

# Mass Spectrometric Fingerprints of Organic Compounds in Sulfate-Rich Ice Grains: Implications for Europa Clipper

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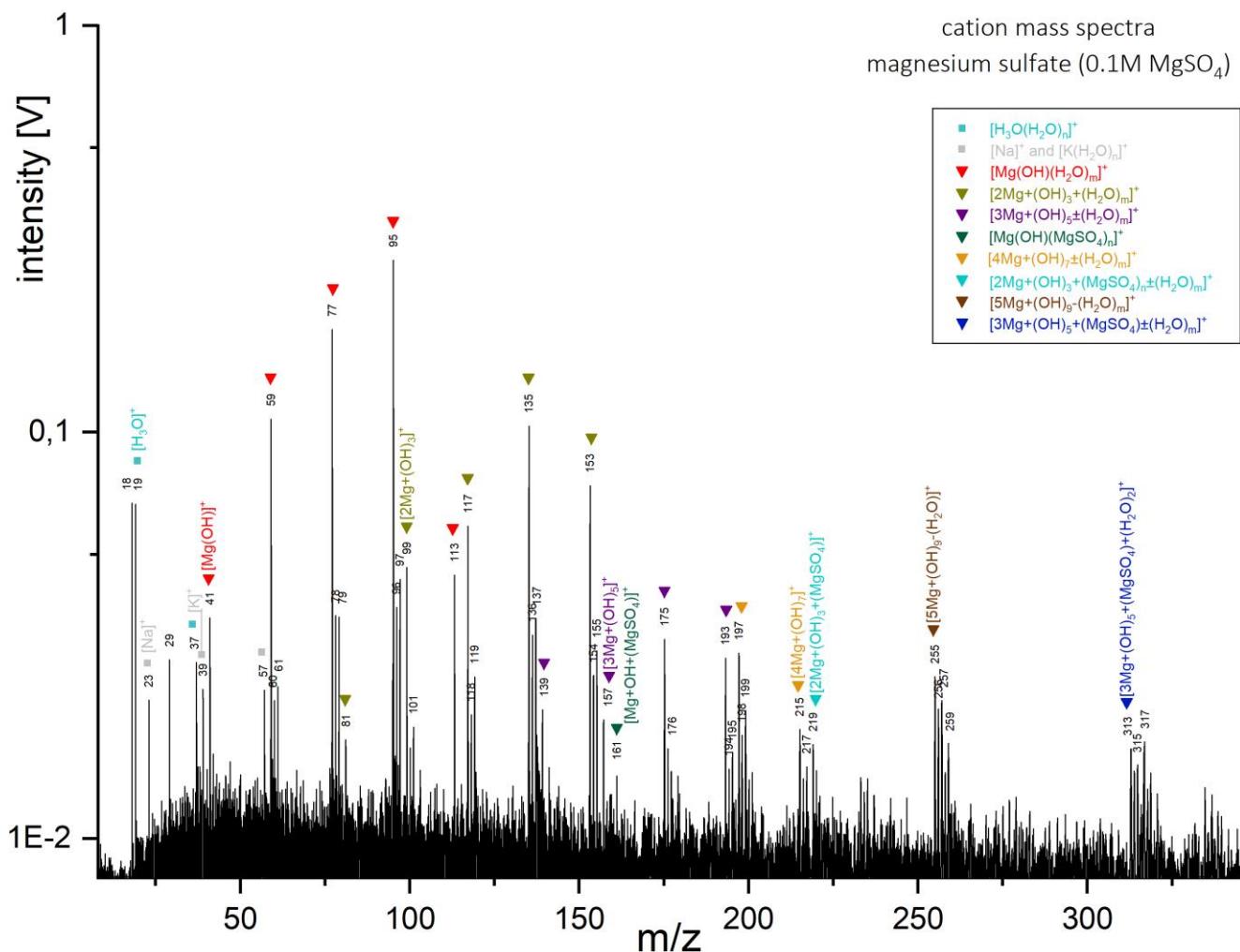
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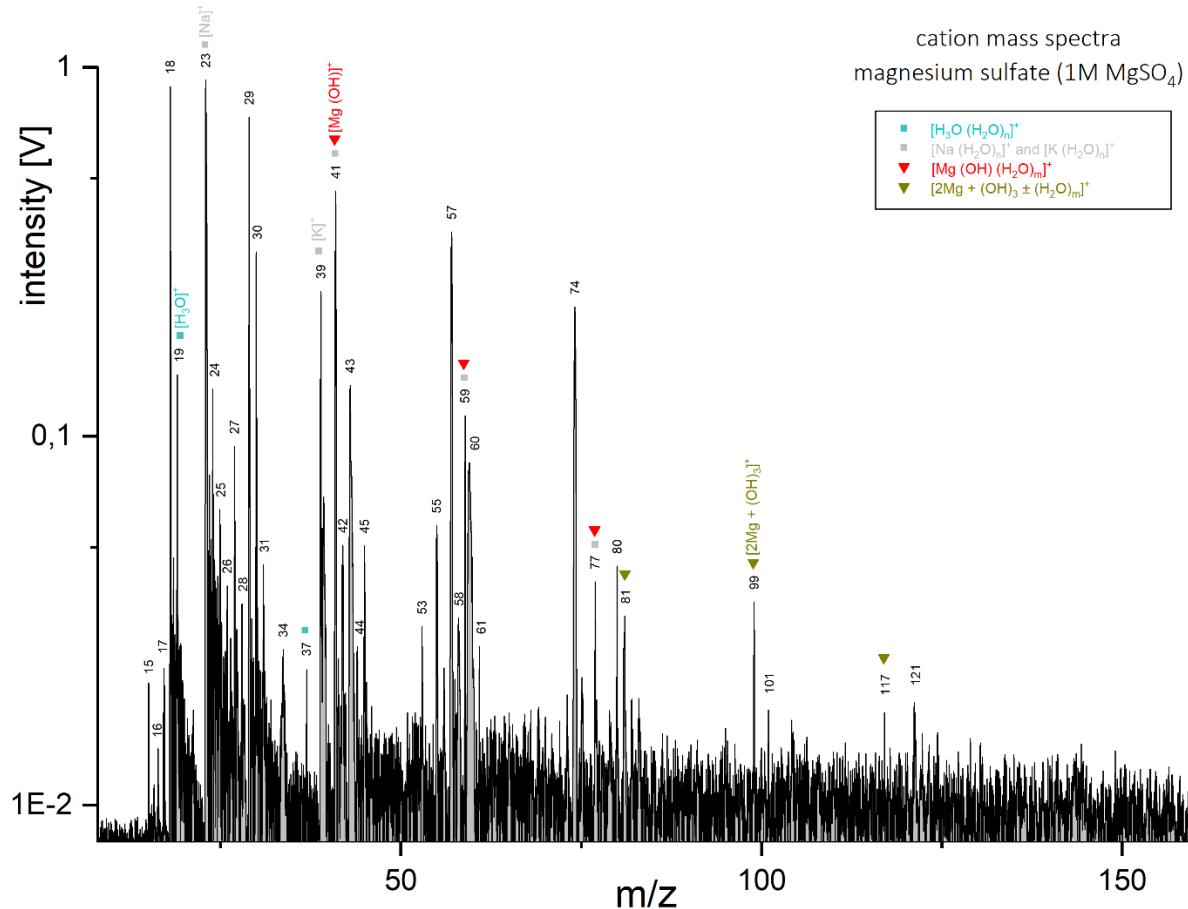
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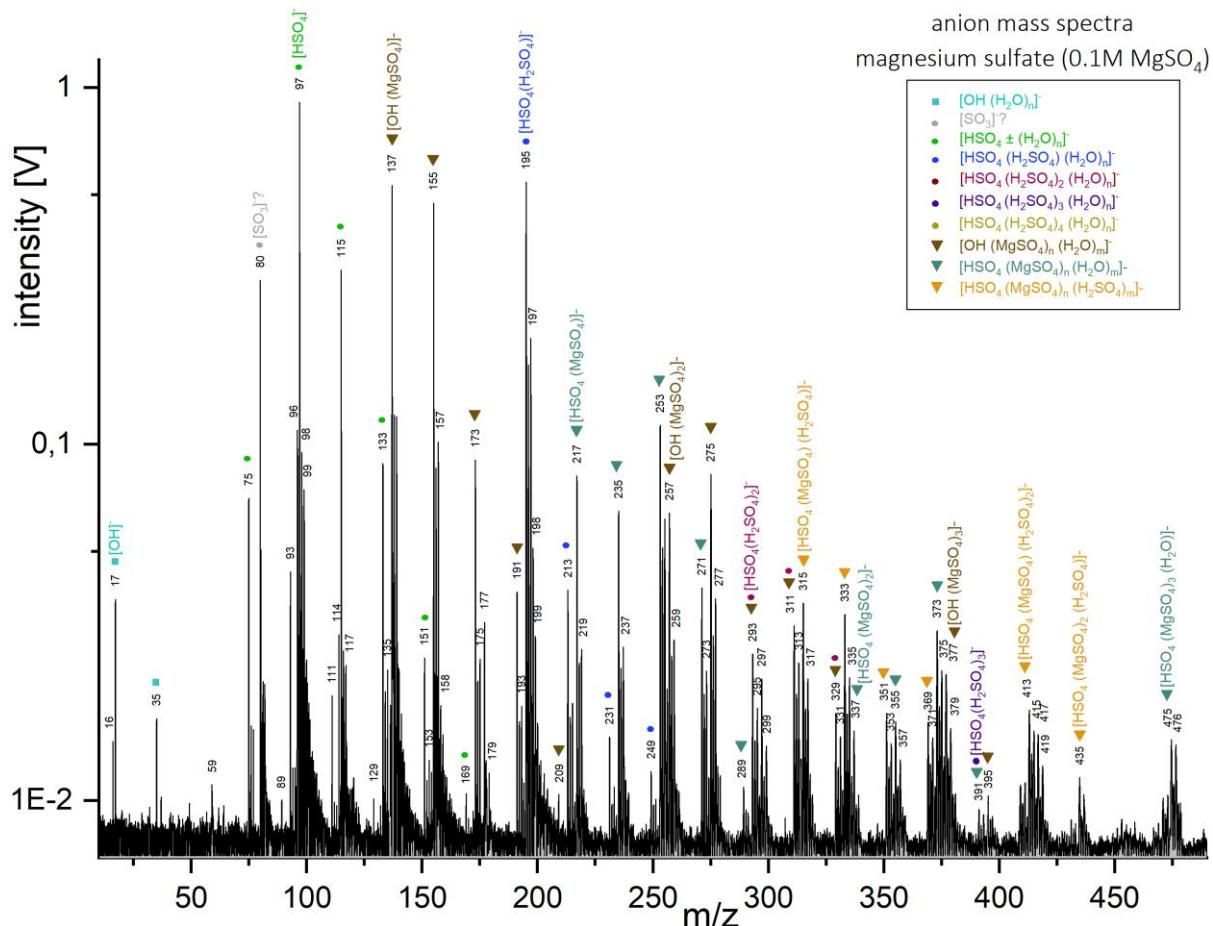
## Supplementary Information



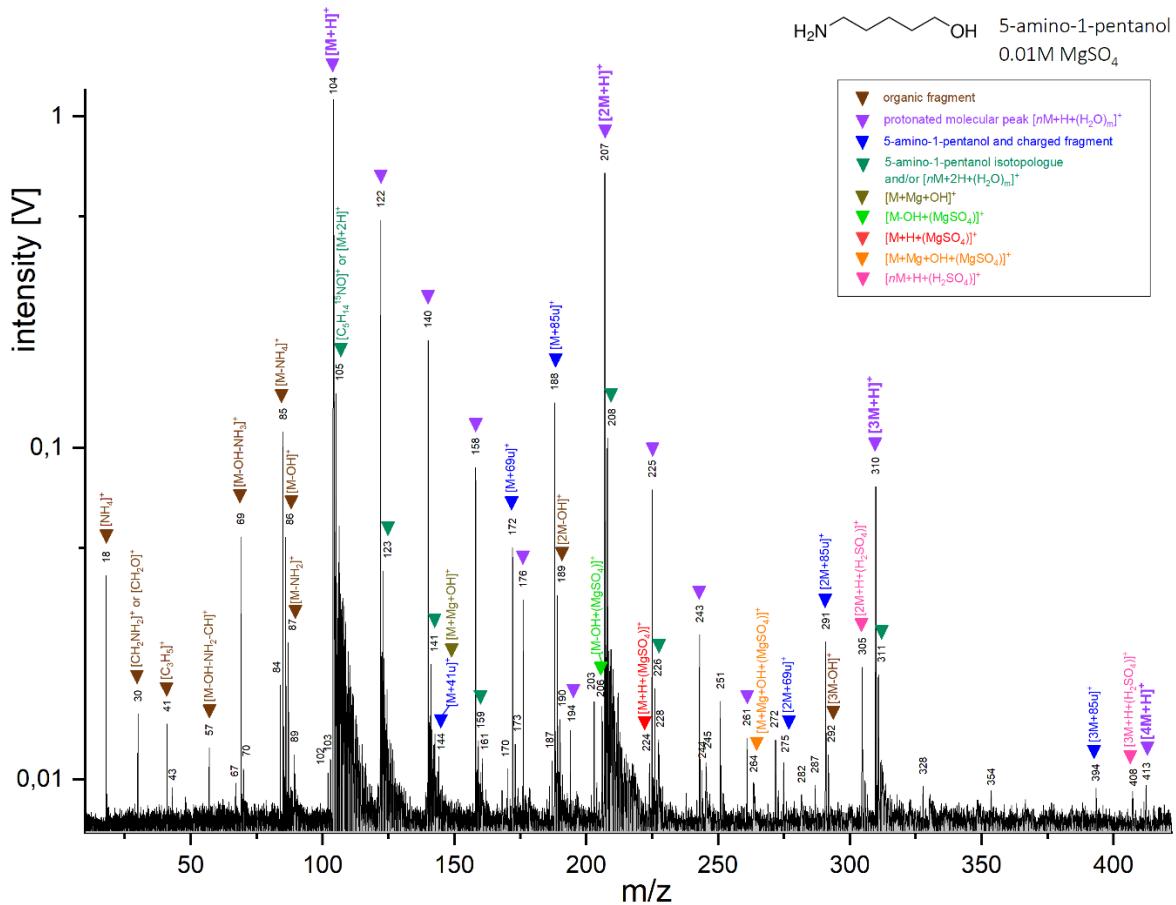
**Figure S1.** Baseline corrected cation mass spectrum of magnesium sulfate ( $\text{MgSO}_4$ ) at a concentration of 0.1M, generated with a delay time of  $5.0 \mu\text{s}$ .



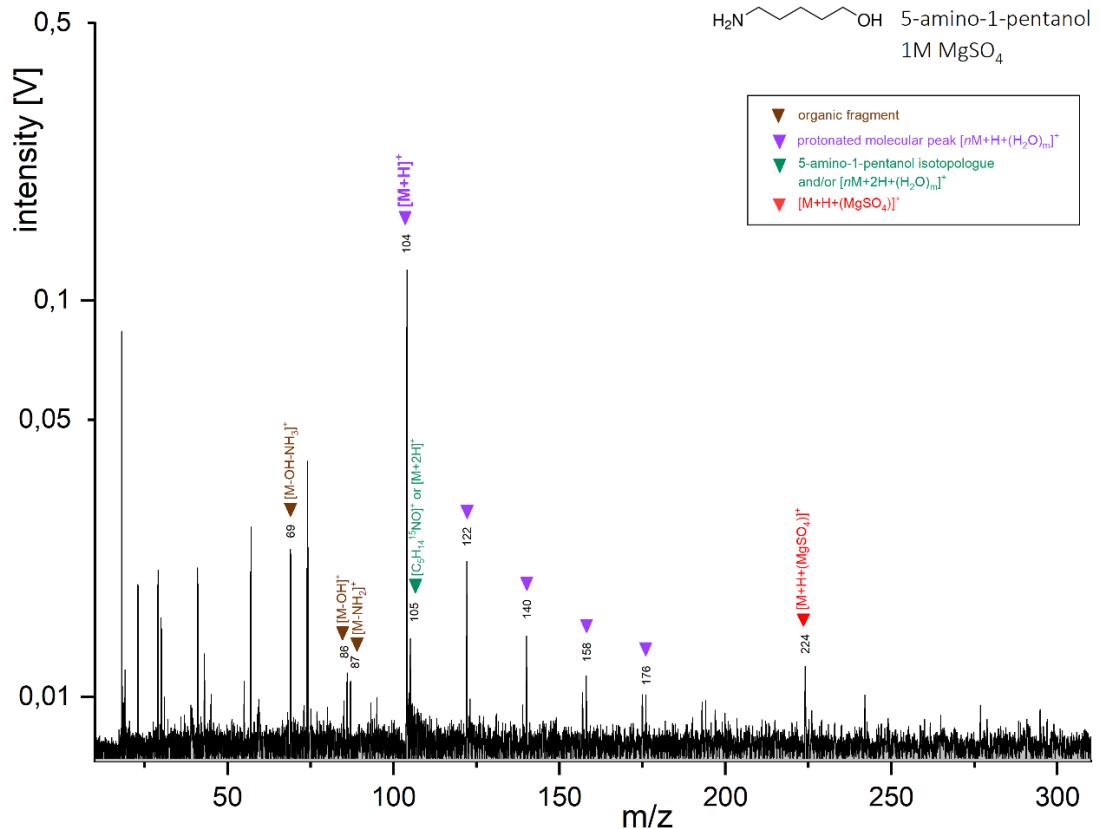
**Figure S2.** Baseline corrected cation mass spectrum of magnesium sulfate ( $\text{MgSO}_4$ ) at a concentration of 1M, generated with a delay time of  $6.0\ \mu\text{s}$ .



