

Supporting Information

Structural elucidation of sulfaquinoxaline metabolism products and their occurrence in biological samples using high-resolution Orbitrap mass spectrometry

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Abstract

This Supporting Information section come experimental data obtained with mass spectrometry techniques used to support the proposed molecular structure of SQX metabolites and to ensure the presence of SQX and their metabolism products in real samples.

Figure S-1. Fragmentation pattern for SQX-OH.

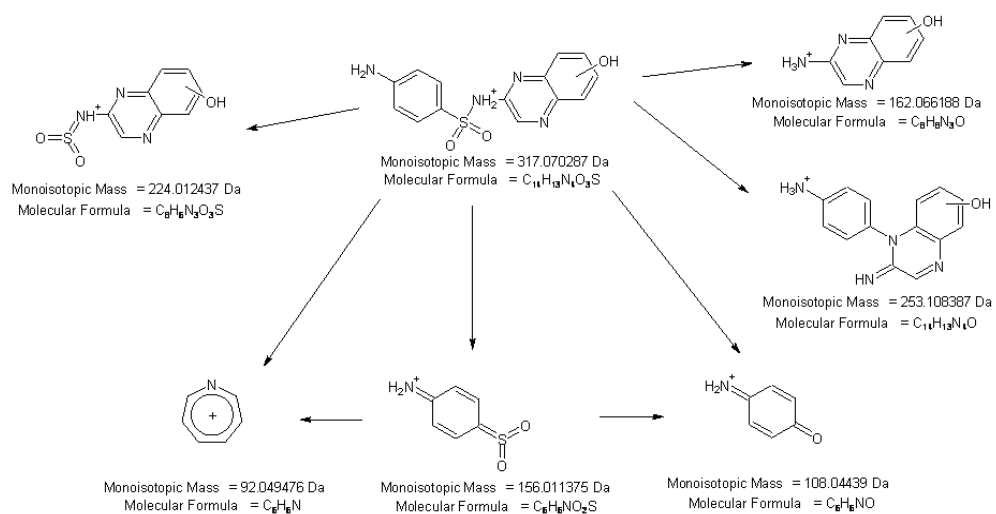


Figure S-2. Fragmentation pattern for N⁴-acetyl-SQX.

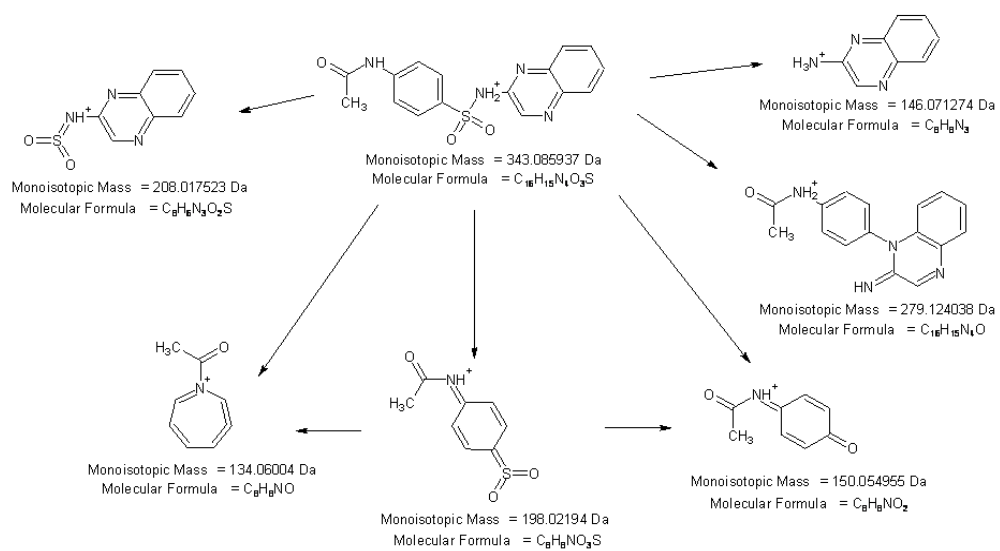


Figure S-3. Fragmentation pattern for N⁴-acetyl-SQX-OH.

