Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Data

Degradation of aquatic sulfadiazine by Fe^0/persulfate: Kinetics, mechanisms, and degradation pathway

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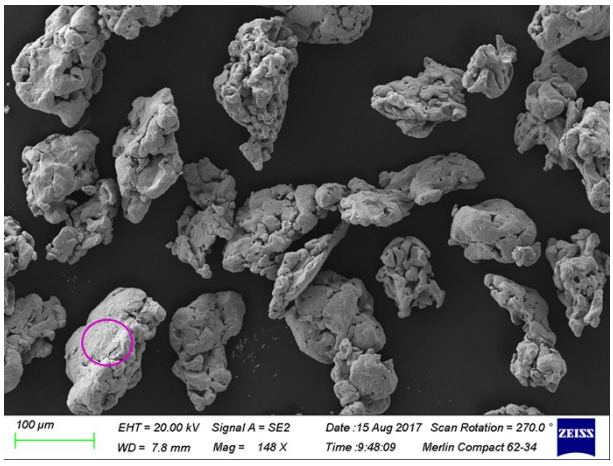
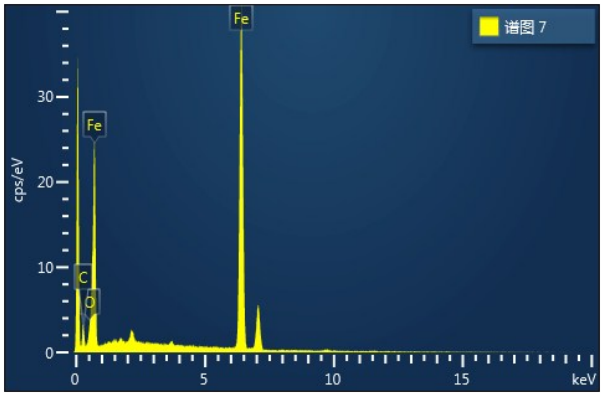


(a)



Element	wt%	atom%
O	2.41	7.93
Fe	97.59	92.07
Total:	100.00	100.00

(b)

Fig. S1 SEM (a) of Fe^0 particles in addition to their corresponding X-ray spectra (b)

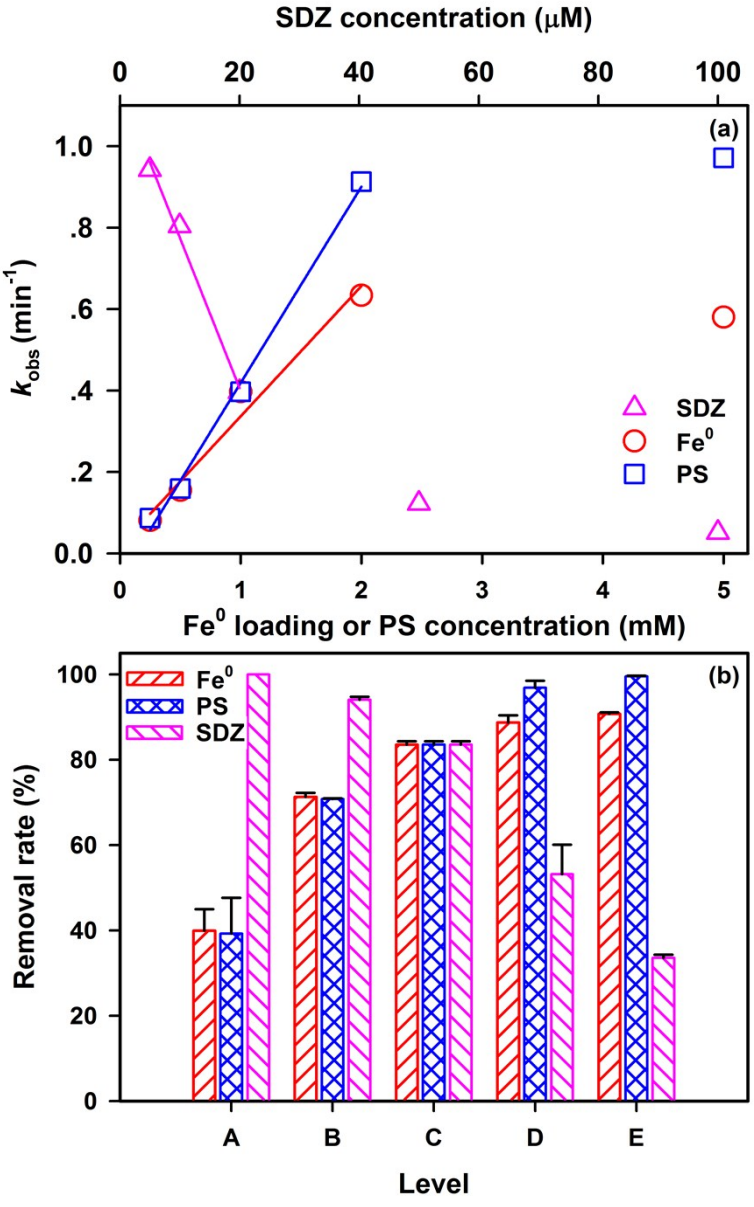


Fig. S2 Effects of treatment factors on rate constant (a) and removal rate (b) of aquatic SDZ degradation by Fe^0/PS. Reaction conditions: initial pH 7.0, rpm = 600, and T = 20 ± 1 °C.

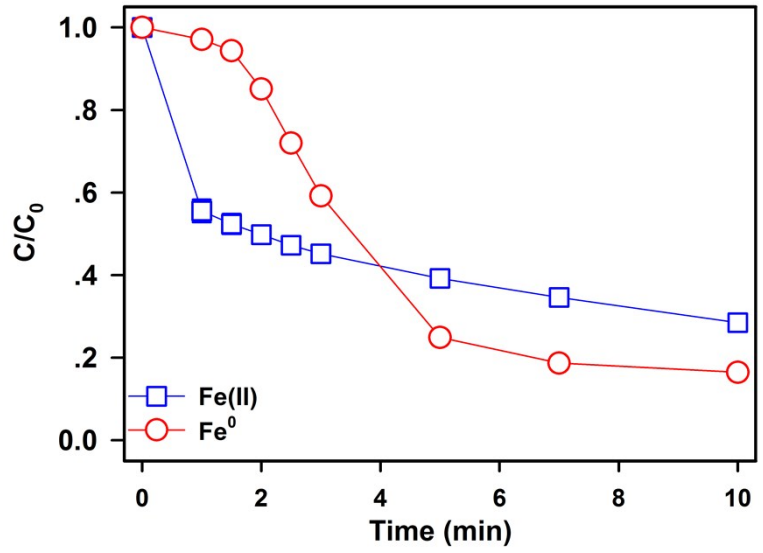


Fig. S3 Comparing experiment of aquatic SDZ degradation by Fe^0/PS and Fe(II)/PS. Reaction conditions: $[SDZ]_0$ = 20 μM, $[Fe^0]_0$ = 1 mM, $[Fe(II)]_0$ = 1 mM, [PS] = 1 mM, initial pH 7.0, rpm = 600, and T = 20 ± 1 °C.

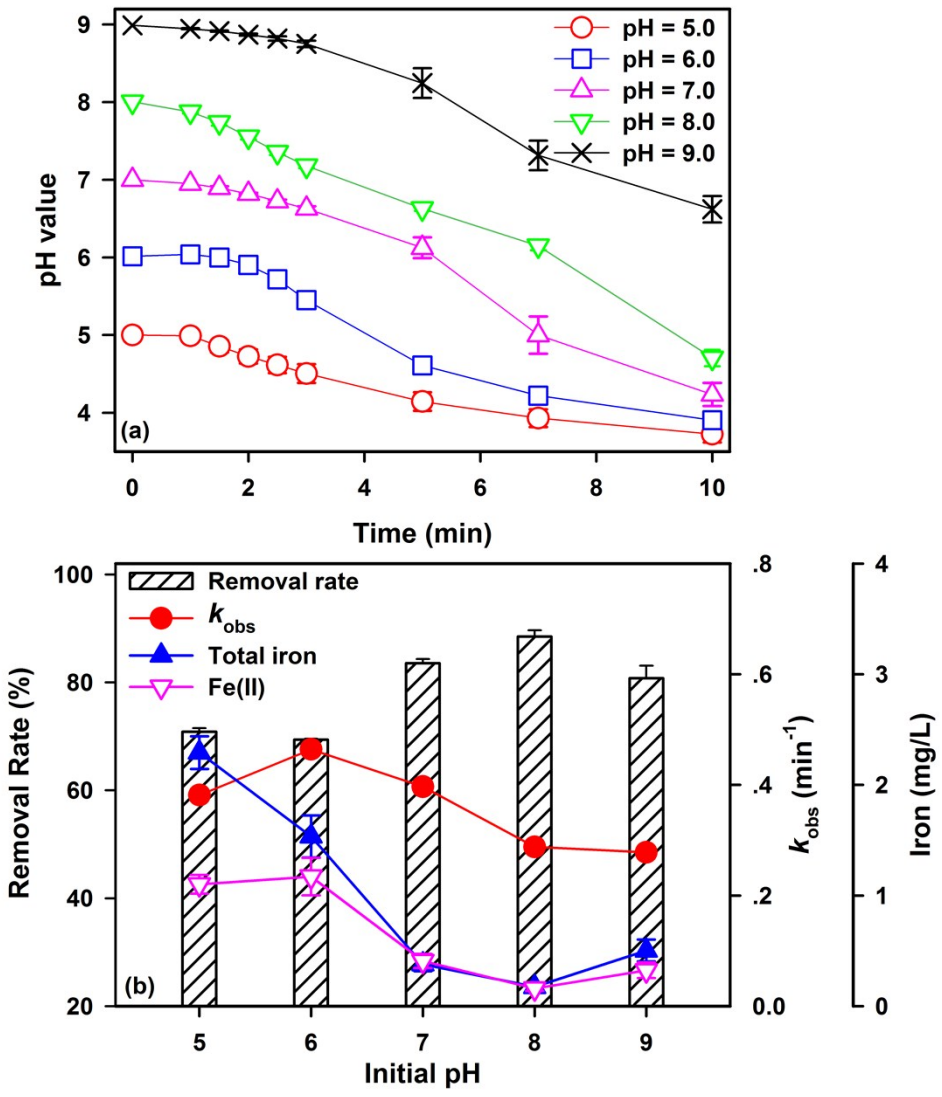


Fig. S4 The variation of pH value at different initial pH (a), and the rate constant, the final removal rate of aquatic SDZ degradation, the concentration of total dissolving iron and dissolving Fe(II) by the end of the reaction at different initial pH (b) in the Fe^0/PS system. Reaction conditions: $[SDZ]_0$ = 20 μM, $[Fe^0]_0$ = 1 mM, [PS] = 1 mM, rpm = 600, and T = 20 ± 1 °C.