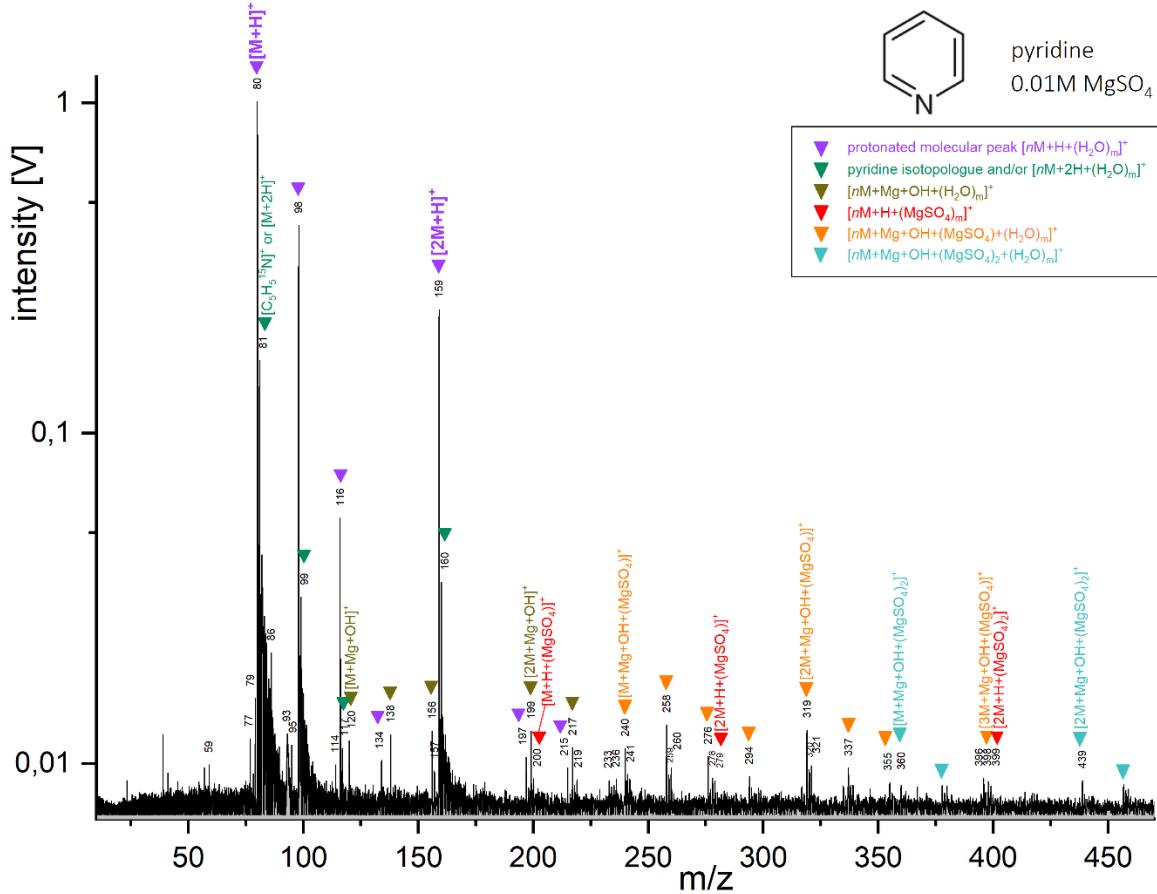
**Figure S3.** Baseline corrected anion mass spectrum of magnesium sulfate ( $\text{MgSO}_4$ ) at a concentration of 0.1M, generated with a delay time of  $6.0\ \mu\text{s}$ .



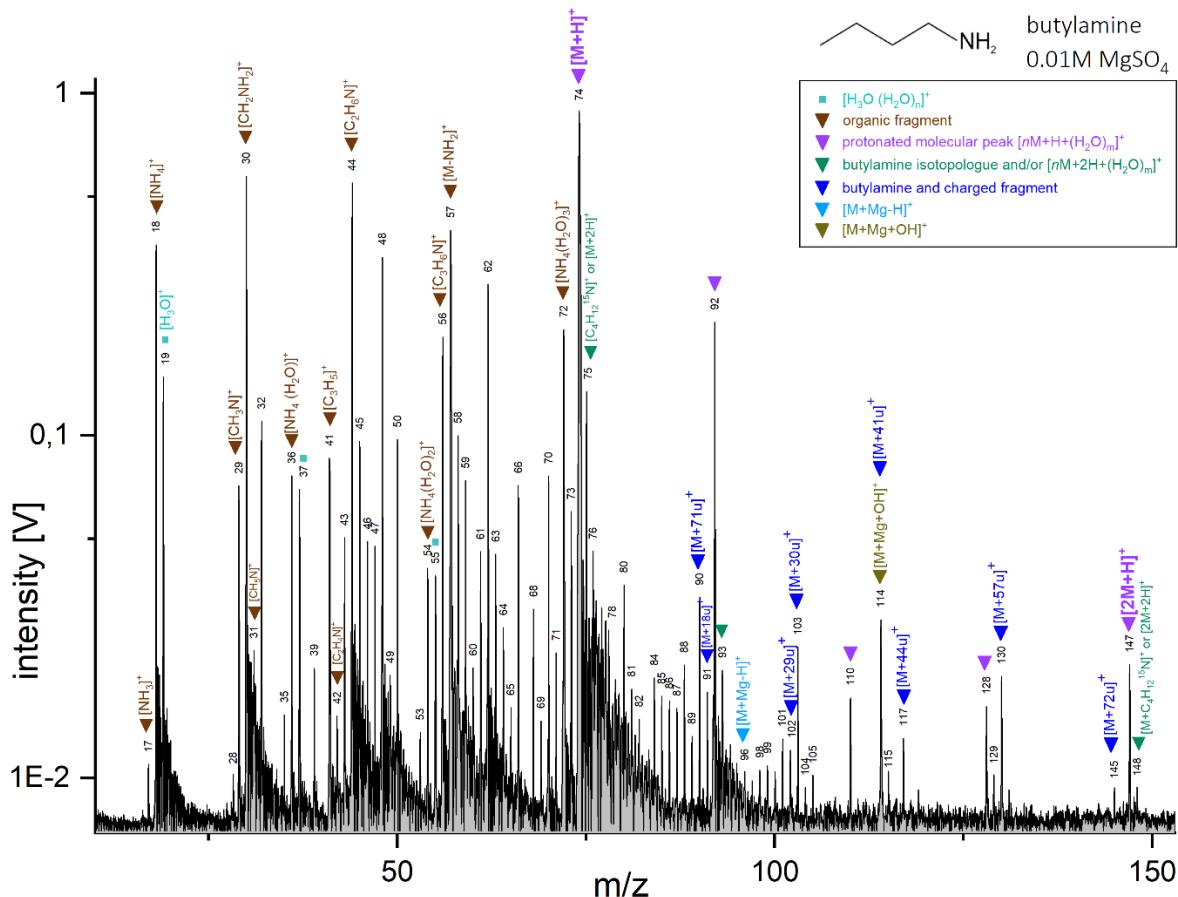
**Figure S4.** Baseline corrected cation mass spectrum of 5-amino-1-pentanol (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 6.4  $\mu\text{s}$ .



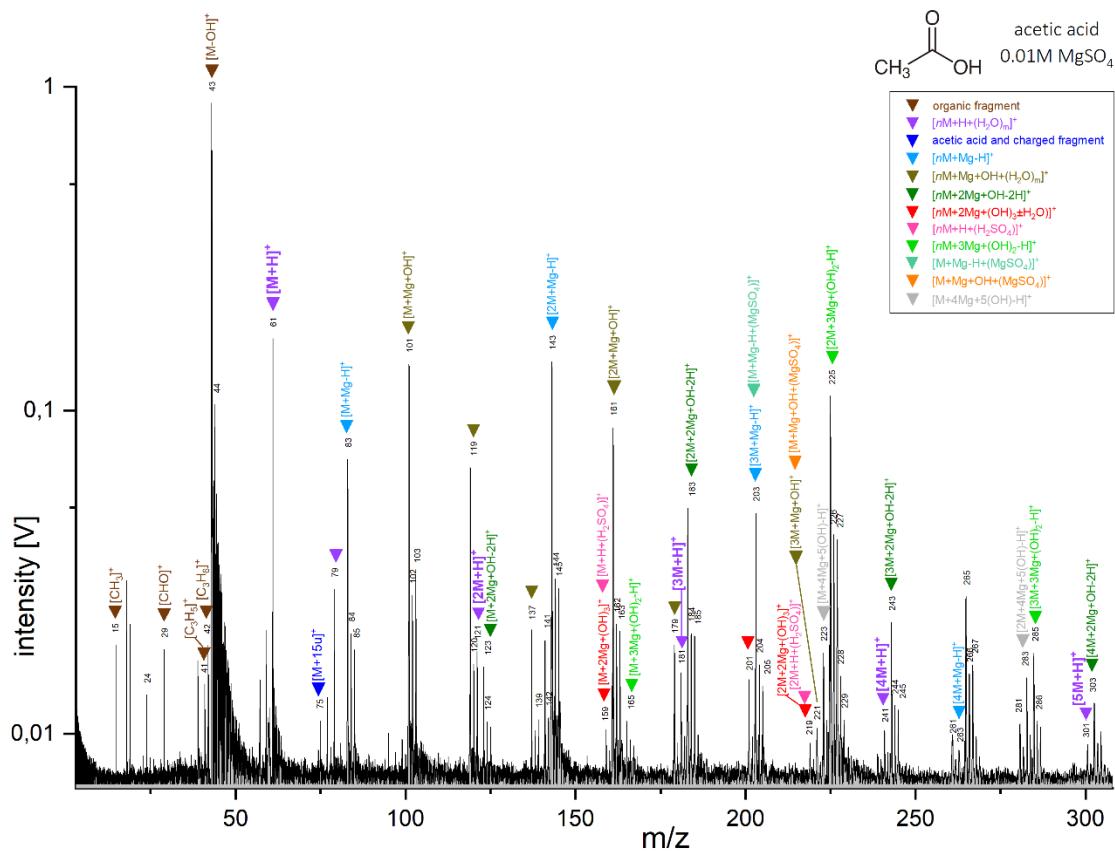
**Figure S5.** Baseline corrected cation mass spectrum of 5-amino-1-pentanol (concentration 0.1 wt%) in 1M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 7.2  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



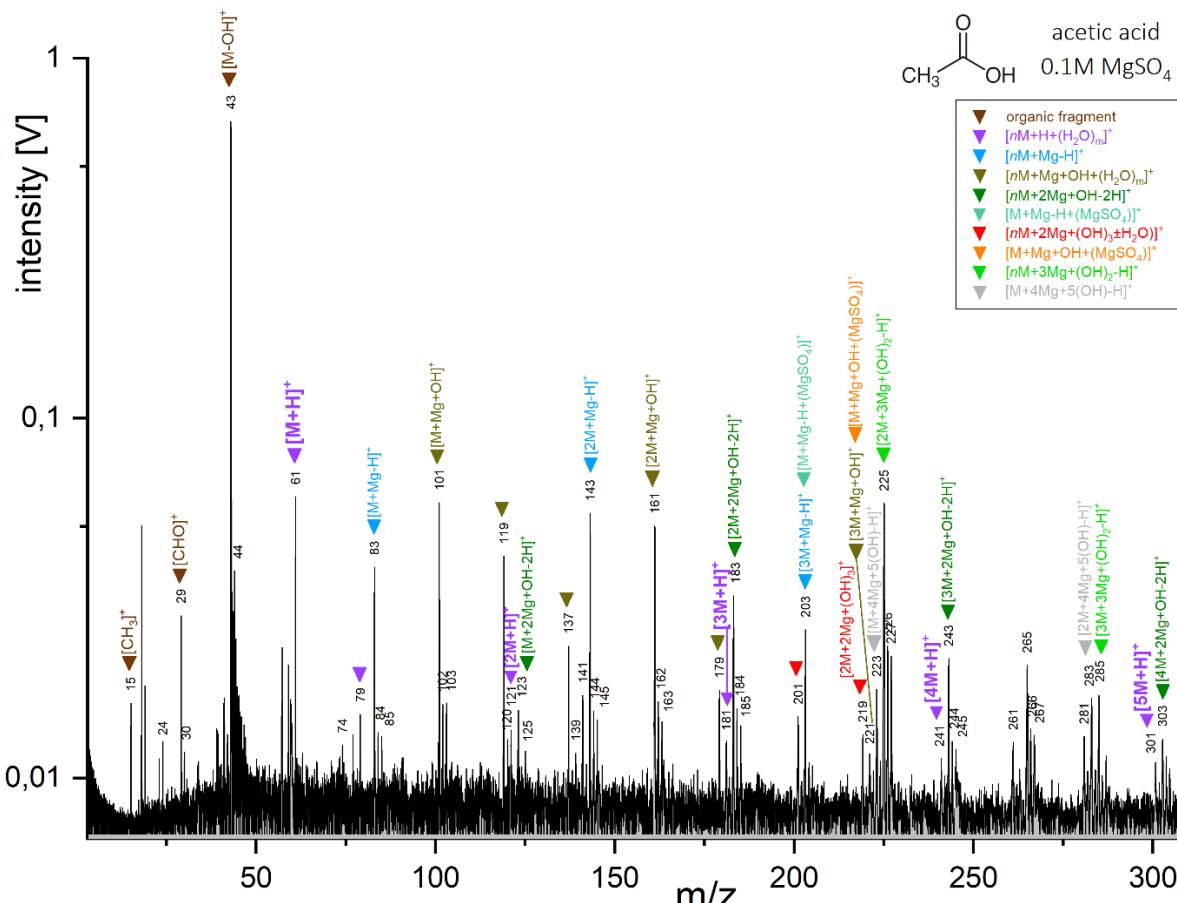
**Figure S6.** Baseline corrected cation mass spectrum of pyridine (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 6.0  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



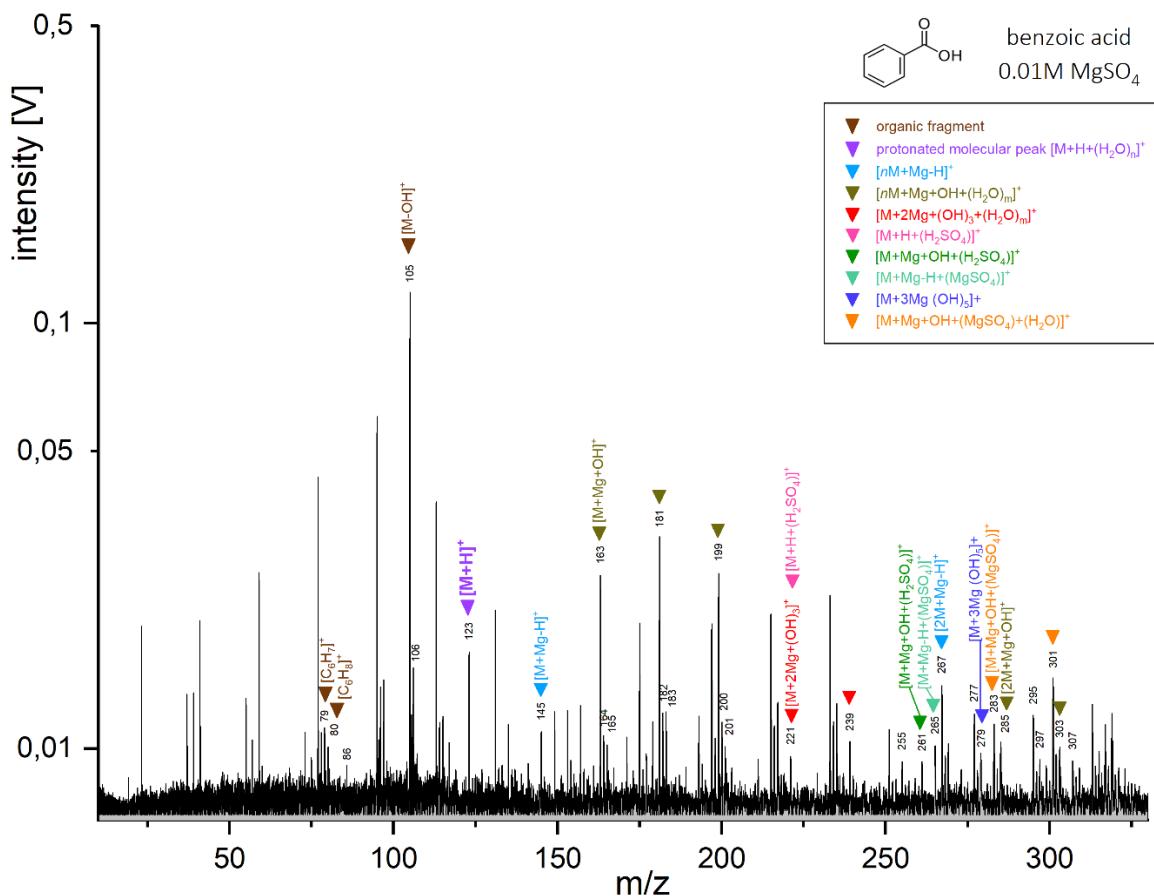
**Figure S7.** Baseline corrected cation mass spectrum of butylamine (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.5  $\mu\text{s}$ .



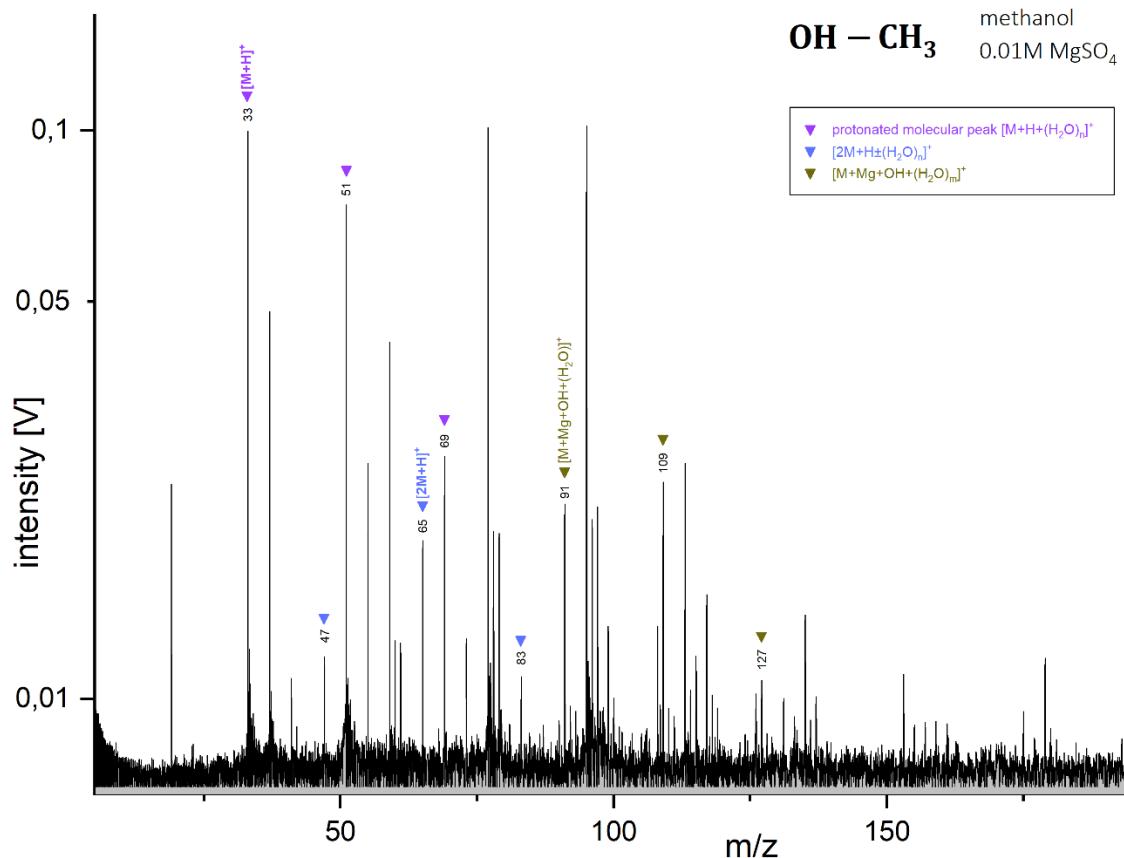
**Figure S8.** Baseline corrected cation mass spectrum of acetic acid (concentration 5 wt%) in 0.01M magnesium sulfate ( $MgSO_4$ ), generated with a delay time of 5.0  $\mu$ s. Unlabeled peaks originate exclusively from the  $MgSO_4$  matrix.



