

Results : Helsinki		impact ESI-QTOF		
Case	Findings in urine by UPLC-QTOF*	detected (diagnostic ion concept)	additional findings	false positives
934	tramadol O-desmethyltramadol caffeine	✓ ✓ ✓		none
936	methadone EDDP caffeine	✓ ✓ ✓	cotinine	none
943	zopiclone paracetamol caffeine	✓ ✓ ✓		none
945	cocaine benzoylecgonine ecgonine methyl ester cocaethylen citalopram norcitalopram zopiclone temazepam cotinine	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	alprazolam caffeine	none
946	codeine morphine tramadol O-desmethyltramadol paracetamol	✓ ✓ ✓ ✓ ✓		none
954	pregabalin carboxy-THC EDDP quetiapine hydroxyquetiapine paracetamol temazepam oxazepam cotinine	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	alprazolam caffeine	none

Results : Helsinki		impact ESI-QTOF		
Case	Findings in urine by UPLC-QTOF*	detected (diagnostic ion concept)	additional findings	false positives
956	pregabalin citalopram norcitalopram mirtazapin diazepam temazepam oxazepam	✓ ✓ ✓ ✓ ✓ ✓ ✓	caffeine cotinine paracetamol	none
962	citalopram norcitalopram codeine morphine paracetamol lamotrigine alprazolam	✓ ✓ ✓ ✓ ✓ ✓ ✓	caffeine	none
970	fenatnyl norfentanyl paracetamol	✓ ✓ ✓		
974	zopiclone diazepam nordiazepam temazepam oxazepam	✓ ✓ ✓ ✓ ✓	cotinine	none
H382	fentanyl oxycodone mirtazapine cotinine midazolam nordiazepam oxazepam caffeine	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	norfentanyl	none

*) result list reduced to compounds of this work

xxx shown as example chromatogram

Sample preparation: for samples analysed on impact:

Urine samples where extracted with mixed mode SPE, see e.g. Anal Bioanal Chem (18 August 2013) DOI 10.1007/s00216-013-7272-8. Reconstituted samples were diluted 1:10 before analysis on impact.

Fig. 7/01

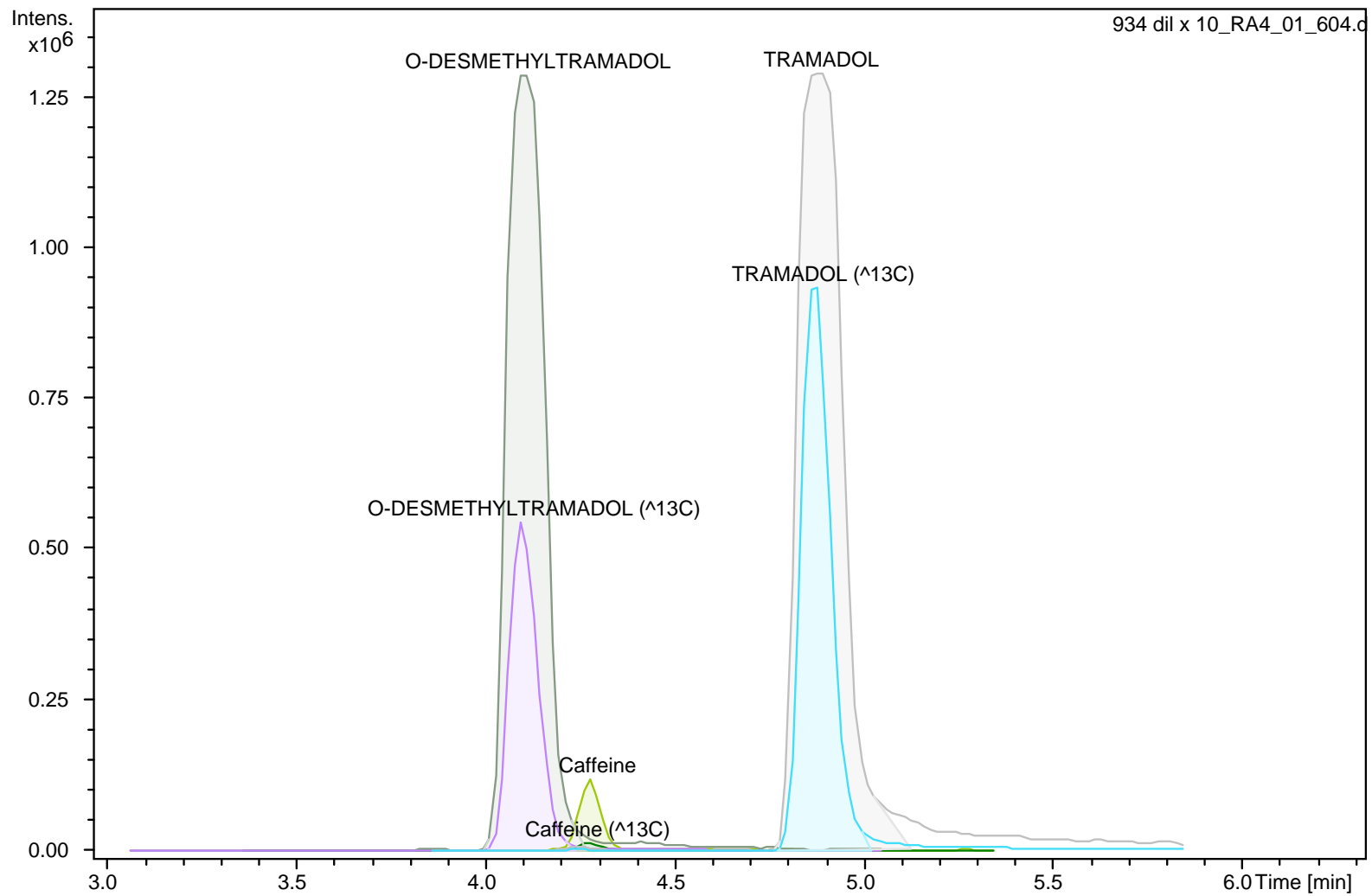
Results : Freiburg		impact ESI-QTOF			
Sample	Compound	Result type	detected (diagnostic ion concept)	additional findings	false positives
T1106562	Serum, roadside testing				
	Amphetamin 147 ng/ml	GC-MS	✓	cotinine	none
	Cocain 1,1 ng/ml	GC-MS	✓	caffeine	
	Benzoyllecgonine 148 ng/ml	GC-MS	✓		
	Ecgoninemethylester 4,0 ng/ml	GC-MS	✓		
T1200778	Serum roadside testing				
	Cocain 2,0 ng/ml	GC-MS	✓	cocaethylen	none
	Benzoyllecgonine 482 ng/ml	GC-MS	✓	cotinine	
	Ecgoninemethylester 48 ng/ml	GC-MS	✓	caffeine	
	THC 3,1 ng/ml	GC-MS	(not in DB)		
	11-OH-THC 2,2 ng/ml	GC-MS	(not in DB)		
	THC-COOH 36 ng/ml	GC-MS	nd *)		
T1210160	Serum roadside testing**)				
	Quetiapin 110 ng/ml	LC-MS/MS	✓	cotinine	Tramadol
	Venlafaxin 100 ng/ml	LC-MS/MS	✓	caffeine	
	Desmethylvenlafaxin ca. 500 ng/ml	LC-MS/MS	✓	zopiclone	
T1210408	Serum roadside testing				
	Morphin 91 ng/ml	LC-MS/MS	✓	6-MAM	none
	Codein 17 ng/ml	LC-MS/MS	✓	cotinine	
	Diazepam 410 ng/ml	LC-MS/MS	✓	caffeine	
	Nordazepam >1000 ng/ml	LC-MS/MS	✓	Paracetamol	
	Temazepam 220 ng/ml	LC-MS/MS	✓		
	Oxazepam 280 ng/ml	LC-MS/MS	✓		
	Flunitrazepam 30 ng/ml	LC-MS/MS	✓		
	7-Aminoflunitrazepam 32 ng/ml	LC-MS/MS	✓		
GS 250 Se	Post mortem serum				
	THC / Metabolites	LC-MS/MS	nd *)	Amphetamin	
	Benzoyllecgonine	LC-MS/MS	✓	cotinine	
	Venlafaxin	LC-MS/MS	✓	Ecgoninemethylester	Tramadol
	Desmethylvenlafaxin	LC-MS/MS	✓		
	Nicotin	LC-MS/MS	(not in DB)		
	Caffeine	LC-MS/MS	✓		
	Methadon	LC-MS/MS	✓		
EDDP	LC-MS/MS	✓			
GS 250 U	Post mortem urine				
	Cotinin	LC-MS/MS	✓	Amphetamin	Tramadol
	Nicotin	LC-MS/MS	(not in DB)	Carboxy-THC***)	
	Caffeine	LC-MS/MS	✓	EDDP***)	
	Theobromin	LC-MS/MS	(not in DB)	Methadone***)	
	Venlafaxin	LC-MS/MS	✓		
	Desmethylvenlafaxin	LC-MS/MS	✓		
	Benzoyllecgonine,	LC-MS/MS	✓		
	Methylecgonin	LC-MS/MS	✓		

