

Table S1. Crystallographic Data for **2** and **3**

	2	3
empirical formula	C ₄₀ H ₅₂ F ₁₂ Fe ₂ N ₈ O ₁₂ S ₄	C ₂₀ H ₂₆ F ₆ FeN ₄ O ₆ S ₂
formula weight	1304.84	652.42
T	173(2) K	173(2) K
crystal system	Monoclinic	Monoclinic
space group	Pna2 ₁	C2/c
unit cell dimensions	<i>a</i> = 16.353(2)	<i>a</i> = 17.232(2) Å
	<i>b</i> = 18.707(3)	<i>b</i> = 9.540(1) Å
	<i>c</i> = 18.231(3)	<i>c</i> = 18.263(2) Å
<i>V</i>	5577(1) Å ³	2667(1) Å ³
<i>Z</i>	4	4
<i>D</i> (calc)	1.554 g cm ⁻³	1.624 g cm ⁻³
λ	0.71073 Å	0.71073 Å
μ	0.772 mm ⁻¹	0.807 mm ⁻¹
<i>R</i> _I ^a	0.0465	0.0369
<i>wR</i> ₂ ^b	0.0857	0.0919

$$^a R_I = \sum ||F_o| - |F_c|| / \sum |F_o|, \quad ^b wR_2 = (\sum [w(F_o^2 - F_c^2)^2] / \sum [wF_o^4])^{1/2},$$

$$\text{where } w = 1/\sigma^2(F_o^2) + (aP)^2 + bP.$$

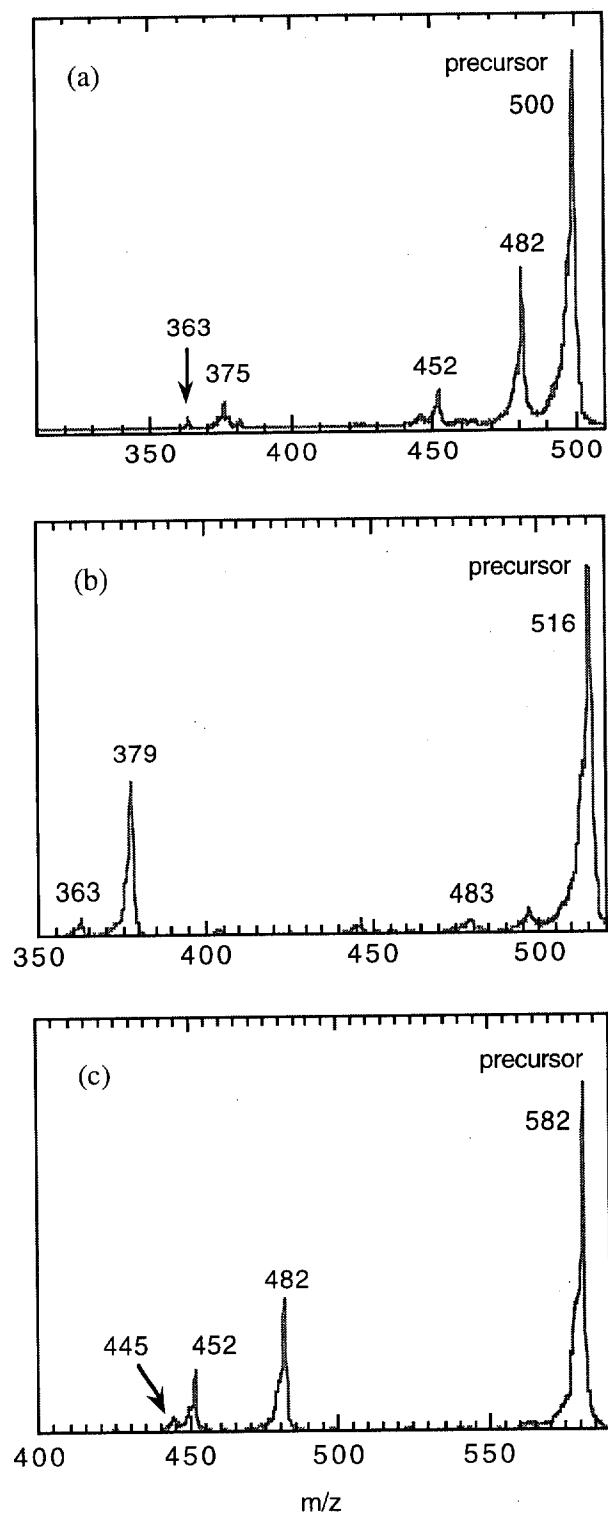


Figure S1 (Chen et al.)