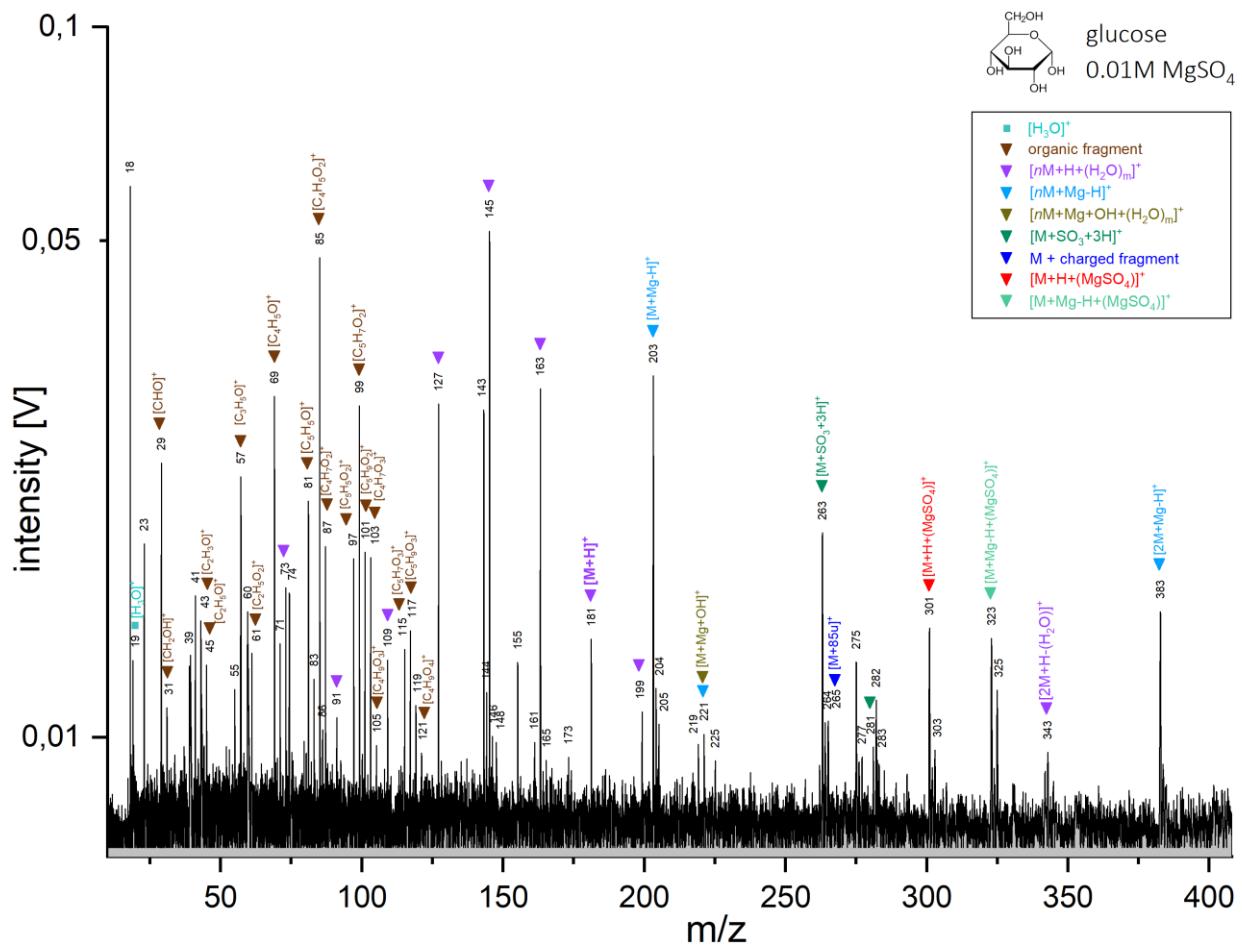
**Figure S9.** Baseline corrected cation mass spectrum of acetic acid (concentration 5 wt%) in 0.1M magnesium sulfate ( $MgSO_4$ ), generated with a delay time of 5.0  $\mu$ s. Unlabeled peaks originate exclusively from the  $MgSO_4$  matrix.



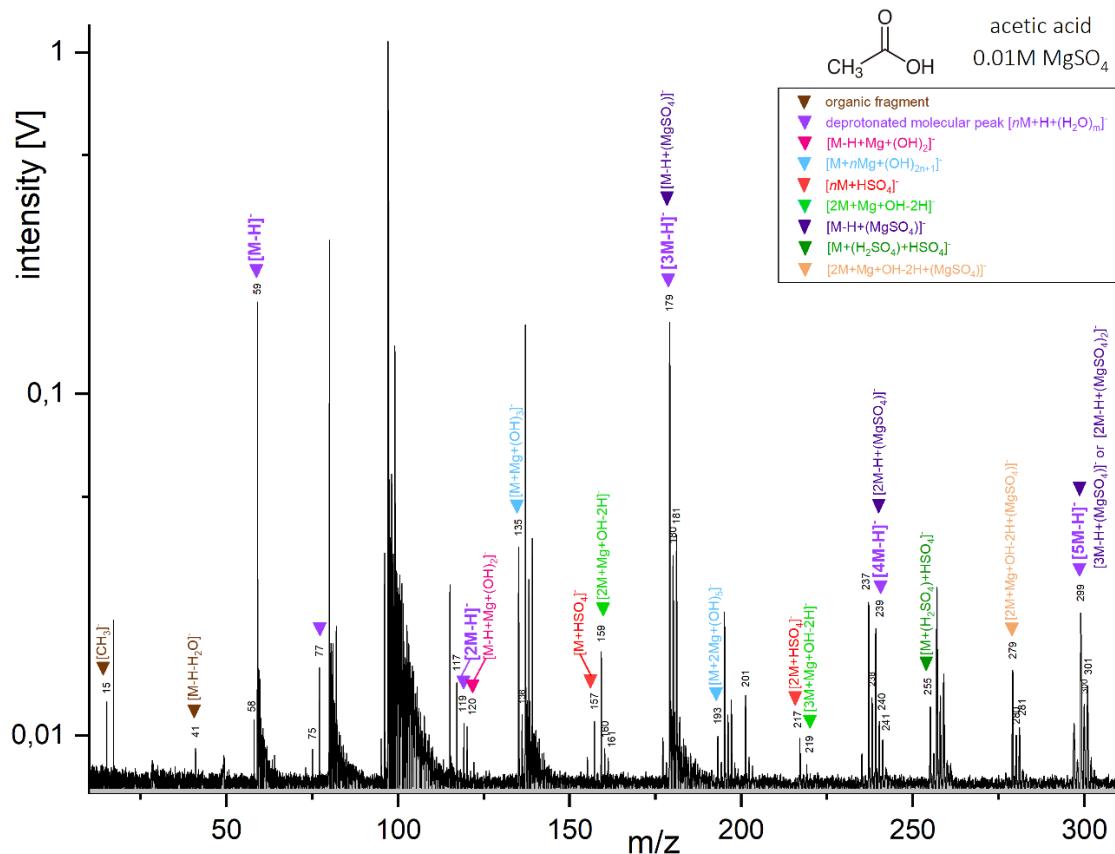
**Figure S10.** Baseline corrected cation mass spectrum of benzoic acid (concentration 0.17 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.8  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



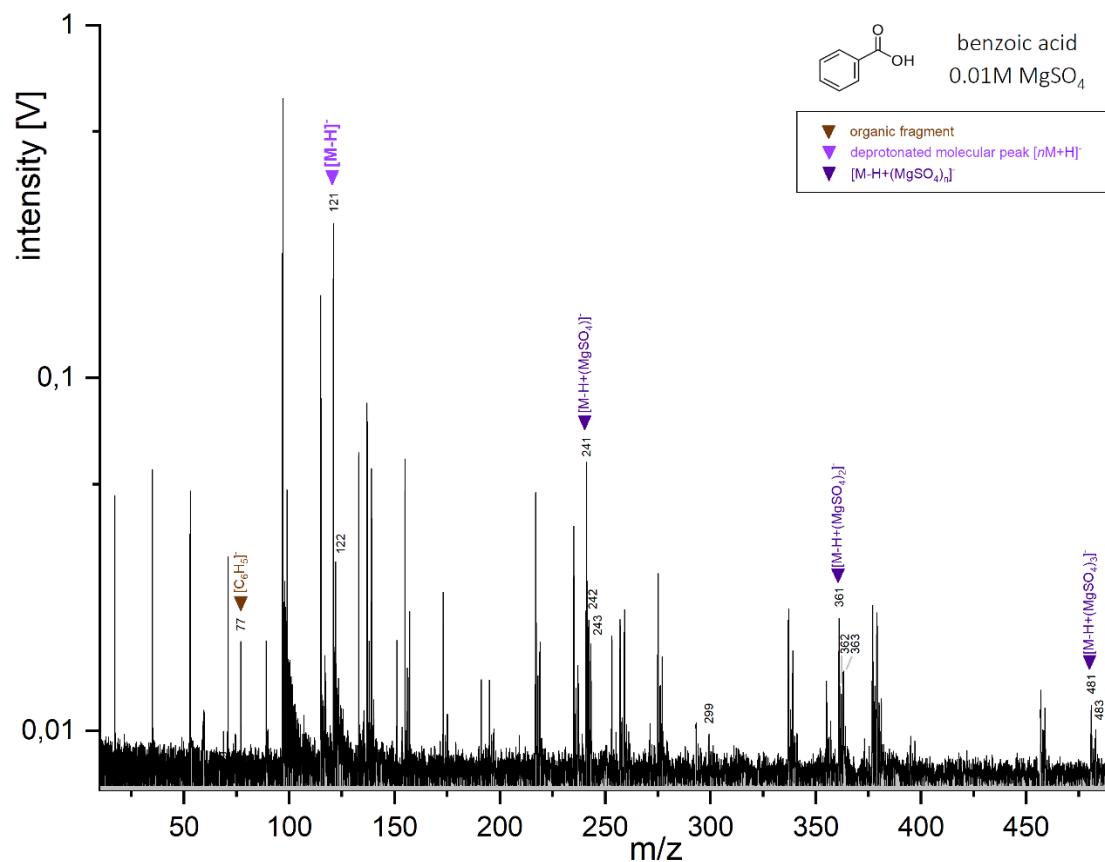
**Figure S11.** Baseline corrected cation mass spectrum of methanol (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.5  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



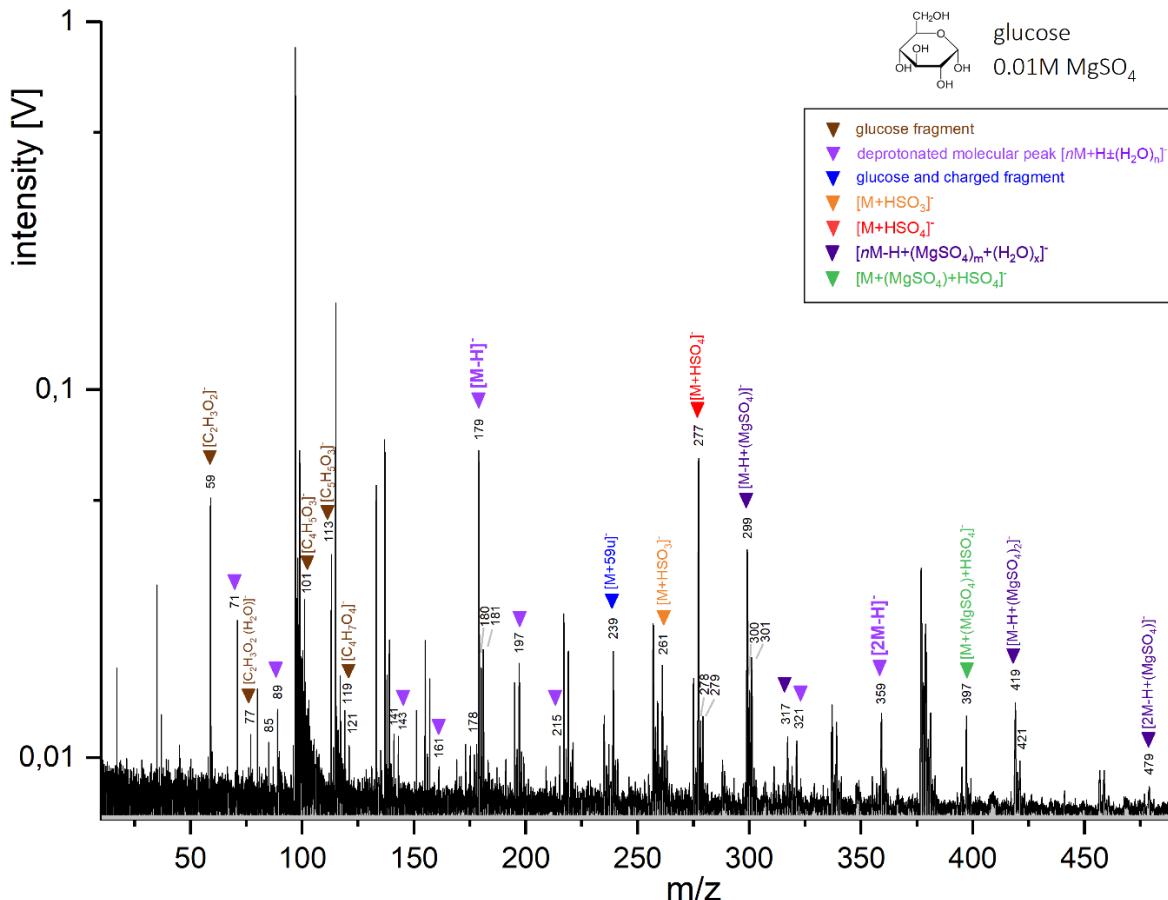
**Figure S12.** Baseline corrected cation mass spectrum of glucose (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 6.0  $\mu\text{s}$ .



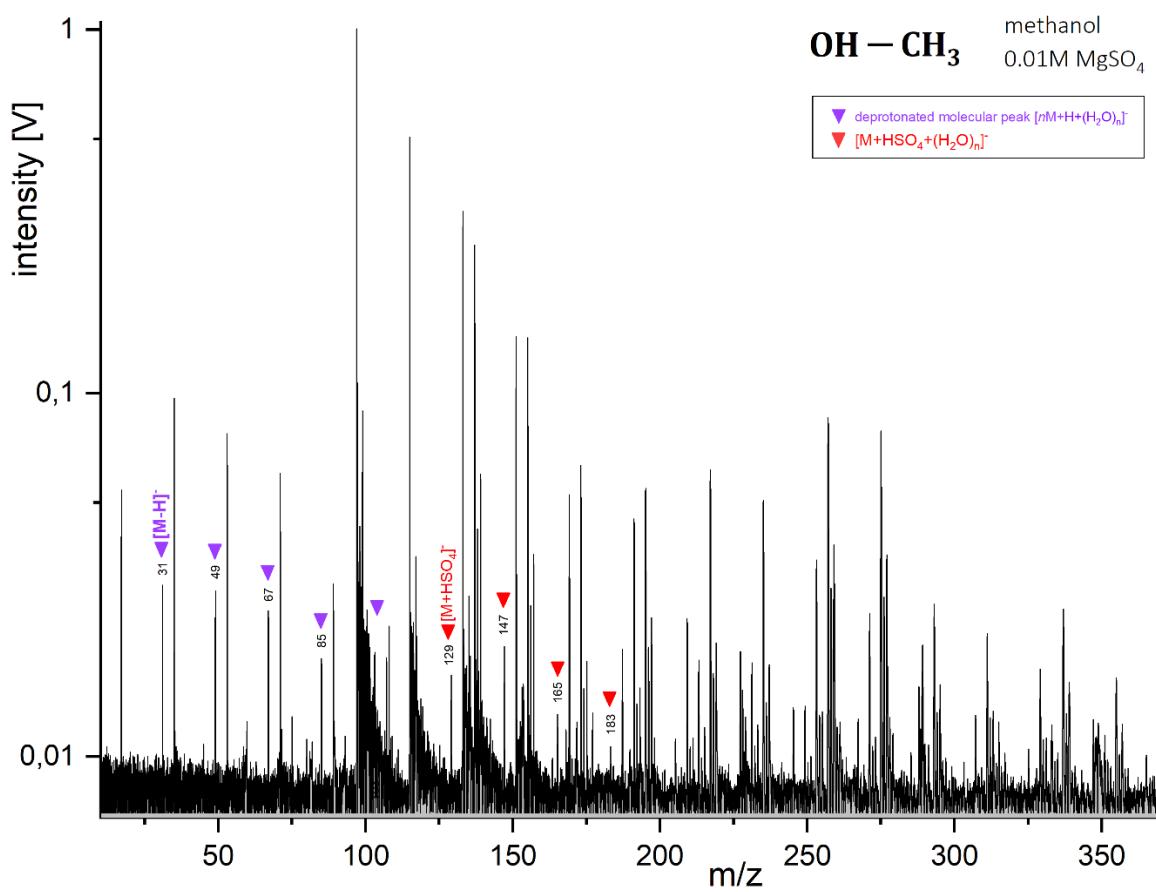
**Figure S13.** Baseline corrected anion mass spectrum of acetic acid (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.0  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



