metabolites

Supplementary Material

Supplemental Table S1. Overview of internal standards.

Chemical	Isotope label	Supplier	Catalogue number
Acetaminophen	ring-D_4	Toronto Research Chemicals	A161222
Diclofenac	ring-$^{13}C_6$	Sigma-Aldrich	35361
Naproxen	methoxy-D_3	Sigma-Aldrich	32104
Caffeine	trimethyl-$^{13}C_3$	Sigma-Aldrich	C-082
Cotinine	N-methyl-D_3	Sigma-Aldrich	C-035

Supplemental Table S2. Overview of LC-MS analytical parameters.

Setting	Value
Analytical setup:	
LC pump	Dionex Ultimate 3000 RS Binary Pump (Cat. No. HPG-3400RS)
LC autosampler	Dionex Ultimate 3000 TS Autosampler (Cat. No. WPS-3000TRS)
LC column oven	Dionex Ultimate 3000 RS Column Compartment (Cat. No. TCC-3000RS)
LC operation software	Dionex Chromeleon Software (version 6.80 SR10, Build 2818)
MS instrument	SCIEX TripleTOF® 5600 Mass Spectrometer (Cat. No. 1032150)
MS calibration device	SCIEX Calibrant Delivery System (Cat. No. ISG-002019)
MS operation software	SCIEX Analyst TF Software (version 1.7.1, Build 1163)
LC parameters:	
Autosampler temperature	6 °C
Column temperature	40 °C
Analytical column	Dr. Maisch ReproSil Gold 120, 2.5 µm, 120 Å, 2.0 × 150 mm (Cat. No. r125.9g.s1502)
Trapping column	Dr. Maisch ReproSil-Pur 120 C18-AQ, 2.4 µm, 120 Å, 2.0 × 5 mm (Cat. No. r124.aq.v0002)
Mobile phase A	5 mM ammonium formate (Fluka; Cat. No. 17843) and 0.1% formic acid (Merck; Cat. No. 1.00264.0100) in water (Chemsolute; Cat. No. 470.2500)
Mobile phase B	Methanol (Fisher Science; Cat. No. M/4058/17)
Trapping settings	0.3 mL/min at 2% B
Flow rate	0.3 mL/min
LC program	0.00 min: 5% B 0.20 min: column switch 0.50 min: 5% B 12.50 min: 80% B 14.00 min: 100% B 17.00 min: 100% B 17.01 min: 5% B 19.00 min: 5% B
MS parameter:	
Source temperature (TEM)	500 °C
Curtain gas (CUR)	35 psi
Nebulizer gas (GS1)	40 psi
Heater gas (GS2)	40 psi
IonSpray voltage floating (ISVF)	5,200 V
Declustering potential (DP)	80 V
Collision energy (CE) MS1	10 V
Collision energy (CE) MS2	40 V
Collision energy spread (CES) MS1	0 V
Collision energy spread (CES) MS2	30 V
Accumulation time MS1	50 ms
Accumulation time MS2	23 ms
TOF MS1 range	m/z 100-1,250
TOF MS2 range	m/z 40-1,250
SWATH precursor isolation windows	Experiment 1: m/z 100-115 Experiment 2: m/z 114-129 Experiment 3: m/z 128-143 Experiment 4: m/z 142-157 Experiment 5: m/z 156-171

	Experiment 6: m/z 170-185
	Experiment 7: m/z 184-199
	Experiment 8: m/z 198-213
	Experiment 9: m/z 212-227
	Experiment 10: m/z 226-241
	Experiment 11: m/z 240-255
	Experiment 12: m/z 254-269
	Experiment 13: m/z 268-283
	Experiment 14: m/z 282-297
	Experiment 15: m/z 296-311
	Experiment 16: m/z 310-325
	Experiment 17: m/z 324-339
	Experiment 18: m/z 338-353
	Experiment 19: m/z 352-367
	Experiment 20: m/z 366-381
	Experiment 21: m/z 380-395
	Experiment 22: m/z 394-409
	Experiment 23: m/z 408-423
	Experiment 24: m/z 422-437
	Experiment 25: m/z 436-451
	Experiment 26: m/z 450-465
	Experiment 27: m/z 454-479
	Experiment 28: m/z 478-493
	Experiment 29: m/z 492-507
	Experiment 30: m/z 506-521
	Experiment 31: m/z 520-535
	Experiment 32: m/z 534-549
	Experiment 33: m/z 548-563
	Experiment 34: m/z 562-577
	Experiment 35: m/z 576-591
	Experiment 36: m/z 590-605
	Experiment 37: m/z 604-900
	Experiment 38: m/z 899-1,250
Total cycle time	± 1.0 s

Supplemental Table S3. Overview of PeakView chemical identification settings.

Setting	Value
Calculations:	
Do not calculate details for XIC with intensity < N counts or S:N < M	N = 1000, M = 100
Default XIC width (Da)	0.01
Default retention time width	0.2
Default threshold (cps)	100
Default threshold (ratio of control)	1
Non-targeted peak finding	Not selected
Formula Finder	Not selected
Library searching:	
Algorithm to use during library search	Candidate search
Results sorted by	Fit
Libraries to search	Sciex Forensics version 1.1 Custom spectral library
Precursor mass tolerance	0.4 Da
Collision energy tolerance	Not selected
Retention time tolerance	Not selected
Mass tolerance	0.4 Da
Use polarity	Selected
Use collision energy spread	Not selected
Use compound specific purity	Not selected
Maximum number of hits	5
Intensity threshold	0.05
Minimal purity	10%
Intensity factor	5
Confidence settings:	
Mass error – hit	< 5 ppm
Mass error – potential hit	< 10 ppm
Mass error – contribution to combined score	40%
Isotope ratio – hit	< 10%
Isotope ratio – potential hit	< 20%
Isotope ratio – contribution to combined score	10%
Library score – hit	> 70
Library score – potential hit	> 30
Library score – contribution to combined score	50%
Combined score for a positive identification	≥ 80%

Supplemental Table S4. Overview of MarkerView data (pre)processing settings.

Setting	Value
Feature finding:	
Experiment	MS1-only or all MS2 experiments
Minimum retention time	0.50 min
Maximum retention time	16.00 min
Subtraction offset	15 scans
Subtraction multiplication factor	1.3
Noise threshold	5
Minimum spectral peak width	5 ppm
Minimum retention time peak width	5 scans
Assign charge states	Enabled
Feature alignment:	
Retention time tolerance	0.50 min
Mass tolerance	0.01 Da
Feature filtering:	
Maximum number of peaks	8,000,000*
Remove peaks in < N samples	Disabled
Isotope filtering	Disabled
Intensity threshold	5
Use exclusion list	Disabled
Retention time filtering	Disabled
Use area integrated from raw data, not from original peak finding	Disabled
*MS1-level normalization**:*	
Normalization method	Most-Likely Ratio
*MS2-level normalization**:*	
Normalization feature m/z value (diclofenac-$^{13}C_6$ fragment ion)	256.04
Normalization feature experiment (diclofenac-$^{13}C_6$ fragment ion)	16
Normalization feature retention time (diclofenac-$^{13}C_6$ fragment ion)	13 min
Principle component analysis:	
PCA preprocessing - Weighting	None
PCA preprocessing - Scaling	Pareto
Perform PCA-DA (supervised)	Disabled
Principle component analysis-discriminant analysis:	
PCA preprocessing - Weighting	None
PCA preprocessing - Scaling	Pareto
Perform PCA-DA (supervised)	Enabled
T-test:	
Samples per group for "first to last" comparison	Disabled
Use Welch t-test	Disabled

*: This parameter was set high enough to prevent peaks from getting filtered at this stage.
**: Normalization was performed after feature peak list generation.

Supplemental Table S5. Baseline characteristics of the stable liver (LKR) and kidney transplant recipients (KTR) included in this study.

Variable*	LTR	KTR
Samples, number	316	570
Females, %	43%	42%
Age, years	55.0 (14.6)	55.4 (13.1)
Body mass index (BMI), kg/m^2	26.7 (4.9)	27.4 (5.0)
Body length, cm	172 (10)	173 (10)
Body weight, kg	79.6 (17.0)	81.7 (16.6)
Waist circumference, cm	97.2 (15.8)	99.6 (14.2)
Hip circumference, cm	102.3 (10.4)	102.4 (10.3)
Serum albumin, g/L	44.0 (3.4)	43.3 (2.9)
Estimated glomerular filtration rate (eGFR), mL/min/1.73m^2	74.9 (26.2)	53.1 (19.2)

Abbreviations: BMI, body mass index; LTR, liver transplant recipient; KTR, kidney transplant recipient.
*: continuous variables are presented as mean (standard deviation).

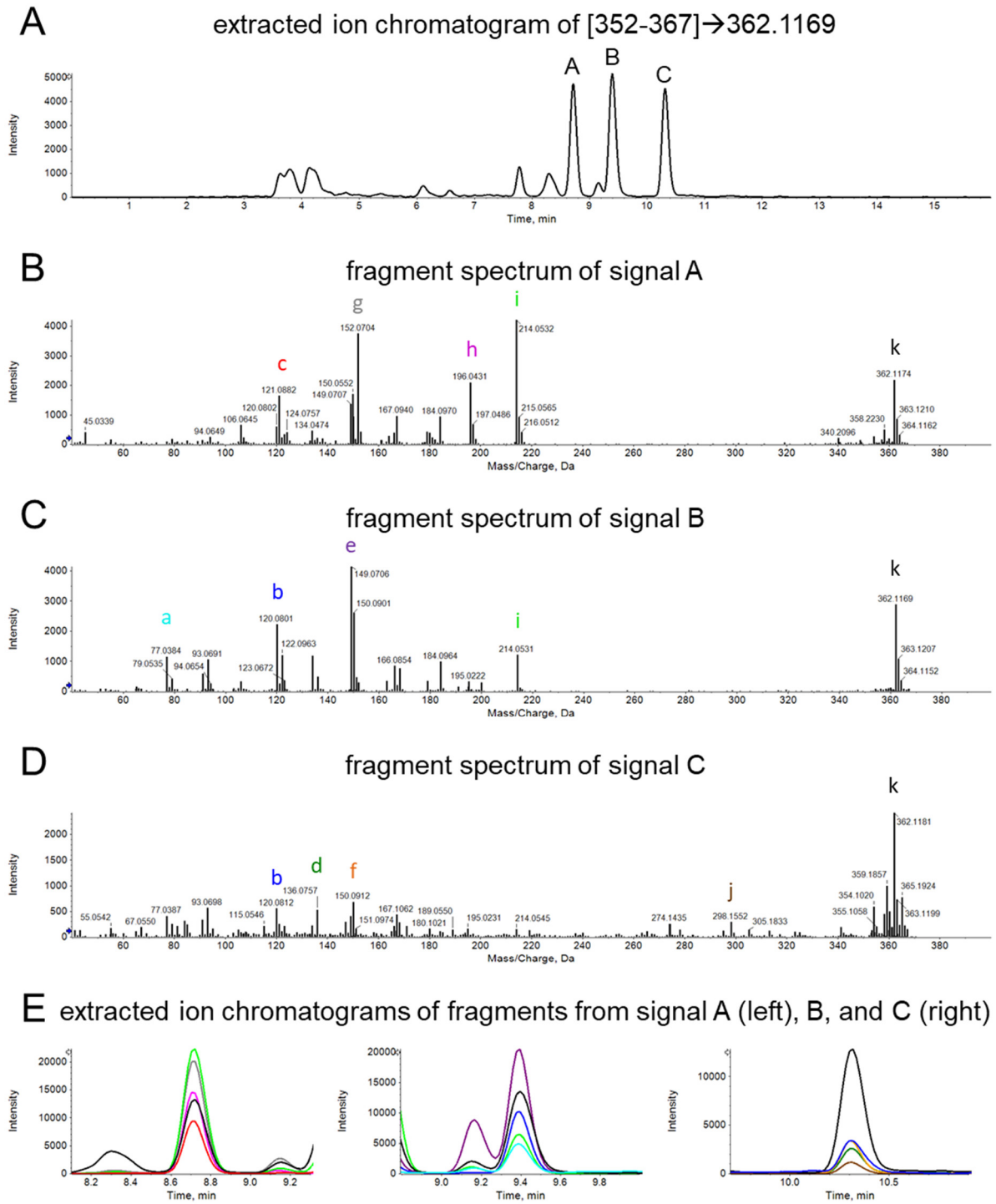
Supplemental Table S6. Quantitative data for cocaine and selected cocaine metabolites in the urine of samples in which benzoylecgonine was identified.

