

SI-7: Concentration pattern and MS/MS spectra of identified transformation products

Azoxystrobin – Azoxystrobin Acid

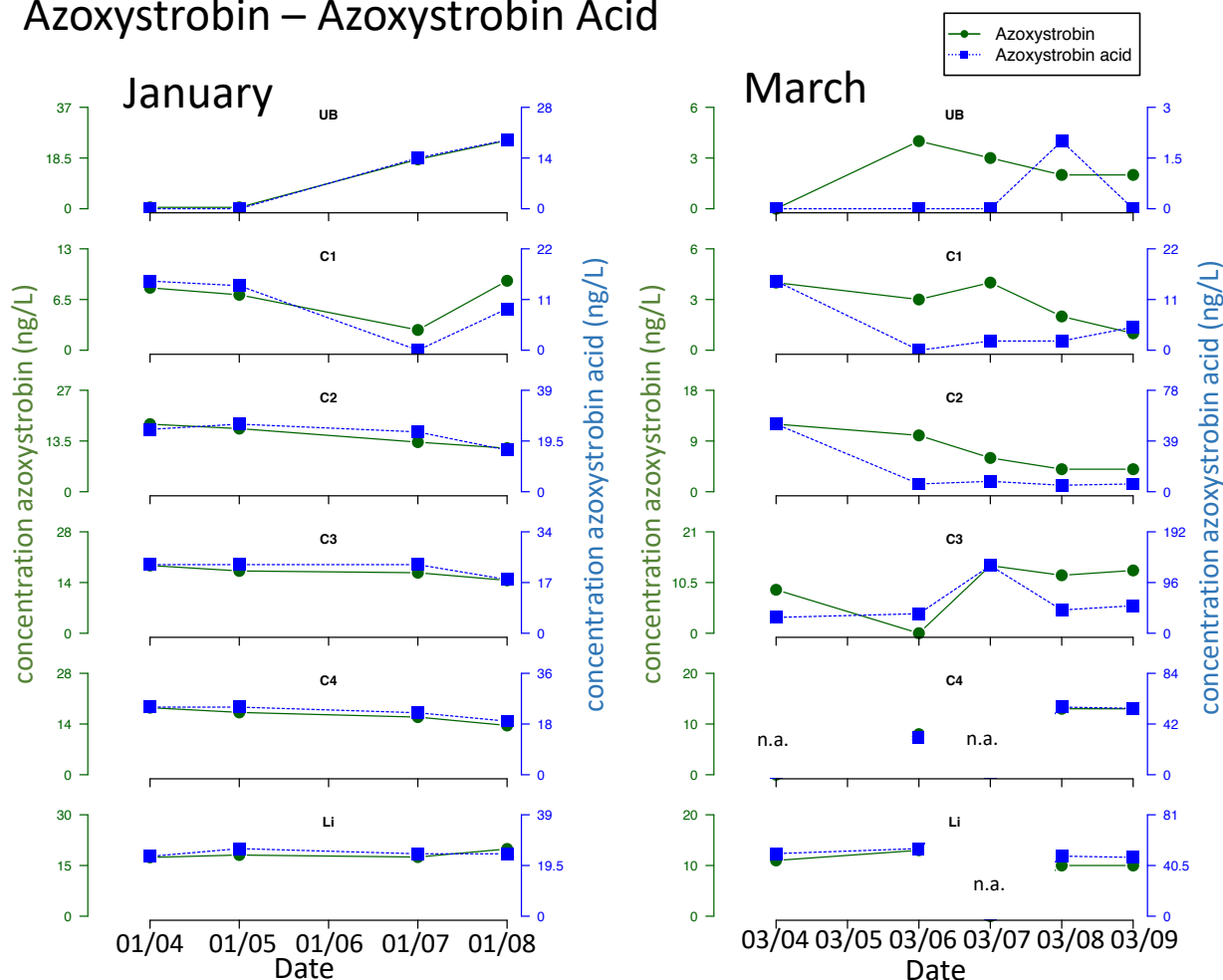


Figure SI-7.1a. Concentration profile over the six sampling locations during the two rain events of azoxystrobin and its transformation product azoxystrobin acid. UB: Ulatis Creek, C1-C4: Cache Slough locations 1-4, LI: Liberty Island. n.a.: no sample available