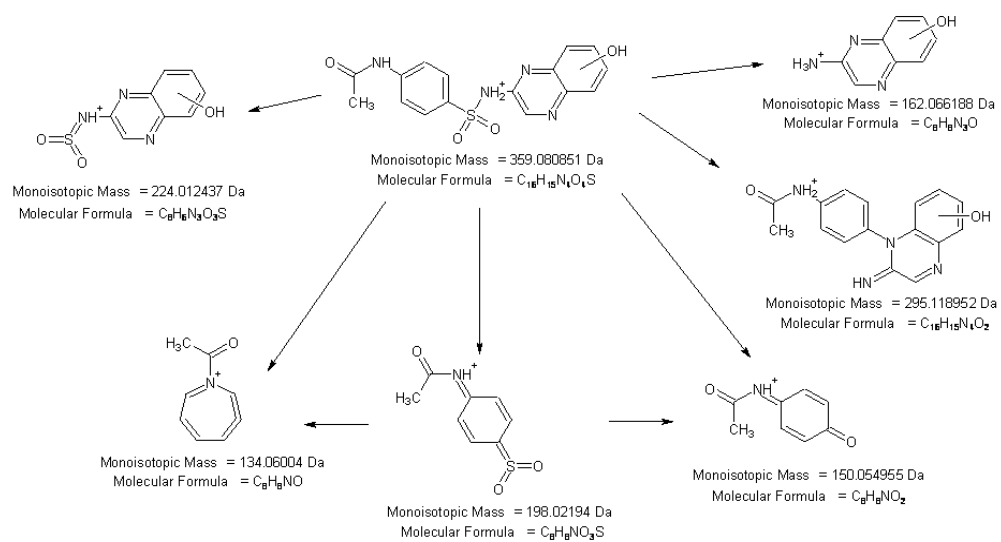


Figure S-4. Fragmentation pattern for N⁴-formyl-SQX.

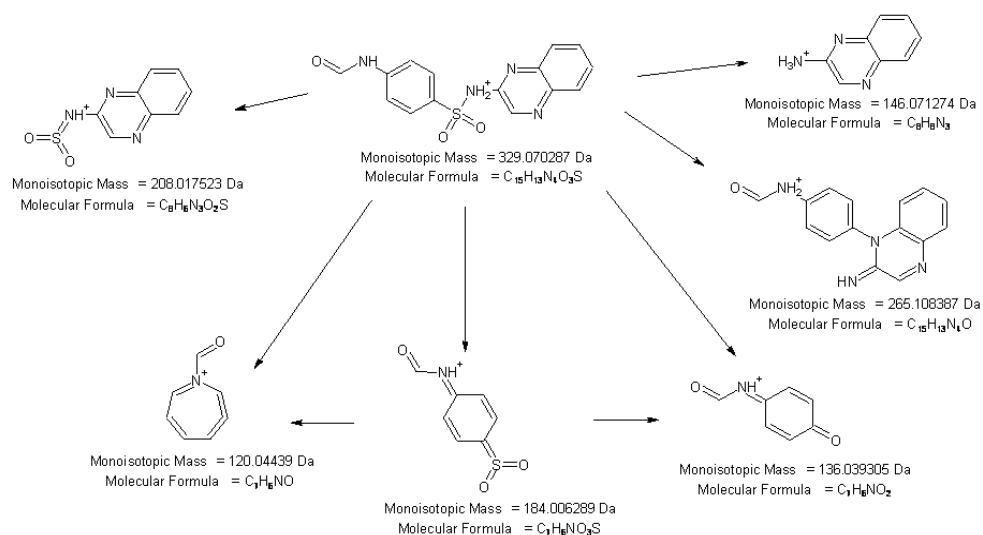


Figure S-5. Fragmentation pattern for N⁴-formyl-SQX-OH.

