Supporting Information

Anaerobic Transformation of the Iodinated X-ray Contrast Medium Iopromide, Its Aerobic Transformation Products, and Transfer to Further Iodinated X-ray Contrast Media

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40 pages, 29 tables, 12 figures

Content

Materials and methods

Chemicals, standards and solvents

Iopromide and DAMI were provided by Schering (Berlin, Germany). Iopromide-d3 was purchased from Toronto Research Chemicals (Toronto, Canada). DDPI was isolated by Schulz et al. (2008) from batch experiments conducted in the BfG laboratory. Diatrizoate and formic acid (eluent additive for LC-MS) were purchased from Sigma-Aldrich (Steinheim, Germany). Methanol (hypergrade for LC-MS) and sulfuric acid (98%, p.a.) were purchased from Merck (Darmstadt, Germany). Heptane and acetone (for residue analysis) were purchased from LGC Standards (Wesel, Germany). Ultrapure water was obtained from a Milli-Q water purification system (Millipore, Darmstadt, Germany). Nitric acid (65%, p.a.) was purchased from Merck (Darmstadt, Germany) and sub-boiled prior to use by means of a Savillex (Eden Prairie, MN, USA) DST-1000 sub-boiling unit.

Preparation, incubation and sampling of batch experiments using anaerobic techniques

The sediment for the batch experiments was taken from a sulfate reducing zone of a polishing pond that has been fed by treated wastewater from a conventional municipal WWTP with nitrification and denitrification (hydraulic retention time (biology): 24 h, solid retention time: 20 d) for several years. From this sediment 10 cm cores were taken by a cylindrical tube. The tube was immediately air tightly closed and transported to the lab of BfG, where it was transferred to the batch bottles in a glove box under argon atmosphere.

Rhine water was taken in Koblenz (km 590.3), Germany. Prior to the preparation of the anaerobic batch experiments, the water was purged with argon for 45 minutes.

After adding oxygen free Rhine water to the anaerobic sediment in the glove box, all bottles were closed with butyl stoppers and purged with argon for another 20 – 30 min. The batch experiments were incubated for 43 d in the dark at room temperature (22±1°C) on a shaking device (KS 260 B, IKA Werke, Staufen, Germany) at 150 rpm. Strictly anaerobic (sulfate-reducing) conditions in the batch experiments were confirmed by monitoring the redox potential and the concentrations of oxygen, sulfate and sulfide in the blank replicates.

Gas-tight syringes (Omnifix®, B. Braun, Melsungen, Germany) which had been extensively purged with argon were used for sampling. The samples were taken by injecting 1 – 1.5 mL of argon into the bottles through the butyl stoppers and withdrawing the same volume of the aqueous phase. They were passed through 0.45 µm regenerated cellulose syringe filters (C. Roth, Karlsruhe, Germany) into 1.5 mL HPLC glass vials.

Q-ToF-MS parameters for the identification of transformation products

The Dual AJS (Agilent Jet Stream) ESI source was operated in positive ionization mode. The source parameters were set as follows: capillary voltage, 3500 V; nozzle voltage, 0 V; fragmentor, 370 V; Octopole RF peak, 750 V; gas temperature, 180°C; gas flow, 16 L/min; nebulizer gas, 40 psig; sheath

gas temperature, 350°C; sheath gas flow, 12 L/min. Data dependent acquisition was used to gain MS^2 spectra as follows: a full scan (100 – 1000 m/z, positive mode) was performed followed by MS^2 for the three most intense ions with an intensity of >100. Collision induced dissociation (CID) with collision energies (CEs) of 10 V, 20 V and 30 V each was used for fragmentation. Active exclusion was applied (exclusion of masses for which three MS^2 experiments have been performed; exclusion duration: 0.2 min, i.e. half width of average chromatographic peaks) enabling also MS^2 experiments for less abundant ions (e.g., during co-elution of different substances). In addition, targeted MS^2 experiments were performed for TPs with too low abundances, and CEs of 40 V, 50 V and 60 V were applied for those TPs for which a fragmentation was not obtained with the lower CEs.

Each acquired MS spectrum was mass-recalibrated in real time. For this a reference mass solution prepared from the reference mass solution kit G1969-85001 (Agilent Technologies) was injected through the reference sprayer of the Dual AJS ESI source with a 1260 Infinity isocratic pump from Agilent Technologies. The flow rate was 10 µL/min (achieved with a flow splitter with a splitting ratio 1/100).

Quantification of iodinated TPs via LC-ICP-MS

For quantification of iodinated TPs an HPLC 1260 Infinity system coupled with a 7700 ICP-Q-MS from Agilent Technologies (Waldbronn, Germany) was used. Coupling was carried out with a peltier-cooled double-pass glass Scott spray-chamber (5 °C) and a PFA-ST ES-2040 nebulizer (Elemental Scientific Inc., Omaha, NE, USA).

A Hydro-RP column (250 mm x 3 mm, 4 µm; Phenomenex, Aschaffenburg, Germany) was used for chromatographic separation. Mobile phase A contained 0.1% formic acid in ultrapure water. Mobile phase B consisted of 0.1% formic acid in methanol. The gradient of A was as follows: 0 – 10 min, 80%; 10.5 – 20 min, 10%; 20.1 – 30 min, 80%. The column oven was set to 40 °C, flow rate to 0.4 mL/min and injection volume was 20 µL.

By means of a T-piece (PEEK TEE P727, Upchurch Scientific, IDEX Health & Science LLC, Home of 244 Upchurch Scientific, Ismatec Products; Oak Harbor, WA, USA) and a peristaltic pump (Gilson, MiniPuls 3) an internal standard (10 µg Ce/L in 6.5% HNO3 (v/v)) was added post-column to control the spray, to enable correction of a potential drift as well as to abet ionization in the ICP source.

The following ICP-MS parameters were applied: Power, 1550 W; carrier gas flow rate, 0.75 L/min; aux gas flow rate, 0.9 L/min; cool gas flow rate, 15 L/min; sampling time, 0.1 s; sampling period, 0.204 s; acquisition time, 30 min; acquisition mode, TRA. The monitored isotopes were ^{127}I and ^{140}Ce. An external calibration was prepared by diluting diatrizoate in ultrapure water (1 µg/L – 500 µg/L, 10 points). The limit of quantification (LOQ) was estimated as the lowest concentration with a signal to noise ratio > 10 that was in the linear range of the calibration curve.

Whether the species- and matrix-unspecific is valid for the model substances and similar compounds was tested by injecting solutions of 52 nmol/L, which corresponds to an organic-bound iodine concentration of 20 µg/L, in ultrapure water. The ICMs iopromide, iomeprol, iopamidol, iohexol and diatrizoate were tested as well as three structurally related triiodinated aromatic compounds, DAMI, 5-amino-2,4,6-triiodisophthalic acid (ATIA) and 3,5-Diamino-2,4,6-triiodibenzoic acid. The solutions

were injected without chromatographic separation into the ICP-MS instrument. Defining the signal intensity of diatrizoate as 100%, the intensities of the other analytes were between 103% and 112%.

Quantification of iodide via IC-MS

A 940 Professional IC Vario with chemical suppressor from Metrohm (Filderstadt, Germany) was coupled with an API 4000 triple quadrupole mass spectrometer from Sciex (Darmstadt, Germany). A MetroSep A Supp 5 column (150 mm x 4 mm, 5 µm) connected to a MetroSep A Supp 4/5 guard column (5 mm x 4 mm; both Metrohm, Filderstadt, Germany) was used for chromatographic separation. Mobile phase A was ultrapure water, mobile phase B was a carbonate buffer (8 mM Na_2CO_3 and 2.5 mM $NaHCO_3$ dissolved in 30% MeoH / 70% ultrapure water). The following gradient of mobile phase A was applied: 0 – 2 min, 70%; 5 – 20 min, 36%; 20,1 – 42 min, 60%. The flow rate was set to 0.7 mL/min, of which 0.35 mL/min were diverted post-column into the waste. The column temperature was 50 °C. The ESI source of the mass spectrometer was operated in negative ionization mode using multiple reaction monitoring. The monitored mass transition was Q1: 126.9 Da, Q3: 126.9 Da, DP: -120 V, CE: -75 eV, CXP: -1 V.

Calculation of response factors and concentrations in batch samples

Example: Iopromide TP 665 isomer with RT 8.3 min (without co-elution)

1. Select samples in which the TP isomer was detected via LC-Q-ToF-MS
2. Determine iodine concentration of the isomer ($c_{LC\text{-}ICP\text{-}MS,\mu gI/L}$) in selected samples by LC-ICP-MS
3. Calculate molar TP concentration of the isomer ($c_{LC\text{-}ICP\text{-}MS}$) from $c_{LC\text{-}ICP\text{-}MS,\mu gI/L}$:

   $$c_{LC\text{-}ICP\text{-}MS}=\frac{c_{LC\text{-}ICP\text{-}MS,\mu gI/L}}{2\times 127 g/mol}\times 1000,$$

   where 2 is the number of iodine atoms in the molecule, 127 g/mol is the molar mass of iodine and the multiplication by 1000 is for the translation from µg/L to nmol/L
4. Divide $c_{LC\text{-}ICP\text{-}MS}$ by normalized LC-Q-ToF-MS peak area ($A_{LC\text{-}Q\text{-}ToF\text{-}MS}$) to obtain response factor (RF):

   $$RF=\frac{c_{LC\text{-}ICP\text{-}MS}}{A_{LC\text{-}Q\text{-}ToF\text{-}MS}}$$
5. Calculate arithmetic mean and standard deviation of obtained RFs
6. Multiply $A_{LC\text{-}Q\text{-}ToF\text{-}MS}$ of each sample by arithmetic mean of RF:

   $$c_{calc}=A_{LC\text{-}Q\text{-}ToF\text{-}MS}\times RF$$

Table S1. Example for calculation of response factors and concentrations in batch samples (TP or TP isomer without co-elution)

	1.		2.	3.	4.	6.
Sample	**$A_{LC\text{-}Q\text{-}ToF\text{-}MS}$**		**$c_{LC\text{-}ICP\text{-}MS}$ / µg I/L**	**$c_{LC\text{-}ICP\text{-}MS}$ / nmol/L**	**RF**	**c_{calc} / nmol/L**
Replicate 1, 0d	0.0047		*<10*	*<39*		*<15*
Replicate 1, 5d	0.0652		33	129	1972	112
Replicate 1, 13d	0.0333		19	75	2259	57
Replicate 1, 20d	0.0125		*<10*	*<39*		21
Replicate 1, 29d	*not detected*					
Replicate 1, 43d	*not detected*					
Replicate 2, 0d	0.0058		*<10*	*<39*		*<15*
Replicate 2, 5d	0.0745		30	117	1566	127
Replicate 2, 13d	0.1116		46	183	1640	191
Replicate 2, 20d	0.0928		34	136	1463	159
Replicate 2, 29d	0.0023		*<10*	*<39*		*<15*
Replicate 2, 43d	*not detected*					
Replicate 3, 0d	0.0045		*<10*	*<39*		*<15*
Replicate 3, 5d	0.0766		30	120	1562	131
Replicate 3, 13d	0.1128		48	189	1678	193
Replicate 3, 20d	0.1047		42	164	1569	179
Replicate 3, 29d	0.0029		*<10*	*<39*		*<15*
Replicate 3, 43d	*not detected*					
				n =	8	
		5.		arithmetic mean (rounded do tens)	1710	
				standard deviation (rounded do tens)	270	
				relative standard deviation	16%	

Example: Iopromide TP 665 isomer with RT 5.7 – 7.7 min (with co-elution of iopromide isomers at 5.9 and 6.3 min)

Note: this calculation can be applied if the concentrations of the co-eluting isomers are known (e.g. because their response factors could be determined from samples taken at earlier incubation times).

1. Select samples in which the TP isomer was detected via LC-Q-ToF-MS

2. Determine total iodine concentration of targeted TP isomer and co-eluting isomer ($c_{LC\text{-}ICP\text{-}MS,tot,\mu gI/L}$) in selected samples by LC-ICP-MS
3. Subtract iodine concentration of co-eluting isomer ($c_{coe,\mu gI/L}$), which could be determined from samples taken at earlier incubation times or, for the target substances themselves, via LC-Q-ToF-MS, from $c_{LC\text{-}ICP\text{-}MS,tot,\mu gI/L}$
4. Calculate molar concentration of the difference:

   $$c_{LC\text{-}ICP\text{-}MS,tot}\text{-}c_{coe}=\frac{c_{LC\text{-}ICP\text{-}MS,\mu gI/L}-c_{coe,\mu g/L}}{2\times 127 g/mol}\times 1000,$$

   where 2 is the number of iodine atoms in the targeted isomer, 127 g/mol is the molar mass of iodine and the multiplication by 1000 is for the translation from µg/L to nmol/L
5. Divide molar difference of $c_{LC\text{-}ICP\text{-}MS,tot}$ and c_{coe} calculated in point 4. by normalized LC-Q-ToF-MS peak area ($A_{LC\text{-}Q\text{-}ToF\text{-}MS}$) to obtain response factor (RF):

   $$RF=\frac{c_{LC\text{-}ICP\text{-}MS,tot}-c_{coe}}{A_{LC\text{-}Q\text{-}ToF\text{-}MS}}$$
6. Calculate arithmetic mean and standard deviation of obtained RFs, ignore apparent outliers (in this example those where the TP 665 isomer was less than 20% of the total concentration of itself and the co-eluting iopromide isomer)
7. Multiply $A_{LC\text{-}Q\text{-}ToF\text{-}MS}$ of each sample by arithmetic mean of RF:

   $$c_{calc}=A_{LC\text{-}Q\text{-}ToF\text{-}MS}\times RF$$

Table S2. Example for calculation of response factors and concentrations in batch samples (TP or TP isomer with co-elution)

	1.		2.		3.	4.	5.	7.
Sample	**$A_{LC\text{-}Q\text{-}ToF\text{-}MS}$**		**$c_{LC\text{-}ICP\text{-}MS,tot}$ / µg l/L**	**c_{coe} / µg l/L**	**$c_{LC\text{-}ICP\text{-}MS,tot}$ - c_{coe} / µg l/L (% of $c_{LC\text{-}ICP\text{-}MS,tot}$)**	**$c_{LC\text{-}ICP\text{-}MS,tot}$ - c_{coe} / nmol/L**	**RF**	**c_{calc} / nmol/L**
Replicate 1, 0d	0.0178		972	851	121 (12)	476	26668	30
Replicate 1, 5d	0.3155		474	304	170 (36)	669	2125	536
Replicate 1, 13d	0.1938		109	25	84 (77)	331	1706	329
Replicate 1, 20d	0.0373		17	*<10*	17 (100)	67	1788	63
Replicate 1, 29d	*not detected*							
Replicate 1, 43d	*not detected*							
Replicate 2, 0d	0.0233		842	880	0 (0)			40
Replicate 2, 5d	0.2962		579	434	145 (25)	571	1929	504
Replicate 2, 13d	0.3793		302	147	155 (51)	610	1613	645
Replicate 2, 20d	0.1756		71	13	58 (81)	228	1296	298
Replicate 2, 29d	*not detected*							
Replicate 2, 43d	*not detected*							
Replicate 3, 0d	0.0218		855	787	68 (8)	268	12307	37
Replicate 3, 5d	0.2897		595	461	134 (22)	528	1816	492
Replicate 3, 13d	0.3852		327	158	170 (52)	669	1733	655
Replicate 3, 20d	0.1980		81	16	65 (80)	256	1292	337
Replicate 3, 29d	*not detected*							
Replicate 3, 43d	*not detected*							
						n =	9	
		6.				arithmetic mean (rounded do tens)	1700	
						standard deviation (rounded do tens)	270	
						relative standard deviation	16%	

Enrichment of bank filtrate samples via solid phase extraction (SPE)

No analytical standards were available to test suitable SPE methods for the enrichment of the compounds in the data base. In order to have the highest chance to detect the suspected TPs, two different methods were applied which were used earlier for the enrichment of ICMs.[1, 2]

SPE method 1: A sample volume of 450 mL, to which 1 ng of iopromide-d_3 had been added as internal standard, was loaded by gravity onto Oasis HLB 200 cartridges (Waters, Eschborn, Germany) preconditioned with 1 x 2 mL heptane, 1 x 2 mL acetone, 3 x 2 mL methanol, 4 x 2 mL ultrapure water. The loaded cartridges were dried with nitrogen gas. The analytes were eluted with 4 x 2 mL acetone and the organic phase was reduced to 100 µL by evaporation under a light nitrogen gas flow. 400 µL of ultrapure water were added.

SPE method 2: A sample volume of 450 mL was adjusted to pH 2.6 – 2.8 using 3.5 M sulfuric acid and 1 ng of iopromide-d_3 was added as internal standard. The samples were loaded by gravity onto Bakerbond SDB1 cartridges (200 mg, 3 mL, J.T. Baker, Deventer, the Netherlands), which had been preconditioned with 2 x 2.5 mL methanol and 4 x 2 mL ultrapure water. The loaded cartridges were dried with nitrogen gas. The analytes were eluted with 4 x 2 mL methanol and the organic phase was reduced to 100 µL by evaporation under a light nitrogen gas flow. 400 µL of ultrapure water were added.