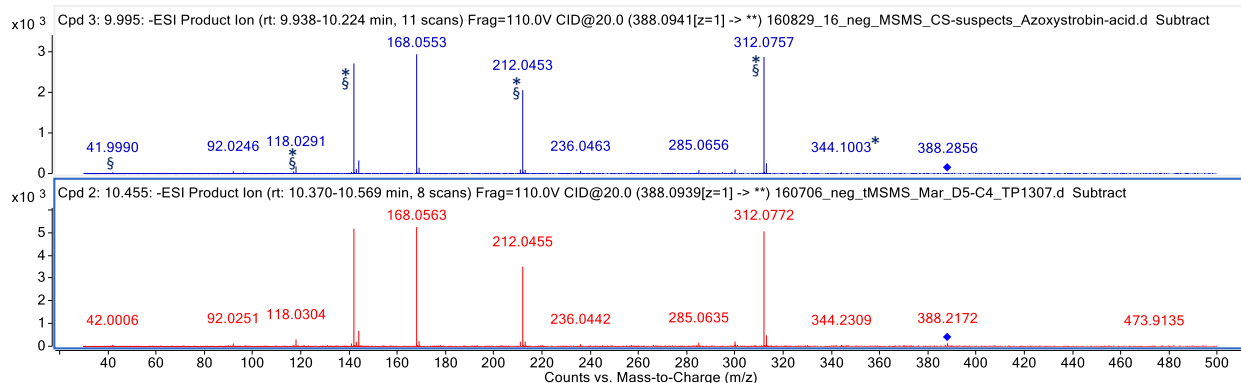


Figure SI-7.1b. MS/MS spectra of azoxystrobin acid in ESI- at collision energy (CE) 20. Top: in reference standard, bottom: in environmental sample. Retention time: 10 min. § predicted by Agilent MSC (score 71.1); * predicted by CFM-ID.

