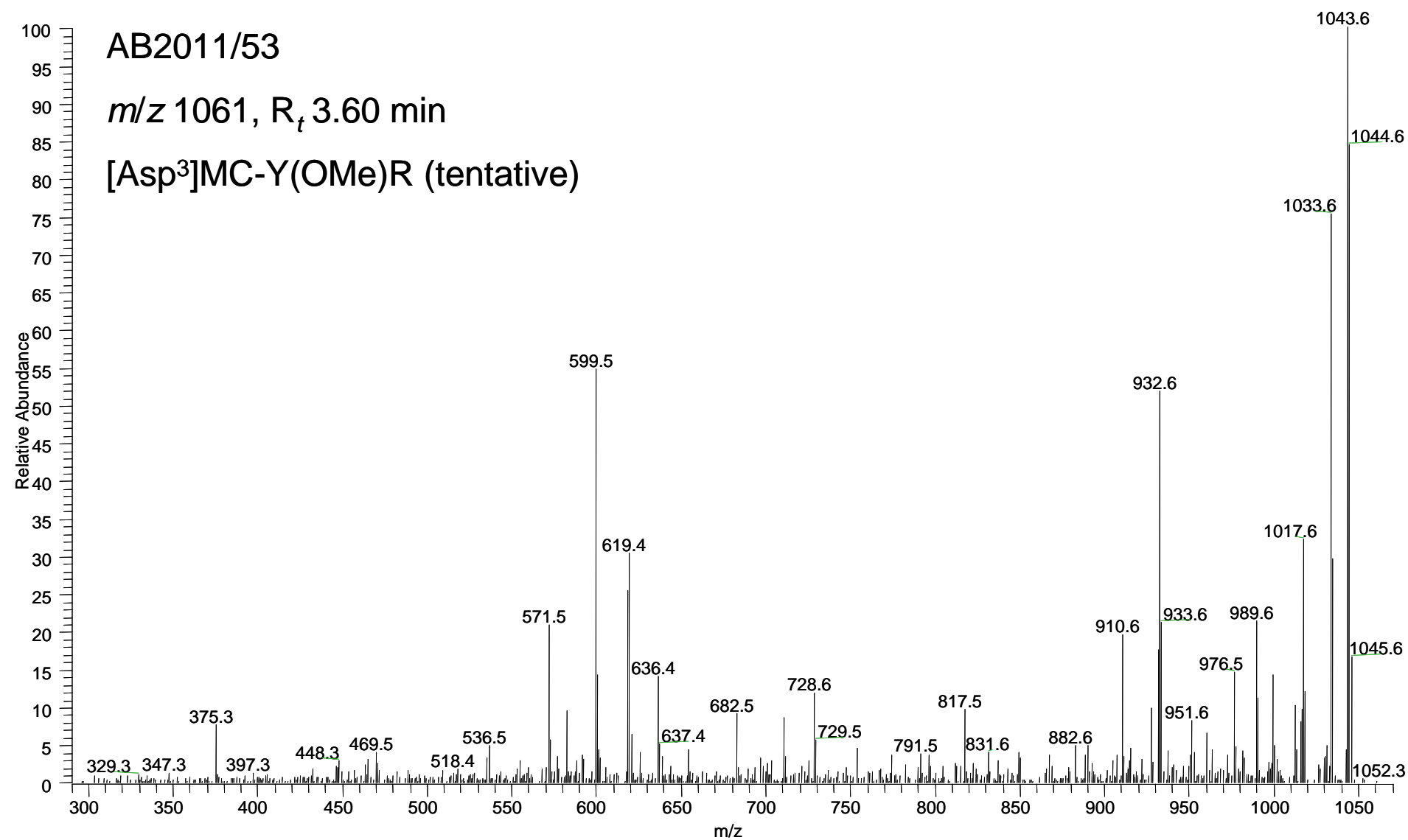
Figure S2bi. MS² spectrum of tentative [Asp³]MC-Y(OMe)R from *M. aeruginosa* AB2011/53

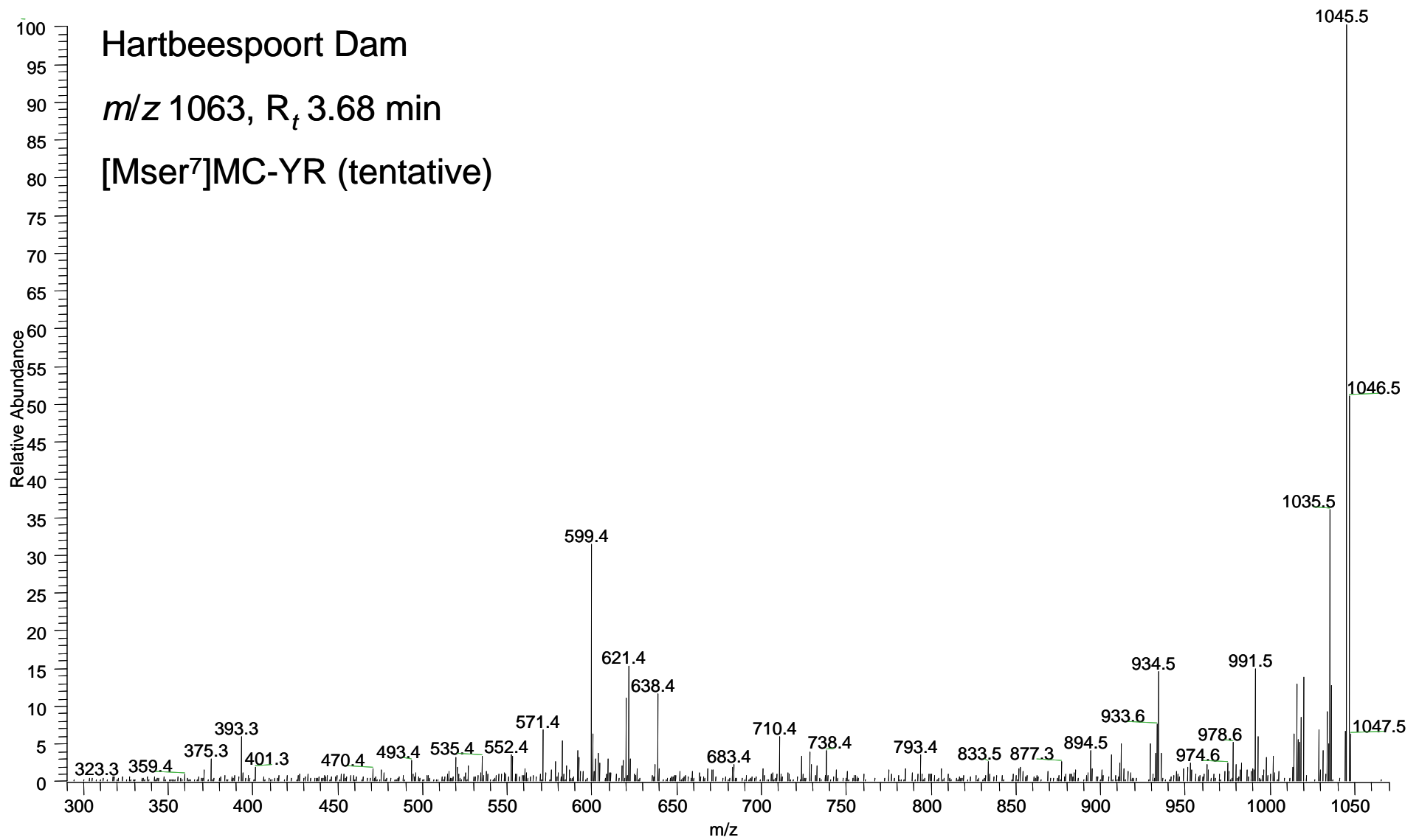