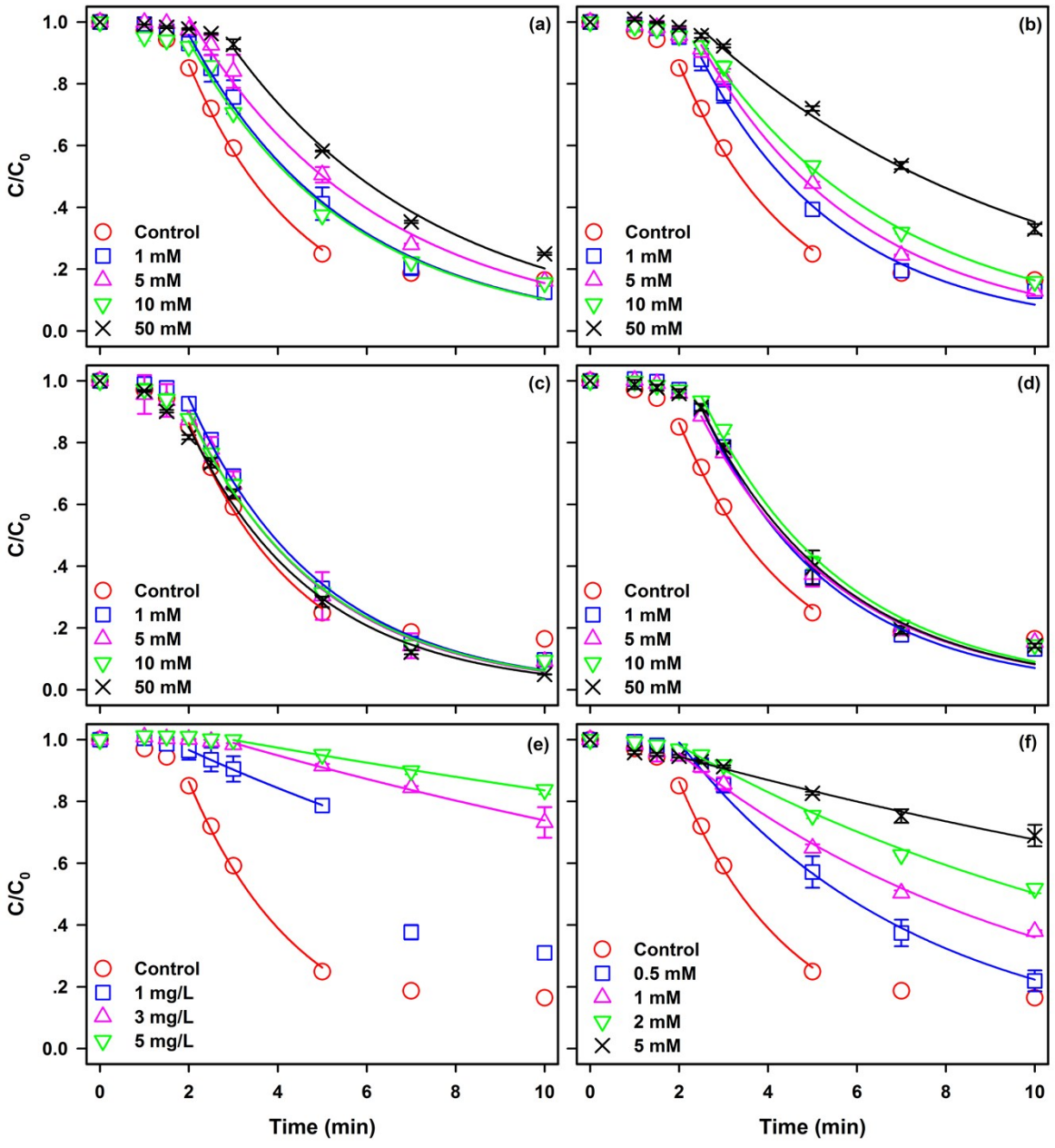


Fig. S5 Effects of SO_4^{2-} (a), NO_3^- (b), Cl^- (c), ClO_4^- (d), humic acid (e), and HCO_3^- (f) on degradative kinetics of aquatic SDZ by Fe^0/PS. Reaction conditions: $[SDZ]_0$ = 20 μM, $[Fe^0]_0$ = 1 mM, [PS] = 1 mM, initial pH = 7.0, rpm = 600, and T = 20 ± 1 °C.