Suspect screening of anaerobic TPs in bank filtrate samples

Table S3. Database of experimental and predicted anaerobic TPs of ICMs and of their aerobic TPs

Anaerobic TP	**Elemental compsotion**	**Experimental / predicted**	**Source**
Iopromide TP 665	$C_{18}H_{25}I_2N_3O_8$	experimental	
Iopromide TP 539	$C_{18}H_{26}IN_3O_8$	experimental	
Iopromide TP 467	$C_{15}H_{22}IN_3O_6$	experimental	
Iopromide TP 413	$C_{18}H_{27}N_3O_8$	experimental	
Iopromide TP 341	$C_{15}H_{23}N_3O_6$	experimental	
DDPI TP 517	$C_{12}H_{13}I_2N_3O_4$	experimental	
DDPI TP 445	$C_9H_9I_2N_3O_2$	experimental	
DDPI TP 391	$C_{12}H_{14}IN_3O_4$	experimental	
DDPI TP 319	$C_9H_{10}IN_3O_2$	experimental	
DDPI TP 265	$C_{12}H_{15}N_3O_4$	experimental	
DDPI TP 193	$C_9H_{11}N_3O_2$	experimental	
DAMI TP 593	$C_{15}H_{21}I_2N_3O_6$	experimental	
DAMI TP 467	$C_{15}H_{22}IN_3O_6$	experimental	
DAMI TP 341	$C_{15}H_{23}N_3O_6$	experimental	
DAMI TP 380	$C_{11}H_{13}IN_2O_5$	experimental	
DAMI TP 254	$C_{11}H_{14}N_2O_5$	experimental	
Diatrizoate TP 488	$C_{11}H_{10}I_2N_2O_4$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 362	$C_{11}H_{11}IN_2O_4$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 320	$C_9H_9IN_2O_3$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 278	$C_7H_7IN_2O_2$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 236	$C_{11}H_{12}N_2O_4$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 194	$C_9H_{10}N_2O_3$	experimental	Redeker et al. (2014)[3]
Diatrizoate TP 152	$C_7H_8N_2O_2$	experimental	Redeker et al. (2014)[3]
Iopromide TP 805 A or B -1I	$C_{18}H_{23}I_2N_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 805 A or B -2I	$C_{18}H_{24}IN_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 805 A or B -3I	$C_{18}H_{25}N_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 805 A or B -1I $-C_3H_4O_2$	$C_{15}H_{19}I_2N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 805 A or B -2I $-C_3H_4O_2$	$C_{15}H_{20}IN_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 805 A or B -3I $-C_3H_4O_2$	$C_{15}H_{21}N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -I	$C_{18}H_{21}I_2N_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -2I	$C_{18}H_{22}IN_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -3I	$C_{18}H_{23}N_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -1I $-C_3H_4O_2$	$C_{15}H_{17}I_2N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -2I $-C_3H_4O_2$	$C_{15}H_{18}IN_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 819 -3I $-C_3H_4O_2$	$C_{15}H_{19}N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -I	$C_{18}H_{19}I_2N_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -2I	$C_{18}H_{20}IN_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -3I	$C_{18}H_{21}N_3O_{10}$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -1I $-C_3H_4O_2$	$C_{15}H_{15}I_2N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -2I $-C_3H_4O_2$	$C_{15}H_{16}IN_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 817 -3I $-C_3H_4O_2$	$C_{15}H_{17}N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 731 A or B -I	$C_{15}H_{17}I_2N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]

Iopromide TP 731 A or B -2I	$C_{15}H_{18}IN_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 731 A or B -3I	$C_{15}H_{19}N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 731 A or B -1I -$C_3H_4O_2$	$C_{12}H_{13}I_2N_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 731 A or B -2I -$C_3H_4O_2$	$C_{12}H_{14}IN_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 731 A or B -3I -$C_3H_4O_2$	$C_{12}H_{15}N_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -I	$C_{15}H_{15}I_2N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -2I	$C_{15}H_{16}IN_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -3I	$C_{15}H_{17}N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -1I -$C_3H_4O_2$	$C_{12}H_{11}I_2N_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -2I -$C_3H_4O_2$	$C_{12}H_{12}IN_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 729 -3I -$C_3H_4O_2$	$C_{12}H_{13}N_3O_5$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -I	$C_{17}H_{17}I_2N_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -2I	$C_{17}H_{18}IN_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -3I	$C_{17}H_{19}N_3O_9$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -1I -$C_3H_4O_2$	$C_{14}H_{13}I_2N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -2I -$C_3H_4O_2$	$C_{14}H_{14}IN_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 787 -3I -$C_3H_4O_2$	$C_{14}H_{15}N_3O_7$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -I	$C_{16}H_{17}I_2N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -2I	$C_{16}H_{18}IN_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -3I	$C_{16}H_{19}N_3O_8$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -1I -$C_3H_4O_2$	$C_{13}H_{13}I_2N_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -2I -$C_3H_4O_2$	$C_{13}H_{14}IN_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 759 -3I -$C_3H_4O_2$	$C_{13}H_{15}N_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -I	$C_{14}H_{15}I_2N_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -2I	$C_{14}H_{16}IN_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -3I	$C_{14}H_{17}N_3O_6$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -1I -$C_3H_4O_2$	$C_{11}H_{11}I_2N_3O_4$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -2I -$C_3H_4O_2$	$C_{11}H_{12}IN_3O_4$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopromide TP 701 A or B -3I -$C_3H_4O_2$	$C_{11}H_{13}N_3O_4$	predicted	aerobic precursor TP: Schulz et al. (2008)[4]
Iopamidol -I	$C_{17}H_{23}I_2N_3O_8$	predicted	
Iopamidol -2I	$C_{17}H_{24}IN_3O_8$	predicted	
Iopamidol -3I	$C_{17}H_{25}N_3O_8$	predicted	
Iopamidol -1I -$C_3H_4O_2$	$C_{14}H_{19}I_2N_3O_6$	predicted	
Iopamidol -2I -$C_3H_4O_2$	$C_{14}H_{20}IN_3O_6$	predicted	
Iopamidol -3I -$C_3H_4O_2$	$C_{14}H_{21}N_3O_6$	predicted	
Iopamidol TP 805 -I	$C_{17}H_{19}I_2N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 805 -2I	$C_{17}H_{20}IN_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 805 -3I	$C_{17}H_{21}N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 805 -1I -$C_3H_4O_2$	$C_{14}H_{15}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 805 -2I -$C_3H_4O_2$	$C_{14}H_{16}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 805 -3I -$C_3H_4O_2$	$C_{14}H_{17}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 791 -I	$C_{17}H_{21}I_2N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 791 -2I	$C_{17}H_{22}IN_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 791 -3I	$C_{17}H_{23}N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 791 -1I -$C_3H_4O_2$	$C_{14}H_{17}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 791 -2I -$C_3H_4O_2$	$C_{14}H_{18}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]

Iopamidol TP 791 -3I -$C_3H_4O_2$	$C_{14}H_{19}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -I	$C_{16}H_{15}I_2N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -2I	$C_{16}H_{16}IN_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -3I	$C_{16}H_{17}N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -1I -$C_3H_2O_2$	$C_{13}H_{13}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -2I -$C_3H_2O_2$	$C_{13}H_{14}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 773 -3I -$C_3H_2O_2$	$C_{13}H_{15}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -I	$C_{16}H_{19}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -2I	$C_{16}H_{20}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -3I	$C_{16}H_{21}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -1I -$C_3H_4O_2$	$C_{13}H_{15}I_2N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -2I -$C_3H_4O_2$	$C_{13}H_{16}IN_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 761 -3I -$C_3H_4O_2$	$C_{13}H_{17}N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -I	$C_{15}H_{15}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -2I	$C_{15}H_{16}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -3I	$C_{15}H_{17}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -1I -$C_3H_4O_2$	$C_{12}H_{11}I_2N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -2I -$C_3H_4O_2$	$C_{12}H_{12}IN_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 745 -3I -$C_3H_4O_2$	$C_{12}H_{13}N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -I	$C_{13}H_{13}I_2N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -2I	$C_{13}H_{14}IN_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -3I	$C_{13}H_{15}N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -1I -$C_3H_4O_2$	$C_{10}H_9I_2N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -2I -$C_3H_4O_2$	$C_{10}H_{10}IN_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 687 -3I -$C_3H_4O_2$	$C_{10}H_{11}N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iopamidol TP 717 -I	$C_{14}H_{16}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 717 -2I	$C_{14}H_{17}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 717 -3I	$C_{14}H_{18}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 717 -1I -$C_3H_4O_2$	$C_{11}H_{12}I_2N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 717 -2I -$C_3H_4O_2$	$C_{11}H_{13}IN_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 717 -3I -$C_3H_4O_2$	$C_{11}H_{14}N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol -1I	$C_{17}H_{23}I_2N_3O_8$	predicted	
Iomeprol -2I	$C_{17}H_{24}IN_3O_8$	predicted	
Iomeprol -3I	$C_{17}H_{25}N_3O_8$	predicted	
Iomeprol -1I -$C_2H_2O_2$	$C_{15}H_{21}I_2N_3O_6$	predicted	
Iomeprol -2I -$C_2H_2O_2$	$C_{15}H_{22}IN_3O_6$	predicted	
Iomeprol -3I -$C_2H_2O_2$	$C_{15}H_{23}N_3O_6$	predicted	
Iomeprol TP 819 -1I	$C_{17}H_{17}I_2N_3O_{11}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 819 -2I	$C_{17}H_{18}IN_3O_{11}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 819 -3I	$C_{17}H_{19}N_3O_{11}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 819 -1I -C_2O_3	$C_{15}H_{17}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 819 -2I -C_2O_3	$C_{15}H_{18}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 819 -3I -C_2O_3	$C_{15}H_{19}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -1I	$C_{17}H_{19}I_2N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -2I	$C_{17}H_{20}IN_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -3I	$C_{17}H_{21}N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -1I -$C_2H_2O_2$	$C_{15}H_{17}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -2I -$C_2H_2O_2$	$C_{15}H_{18}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 805 -3I -$C_2H_2O_2$	$C_{15}H_{19}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 789 -1I	$C_{16}H_{15}I_2N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 789 -2I	$C_{16}H_{16}IN_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 789 -3I	$C_{16}H_{17}N_3O_{10}$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]

Iomeprol TP 789 -1I -C_2O_3	$C_{14}H_{15}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 789 -2I -C_2O_3	$C_{14}H_{16}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 789 -3I -C_2O_3	$C_{14}H_{17}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -1I	$C_{14}H_{13}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -2I	$C_{14}H_{14}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -3I	$C_{14}H_{15}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -1I -C_2O_3	$C_{12}H_{13}I_2N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -2I -C_2O_3	$C_{12}H_{14}IN_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 731 -3I -C_2O_3	$C_{12}H_{15}N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -1I	$C_{14}H_{15}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -2I	$C_{14}H_{16}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -3I	$C_{14}H_{17}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -1I -$C_2H_2O_2$	$C_{12}H_{13}I_2N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -2I -$C_2H_2O_2$	$C_{12}H_{14}IN_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 717 -3I -$C_2H_2O_2$	$C_{12}H_{15}N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -1I	$C_{13}H_{11}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -2I	$C_{13}H_{12}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -3I	$C_{13}H_{13}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -1I -C_2O_3	$C_{11}H_{11}I_2N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -2I -C_2O_3	$C_{11}H_{12}IN_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 701 -3I -C_2O_3	$C_{11}H_{13}N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -1I	$C_{13}H_{13}I_2N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -2I	$C_{13}H_{14}IN_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -3I	$C_{13}H_{15}N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -1I -$C_2H_2O_2$	$C_{11}H_{11}I_2N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -2I -$C_2H_2O_2$	$C_{11}H_{12}IN_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 687 -3I -$C_2H_2O_2$	$C_{11}H_{13}N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -1I	$C_{11}H_9I_2N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -2I	$C_{11}H_{10}IN_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -3I	$C_{11}H_{11}N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -1I -C_2O_3	$C_9H_9I_2N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -2I -C_2O_3	$C_9H_{10}IN_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 643 -3I -C_2O_3	$C_9H_{11}N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -1I	$C_{11}H_{11}I_2N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -2I	$C_{11}H_{12}IN_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -3I	$C_{11}H_{13}N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -1I -$C_2H_2O_2$	$C_9H_9I_2N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -2I -$C_2H_2O_2$	$C_9H_{10}IN_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 629 -3I -$C_2H_2O_2$	$C_9H_{11}N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2009)[5]
Iomeprol TP 791 -1I	$C_{17}H_{21}I_2N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 791 -2I	$C_{17}H_{22}IN_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 791 -3I	$C_{17}H_{23}N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 791 -1I -$C_2H_2O_2$	$C_{15}H_{20}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 791 -2I -$C_2H_2O_2$	$C_{15}H_{21}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 791 -3I -$C_2H_2O_2$	$C_{15}H_{22}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 761 -1I	$C_{16}H_{20}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -1I	$C_{16}H_{18}I_2N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -2I	$C_{16}H_{19}IN_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -3I	$C_{16}H_{20}N_3O_9$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -1I -$C_2H_2O_2$	$C_{14}H_{16}I_2N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -2I -$C_2H_2O_2$	$C_{14}H_{17}IN_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 775 -3I -$C_2H_2O_2$	$C_{14}H_{18}N_3O_7$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]

Iopamidol TP 745 -I	$C_{15}H_{16}I_2N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 745 -2I	$C_{15}H_{17}IN_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 745 -3I	$C_{15}H_{18}N_3O_8$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 745 -1I -$C_3H_4O_2$	$C_{13}H_{14}I_2N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 745 -2I -$C_3H_4O_2$	$C_{13}H_{15}IN_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iopamidol TP 745 -3I -$C_3H_4O_2$	$C_{13}H_{16}N_3O_6$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 657 -2I	$C_{12}H_{13}IN_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 657 -3I	$C_{12}H_{14}N_3O_5$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 657 -1I -$C_2H_2O_2$	$C_{11}H_{12}I_2N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 657 -2I -$C_2H_2O_2$	$C_{11}H_{13}IN_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 657 -3I -$C_2H_2O_2$	$C_{11}H_{14}N_3O_4$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -1I	$C_{10}H_{10}I_2N_3O_3$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -2I	$C_{10}H_{11}IN_3O_3$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -3I	$C_{10}H_{12}N_3O_3$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -1I -CO	$C_9H_{10}I_2N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -2I -CO	$C_9H_{11}IN_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]
Iomeprol TP 599 -3I -CO	$C_9H_{12}N_3O_2$	predicted	aerobic precursor TP: Kormos et al. (2010)[6]

Results and discussion

Primary degradation of iopromide, DDPI and DAMI

Table S4. DT_{50} values for iopromide, DDPI and DAMI in anaerobic batch experiments

Substance	**observed DT_{50} replicate 1**	**observed DT_{50} replicate 2**	**observed DT_{50} replicate 3**	**mean DT_{50}**	**standard deviation DT_{50}**
Iopromide	4 d	5 d	7 d	5.3 d	1.5 d
DDPI	6 d	6.5 d	7 d	6.5 d	0.5 d
DAMI	8 d	10 d	11 d	9.7 d	1.5 d

