

# Biodegradation of dental care antimicrobial agents chlorhexidine and octenidine by ligninolytic fungi

Lucie Linhartová <sup>1,2</sup>, Klára Michalíková <sup>1,2</sup>, Kamila Šředlová <sup>1,2</sup> and Tomáš Cajthaml <sup>1,2,\*</sup>

<sup>1</sup> Laboratory of environmental biotechnology, Institute of Microbiology of the Czech Academy of Sciences, Vídeňská 1083, CZ-14220 Prague 4, Czech Republic; lucie.linhartova@biomed.cas.cz (L.L.);

klara.michalikova@biomed.cas.cz (K.M.); kamila.sredlova@biomed.cas.cz (K.Š.)

<sup>2</sup> Faculty of Science, Institute for Environmental Studies, Charles University, Benátská 2, CZ-12801 Prague 2, Czech Republic

\* Correspondence: cajthaml@biomed.cas.cz

## The list of supporting information:

**Table S1:** Activity of manganese-dependent peroxidase (MnP) from *I. lacteus* and laccase (Lac) from *P. ostreatus* during *in vivo* degradation of octenidine (OCT) and chlorhexidine (CHX).

**Table S2:** Activity of manganese-dependent peroxidase (MnP) from *I. lacteus* and laccase (Lac) from *P. ostreatus* during *in vitro* degradation of octenidine (OCT) and chlorhexidine (CHX).

**Figure S1:** Product ion spectra and suggested fragments of (a)  $m/z$  515.2  $[M+H]^+$  and (b)  $m/z$  258.2  $[M+2H]^{2+}$ .

**Figure S2:** (a) mass spectrum of the peak with  $R_t = 5.9$  min,  $m/z$  439.4  $[M+H]^+$  (b) product ion spectra and suggested fragments of  $m/z$  439.4  $[M+H]^+$ .

**Figure S3:** Product ion spectra and suggested fragments of (a)  $m/z$  567.5  $[M+H]^+$  and (b)  $m/z$  284.3  $[M+2H]^{2+}$ .

**Figure S4:** (a) mass spectrum of the peak with  $R_t = 7.1$  min,  $m/z$  283.2  $[M+H]^+$  (b) product ion spectra and suggested fragments of  $m/z$  565.5  $[M+H]^+$ .

**Figure S5:** Product ion spectra and suggested fragments of (a)  $m/z$  565.5  $[M+H]^+$  and (b)  $m/z$  283.3  $[M+2H]^{2+}$ .

**Table S1.** Activity of manganese-dependent peroxidase (MnP) from *I. lacteus* and laccase (Lac) from *P. ostreatus* during *in vivo* degradation of octenidine (OCT) and chlorhexidine (CHX).