- *) ok due to sample preparation, not extractable with chlorbutan
- ***) sample analysis was not completed
- ***) reported for serum
- xxx shown as example chromatogram

Results : Freiburg		impact ESI-QTOF			
Sample	Compound	Result type	detected (diagnostic ion concept)	additional findings	false positives
GS 548 Se	Post mortem serum				
	Promethazine	Toxtyper	✓	Cotinine	none
	Fentanyl	Toxtyper	✓	Caffeine	
	Diazepam	Toxtyper	✓	Olanzapine	
	Methadon	Toxtyper	✓		
	Nordazepam	Toxtyper	✓		
	Mirtazapin	Toxtyper	✓		
	Methadon 32 ng/ml	LC-MS/MS	✓		
	EDDP 10 ng/ml	LC-MS/MS	✓		
	Pregabalin 1.8 µg/ml	LC-MS/MS	nd*)		
	Promethazin 402 ng/ml	LC-MS/MS	✓		
	Fentanyl 74 ng/ml	LC-MS/MS	✓		
	Norfentanyl 10 ng/ml	LC-MS/MS	✓		
	Phenothiazin 27 ng/ml	LC-MS/MS	✓		
	Mirtazapin 48 ng/ml	LC-MS/MS	✓		
	Diazepam	LC-MS/MS	✓		
	Nordazepam	LC-MS/MS	✓		
	Oxazepam	LC-MS/MS	✓		
	Temazepam	LC-MS/MS	✓		
	Lorazepam	LC-MS/MS	(not in DB)		
GS 548 U	Post mortem urine				
	EDDP	Toxtyper	✓	Norfentanyl	none
	Methadon	Toxtyper	✓		
	Fentanyl	Toxtyper	✓		
	Mirtazapin	Toxtyper	✓		
	Nicotin	Toxtyper	(not in DB)		
	Mirtazapin	GC-MS	✓		
	Promethazin	GC-MS	✓		
	Pregabalin	GC-MS	✓		
	Coffein	GC-MS	✓		
	Methadon	GC-MS	✓		
	EDDP	GC-MS	✓		
	Nicotin	GC-MS	(not in DB)		
	Cotinin	GC-MS	✓		
Diazepam	GC-MS	✓			
Nordazepam	GC-MS	✓			
Oxazepam	GC-MS	✓			
Temazepam	GC-MS	✓			

Sample preparation for samples analysed on impact:
Serum samples (1 mL) were extracted by alkaline liquid-liquid-extraction. Urine samples (100 µL) were precipitated with 500 µL ACN. Residue was reconstituted in 25 µL eluent A/B 50/50.

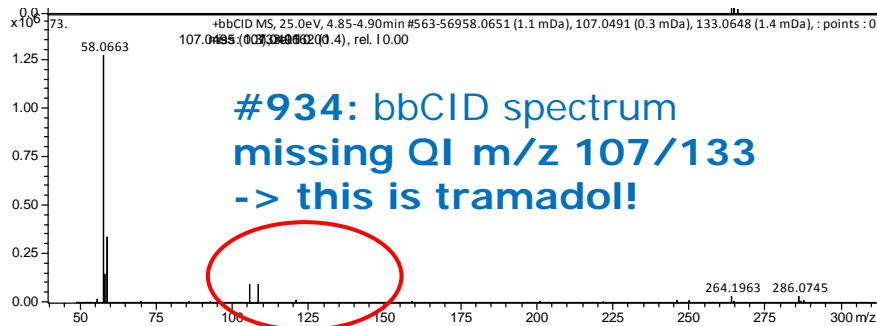
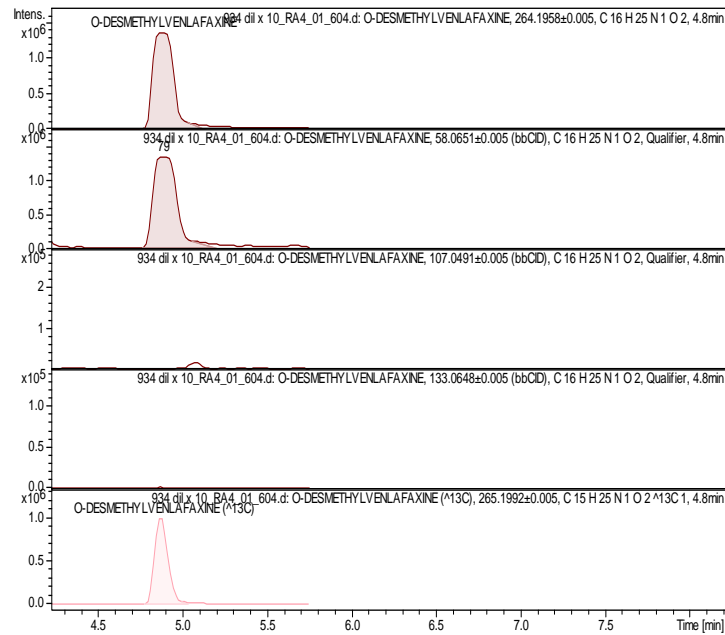
Fig. 7/02



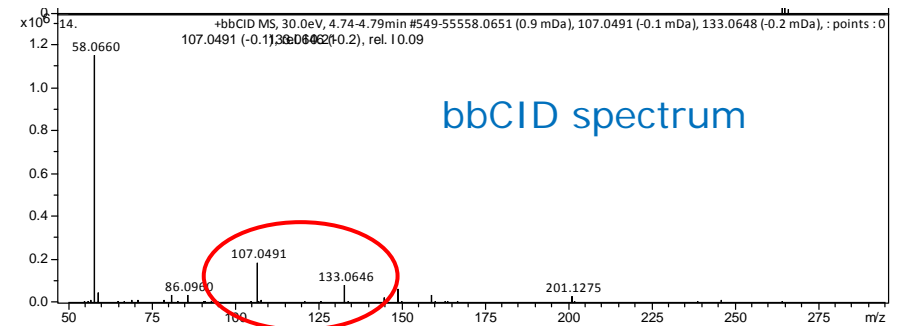
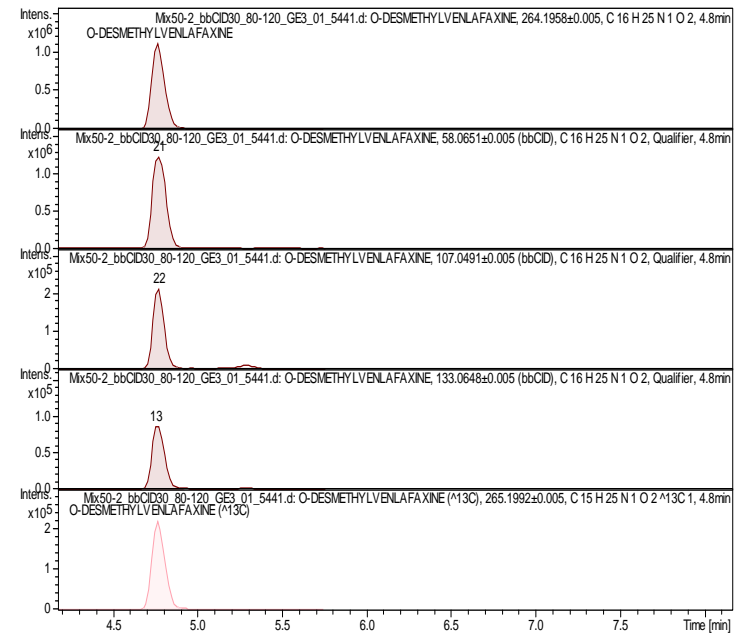
Authentic case examples: Helsinki #934