Identification of transformation products

Table S5. Precursor and product ions of the iopromide peaks with RT 5.9 min and 6.3 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
791.8758	*5.9, 6.3*	*$C_{18}H_{25}I_3N_3O_8$*	*1.5*		*$[M+H]^+$*
773.8641	5.9, 6.3	$C_{18}H_{23}I_3N_3O_7$	3.0	H_2O	$[M+H-H_2O]^+$ or $[M+H-H_2O]^+$
700.8119	5.9, 6.3	$C_{15}H_{16}I_3N_2O_6$	2.6	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
686.7961	5.9, 6.3	$C_{14}H_{14}I_3N_2O_6$	2.8	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$
572.9008	5.9, 6.3	$C_{15}H_{15}I_2N_2O_6$	1.1	$C_3H_{10}INO_2$	$[M+H-H_2O-C_3H_7NO-HI]^+$
558.8842	5.9, 6.3	$C_{14}H_{13}I_2N_2O_6$	2.7	$C_4H_{12}INO_2$	$[M+H-H_2O-C_4H_9NO-HI]^+$
545.9142	5.9, 6.3	$C_{14}H_{16}I_2N_2O_5$	0.2	$C_4H_9INO_3$	$[M+H-H_2O-C_3H_7NO-I-CO]^{\cdot+}$
541.8828	5.9, 6.3	$C_{14}H_{12}I_2N_2O_5$	0.4	$C_4H_{13}INO_3$	$[M+H-H_2O-C_3H_7NO-HI-CH_3O]^{\cdot+}$
531.8971	5.9, 6.3	$C_{13}H_{14}I_2N_2O_5$	2.9	$C_5H_{11}INO_3$	$[M+H-H_2O-C_4H_9NO-I-CO]^{\cdot+}$
527.8659	5.9, 6.3	$C_{13}H_{10}I_2N_2O_5$	2.8	$C_5H_{15}INO_3$	$[M+H-H_2O-C_4H_9NO-HI-CH_3O]^{\cdot+}$
444.9875	5.9, 6.3	$C_{15}H_{14}IN_2O_6$	3.6	$C_3H_{11}I_2NO_2$	$[M+H-H_2O-C_3H_7NO-HI-HI]^+$
413.9689	5.9, 6.3	$C_{14}H_{11}IN_2O_5$	2.1	$C_4H_{14}I_2NO_3$	$[M+H-H_2O-C_3H_7NO-HI-CH_3O-HI]^{\cdot+}$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S6. Precursor and product ions of the iopromide TP 665 signals with RT 5.9 – 7.7 min, 8.3 min and 9.2 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
665.9790	*5.9-7.7, 8.3, 9.2*	*$C_{18}H_{26}I_2N_3O_8$*	*2.1*		*$[M+H]^+$*
647.9677	5.9-7.7, 8.3, 9.2	$C_{18}H_{24}I_2N_3O_7$	3.3	H_2O	$[M+H-H_2O]^+$ or $[M+H-H_2O]^+$
574.9141	5.9-7.7, 8.3, 9.2	$C_{15}H_{17}I_2N_2O_6$	5.1	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
560.9003	5.9-7.7, 8.3, 9.2	$C_{14}H_{15}I_2N_2O_6$	2.0	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$
447.0039	5.9-7.7, 8.3, 9.2	$C_{15}H_{16}IN_2O_6$	2.0	$C_3H_{10}INO_2$	$[M+H-H_2O-C_3H_7NO-HI]^+$
432.9870	5.9-7.7, 8.3, 9.2	$C_{14}H_{14}IN_2O_6$	4.9	$C_4H_{12}INO_2$	$[M+H-H_2O-C_4H_9NO-HI]^+$
415.9848	5.9-7.7	$C_{14}H_{13}IN_2O_5$	3.8	$C_4H_{13}INO_3$	$[M+H-H_2O-C_3H_7NO-HI-CH_3O]^{\cdot+}$
406.0003	5.9-7.7	$C_{13}H_{15}IN_2O_5$	4.3	$C_5H_{11}INO_3$	$[M+H-H_2O-C_4H_9NO-I-CO]^{\cdot+}$
401.9686	5.9-7.7, 8.3, 9.2	$C_{13}H_{11}IN_2O_5$	5.3	$C_5H_{15}INO_3$	$[M+H-H_2O-C_4H_9NO-HI-CH_3O]^{\cdot+}$
359.9342	8.3, 9.2	$C_{11}H_7INO_5$	5.8	$C_7H_{19}IN_2O_3$	$[M+H-H_2O-C_3H_7NO-HI-C_4H_9NO]^+$
247.0697	8.3	$C_{12}H_{11}N_2O_4$	6.5	$C_6H_{15}I_2NO_4$	$[M+H-H_2O-C_4H_9NO-I-CO-HI-CH_3O]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S7. Precursor and product ions of the iopromide TP 539 signals with RT 4.8 min, 5.2 min and 10.0 – 12.0 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
540.0826	*4.8, 5.2, 10.0-12.0*	*$C_{18}H_{27}IN_3O_8$*	*2.1*		*$[M+H]^+$*
522.0705	4.8, 5.2, 10.0-12.0	$C_{18}H_{25}IN_3O_7$	5.1	H_2O	$[M+H-H_2O]^+$ or $[M+H-H_2O]^+$
449.0193	4.8, 5.2, 10.0-12.0	$C_{15}H_{18}IN_2O_6$	2.4	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
435.0033	4.8, 5.2, 10.0-12.0	$C_{14}H_{16}IN_2O_6$	3.3	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$ or $[M+H-H_2O-C_4H_9NO]^+$
361.9509	4.8, 5.2	$C_{11}H_9INO_5$	3.0	$C_7H_{18}N_2O_3$	$[M+H-H_2O-C_4H_9NO-C_3H_7NO]^+$
345.9563	4.8, 5.2	$C_{11}H_9INO_4$	2.4	$C_7H_{18}N_2O_4$	$[M+H-H_2O-C_3H_7NO-C_4H_9NO_2]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2]^+$
321.1062	10.0-12.0	$C_{15}H_{17}N_2O_6$	5.9	$C_3H_{10}INO_2$	$[M+H-H_2O-C_3H_7NO-HI]^+$
307.0893	10.0-12.0	$C_{14}H_{15}N_2O_6$	10.3	$C_4H_{12}INO_2$	$[M+H-H_2O-C_4H_9NO-HI]^+$
294.1183	10.0-12.0	$C_{14}H_{18}N_2O_5$	9.3	$C_4H_9INO_3$	$[M+H-H_2O-C_3H_7NO-I-CO]^{\cdot+}$
280.1049	10.0-12.0	$C_{13}H_{16}N_2O_5$	1.7	$C_5H_{11}INO_3$	$[M+H-H_2O-C_4H_9NO-I-CO]^{\cdot+}$
276.0730	10.0-12.0	$C_{13}H_{12}N_2O_5$	3.9	$C_5H_{15}INO_3$	$[M+H-H_2O-C_4H_9NO-HI-CH_3O]^{\cdot+}$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S8. Precursor and product ions of iopromide TP 413 (RT 6.5 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
414.1862	*6.5*	*$C_{18}H_{28}N_3O_8$*	*2.2*		*$[M+H]^+$*
396.1758	6.5	$C_{18}H_{26}N_3O_7$	1.8	H_2O	$[M+H-H_2O]^+$ or $[M+H-H_2O]^+$
323.1236	6.5	$C_{15}H_{19}N_2O_6$	0.5	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
309.1074	6.5	$C_{14}H_{17}N_2O_6$	2.3	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$
236.0538	6.5	$C_{11}H_{10}NO_5$	6.6	$C_7H_{18}N_2O_3$	$[M+H-H_2O-C_4H_9NO-C_3H_7NO]^+$
220.0597	6.5	$C_{11}H_{10}NO_4$	3.2	$C_7H_{18}N_2O_4$	$[M+H-H_2O-C_3H_7NO-C_3H_6O_2-CH_3N]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2]^+$
190.0490	6.5	$C_{10}H_8NO_3$	4.7	$C_8H_{20}N_2O_5$	$[M+H-H_2O-C_3H_7NO-C_3H_6O_2-CH_3N-CH_2O]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2-CH_2O]^+$
162.0532	6.5	$C_9H_8NO_2$	5.9	$C_9H_{20}N_2O_6$	$[M+H-H_2O-C_3H_7NO-C_3H_6O_2-C_3H_5NO_2]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S9. Precursor and product ions of the iopromide TP 467 signals with RT 3.7 min, 3.9 min and 5.5 – 6.8 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
468.0615	*3.7, 3.9, 5.5-6.8*	*$C_{15}H_{23}IN_3O_6$*	*2.4*		*$[M+H]^+$*
376.9973	3.7, 3.9	$C_{12}H_{14}IN_2O_4$	5.2	$C_3H_9NO_2$	$[M+H-C_3H_9NO_2]^+$
362.9817	3.7, 3.9, 5.5-6.8	$C_{11}H_{12}IN_2O_4$	2.8	$C_4H_{11}NO_2$	$[M+H-C_4H_{11}NO_2]^+$ or $[M+H-H_2O-C_4H_9NO]^+$
289.9292	3.9	$C_8H_5INO_3$	5.7	$C_7H_{18}N_2O_3$	$[M+H-H_2O-C_4H_9NO-C_3H_7NO]^+$
261.9518	3.7, 3.9, 5.5-6.8	$C_7H_5INO_2$	0.4	$C_8H_{18}IN_2O_4$	$[M+H-H_2O-C_4H_9NO-C_3H_7NO-CO]^+$
260.9518	3.7	$C_7H_6IN_2O$	1.0	$C_8H_{17}NO_5$	$[M+H-C_5H_{11}NO_3-C_3H_6O_2]^+$
245.9405	3.7, 3.9	C_7H_5INO	0.5	$C_8H_{18}N_2O_5$	$[M+H-C_5H_{11}NO_3-C_3H_7NO_2]^+$
243.9236	5.5-6.8	C_7H_3INO	7.3	$C_8H_{20}N_2O_5$	$[M+H-H_2O-C_3H_7NO-C_5H_{11}NO_3]^+$ or $[M+H-H_2O-C_4H_9NO-C_4H_9NO_3]^+$
217.9454	3.7, 3.9	C_6H_5IN	3.2	$C_9H_{18}N_2O_6$	$[M+H-C_5H_{11}NO_3-C_3H_7NO_2-CO]^+$
134.0467	3.9	$C_7H_6N_2O$	5.7	$C_8H_{17}INO_5$	$[M+H-C_5H_{11}NO_3-C_3H_6O_2-I]^{\cdot+}$
133.0389	3.9	$C_7H_5N_2O$	5.6	$C_8H_{18}INO_5$	$[M+H-C_5H_{11}NO_3-C_3H_6O_2-HI]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S10. Precursor and product ions of iopromide TP 341 (RT 3.4 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
342.1657	*3.4*	*$C_{15}H_{24}N_3O_6$*	*0.8*		*$[M+H]^+$*
251.1024	3.4	$C_{12}H_{15}N_2O_4$	1.0	$C_3H_9NO_2$	$[M+H\text{-}C_3H_9NO_2]^+$
237.0865	3.4	$C_{11}H_{13}N_2O_4$	1.8	$C_4H_{11}NO_2$	$[M+H\text{-}C_4H_{11}NO_2]^+$ $[M+H\text{-}H_2O\text{-}C_4H_9NO]^+$
209.916	3.4	$C_{10}H_{13}N_2O_3$	2.1	$C_5H_{11}NO_3$	$[M+H\text{-}C_4H_{11}NO_2\text{-}CO]^+$
164.0346	3.4	$C_8H_6NO_3$	2.3	$C_7H_{18}N_2O_3$	$[M+H\text{-}H_2O\text{-}C_4H_9NO\text{-}C_3H_7NO]^+$
148.0375	3.4	$C_8H_6NO_2$	12.0	$C_7H_{18}N_2O_4$	$[M+H\text{-}C_3H_9NO_2\text{-}C_4H_9NO_2]^+$ or $[M+H\text{-}C_4H_{11}NO_2\text{-}C_3H_7NO_2]^+$
135.0545	3.4	$C_7H_7N_2O$	6.0	$C_8H_{17}NO_5$	$[M+H\text{-}C_4H_{11}NO_2\text{-}CO\text{-}C_3H_6O_2]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S11. Precursor and product ions of DDPI (RT 7.8 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
643.8029	*7.8*	*$C_{12}H_{13}I_3N_3O_4$*	*0.9*		*$[M+H]^+$*
626.7742	7.8	$C_{12}H_{10}I_3N_2O_4$	4.3	H_3N	$[M+H\text{-}NH_3]^+$
612.7616	7.8	$C_{11}H_8I_3N_2O_4$	0.1	CH_5N	$[M+H\text{-}CH_5N]^+$
516.8963	7.8	$C_{12}H_{13}I_2N_3O_4$	3.9	I	$[M+H\text{-}I]^{\cdot+}$
498.8610	7.8	$C_{12}H_9I_2N_2O_4$	7.3	H_4IN	$[M+H\text{-}NH_3\text{-}HI]^+$
483.8618	7.8	$C_{11}H_8I_2N_3O_3$	6.5	CH_5IO	$[M+H\text{-}HI\text{-}CH_4O]^+$
471.8782	7.8	$C_{11}H_{10}I_2N_2O_3$	1.5	CH_3INO	$[M+H\text{-}NH_3\text{-}CO\text{-}I]^{\cdot+}$
467.8451	7.8	$C_{11}H_6I_2N_2O_3$	2.4	CH_7INO	$[M+H\text{-}NH_3\text{-}HI\text{-}CH_3O]^{\cdot+}$
457.8577	7.8	$C_{10}H_8I_2N_2O_3$	9.2	C_2H_5INO	$[M+H\text{-}CH_5N\text{-}CO\text{-}I]^{\cdot+}$
389.9931	7.8	$C_{12}H_{13}IN_3O_4$	3.7	I_2	$[M+H\text{-}I\text{-}I]^+$
357.9680	7.8	$C_{11}H_9IN_3O_3$	1.0	CH_4I_2O	$[M+H\text{-}I\text{-}HI\text{-}CH_3O]^{\cdot\cdot+}$
330.9557	7.8	$C_{10}H_8IN_2O_3$	6.4	$C_2H_5I_2NO$	$[M+H\text{-}HI\text{-}I\text{-}C_2H_4NO]^+$
329.9694	7.8	$C_{10}H_9IN_3O_2$	12.2	$C_2H_4I_2O_2$	$[M+H\text{-}I\text{-}I\text{-}CH_4O\text{-}CO]^+$
230.0554	7.8	$C_{11}H_8N_3O_3$	3.6	CH_5I_3O	$[M+H\text{-}I\text{-}I\text{-}CH_4O\text{-}HI]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S12. Precursor and product ions of the DDPI TP 517 signals with RT 7.4 min, 7.6 min and 9.3 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
517.9056	*7.4, 7.6, 9.3*	*$C_{12}H_{14}I_2N_3O_4$*	*2.4*		*$[M+H]^+$*
500.8815	7.4, 7.6, 9.3	$C_{12}H_{11}I_2N_2O_4$	2.4	H_3N	$[M+H-H_3N]^+$
486.8633	7.4, 7.6, 9.3	$C_{11}H_9I_2N_2O_4$	2.8	CH_5N	$[M+H-CH_5N]^+$
428.8573	7.6	$C_9H_7I_2N_2O_2$	4.3	$C_3H_7NO_2$	$[M+H-NH_3-C_3H_4O_2]^+$
391.0010	7.4, 7.6, 9.3	$C_{12}H_{14}IN_3O_4$	3.5	I	$[M+H-I]^{\cdot+}$
389.9929	7.4	$C_{12}H_{13}IN_3O_4$	4.1	HI	$[M+H-HI]^+$
372.9677	7.6, 9.3	$C_{12}H_{10}IN_2O_4$	0.8	H_4IN	$[M+H-NH_3-HI]^+$
358.9510	7.6, 9.3	$C_{11}H_8IN_2O_4$	3.7	CH_6IN	$[M+H-CH_5N-HI]^+$
357.9665	7.4	$C_{11}H_9IN_3O_3$	5.1	CH_5IO	$[M+H-HI-CH_4O]^+$
345.9794	9.3	$C_{11}H_{11}IN_2O_3$	4.3	CH_3INO	$[M+H-NH_3-CO-I]^{\cdot+}$
341.9466	7.4, 7.6, 9.3	$C_{11}H_7IN_2O_3$	8.7	CH_7INO	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
331.9654	7.6	$C_{10}H_9IN_2O_3$	0.5	C_2H_5INO	$[M+H-I-C_2H_5NO]^{\cdot+}$
327.9337	7.6, 9.3	$C_{10}H_5IN_2O_3$	0.7	C_2H_9INO	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
264.0974	7.4, 7.6	$C_{12}H_{14}N_3O_4$	1.8	I_2	$[M+H-I-I]^+$
232.0709	7.4, 7.6, 9.3	$C_{11}H_{10}N_3O_3$	3.3	CH_4I_2O	$[M+H-I-HI-CH_3O]^{\cdot\cdot+}$
219.0752	7.6, 9.3	$C_{11}H_{11}N_2O_3$	5.6	CH_3I_2NO	$[M+H-NH_3-CO-I-I]^{\cdot\cdot+}$
205.0602	7.4, 7.6, 9.3	$C_{10}H_9N_2O_3$	2.8	$C_2H_5I_2NO$	$[M+H-HI-I-C_2H_4NO]^{\cdot\cdot+}$
203.0455	7.6	$C_{10}H_7N_2O_3$	1.9	$C_2H_7I_2NO$	$[M+H-I-HI-CH_3O-CH_3N]^+$
187.0490	7.6	$C_{10}H_7N_2O_2$	6.4	$C_2H_7I_2NO_2$	$[M+H-I-HI-CH_3O-CH_3NO]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S13. Precursor and product ions of the DDPI TP 391 signals with RT 5.5 min, 10.3 min and 10.8 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
392.0092	*5.5, 10.3, 10.8*	*$C_{12}H_{15}IN_3O_4$*	*2.5*		*$[M+H]^+$*
374.9832	5.5, 10.3, 10.8	$C_{12}H_{12}IN_2O_4$	1.2	H_3N	$[M+H-NH_3]^+$
360.9675	5.5, 10.3, 10.8	$C_{11}H_{10}IN_2O_4$	1.3	CH_5N	$[M+H-CH_5N]^+$
346.9854	5.5	$C_{11}H_{12}IN_2O_3$	9.6	CH_3NO	$[M+H-CH_3NO]^+$
334.9891	10.3, 10.8	$C_{10}H_{12}IN_2O_3$	1.2	C_2H_3NO	$[M+H-CH_3N-CO]^+$
317.9594	5.5	$C_{10}H_9INO_3$	8.7	$C_2H_6N_2O$	$[M+H-CH_5N-CHNO]^+$
302.9622	10.3, 10.8	$C_9H_8IN_2O_2$	1.0	$C_3H_7NO_2$	$[M+H-NH_3-C_3H_4O_2]^+$
265.1044	5.5, 10.3, 10.8	$C_{12}H_{15}N_3O_4$	4.9	I	$[M+H-I]^{\cdot+}$
264.0965	10.3, 10.8	$C_{12}H_{14}N_3O_4$	5.2	HI	$[M+H-HI]^+$
235.0950	5.5, 10.3	$C_{11}H_{13}N_3O_3$	0.6	CH_2IO	$[M+H-I-CH_2O]^{\cdot+}$
234.0863	5.5	$C_{11}H_{12}N_3O_3$	4.3	CH_3IO	$[M+H-I-CH_3O]^+$
233.0567	10.3	$C_{11}H_9N_2O_4$	3.1	CH_6IN	$[M+H-CH_5N-HI]^+$
232.0708	10.3, 10.8	$C_{11}H_{10}N_3O_3$	3.7	CH_5IO	$[M+H-HI-CH_4O]^+$
220.0819	10.8	$C_{11}H_{12}N_2O_3$	10.7	CH_3INO	$[M+H-I-CH_3NO]^{\cdot+}$
208.0827	10.8	$C_{10}H_{12}N_2O_3$	7.4	C_2H_3INO	$[M+H-I-C_2H_3NO]^{\cdot+}$
206.0920	5.5, 10.8	$C_{10}H_{12}N_3O_2$	2.0	$C_2H_3IO_2$	$[M+H-I-CH_3O-CO]^+$
206.0692	10.3	$C_{10}H_{10}N_2O_3$	2.9	C_2H_5INO	$[M+H-I-CH_2O-CH_3N]^{\cdot+}$