Figure S2bj. MS² spectrum of tentative [Mser⁷]MC-YR from Hartbeespoort Dam

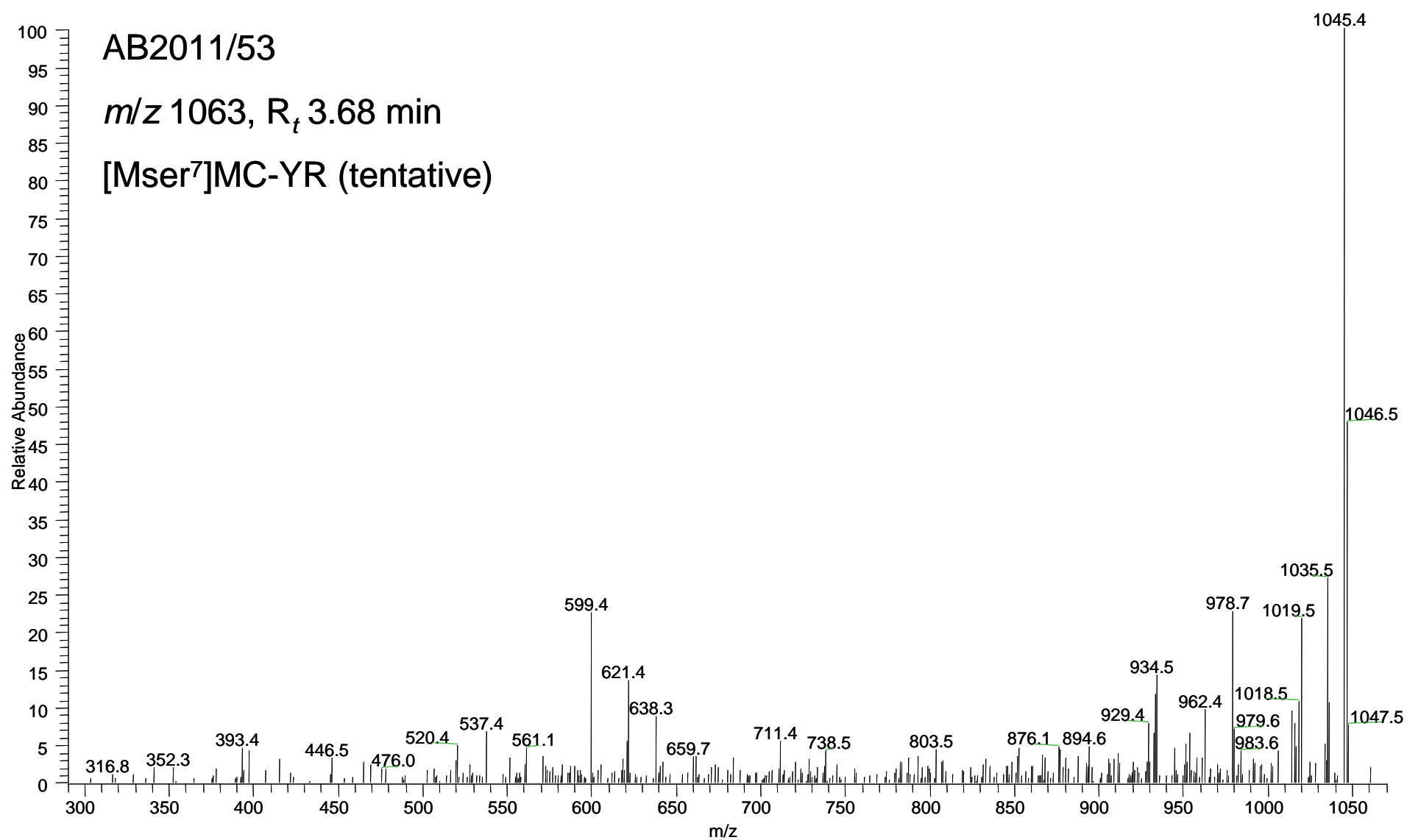
Figure S2bk. MS² spectrum of