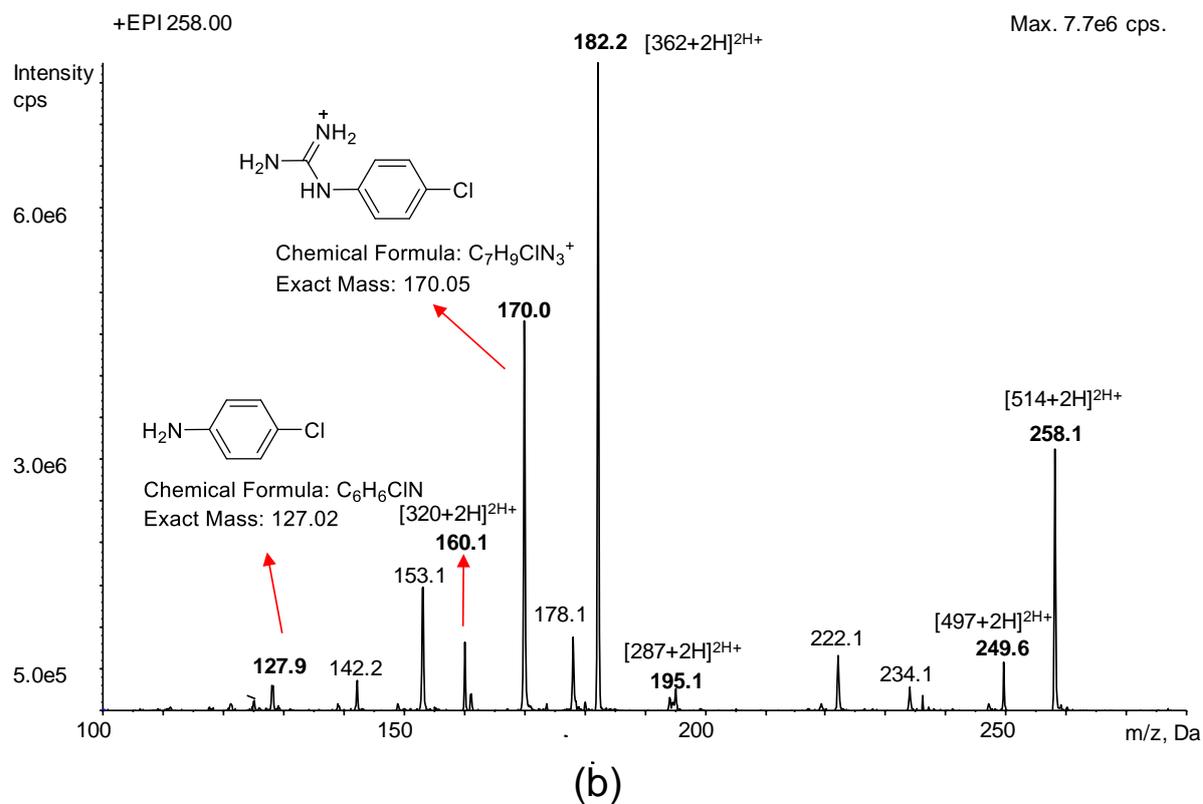
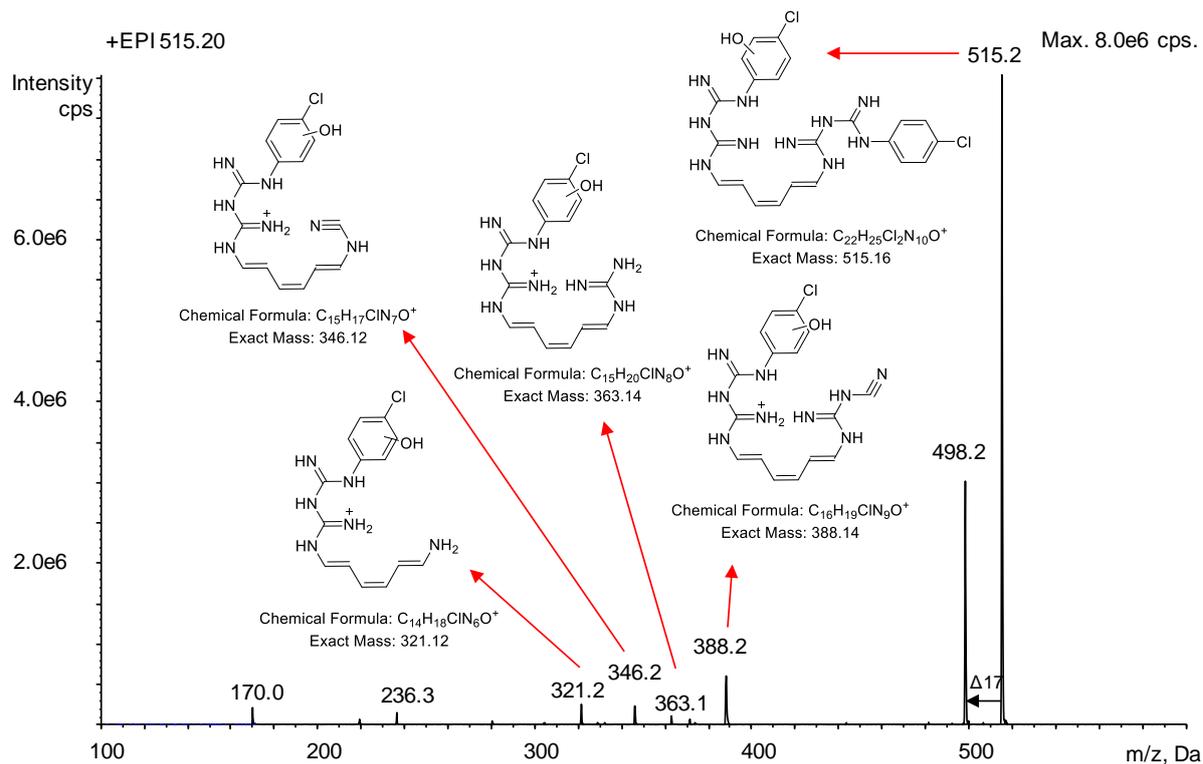
Degradation Time	OCT		CHX	
	MnP (U/l)	Lac (U/l)	MnP (U/l)	Lac (U/l)
0 d	3.6 ± 0.4	31.5 ± 0.5	4.6 ± 0.5	33 ± 4
3 d	3.0 ± 0.4	17.2 ± 0.5	6.2 ± 0.5	15 ± 3
7 d	1.5 ± 0.5	14.1 ± 0.1	5.7 ± 0.3	14.1 ± 0.7
14 d	2.5 ± 0.9	10.8 ± 0.1	6.3 ± 0.5	9.1 ± 0.4
21 d	2.5 ± 0.5	1.8 ± 0	4 ± 1	5.1 ± 0.1