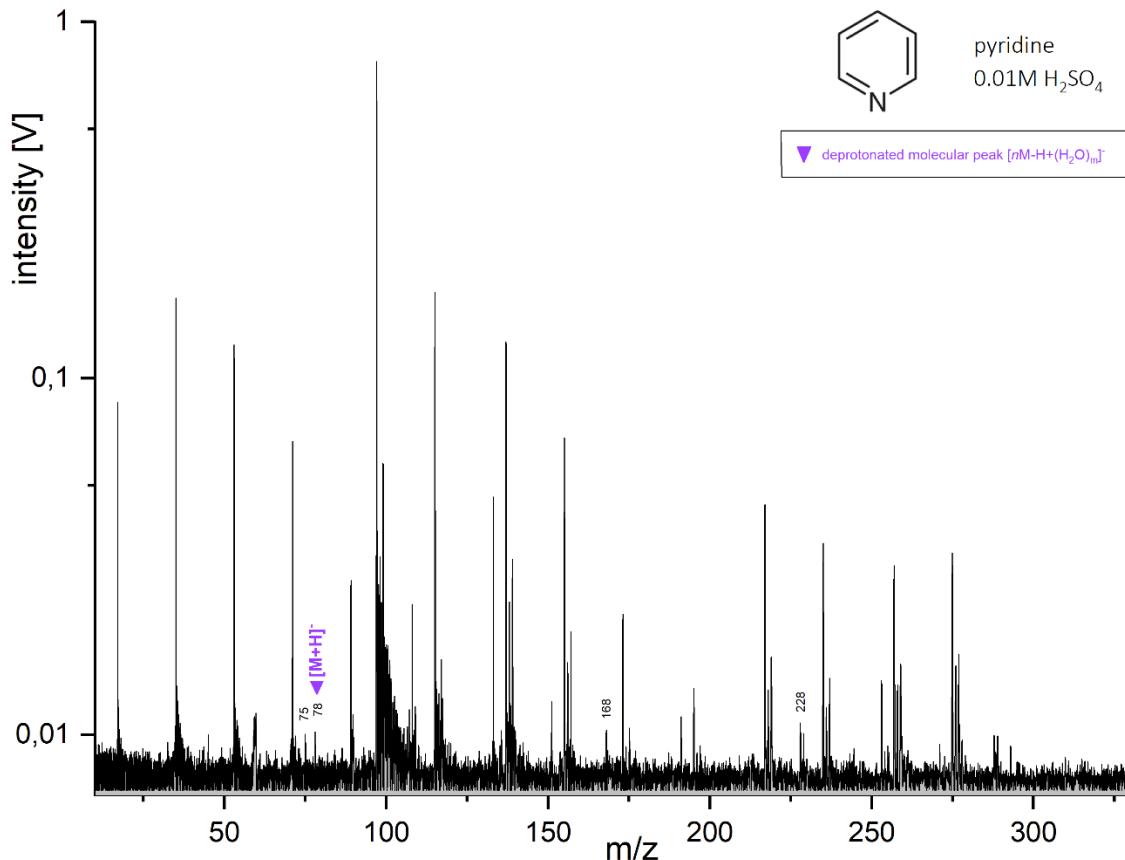
**Figure S14.** Baseline corrected anion mass spectrum of benzoic acid (concentration 0.17 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.8  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



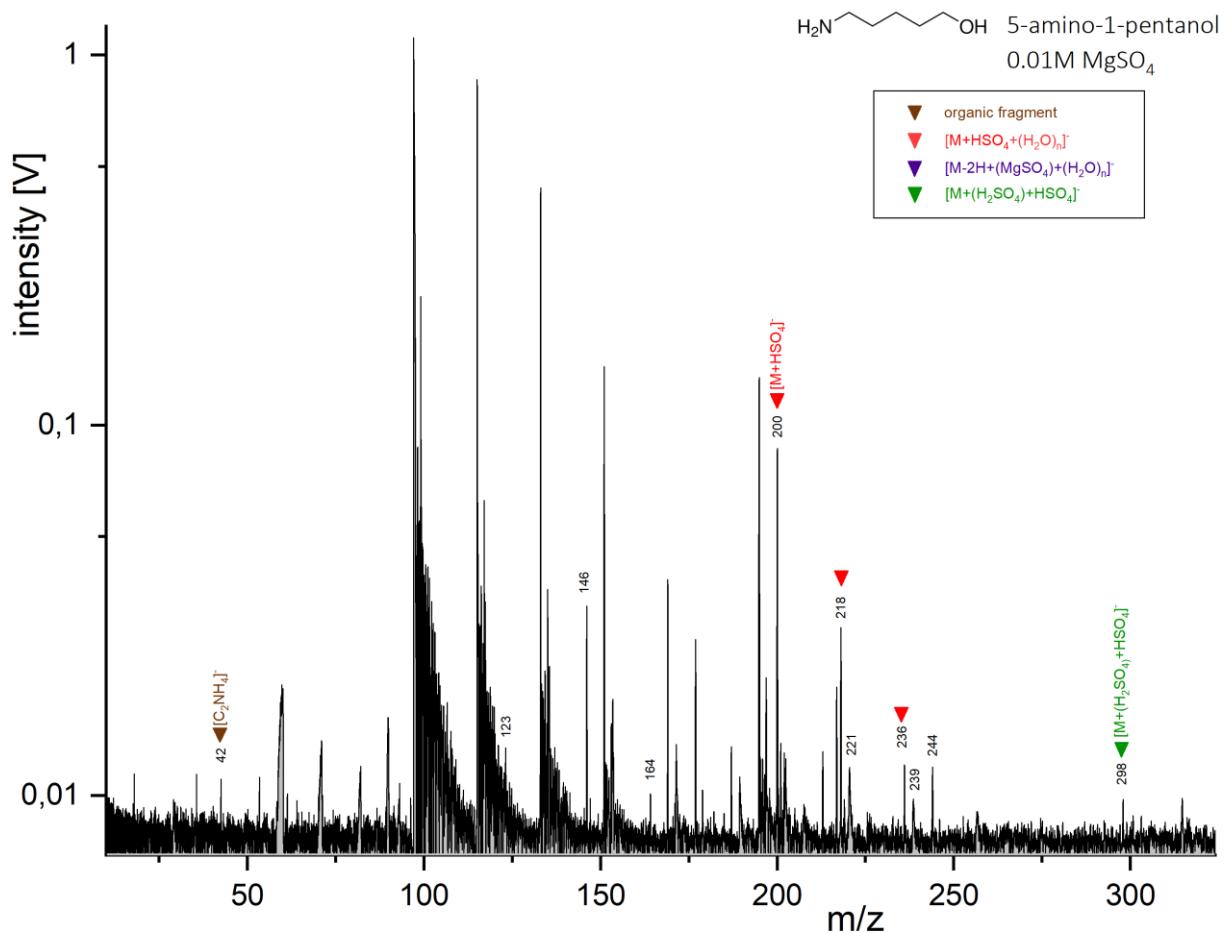
**Figure S15.** Baseline corrected anion mass spectrum of glucose (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 6.0  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



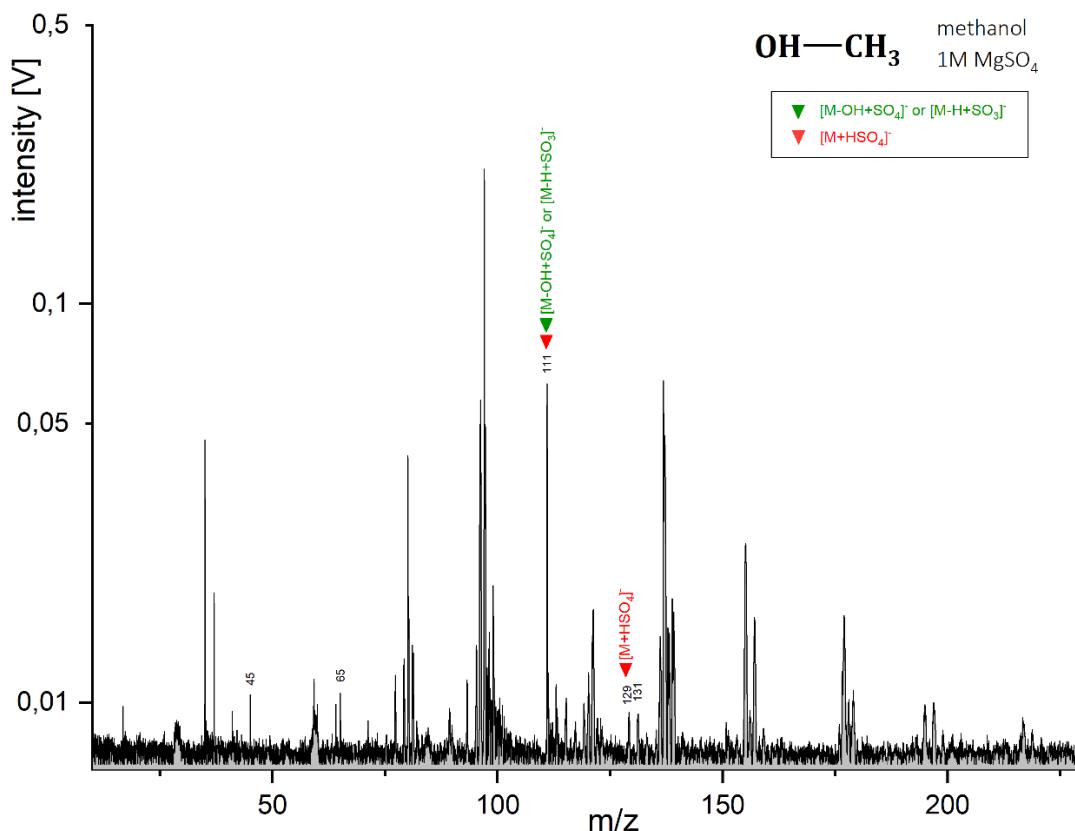
**Figure S16.** Baseline corrected anion mass spectrum of methanol (concentration 5 wt%) in 0.01M magnesium sulfate (MgSO<sub>4</sub>), generated with a delay time of 6.3  $\mu$ s. Unlabeled peaks originate exclusively from the MgSO<sub>4</sub> matrix.



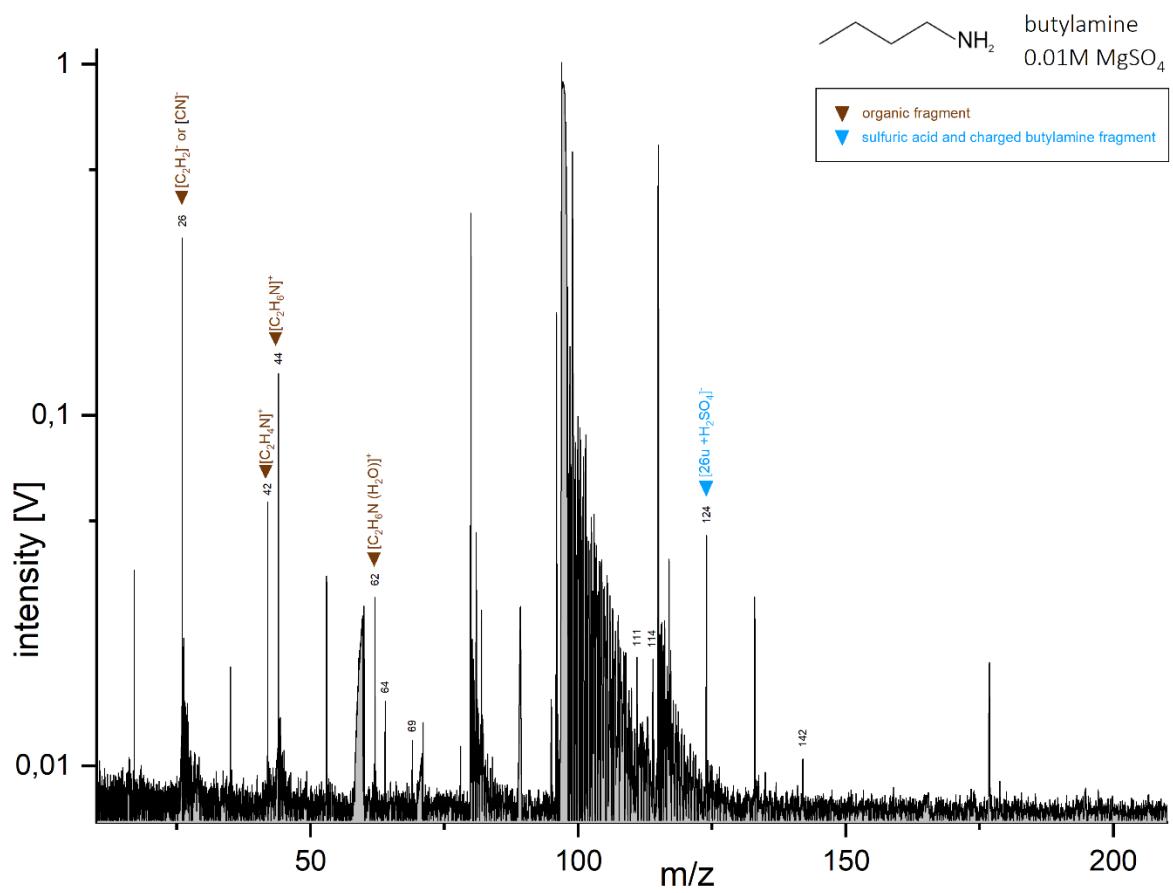
**Figure S17.** Baseline corrected anion mass spectrum of pyridine (concentration 5 wt%) in 0.01M magnesium sulfate (MgSO<sub>4</sub>), generated with a delay time of 5.8  $\mu$ s. Unlabeled peaks originate exclusively from the MgSO<sub>4</sub> matrix.



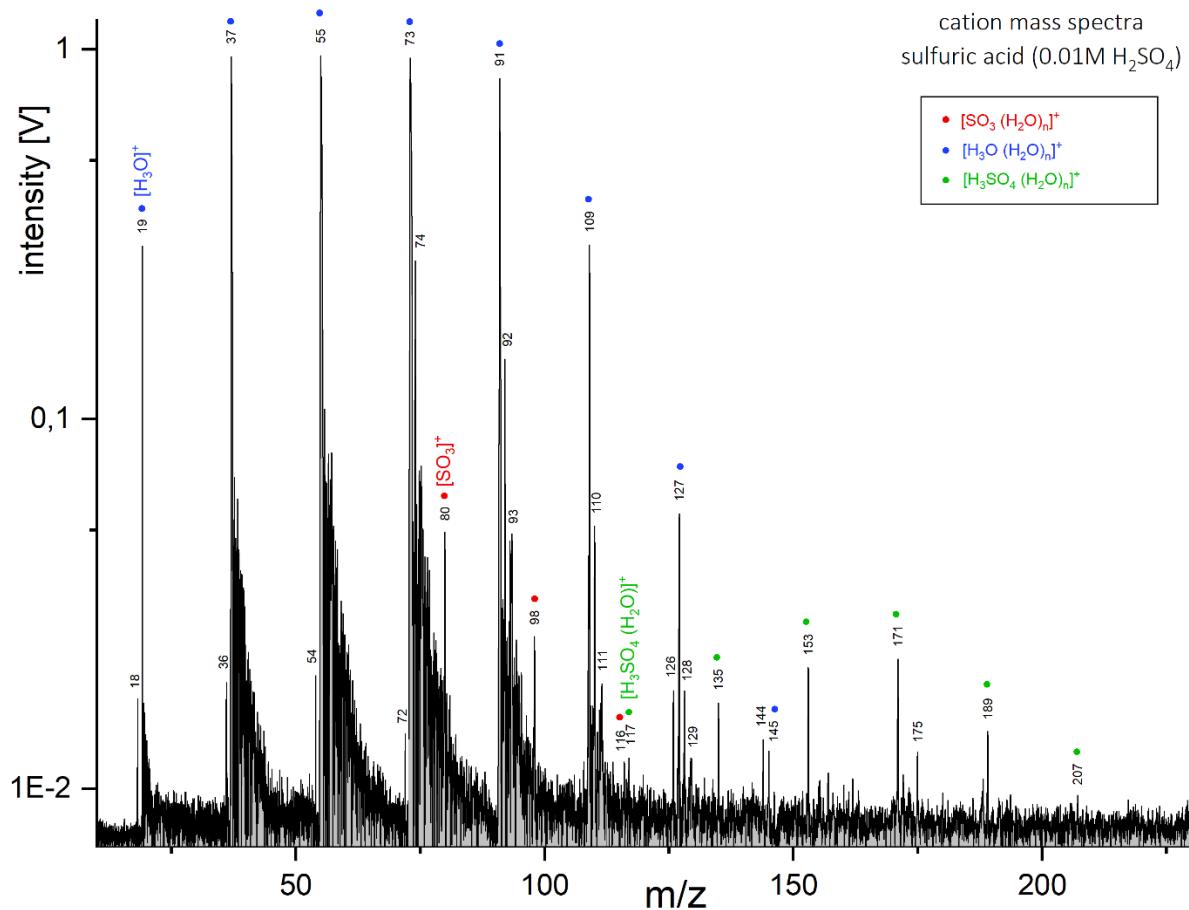
**Figure S18.** Baseline corrected anion mass spectrum of 5-amino-1-pentanol (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 6.1  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



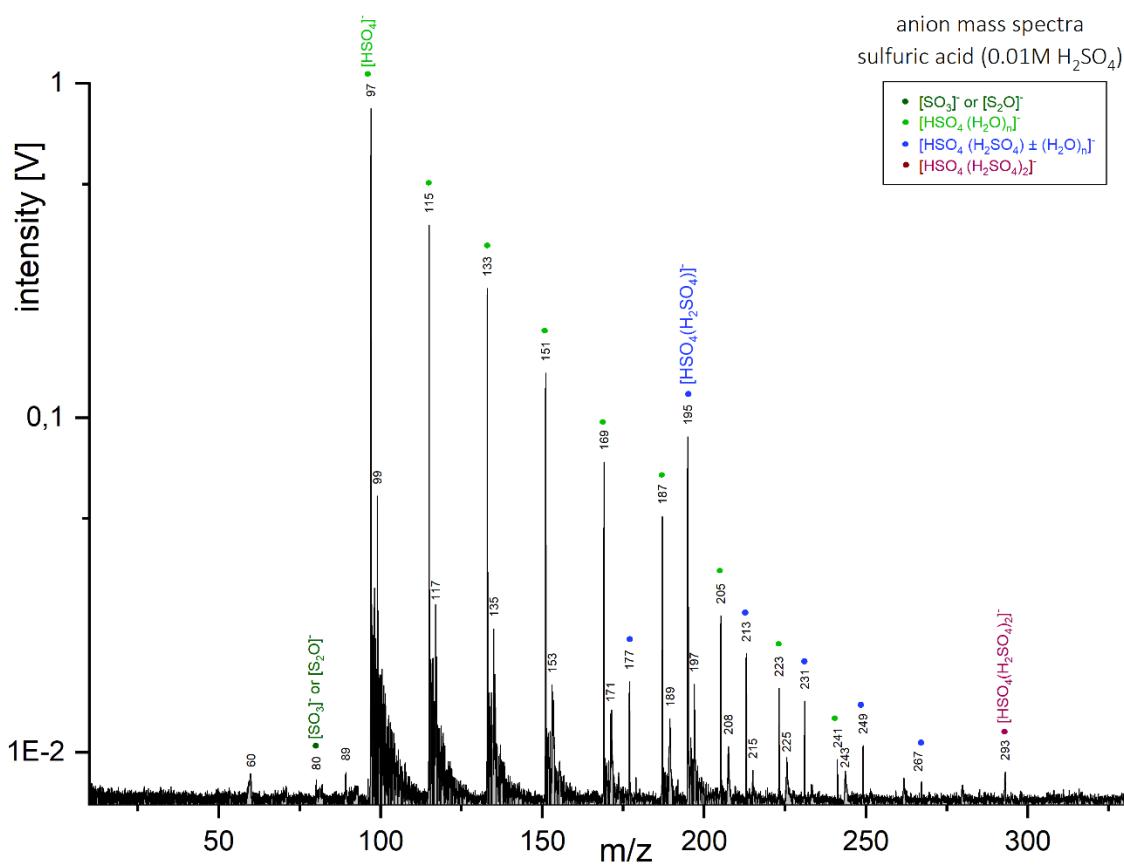
**Figure S19.** Baseline corrected anion mass spectrum of methanol (concentration 5 wt%) in 1M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 9.3  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