205.0587	10.3	$C_{10}H_9N_2O_3$	10.1	C_2H_6INO	$[M+H-I-CH_2O-CH_4N]^+$
203.0450	10.3, 10.8	$C_{10}H_7N_2O_3$	0.6	C_2H_8INO	$[M+H-HI-CH_4O-CH_3N]^+$
202.0371	10.3	$C_{10}H_6N_2O_3$	1.1	C_2H_9INO	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
190.0731	5.5, 10.3, 10.8	$C_{10}H_{10}N_2O_2$	3.0	$C_2H_5INO_2$	$[M+H-HI-CHNO-CH_3O]^{\cdot+}$
176.0580	10.8	$C_9H_8N_2O_2$	0.2	$C_3H_7INO_2$	$[M+H-HI-CHNO-CH_3O-CH_2]^{\cdot+}$ or $[M+H-HI-CH_2NO-CH_2O-CH_2]^{\cdot+}$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S14. Precursor and product ions of DDPI TP 265 (RT 10.7 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
266.1131	*10.7*	*$C_{12}H_{16}N_3O_4$*	*1.6*		*$[M+H]^+$*
249.0864	10.7	$C_{12}H_{13}N_2O_4$	2.3	H_3N	$[M+H-NH_3]^+$
235.0711	10.7	$C_{11}H_{11}N_2O_4$	1.0	CH_5N	$[M+H-CH_5N]^+$
209.0924	10.7	$C_{10}H_{13}N_2O_3$	1.7	C_2H_3NO	$[M+H-C_2H_3NO]^+$
177.0651	10.7	$C_9H_9N_2O_2$	4.2	$C_3H_7NO_2$	$[M+H-NH_3-C_3H_4O_2]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S15. Precursor and product ions of the DDPI TP 445 signals with RT 4.6 min and 5.4 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
445.8845	*4.6, 5.4*	*$C_9H_{10}I_2N_3O_2$*	*2.7*		*$[M+H]^+$*
414.8413	5.4	$C_8H_5I_2N_2O_2$	5.3	CH_5N	$[M+H-CH_5N]^+$
318.9801	4.6, 5.4	$C_9H_{10}IN_3O_2$	3.5	I	$[M+H-I]^{\cdot+}$
317.9701	4.6, 5.4	$C_9H_9IN_3O_2$	10.4	HI	$[M+H-HI]^+$
289.9533	4.6	$C_8H_7IN_2O_2$	4.7	CH_3IN	$[M+H-I-CH_3N]^{\cdot+}$
288.9451	4.6, 5.4	$C_8H_6IN_2O_2$	6.1	CH_4IN	$[M+H-HI-CH_3N]^+$
274.9660	5.4	$C_8H_8IN_2O$	5.8	CH_2INO	$[M+H-HI-CHNO]^+$
272.9501	4.6	$C_8H_6IN_2O$	6.7	CH_4INO	$[M+H-HI-CH_3NO]^+$
261.9597	4.6, 5.4	$C_7H_7IN_2O$	0.2	C_2H_3INO	$[M+H-I- CH_2H_3NO]^{\cdot+}$
260.9512	5.4	$C_7H_6IN_2O$	2.8	C_2H_4INO	$[M+H-HI-CH_2H_3NO]^+$
192.0759	4.6, 5.4	$C_9H_{10}N_3O_2$	4.4	I_2	$[M+H-I-I]^+$
175.0501	4.6, 5.4	$C_9H_7N_2O_2$	0.6	H_3I_2N	$[M+H-I-I-NH_3]^+$
163.0502	5.4	$C_8H_7N_2O_2$	0.0	CH_3I_2N	$[M+H-I-I-CH_3N]^+$
135.0553	5.4	$C_7H_7N_2O$	0.1	$C_2H_3I_2NO$	$[M+H-I-I-C_2H_3NO]^+$
134.0473	5.4	$C_7H_6N_2O$	1.2	$C_2H_4I_2NO$	$[M+H-HI-I-C_2H_3NO]^{\cdot+}$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S16. Precursor and product ions of the DDPI TP 319 signals with RT 3.9 min and 5.7 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
319.9885	*3.9, 5.7*	*$C_9H_{11}IN_3O_2$*	*1.7*		*$[M+H]^+$*
302.9622	3.9	$C_9H_8IN_2O_2$	1.0	H_3N	$[M+H\text{-}NH_3]^+$ or $[M+H\text{-}NH_3]^+$
288.9458	3.9	$C_8H_6IN_2O_2$	3.6	CH_5N	$[M+H\text{-}CH_5N]^+$
193.0845	3.9, 5.7	$C_9H_{11}N_3O_2$	0.4	I	$[M+H\text{-}I]^{\cdot+}$
192.0758	3.9, 5.7	$C_9H_{10}N_3O_2$	5.0	HI	$[M+H\text{-}HI]^+$
164.0576	3.9, 5.7	$C_8H_8N_2O_2$	2.6	CH_3IN	$[M+H\text{-}I\text{-}CH_3N]^{\cdot+}$
163.0500	3.9, 5.7	$C_8H_7N_2O_2$	1.3	CH_4IN	$[M+H\text{-}HI\text{-}CH_3N]^+$
149.0699	3.9	$C_8H_9N_2O$	7.0	CH_2INO	$[M+H\text{-}HI\text{-}CHNO]^+$
136.0620	3.9, 5.7	$C_7H_8N_2O$	8.2	C_2H_3INO	$[M+H\text{-}I\text{-}C_2H_3NO]^{\cdot+}$
135.0547	3.9, 5.7	$C_7H_7N_2O$	4.4	C_2H_4INO	$[M+H\text{-}HI\text{-}C_2H_3NO]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S17. Precursor and product ions of DDPI TP 193 (RT 4.2 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
194.0926	*4.2*	*$C_9H_{12}N_3O_2$*	*1.0*		*$[M+H]^+$*
177.0657	4.2	$C_9H_9N_2O_2$	0.9	H_3N	$[M+H\text{-}NH_3]^+$ oder $[M+H\text{-}NH_3]^+$
163.0498	4.2	$C_8H_7N_2O_2$	2.5	CH_5N	$[M+H\text{-}CH_5N]^+$
151.0861	4.2	$C_8H_{11}N_2O$	3.2	CHNO	$[M+H\text{-}CHNO]^+$
149.0699	4.2	$C_8H_9N_2O$	7.0	CH_3NO	$[M+H\text{-}CH_3NO]^+$
137.0705	4.2	$C_7H_9N_2O$	3.2	C_2H_3NO	$[M+H\text{-}C_2H_3NO]^+$
135.0538	4.2	$C_7H_7N_2O$	11.0	C_2H_5NO	$[M+H\text{-}C_2H_5NO]^+$
120.0442	4.2	C_7H_6NO	1.6	$C_2H_6N_2O$	$[M+H\text{-}C_2H_3NO\text{-}NH_3]^+$ or $[M+H\text{-}C_2H_3NO\text{-}NH_3]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B, red: fragment originates from chain C

Table S18. Precursor and product ions of the DAMI peaks with RT 5.7 min, 5.9 min, 7.6 min and 8.3 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
719.8552	*5.7, 5.9, 7.6, 8.3*	*$C_{15}H_{21}I_3N_3O_6$*	*1.0*		*$[M+H]^+$*
701.8419	5.7, 5.9, 7.6, 8.3	$C_{15}H_{19}I_3N_3O_5$	4.9	H_2O	$[M+H\text{-}H_2O]^+$ or $[M+H\text{-}H_2O]^+$
628.7904	5.7, 5.9, 7.6, 8.3	$C_{12}H_{12}I_3N_2O_4$	3.5	$C_3H_9NO_2$	$[M+H\text{-}H_2O\text{-}C_3H_7NO]^+$
614.7763	5.7, 5.9, 7.6, 8.3	$C_{11}H_{10}I_3N_2O_4$	1.0	$C_4H_{11}NO_2$	$[M+H\text{-}H_2O\text{-}C_4H_9NO]^+$
500.8791	5.7, 5.9, 7.6	$C_{12}H_{11}I_2N_2O_4$	2.4	$C_3H_{10}INO_2$	$[M+H\text{-}H_2O\text{-}C_3H_7NO\text{-}HI]^+$
314.9611	5.7, 5.9, 7.6, 8.3	$C_{10}H_8IN_2O_2$	4.5	$C_5H_{13}I_2NO_4$	$[M+H\text{-}H_2O\text{-}C_4H_9NO\text{-}I\text{-}CO\text{-}H_2O\text{-}I^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S19. Precursor and product ions of the DAMI TP 593 signals with RT 4.3 min, 4.5 min, 5.1 min, 5.3 min and 7.9 – 9.6 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
593.9579	*4.3, 4.5, 5.1, 5.3, 7.9 – 9.6*	*$C_{15}H_{22}I_2N_3O_6$*	*2.3*		*$[M+H]^+$*
575.9460	4.3, 4.5, 5.1, 5.3, 7.9 – 9.6	$C_{15}H_{20}I_2N_3O_5$	4.7	H_2O	$[M+H-H_2O]^+$ oder $[M+H-H_2O]^+$
502.8951	4.3, 4.5, 5.1, 5.3, 7.9 – 9.6	$C_{12}H_{13}I_2N_2O_4$	1.7	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
488.8800	4.3, 4.5, 5.1, 5.3, 7.9 – 9.6	$C_{11}H_{11}I_2N_2O_4$	0.6	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S20. Precursor and product ions of the DAMI TP 467 signals with RT 3.7 min, 3.9 min, 4.3 min and 5.0 – 7.0 min obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
468.0616	*3.7, 3.9, 4.3, 5.0 – 7.0*	*$C_{15}H_{23}IN_3O_6$*	*2.2*		*$[M+H]^+$*
450.0525	4.3, 5.0 – 7.0	$C_{15}H_{21}IN_3O_5$	1.0	H_2O	$[M+H-H_2O]^+$ or $[M+H-H_2O]^+$
376.9980	3.7, 3.9, 4.3, 5.0 – 7.0	$C_{12}H_{14}IN_2O_4$	3.4	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
362.9824	3.7, 3.9, 4.3, 5.0 – 7.0	$C_{11}H_{12}IN_2O_4$	3.4	$C_4H_{11}NO_2$	$[M+H-H_2O-C_4H_9NO]^+$ or $[M+H-H_2O-C_4H_9NO]^+$
289.9288	3.9, 4.3, 5.0 – 7.0	$C_8H_5INO_3$	7.1	$C_7H_{18}N_2O_3$	$[M+H-H_2O-C_4H_9NO-C_3H_7NO]^+$
273.9330	4.3	$C_8H_5INO_2$	10.8	$C_7H_{18}N_2O_4$	$[M+H-H_2O-C_3H_7NO-C_4H_9NO_2]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2]^+$
245.9414	3.7	C_7H_5INO	1.5	$C_8H_{18}N_2O_5$	$[M+H-H_2O-C_3H_7NO-C_4H_9NO_2-CO]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2-CO]^+$
243.9247	3.9, 4.3, 5.0 – 7.0	C_7H_3INO	2.8	$C_8H_{20}N_2O_5$	$[M+H-H_2O-C_3H_7NO-C_4H_9NO_2-CH_2O]^+$ or $[M+H-H_2O-C_4H_9NO-C_3H_7NO_2-CH_2O]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S21. Precursor and product ions of the DAMI TP 341 (RT 3.5 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
342.1650	*3.5*	*$C_{15}H_{24}N_3O_6$*	*2.8*		*$[M+H]^+$*
251.1025	3.5	$C_{12}H_{15}N_2O_4$	0.5	$C_3H_9NO_2$	$[M+H-C_3H_9NO_2]^+$
237.0863	3.5	$C_{11}H_{13}N_2O_4$	2.9	$C_4H_{11}NO_2$	$[M+H-C_4H_{11}NO_2]^+$
164.0337	3.5	$C_8H_6NO_3$	3.2	$C_7H_{18}N_2O_3$	$[M+H-C_3H_9NO_2-C_4H_9NO]^+$ or $[M+H-C_4H_{11}NO_2-H_2O-C_3H_7NO]^+$
148.0380	3.5	$C_8H_6NO_2$	8.8	$C_7H_{18}N_2O_4$	$[M+H-C_3H_9NO_2-C_4H_9NO_2]^+$ or $[M+H-C_4H_{11}NO_2-H_2O-C_3H_7NO_2]^+$
108.0443	3.5	C_6H_6NO	0.8	$C_9H_{18}N_2O_5$	$[M+H-C_3H_9NO_2-C_4H_9NO-CO-CO]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

Table S22. Precursor and product ions of DAMI TP 380 (RT 5.2 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
380.9929	*5.2*	*$C_{11}H_{14}IN_2O_5$*	*3.4*		*$[M+H]^+$*
362.9816	5.2	$C_{11}H_{12}IN_2O_4$	5.5	H_2O	$[M+H-H_2O]^+$
289.9301	5.2	$C_8H_5INO_3$	2.6	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
261.9356	5.2	$C_7H_5INO_2$	1.3	$C_4H_9NO_3$	$[M+H-H_2O-C_3H_7NO-CO]^+$
135.0306	5.2	$C_7H_5NO_2$	6.5	$C_4H_9INO_3$	$[M+H-H_2O-C_3H_7NO-CO-I]^{\cdot+}$

[1)] color code: green: fragment originates from chain B

Table S23. Precursor and product ions of DAMI TP 254 (RT 4.7 min) obtained by MS^2 experiments using LC-Q-ToF-MS.

m/z	Observed at RT	Ion Formula	Mass error / ppm	Loss Formula	Proposed fragmentation[1)]
255.0977	*4.7*	*$C_{11}H_{15}N_2O_5$*	*0.6*		*$[M+H]^+$*
237.0858	4.7	$C_{11}H_{13}N_2O_4$	5.0	H_2O	$[M+H-H_2O]^+$
164.0342	4.7	$C_8H_6NO_3$	0.3	$C_3H_9NO_2$	$[M+H-H_2O-C_3H_7NO]^+$
136.0389	4.7	$C_7H_6NO_2$	3.0	$C_4H_9NO_3$	$[M+H-H_2O-C_3H_7NO-CO]^+$
108.0439	4.7	C_6H_6NO	4.5	$C_5H_9NO_4$	$[M+H-H_2O-C_3H_7NO-CO-I-CO]^+$

[1)] color code: blue: fragment originates from chain A, green: fragment originates from chain B