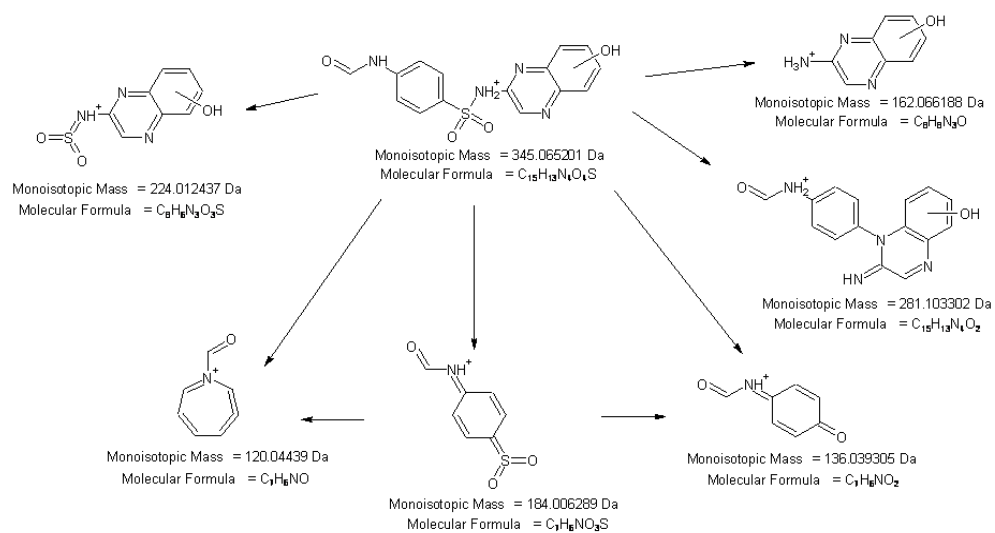
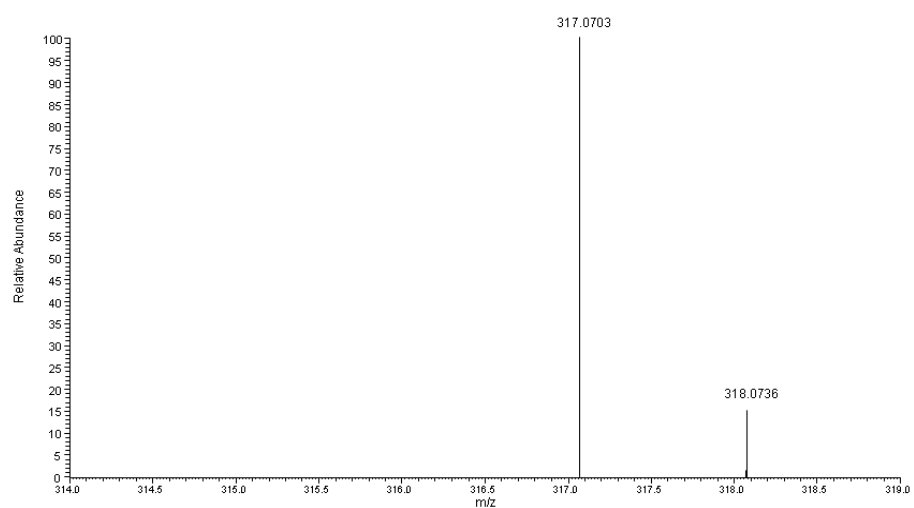


Figure S-6. SQX-OH isotope pattern simulation (A) and experimental isotope pattern (B) ($\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_3\text{S}$)

(A)



(B)

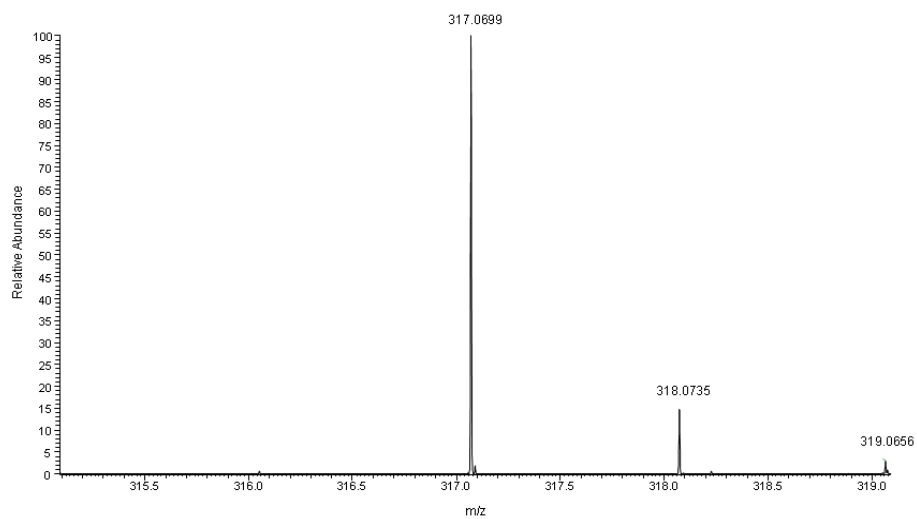


Figure S-7. Substructure-specific fragment for SQX-OH formed at in-source CID fragmentation: experimental isotope pattern ($\text{C}_8\text{H}_8\text{N}_3\text{O}$).