Trifloxystrobin – Trifloxystrobin Acid

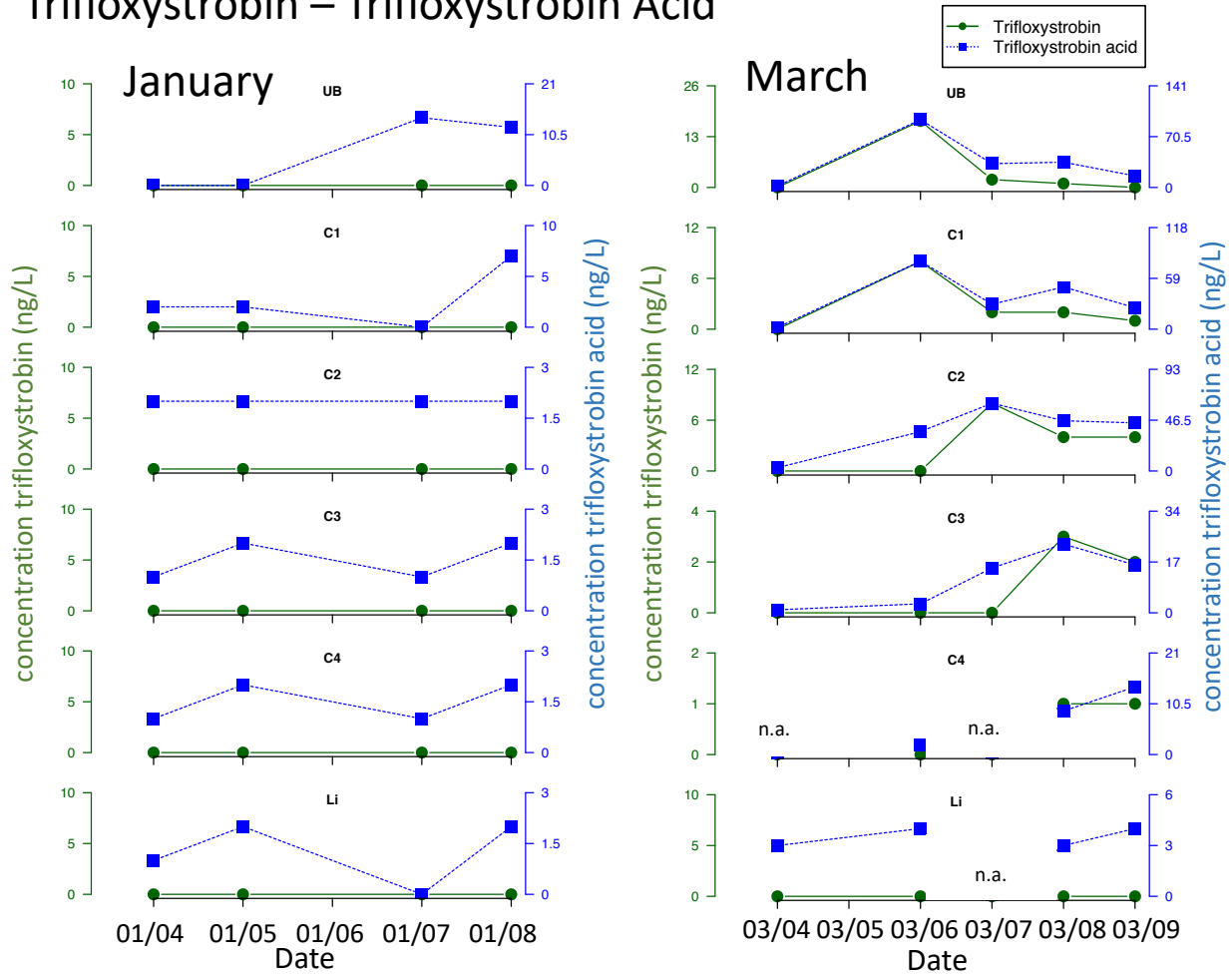


Figure SI-7.2a. Concentration profile over the six sampling locations during the two rain events of trifloxystrobin and its transformation product trifloxystrobin acid. UB: Ulatis Creek, C1-C4: Cache Slough locations 1-4, Li: Liberty Island. n.a.: no sample available

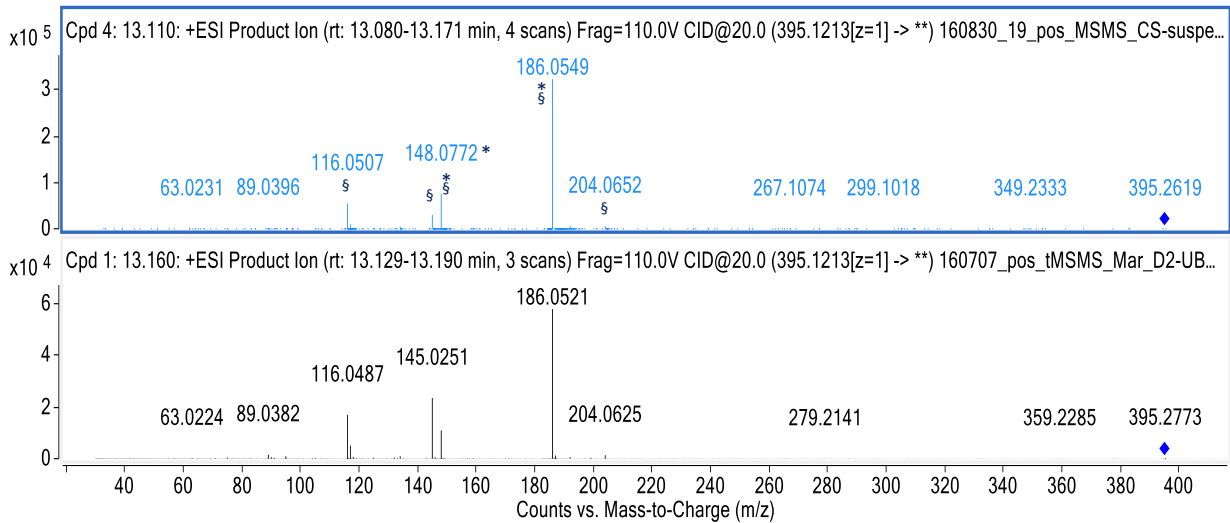


Figure SI-7.2b. MS/MS spectra of trifloxystrobin acid in ESI+ at collision energy (CE) 20. Top: in reference standard, bottom: in environmental sample. Retention time: 13.1 min.