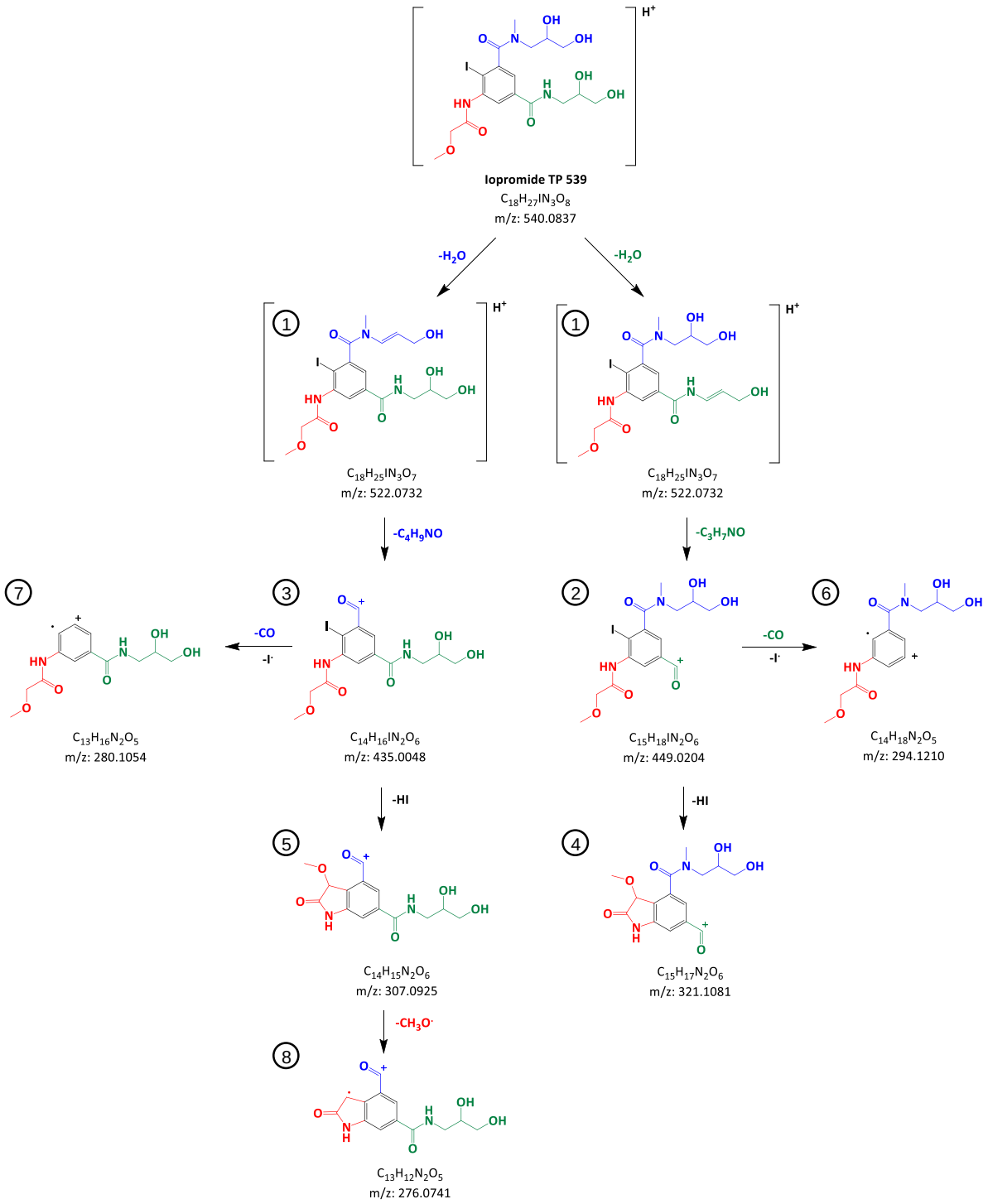

Figure S1. Proposed fragmentation pathway of iopromide TP 539 (RT 10.0 – 12.0 min) with elemental compositions and theoretical *m/z* ratios. The position of the iodine atom has been assigned arbitrarily. Numbers correspond to the peaks in Figure S2.

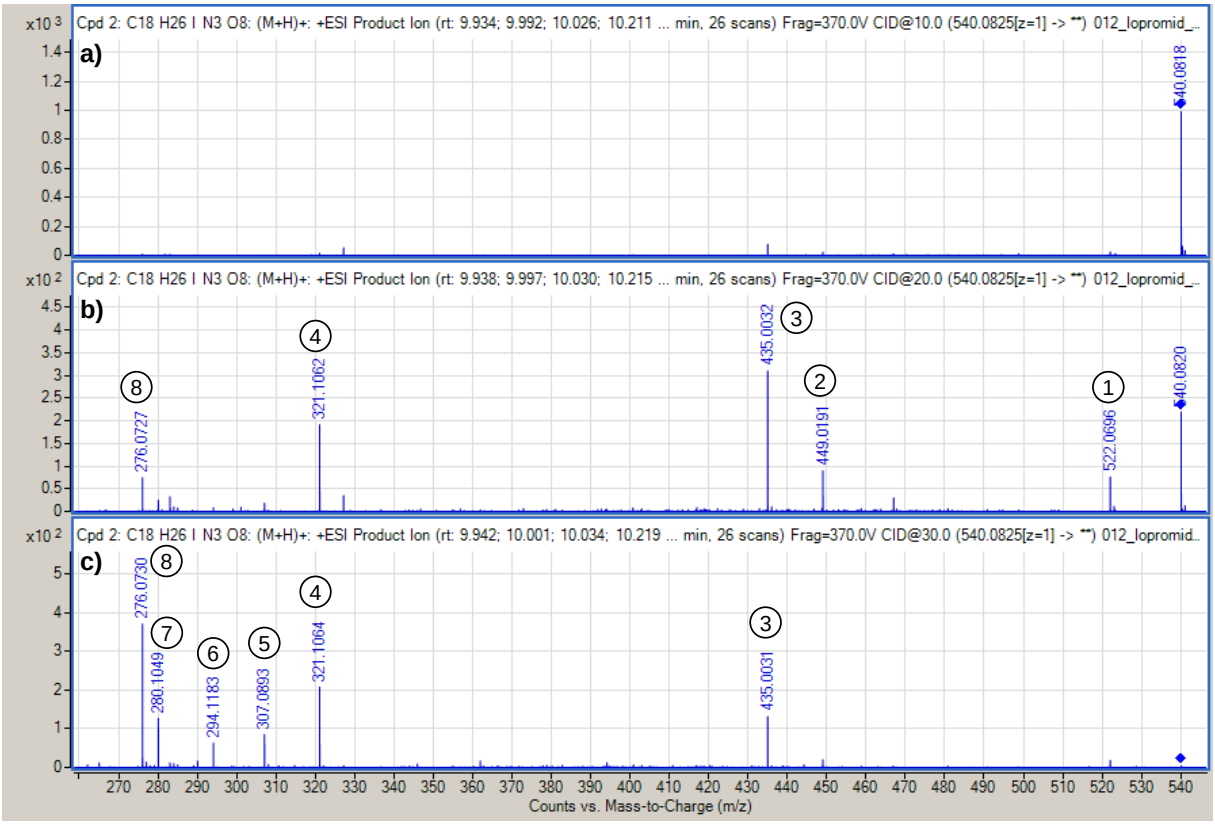

Figure S2. MS^2 spectra of iopromide TP 539 (RT 10.0 – 12.0 min) with collision energies a) 10 V, b) 20 V and c) 30 V.

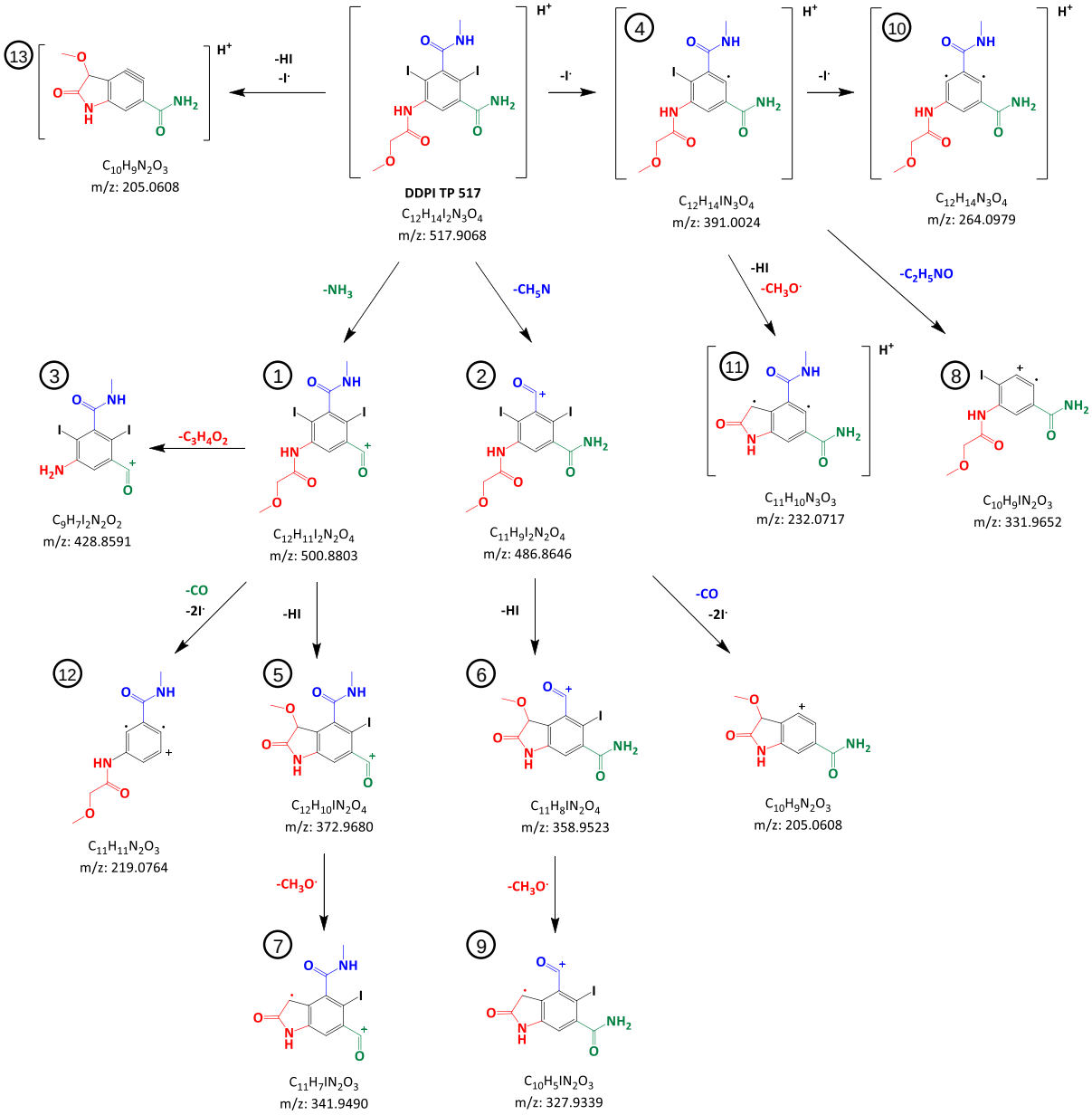

Figure S3. Proposed fragmentation pathway of DDPI TP 517 (RT 7.4 min) with elemental compositions and theoretical m/z ratios. The position of the iodine atoms has been assigned arbitrarily. Numbers correspond to the peaks in Figure S4.

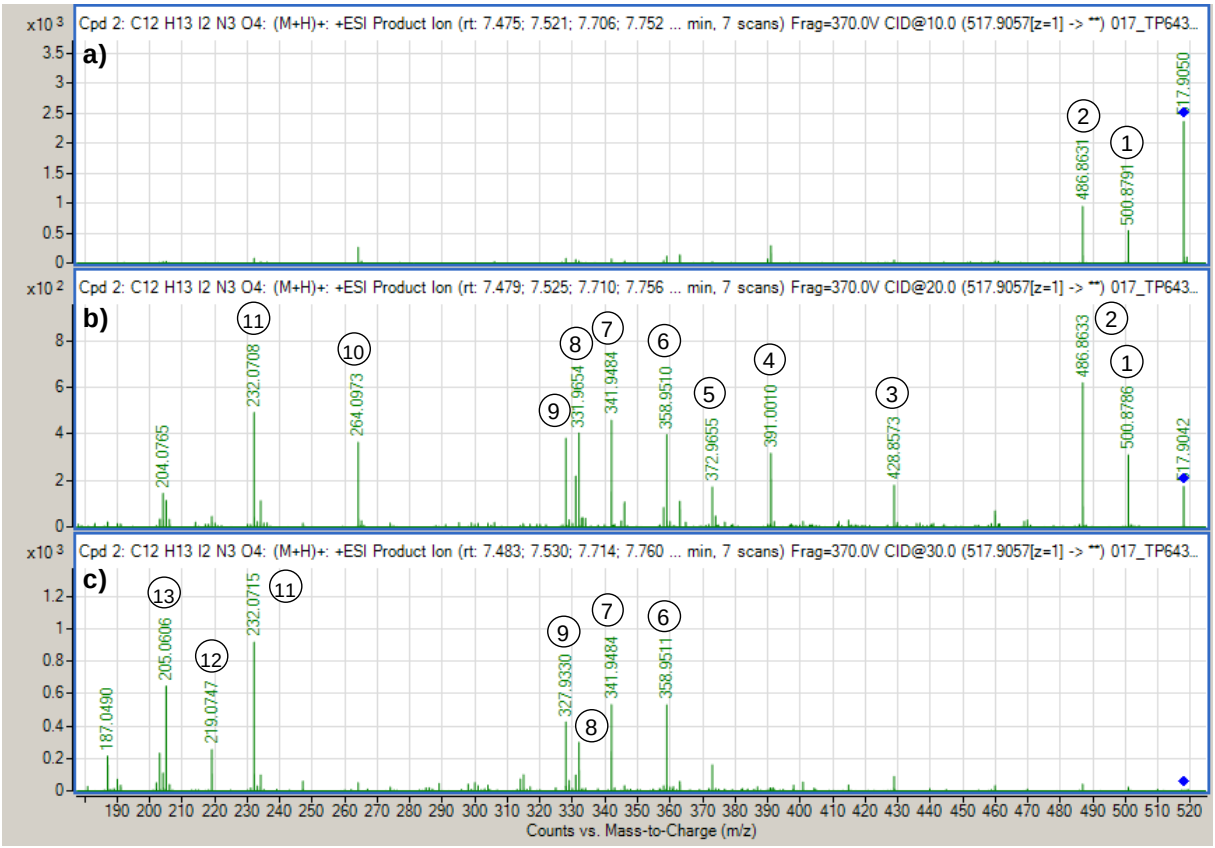

Figure S4. MS^2 spectra of DDPI TP 517 (RT 7.4 min) with collision energies a) 10 V, b) 20 V and c) 30 V.

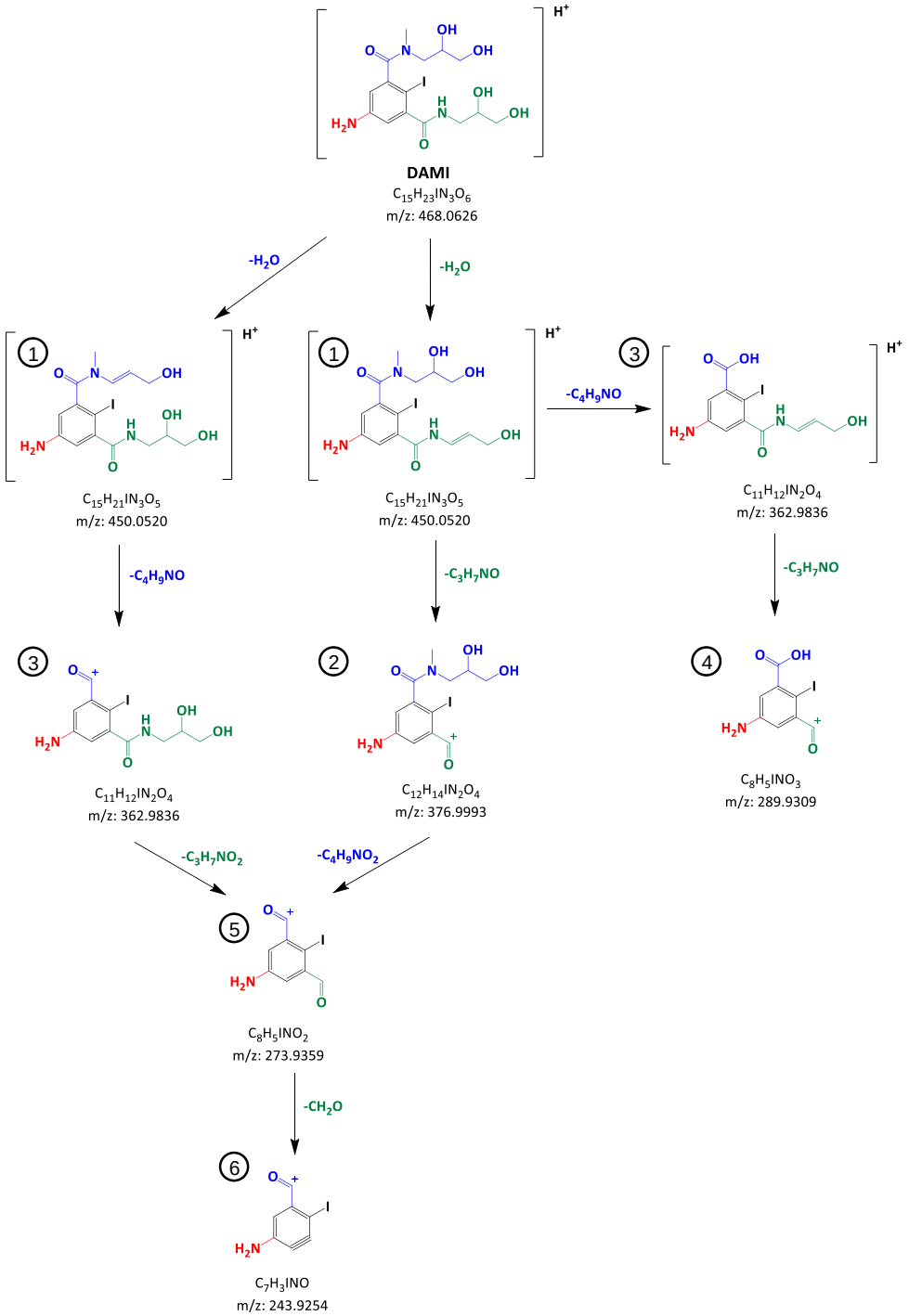

Figure S5. Proposed fragmentation pathway of DAMI TP 467 (RT 3.9 min) with elemental compositions and theoretical m/z ratios. The position of the iodine atom has been assigned arbitrarily. Numbers correspond to the peaks in Figure S6.