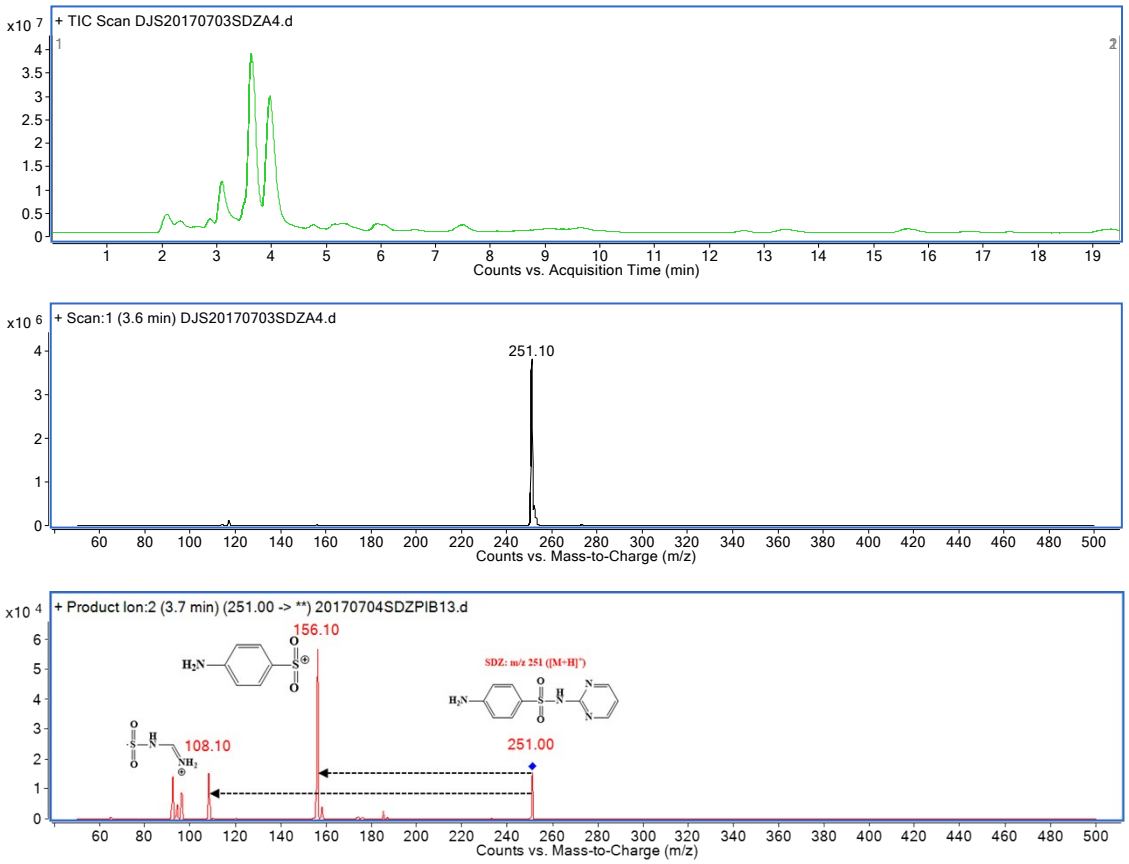


Fig. S6 Identification of SDZ (m/z^+ 251)
Product ion 156 and 108

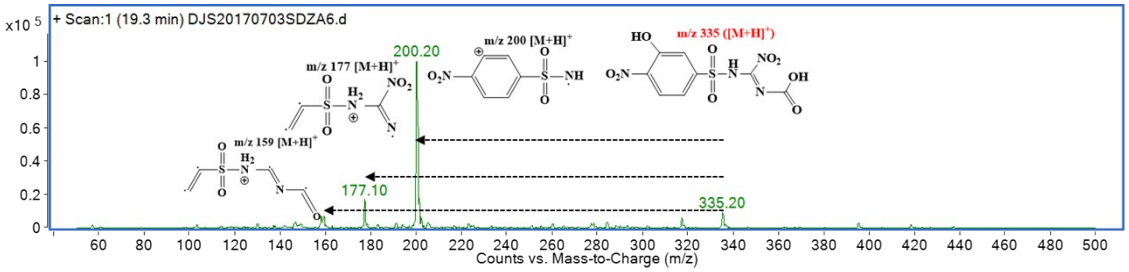


Fig. S7 Identification of P13 (m/z^+ 335)
Product ion 200 , 177, and 159

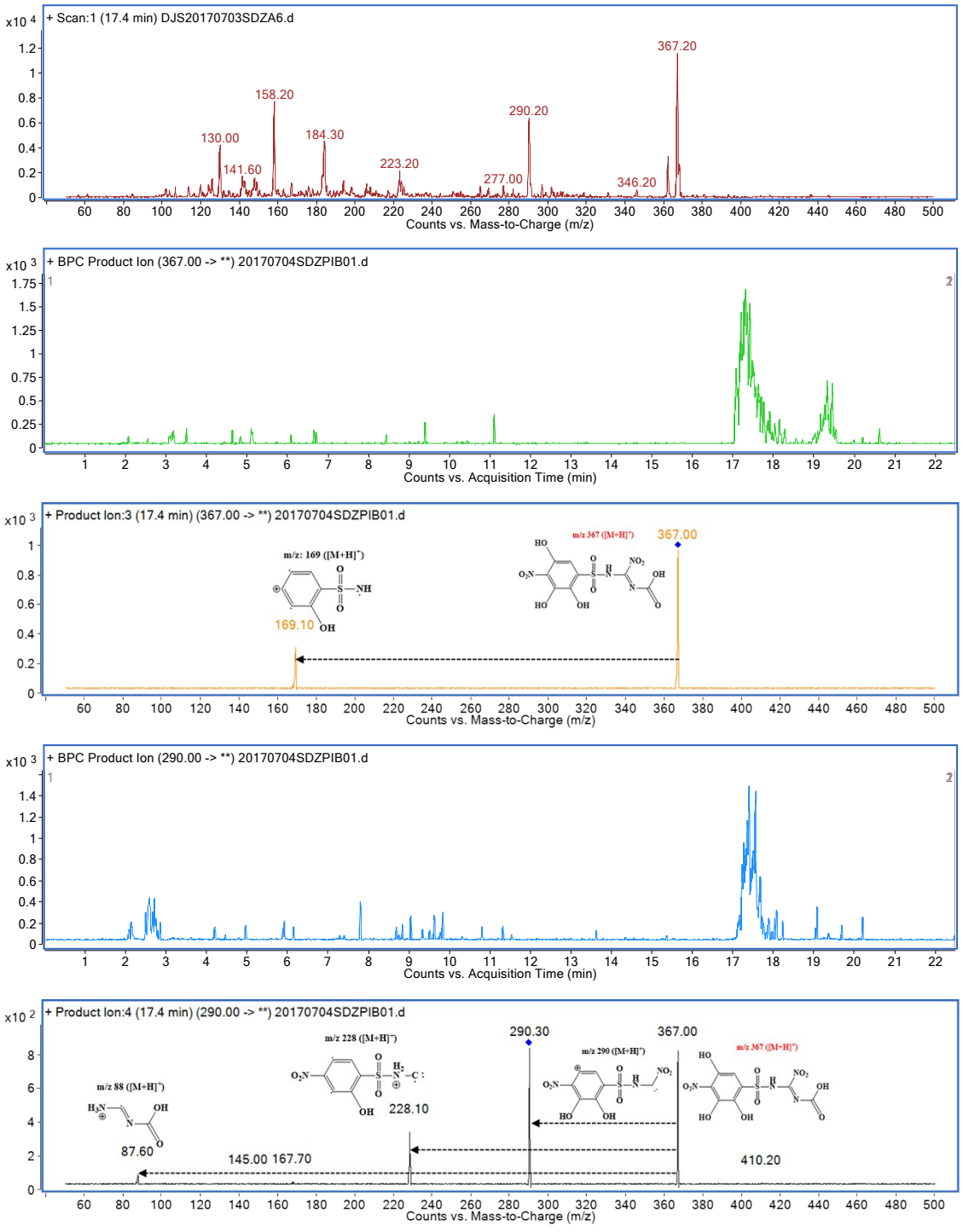


Fig. S8 Identification of P14 (m/z^+ 367)
Product ion 290, 228, 169 and 88

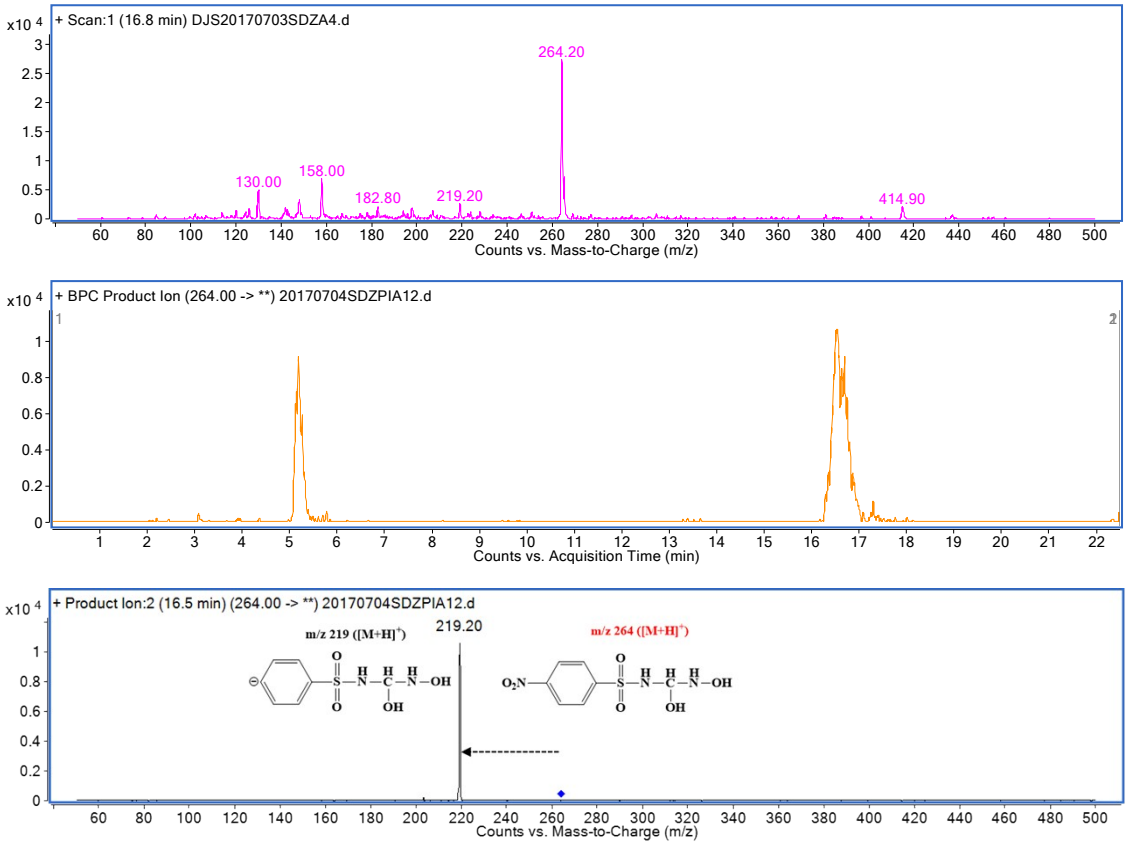