tentative [Mser⁷]MC-YR from *M. aeruginosa* AB2011/53

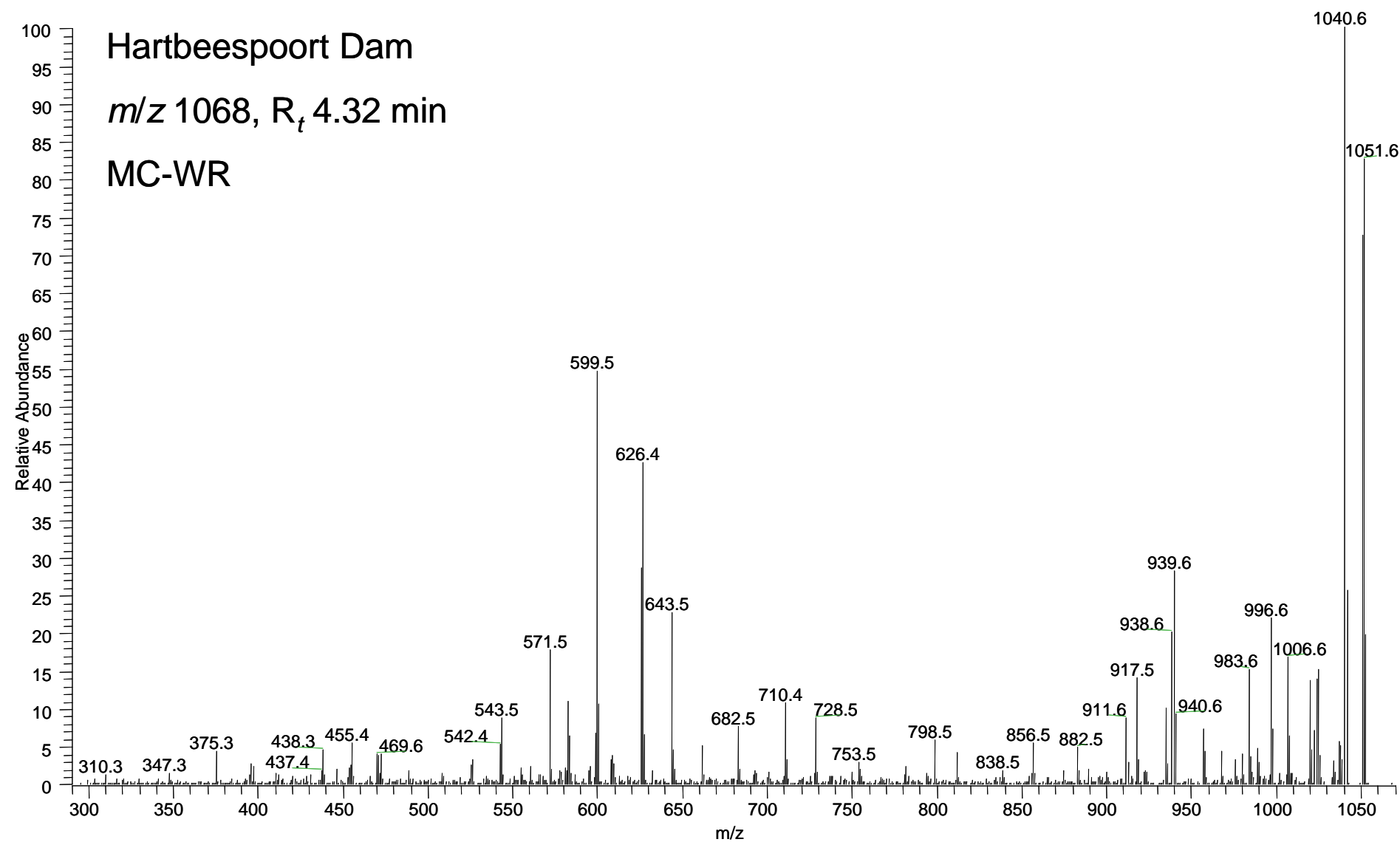
Figure S2bl. MS² spectrum of confirmed MC-WR from Hartbeespoort Dam