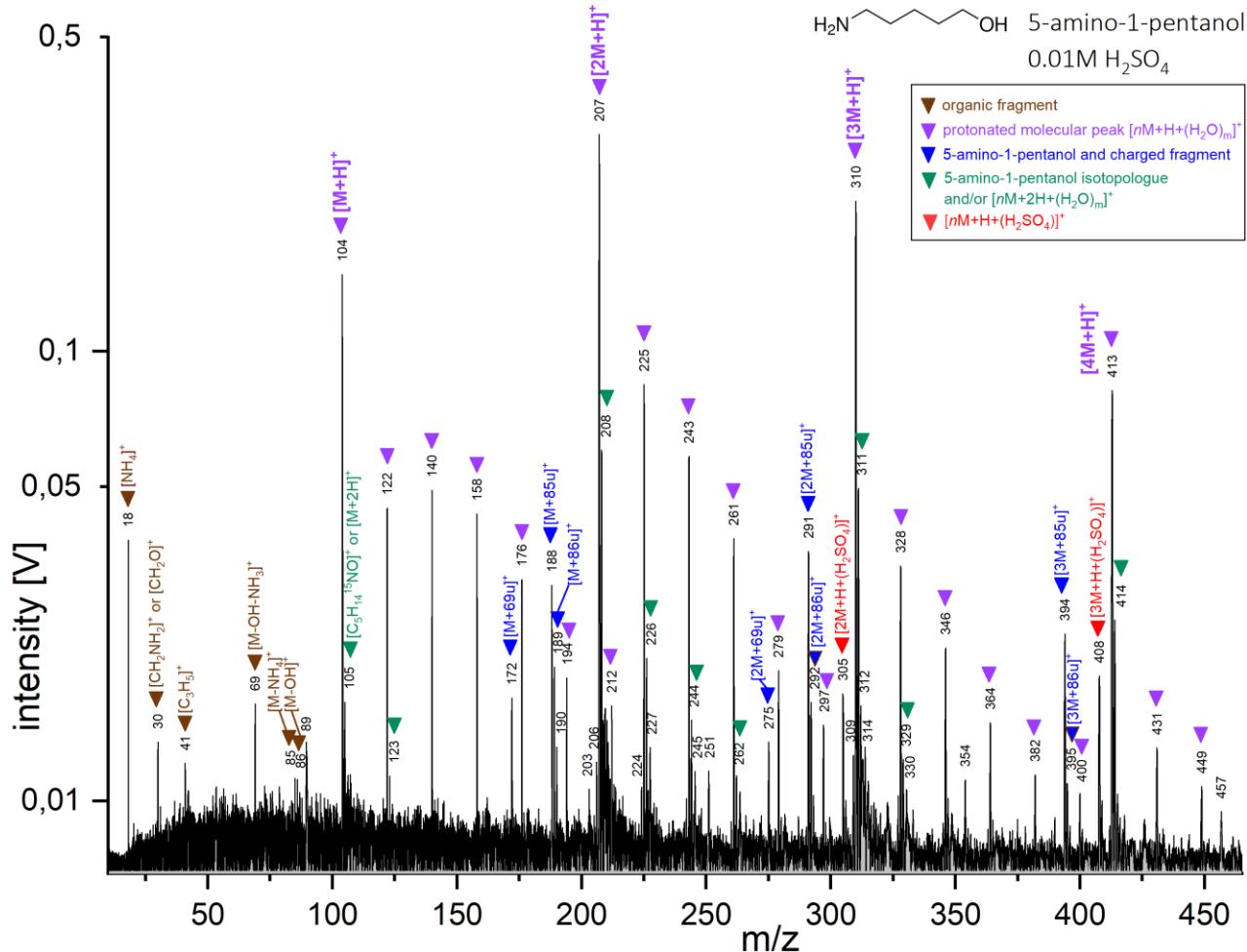
**Figure S20.** Baseline corrected anion mass spectrum of butylamine (concentration 5 wt%) in 0.01M magnesium sulfate ( $\text{MgSO}_4$ ), generated with a delay time of 5.5  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{MgSO}_4$  matrix.



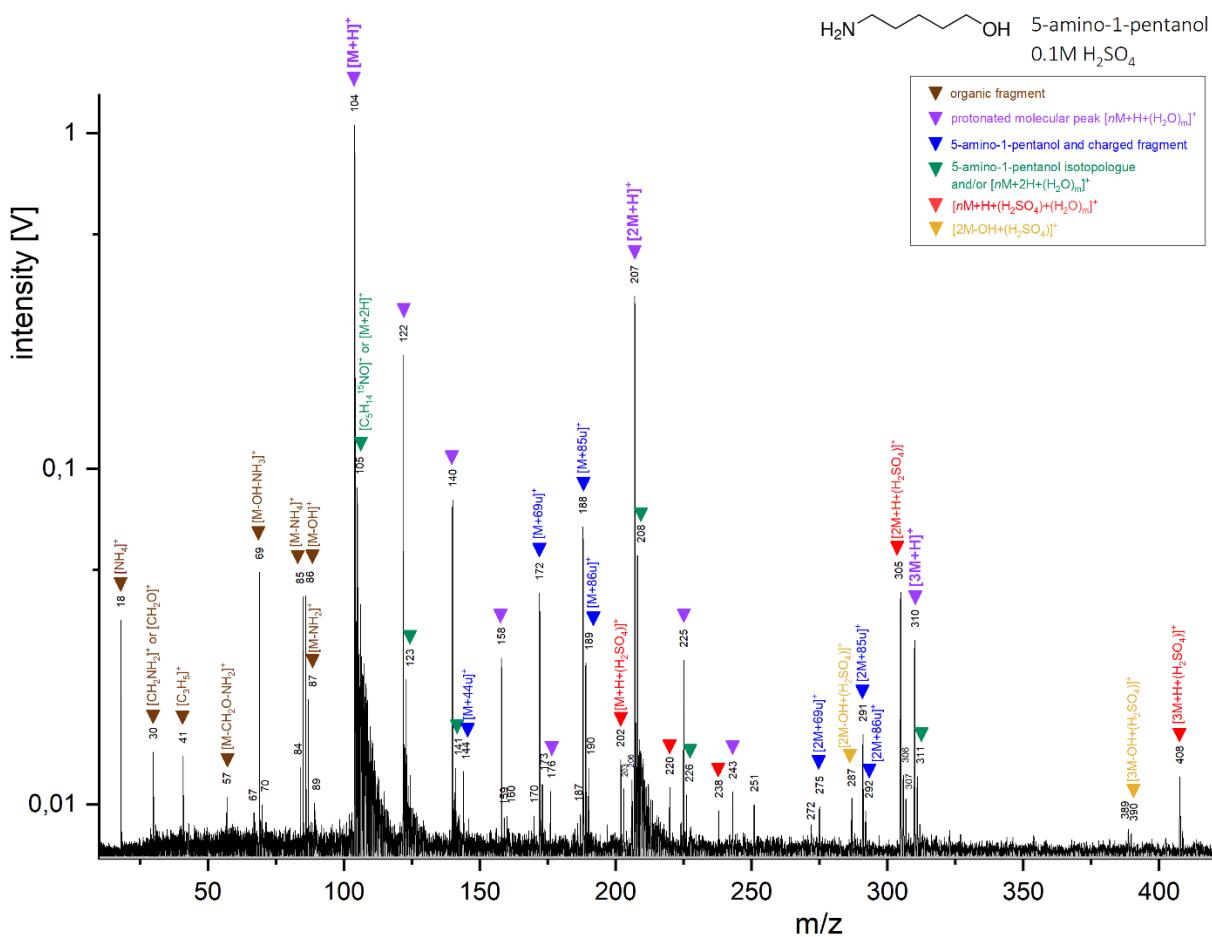
**Figure S21.** Baseline corrected cation mass spectrum of sulfuric acid ( $\text{H}_2\text{SO}_4$ ) at a concentration of 0.01M, generated with a delay time of 6.0  $\mu\text{s}$ .



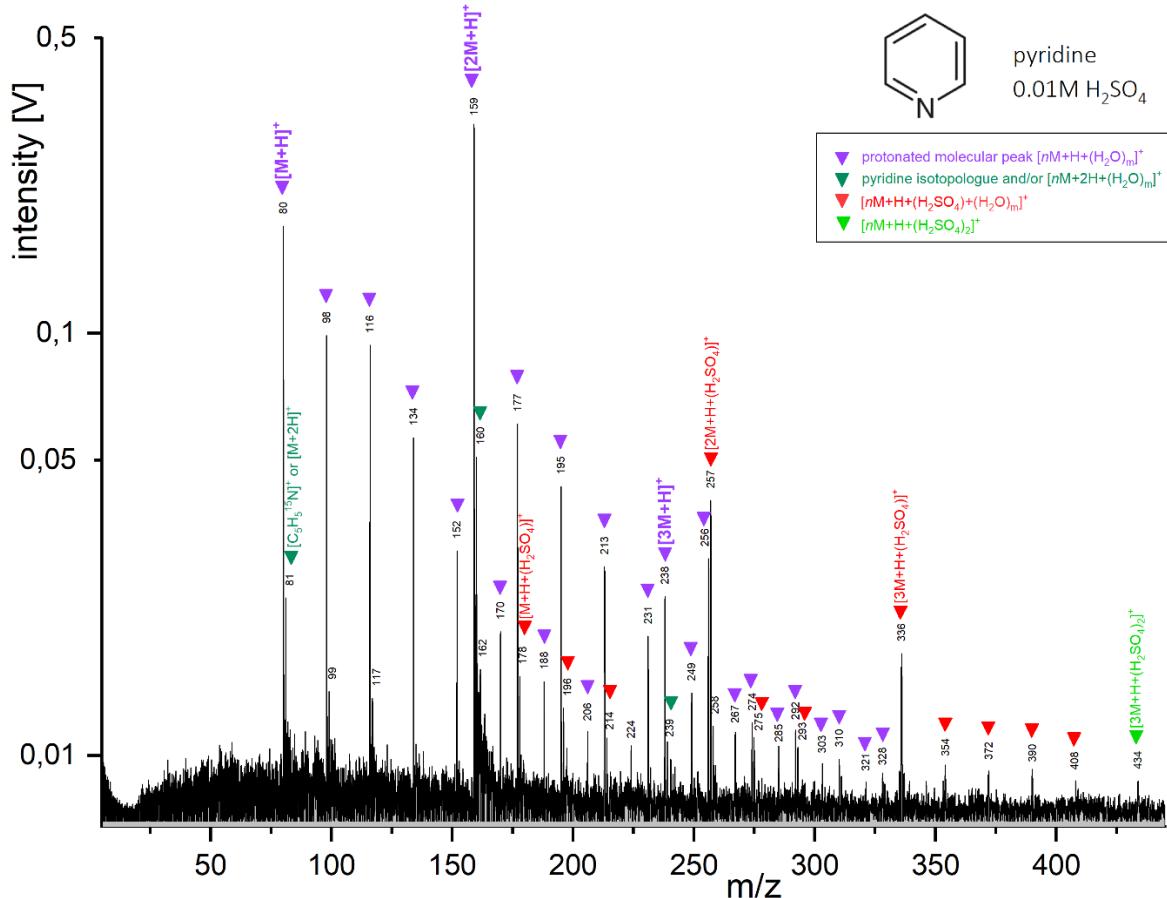
**Figure S22.** Baseline corrected anion mass spectrum of sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) at a concentration of 0.01M, generated with a delay time of 6.2μs.



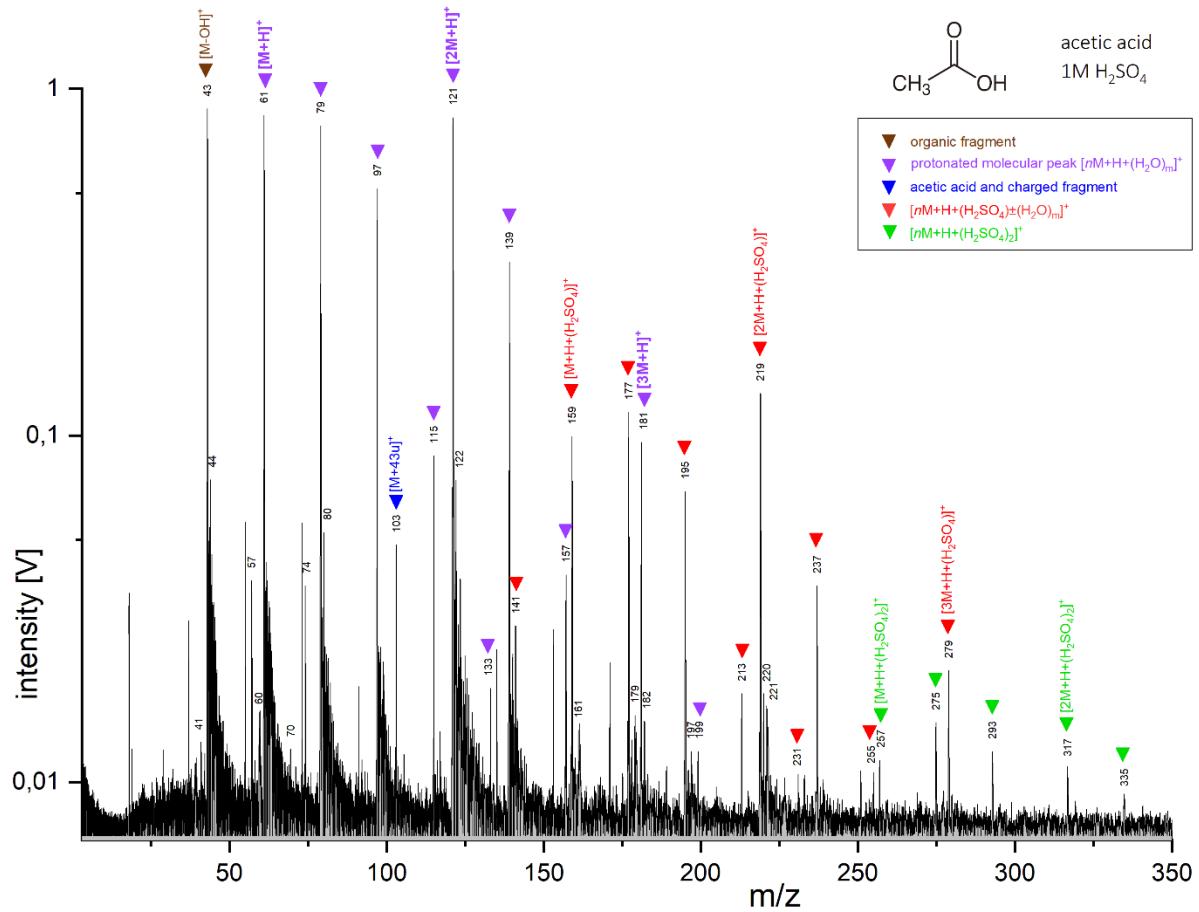
**Figure S23.** Baseline corrected cation mass spectrum of 5-amino-1-pentanol (concentration 5wt%) in 0.01M sulfuric acid (H<sub>2</sub>SO<sub>4</sub>), generated with a delay time of 6.8μs.



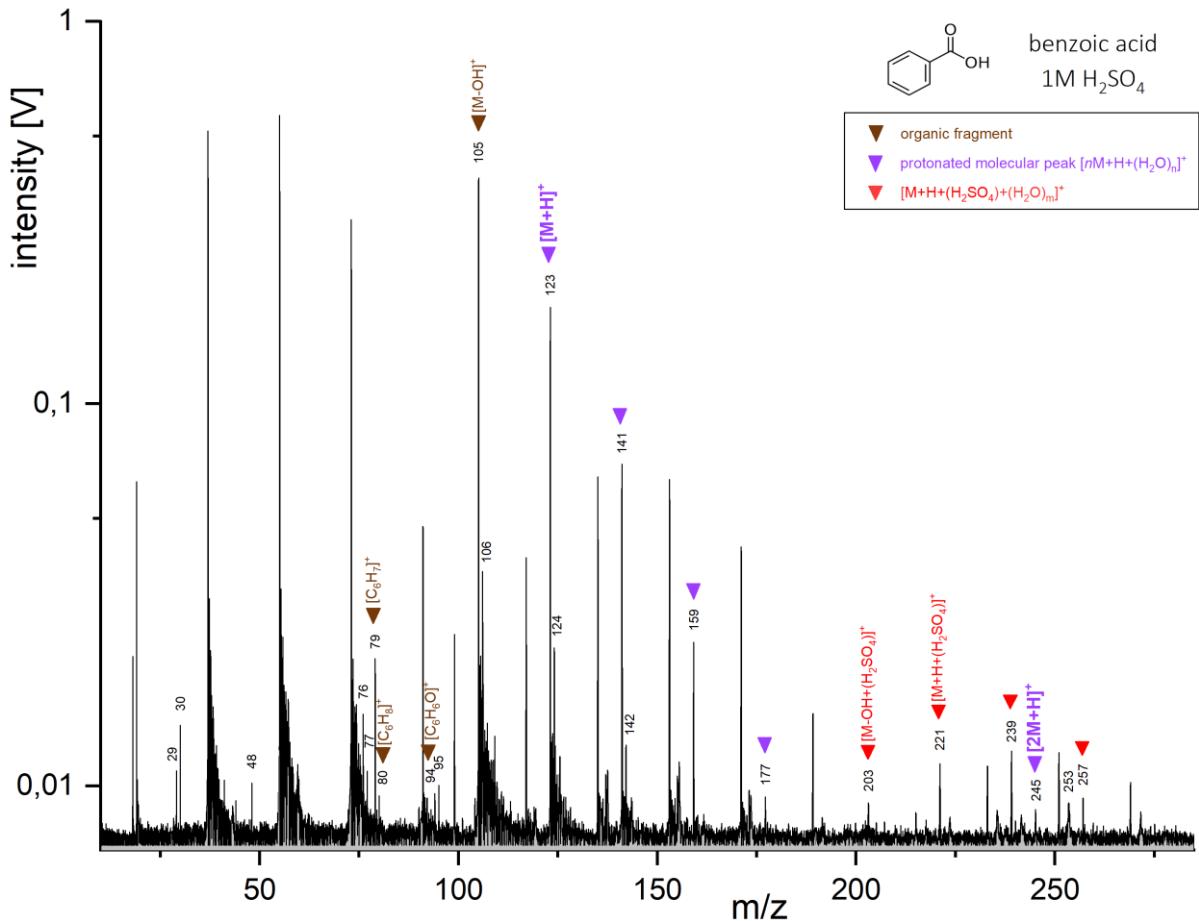
**Figure S24.** Baseline corrected cation mass spectrum of 5-amino-1-pentanol (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.8 $\mu\text{s}$ .