Sample	Cocaine	Benzoylecgonine	Ecgonine methyl ester	Cocaethylene
X-1	<25 ng/mL	<25 ng/mL	<25 ng/mL	<25 ng/mL
X-2	<25 ng/mL	<25 ng/mL	<25 ng/mL	<25 ng/mL
X-3	<25 ng/mL	<25 ng/mL	<25 ng/mL	<25 ng/mL
X-4	<25 ng/mL	<25 ng/mL	<25 ng/mL	<25 ng/mL
X-5	<25 ng/mL	1251 ng/mL	229 ng/mL	<25 ng/mL
Y-1	<25 ng/mL	1524 ng/mL	200 ng/mL	<25 ng/mL
Y-2	1167 ng/mL	137 ng/mL	6332 ng/mL	<25 ng/mL

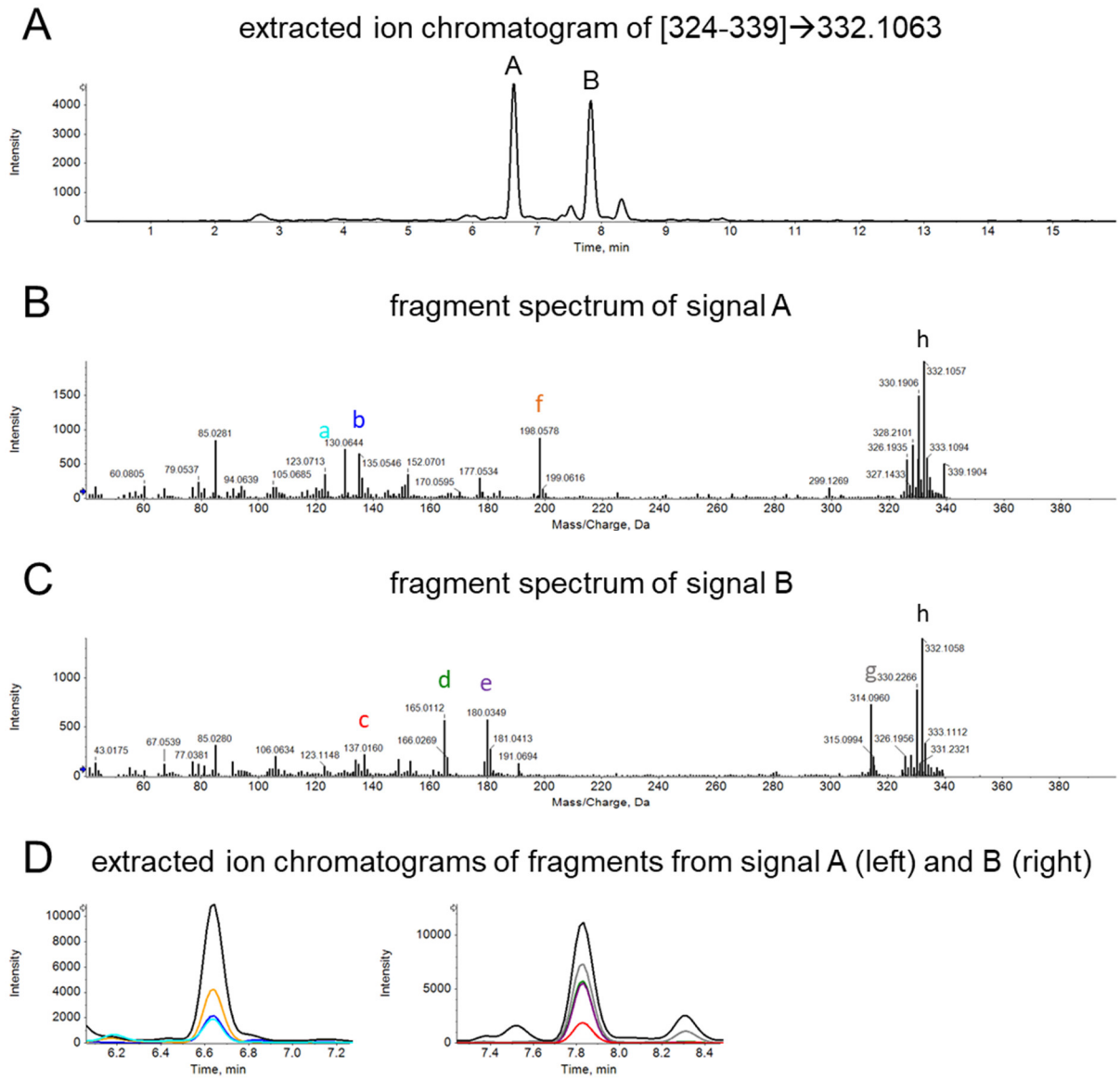
Supplemental Table S7. P-value matrix for differences in MS1-level ratios of possible phase I metabolites of omeprazole when comparing omeprazole and esomeprazole users among liver transplant recipients (in grey) and kidney transplant recipients (in black). With regard to drug use, only "double-positive" subjects were included, and subjects were assigned as omeprazole or esomeprazole user based on information present in the clinical database.

m/z		**268**	**310**	**316**		**330**	**332**		**360**		**362**			**376**				**378**			**392**
	RT	**5.6**	**6.7**	**7.9**	**8.8**	**9.8**	**6.7**	**7.9**	**8.3**	**9.2**	**8.7**	**9.3**	**10.3**	**6.3**	**7.2**	**8.2**	**7.7**	**8.4**	**9.0**	**9.2**	**9.5**	**8.5**
268	**5.6**		ns	ns*	ns*	ns*	ns	ns*	**2e^{-8}**	**2e^{-5}**	ns	ns*	**1e^{-5}**	ns	**2e^{-5}**	ns	**6e^{-8}**	ns*	**9e^{-6}**	**3e^{-6}**	**2e^{-5}**	**2e^{-4}**
310	**6.7**	ns		ns	ns*	ns	ns	**6e^{-5}**	**8e^{-12}**	**2e^{-4}**	ns	ns*	**6e^{-6}**	ns	**1e^{-7}**	ns*	**6e^{-8}**	ns*	**2e^{-4}**	**4e^{-5}**	ns*	ns*
316	**7.9**	ns	ns		ns	ns	ns	**5e^{-5}**	**4e^{-10}**	ns	ns*	ns	ns	ns	**2e^{-6}**	ns*	**1e^{-8}**	ns*	ns	ns*	ns	ns
	8.8	ns	ns*	ns		ns	ns	1e^{-11}	4e^{-17}	ns	ns*	ns	ns	ns*	**8e^{-12}**	ns*	**5e^{-11}**	**1e^{-6}**	ns*	ns*	ns	ns
330	**9.8**	ns	ns	ns	ns		ns	ns*	**4e^{-8}**	ns*	ns	ns	ns*	ns	**3e^{-6}**	ns*	**5e^{-8}**	ns*	ns	**2e^{-4}**	ns*	ns
332	**6.7**	ns	ns	ns	ns	ns		ns*	**3e^{-6}**	ns	ns	ns	ns	ns	ns*	ns	**8e^{-5}**	ns	ns	ns*	ns	ns
	7.9	ns*	ns*	**2e^{-4}**	**4e^{-10}**	ns*	ns*		**2e^{-6}**	**7e^{-8}**	ns	**1e^{-4}**	**1e^{-7}**	**6e^{-5}**	ns*	ns	**4e^{-5}**	ns	**6e^{-10}**	**7e^{-7}**	**2e^{-6}**	**2e^{-8}**
360	**8.3**	**2e^{-4}**	**1e^{-5}**	**2e^{-7}**	**5e^{-12}**	**2e^{-4}**	ns*	ns*		**2e^{-13}**	ns	**2e^{-8}**	**1e^{-11}**	**3e^{-13}**	ns*	ns	ns	**3e^{-7}**	**1e^{-13}**	**1e^{-9}**	**6e^{-10}**	**2e^{-18}**
	9.2	ns*	ns*	ns	ns	ns	ns	**5e^{-5}**	**5e^{-7}**		ns*	ns	ns	**2e^{-4}**	**2e^{-12}**	ns*	**1e^{-12}**	**1e^{-8}**	ns	ns*	ns	ns
362	**8.7**	ns	ns	ns	ns	ns	ns	ns	ns	ns*		ns*	ns*	ns	ns	ns	ns*	ns	ns*	ns*	ns*	ns*
	9.3	ns	ns	ns	ns	ns	ns	ns*	**1e^{-4}**	ns	ns		ns	ns*	**1e^{-6}**	ns*	**7e^{-10}**	**5e^{-5}**	ns	ns*	**6e^{-5}**	ns
	10.3	ns*	**7e^{-6}**	ns	ns	ns*	ns	**7e^{-6}**	**8e^{-8}**	ns	ns*	ns		ns*	**2e^{-10}**	ns*	**1e^{-11}**	**1e^{-7}**	ns	ns*	ns	ns
376	**6.3**	ns	ns	ns	ns*	ns	ns	ns*	**2e^{-6}**	ns*	ns	ns	ns*		**5e^{-9}**	ns	**2e^{-8}**	ns*	ns*	ns*	ns*	**9e^{-5}**
	7.2	ns*	ns*	ns*	**8e^{-6}**	ns*	ns*	ns	ns	**3e^{-7}**	ns	ns*	**1e^{-6}**	ns*		ns	ns*	ns*	**4e^{-11}**	**1e^{-8}**	**2e^{-8}**	**9e^{-16}**
	8.2	ns	ns	ns	ns	ns	ns	ns	ns	ns*	ns	ns	ns*	ns	ns		ns	ns	ns*	**2e^{-4}**	ns*	ns*
378	**7.7**	**2e^{-4}**	**2e^{-4}**	**5e^{-6}**	**2e^{-6}**	**1e^{-4}**	ns*	ns*	ns	**3e^{-7}**	ns*	**1e^{-5}**	**9e^{-8}**	**1e^{-4}**	ns*	ns		**2e^{-6}**	**2e^{-13}**	**4e^{-12}**	**3e^{-11}**	**1e^{-11}**
	8.4	ns*	ns	ns*	**2e^{-4}**	ns*	ns	ns	ns*	**4e^{-5}**	ns	ns*	**5e^{-6}**	ns	ns	ns	ns*		**1e^{-8}**	**9e^{-7}**	**1e^{-6}**	**3e^{-13}**
	9.0	ns	ns	ns	ns	ns	ns	**2e^{-4}**	**3e^{-6}**	ns*	ns	ns	ns*	ns	ns*	ns	**7e^{-6}**	ns*		**ns***	ns	ns
	9.2	ns*	ns*	ns	ns	ns	ns	ns*	ns*	ns	ns	ns	ns	ns	ns*	ns	**3e^{-5}**	ns*	ns		ns	ns*
	9.5	ns	ns*	ns	ns	ns	ns	ns*	**1e^{-4}**	ns	ns	ns	ns	ns	ns*	ns	**3e^{-5}**	ns*	ns	ns		ns
392	**8.5**	ns	ns*	ns	ns	ns	ns	**1e^{-5}**	**6e^{-8}**	ns*	ns	ns	ns	ns	**8e^{-6}**	ns	**6e^{-6}**	**2e^{-6}**	ns	ns	ns	

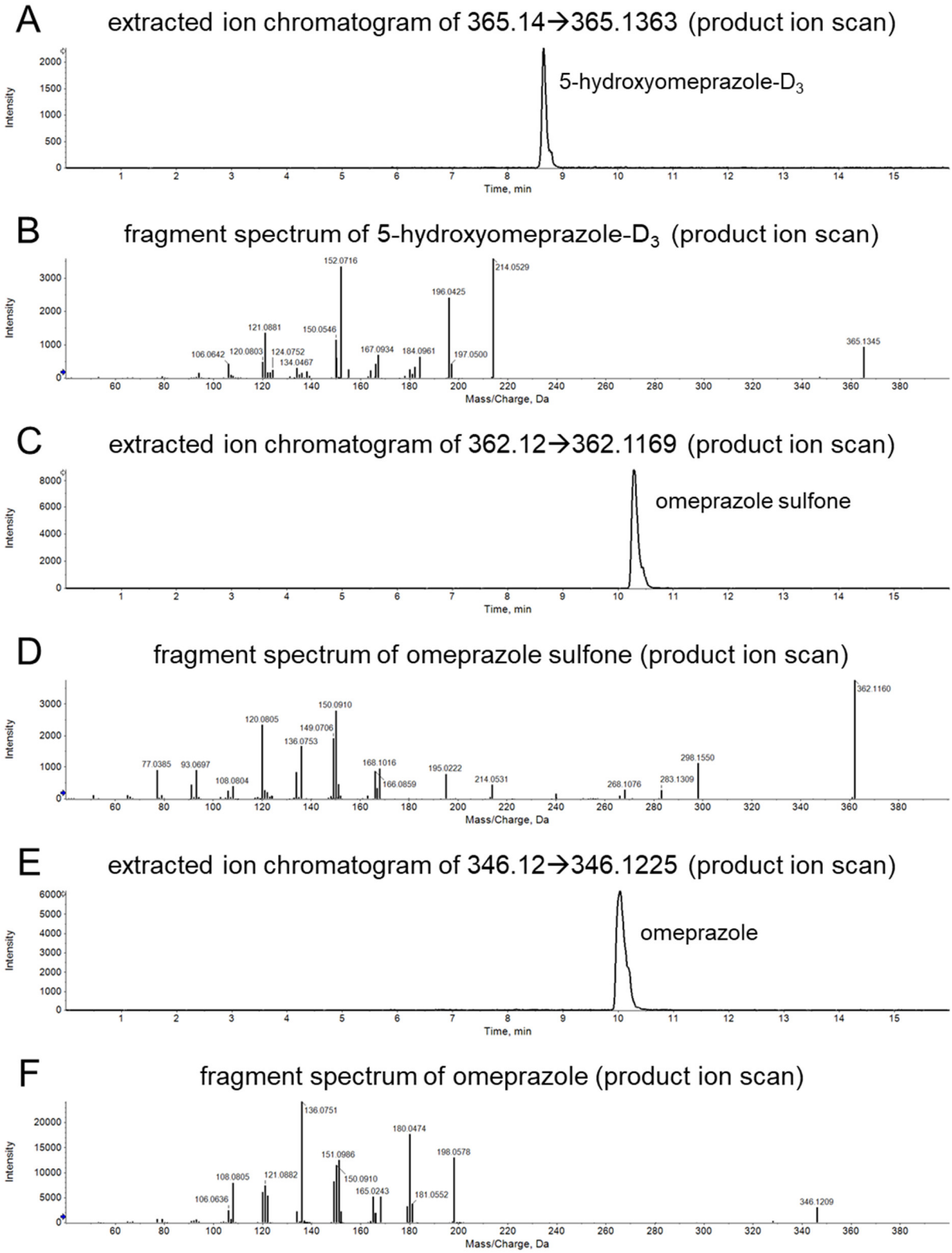
ns: nonsignificant, as was based on Mann-Whitney U nonparametric testing using an alpha of 0.05 and Bonferroni correction. Nonsignificant associations with a P-value between the non-corrected and the Bonferroni-corrected alpha level are indicated with an asterisk (*).