Fig. S9 Identification of P17 (m/z^+ 264)
Product ion 219

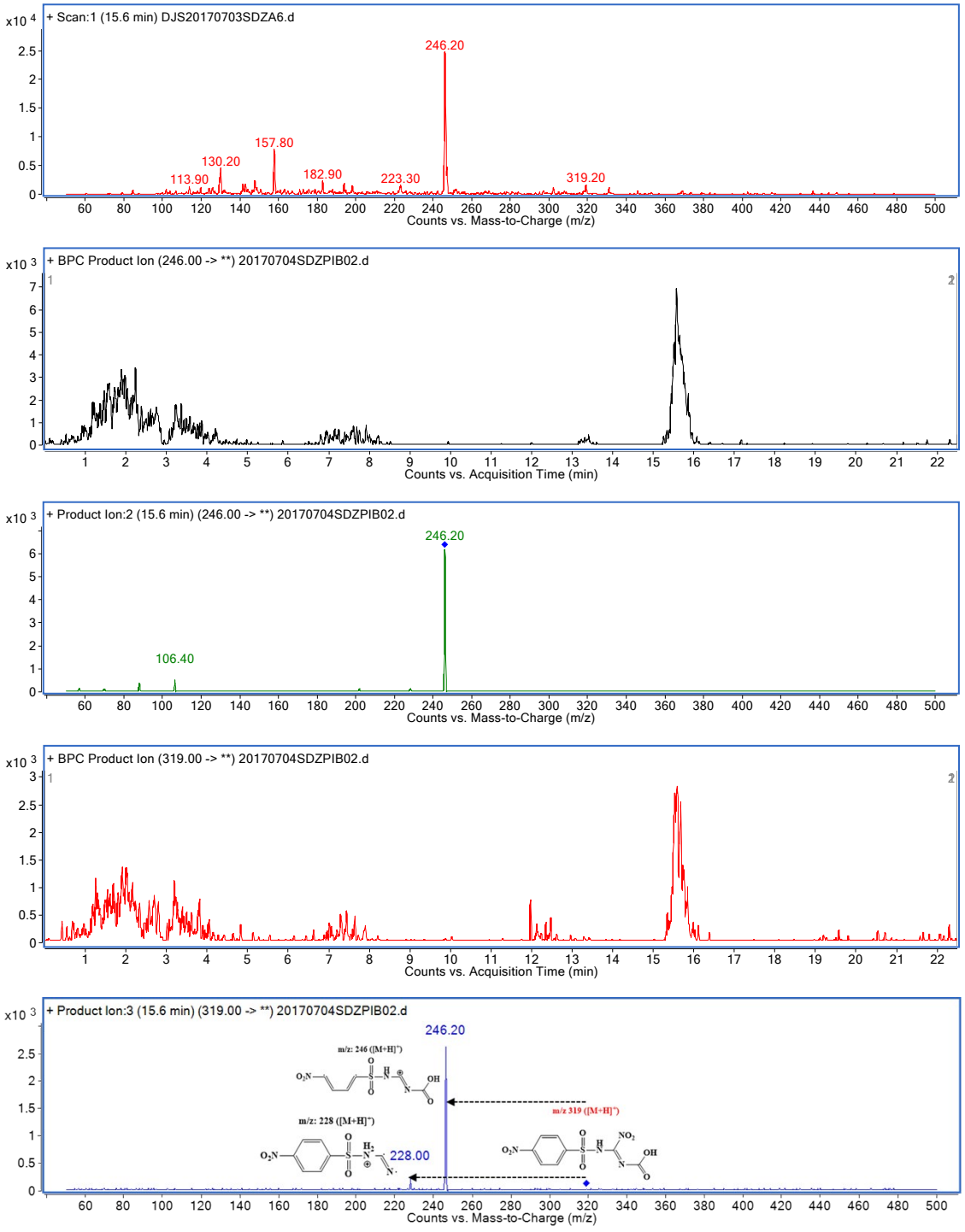


Fig. S10 Identification of P12 (m/z^+ 319)
Product ion 246 and 228

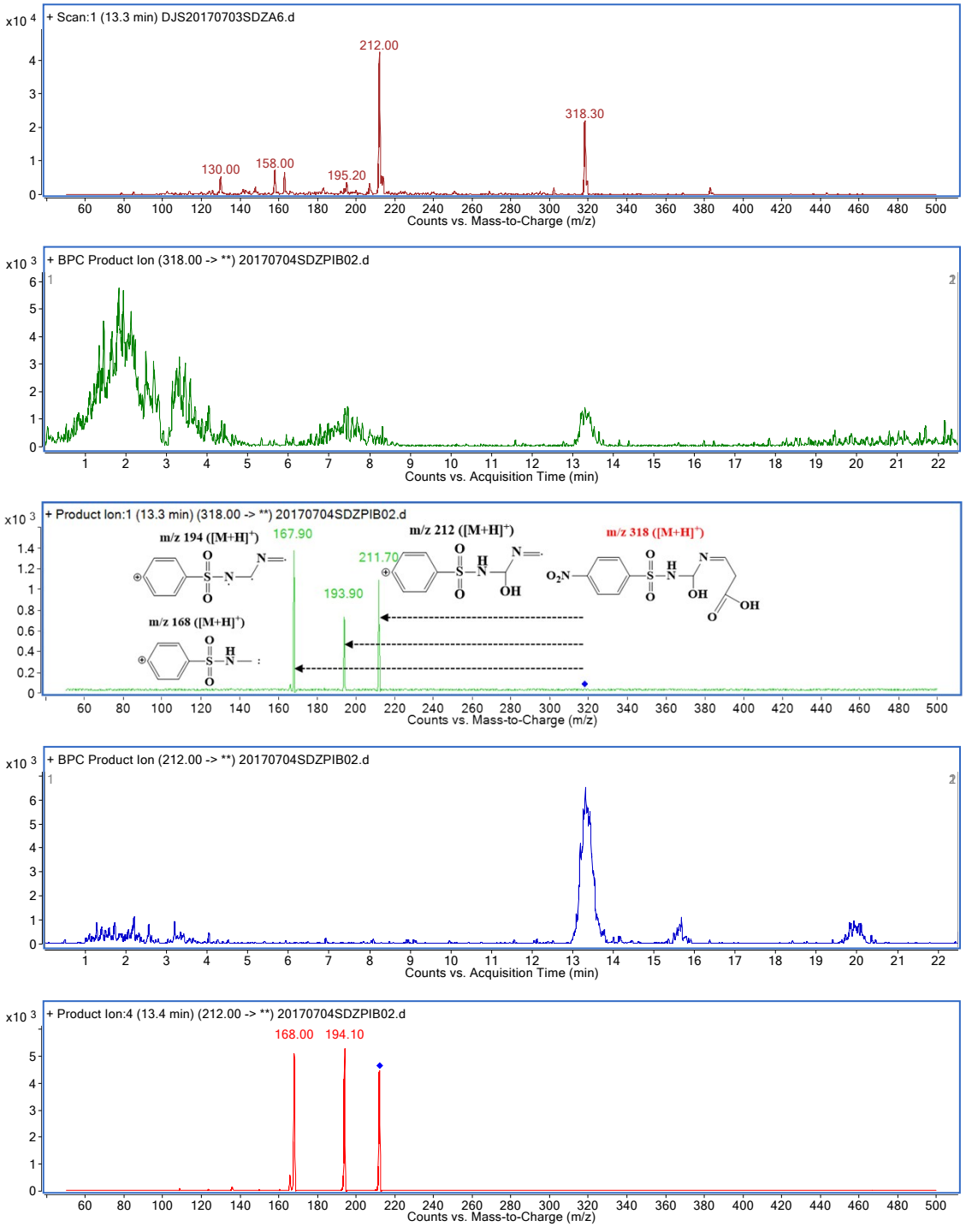


Fig. S11 Identification of P15 (m/z^+ 318)
Product ion 212, 194, and 168

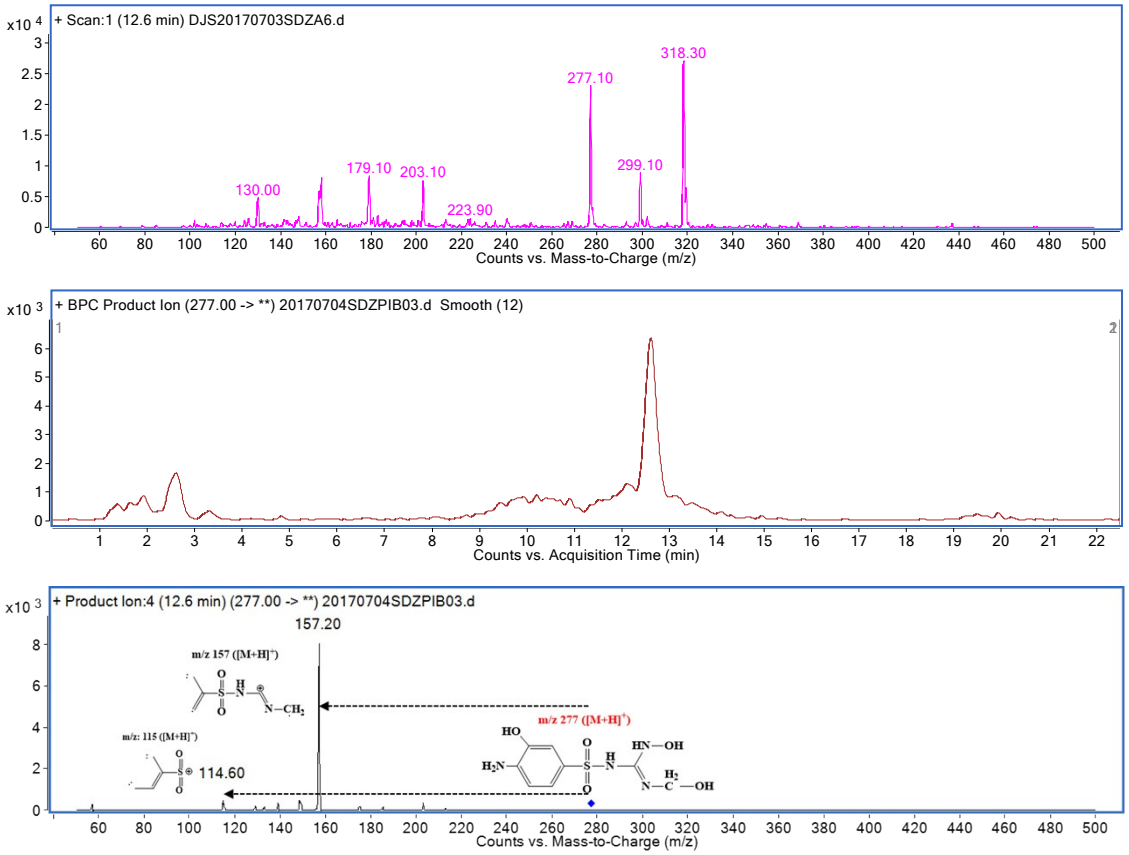


Fig. S12 Identification of P20 (m/z^+ 277)
