

RT (min.)	m/z monoisotopic molecular ion	m/z monoisotopic fragment ions	[M+H ⁺] chemical formulae	Δm (ppm)	Intra scan Relative Abundance
1.81	431.05748		C ₁₄ H ₂₁ O ₅ N ₆ Se	-0.46	8.0%
	a	296.00369	C ₉ H ₁₄ O ₅ NSe	1.75	
	b	250.09348	C ₁₀ H ₁₂ O ₃ N ₅ Se	0.06	
	c	235.98239	C ₇ H ₁₀ O ₃ NSe	1.48	
	d	181.97173	C ₄ H ₈ O ₂ NSe	1.39	
	e	136.06183	C ₅ H ₆ N ₅	0.43	
	f	135.96632	C ₃ H ₆ NSe	2.37	
		97.02838	C ₅ H ₅ O ₂	-0.27	

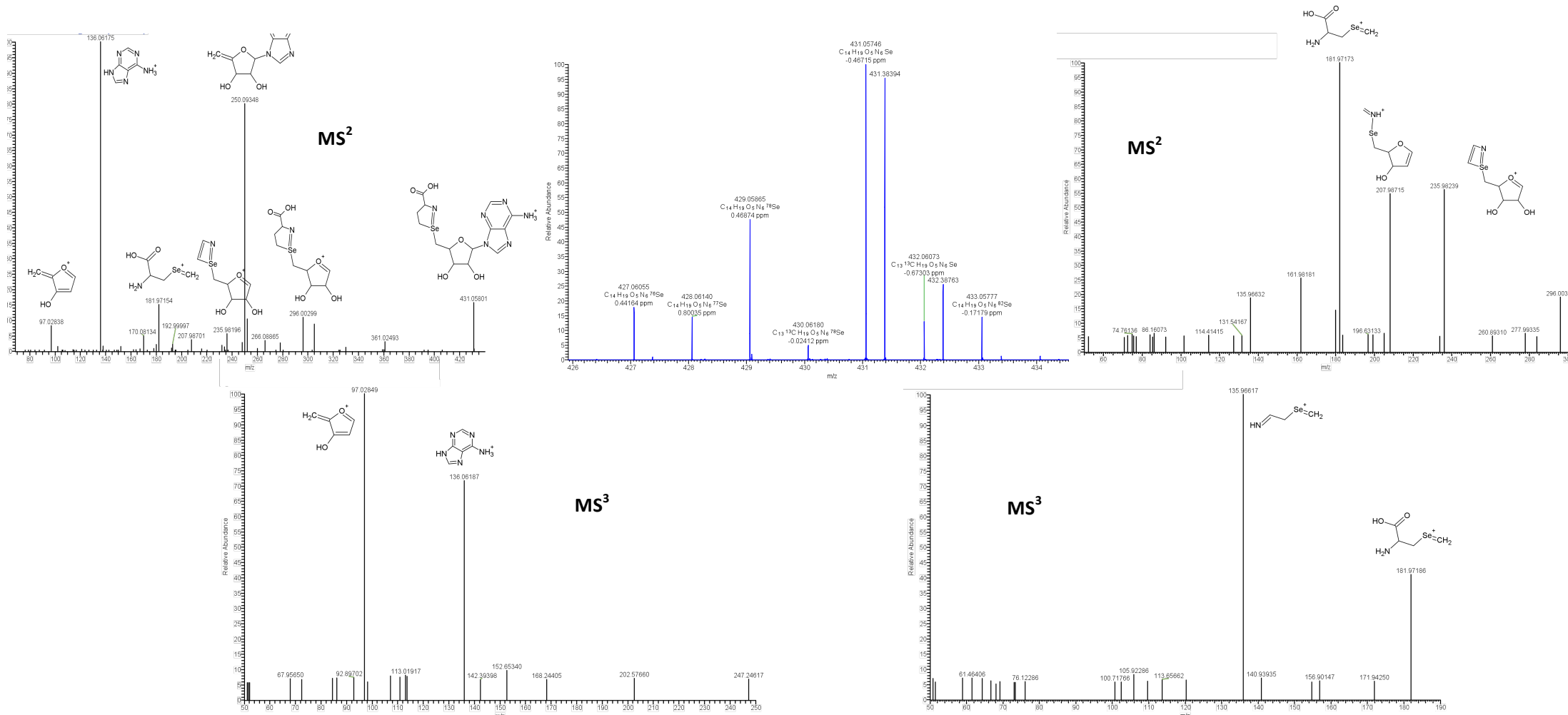
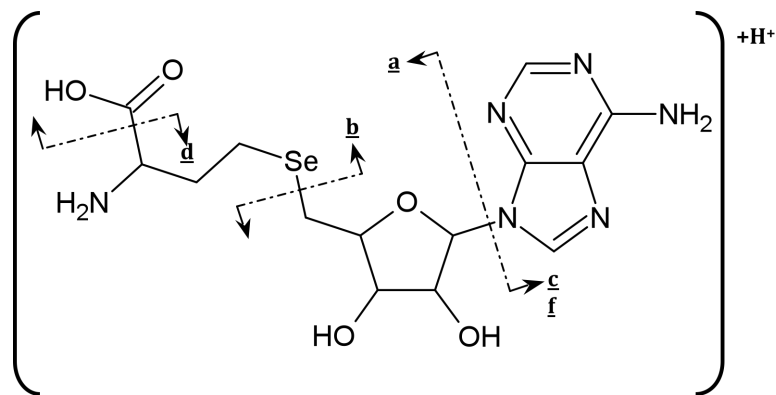


Fig. 1 SI: example of MS tree (Se pattern and exact mass, CID, HCD MS_n) on line on F9 (selenometabolite 9 (table 1)).