Data are means ± SD (n=3).

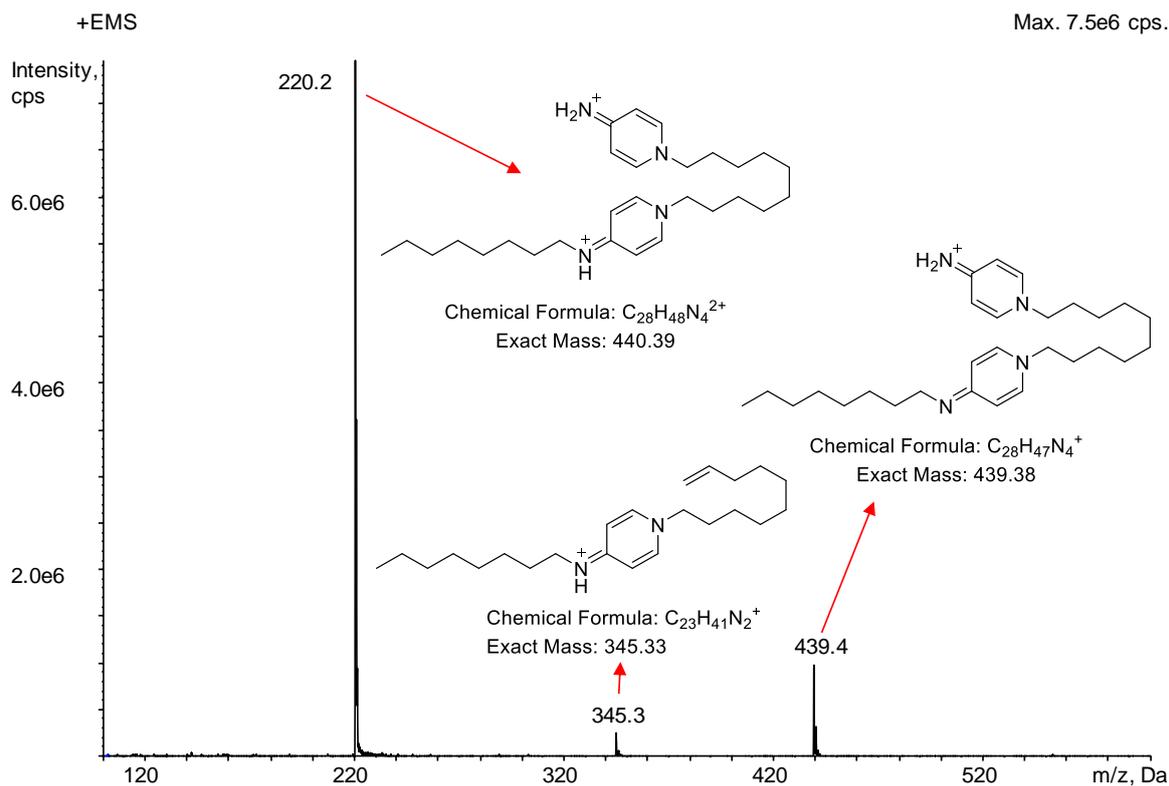
**Table S2.** Activity of manganese-dependent peroxidase (MnP) from *I. lacteus* and laccase (Lac) from *P. ostreatus* during *in vitro* degradation of octenidine (OCT) and chlorhexidine (CHX).