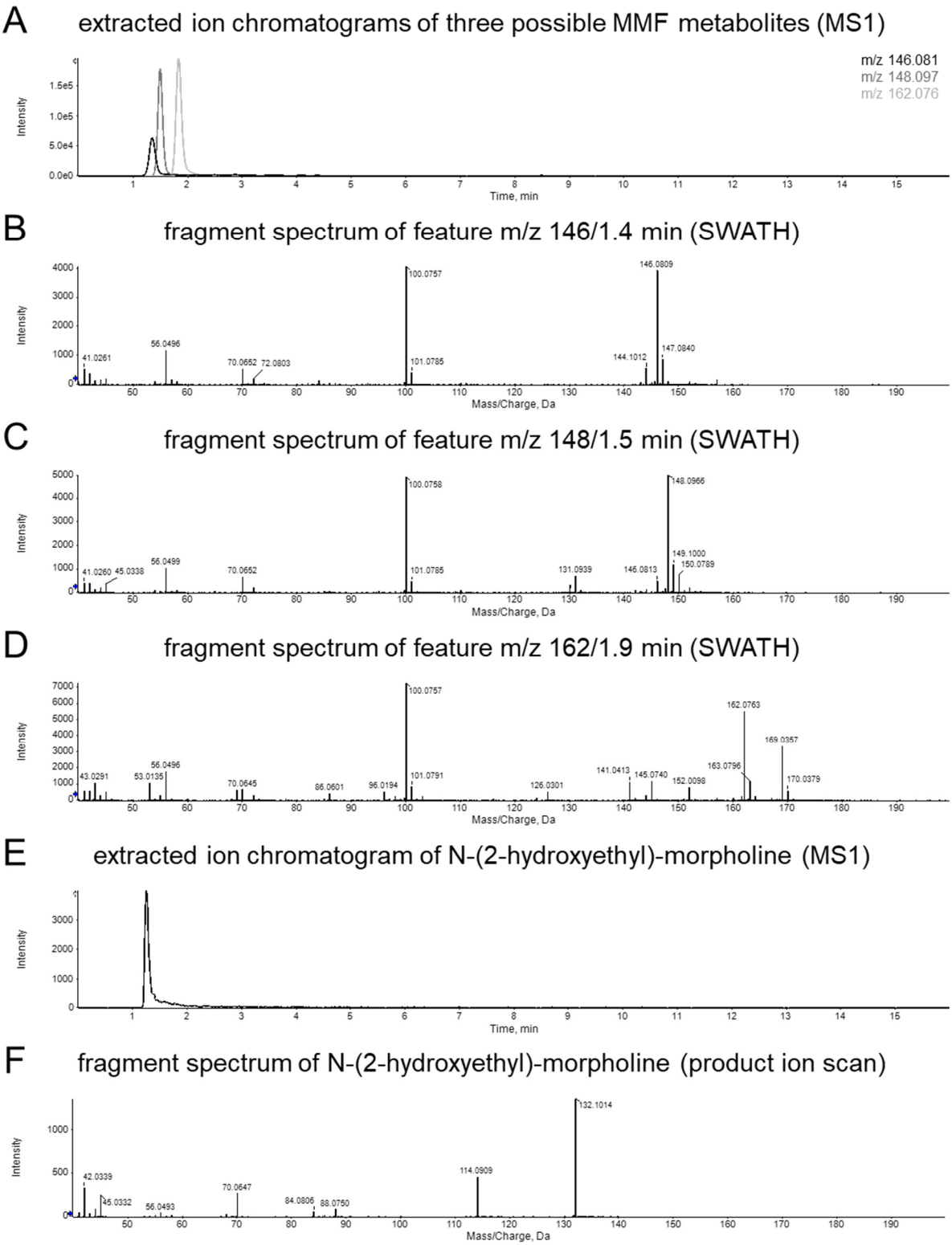
Supplemental Figure S1. Exemplary (**A**, **E**) extracted ion chromatograms and (**B**, **C**, **D**) fragment spectra of three possible oxidation products (+16) of omeprazole as observed in one of the omeprazole-positive samples. Quantifier traces for signals A, B, and C are respectively indicated in light green (m/z 214.0532, i), light green (m/z 214.0532, i), and brown (m/z 298.1550, j). The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



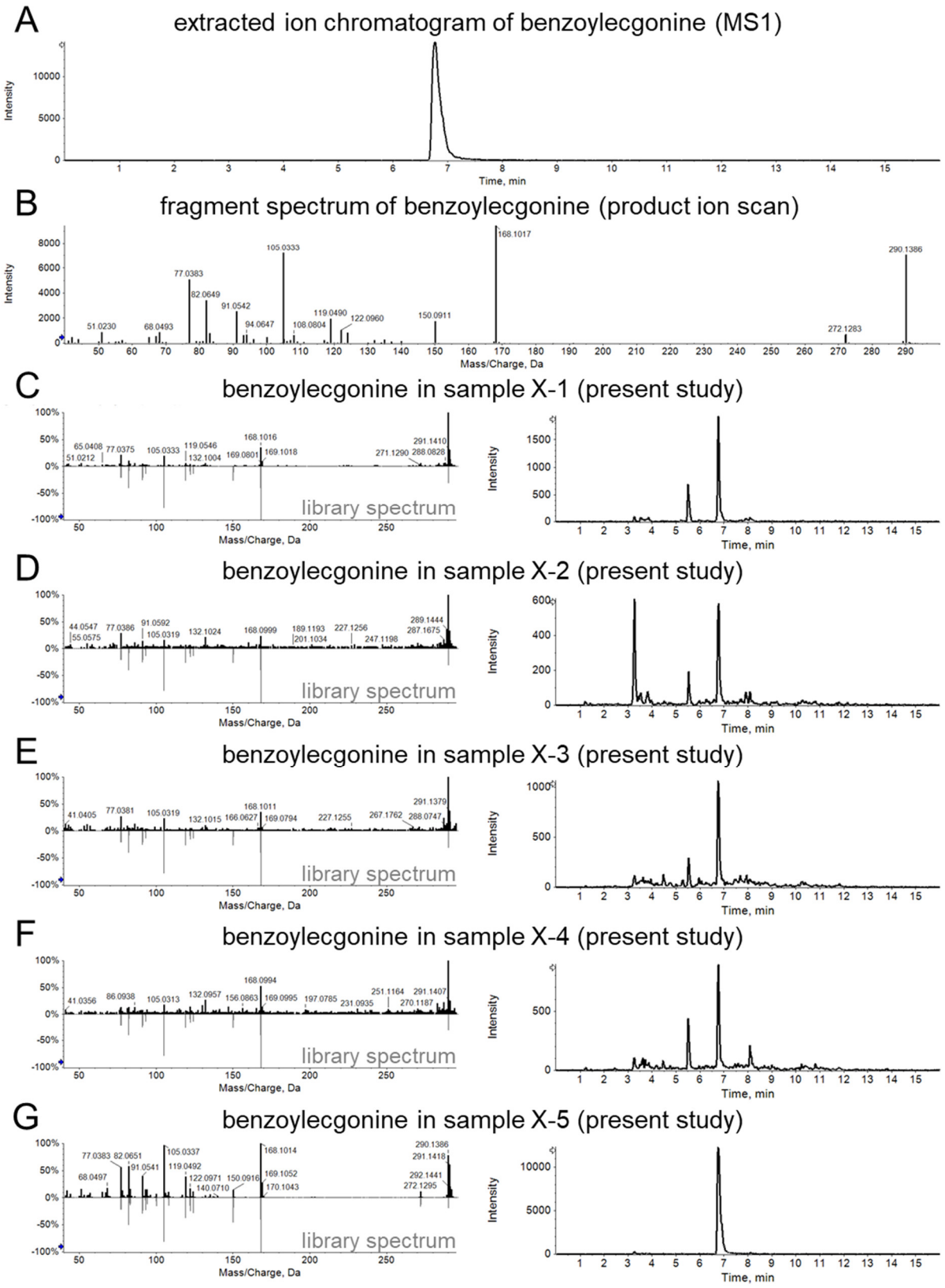
Supplemental Figure S2. Exemplary (**A**, **D**) extracted ion chromatograms and (**B**, **C**) fragment spectra of two possible oxidation products (-14) of omeprazole as observed in one of the omeprazole-positive samples. Quantifier traces for signals A and B are respectively indicated in orange (m/z 198.0583, f) and dark green (m/z 165.0117, d). The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



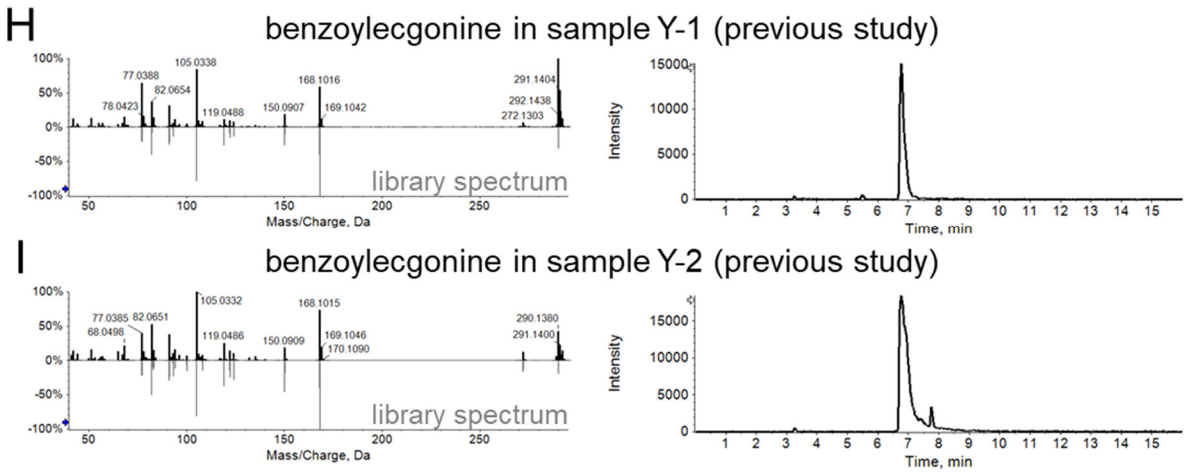
Supplemental Figure S3. (**A**, **C**, **E**) Extracted ion chromatograms and (**B**, **D**, **F**) fragment spectra of (**A**, **B**) 5-hydroxyomeprazole-D3 (Toronto Research Chemicals, Cat. No. H948864), (**C**, **D**) omeprazole sulfone (Sigma-Aldrich, Cat. No. O0151000), and (**E**, **F**) omeprazole (crushed granules from a omeprazole capsule from the company Healthypharm). The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