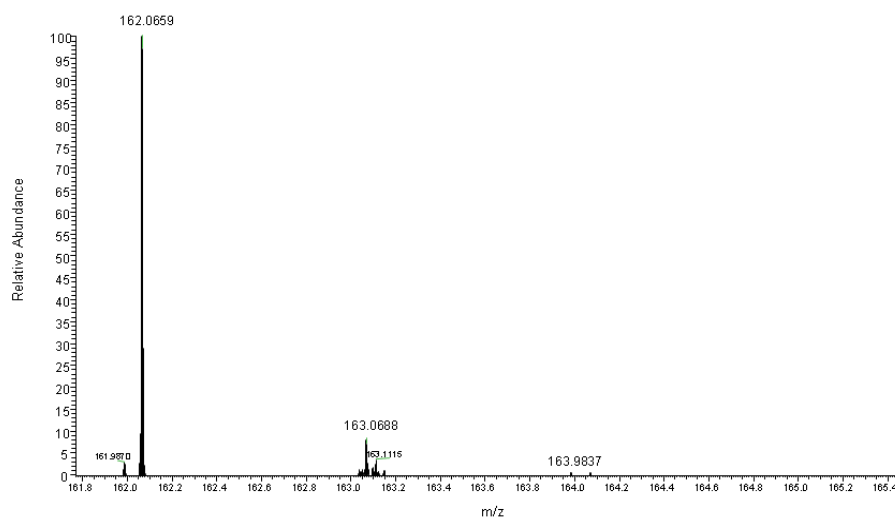


Figure S-8. MS/MS spectrum of SQX in poultry liver

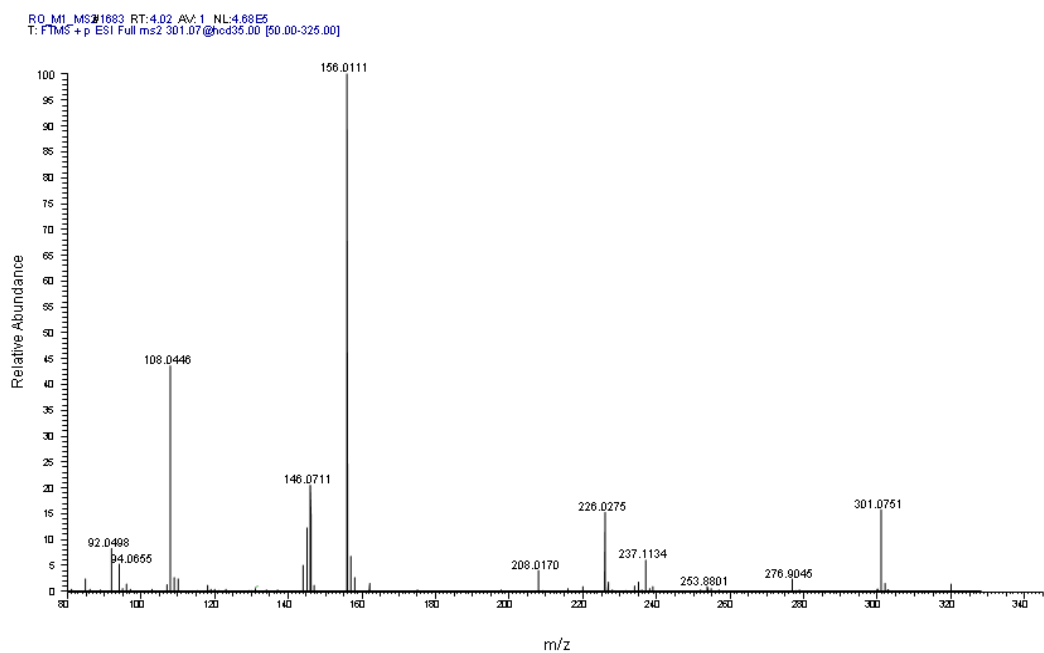


Figure S-9. MS/MS spectrum of SQX-OH in ovine liver

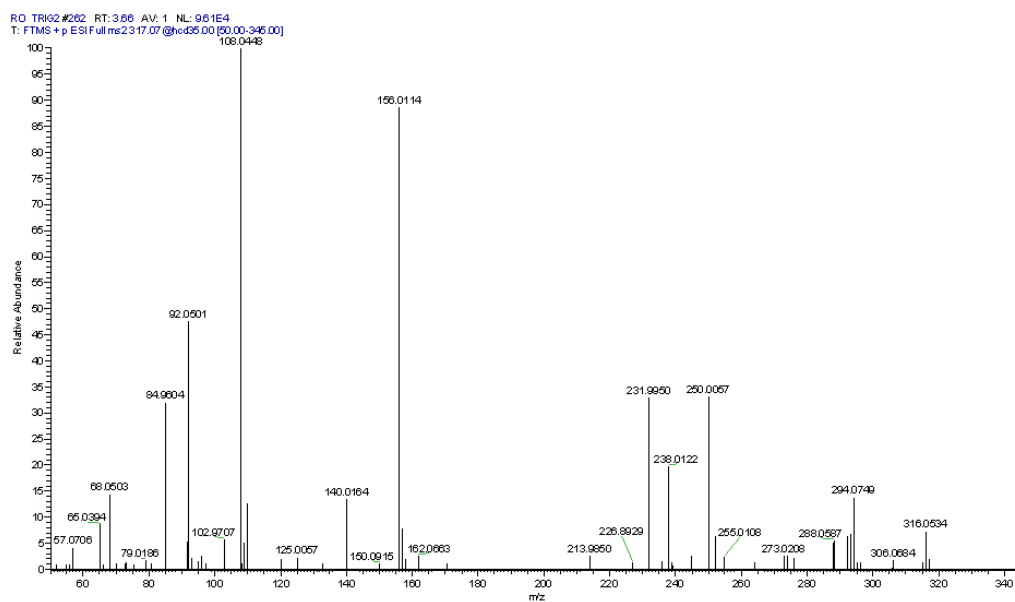


Figure S-10. MS/MS spectrum of N⁴-acetyl-SQX-OH in poultry liver