Degradation Time	OCT		CHX	
	MnP (U/l)	Lac (U/l)	MnP (U/l)	Lac (U/l)
0 h	60 ± 1	120 ± 2	60 ± 2	120 ± 7
2 h	58 ± 2	119 ± 3	59 ± 4	118 ± 5
4 h	57 ± 2	118 ± 8	57 ± 5	116 ± 5
8 h	58 ± 2	105 ± 12	57 ± 3	110 ± 8
24 h	58 ± 8	79 ± 1	56 ± 5	86 ± 7
48 h	52 ± 4	55 ± 2	54 ± 3	62 ± 3
96 h	30 ± 5	47 ± 1	32 ± 7	42 ± 5
192 h	17 ± 2	33 ± 0	21 ± 4	31 ± 4

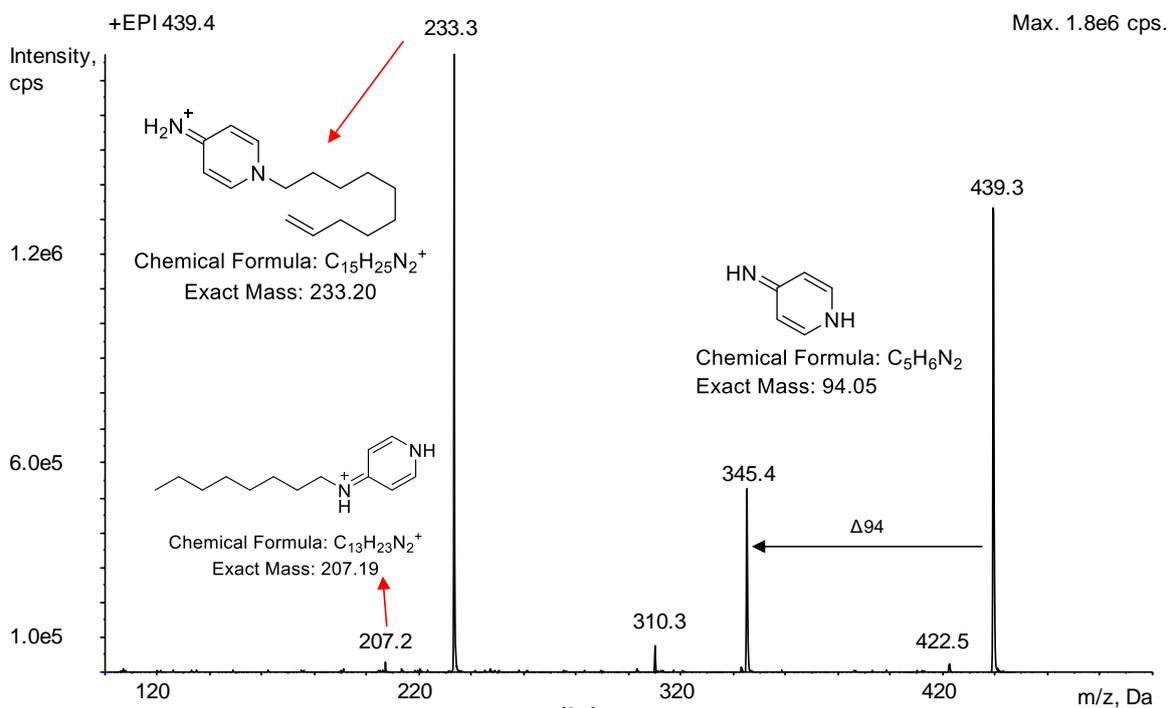
Data are means ± SD (n=3).



**Figure S1:** Product ion spectra and suggested fragments of (a)  $m/z$  515.2  $[M+H]^+$  and (b)  $m/z$  258.2  $[M+2H]^{2+}$ .