Fig. 7/03

Sample #934:

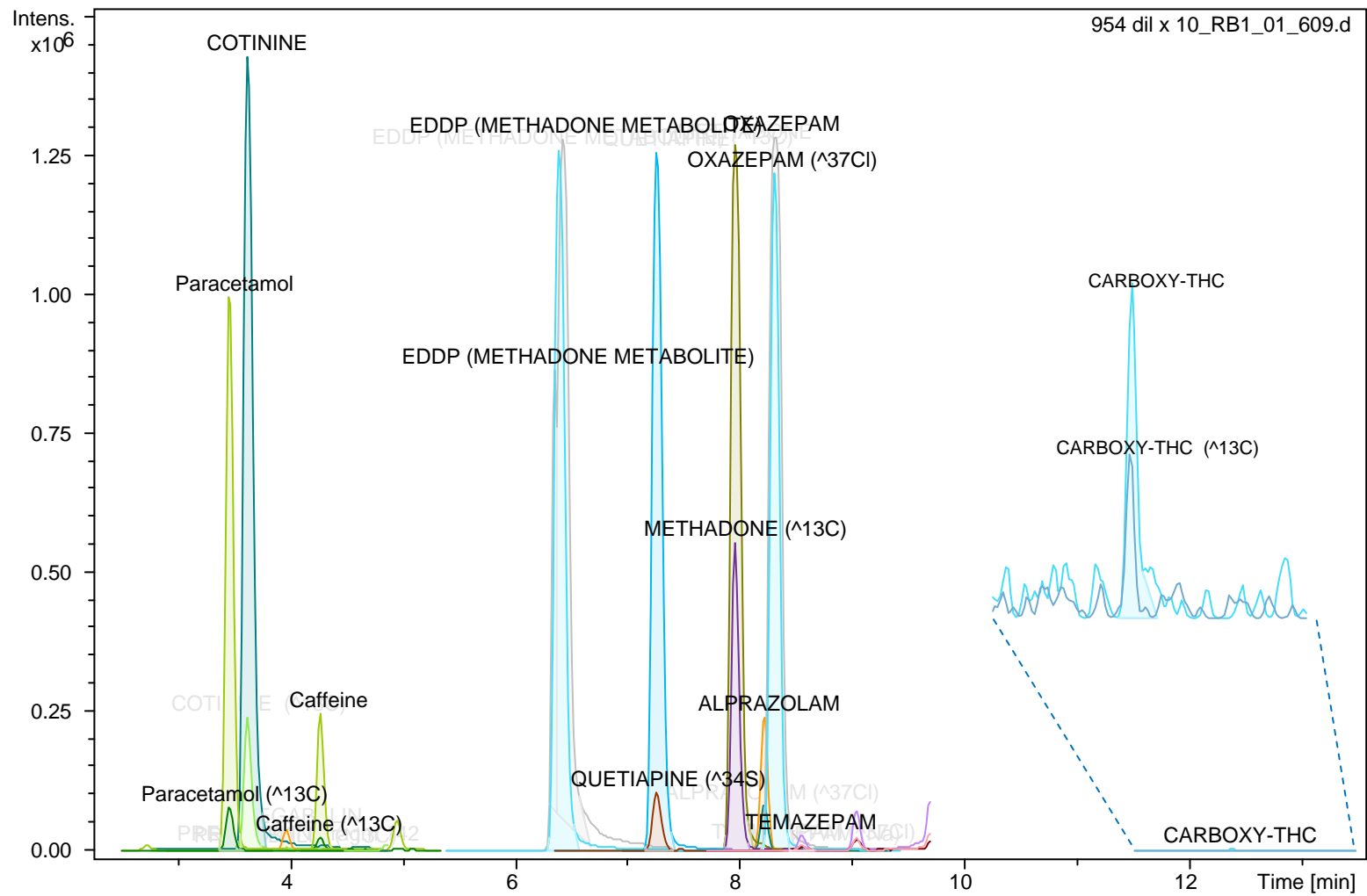


O-desmethyl venlafaxine :



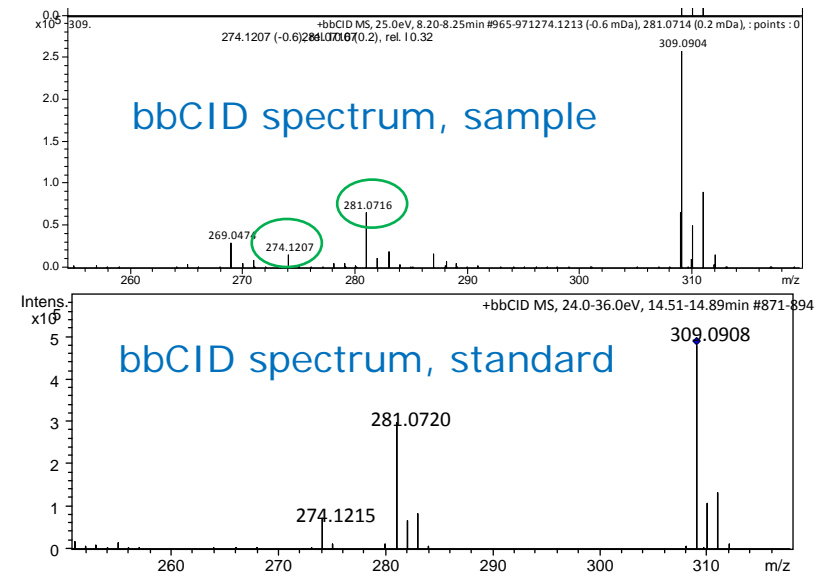
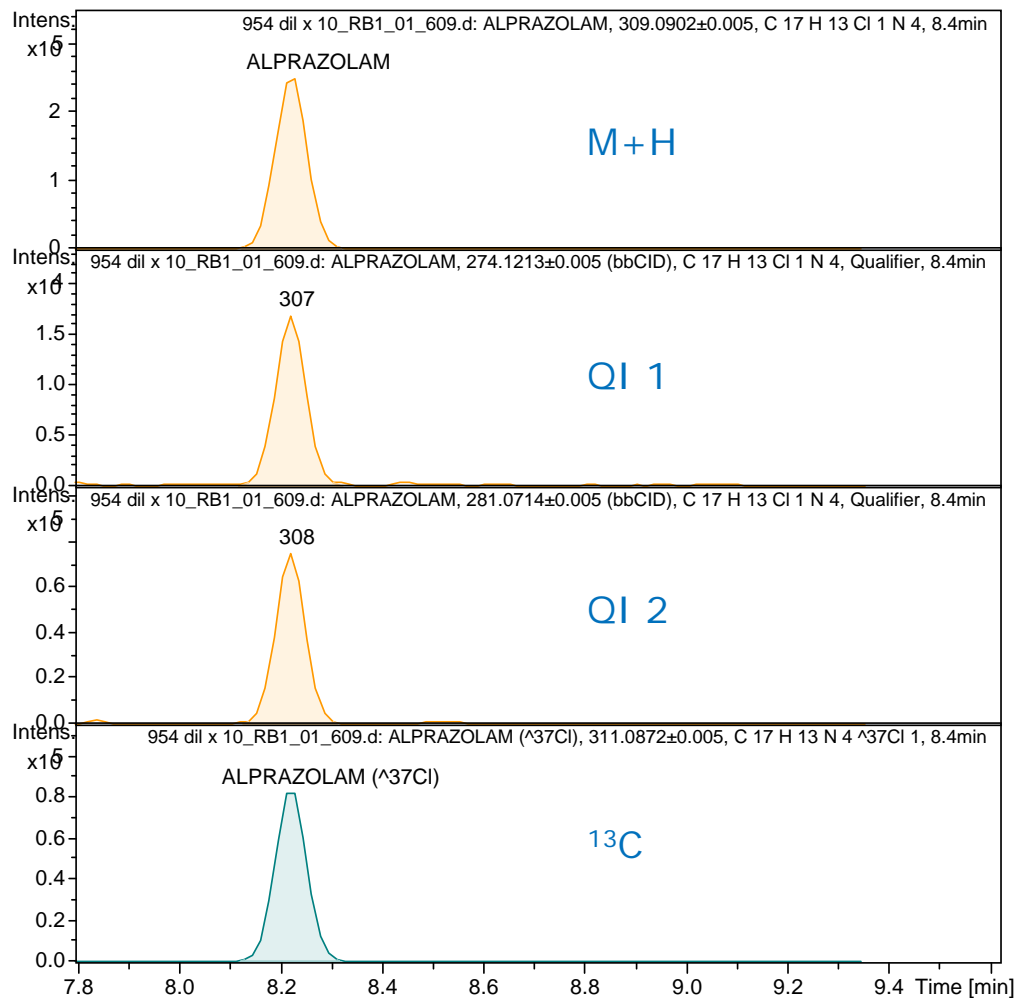
Authentic case examples: Helsinki #934: removing FP O-desmethyl venlafaxine (same sum formula & RT as tramadol)