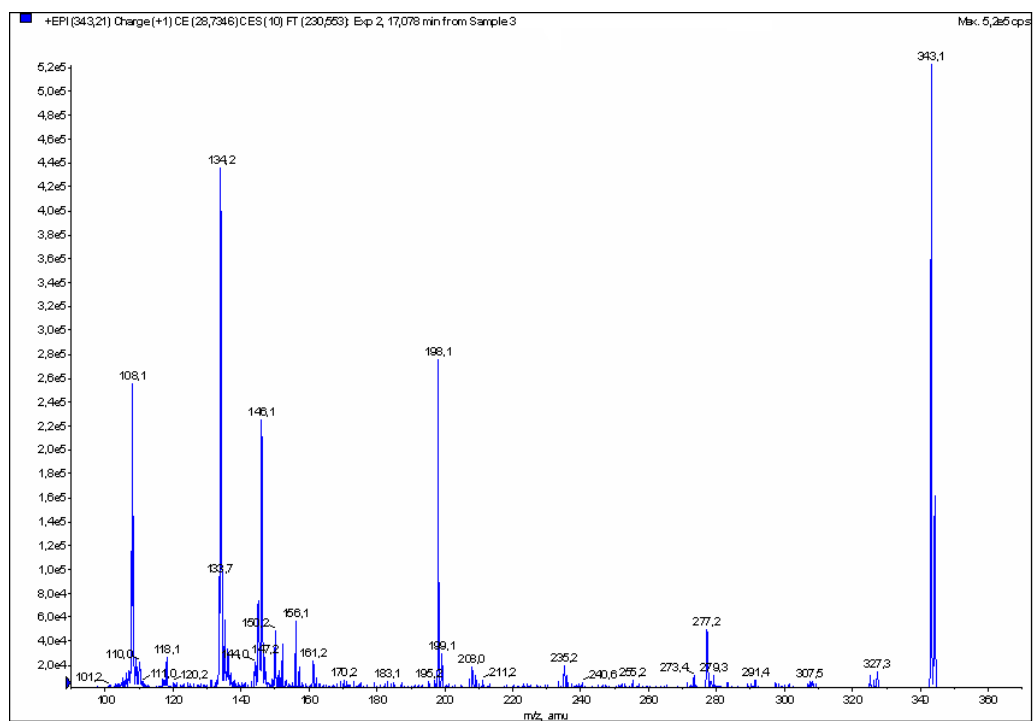


Figure S-11. Total ion chromatogram of fish sample and MS/MS spectrum of SQX.

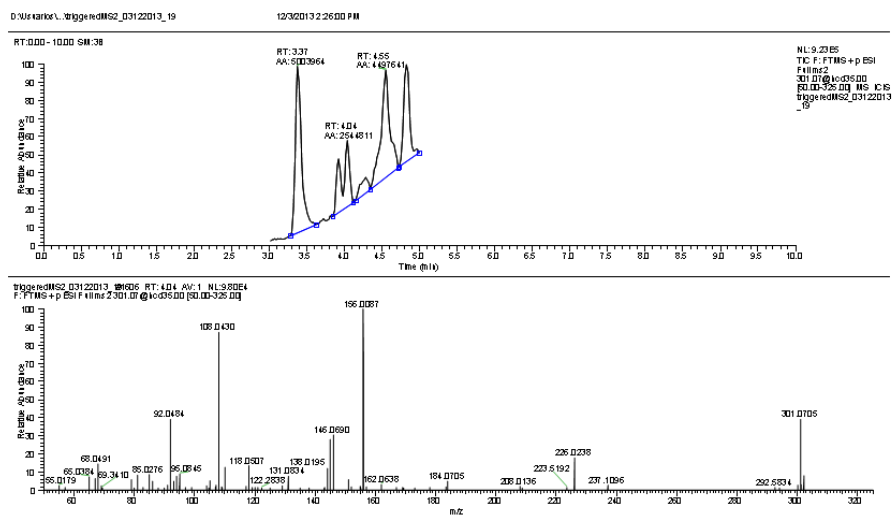


Figure S-12. Total ion chromatogram of poultry liver sample and MS/MS spectrum of presumable N⁴-formyl-SQX.