§ predicted by Agilent MSC (score 84.2); * predicted by CFM-ID.

Norflurazon– Norflurazon-desmethyl

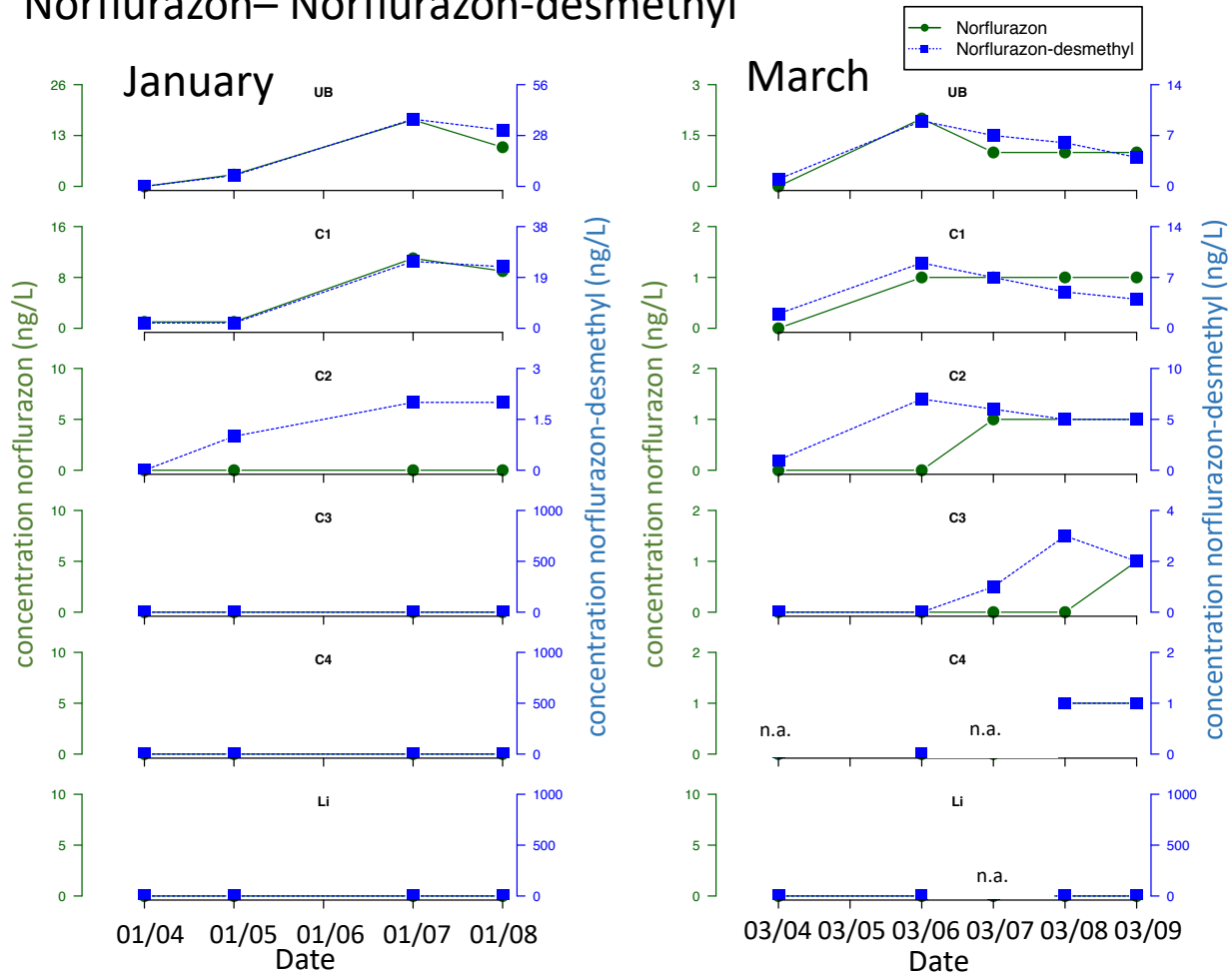


Figure SI-7.3a. Concentration profile over the six sampling locations during the two rain events of norflurazon and its transformation product norflurazon-desmethyl. UB: Ulatis Creek, C1-C4: Cache Slough locations 1-4, LI: Liberty Island. n.a.: no sample available