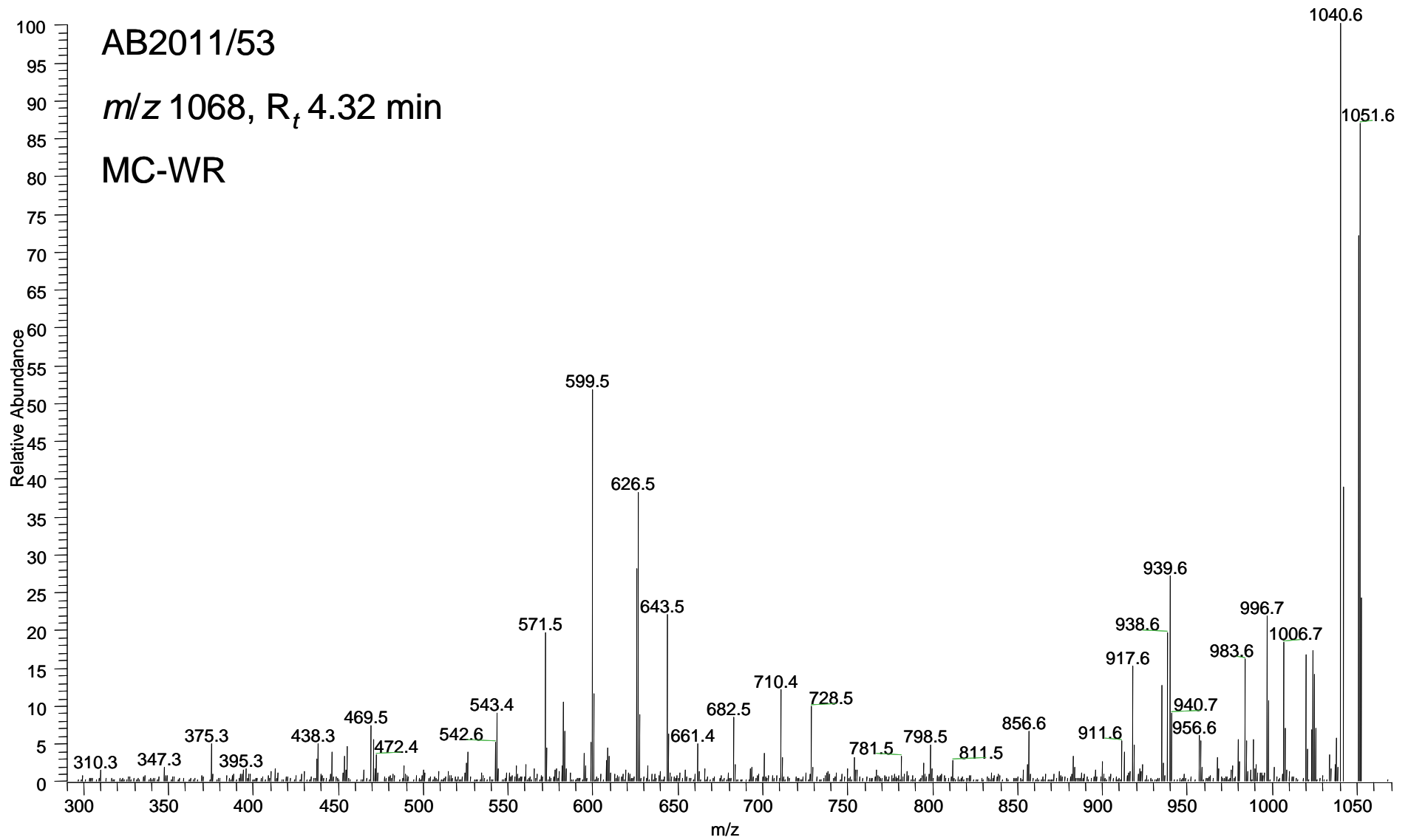
Figure S2bm. MS² spectrum of confirmed MC-WR from *M. aeruginosa* AB2011/53

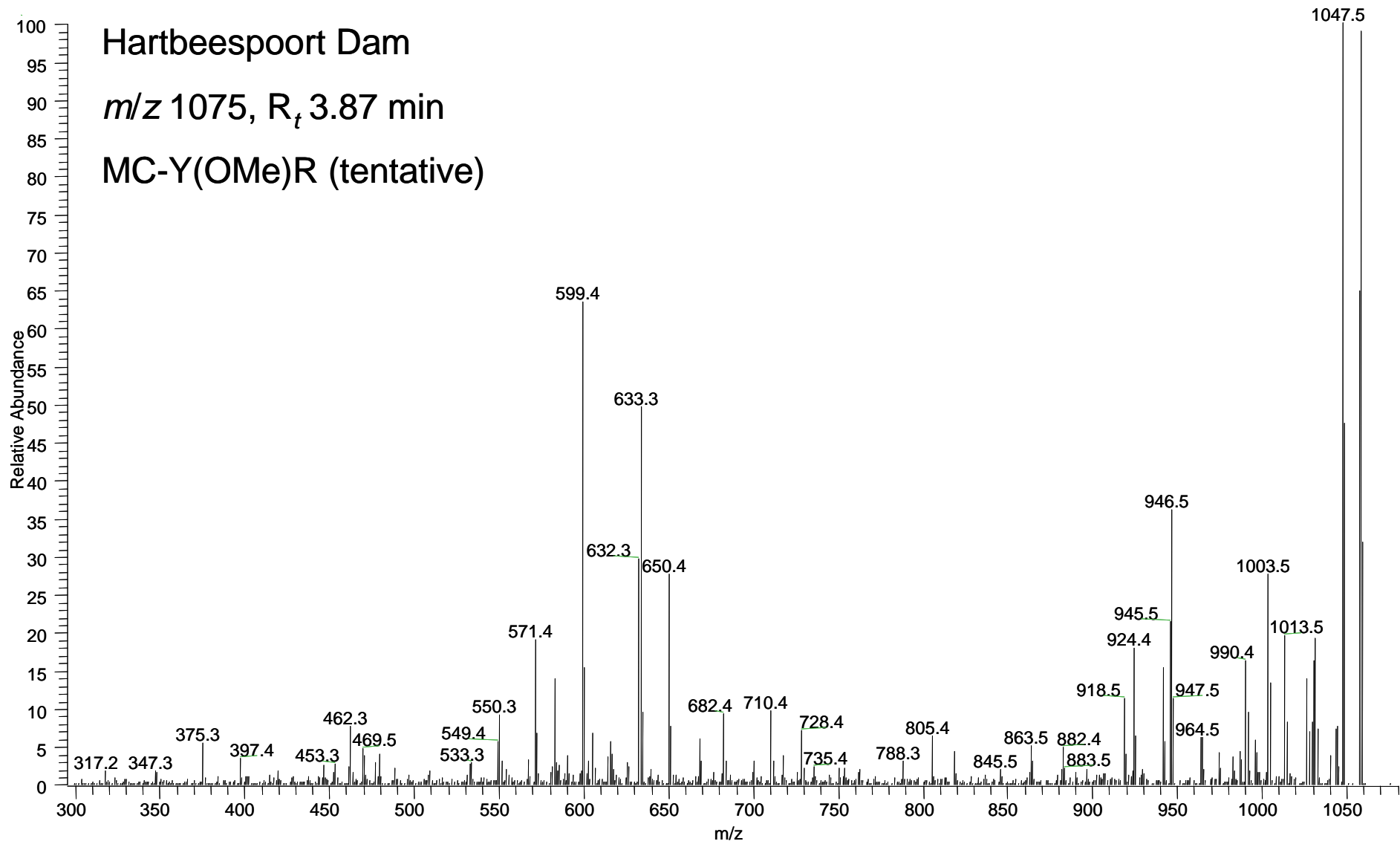