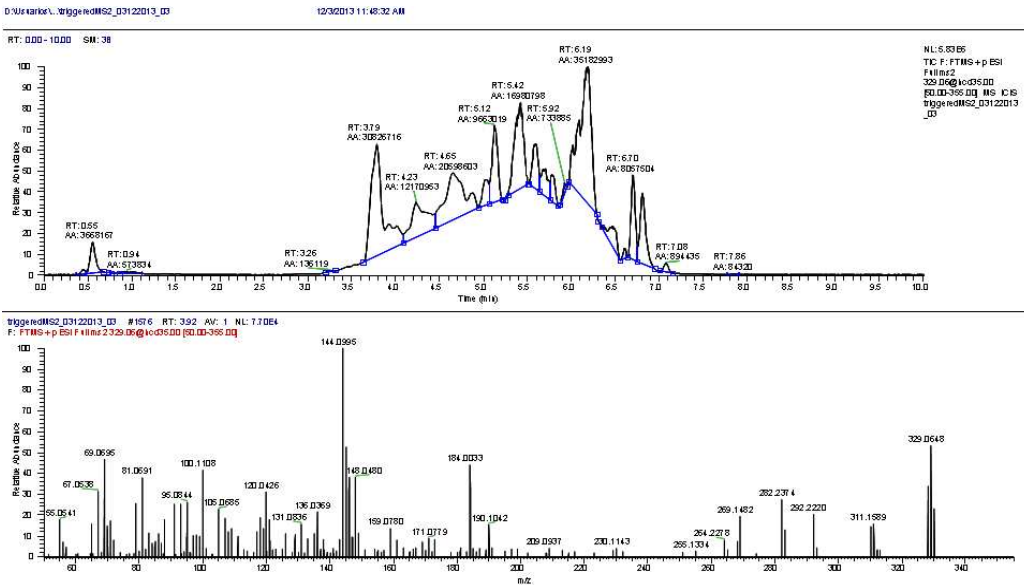


Figure S-13. Total ion chromatogram of poultry liver sample and MS/MS spectrum of N⁴-acetyl-SQX.

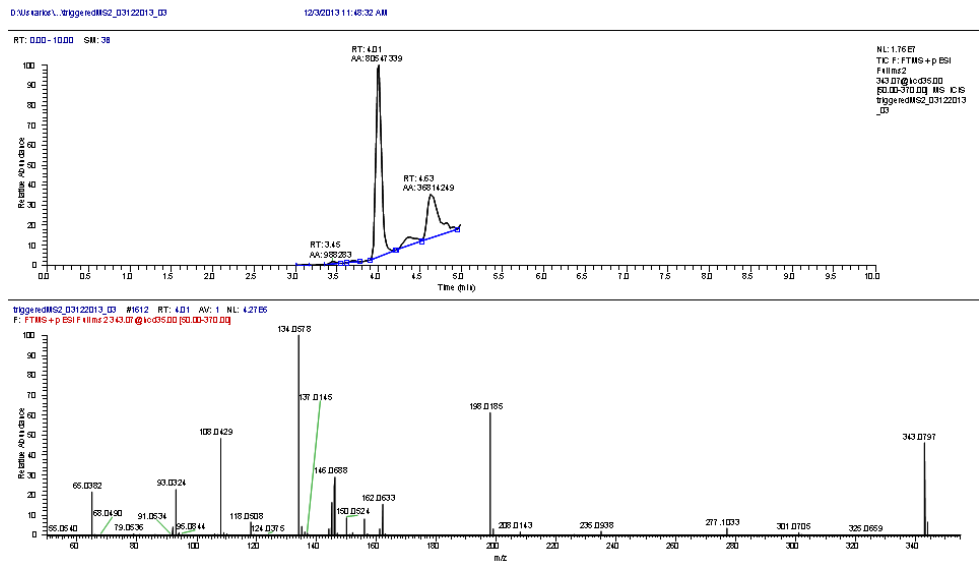


Figure S-14. Total ion chromatogram of poultry liver sample and MS/MS spectrum of presumable N⁴-formyl-SQX-OH.