Fig. 7/04



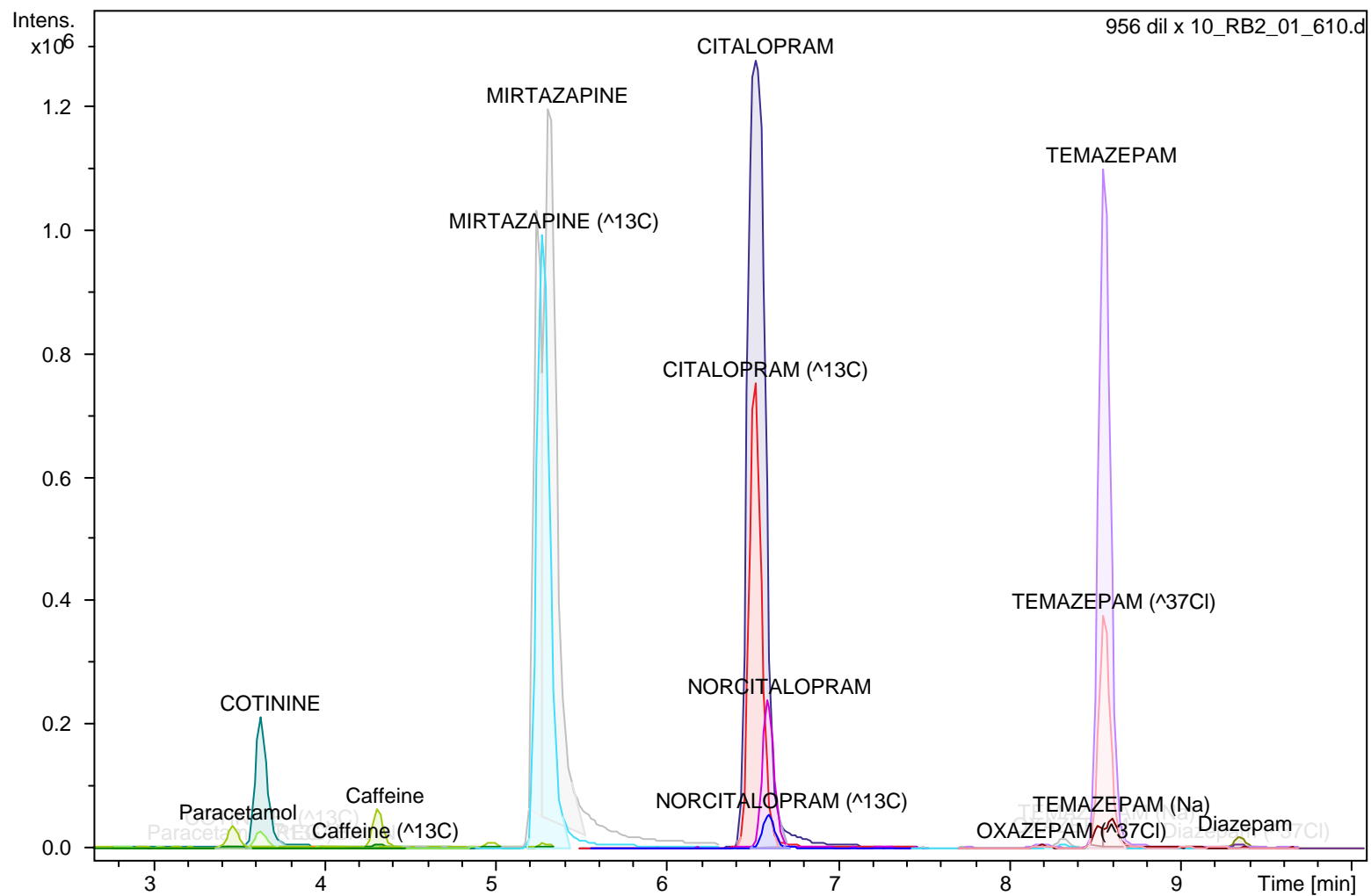
Authentic case examples: Helsinki #954

Fig. 7/05



Authentic case examples: Helsinki #954: additional finding alprazolam: confirmed on QI traces and in bbCID spectrum