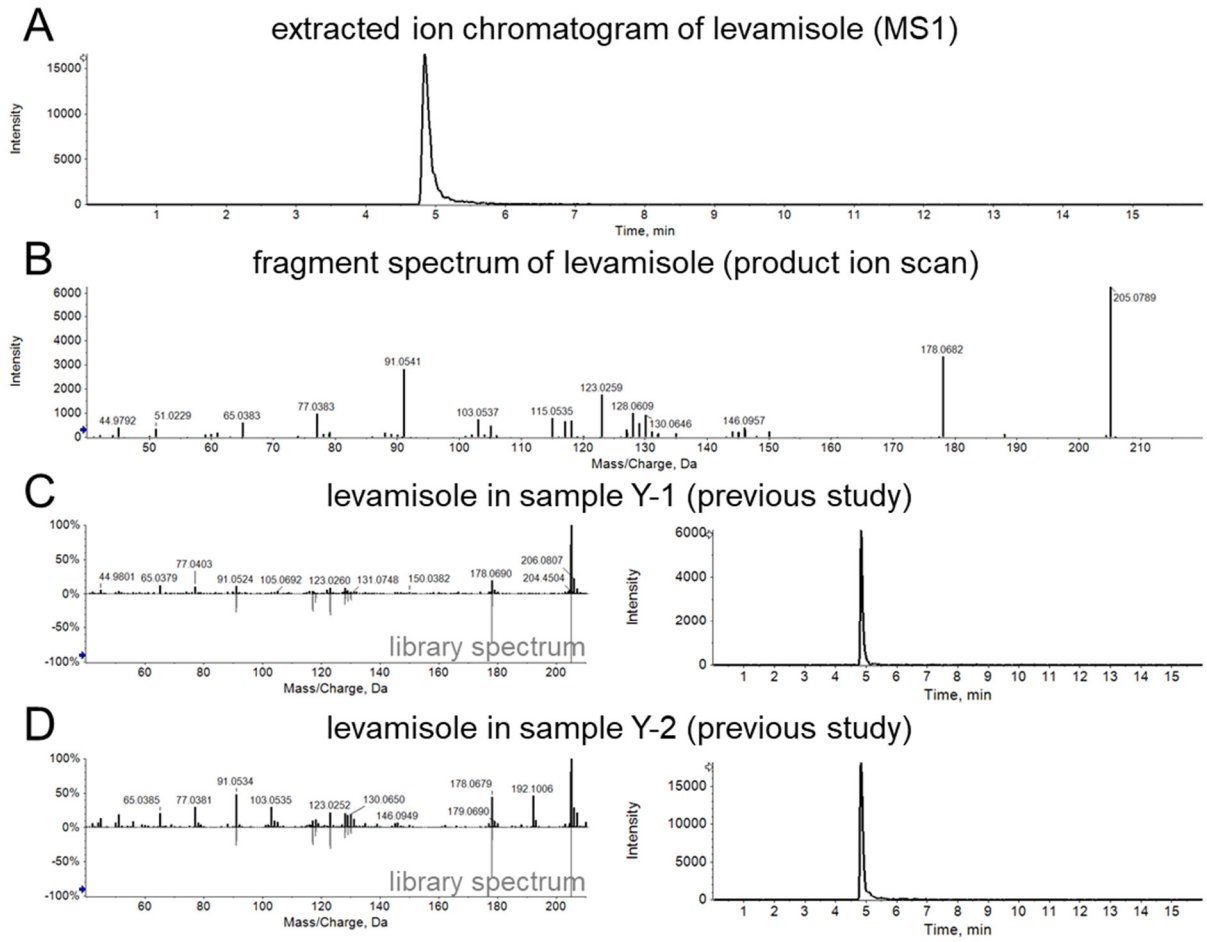
Supplemental Figure S4. Exemplary (**A**) extracted ion chromatograms and (**B**, **C**, **D**) fragment spectra of three possible biotransformation products of MMF's mofetil moiety. (**E**) Extracted ion chromatogram and (**F**) fragment spectrum of N-(2-hydroxyethyl)-morpholine (Sigma-Aldrich, Cat. No. H28203), which was not detected but has been described as possible biotransformation product of MMF's mofetil moiety. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



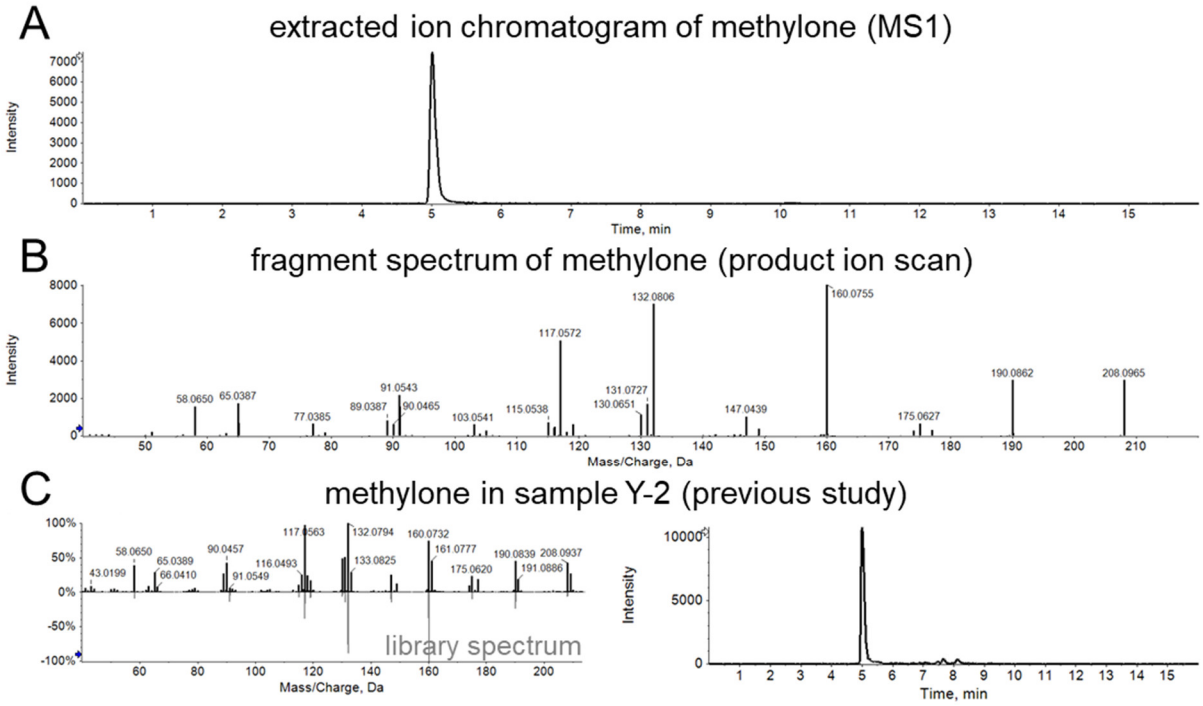
Supplemental Figure S5. (**A**) Extracted ion chromatogram and (**B**) fragment spectrum of benzoylecgonine (Lipomed, Cat. No. COC-204-FB) and (**C**-**I**) spectral library matching results of benzoylecgonine-positive samples. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



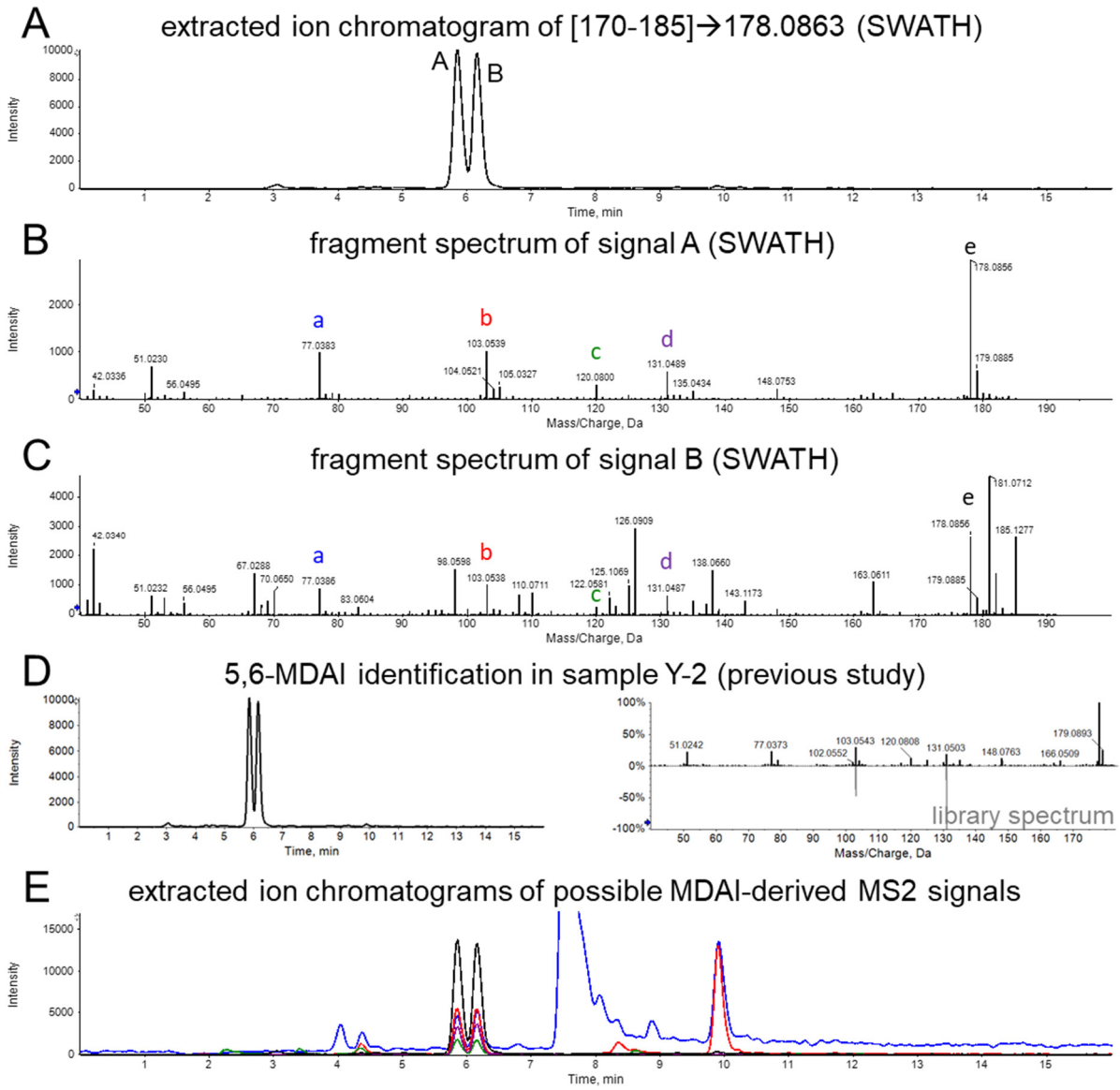
Supplemental Figure S5. *Cont*.



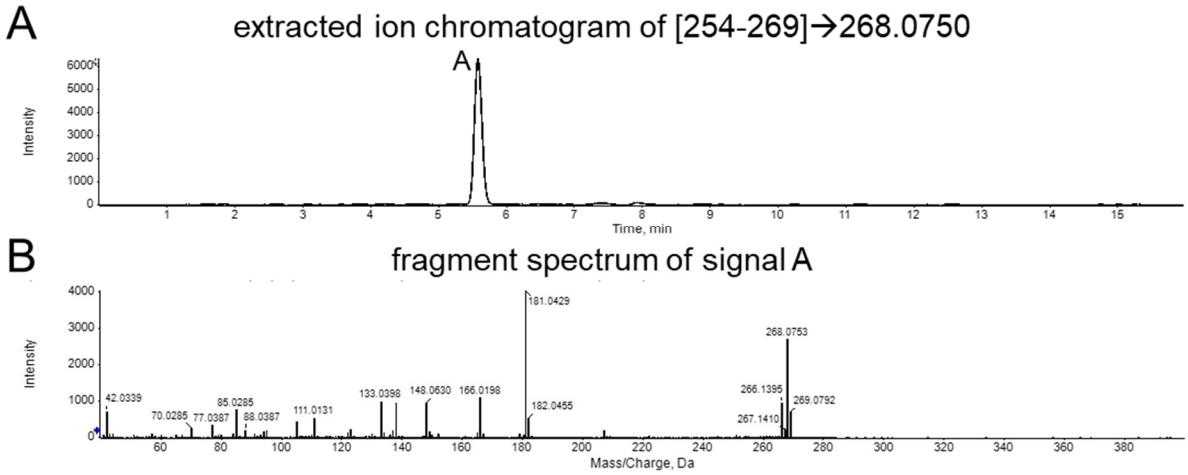
Supplemental Figure S6. (**A**) Extracted ion chromatogram and (**B**) fragment spectrum of levamisole (Sigma-Aldrich, Cat. No. L9756) and (**C**-**D**) spectral library matching results of levamisole-positive samples. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



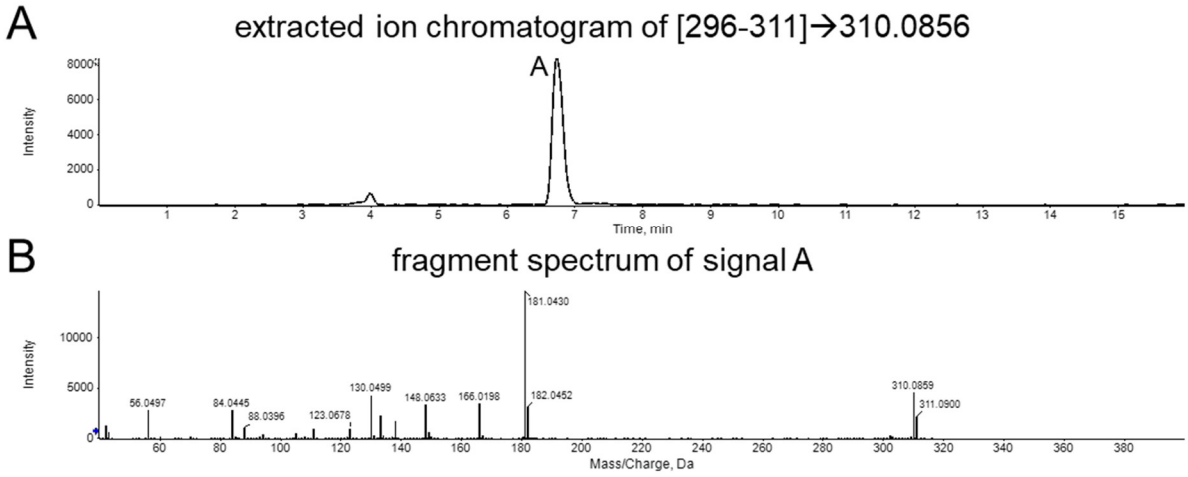
Supplemental Figure S7. (**A**) Extracted ion chromatogram and (**B**) fragment spectrum of methylone (Lipomed, Cat. No. MTY-1289-HC) and (**C**) spectral library matching result of the methylone-positive sample. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