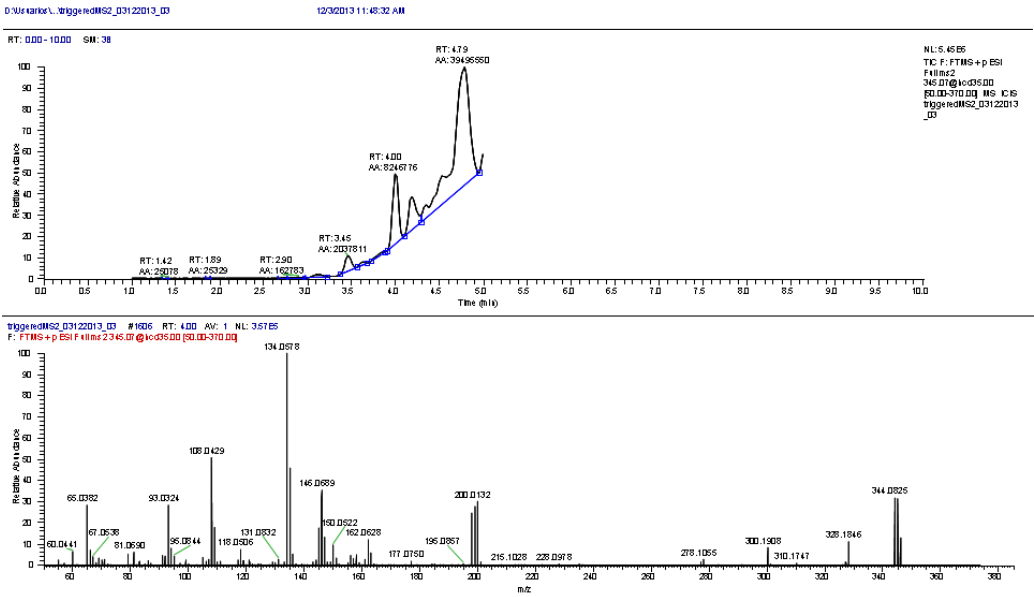


Figure S-15. Mass spectrum in negative ionization of photodegradation product
m/z 160.0516.

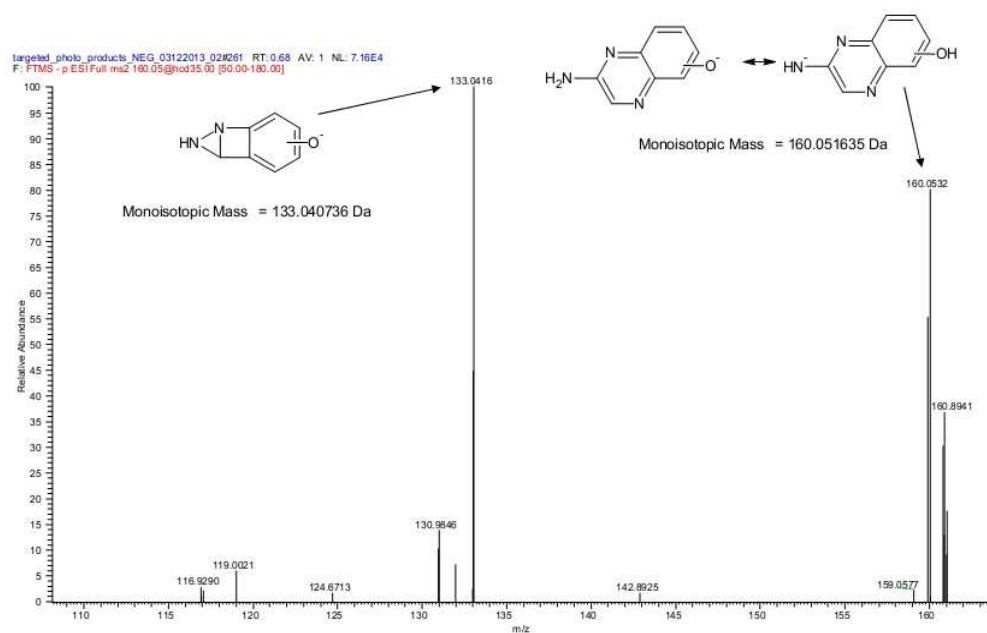


Figure S-16. SQX-OH MS/MS spectrum obtained in HPLC-LIT-MS/MS system.