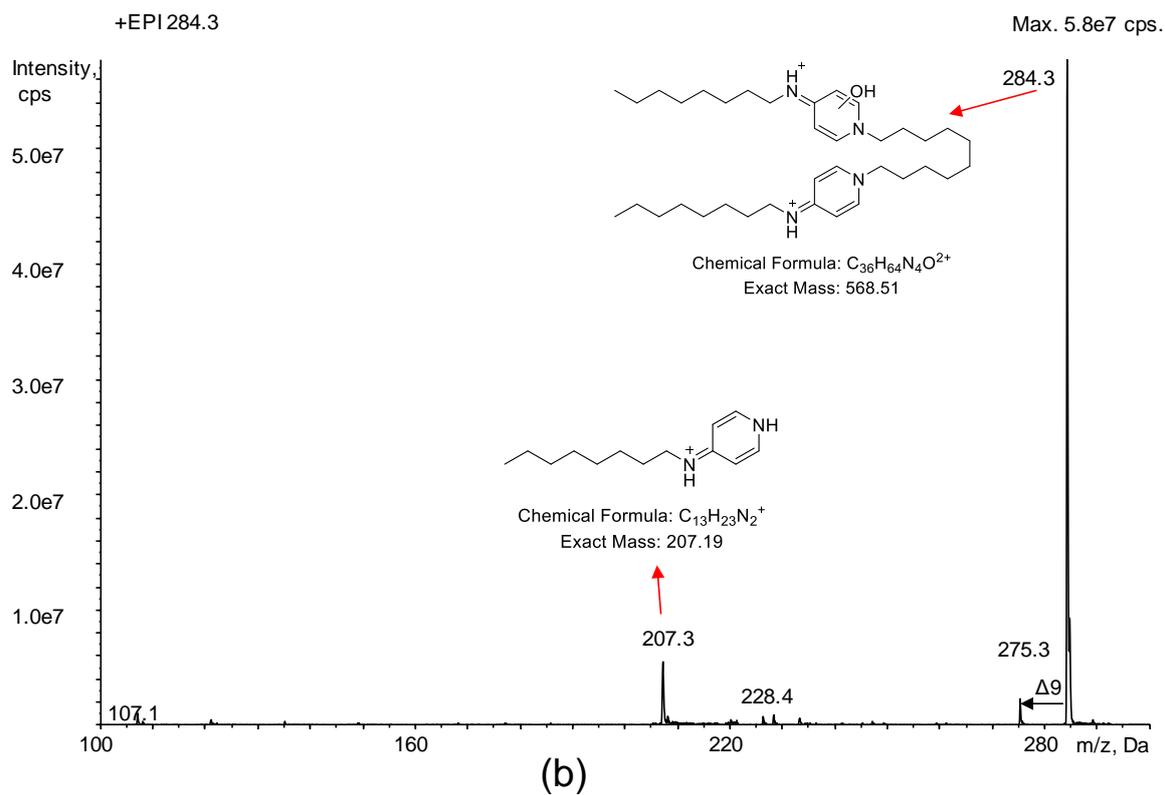
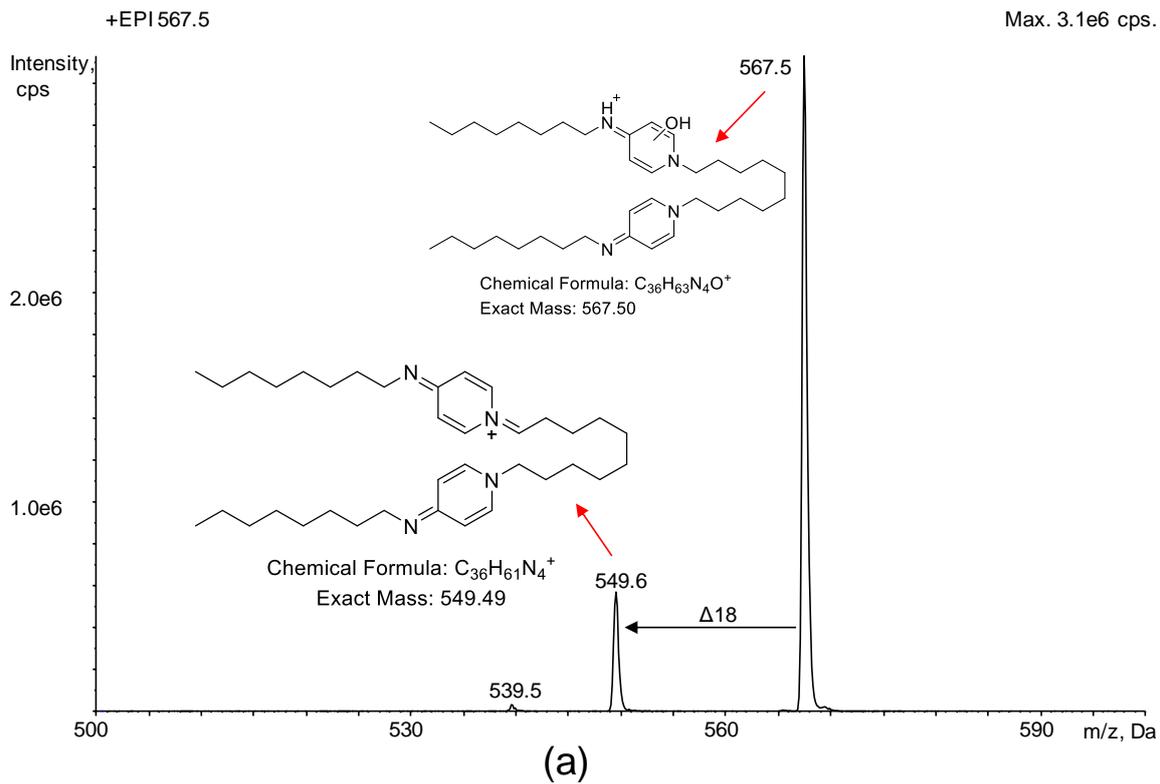