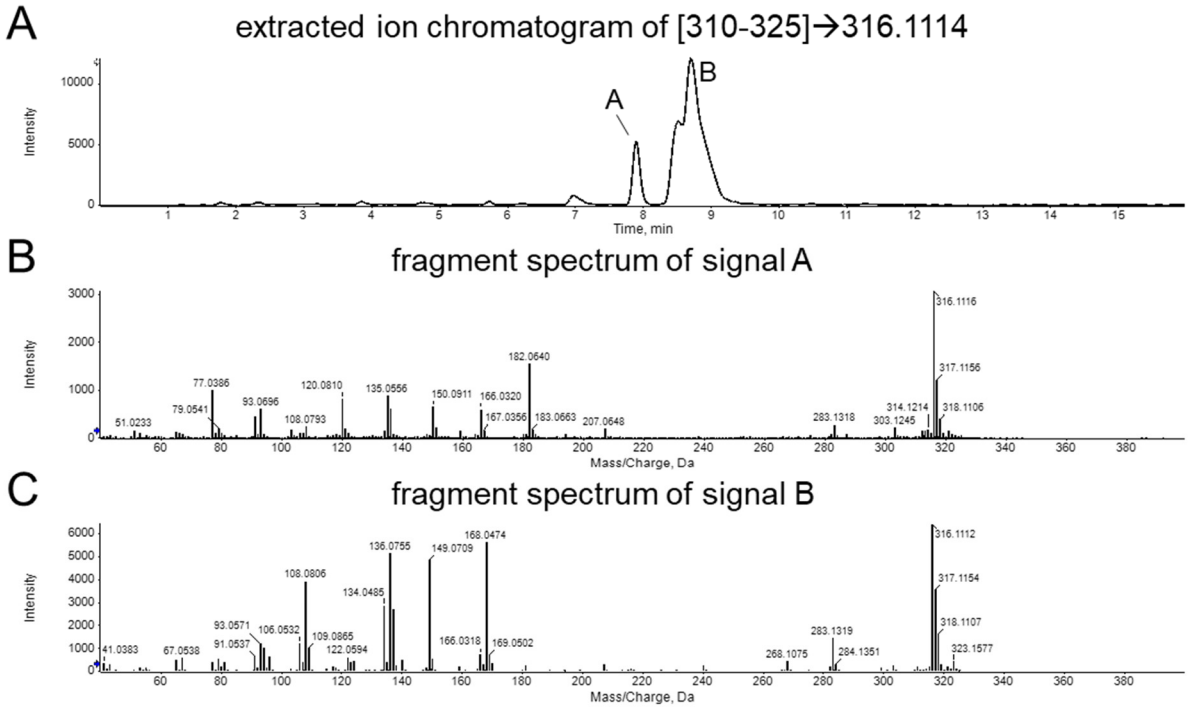
Supplemental Figure S8. (**A**) Extracted ion chromatogram and (**B**) fragment spectra (**C**) of two possible methylenedioxy-2-aminoindanes (MDAI) as well as (**D**) spectral library matching result for 5,6-MDAI, and (**E**) extracted ion chromatograms of presumed MDAI-derived fragments, as observed in the 5,6-MDAI-positive sample. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



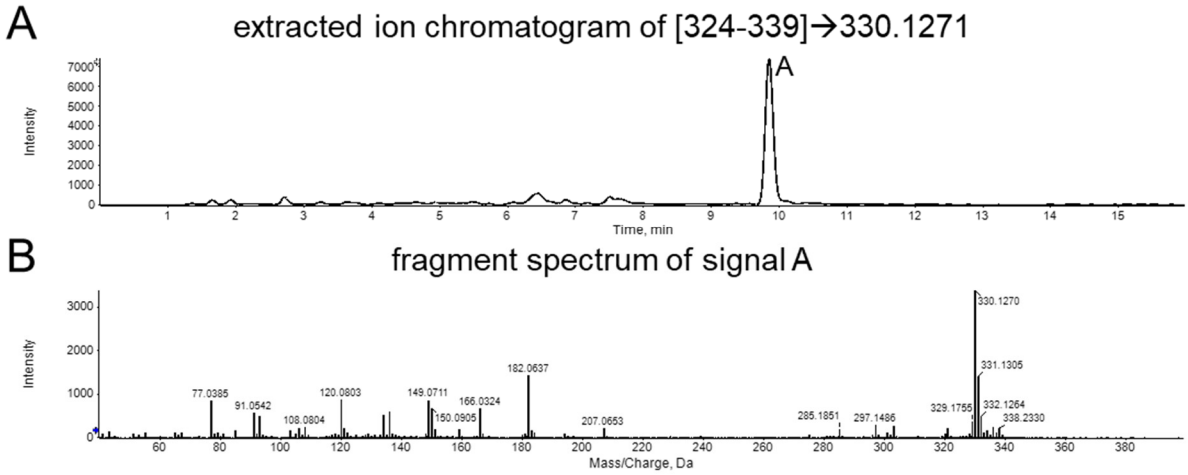
Supplemental Figure S9. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible cysteine metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



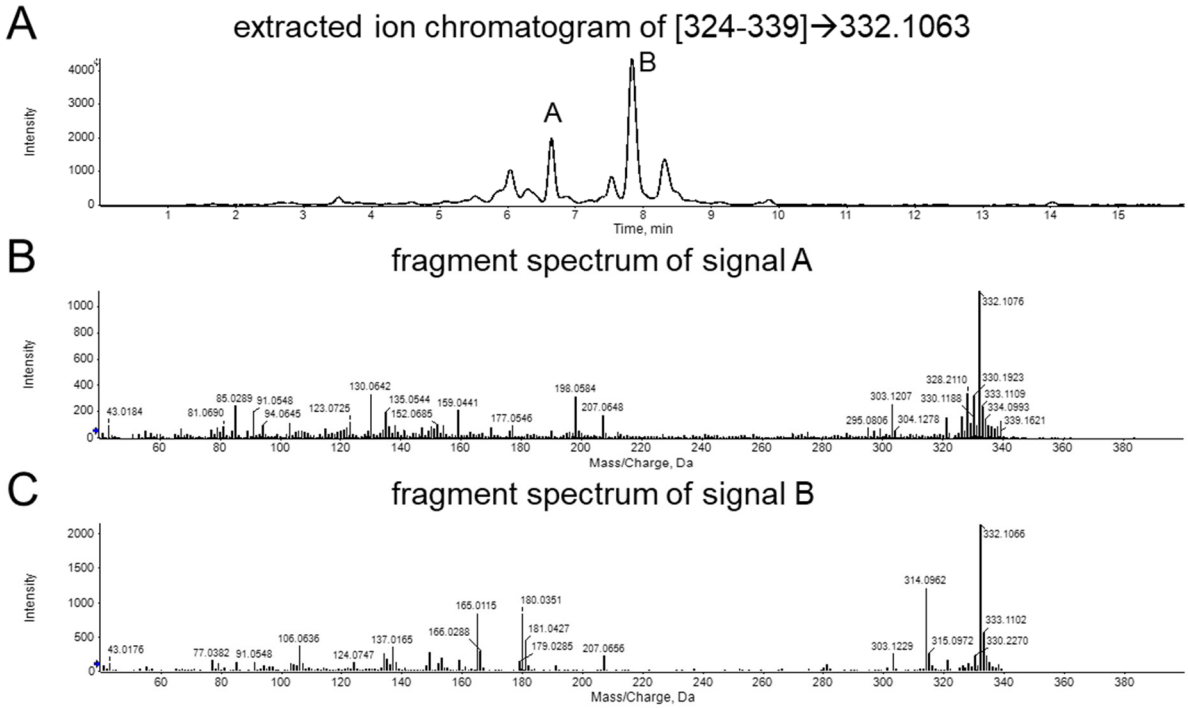
Supplemental Figure S10. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible mercapturate metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



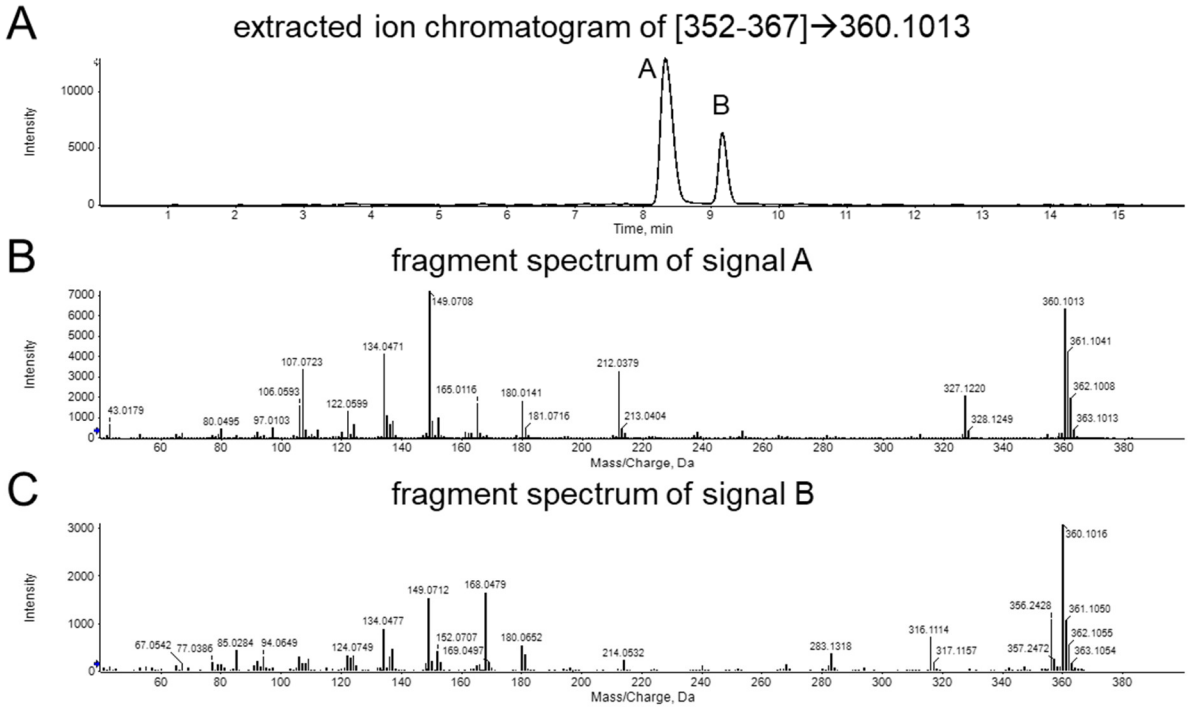
Supplemental Figure S11. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**) fragment spectra of possible demethylated and dehydroxylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



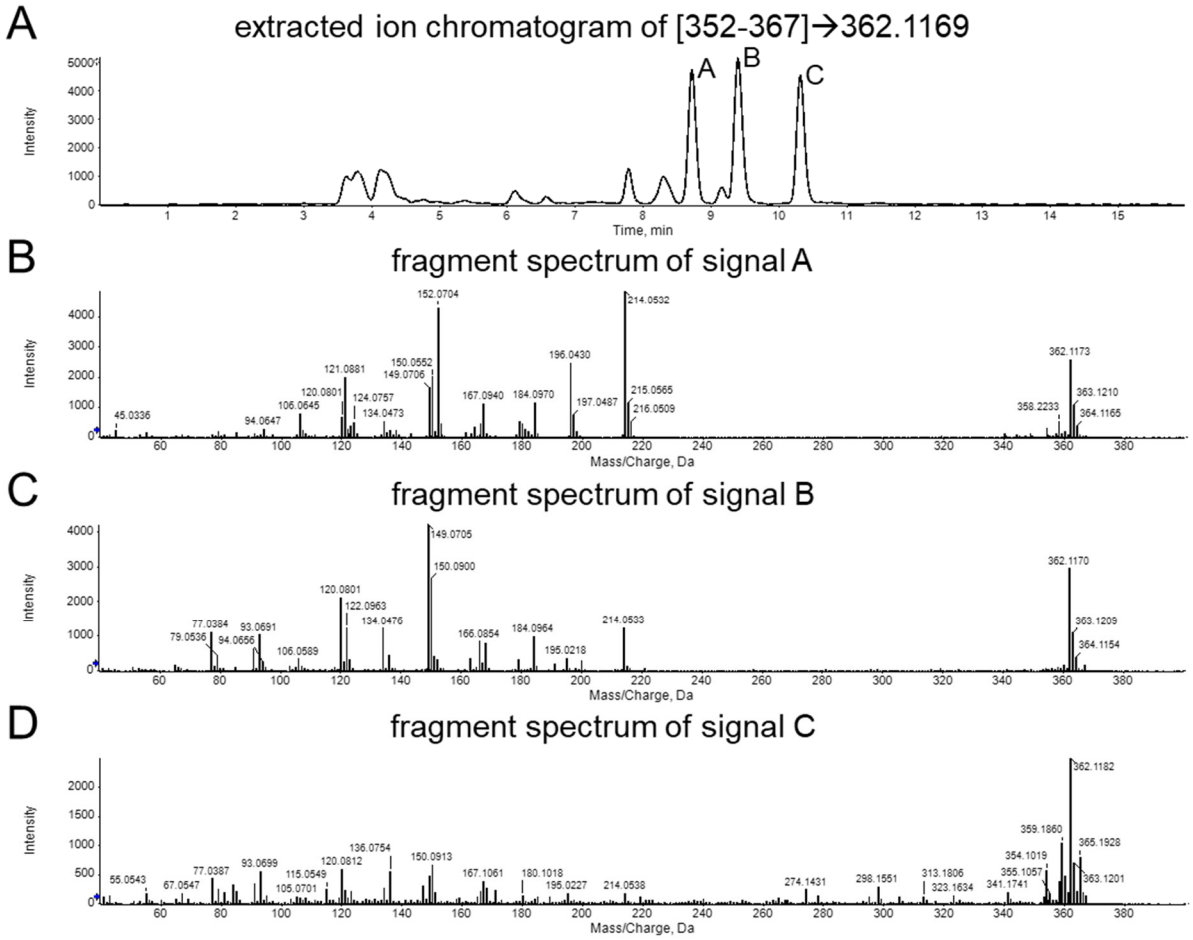
Supplemental Figure S12. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible dehydroxylated metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