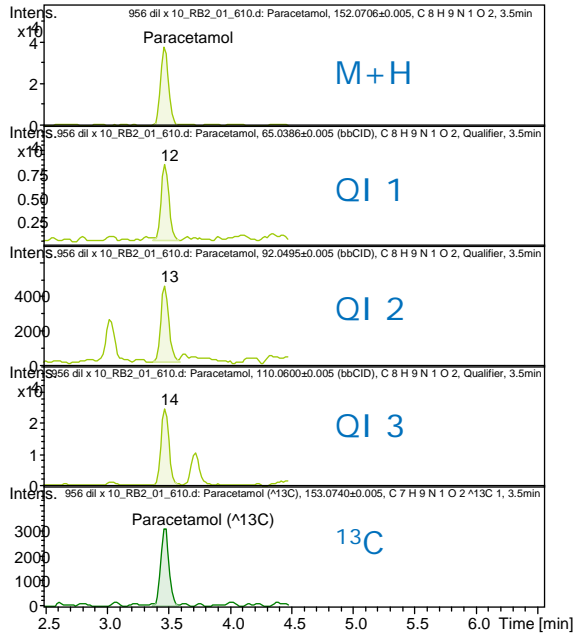
Fig. 7/06



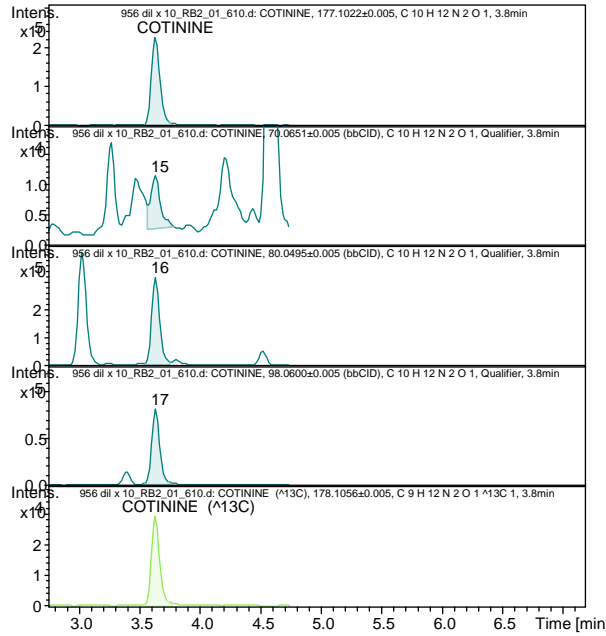
Authentic case examples: Helsinki #956

Fig. 7/07

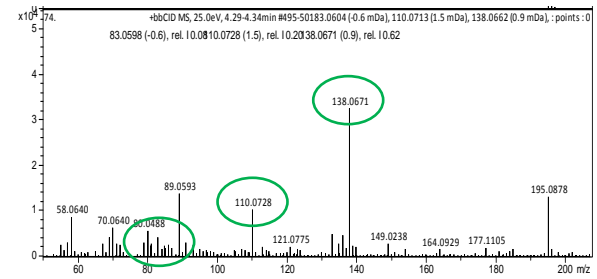
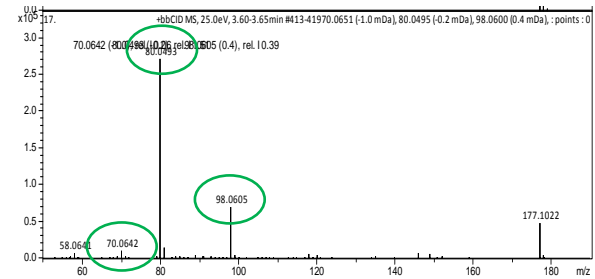
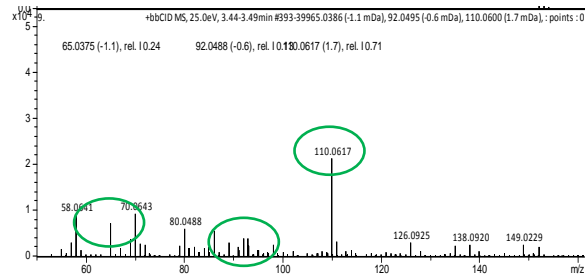
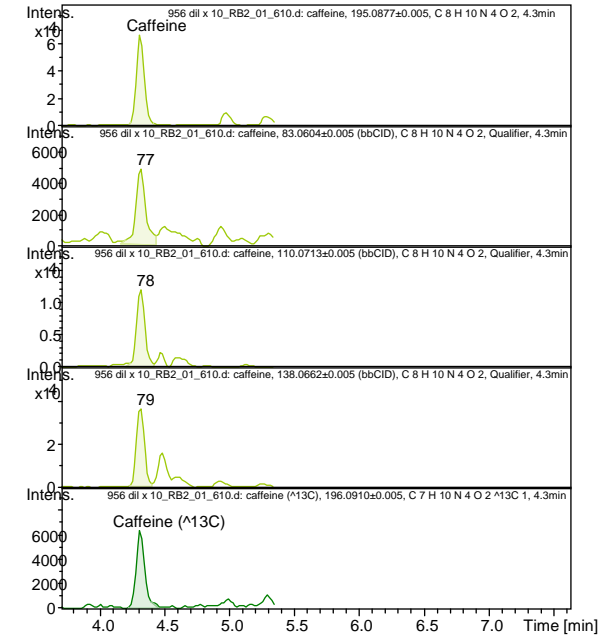
Paracetamol