(a)

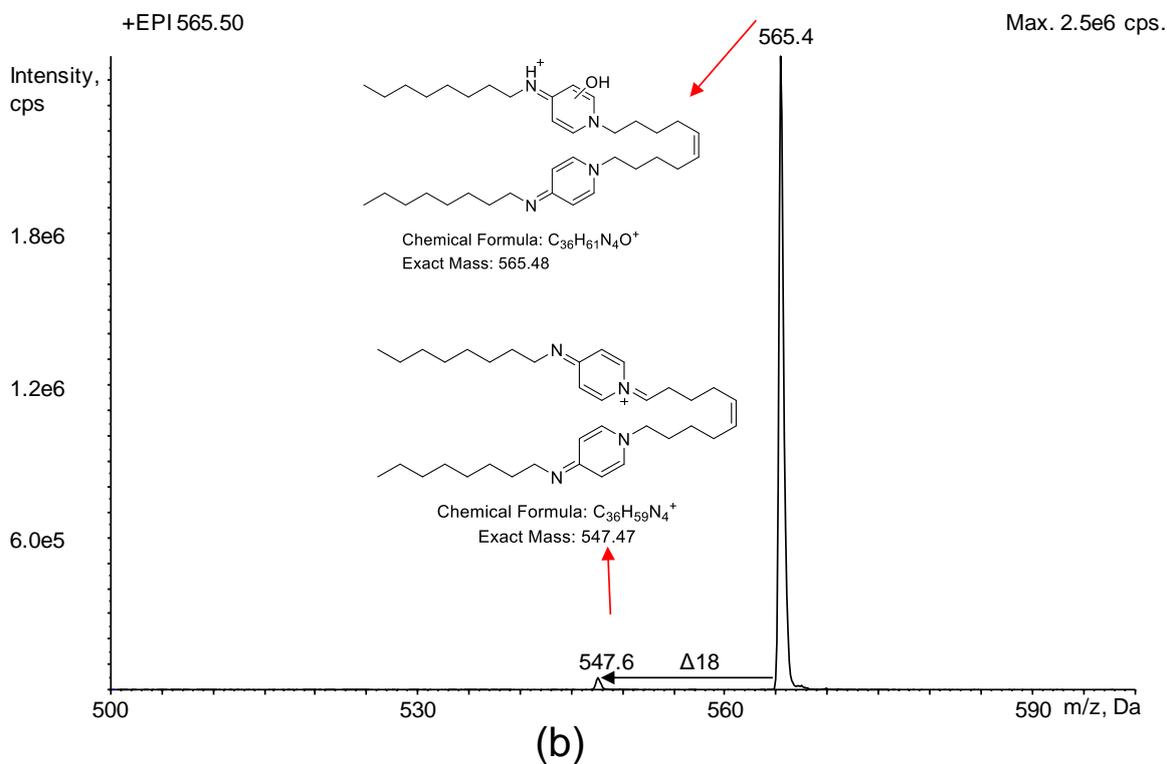
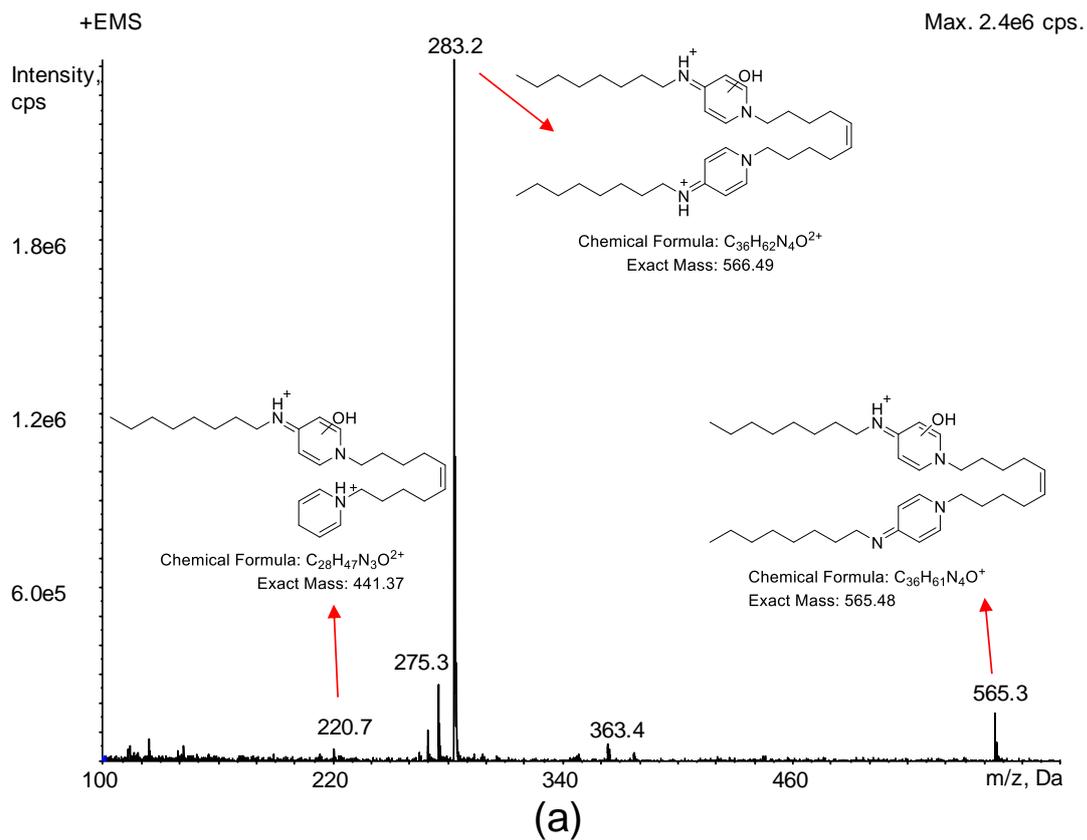