Figure S2bn. MS² spectrum of tentative MC-Y(OMe)R from Hartbeespoort Dam

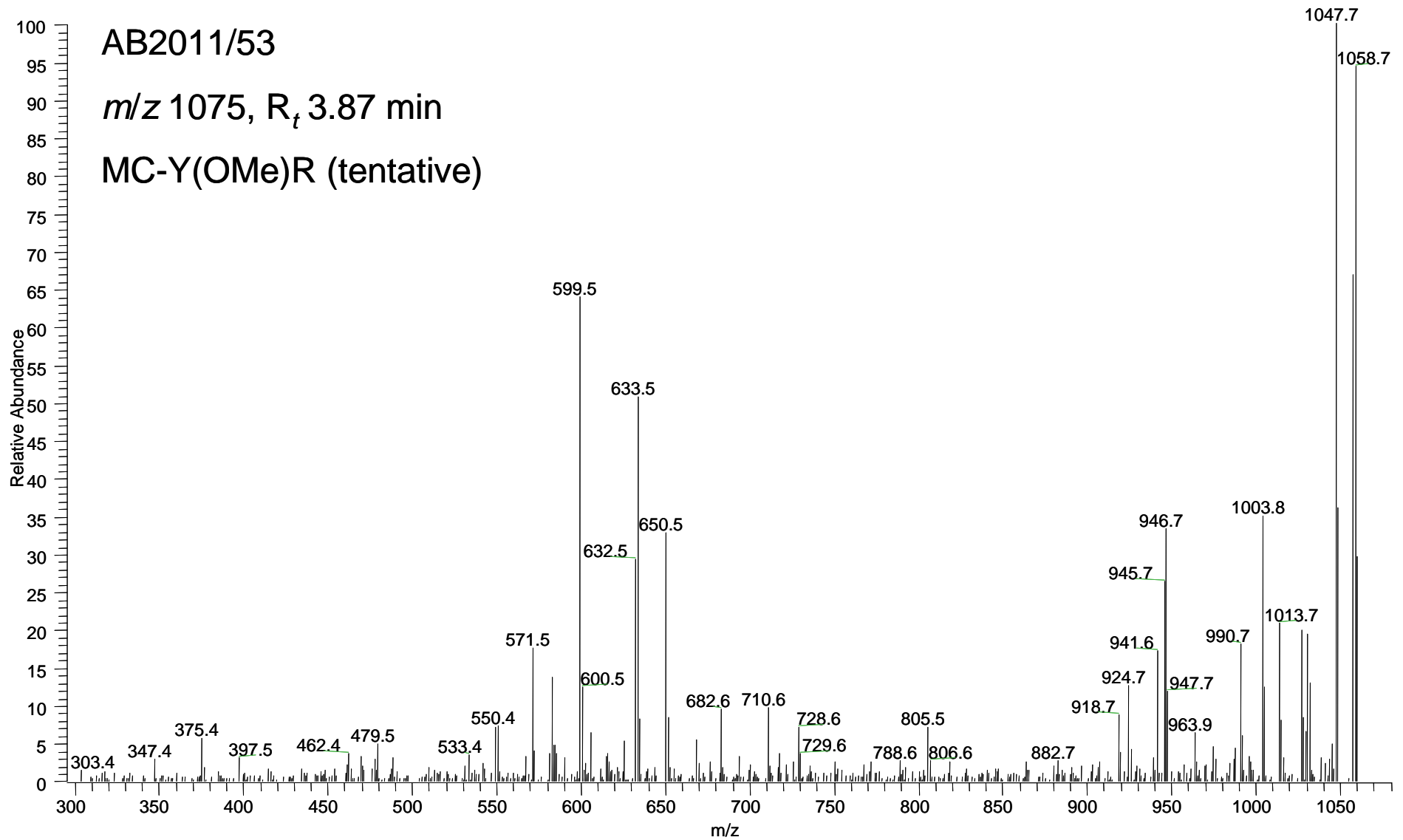
Figure S2bo. MS² spectrum of