Cotinin

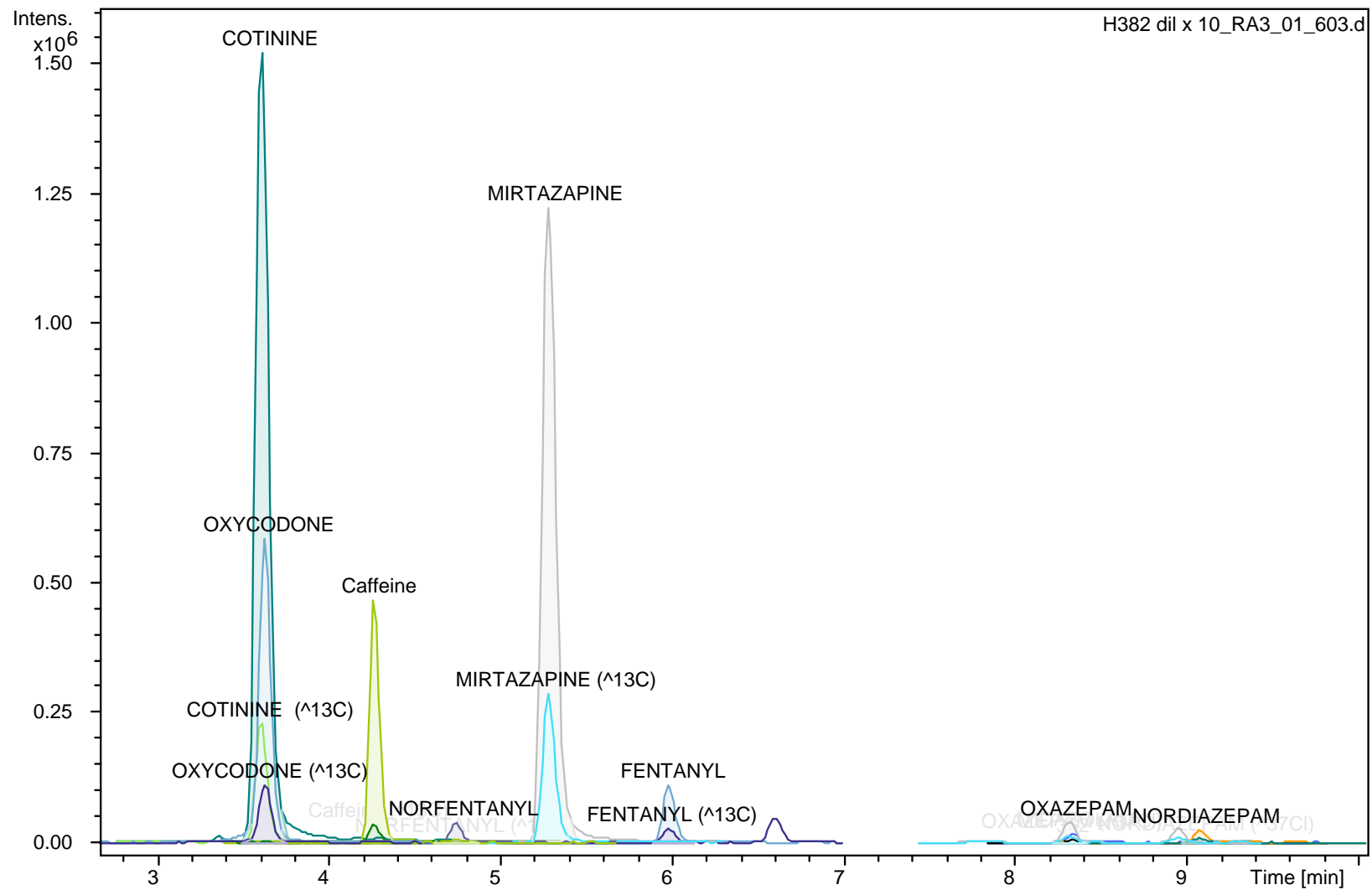


Caffeine



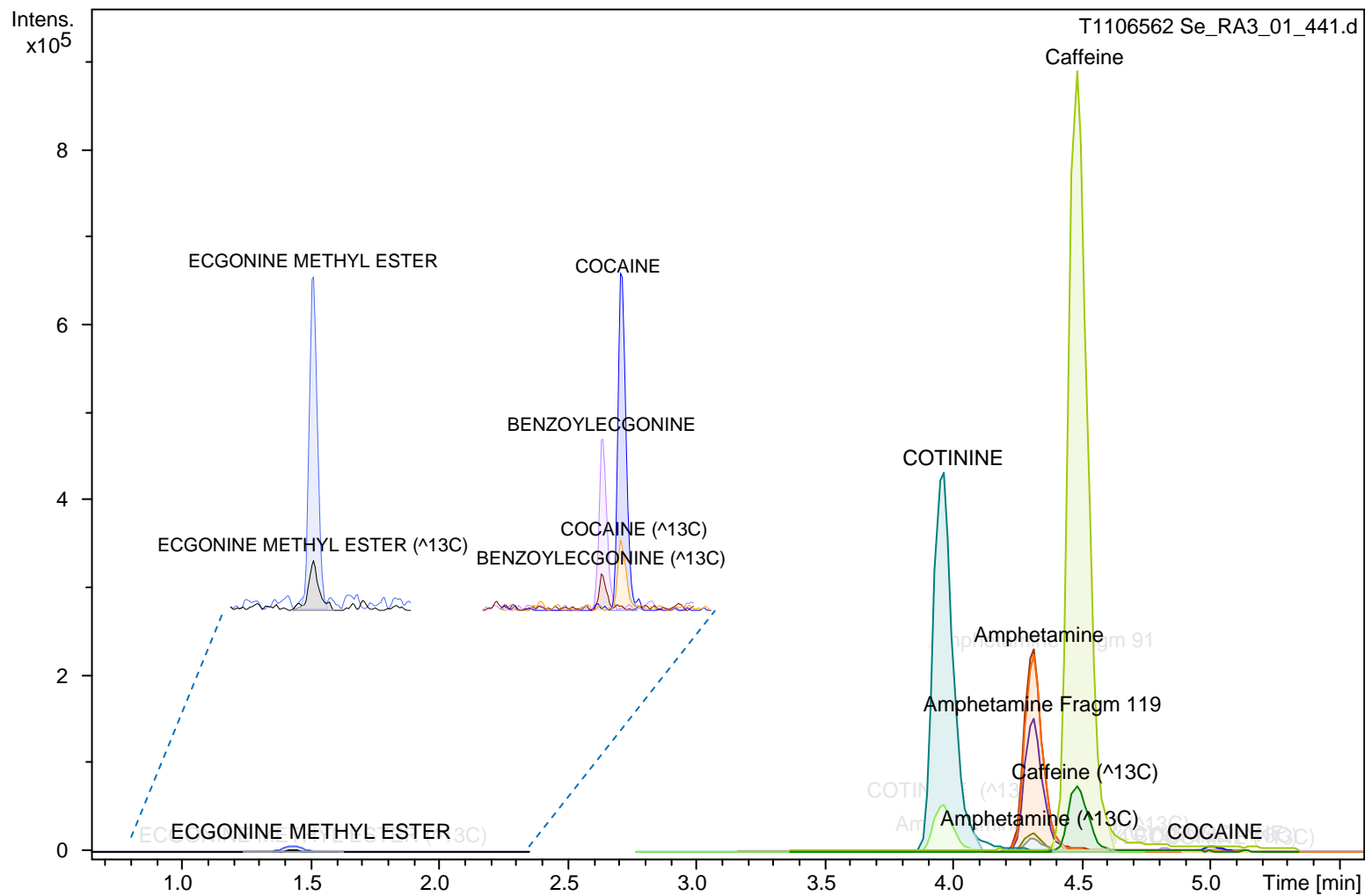
Authentic case examples: Helsinki #956:
additional findings paracetamol, cotinine, caffeine:
confirmed on QI traces and in bbCID spectra

Fig. 7/08

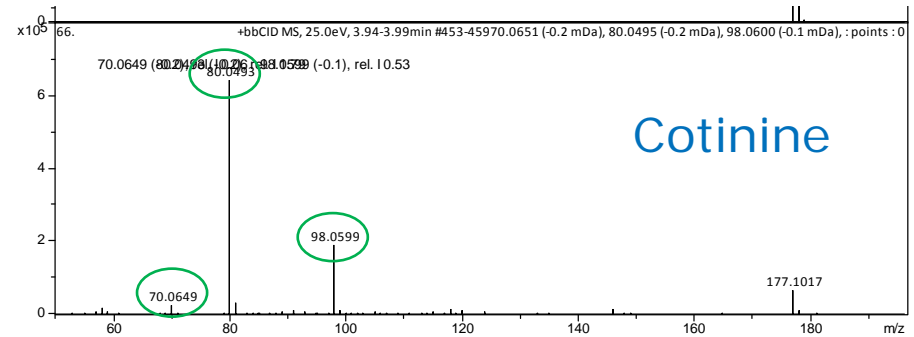
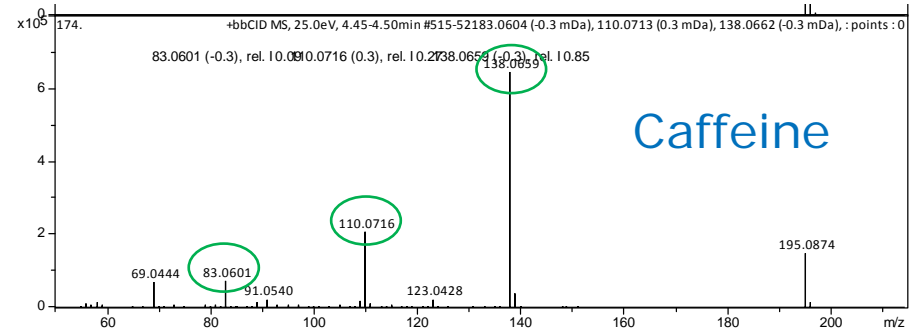
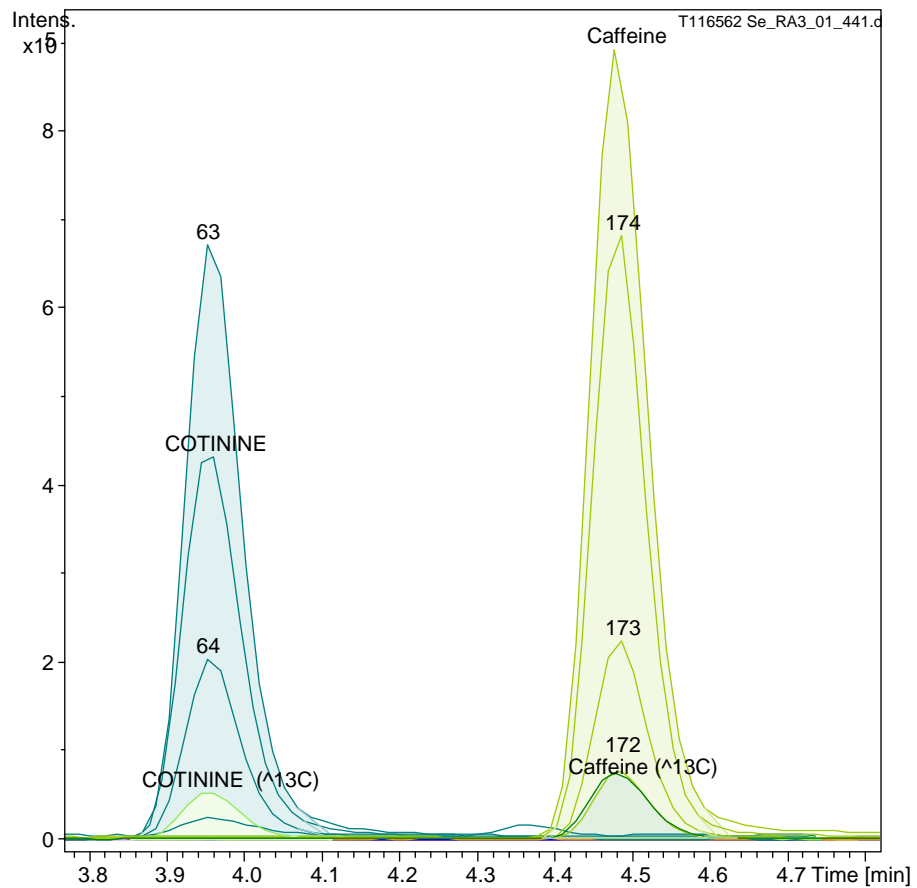