Product ion 157 and 114

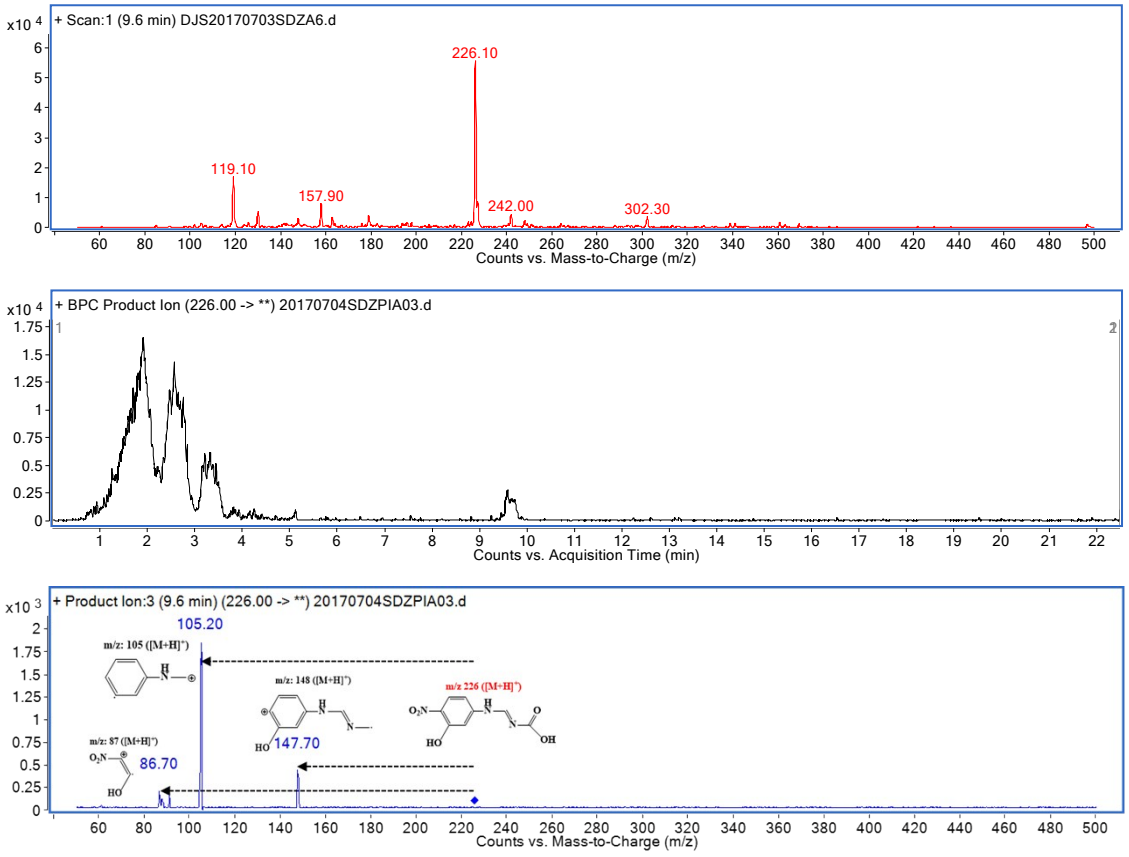


Fig. S13 Identification of P2 (m/z^+ 226)
Product ion 148, 105, and 87

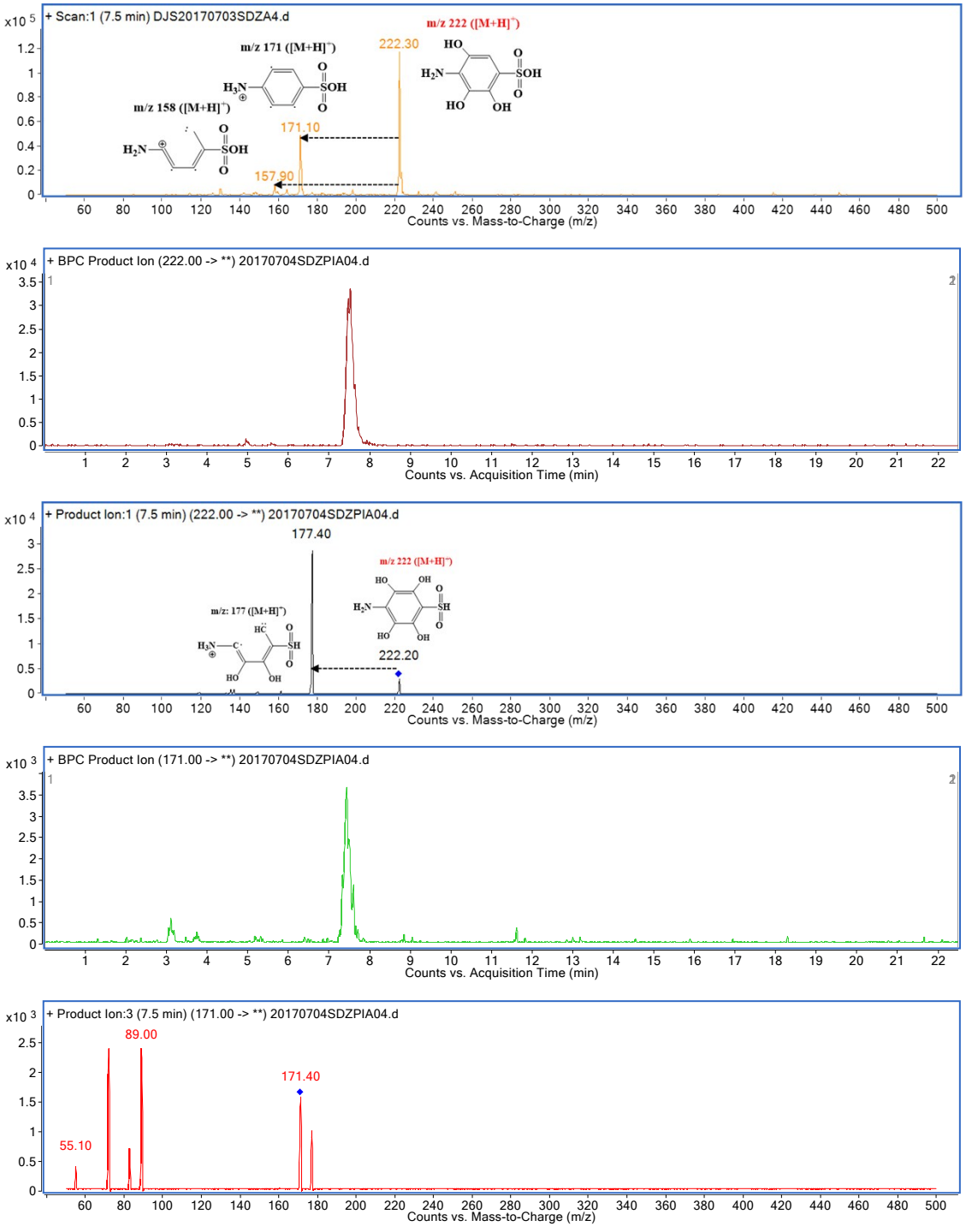


Fig. S14 Identification of P4 (m/z^+ 222)
Product ion 177, 171, and 89

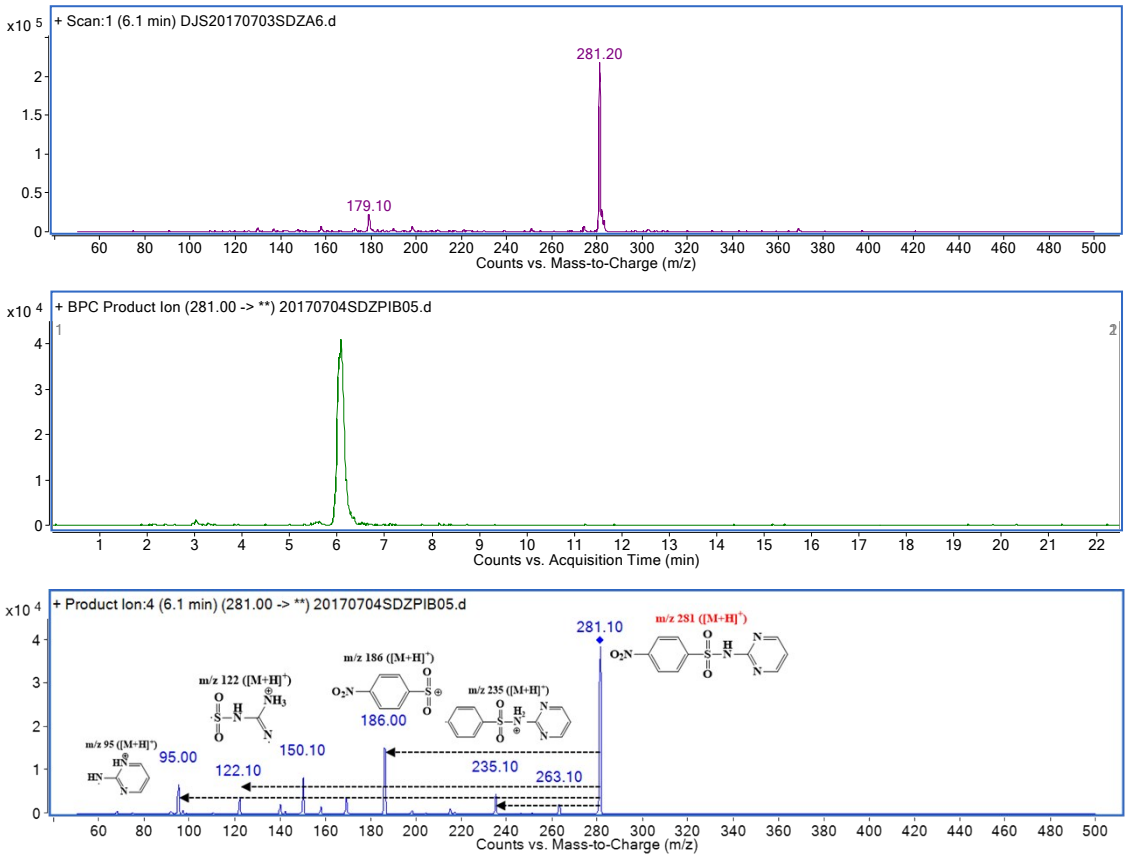


Fig. S15 Identification of P11 (m/z^+ 281)
Product ion 263, 235, 186, 150, 122, and 95