tentative MC-Y(OMe)R from *M. aeruginosa* AB2011/53

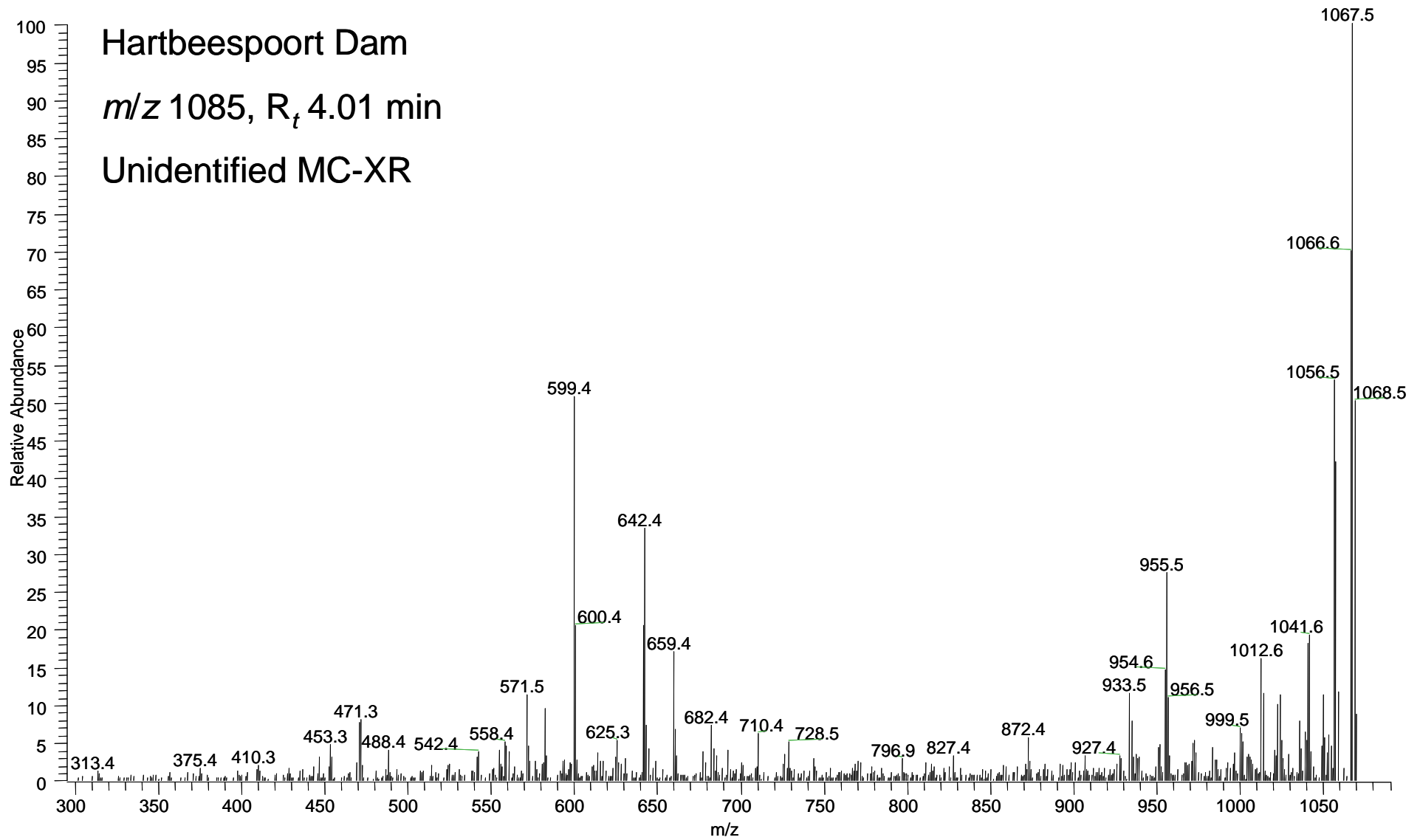
Figure S2bp. MS² spectrum of unidentified MC-XR from Hartbeespoort Dam