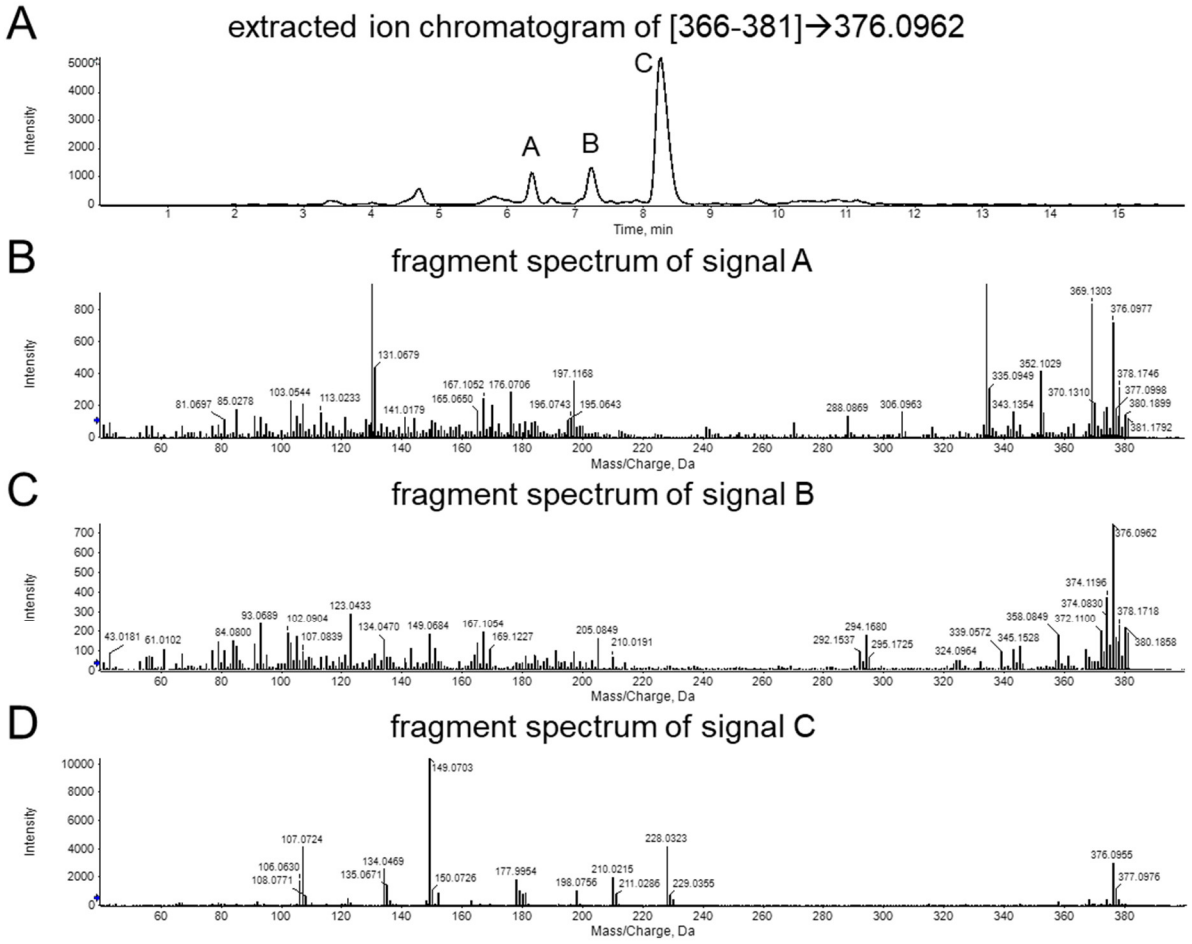
Supplemental Figure S13. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**) fragment spectra of possible demethylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



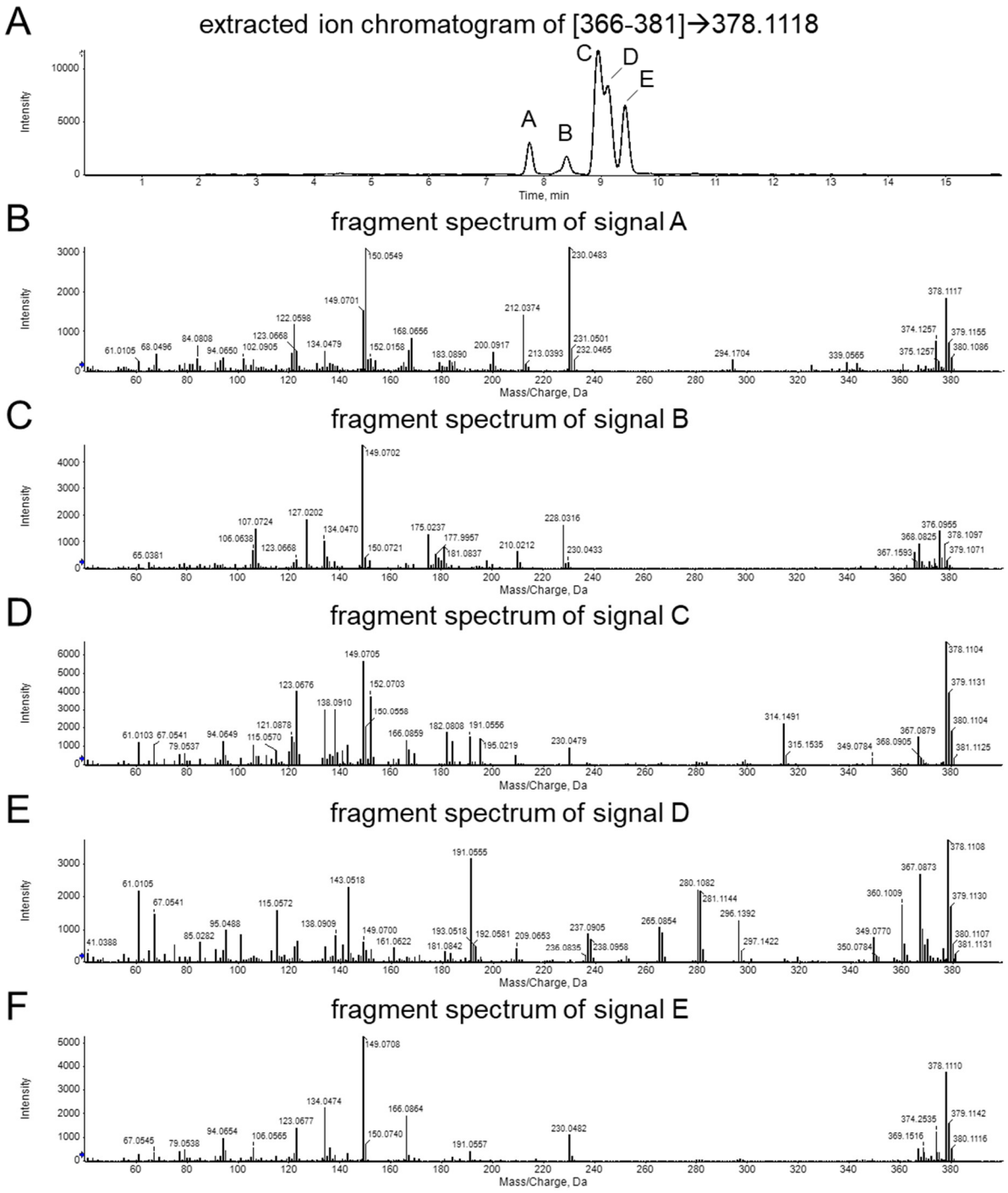
Supplemental Figure S14. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**) fragment spectra of possible dehydroxylated and carboxylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



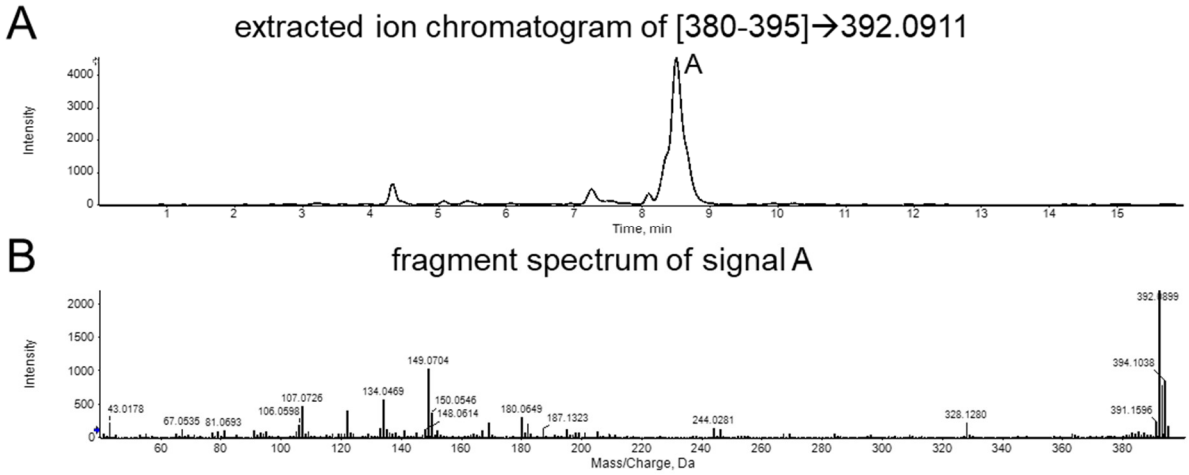
Supplemental Figure S15. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**) fragment spectra of possible hydroxylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



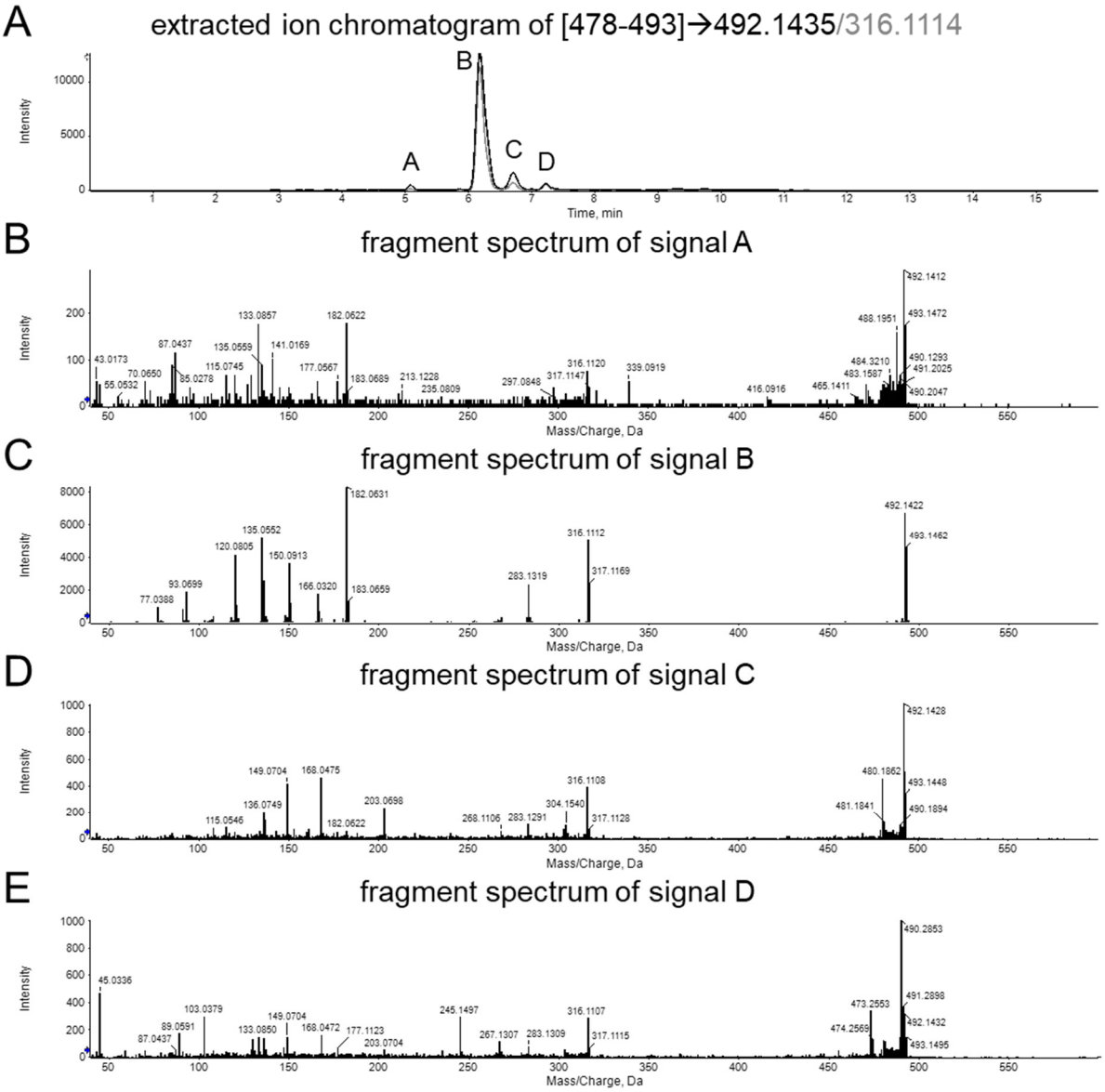
Supplemental Figure S16. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**) fragment spectra of possible carboxylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