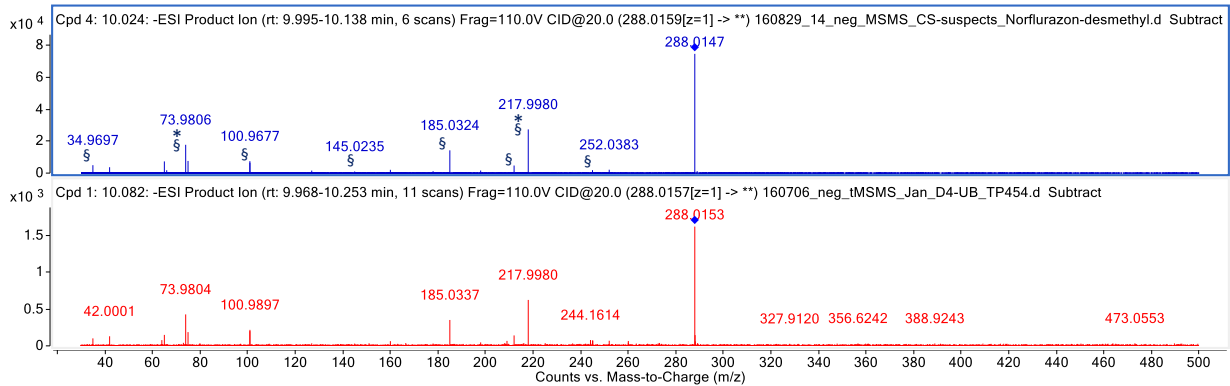


Figure SI-7.3b. MS/MS spectra of norflurazon-desmethyl in ESI- at collision energy (CE) 20. Top: in reference standard, bottom: in environmental sample. Retention time: 10 min. § predicted by Agilent MSC (score 72.1); * predicted by CFM-ID.