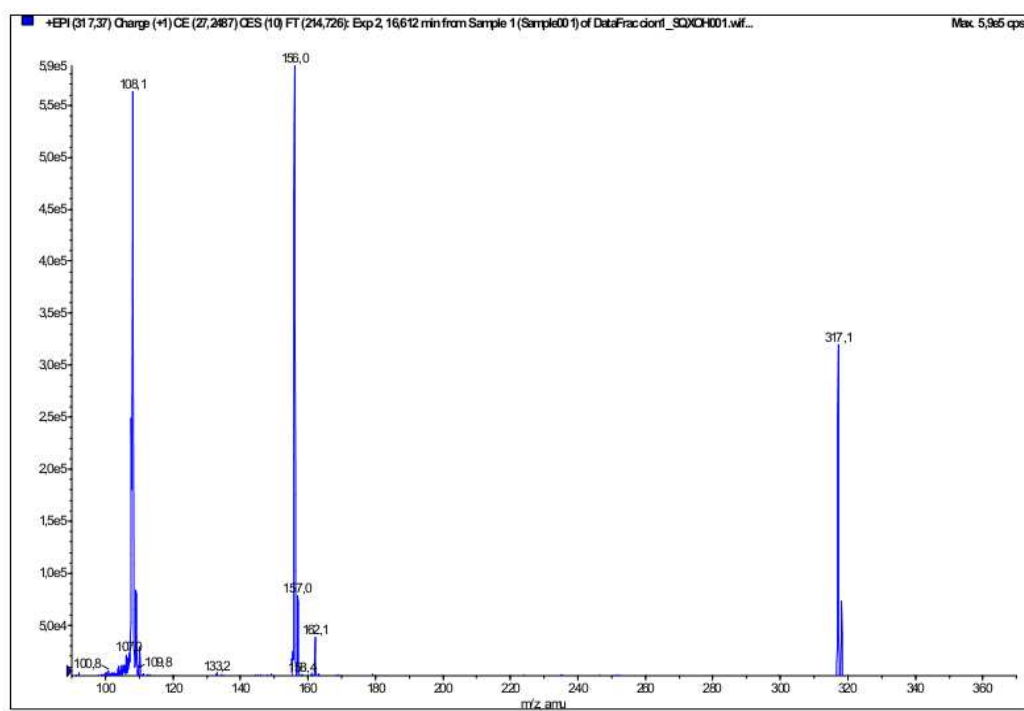


Figure S-17. SQX-OH MS spectrum obtained in HPLC-LIT-MS/MS system.

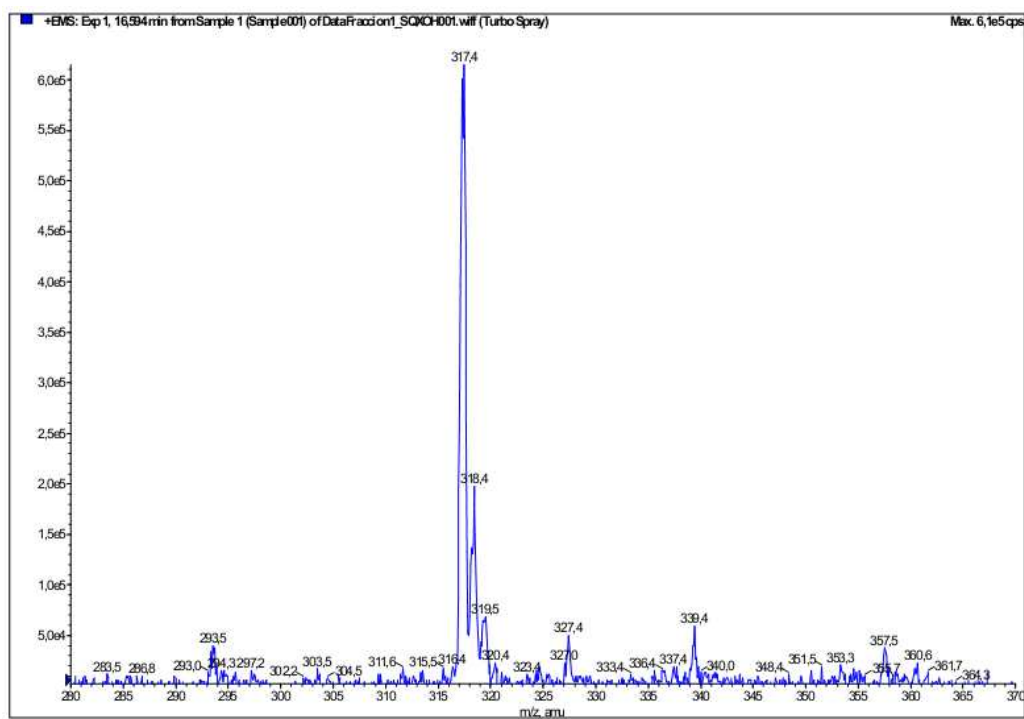


Figure S-18. N⁴-acetyl-SQX MS/MS spectrum obtained in HPLC-LIT-MS/MS system.