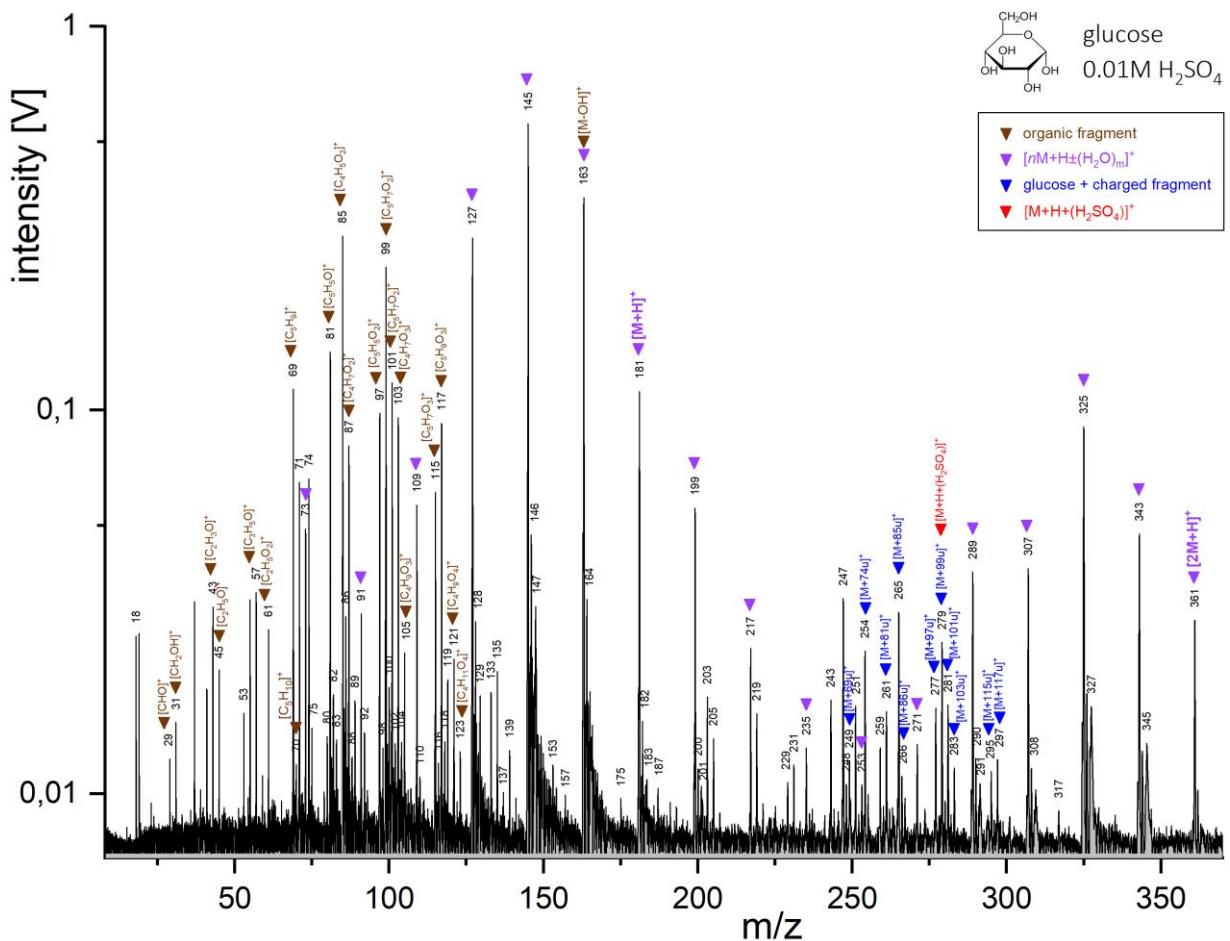
**Figure S25.** Baseline corrected cation mass spectrum of pyridine (concentration 5wt%) in 0.01M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.2 $\mu\text{s}$ .



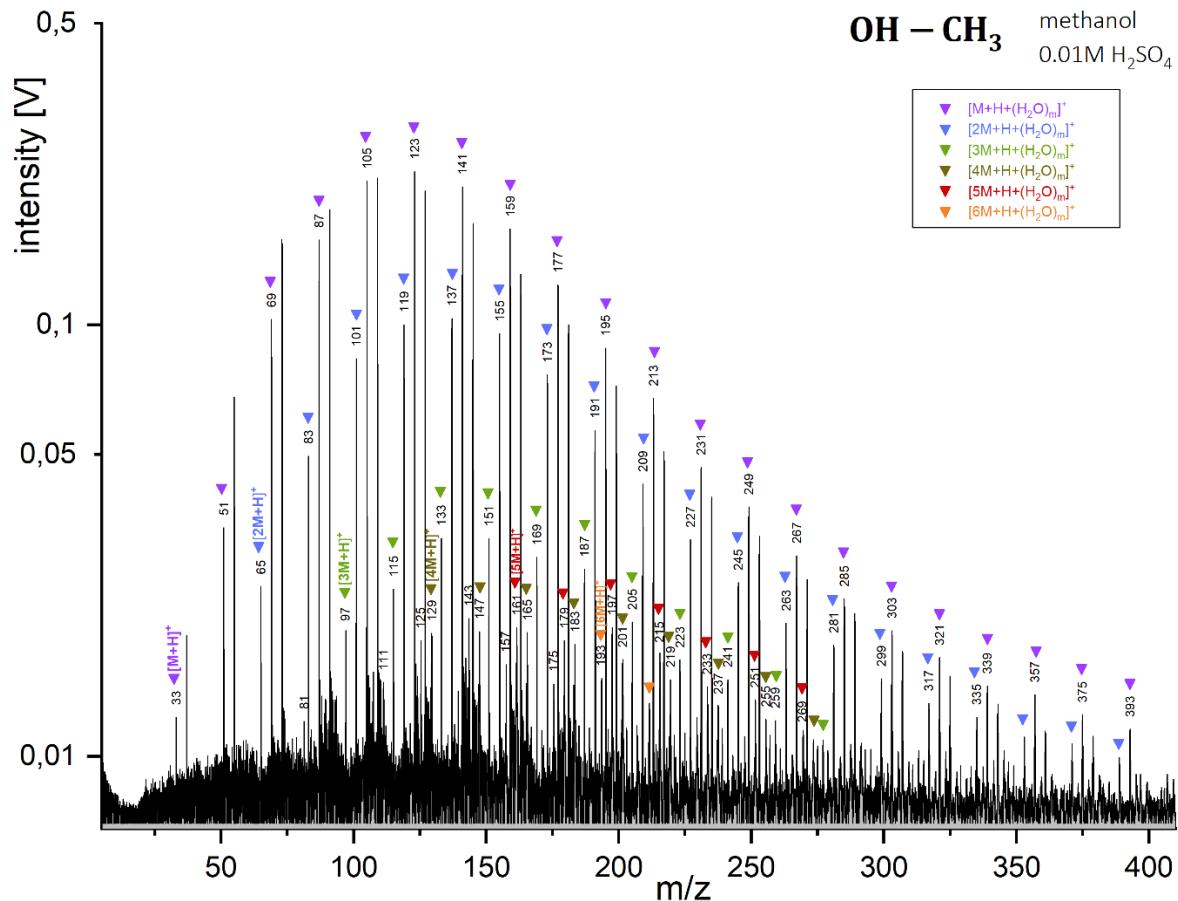
**Figure S26.** Baseline corrected cation mass spectrum of acetic acid (concentration 5wt%) in 1M sulfuric acid (H<sub>2</sub>SO<sub>4</sub>), generated with a delay time of 6.4μs.



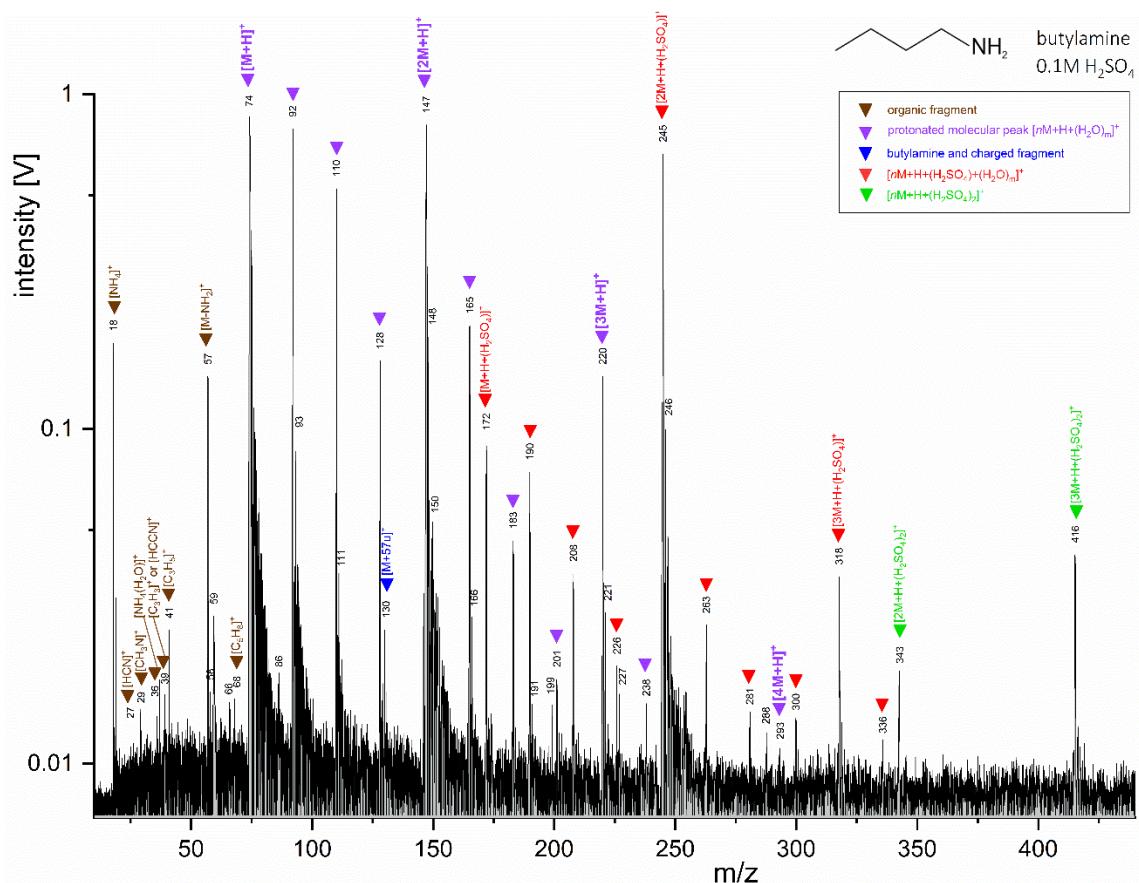
**Figure S27.** Baseline corrected cation mass spectrum of benzoic acid (concentration 0.17wt%) in 1M sulfuric acid (H<sub>2</sub>SO<sub>4</sub>), generated with a delay time of 6.0 μs. Unlabeled peaks originate exclusively from the H<sub>2</sub>SO<sub>4</sub> matrix.



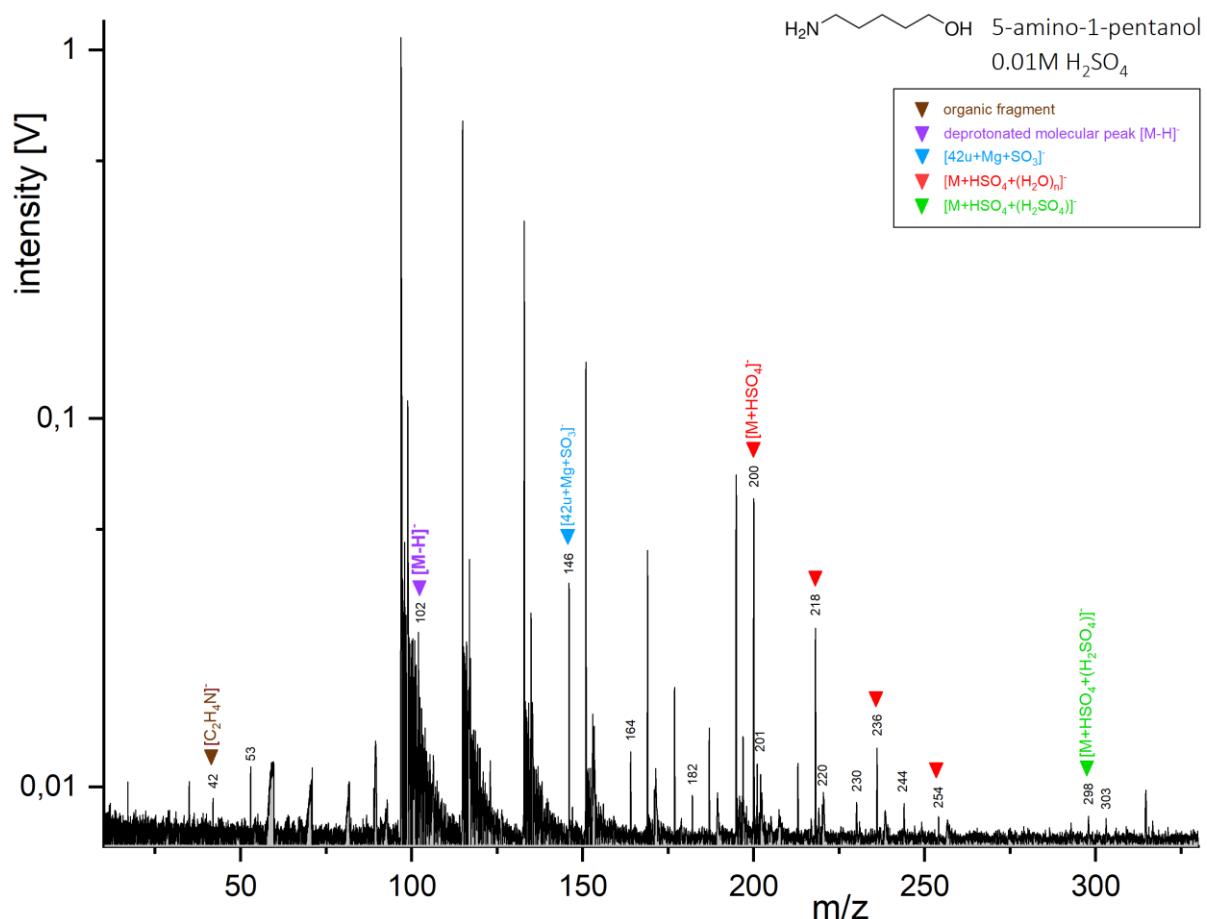
**Figure S28.** Baseline corrected cation mass spectrum of glucose (concentration 5wt%) in 0.01M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.0 $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



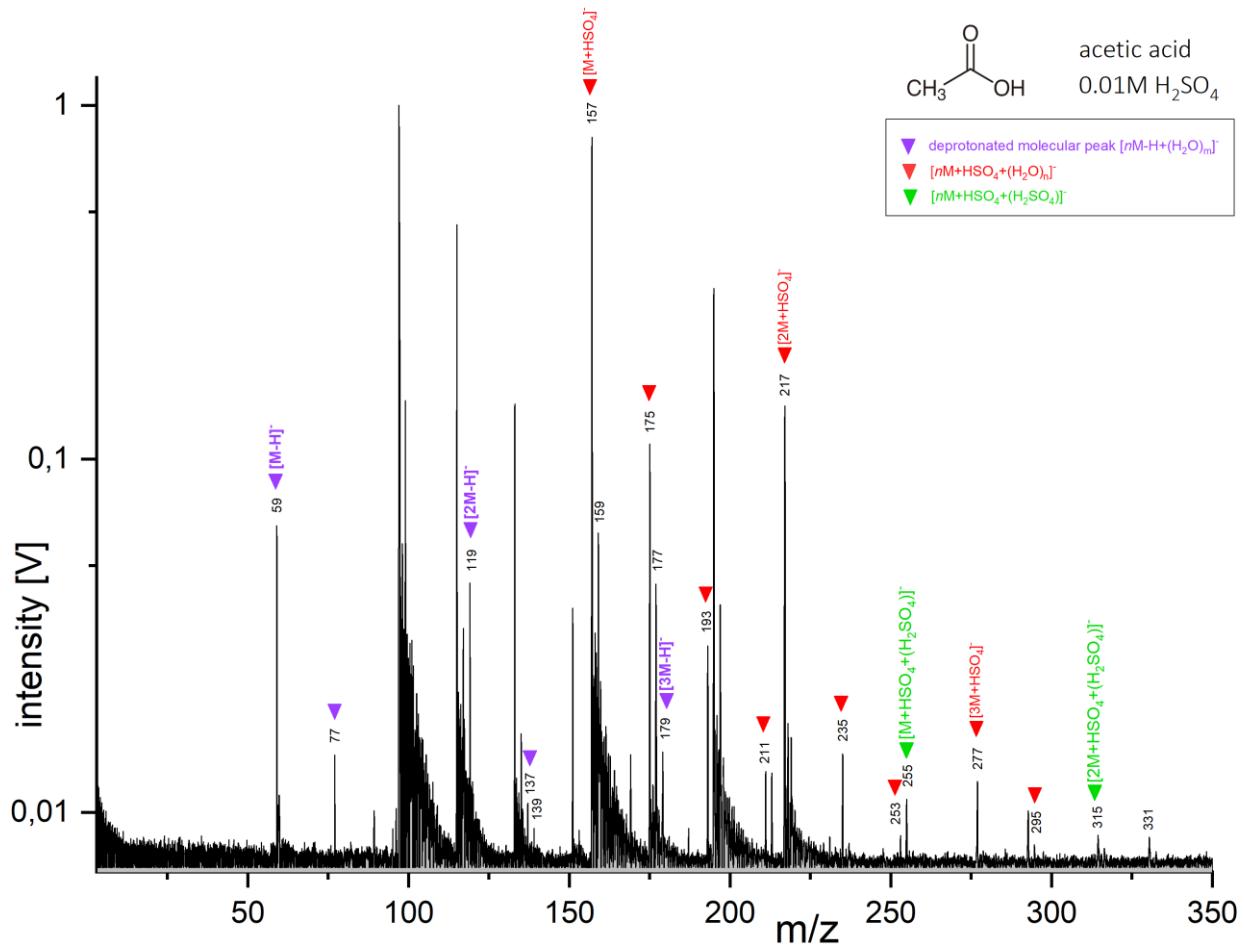
**Figure S29.** Baseline corrected cation mass spectrum of methanol (concentration 5wt%) in 0.01M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.7 $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