Authentic case examples: Helsinki #H382

Fig. 7/09

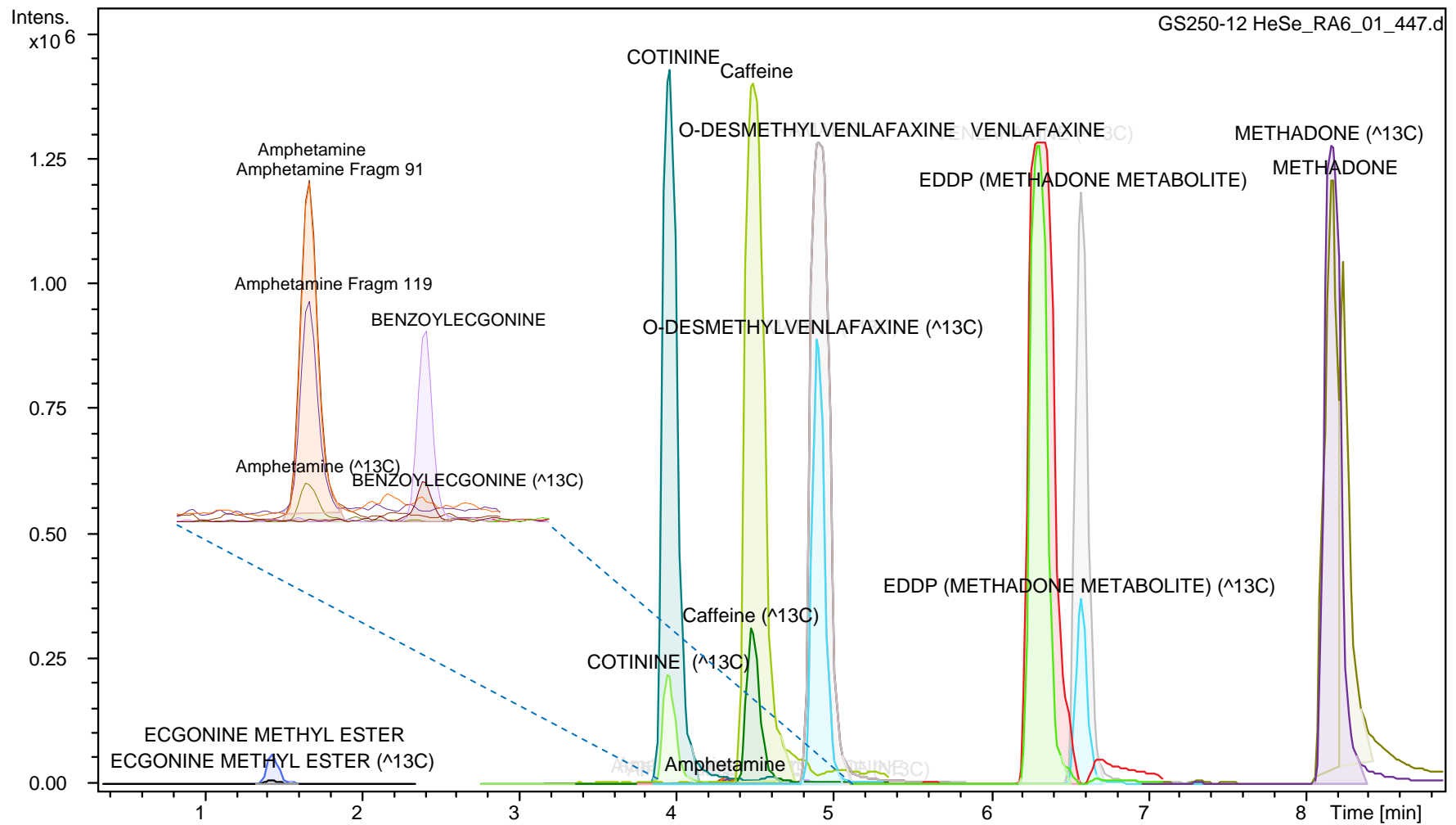


Authentic case examples: Freiburg, T1106562



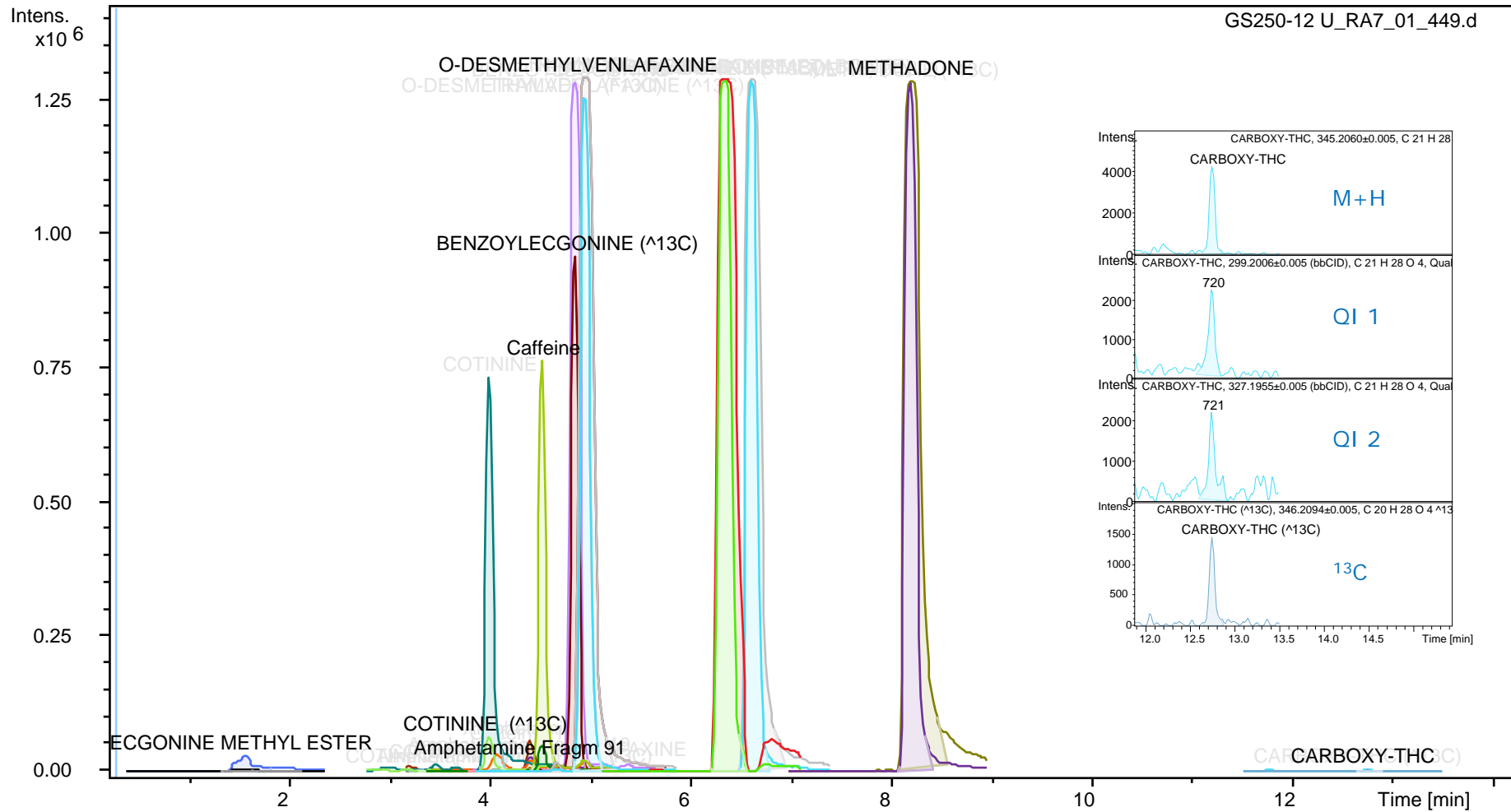
Authentic case examples: Freiburg, T1106562
 additional finding cotinine, caffeine:
 confirmed on QI traces and in bbCID spectra