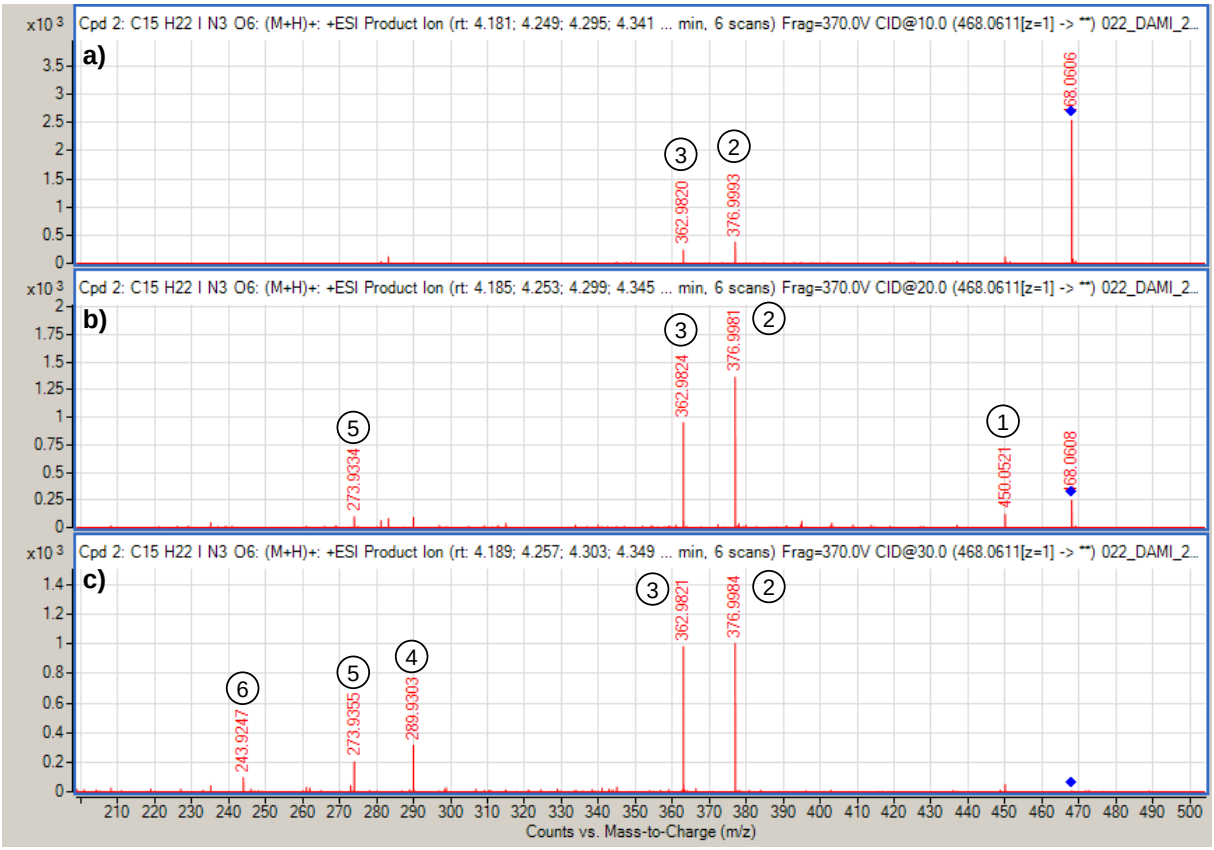

Figure S6. MS^2 spectra of DAMI TP 467 (RT 3.9 min) with collision energies a) 10 V, b) 20 V and c) 30 V.

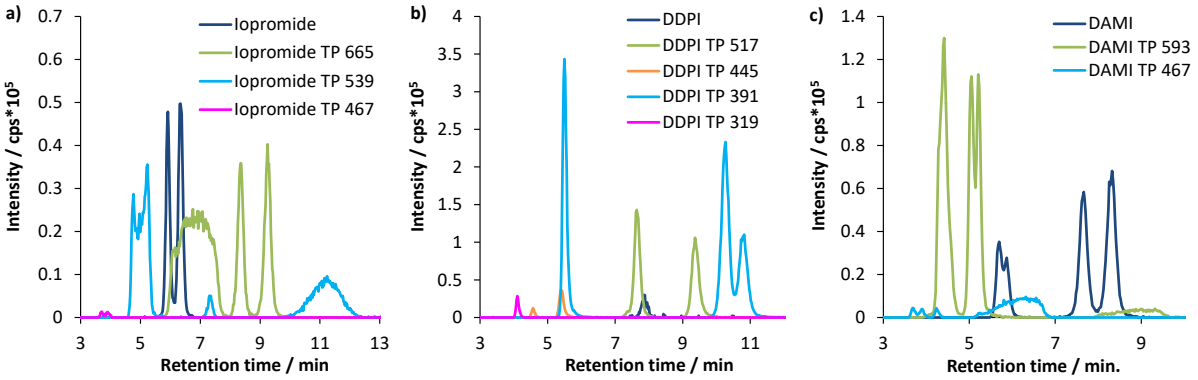

Figure S7. EICs of a) iopromide, b) DDPI, c) DAMI and their iodinated anaerobic TPs showing co-eluting signals as well as the higher number of isomers of DAMI and its TPs compared to iopromide, DDPI and their TPs.

Investigation of mass balances

Table S24. Response factors based on LC-ICP-MS measurements to convert LC-Q-ToF-MS peak areas of the iodinated TPs into concentrations and limits of quantification (LOQs).

Isomer	**Iopromide TP 665 (5.7 – 7.7 min)**	**Iopromide TP 665 (8.3 min)**	**Iopromide TP 665 (9.3 min)**	
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 1700 270 (16) 9	 1710 270 (16) 8	 1900 280 (15) 8	
LOQ / µg /L (nmol/L) LC-ICP-MS	30 (40)	30 (40)	30 (40)	
LOQ / µg /L (nmol/L) LC-Q-ToF-MS	25 (40)	10 (15)	10 (15)	
Isomer	**Iopromide TP 539 (4.5 – 5.5 min)**	**Iopromide TP 539 (7.3 min)**	**Iopromide TP 539 (10 – 12.5 min)**	
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 1540 210 (15) 15	 - [a)]	 1800 150 (9) 15	
LOQ / µg/L (nmol/L) LC-ICP-MS	45 (80)	45 (80)	45 (80)	
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	15 (30)	- [c)]	10 (20)	
Isomer	**Iopromide TP 467 (3.7 min)**	**Iopromide TP 467 (3.9 min)**		
Response factor / nmol/L - Arithmetic mean - Standard deviation	 - [b)]	 - [b)]		
LOQ / µg/L (nmol/L) LC-ICP-MS	40 (80)	40 (80)		
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	- [c)]	- [c)]		

Isomer	**DDPI TP 517 (7.2 – 8.2 min)**	**DDPI TP 517 (9.4 min)**		
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 720 100 (14) 9	 960 80 (8) 9		
LOQ / µg/L (nmol/L) LC-ICP-MS	20 (40)	20 (40)		
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	3.5 (7)	4 (8)		
Isomer	**DDPI TP 445 (4.6 min)**	**DDPI TP 445 (5.4 min)**		
Response factor / nmol/L - Arithmetic mean - Standard deviation	- [b)]	- [a)]		
LOQ / µg/L (nmol/L) LC-ICP-MS	20 (40)	20 (40)		
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	- [c)]	- [c)]		
Isomer	**DDPI TP 391 (5.5 min)**	**DDPI TP 391 (10.3 min)**	**DDPI TP 391 (10.8 min)**	
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 770 130 (15) 8	 550 220 (40) 8	 1020 210 (21) 10	
LOQ / µg/L (nmol/L) LC-ICP-MS	35 (80)	35 (80)	35 (80)	
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	1.5 (4)	1.5 (4)	2 (5.5)	
Isomer	**DDPI TP 319 (3.9 min)**	**DDPI TP 319 (5.7 min)**		
Response factor / nmol/L - Arithmetic mean - Standard deviation	- [b)]	- [a)]		
LOQ / µg/L (nmol/L) LC-ICP-MS	25 (80)	25 (80)		
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	- [c)]	- [c)]		

Isomer	**DAMI TP 593 (4.4 min)**	**DAMI TP 593 (5.1 min)**	**DAMI TP 593 (5.3 min)**	**DAMI TP 593 (7.9 – 9.6 min)**
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 1290 60 (5) 4	 1400 210 (15) 7	 1850 110 (6) 7	 2580 130 (5) 4
LOQ / µg/L (nmol/L) LC-ICP-MS	25 (40)	25 (40)	25 (40)	25 (40)
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	25 (40)	2.5 (4)	5 (8)	40 (70)
Isomer	**DAMI TP 467 (3.7 min)**	**DAMI TP 467 (3.9 min)**	**DAMI TP 467 (4.3 min)**	**DAMI TP 467 (5 – 7 min)**
Response factor / nmol/L - Arithmetic mean - Standard deviation (relative / %) - n =	 - [a)]	 - [a)]	 2450 380 (16) 3	 1800 210 (12) 6
LOQ / µg/L (nmol/L) LC-ICP-MS	40 (80)	40 (80)	40 (80)	40 (80)
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	- [c)]	- [c)]	2 (4)	8 (16)
Isomer	**DAMI TP 380 (5.2 min)**			
Response factor / nmol/L - Arithmetic mean - Standard deviation	- [a)]			
LOQ / µg/L (nmol/L) LC-ICP-MS	30 (80)			
LOQ / µg/L (nmol/L) LC-Q-ToF-MS	- [c)]			

[a)] response factor could not be assessed due to coelution, [b)] response factor could not be assessed because isomer concentration was <LOQ (LC-ICP-MS) in all samples, [c)] LOQ (LC-Q-ToF-MS) could not be calculated because of missing response factor

Detection of anaerobic ICM TPs in bank filtration samples

Table S25. Fragments of the detected (experimental and predicted) anaerobic TPs and their precursor substances in well 1.

Substance	RT / min	Fragment m/z	Ion Formula	Mass error / ppm	Proposed fragmentation (see also Tables S 7 and S 8)
DDPI	8.2	*643.8029*	*$C_{12}H_{13}I_3N_3O_4$*	*0.9*	*$[M+H]^+$*
		357.9642	$C_{11}H_9IN_3O_3$	11.4	$[M+H-I-HI-CH_3O]^+$
		498.8426	$C_{12}H_9I_2N_2O_4$	22.0	$[M+H-NH_3-HI]^+$
		330.9556	$C_{10}H_8IN_2O_3$	5.5	$[M+H-CH_5N-CO-I-I]^+$
		453.8465[1)]	$C_{10}H_4I_2N_2O_3$	35.0	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
DDPI TP 517	8.0	*517.9054*	*$C_{12}H_{14}I_2N_3O_4$*	*2.8*	*$[M+H]^+$*
		327.9242	$C_{10}H_5IN_2O_3$	29.7	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		232.0846	$C_{11}H_{10}N_3O_3$	55.7[3)]	$[M+H-I-HI-CH_3O]^+$
		331.9673	$C_{10}H_9IN_2O_3$	6.2	$[M+H-I-C_2H_5NO]^{\cdot+}$
		341.9518	$C_{11}H_7IN_2O_3$	6.4	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
	9.7	*517.9067*	*$C_{12}H_{14}I_2N_3O_4$*	*0.4*	*$[M+H]^+$*
		327.9337	$C_{10}H_5IN_2O_3$	0.7	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		205.0675	$C_{10}H_9N_2O_3$	32.8	$[M+H-CH_5N-CO-I-I]^{\cdot\cdot+}$
		219.0855	$C_{11}H_{11}N_2O_3$	9.1	$[M+H-NH_3-CO-I-I]^{\cdot\cdot+}$
		372.9427	$C_{12}H_{10}IN_2O_4$	67.8[3)]	$[M+H-NH_3-HI]^+$
Iomeprol TP 629	4.7	*629.7869*	*$C_{11}H_{13}I_3N_3O_4$*	*1.5*	*$[M+H]^+$*
		330.9596	$C_{10}H_8IN_2O_3$	6.7	$[M+H-NH_3-CO-I-I]^+$
		457.8701	$C_{10}H_8I_2N_2O_3$	18.0	$[M+H-NH_3-CO-I]^{\cdot+}$
		501.8853[2)]	$C_{11}H_{10}I_2N_3O_4$	19.5	$[M+H-HI]^+$
		357.9719	$C_{11}H_7IN_2O_4$	76.6[3)]	$[M+H-NH_3-HI-I]^{\cdot+}$
		484.8546	$C_{11}H_7I_2N_2O_4$	11.6	$[M+H-NH_3-HI]^+$
Iomeprol TP 629 -1I	3.9	*503.8878*	*$C_{11}H_{12}I_2N_3O_4$*	*6.7*	*$[M+H]^+$*
		205.0644	$C_{10}H_9N_2O_3$	17.6	$[M+H-HI-I-CH_2NO]^+$
		375.9770	$C_{11}H_{11}IN_3O_4$	5.0	$[M+H-HI]^+$
		177.0741	$C_9H_9N_2O_2$	46.6	$[M+H-I-I-CHNO-CH_2O]^+$
		206.0732	$C_{10}H_{10}N_2O_3$	22.4	$[M+H-HI-I-CHNO]^{\cdot+}$
		331.9598	$C_{10}H_9IN_2O_3$	16.5	$[M+H-CH_3NO-I]^{\cdot+}$
		318.9783	$C_9H_{10}IN_3O_2$	9.2	$[M+H-I-C_2H_2O_2]^{\cdot+}$
	4.6	*503.8896*	*$C_{11}H_{12}I_2N_3O_4$*	*3.1*	*$[M+H]^+$*
		375.9759	$C_{11}H_{11}IN_3O_4$	8.0	$[M+H-HI]^{\cdot+}$
		205.0697	$C_{10}H_9N_2O_3$	43.4	$[M+H-HI-I-CH_2NO]^+$
		206.0723	$C_{10}H_{10}N_2O_3$	18.0	$[M+H-HI-I-CHNO]^{\cdot+}$
		318.9799	$C_9H_{10}IN_3O_2$	4.2	$[M+H-I-C_2H_2O_2]^{\cdot+}$

	5.0	*503.8903*	*$C_{11}H_{12}I_2N_3O_4$*	*1.7*	*$[M+H]^+$*
		375.9722	$C_{11}H_{11}IN_3O_4$	17.8	$[M+H-HI]^+$
		206.0739	$C_{10}H_{10}N_2O_3$	25.7	$[M+H-HI-I-CHNO]^{\cdot+}$
		205.0665	$C_{10}H_9N_2O_3$	27.9	$[M+H-HI-I-CH_2NO]^+$
Iomeprol TP 629 -2I	4.4	*377.9943*	*$C_{11}H_{13}IN_3O_4$*	*0.7*	*$[M+H]^+$*
		250.0835	$C_{11}H_{12}N_3O_4$	5.1	$[M+H-HI]^{\cdot+}$
		203.0516	$C_{10}H_7N_2O_3$	31.9	$[M+H-HI-CH_3NO-H_2]^+$
		206.0753	$C_{10}H_{10}N_2O_3$	32.5	$[M+H-HI-I-CHNO]^{\cdot+}$
		193.0935	$C_9H_{11}N_3O_2$	46.7	$[M+H-I-C_2H_2O_2]^{\cdot+}$
Diatrizoate	5.4	*614.7747*	*$C_{11}H_{10}N_2O_4I_3$*	*2.3*	*$[M+H]^+$*
		360.9720	$C_{11}H_{10}N_2O_4I$	11.1	$[M+H-I-I]^+$
		233.0559	$C_{11}H_9N_2O_4$	16.3	$[M+H-I-I-HI]^+$