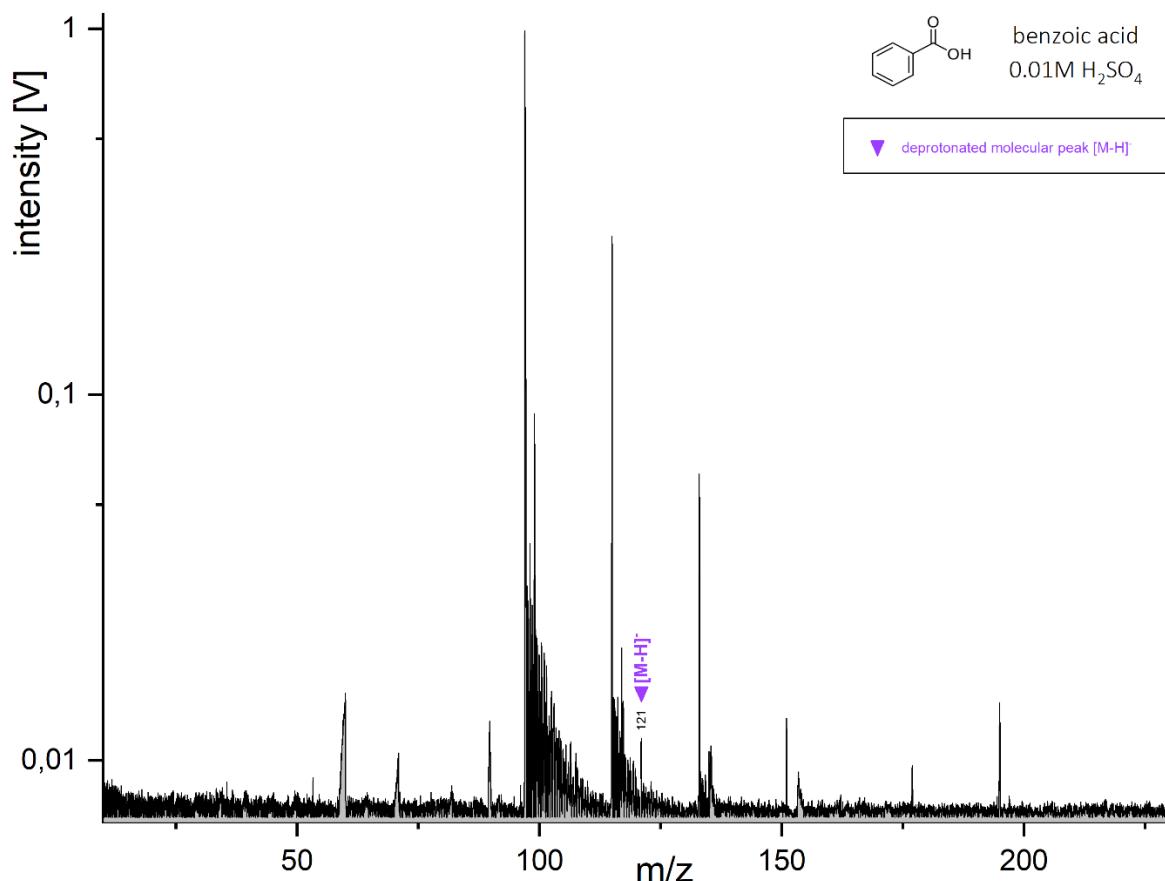
**Figure S30.** Baseline corrected cation mass spectrum of butylamine (concentration 1.3wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.4 $\mu\text{s}$ .



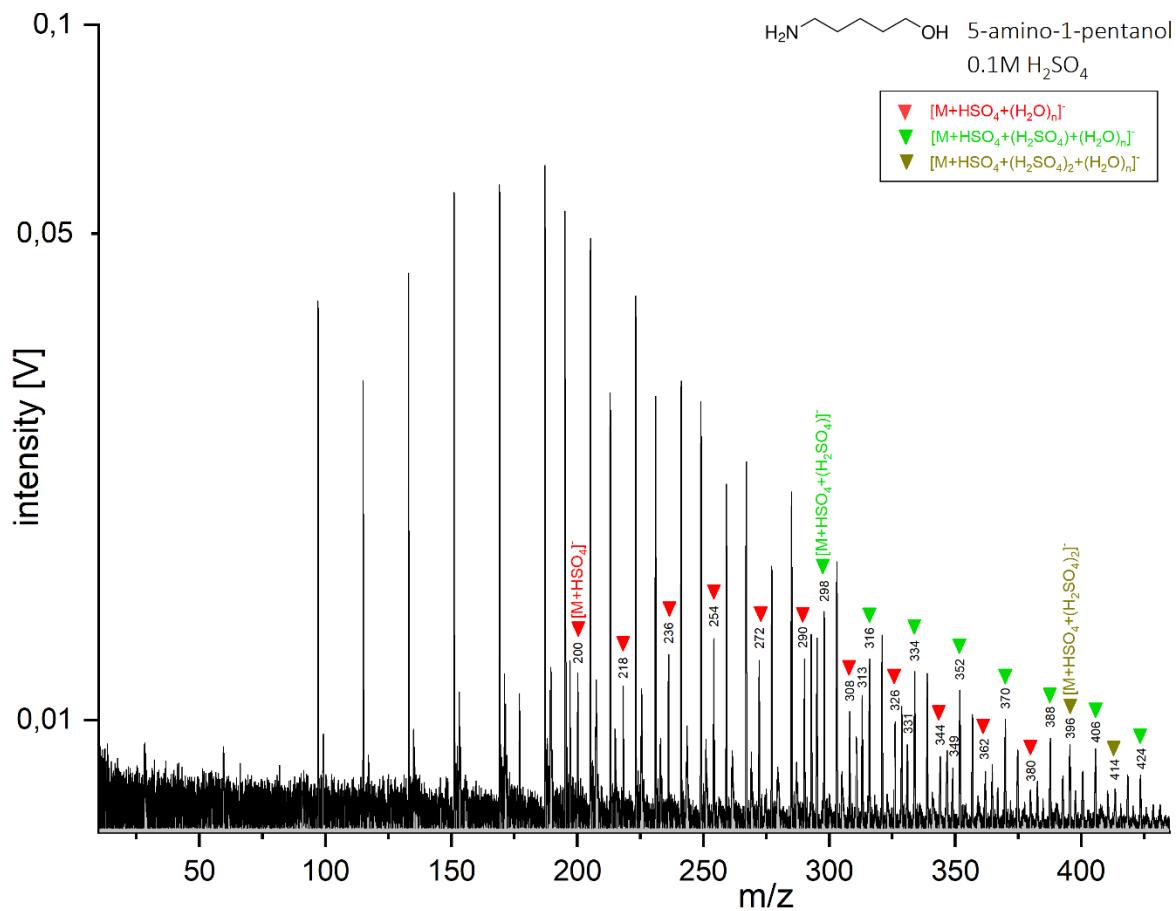
**Figure S31.** Baseline corrected anion mass spectrum of 5-amino-1-pentanol (concentration 5wt%) in 0.01M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.2 $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



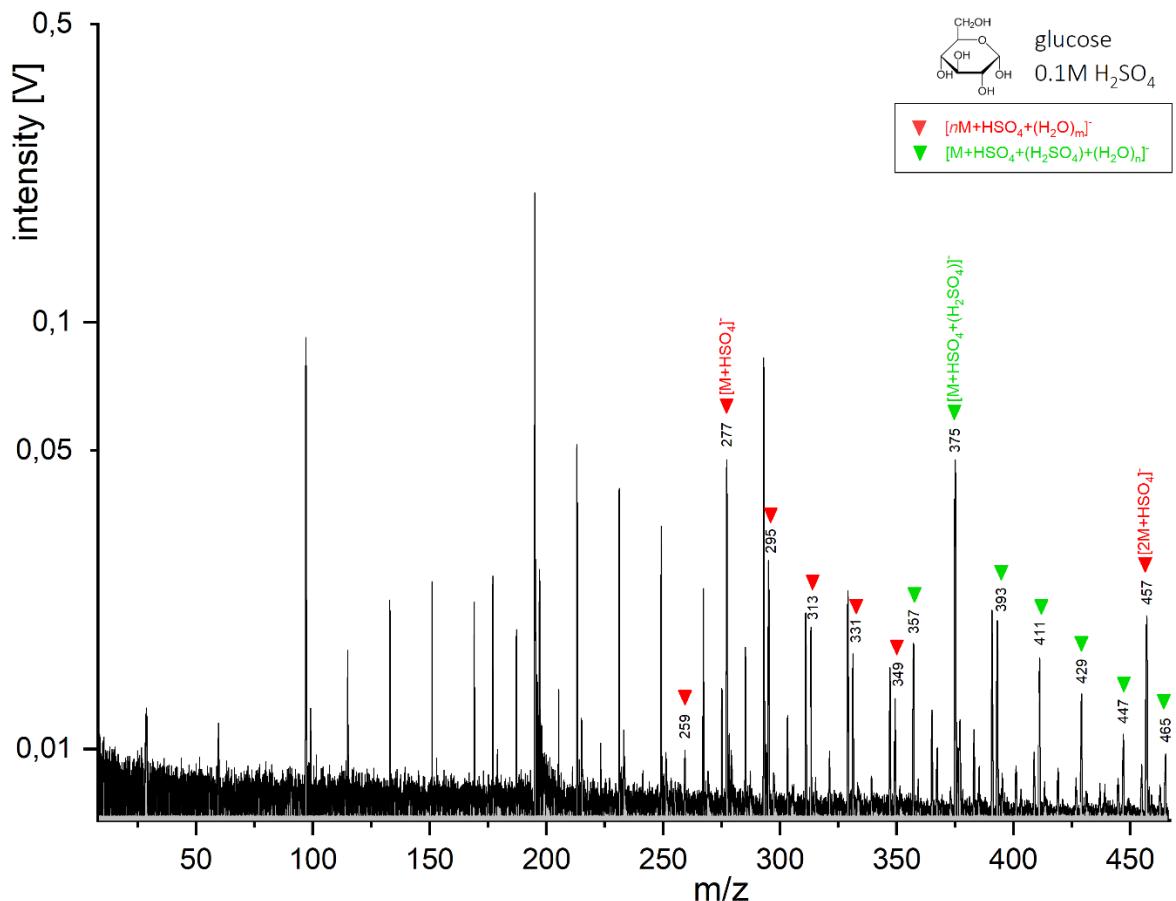
**Figure S32.** Baseline corrected anion mass spectrum of acetic acid (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.4 $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



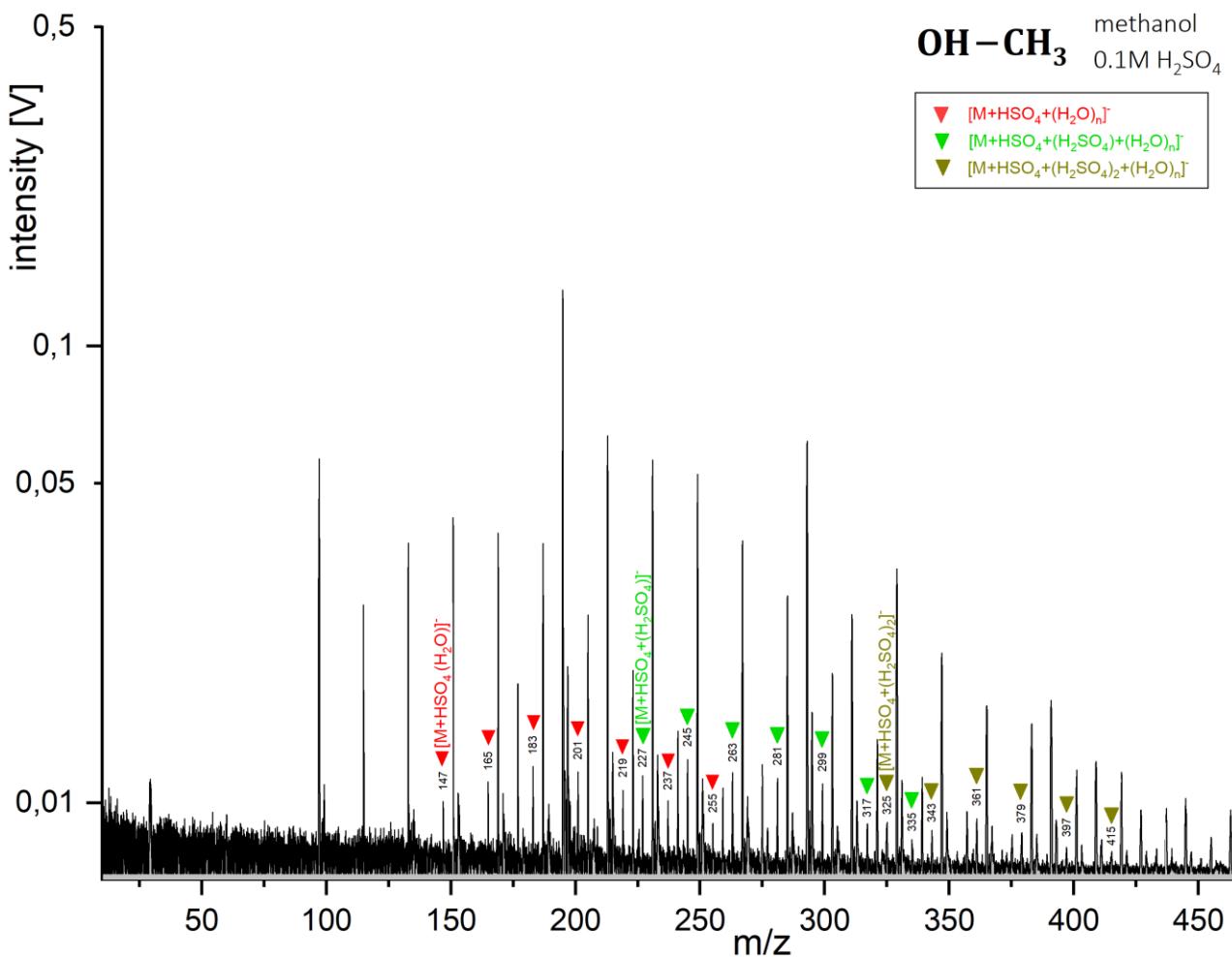
**Figure S33.** Baseline corrected anion mass spectrum of benzoic acid (concentration 0.17wt%) in 1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 5.7  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



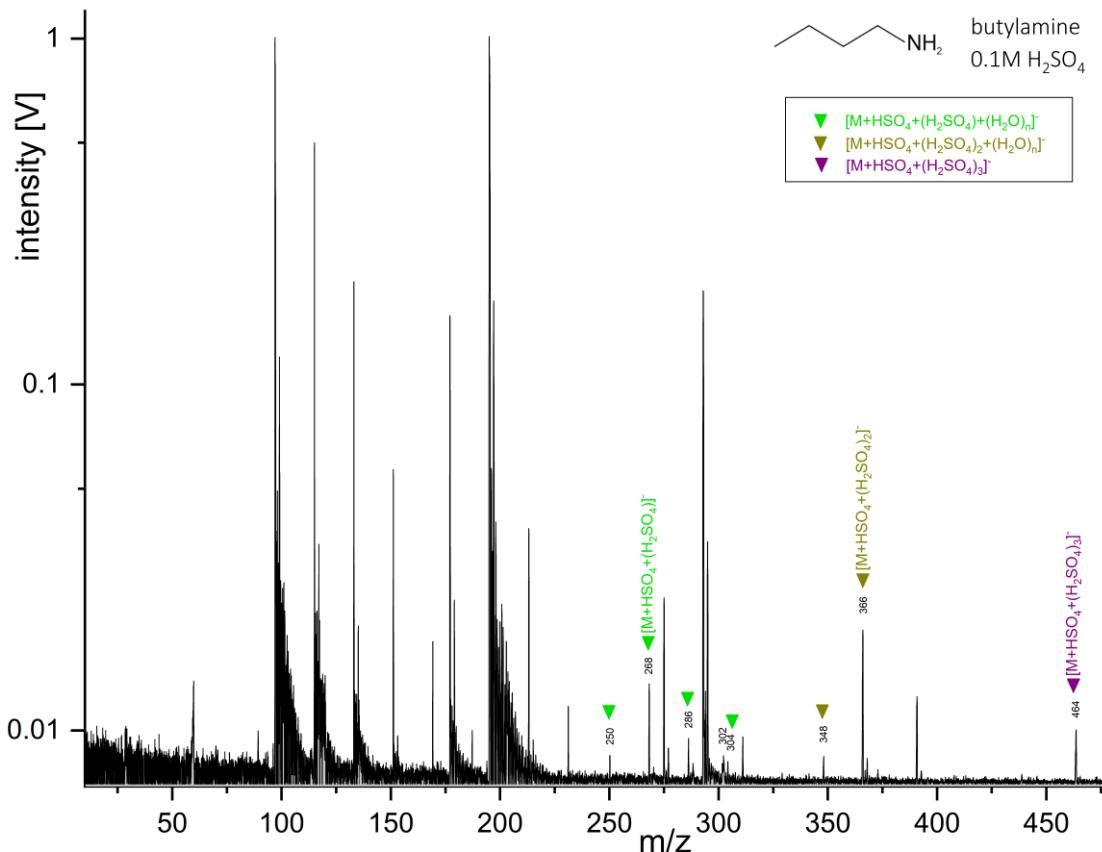
**Figure S34.** Baseline corrected anion mass spectrum of 5-amino-1-pentanol (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of  $6.8\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



**Figure S35.** Baseline corrected anion mass spectrum of glucose (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of  $6.9\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



**Figure S36.** Baseline corrected anion mass spectrum of methanol (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.8  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.