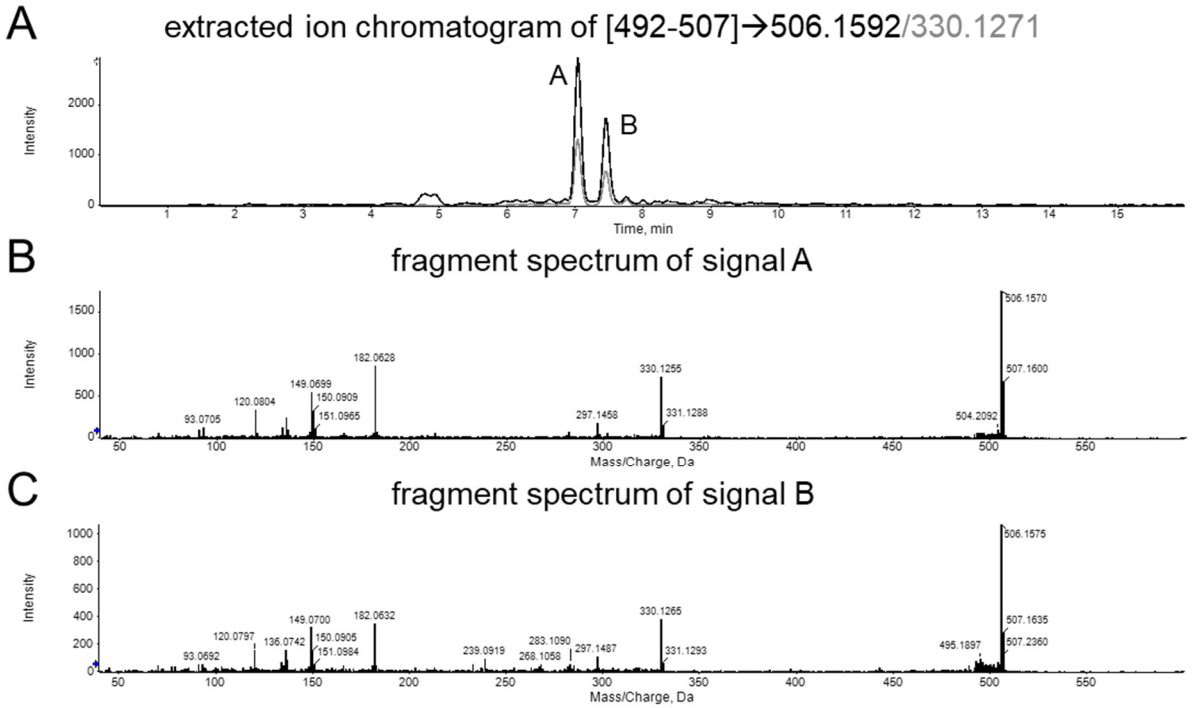
Supplemental Figure S17. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**, **E**, **F**) fragment spectra of possible dihydroxylated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



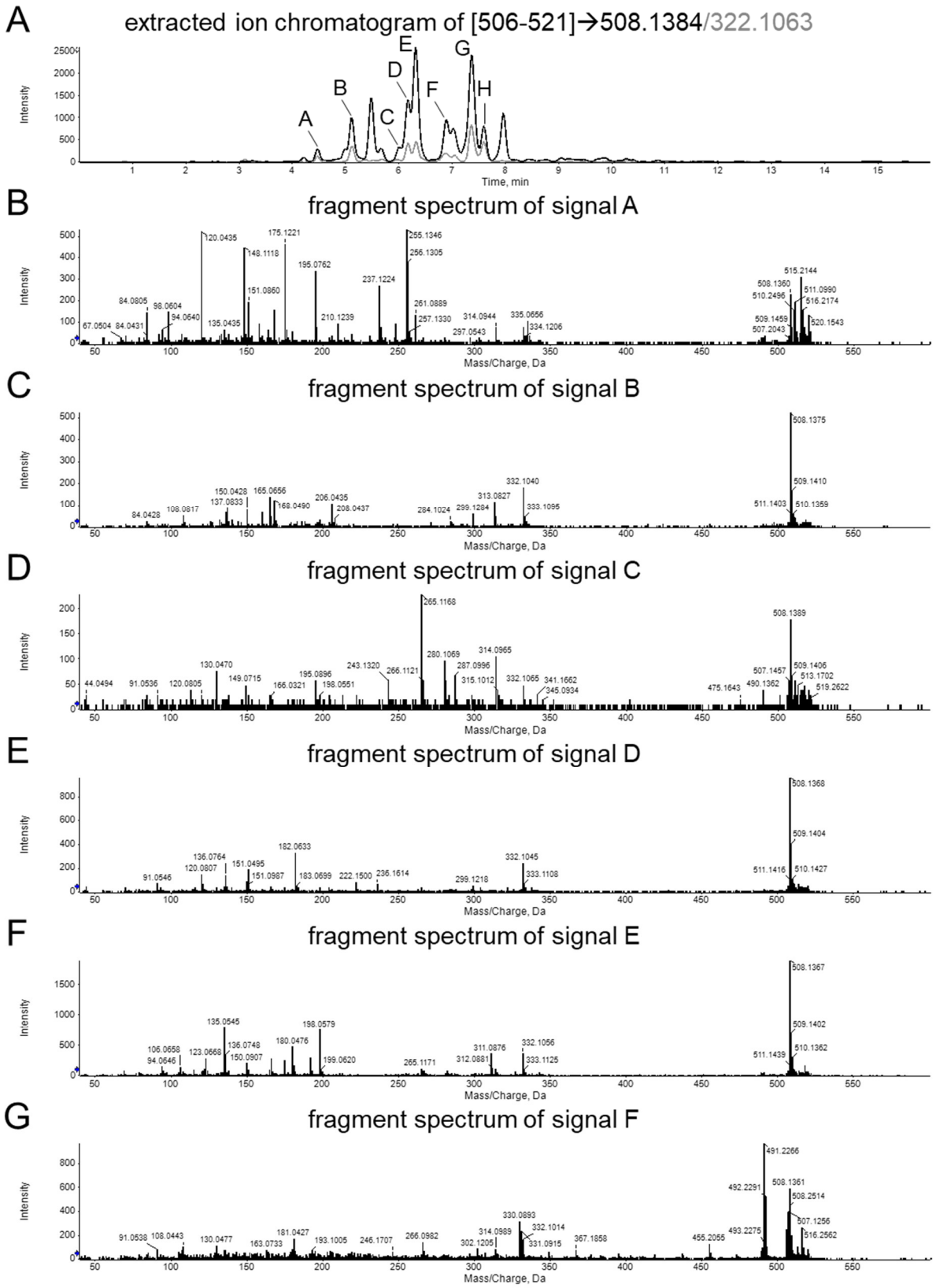
Supplemental Figure S18. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible hydroxylated and carboxylated metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



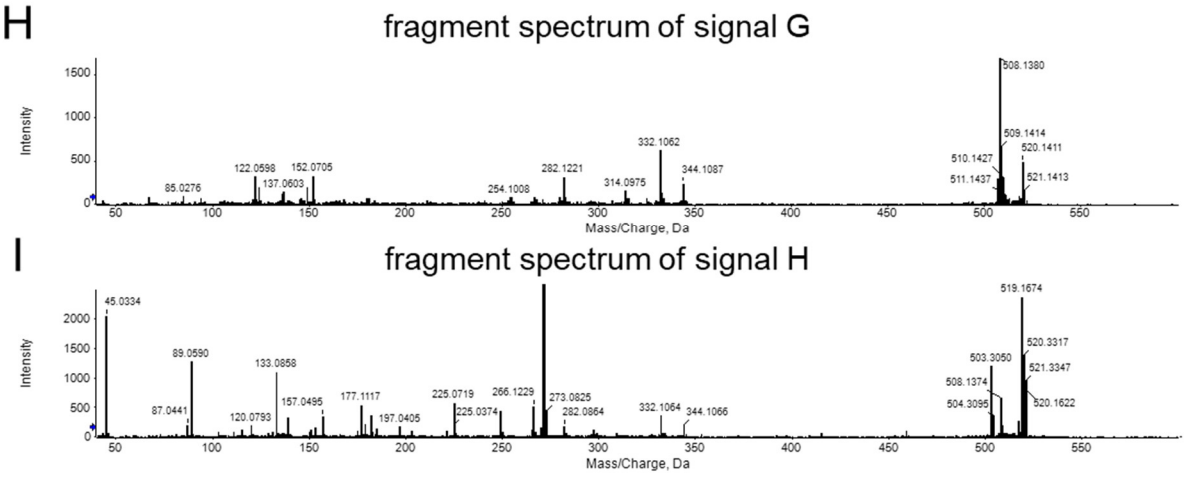
Supplemental Figure S19. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**, **E**) fragment spectra of possible demethylated, dehydroxylated, and glucuronidated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



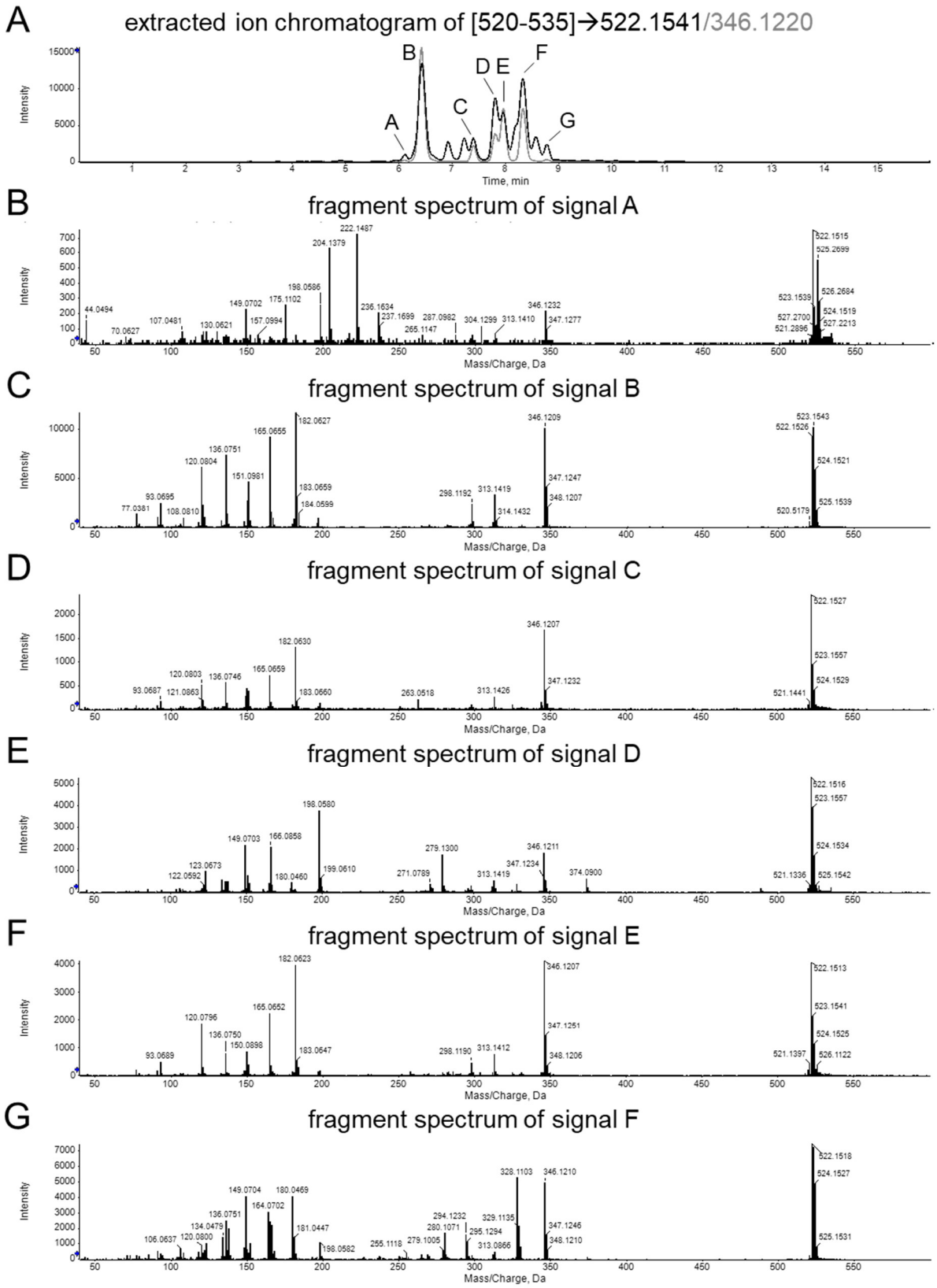
Supplemental Figure S20. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**) fragment spectra of possible dehydroxylated and glucuronidated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