[1)] fragment not observed in batch experiment, but can be explained by molecular structure

[2)] fragment not observed by Kormos et al.[5], but can be explained by reactions in their proposed fragmentation pathway

[3)] fragments with mass error >50 ppm were not included in assigning the confidence levels

Table S26. Fragments of the detected (experimental and predicted) anaerobic TPs and their precursor substances in well 2.

substance	RT / min	Fragment m/z	Ion Formula	Mass error / ppm	Proposed fragmentation (see also Tables S 7 and S 8)
DDPI	8.1	*643.8004*	*$C_{12}H_{13}I_3N_3O_4$*	*4.8*	*$[M+H]$*
		357.9630	$C_{11}H_9IN_3O_3$	14.9	$[M+H-I-HI-CH_3O]^+$
		231.0667[1)]	$C_{11}H_9N_3O_3$	12.4	$[M+H-I-I-I-CH_4O]^{\cdot+}$
		467.8334	$C_{11}H_6I_2N_2O_3$	27.7	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
		330.9521	$C_{10}H_8IN_2O_3$	16.1	$[M+H-CH_5N-CO-I-I]^+$
DDPI TP 517	8.0	*517.9042*	*$C_{12}H_{14}I_2N_3O_4$*	*5.0*	*$[M+H]$*
		341.9455	$C_{11}H_7IN_2O_3$	12.0	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
		327.9362	$C_{10}H_5IN_2O_3$	6.9	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		205.0672	$C_{10}H_9N_2O_3$	31.4	$[M+H-CH_5N-CO-I-I]^{\cdot\cdot+}$
		358.9479	$C_{11}H_8IN_2O_4$	12.4	$[M+H-CH_5N-HI]^+$
		331.9740	$C_{10}H_9IN_2O_3$	26.4	$[M+H-I-C_2H_5NO]^{\cdot+}$
	9.6	*517.9052*	*$C_{12}H_{14}I_2N_3O_4$*	*3.1*	*$[M+H]$*
		327.9279	$C_{10}H_5IN_2O_3$	18.4	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		331.9803	$C_{10}H_9IN_2O_3$	45.3	$[M+H-I-C_2H_5NO]^{\cdot+}$
		219.0789	$C_{11}H_{11}N_2O_3$	11.3	$[M+H-NH_3-CO-I-I]^{\cdot\cdot+}$
		372.9648	$C_{12}H_{10}IN_2O_4$	8.5	$[M+H-NH_3-HI]^+$
		358.9386	$C_{11}H_8IN_2O_4$	38.3	$[M+H-CH_5N-HI]^+$
Iomeprol TP 629	4.7	*629.7856*	*$C_{11}H_{13}I_3N_3O_4$*	*3.6*	*$[M+H]$*
		330.9611	$C_{10}H_8IN_2O_3$	11.0	$[M+H-NH_3-CO-I-I]^+$
		457.8707	$C_{10}H_8I_2N_2O_3$	19.3	$[M+H-NH_3-CO-I]^{\cdot+}$
		501.8900[2)]	$C_{11}H_{10}I_2N_3O_4$	28.8	$[M+H-HI]^+$
		357.9729	$C_{11}H_7IN_2O_4$	79.3[3)]	$[M+H-NH_3-HI-I]^{\cdot+}$

Iomeprol TP 629 -1I	3.9	177.0710	$C_9H_9N_2O_2$	29.1	$[M+H-I-I-CHNO-CH_2O]^+$
	5.0	375.9675	$C_{11}H_{11}IN_3O_4$	30.3	$[M+H-HI]^+$
		205.0676	$C_{10}H_9N_2O_3$	33.3	$[M+H-HI-I-CH_2NO]^+$
		206.0745	$C_{10}H_{10}N_2O_3$	28.7	$[M+H-HI-I-CHNO]^{\cdot+}$
		318.9758	$C_9H_{10}IN_3O_2$	17.0	$[M+H-I-C_2H_2O_2]^{\cdot+}$
Diatrizoate	5.4	*614.7720*	*$C_{11}H_{10}N_2O_4I_3$*	*8.0*	*$[M+H]^+$*
		360.9718	$C_{11}H_{10}N_2O_4I$	10.6	$[M+H-I-I]^+$
		233.0559	$C_{11}H_9N_2O_4$	15.5	$[M+H-I-I-HI]^+$

[1] fragment not observed in batch experiment, but can be explained by molecular structure

[2] fragment not observed by Kormos et al.[5], but can be explained by reactions in their proposed fragmentation pathway

[3] fragments with mass error >50 ppm were not included in assigning the confidence levels

Table S27. Fragments of the detected (experimental and predicted) anaerobic TPs and their precursor substances in well 3.

substance	RT / min	Fragment m/z	Ion Formula	Mass error / ppm	Proposed fragmentation (see also Tables S 7 and S 8)
DDPI	8.1	*643.8033*	*$C_{12}H_{13}I_3N_3O_4$*	*0.3*	*$[M+H]$*
		357.9603	$C_{11}H_9IN_3O_3$	22.4	$[M+H-I-HI-CH_3O]^+$
		330.9567	$C_{10}H_8IN_2O_3$	2.2	$[M+H-CH_5N-CO-I-I]^+$
		231.0697[1]	$C_{11}H_9N_3O_3$	25.3	$[M+H-HI-HI-I-CH_2O]^{\cdot+}$
		329.9729	$C_{10}H_9IN_3O_2$	70.6[3]	$[M+H-CH_5N-CO-I-HI]^{\cdot+}$
		498.8510	$C_{12}H_9I_2N_2O_4$	27.3	$[M+H-NH_3-HI]^+$
		389.9961	$C_{12}H_{13}IN_3O_4$	4	$[M+H-I-I]^+$
DDPI TP 517	8.0	*517.9068*	*$C_{12}H_{14}I_2N_3O_4$*	*0.1*	*$[M+H]$*
		203.0644	$C_{10}H_7N_2O_3$	95.0[3]	$[M+H-I-HI-CH_3O-CH_3N]^+$
		358.9489	$C_{11}H_8IN_2O_4$	9.6	$[M+H-CH_5N-HI]^+$
		205.0657	$C_{10}H_9N_2O_3$	24.0	$[M+H-CH_5N-CO-I-I]^+$
	9.7	*517.9055*	*$C_{12}H_{14}I_2N_3O_4$*	*2.6*	*$[M+H]$*
		327.9504	$C_{10}H_5IN_2O_3$	49.9	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		232.0793	$C_{11}H_{10}N_3O_3$	32.9	$[M+H-I-HI-CH_3O]^+$
		372.9606	$C_{12}H_{10}IN_2O_4$	19.8	$[M+H-NH_3-HI]^+$
		205.0682	$C_{10}H_9N_2O_3$	36.2	$[M+H-CH_5N-CO-I-I]^+$
Iomeprol TP 629	4.7	*629.7855*	*$C_{11}H_{13}I_3N_3O_4$*	*3.7*	*$[M+H]$*
		330.9584	$C_{10}H_8IN_2O_3$	2.8	$[M+H-NH_3-CO-I-I]^+$
		457.8646	$C_{10}H_8I_2N_2O_3$	5.8	$[M+H-NH_3-CO-I]^{\cdot+}$
		501.8805[2]	$C_{11}H_{10}I_2N_3O_4$	9.8	$[M+H-HI]^+$
		329.9768[2]	$C_{10}H_7IN_2O_3$	82.4[3]	$[M+H-NH_3-CO-I-HI]^{\cdot+}$
Iomeprol TP 629 -1I	4.0	*503.8895*	*$C_{11}H_{12}I_2N_3O_4$*	*3.3*	*$[M+H]$*
		205.0677	$C_{10}H_9N_2O_3$	33.8	$[M+H-HI-I-CH_2NO]^+$
		206.0736	$C_{10}H_{10}N_2O_3$	24.3	$[M+H-HI-I-CHNO]^{\cdot+}$
		177.0757	$C_9H_9N_2O_2$	55.6[3]	$[M+H-I-I-CHNO-CH_2O]^+$
		375.9733	$C_{11}H_{11}IN_3O_4$	14.9	$[M+H-HI]^+$

	4.6	*503.8907*	*$C_{11}H_{12}I_2N_3O_4$*	*1.0*	*[M+H]*
		205.0668	$C_{10}H_9N_2O_3$	29.4	$[M+H-HI-I-CH_2NO]^+$
		206.0734	$C_{10}H_{10}N_2O_3$	23.3	$[M+H-HI-I-CHNO]^{\cdot+}$
		375.9737	$C_{11}H_{11}IN_3O_4$	13.8	$[M+H-HI]^+$
		318.9769	$C_9H_{10}IN_3O_2$	13.6	$[M+H-I-C_2H_2O_2]^{\cdot+}$
	5.0	*503.8889*	*$C_{11}H_{12}I_2N_3O_4$*	*4.6*	*[M+H]*
		375.9718	$C_{11}H_{11}IN_3O_4$	18.8	$[M+H-HI]^+$
		205.0670	$C_{10}H_9N_2O_3$	29.9	$[M+H-HI-I-CH_2NO]^+$
		232.0750	$C_{11}H_{10}N_3O_3$	14.4	$[M+H-HI-I-HO]^+$
		206.0766	$C_{10}H_{10}N_2O_3$	38.9	$[M+H-HI-I-CHNO]^{\cdot+}$
		318.9754	$C_9H_{10}IN_3O_2$	18.3	$[M+H-I-C_2H_2O_2]^{\cdot+}$
Iomeprol TP 629 -2I	4.5	*377.9936*	*$C_{11}H_{13}IN_3O_4$*	*2.4*	*[M+H]*
		250.0824	$C_{11}H_{12}N_3O_4$	0.7	$[M+H-HI]^{\cdot+}$
		193.0871	$C_9H_{11}N_3O_2$	13.1	$[M+H-I-C_2H_2O_2]^{\cdot+}$
		203.0506	$C_{10}H_7N_2O_3$	27.0	$[M+H-HI-CH_3NO-H_2]^+$
		206.0729	$C_{10}H_{10}N_2O_3$	20.9	$[M+H-HI-I-CHNO]^{\cdot+}$

[1)] fragment not observed in batch experiment, but can be explained by molecular structure

[2)] fragment not observed by Kormos et al.[5], but can be explained by reactions in their proposed fragmentation pathway

[3)] fragments with mass error >50 ppm were not included in assigning the confidence levels

Table S28. Fragments of the detected (experimental and predicted) anaerobic TPs and their precursor substances in well 4.

substance	RT / min	Fragment m/z	Ion Formula	Mass error / ppm	Proposed fragmentation (see also Tables S 7 and S 8)
DDPI	8.0	*643.8030*	*$C_{12}H_{13}I_3N_3O_4$*	*0.7*	*[M+H]*
		357.9674	$C_{11}H_9IN_3O_3$	2.6	$[M+H-I-HI-CH_3O]^+$
		467.8293	$C_{11}H_6I_2N_2O_3$	36.2	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
		330.9511	$C_{10}H_8IN_2O_3$	19.1	$[M+H-CH_5N-CO-I-I]^+$
		344.9821[1)]	$C_{11}H_{10}IN_2O_3$	26.2	$[M+H-NH_3-CO-I-I]^{\cdot+}$
		231.0701[1)]	$C_{11}H_9N_3O_3$	27.1	$[M+H-HI-HI-I-CH_2O]^{\cdot+}$
DDPI TP 517	7.9	*517.9045*	*$C_{12}H_{14}I_2N_3O_4$*	*4.6*	*[M+H]*
		232.0819	$C_{11}H_{10}N_3O_3$	44.2	$[M+H-I-HI-CH_3O]^+$
		341.9612	$C_{11}H_7IN_2O_3$	33.9	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
		372.9624	$C_{12}H_{10}IN_2O_4$	15	$[M+H-NH_3-HI]^+$
		358.9457	$C_{11}H_8IN_2O_4$	18.5	$[M+H-CH_5N-HI]^+$
	9.7	*517.9018*	*$C_{12}H_{14}I_2N_3O_4$*	*9.8*	*[M+H]*
		327.9304	$C_{10}H_5IN_2O_3$	10.8	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		372.9514	$C_{12}H_{10}IN_2O_4$	44.5	$[M+H-NH_3-HI]^+$
		205.0668	$C_{10}H_9N_2O_3$	29.4	$[M+H-CH_5N-CO-I-I]^+$
		219.0778	$C_{11}H_{11}N_2O_3$	6.3	$[M+H-NH_3-CO-I-I]^+$

Iomeprol TP 629	4.6	*629.7856*	*$C_{11}H_{13}I_3N_3O_4$*	*3.5*	*[M+H]*
		330.9593	$C_{10}H_8IN_2O_3$	5.7	$[M+H-NH_3-CO-I-I]^+$
		457.8656	$C_{10}H_8I_2N_2O_3$	8.1	$[M+H-NH_3-CO-I]^{\cdot+}$
		357.9894	$C_{11}H_7IN_2O_4$	125.5[3)]	$[M+H-NH_3-HI-I]^{\cdot+}$
		329.9734[2)]	$C_{10}H_7IN_2O_3$	72.3[3)]	$[M+H-NH_3-CO-I-HI]^{\cdot+}$
		357.9719	$C_{11}H_7IN_2O_4$	76.7[3)]	$[M+H-NH_3-HI-I]^{\cdot+}$
Iomeprol TP 629 -1I	3.9	*503.8876*	*$C_{11}H_{12}I_2N_3O_4$*	*7.1*	*[M+H]*
		205.0664	$C_{10}H_9N_2O_3$	27.5	$[M+H-HI-I-CH_2NO]^+$
		206.0770	$C_{10}H_{10}N_2O_3$	40.8	$[M+H-HI-I-CHNO]^{\cdot+}$
		177.0702	$C_9H_9N_2O_2$	24.5	$[M+H-I-I-CHNO-CH_2O]^+$
		318.9815	$C_9H_{10}IN_3O_2$	0.8	$[M+H-I-C_2H_2O_2]^{\cdot+}$
		375.9748	$C_{11}H_{11}IN_3O_4$	10.9	$[M+H-HI]^+$
	4.5	*503.8883*	*$C_{11}H_{12}I_2N_3O_4$*	*5.7*	*[M+H]*
		375.9739	$C_{11}H_{11}IN_3O_4$	13.3	$[M+H-HI]^+$
		206.0733	$C_{10}H_{10}N_2O_3$	22.8	$[M+H-HI-I-CHNO]^{\cdot+}$
		205.0653	$C_{10}H_9N_2O_3$	22.1	$[M+H-HI-I-CH_2NO]^+$
		318.9782	$C_9H_{10}IN_3O_2$	9.5	$[M+H-I-C_2H_2O_2]^{\cdot+}$
		232.0776	$C_{11}H_{10}N_3O_3$	26	$[M+H-HI-I-HO]^+$
	5.0	*503.8886*	*$C_{11}H_{12}I_2N_3O_4$*	*5.2*	*[M+H]*
		375.9718	$C_{11}H_{11}IN_3O_4$	18.8	$[M+H-HI]^+$
		205.0660	$C_{10}H_9N_2O_3$	25.5	$[M+H-HI-I-CH_2NO]^+$
		206.0756	$C_{10}H_{10}N_2O_3$	34	$[M+H-HI-I-CHNO]^{\cdot+}$
		232.0776	$C_{11}H_{10}N_3O_3$	25.6	$[M+H-HI-I-HO]^+$
		318.9814	$C_9H_{10}IN_3O_2$	0.5	$[M+H-I-C_2H_2O_2]^{\cdot+}$
Iomeprol TP 629 -2I	4.4	*377.9930*	*$C_{11}H_{13}IN_3O_4$*	*4.0*	*[M+H]*
		250.0852	$C_{11}H_{12}N_3O_4$	11.9	$[M+H-HI]^{\cdot+}$
		193.0931	$C_9H_{11}N_3O_2$	44.2	$[M+H-I-C_2H_2O_2]^{\cdot+}$
		203.0505	$C_{10}H_7N_2O_3$	26.5	$[M+H-HI-CH_3NO-H_2]^+$
		206.0740	$C_{10}H_{10}N_2O_3$	26.2	$[M+H-HI-I-CHNO]^{\cdot+}$
Diatrizoate	5.4	*614.7756*	*$C_{11}H_{10}N_2O_4I_3$*	*2.1*	*$[M+H]^+$*
		360.9777	$C_{11}H_{10}N_2O_4I$	26.9	$[M+H-I-I]^+$

[1)] fragment not observed in batch experiment, but can be explained by molecular structure

[2)] fragment not observed by Kormos et al.[5], but can be explained by reactions in their proposed fragmentation pathway

[3)] fragments with mass error >50 ppm were not included in assigning the confidence levels

Table S29. Fragments of the detected (experimental and predicted) anaerobic TPs and their precursor substances in well 5.