2,4-D – 2,4-dichlorophenol

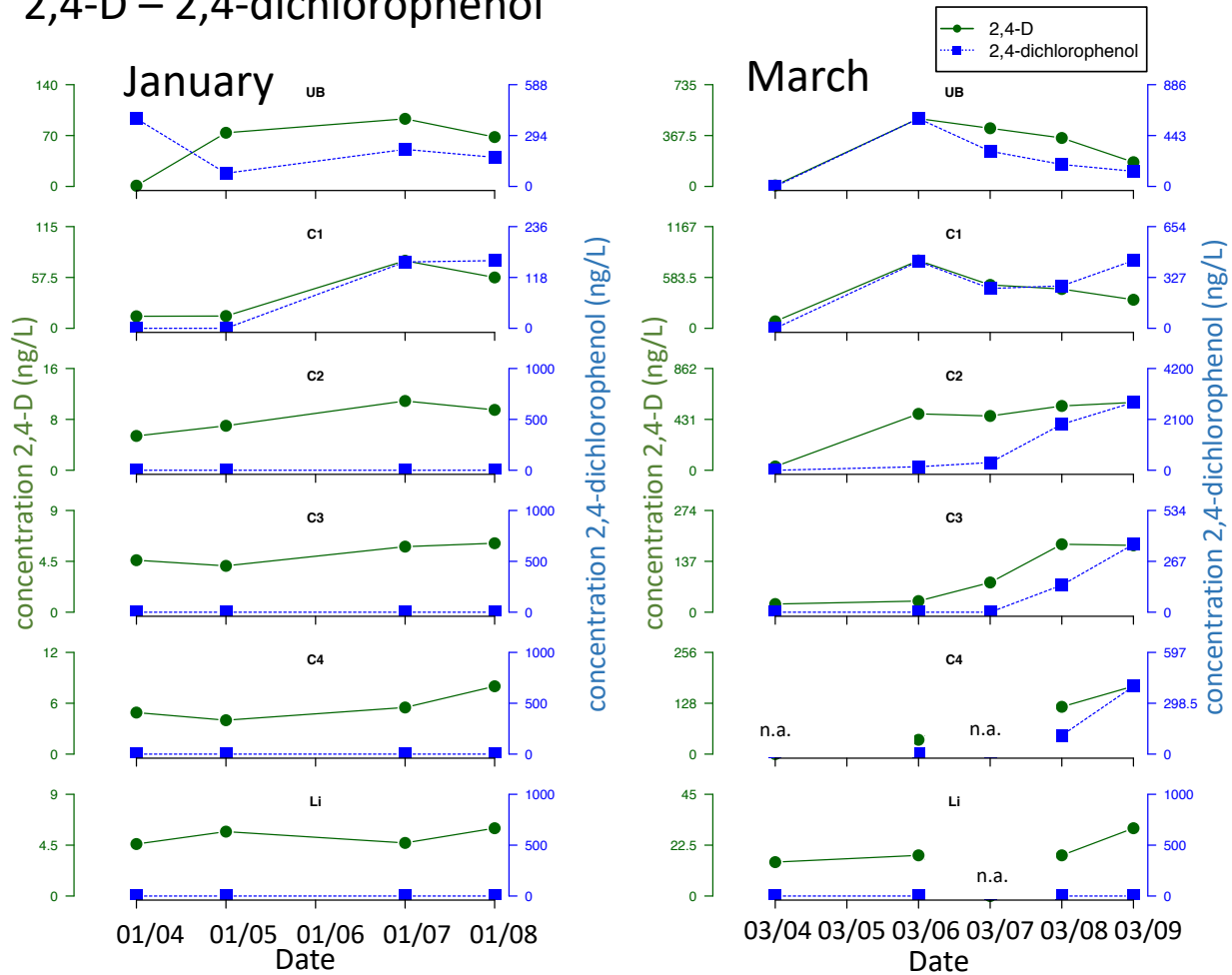


Figure SI-7.4a. Concentration profile over the six sampling locations during the two rain events of 2,4-D and its transformation product 2,4-dichlorophenol. UB: Ulatis Creek, C1-C4: Cache Slough locations 1-4, Li: Liberty Island. n.a.: no sample available

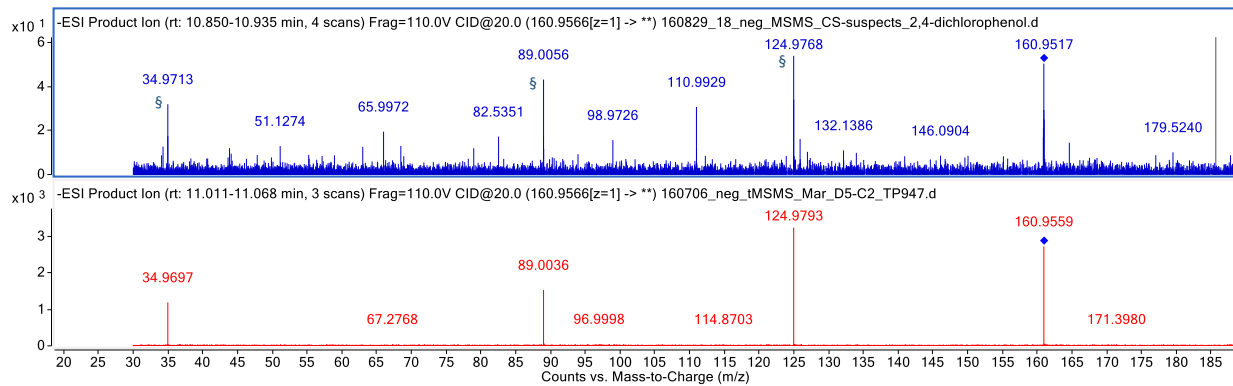


Figure SI-7.4b. MS/MS spectra of 2,4-dichlorophenol in ESI- at collision energy (CE) 20. Top: in reference standard, bottom: in environmental sample. Retention time: 11 min.

§ predicted by Agilent MSC (score 71.6); CFM-ID did not predict the main fragments.