(b)

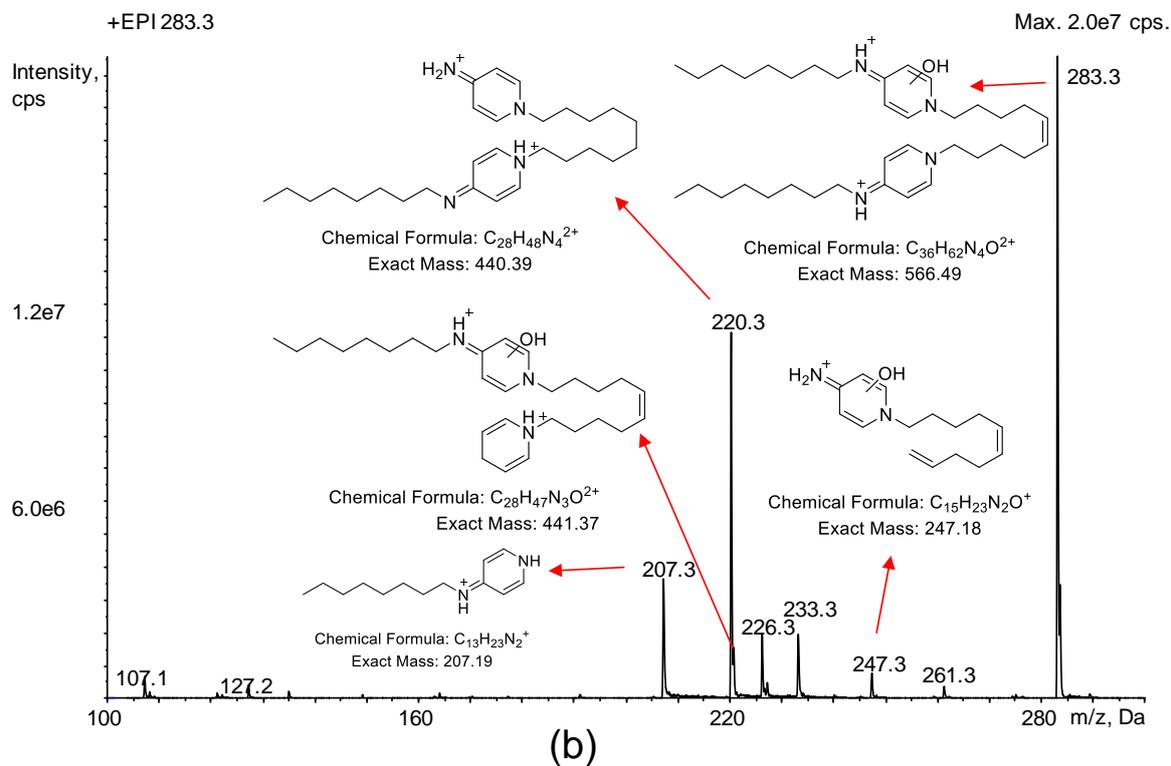
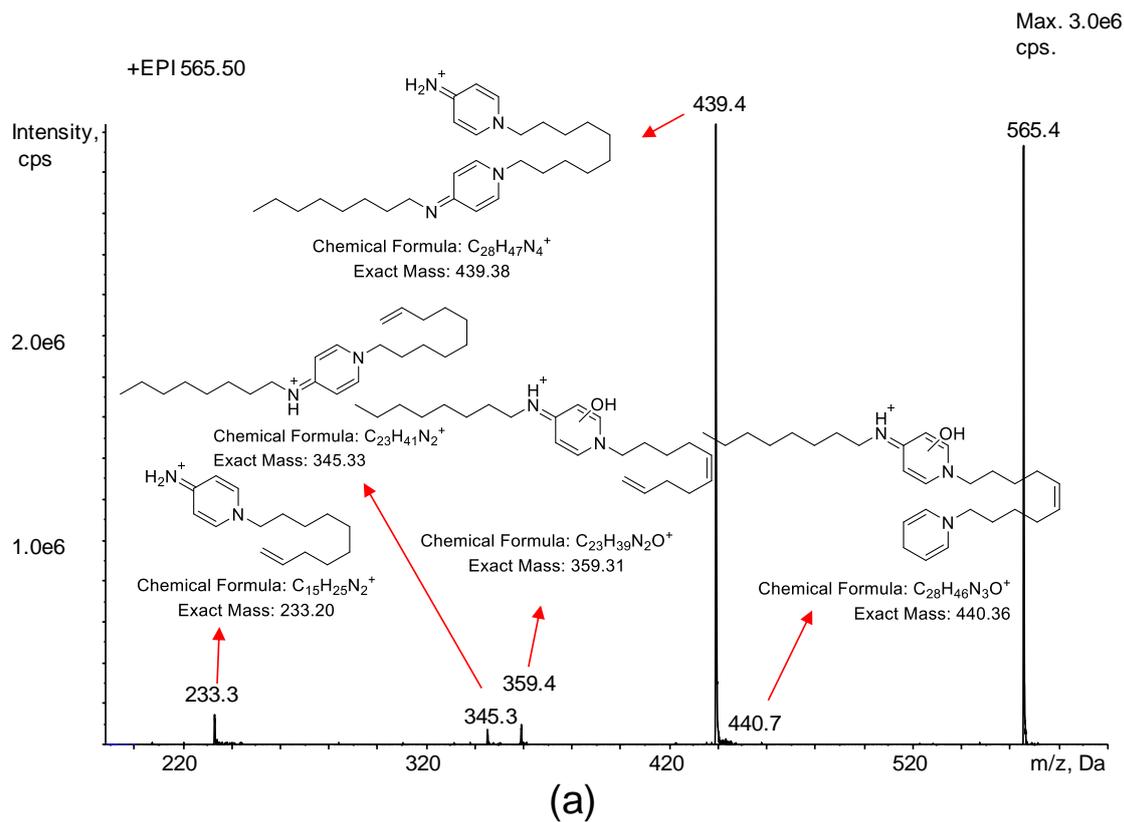
**Figure S2:** (a) mass spectrum of the peak with  $R_t = 5.9$  min,  $m/z$  439.4  $[M+H]^+$  (b) product ion spectra and suggested fragments of  $m/z$  439.4  $[M+H]^+$ .



**Figure S3:** Product ion spectra and suggested fragments of (a)  $m/z$  567.5  $[M+H]^+$  and (b)  $m/z$  284.3  $[M+2H]^{2+}$ .



**Figure S4:** (a) mass spectrum of the peak with  $R_t = 7.1$  min,  $m/z$  283.2  $[M+H]^+$  (b) product ion spectra and suggested fragments of  $m/z$  565.5  $[M+H]^+$ .



**Figure S5:** Product ion spectra and suggested fragments of (a)  $m/z$  565.5  $[M+H]^+$  and (b)  $m/z$  283.3  $[M+2H]^{2+}$ .