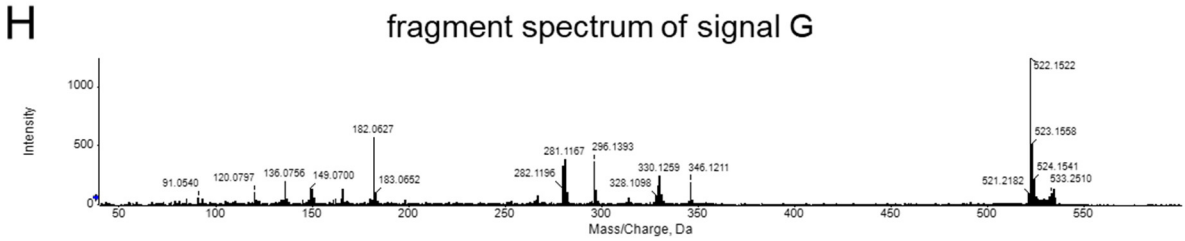
Supplemental Figure S21. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**, **E**, **F**, **G**, **H**, **I**) fragment spectra of possible demethylated and glucuronidated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



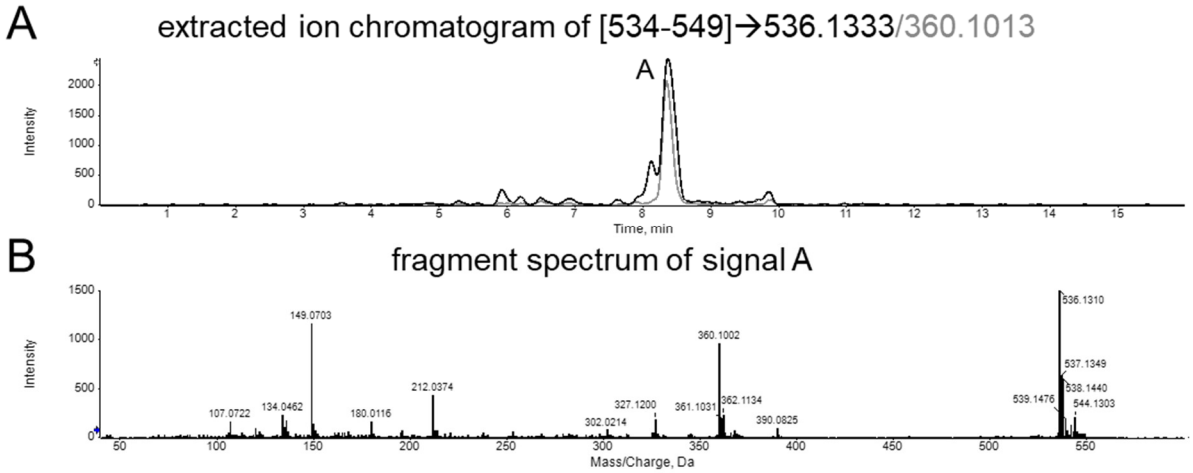
Supplemental Figure S21. *Cont*.



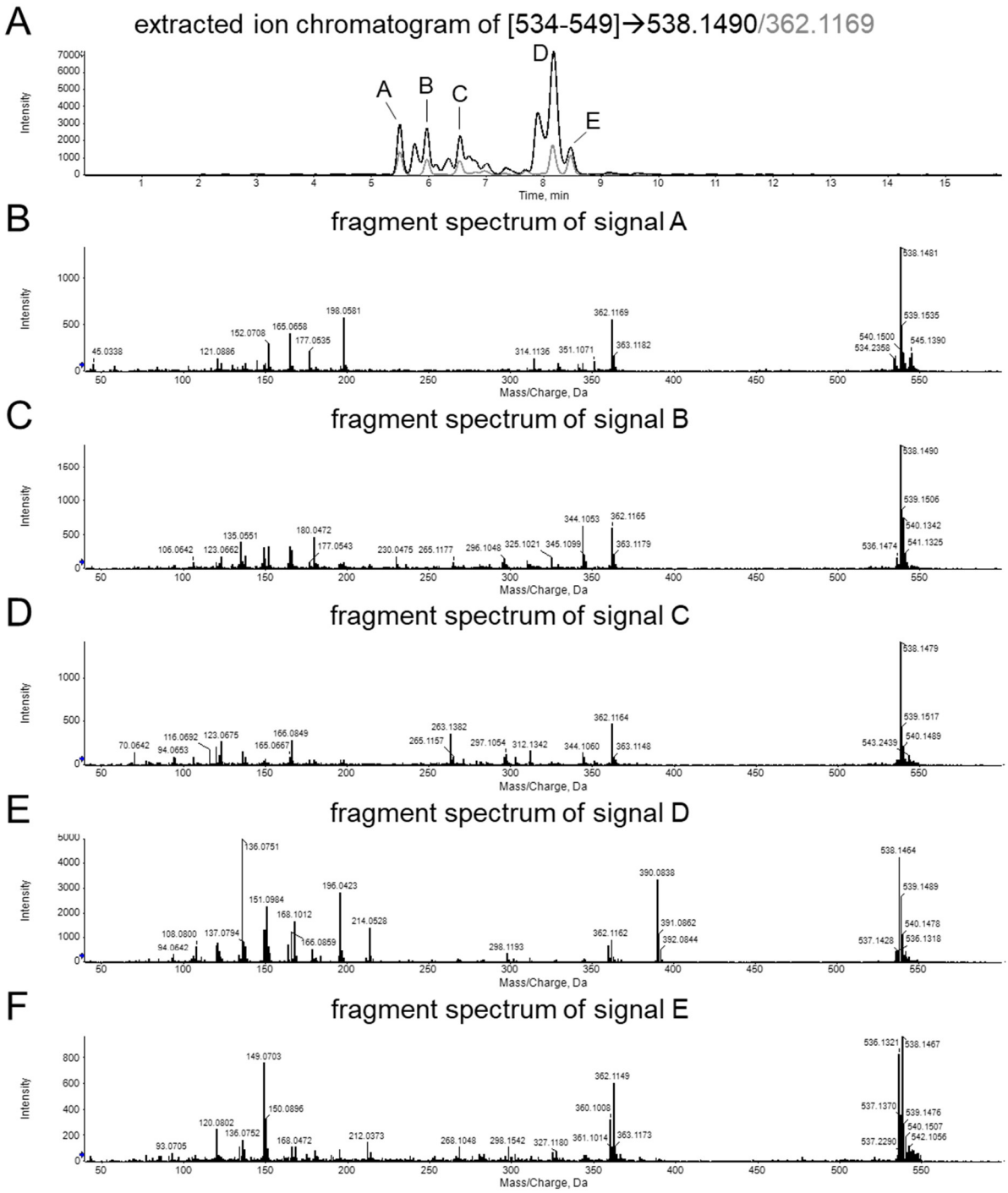
Supplemental Figure S22. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**, **E**, **F**, **G**, **H**) fragment spectra of possible glucuronidated metabolites of omeprazole. The blue arrows on the y-axes indicate thresholds for presenting m/z values.



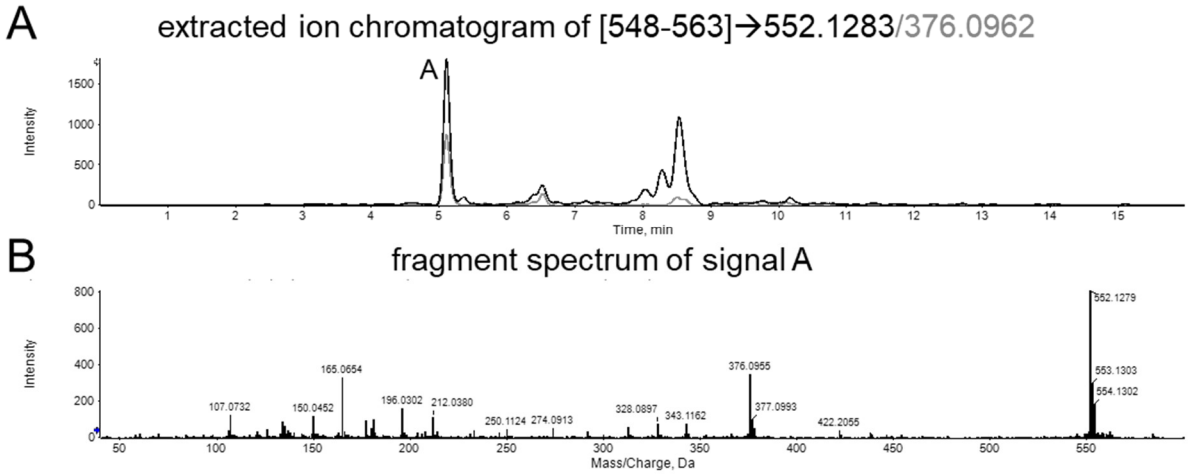
Supplemental Figure S22. *Cont*.



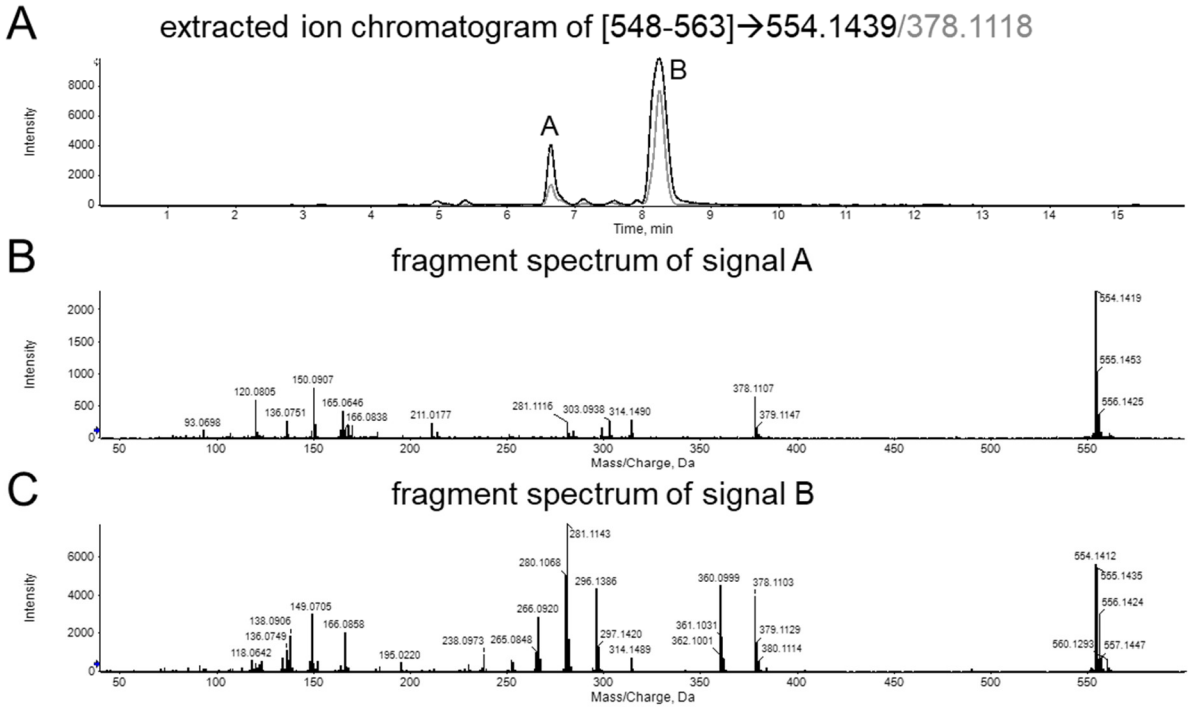
Supplemental Figure S23. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible dehydroxylated, carboxylated, and glucuronidated metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



Supplemental Figure S24. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**, **D**, **E**, **F**) fragment spectra of possible hydroxylated and glucuronidated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



Supplemental Figure S25. Exemplary (**A**) extracted ion chromatogram and (**B**) fragment spectrum of a possible carboxylated and glucuronidated metabolite of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.



Supplemental Figure S26. Exemplary (**A**) extracted ion chromatogram and (**B**, **C**) fragment spectra of possible dihydroxylated and glucuronidated metabolites of omeprazole. The blue and white arrows on the y-axes indicate thresholds for presenting m/z values.