substance	RT / min	Fragment m/z	Ion Formula	Mass error / ppm	Proposed fragmentation (see also Tables S 7 and S 8)
DDPI	8.0	*643.8028*	*$C_{12}H_{13}I_3N_3O_4$*	*1.1*	*[M+H]*
		357.9640	$C_{11}H_9IN_3O_3$	12.1	$[M+H-I-HI-CH_3O]^+$
		330.9509	$C_{10}H_8IN_2O_3$	19.7	$[M+H-CH_5N-CO-I-I]^+$
		498.8325	$C_{12}H_9I_2N_2O_4$	64.4[3)]	$[M+H-NH_3-HI]^+$
		231.0716[1)]	$C_{11}H_9N_3O_3$	33.6	$[M+H-HI-HI-I-CH_2O]^{\cdot+}$
		467.8332	$C_{11}H_6I_2N_2O_3$	27.9	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
DDPI TP 517	7.9	*517.9036*	*$C_{12}H_{14}I_2N_3O_4$*	*6.3*	*[M+H]*
		341.9468	$C_{11}H_7IN_2O_3$	8.2	$[M+H-NH_3-HI-CH_3O]^{\cdot+}$
		205.0607	$C_{10}H_9N_2O_3$	0.2	$[M+H-CH_5N-CO-I-I]^{\cdot\cdot+}$
	9.7	*517.9038*	*$C_{12}H_{14}I_2N_3O_4$*	*5.8*	*[M+H]*
		327.9360	$C_{10}H_5IN_2O_3$	6.3	$[M+H-CH_5N-HI-CH_3O]^{\cdot+}$
		331.9801	$C_{10}H_9IN_2O_3$	44.7	$[M+H-I-C_2H_5NO]^{\cdot+}$
Iomeprol TP 629	4.7	*629.7870*	*$C_{11}H_{13}I_3N_3O_4$*	*1.3*	*[M+H]*
		330.9615	$C_{10}H_8IN_2O_3$	12.4	$[M+H-NH_3-CO-I-I]^+$
		457.8650	$C_{10}H_8I_2N_2O_3$	6.9	$[M+H-NH_3-CO-I]^{\cdot+}$
		357.9719	$C_{11}H_7IN_2O_4$	76.5[3)]	$[M+H-NH_3-HI-I]^{\cdot+}$
		501.8812[2)]	$C_{11}H_{10}I_2N_3O_4$	11.3	$[M+H-HI]^+$
		329.9735[2)]	$C_{10}H_7IN_2O_3$	72.5[3)]	$[M+H-NH_3-CO-I-HI]^{\cdot+}$
Iomeprol TP 629 -1I	3.9	*503.8895*	*$C_{11}H_{12}I_2N_3O_4$*	*3.4*	*[M+H]*
		205.0662	$C_{10}H_9N_2O_3$	26.5	$[M+H-HI-I-CH_2NO]^+$
		206.0749	$C_{10}H_{10}N_2O_3$	30.6	$[M+H-HI-I-CHNO]^{\cdot+}$
		177.0740	$C_9H_9N_2O_2$	46.0	$[M+H-I-I-CHNO-CH_2O]^+$
		318.9808	$C_9H_{10}IN_3O_2$	1.3	$[M+H-I-C_2H_2O_2]^{\cdot+}$
		375.9709	$C_{11}H_{11}IN_3O_4$	21.2	$[M+H-HI]^+$
	4.6	*503.8879*	*$C_{11}H_{12}I_2N_3O_4$*	*6.5*	*[M+H]*
		375.9720	$C_{11}H_{11}IN_3O_4$	18.3	$[M+H-HI]^+$
		206.0753	$C_{10}H_{10}N_2O_3$	32.5	$[M+H-HI-I-CHNO]^{\cdot+}$
		205.0664	$C_{10}H_9N_2O_3$	27.6	$[M+H-HI-I-CH_2NO]^+$
	5.0	*503.8885*	*$C_{11}H_{12}I_2N_3O_4$*	*5.3*	*[M+H]*
		375.9739	$C_{11}H_{11}IN_3O_4$	13.3	$[M+H-HI]^+$
		205.0663	$C_{10}H_9N_2O_3$	27.0	$[M+H-HI-I-CH_2NO]^+$
		206.0747	$C_{10}H_{10}N_2O_3$	29.6	$[M+H-HI-I-CHNO]^{\cdot+}$
		232.0753	$C_{11}H_{10}N_3O_3$	15.7	$[M+H-HI-I-HO]^+$
		318.9798	$C_9H_{10}IN_3O_2$	4.5	$[M+H-I-C_2H_2O_2]^{\cdot+}$
Iomeprol TP 629 -2I	4.4	*377.9921*	*$C_{11}H_{13}IN_3O_4$*	*6.4*	*[M+H]*
		250.0839	$C_{11}H_{12}N_3O_4$	6.5	$[M+H-HI]^{\cdot+}$
		206.0742	$C_{10}H_{10}N_2O_3$	26.7	$[M+H-HI-I-CHNO]^{\cdot+}$
		203.0515	$C_{10}H_7N_2O_3$	31.4	$[M+H-HI-CH_3NO-H_2]^+$
		193.0916	$C_9H_{11}N_3O_2$	36.4	$[M+H-I-C_2H_2O_2]^{\cdot+}$

Diatrizoate	5.4	*614.7720*	*$C_{11}H_{10}N_2O_4I_3$*	*8.0*	*$[M+H]^+$*
		233.0601	$C_{11}H_9N_2O_4$	18.9	$[M+H-I-I-HI]^+$
		360.9705	$C_{11}H_{10}N_2O_4I$	7.0	$[M+H-I-I]^+$

[1)] fragment not observed in batch experiment, but can be explained by molecular structure

[2)] fragment not observed by Kormos et al.[5], but can be explained by reactions in their proposed fragmentation pathway

[3)] fragments with mass error >50 ppm were not included in assigning the confidence levels

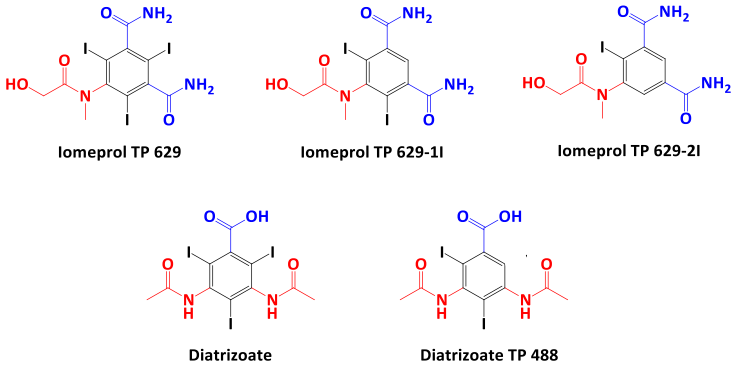

Figure S8. Molecular structures of detected anaerobic TPs not identified in the batch experiments and their precursors.[3, 5]

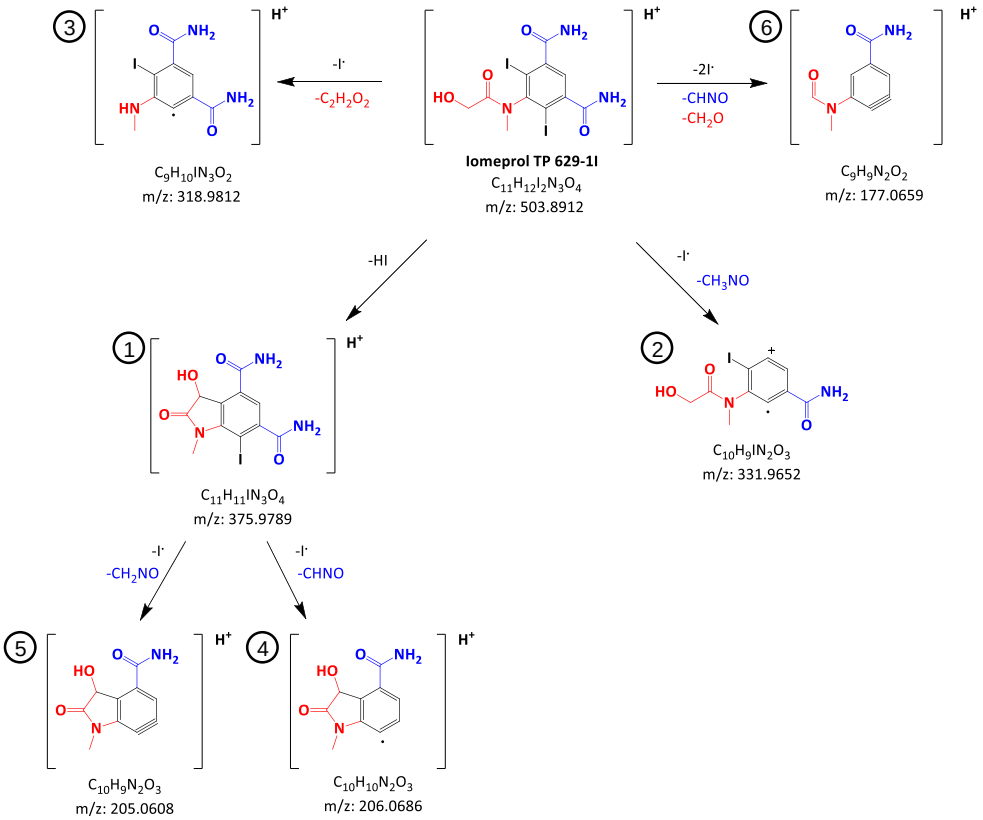

Figure S9. Proposed fragmentation pathway of iomeprol TP 629 -1I (3.9 min, well 1). Numbers correspond to the peaks in Figure S10.

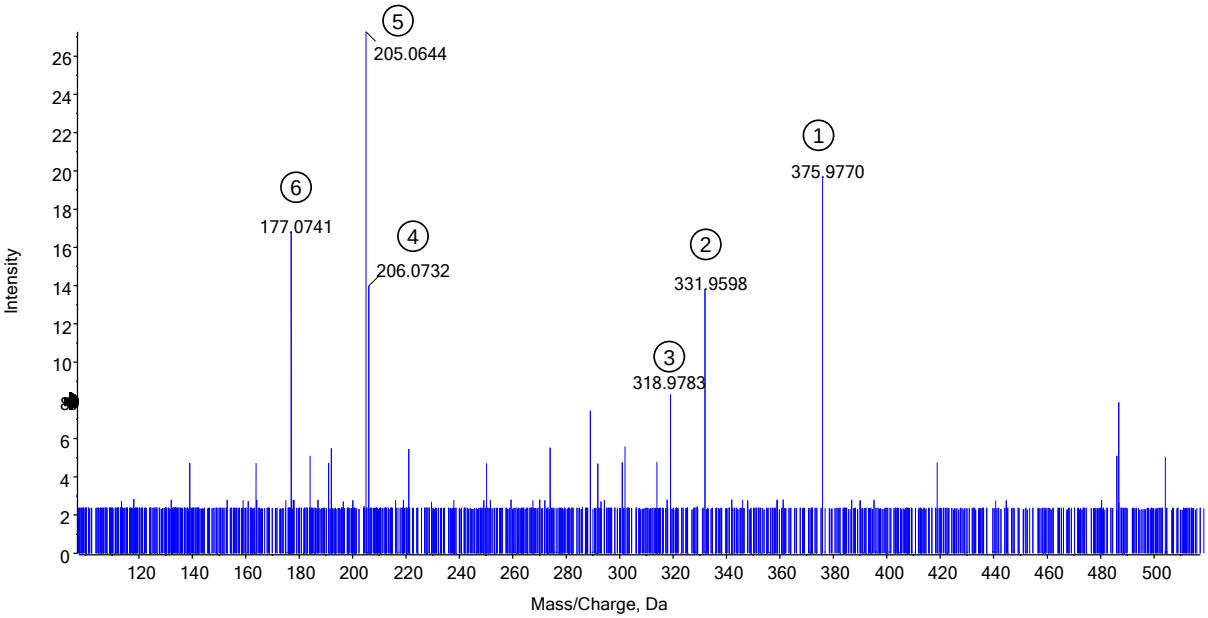

Figure S10. MS^2 spectrum of iomeprol TP 629 -1I (3.9 min, well 1).

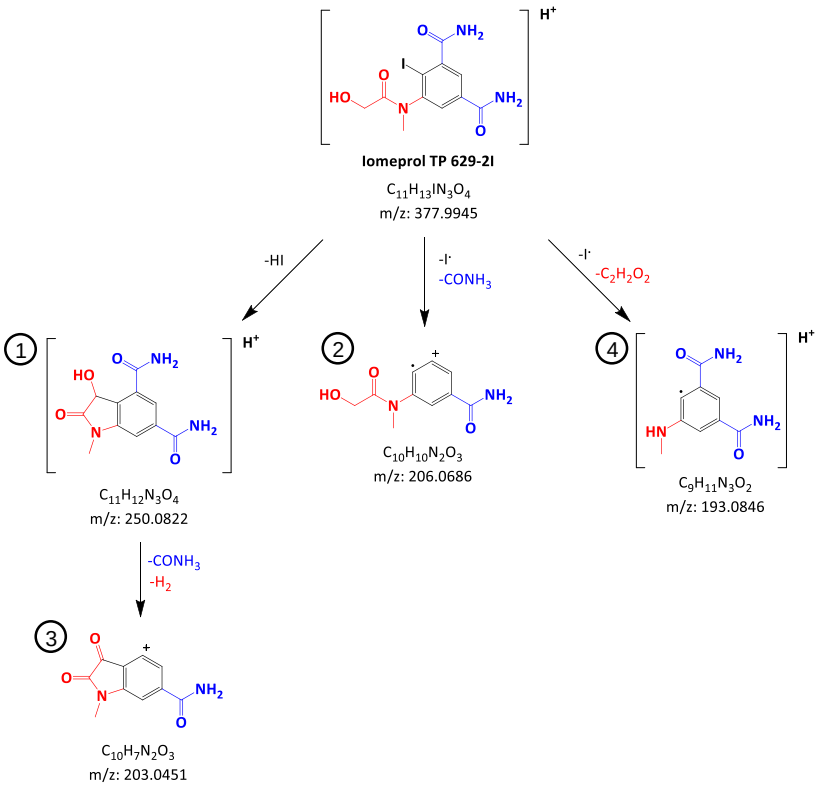

Figure S11. Proposed fragmentation pathway of iomeprol TP 629 -2I (well 3). Numbers correspond to the peaks in Figure S12.

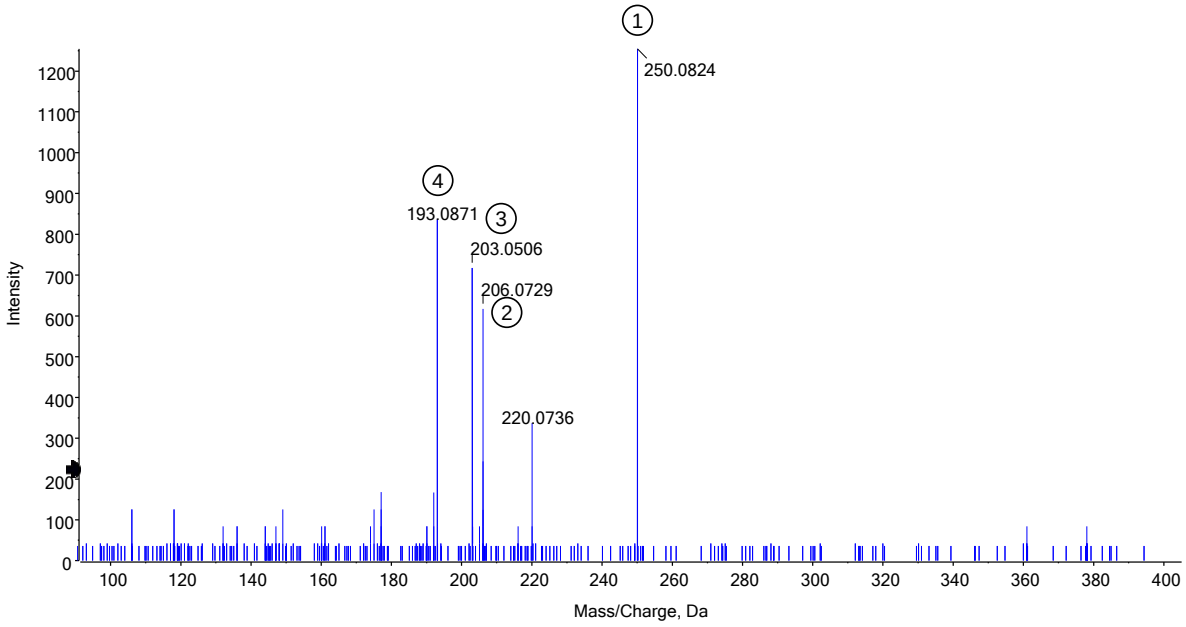

Figure S12. MS^2 spectrum of iomeprol TP 629 -2I (well 3).

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