Fig. 1 SI



RT (min.)	m/z monoisotopic molecular ion	m/z monoisotopic fragment ions	[M+H ⁺] chemical formulae	Δm (ppm)	Intra scan Relative Abundance
2.37	433.07367		C ₁₄ H ₂₁ O ₅ N ₆ Se	0.82	8.0%
	a	298.01917	C ₉ H ₁₆ O ₅ NSe	1.17	
	b	181.97153	C ₄ H ₈ O ₂ NSe	0.28	
	c	136.06183	C ₅ H ₆ N ₅	0.42	
	d	135.9662	C ₃ H ₆ NSe	1.49	

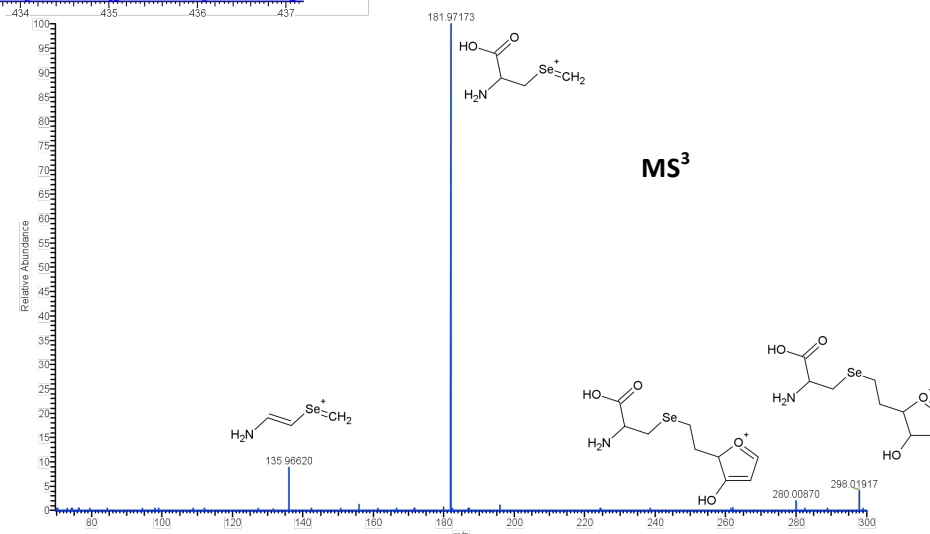
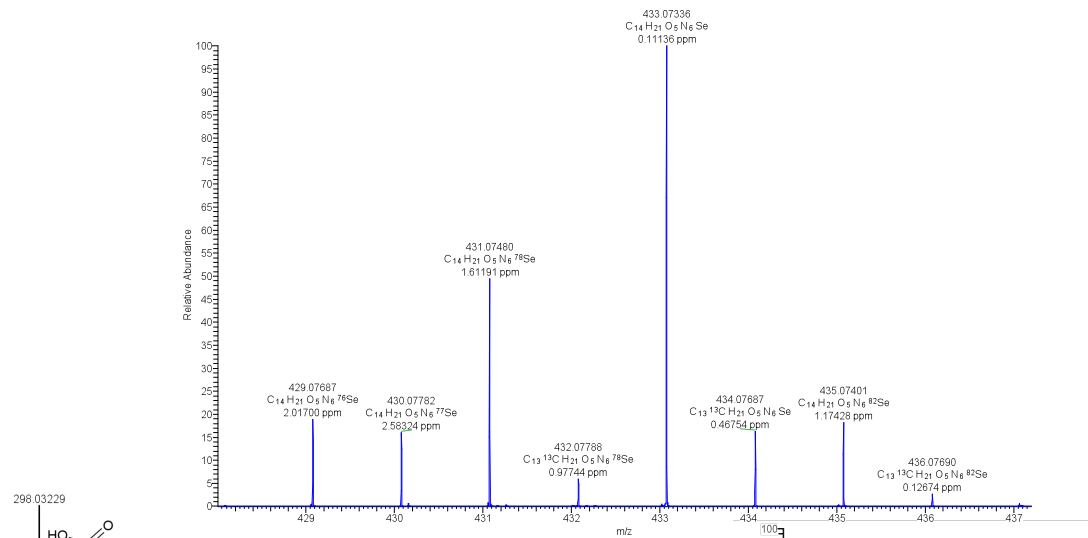
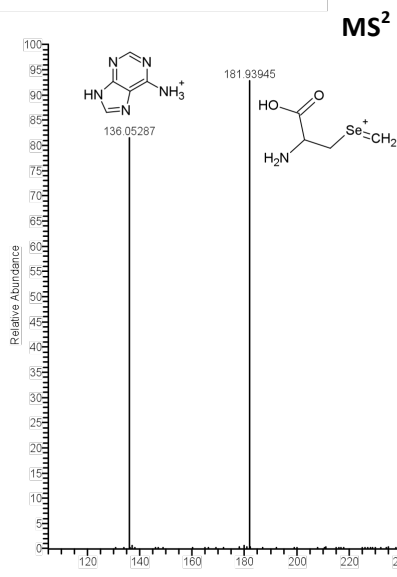