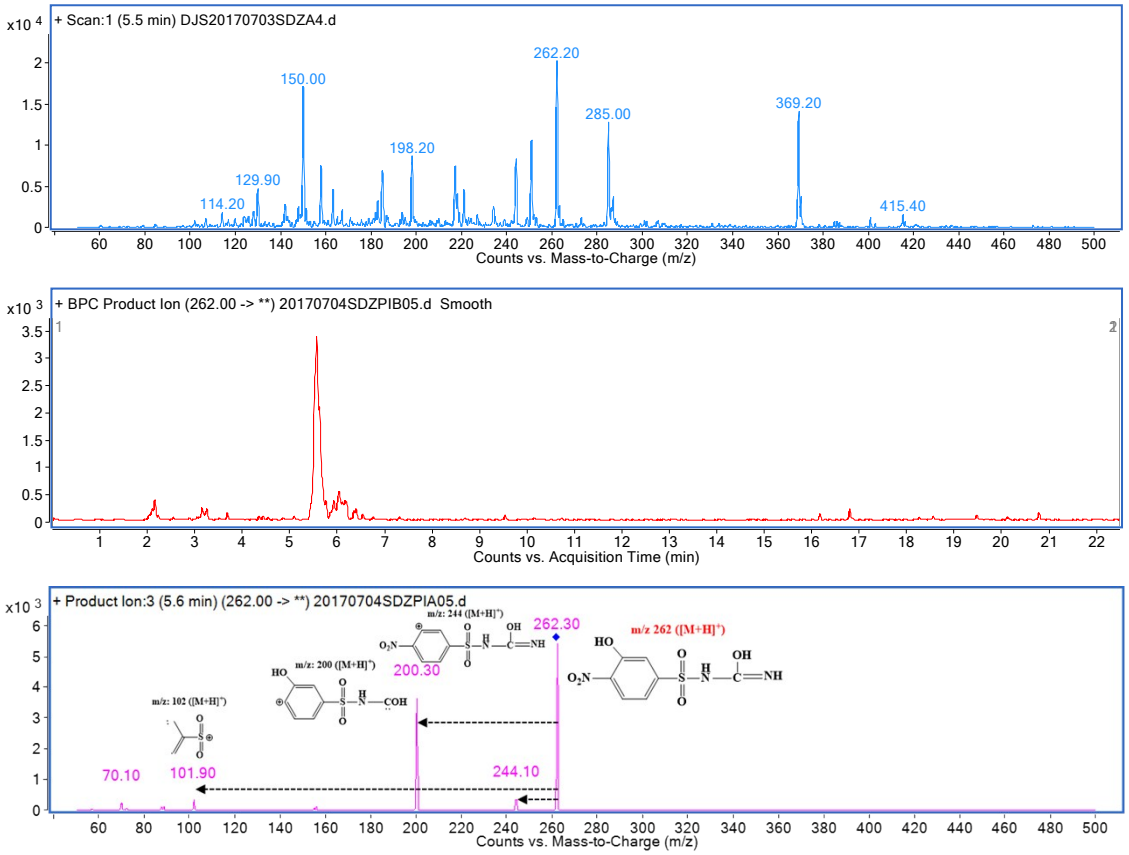


Fig. S16 Identification of P18 (m/z^+ 262)
Product ion 244, 200, and 102

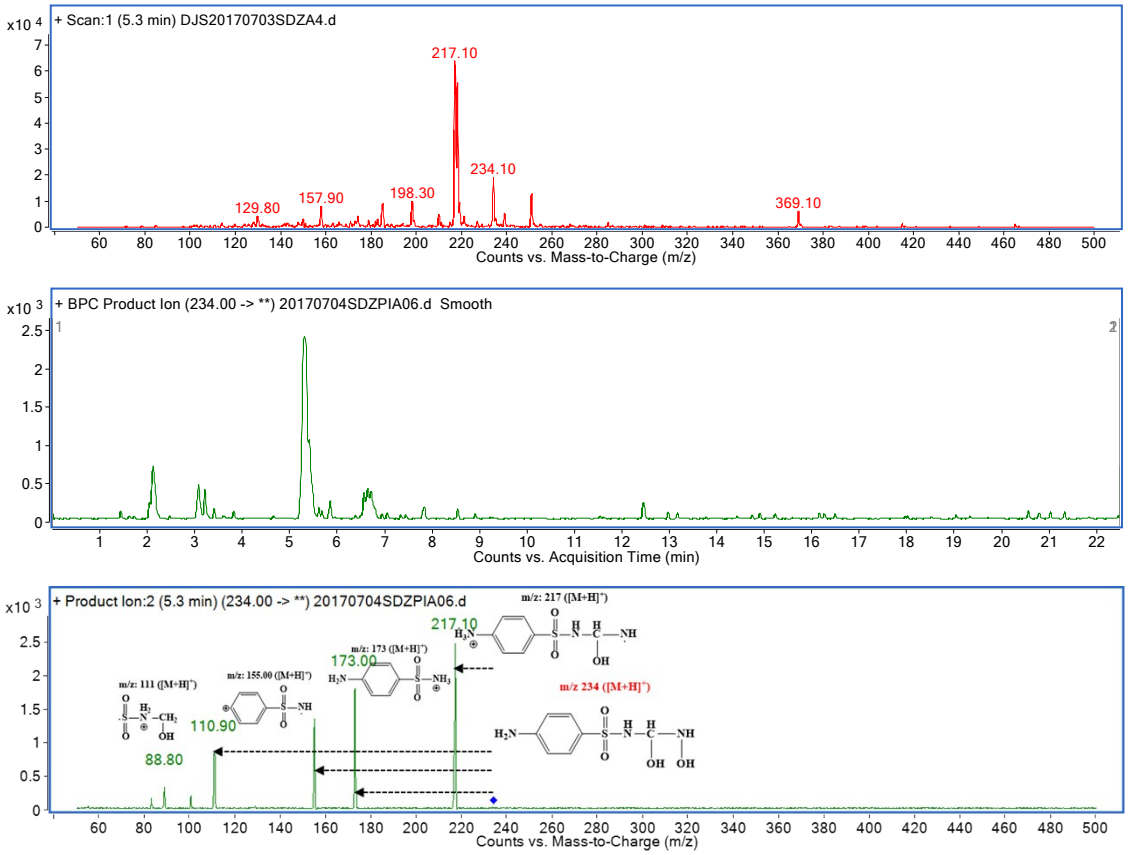


Fig. S17 Identification of P10 (m/z^+ 234)
Product ion 217, 173, 155, and 111

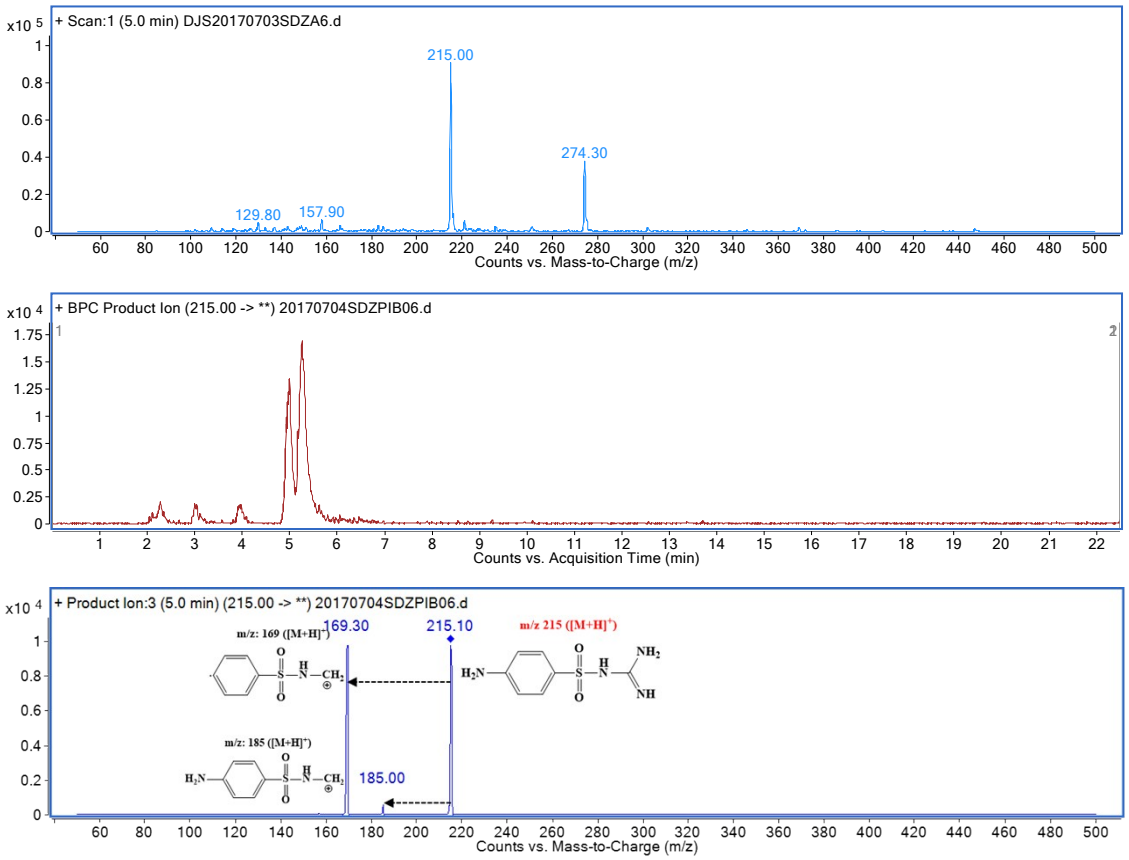


Fig. S18 Identification of P9 (m/z^+ 215)
Product ion 185 and 169

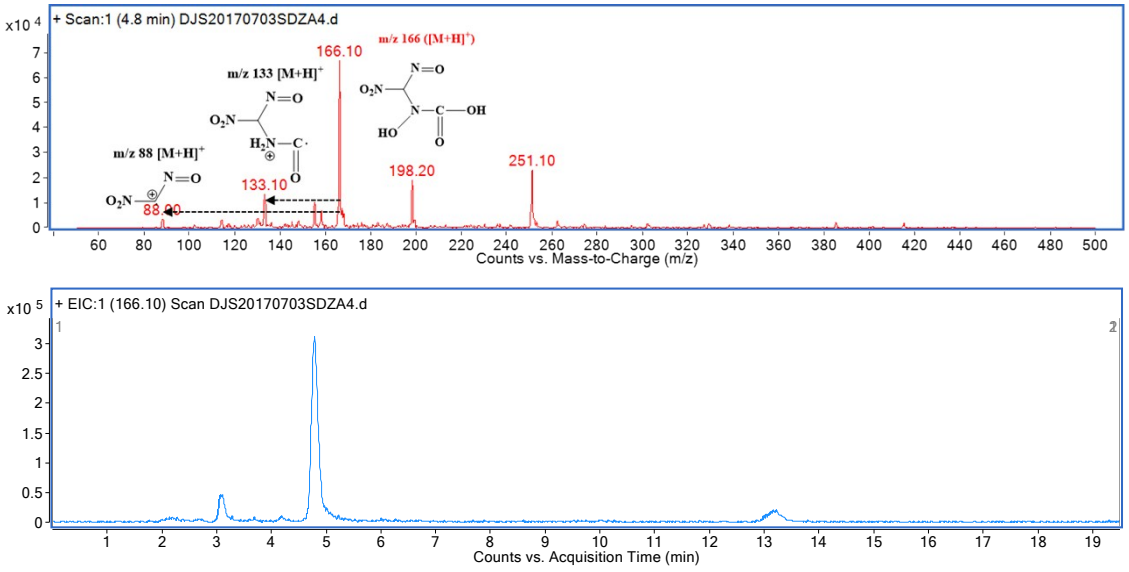


Fig. S19 Identification of P7 (m/z^+ 166)
Product ion 133 and 88

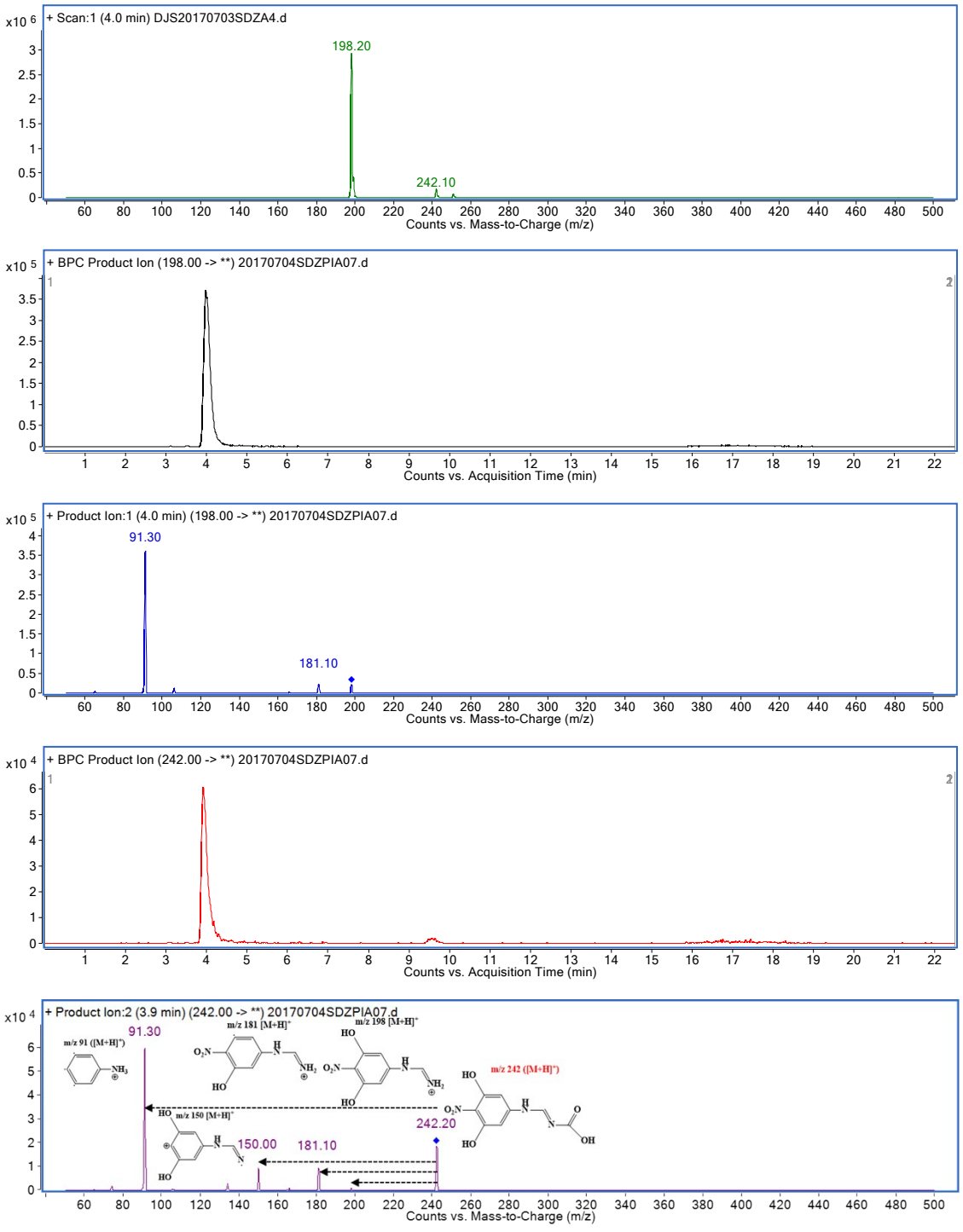


Fig. S20 Identification of P3 (m/z^+ 242)
Product ion 198, 181, 150, and 91

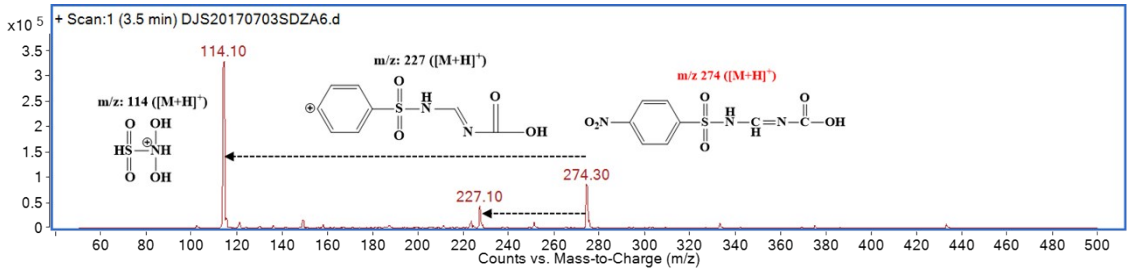


Fig. S21 Identification of P16 (m/z^+ 274)
Product ion 227 and 114

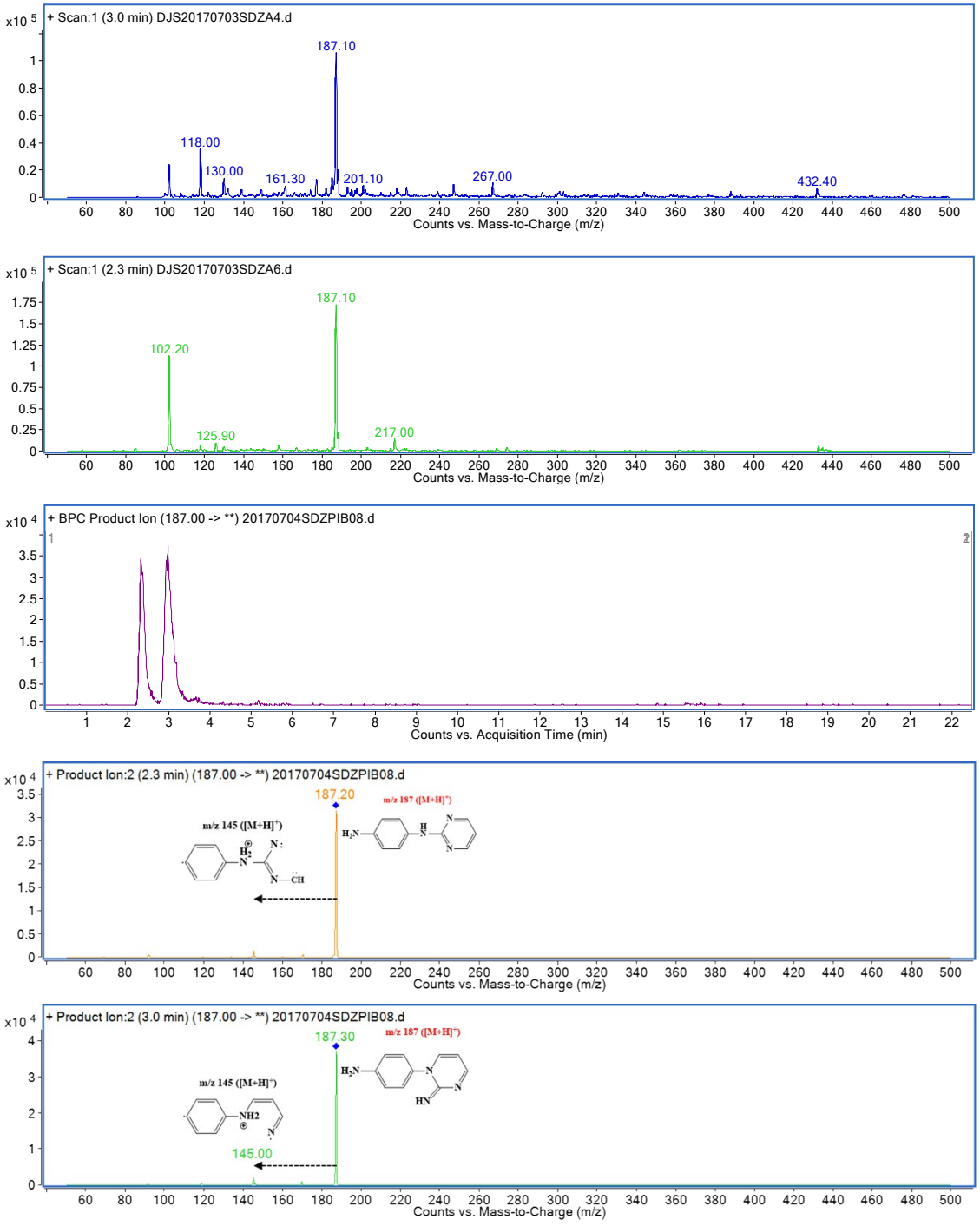