Fig. 7/11



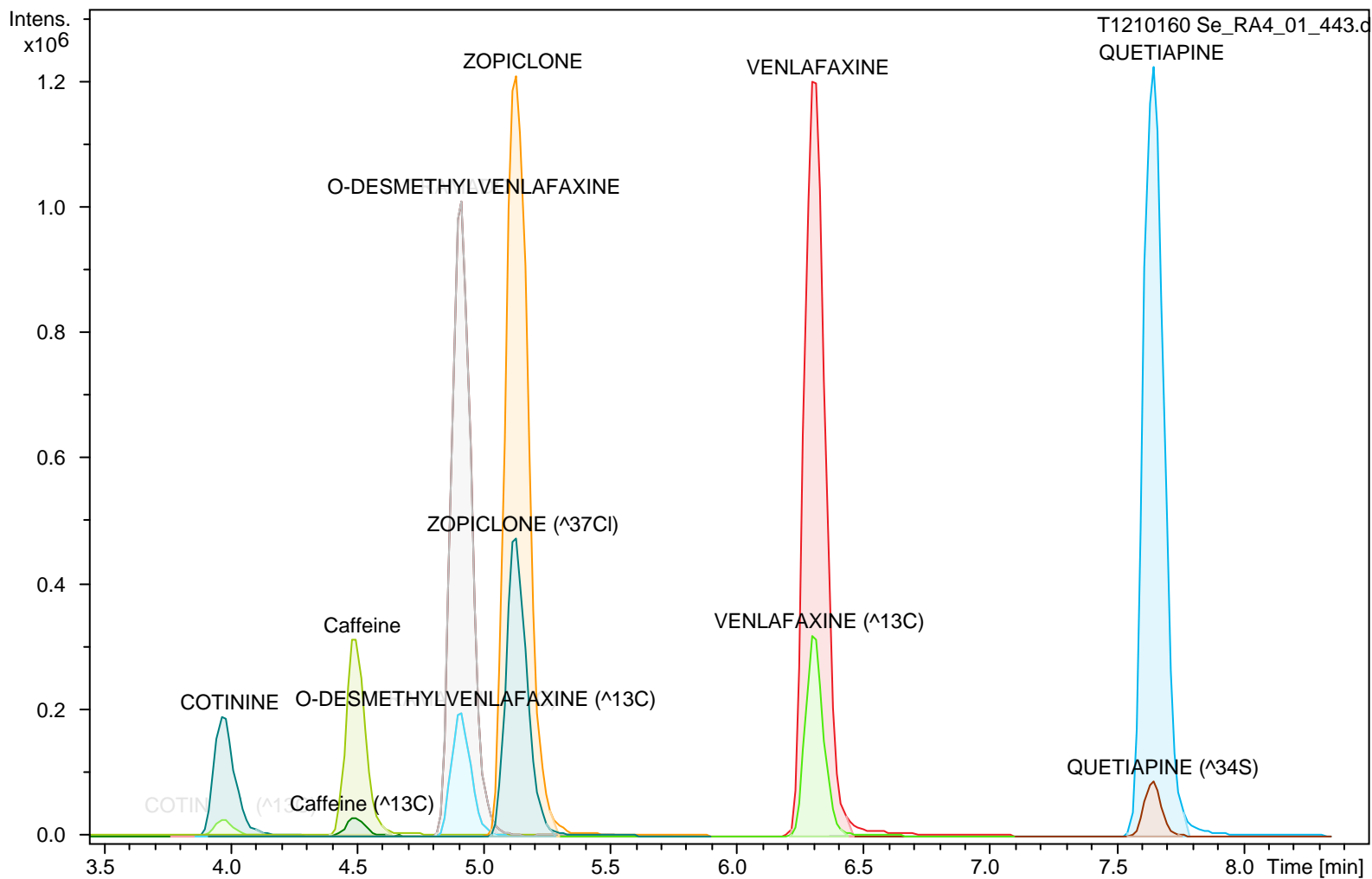
Authentic case examples: Freiburg, GS 250 Serum

Fig. 7/12



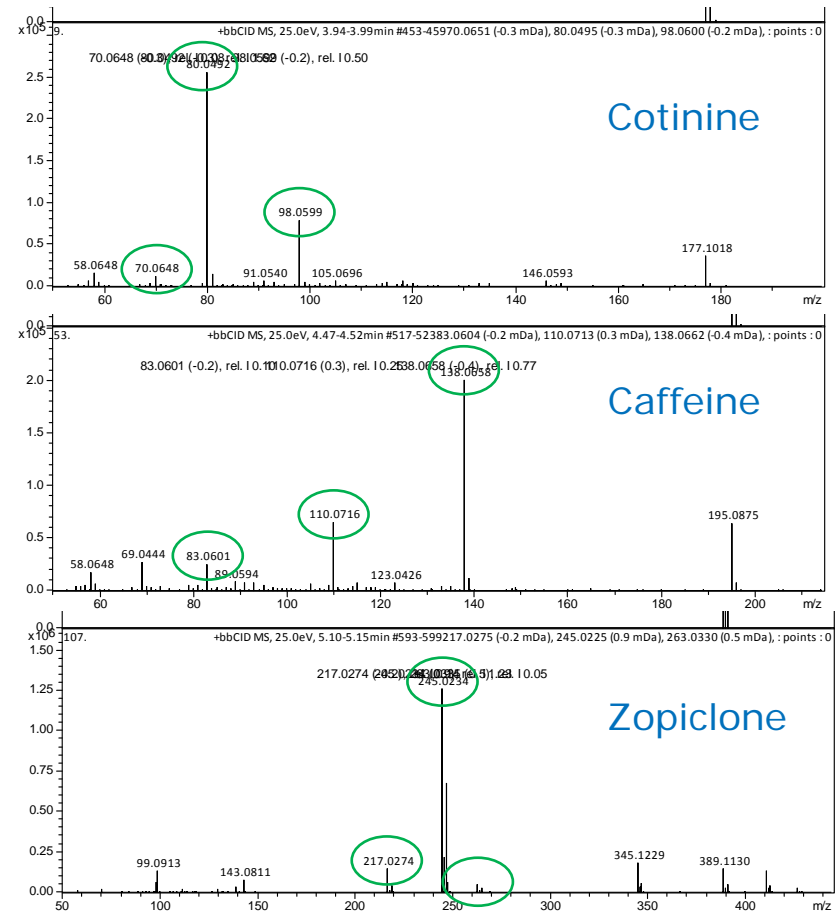
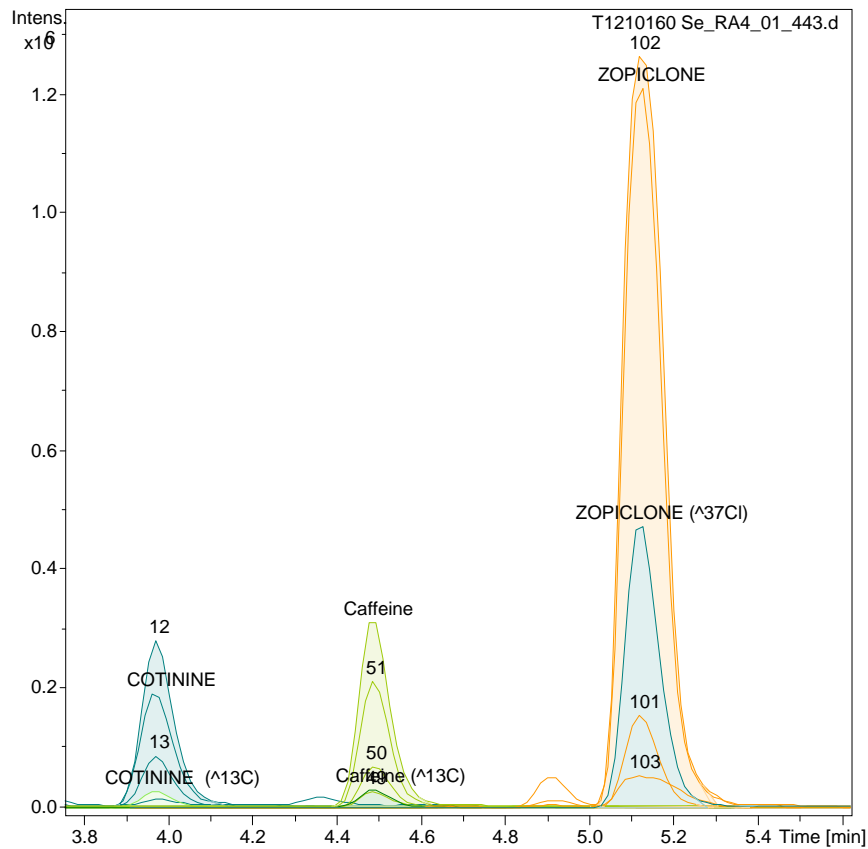
Authentic case examples: Freiburg, GS 250 Urine
 additional finding amphetamine, carboxy-THC:
 confirmed with additional fragment traces or on QI traces

Fig. 7/13



Authentic case examples: Freiburg, T1210160

Fig. 7/14



Authentic case examples: Freiburg, T1210160
 additional finding cotinine, caffeine, zopiclone:
 confirmed on QI traces and in bbCID spectra

Fig. 7/15