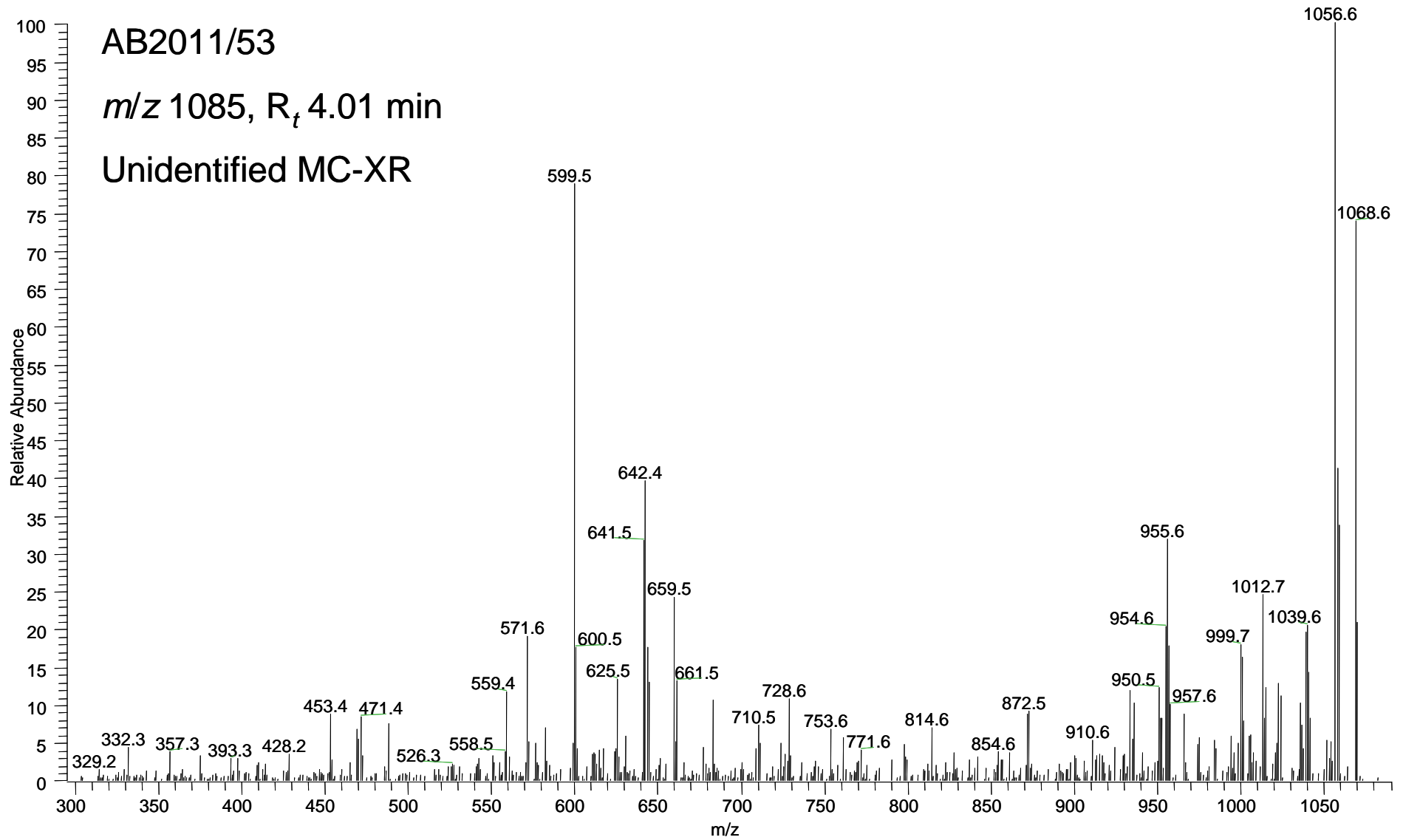
Figure S2bq. MS² spectrum of unidentified MC-XR from *M. aeruginosa* AB2011/53

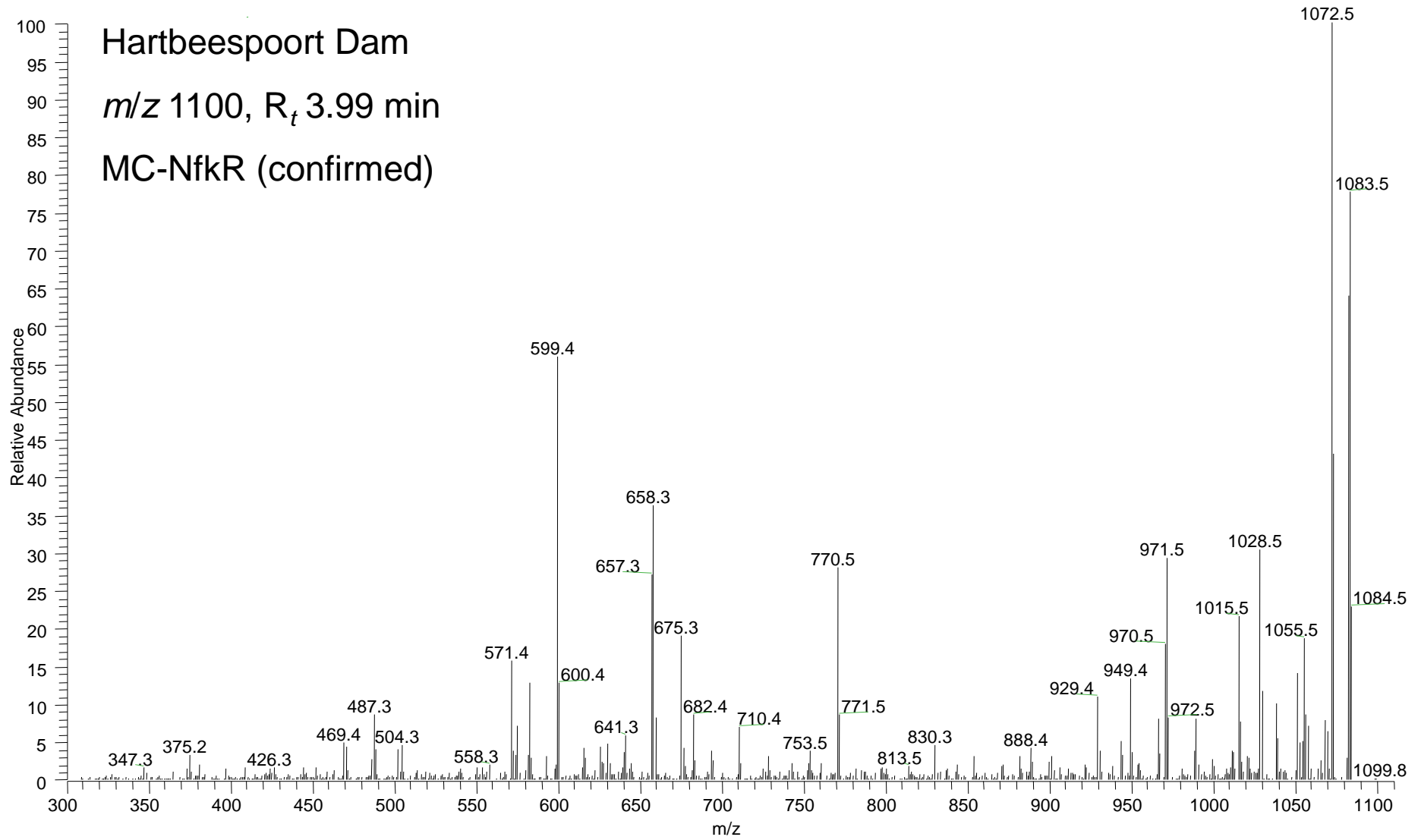
Figure S2br. MS² spectrum of confirmed MC-NfkR from Hartbeespoort Dam

Figure S2bs. MS² spectrum of confirmed MC-NfkR from *M. aeruginosa* AB2011/53