**Figure S37.** Baseline corrected anion mass spectrum of butylamine (concentration 5wt%) in 0.1M sulfuric acid ( $\text{H}_2\text{SO}_4$ ), generated with a delay time of 6.4  $\mu\text{s}$ . Unlabeled peaks originate exclusively from the  $\text{H}_2\text{SO}_4$  matrix.

m/z		pure H <sub>2</sub> O	MgSO <sub>4</sub>			H <sub>2</sub> SO <sub>4</sub>		
			0.01M	0.1M	1M	0.01M	0.1M	1M
5-amino-1-pentanol	18	[NH <sub>4</sub> ] <sup>+</sup>	[NH <sub>4</sub> ] <sup>+</sup>	[NH <sub>4</sub> ] <sup>+</sup>		[NH <sub>4</sub> ] <sup>+</sup>	[NH <sub>4</sub> ] <sup>+</sup>	[NH <sub>4</sub> ] <sup>+</sup>
	25, 29							UI
	30	[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>	[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>	[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>		[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>	[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>	[CH <sub>2</sub> NH <sub>2</sub> ] <sup>+</sup> or [CH <sub>2</sub> O] <sup>+</sup>
	31							[CH <sub>3</sub> O] <sup>+</sup>
	36	[NH <sub>4</sub> (H <sub>2</sub> O)] <sup>+</sup>		[NH <sub>4</sub> (H <sub>2</sub> O)] <sup>+</sup>				[NH <sub>4</sub> (H <sub>2</sub> O)] <sup>+</sup>
	41		[C <sub>3</sub> H <sub>5</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> ] <sup>+</sup>		[C <sub>3</sub> H <sub>5</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> ] <sup>+</sup>
	42							UI
	43		UI	UI				UI
	44							UI
	45							[C <sub>2</sub> H <sub>5</sub> O] <sup>+</sup>
	48	[CH <sub>2</sub> NH <sub>2</sub> (H <sub>2</sub> O)] <sup>+</sup>		[CH <sub>2</sub> NH <sub>2</sub> (H <sub>2</sub> O)] <sup>+</sup>				
	54	[NH <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sup>+</sup>						[NH <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sup>+</sup>
	56			UI				
	57	[M-CH <sub>2</sub> O-NH <sub>2</sub> ] <sup>+</sup>	[M-CH <sub>2</sub> O-NH <sub>2</sub> ] <sup>+</sup>	[M-CH <sub>2</sub> O-NH <sub>2</sub> ] <sup>+</sup>			[M-CH <sub>2</sub> O-NH <sub>2</sub> ] <sup>+</sup>	[M-CH <sub>2</sub> O-NH <sub>2</sub> ] <sup>+</sup>
	58			UI				UI
	62			UI				
	66	UI						
	67		UI					UI
	69	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>	[M-OH-NH <sub>3</sub> ] <sup>+</sup>
	70	UI	UI	UI			UI	UI
Acetic acid	72, 80	UI						
	84	UI	UI	UI			UI	UI
	85	[M-NH <sub>4</sub> ] <sup>+</sup>	[M-NH <sub>4</sub> ] <sup>+</sup>	[M-NH <sub>4</sub> ] <sup>+</sup>		[M-NH <sub>4</sub> ] <sup>+</sup>	[M-NH <sub>4</sub> ] <sup>+</sup>	[M-NH <sub>4</sub> ] <sup>+</sup>
	86	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>	[M-OH] <sup>+</sup>
	87	[M-NH <sub>2</sub> ] <sup>+</sup>	[M-NH <sub>2</sub> ] <sup>+</sup>	[M-NH <sub>2</sub> ] <sup>+</sup>	[M-NH <sub>2</sub> ] <sup>+</sup>		[M-NH <sub>2</sub> ] <sup>+</sup>	[M-NH <sub>2</sub> ] <sup>+</sup>
	88	UI						UI
	89		UI			UI	UI	
	90	UI						UI
Acetic acid	98							UI
	102	UI	UI	UI				UI
	103	UI	UI					UI
	15		[CH <sub>3</sub> ] <sup>+</sup>	[CH <sub>3</sub> ] <sup>+</sup>				
Acetic acid	24		UI	UI				

Acetic acid	29		$[CHO]^+$	$[CHO]^+$		
	30, 34			UI		
	41		$[C_3H_5]^+$			UI
	42	UI	$[C_3H_6]^+$		UI	UI
	43	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$
	44	UI	UI	UI	UI	UI
	57	UI			UI	UI
	23	UI				
Benzoic acid	29					UI
	30					UI
	41	$[C_3H_5]^+$				
	43	UI				
	48					UI
	59, 61	UI				
	74				UI	
	76					UI
	77	UI			UI	UI
	79	$[C_6H_7]^+$	$[C_6H_7]^+$		$[C_6H_7]^+$	$[C_6H_7]^+$
	80	$[C_6H_8]^+$	$[C_6H_8]^+$		$[C_6H_8]^+$	$[C_6H_8]^+$
	86		UI			
	92					UI
	93	$[C_7H_9]^+$				
Butylamine	94				$[C_6H_6O]^+$	$[C_6H_6O]^+$
	95	UI			UI	UI
	104	UI				
	105	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$
	106	UI			UI	UI
	17		$[NH_3]^+$	$[NH_3]^+$		
	18	$[NH_4]^+$	$[NH_4]^+$	$[NH_4]^+ ?$	$[NH_4]^+$	$[NH_4]^+$
	25					UI
Butylamine	27					$[HCN]^+$
	28		UI	UI		$[HCN]^+$
	29	$[CH_3N]^+$	$[CH_3N]^+$			$[CH_3N]^+$
	30		$[CH_2NH_2]^+$ or $[CH_2O]^+$	$[CH_2NH_2]^+$ or $[CH_2O]^+$		
	31		$[CH_5N]^+$	$[CH_5N]^+$		
	32		UI	UI		

Butylamine	33			UI
	34		UI	
	35	UI	UI	
	36	$[\text{NH}_4(\text{H}_2\text{O})]^+$	$[\text{NH}_4(\text{H}_2\text{O})]^+$	$[\text{NH}_4(\text{H}_2\text{O})]^+$
	39			$[\text{C}_3\text{H}_3]^+$ or $[\text{HCCN}]^+$
	41	$[\text{C}_3\text{H}_5]^+$	$[\text{C}_3\text{H}_5]^+$	$[\text{C}_3\text{H}_5]^+$
	42		$[\text{C}_2\text{H}_4\text{N}]^+$	$[\text{C}_2\text{H}_4\text{N}]^+$
	43		UI	UI
	44		$[\text{C}_2\text{H}_6\text{N}]^+$	$[\text{C}_2\text{H}_6\text{N}]^+$
	45, 46, 47, 48		UI	UI
	49		UI	
	50, 53		UI	UI
	54	$[\text{NH}_4(\text{H}_2\text{O})_2]^+$	$[\text{NH}_4(\text{H}_2\text{O})_2]^+$	$[\text{NH}_4(\text{H}_2\text{O})_2]^+$
	56		$[\text{C}_3\text{H}_6\text{N}]^+$	$[\text{C}_3\text{H}_6\text{N}]^+$
	57	$[\text{M-NH}_2]^+$	$[\text{M-NH}_2]^+$	$[\text{M-NH}_2]^+$
	58	UI	UI	UI
	59		UI	UI
	60		UI	UI
	61-65		UI	
	66		UI	UI
	67-71		UI	UI
	68			$[\text{C}_3\text{H}_5\text{N}_2]^+$ or $[\text{C}_5\text{H}_9]^+$
	72	$[\text{NH}_4(\text{H}_2\text{O})_3]^+$	$[\text{NH}_4(\text{H}_2\text{O})_3]^+$	
Glucose	15			$[\text{CH}_3]^+$
	18			UI
	27			UI
	29	$[\text{CHO}]^+$	$[\text{CHO}]^+$	$[\text{CHO}]^+$
	31	$[\text{CH}_2\text{OH}]^+$	$[\text{CH}_2\text{OH}]^+$	$[\text{CH}_2\text{OH}]^+$
	33			UI
	39			UI
	41			UI
	43	$[\text{C}_2\text{H}_3\text{O}]^+$	$[\text{C}_2\text{H}_3\text{O}]^+$	$[\text{C}_2\text{H}_3\text{O}]^+$
	45	$[\text{C}_2\text{H}_5\text{O}]^+$	$[\text{C}_2\text{H}_5\text{O}]^+$	$[\text{C}_2\text{H}_5\text{O}]^+$
	53			UI
	55		UI	UI

Glucose	57	[C <sub>3</sub> H <sub>5</sub> O] <sup>+</sup>					
	58					UI	UI
	59				UI	UI	UI
	60	UI				UI	
	61	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>
	63					UI	UI
	69	[C <sub>4</sub> H <sub>5</sub> O] <sup>+</sup>					
	70	[C <sub>5</sub> H <sub>10</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>10</sub> ] <sup>+</sup>			[C <sub>5</sub> H <sub>10</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>10</sub> ] <sup>+</sup>
	71	UI	UI		UI	UI	UI
	73	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>
	74		UI		UI	UI	UI
	75	UI	UI		UI	UI	UI
	79	UI				UI	UI
	80				UI	UI	UI
	81	[C <sub>5</sub> H <sub>5</sub> O] <sup>+</sup>					
	82	UI			UI	UI	UI
	83	UI	UI		UI	UI	UI
	85	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>
	86		UI	UI	UI	UI	UI
	87	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>
	88	UI			UI	UI	UI
	89	UI	UI		UI	UI	UI
	91	[M+H-(H <sub>2</sub> O) <sub>5</sub> ] <sup>+</sup>					
	92				UI	UI	UI
	93	UI	UI	UI		UI	UI
	97	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> ] <sup>+</sup>
	98				UI	UI	UI
	99	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ] <sup>+</sup>
	100				UI	UI	UI
	101	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>	[C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup>
	102				UI	UI	UI
	103	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> ] <sup>+</sup>
	104				UI	UI	UI
	105	[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> ] <sup>+</sup>		[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> ] <sup>+</sup>	[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> ] <sup>+</sup>
	109	[M+H-(H <sub>2</sub> O) <sub>4</sub> ] <sup>+</sup>					
	110				UI	UI	UI
	111				UI	UI	UI

		$[C_5H_7O_3]^+$	$[C_5H_7O_3]^+$	$[C_5H_7O_3]^+$	$[C_5H_7O_3]^+$	$[C_5H_7O_3]^+$	$[C_5H_7O_3]^+$
115					UI	UI	UI
116					$[C_5H_9O_3]^+$	$[C_5H_9O_3]^+$	$[C_5H_9O_3]^+$
117		$[C_5H_9O_3]^+$	$[C_5H_9O_3]^+$	$[C_5H_9O_3]^+$			
118					UI	UI	UI
119	UI	UI	UI		UI	UI	UI
121	$[C_4H_9O_4]^+$	$[C_4H_9O_4]^+$			$[C_4H_9O_4]^+$	$[C_4H_9O_4]^+$	$[C_4H_9O_4]^+$
123	$[C_4H_{11}O_4]^+$	$[C_4H_{11}O_4]^+$			$[C_4H_{11}O_4]^+$	$[C_4H_{11}O_4]^+$	$[C_4H_{11}O_4]^+$
127	$[M+H-(H_2O)_3]^+$	$[M+H-(H_2O)_3]^+$	$[M+H-(H_2O)_3]^+$		$[M+H-(H_2O)_3]^+$	$[M+H-(H_2O)_3]^+$	$[M+H-(H_2O)_3]^+$
128	UI				UI	UI	UI
129					UI		UI
130	UI					UI	UI
133	UI				UI	UI	UI
135	UI				UI	UI	UI
137					UI	UI	UI
139		UI			UI		UI
141			UI		UI	UI	UI
143		UI	UI			UI	
144		UI					
145	$[M+H-(H_2O)_2]^+$	$[M+H-(H_2O)_2]^+$	$[M+H-(H_2O)_2]^+$		$[M+H-(H_2O)_2]^+$	$[M+H-(H_2O)_2]^+$	$[M+H-(H_2O)_2]^+$
146	UI	UI				UI	UI
147					UI		
148	UI	UI				UI	UI
151					UI	UI	UI
153					UI	UI	UI
155		UI					
157					UI	UI	UI
159					UI		
161		UI					
163	$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$		$[M-OH]^+$	$[M-OH]^+$	$[M-OH]^+$
164	UI				UI	UI	UI
165		UI					
167							UI
173		UI					
169, 175					UI		
<b>Methanol</b>	15	$[CH_3]^+$					$[CH_3]^+$
	18						$[NH_4]^+$

Pyridine	23	UI			
	39			[HC <sub>2</sub> N] <sup>+</sup> or [C <sub>3</sub> H <sub>3</sub> ] <sup>+</sup>	
	41	UI			
	43			[C <sub>2</sub> H <sub>5</sub> N] <sup>+</sup>	
	53	[C <sub>3</sub> H <sub>3</sub> N] <sup>+</sup>			[C <sub>3</sub> H <sub>3</sub> N] <sup>+</sup>
	59, 77	UI	UI		
	79	UI	UI	UI	UI

**Table S1.** Fragment peaks, and their respective mass, detected in cation mode for the investigated organics in pure water matrix (Napoleoni et al. 2022), in 0.01M, 0.1M and 1M MgSO<sub>4</sub> and 0.01M, 0.1M and 1M H<sub>2</sub>SO<sub>4</sub> matrices, at all investigated delay times and laser power intensities. UI stands for unidentified ion species. Species written in blue are tentative identifications.

m/z		pure H <sub>2</sub> O	MgSO <sub>4</sub>			H <sub>2</sub> SO <sub>4</sub>		
			0.01M	0.1M	1M	0.01M	0.1M	1M
<b>5-amino-1-pentanol</b>	16	[NH <sub>2</sub> ] <sup>-</sup>						
	26	[C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> or [CN] <sup>-</sup>						
	27		UI					
	42	[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>	[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>			[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>		
	43	UI		UI				
	44, 45, 46	UI						
	53					UI		
	59, 60	UI						
	61	UI		UI				
	62, 63, 64, 77, 78, 79, 80, 81, 83	UI						
	93					UI		
	95, 97, 98	UI						
<b>Acetic acid</b>	15	[CH <sub>3</sub> ] <sup>-</sup>						
	36	UI						
	41	[M-H <sub>3</sub> O] <sup>-</sup>	[M-H <sub>3</sub> O] <sup>-</sup>					
	54	UI						
	58	UI	UI	UI				
<b>Benzoic acid</b>	59	UI						
	77	[M-COOH] <sup>-</sup>	[M-COOH] <sup>-</sup>	[M-COOH] <sup>-</sup>	[M-COOH] <sup>-</sup>			
	95	[M-COOH+(H <sub>2</sub> O)] <sup>-</sup>						
	113	[M-COOH+(H <sub>2</sub> O) <sub>2</sub> ] <sup>-</sup>						
<b>Butylamine</b>	16	[NH <sub>2</sub> ] <sup>-</sup>						
	26	[C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> or [CN] <sup>-</sup>	[C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> or [CN] <sup>-</sup>	[C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> or [CN] <sup>-</sup>	[C <sub>2</sub> H <sub>2</sub> ] <sup>-</sup> or [CN] <sup>-</sup>			
	32	[N <sub>2</sub> H <sub>4</sub> ] <sup>-</sup>						
	42		[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>	[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>	[C <sub>2</sub> H <sub>4</sub> N] <sup>-</sup>			
	44	[C <sub>2</sub> H <sub>6</sub> N] <sup>-</sup>	[C <sub>2</sub> H <sub>6</sub> N] <sup>-</sup>	[C <sub>2</sub> H <sub>6</sub> N] <sup>-</sup>				
	49	UI						

	53		UI	
	60		UI	
	61			UI
	62	UI	$[C_2H_4N(H_2O)]^-$	$[C_2H_4N(H_2O)]^-$
	64		UI	UI
	66	UI		UI
	67	UI		
	68			UI
	69		UI	UI
	70	UI		
	71			UI
Glucose	31	UI		
	41			UI
	43	UI		UI
	45	UI		UI
	55, 57	UI		
	58	$[C_4H_{10}]^-$		
	59	$[C_2H_3O_2]^-$	$[C_2H_3O_2]^-$	$[C_2H_3O_2]^-$
	62	UI		
	71	$[C_3H_5O_2]^-$ or $[M-H-(H_2O)_6]^-$	$[C_3H_5O_2]^-$ or $[M-H-(H_2O)_6]^-$	$[C_3H_5O_2]^-$ or $[M-H-(H_2O)_6]^-$
	73	$[C_3H_5O_2]^-$		
	75	UI		
	77	$[C_2H_5O_3]^-$	$[C_2H_5O_3]^-$	
	78, 83, 84	UI		
	85	UI	UI	
	87	$[C_4H_7O_2]^-$		
	89	$[C_3H_5O_3]^-$ or $[M-$ $H-(H_2O)_5]^-$	$[C_3H_5O_3]^-$ or $[M-$ $H-(H_2O)_5]^-$	$[C_3H_5O_3]^-$ or $[M-$ $H-(H_2O)_5]^-$
	90, 95, 97, 99, 100	UI		
	101	$[C_4H_5O_3]^-$	$[C_4H_5O_3]^-$	
	102, 103, 105	UI		

107	$[C_3H_7O_4]^-$ or $[M-H-(H_2O)_4]^-$		
112	UI		
113	$[C_5H_5O_3]^-$	$[C_5H_5O_3]^-$	
114	UI		
119	$[C_4H_7O_4]^-$	$[C_4H_7O_4]^-$	
120	UI		
121		UI	
125	$[M-H-(H_2O)_3]^-$		
131	UI		
135	$[C_5H_{11}O_4]^-$		
137	$[C_4H_9O_5]^-$		
141		UI	
143	$[M-H-(H_2O)_2]^-$	$[M-H-(H_2O)_2]^-$	
149, 155	UI		
159			
161	$[M-H-(H_2O)]^-$	$[M-H-(H_2O)]^-$	
167	UI		
171			
177		UI	
178		UI	
<b>Methanol</b>			
22, 33	UI		
42	$[C_2H_4N]^-$		
44, 45, 59	UI		
61	$[C_5H]^-$		
63	UI		
75		UI	
77	UI		

**Table S2.** Fragment peaks, and their respective mass, detected in anion mode for the investigated organics in pure water matrix (Napoleoni et al. 2022), in 0.01M, 0.1M and 1M MgSO<sub>4</sub> and 0.01M, 0.1M and 1M H<sub>2</sub>SO<sub>4</sub> matrices, at all investigated delay times and laser power intensities. UI stands for unidentified ion species.