Fig. S22 Identification of P1 (m/z^+ 187)
Product ion 145

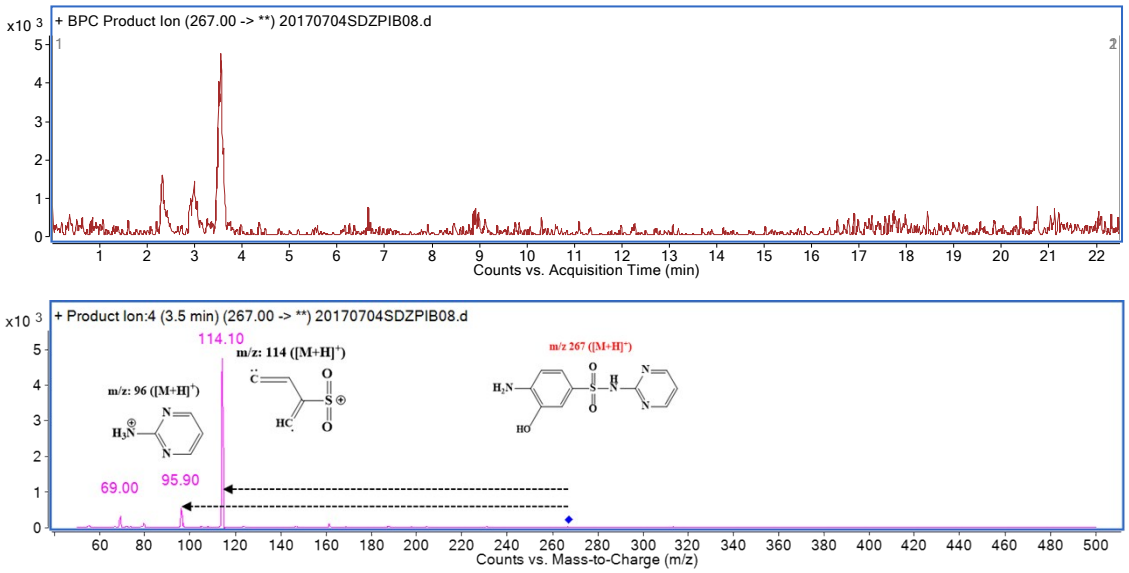


Fig. S23 Identification of P19 (m/z^+ 267)
Product ion 114 and 96

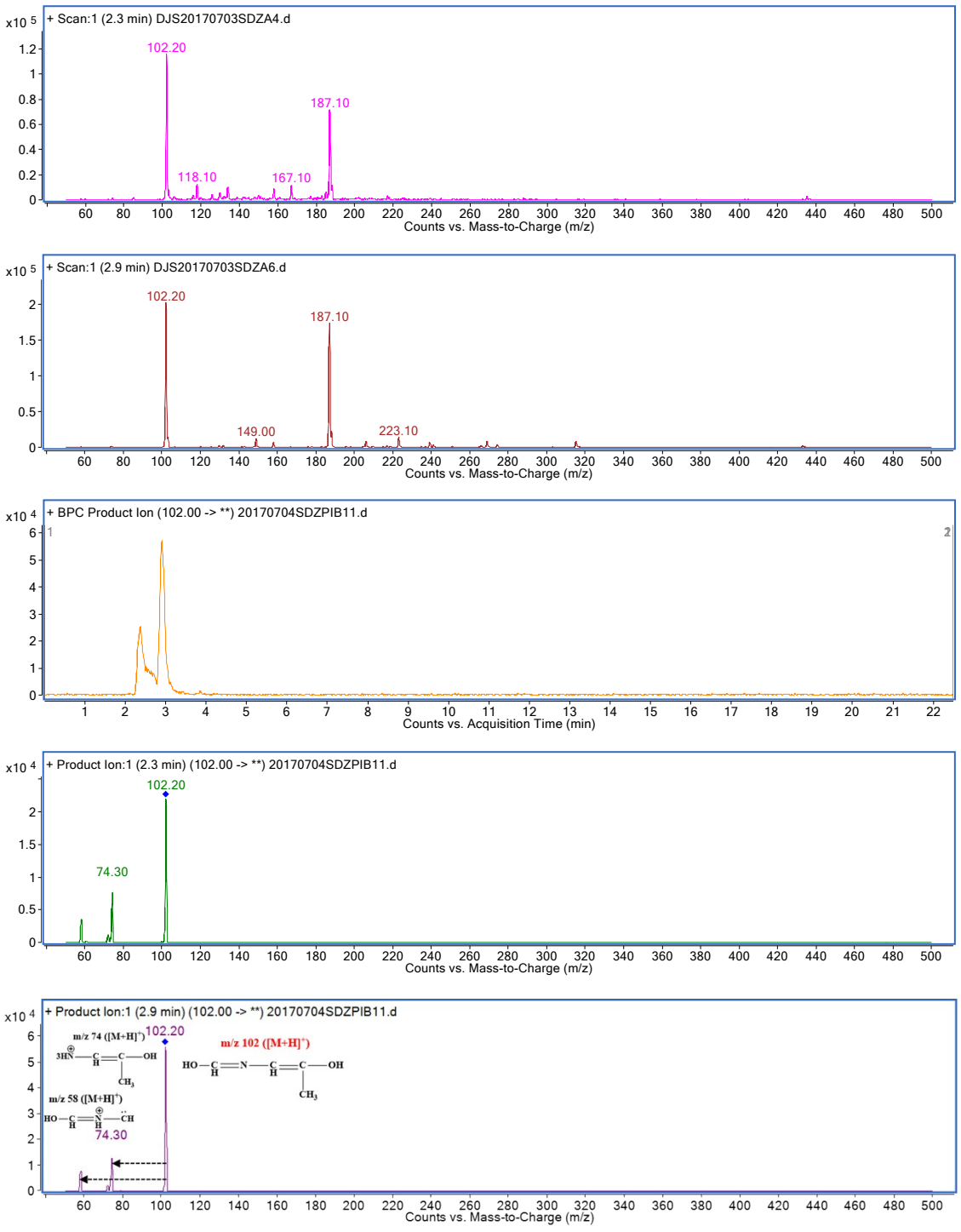


Fig. S24 Identification of P8 (m/z^+ 102)
Product ion 74 and 58

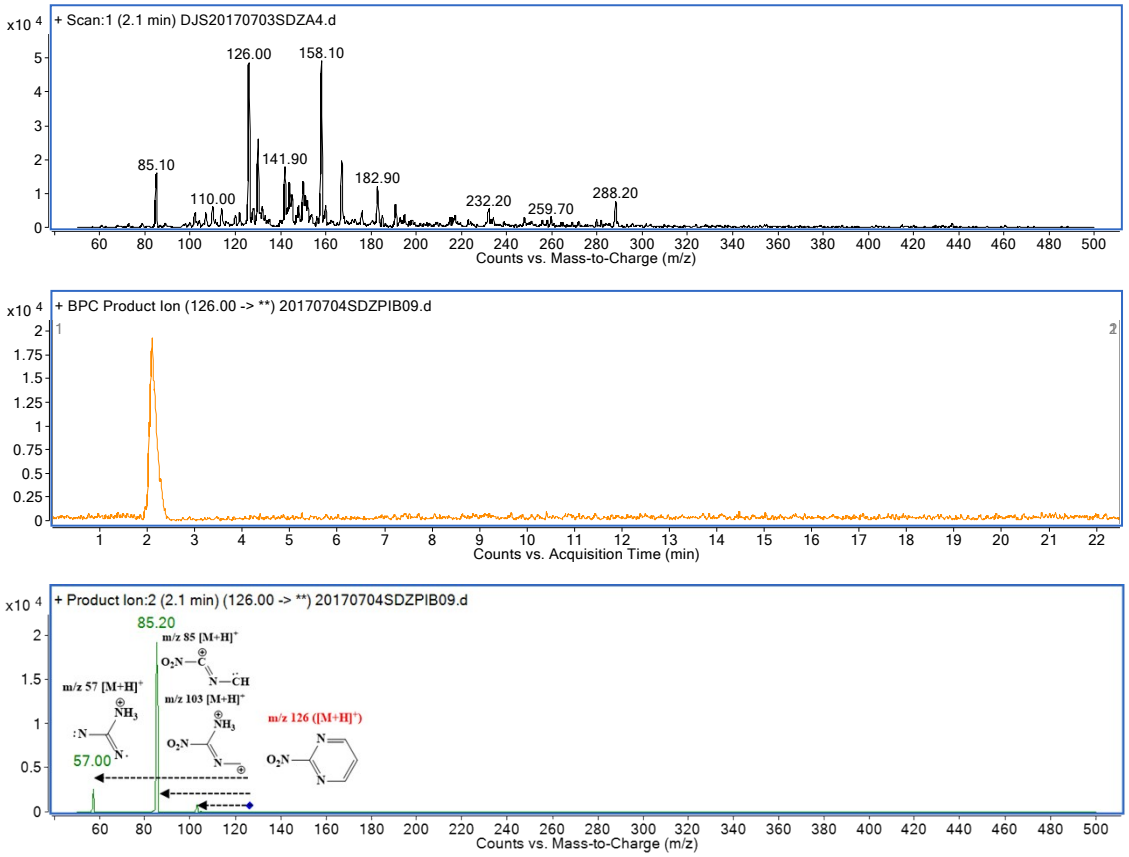


Fig. S25 Identification of P6 (m/z^+ 126)
Product ion 85 and 57

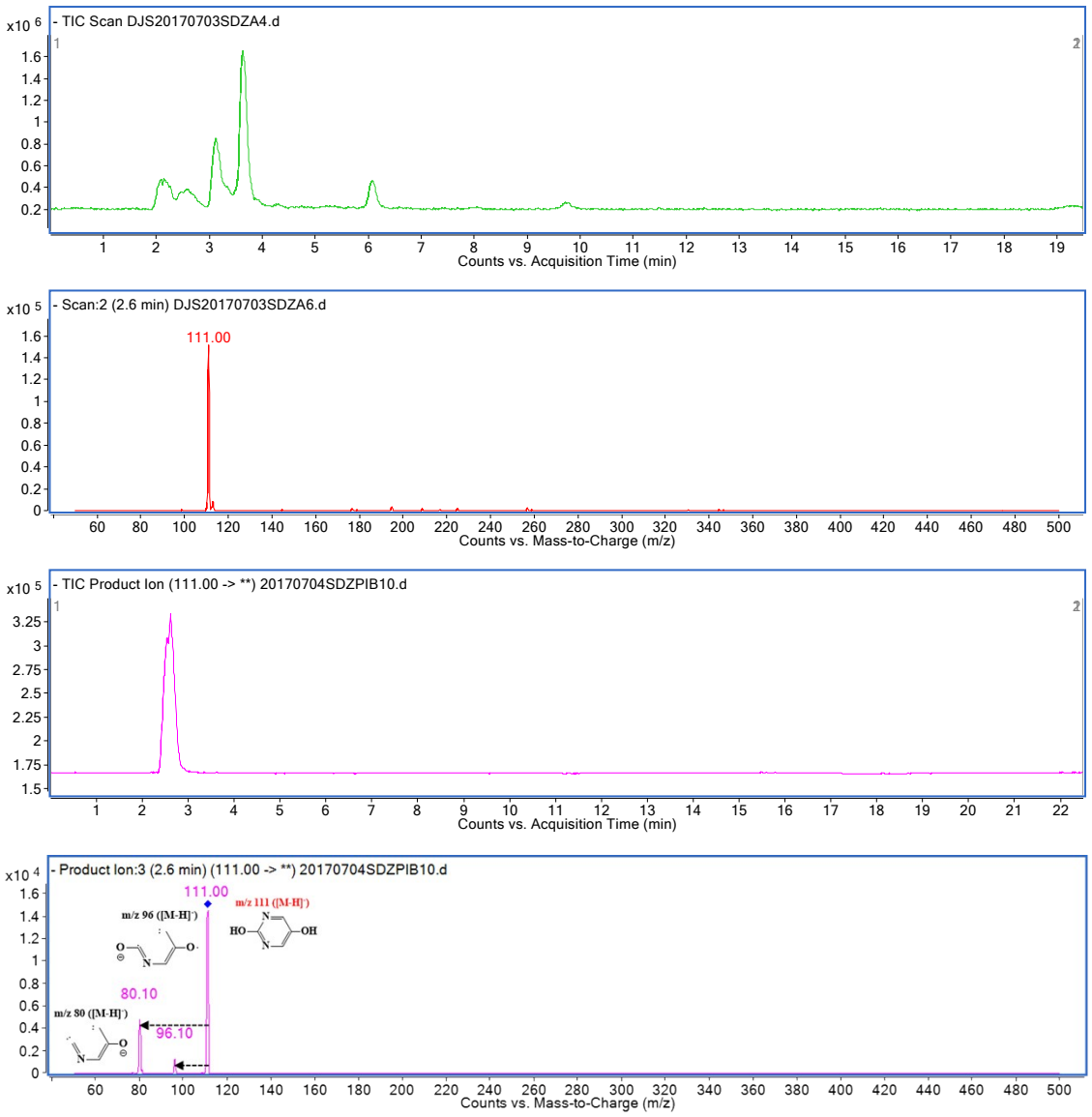


Fig. S26 Identification of P5 (m/z- 111)
Product ion 96 and 80

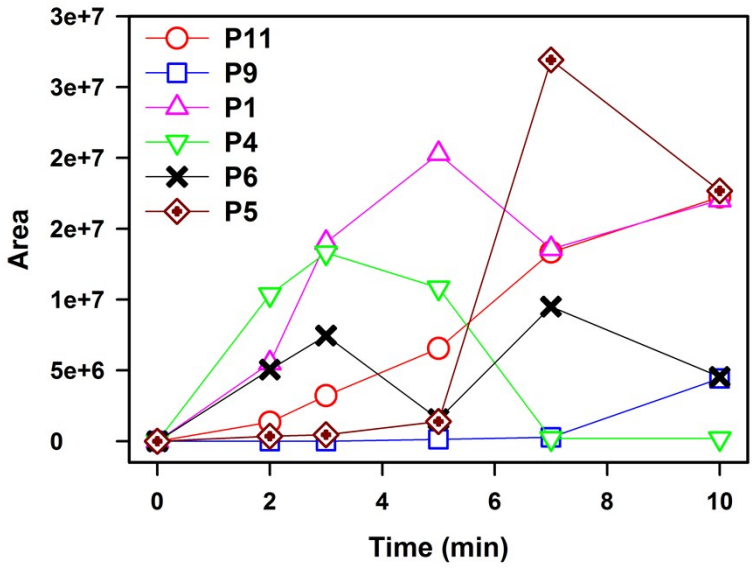


Fig. S27 Peak area for typical compounds of three pathways via $\bullet SO_4^-$ detected by UHPLC-MS/MS

Table S1 Summary of pseudo-first-order rate constants for SDZ removal by Fe^0/PS in the

presence of various background materials

Concentration of aquatic matrixes	k_{obs} (min^{-1})
Control (0 mM)	0.3969
Sulfate (1 mM)	0.2773
Sulfate (5 mM)	0.2348
Sulfate (10 mM)	0.2768
Sulfate (50 mM)	0.2156
Chloride (1 mM)	0.3378
Chloride (5 mM)	0.3388
Chloride (10 mM)	0.3338
Chloride (50 mM)	0.3522
Nitrate (1 mM)	0.3117
Nitrate (5 mM)	0.2743
Nitrate (10 mM)	0.233
Nitrate (50 mM)	0.1359
Perchlorate (1 mM)	0.3413
Perchlorate (5 mM)	0.3164
Perchlorate (10 mM)	0.3128
Perchlorate (50 mM)	0.3186
Humic acid (1 mg/L as TOC)	0.0681
Humic acid (3 mg/L as TOC)	0.0418
Humic acid (5 mg/L as TOC)	0.0254
Bicarbonate (0.5 mM)	0.1862
Bicarbonate (1 mM)	0.1221
Bicarbonate (2 mM)	0.0836
Bicarbonate (5 mM)	0.0418