Fig. 2 SI: example of MS tree (Se pattern and exact mass, CID, HCD MSn) on line on F9 selenometabolite 25 (table 2)).

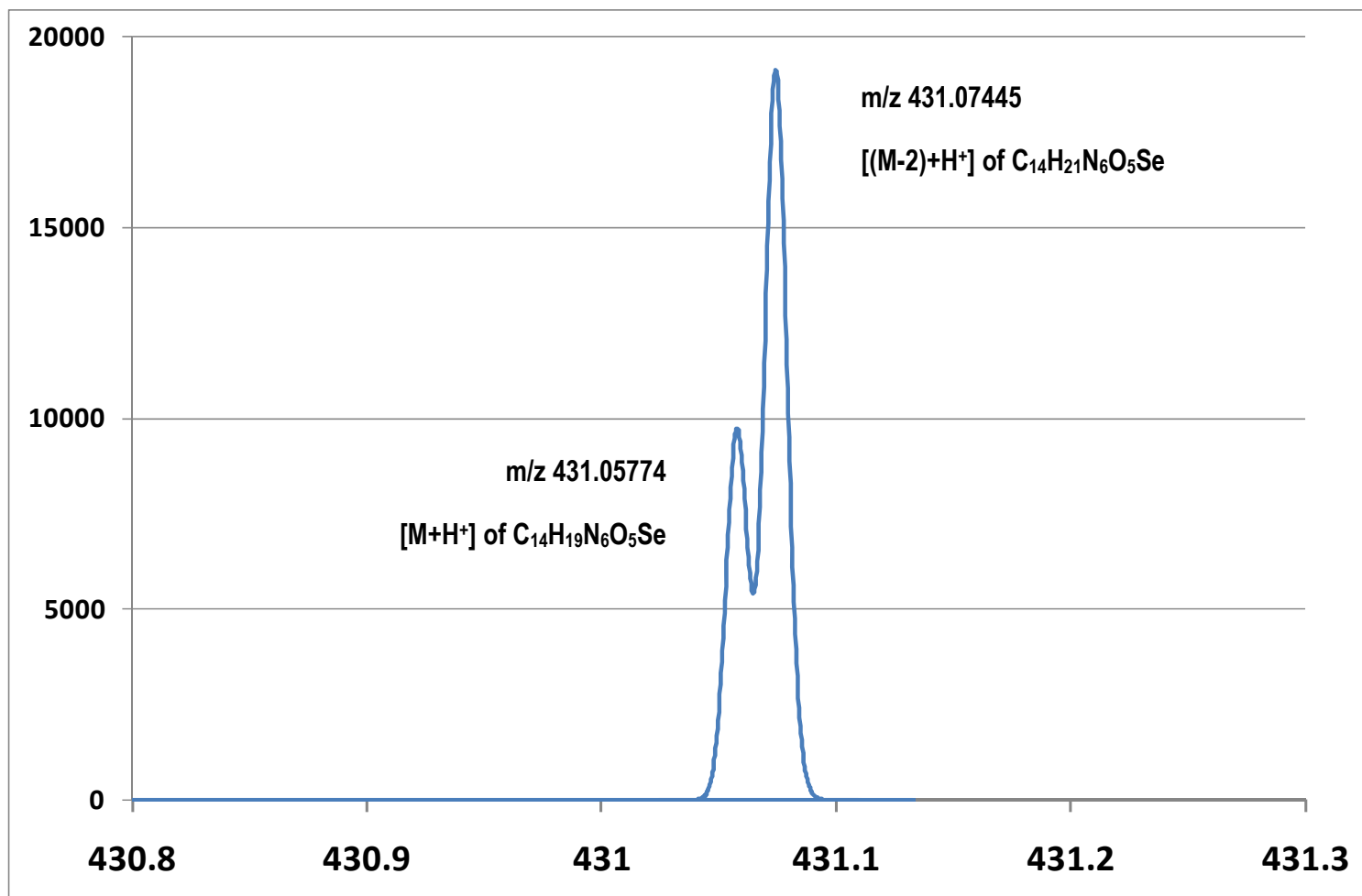


Fig. 3 SI: Mass resolution required for separation of Selenoadenosyl homocysteine homologues (references 9 and 25 in tables 1 and 2).

Fig. 3 SI