

## SUPPLEMENTARY MATERIALS

# Evaluation of Solvent Compatibilities for Headspace-SIFT-MS Analysis of Pharmaceutical Products

Mark J. Perkins <sup>1</sup>, Leslie P. Silva <sup>2</sup>, and Vaughan S. Langford <sup>3,\*</sup>

<sup>1</sup> Element Materials Technology, Girton, Cambridge CB3 0NA, UK

<sup>2</sup> Syft Technologies Inc., Los Angeles, CA, USA

<sup>3</sup> Syft Technologies Limited, Christchurch 8011, New Zealand

\* Correspondence: vaughan.langford@syft.com; Tel.: +64-3-3386701

## Contents

### Tables

#### A. Materials and Methods

Table S1. Reagent ions, primary product ion mass-to-charge ratios (m/z), and branching ratio (in parentheses, %) for the analytes.	3
--	---

#### B. Linearity

Table S2. Mix 1 in <u>water</u> across both concentration ranges.	4
Table S3. Mix 2 in <u>water</u> across the low concentration range.	5
Table S4a. Mix 1 in 5% <u>DMAC</u> :95% water across the high concentration range.	6
Table S4b. Mix 1 in 10% <u>DMAC</u> :90% water across the high concentration range.	7
Table S4c. Mix 1 in 25% <u>DMAC</u> :75% water across the high concentration range.	8
Table S4d. Mix 1 in 50% <u>DMAC</u> :50% water across the high concentration range.	9
Table S5. Mix 1 in 5% <u>DMF</u> :95% water across the high concentration range.	10
Table S6a. Mix 1 in 5% <u>DMI</u> :95% water across both concentration ranges.	11
Table S6b. Mix 1 in 10% <u>DMI</u> :90% water across both concentration ranges.	12
Table S6c. Mix 1 in 25% <u>DMI</u> :75% water across the high concentration range.	13
Table S6d. Mix 1 in 50% <u>DMI</u> :50% water across the high concentration range.	14
Table S6e. Mix 1 in 75% <u>DMI</u> :25% water across the high concentration range.	15
Table S6f. Mix 1 in 100% <u>DMI</u> across the high concentration range.	16
Table S7a. Mix 2 in 10% <u>DMI</u> :90% water across the low concentration range.	17
Table S7b. Mix 2 in 100% <u>DMI</u> across the high concentration range.	18
Table S8a. Mix 1 in 5% <u>DMSO</u> :95% water across the high concentration range.	19
Table S8b. Mix 1 in 10% <u>DMSO</u> :90% water across the high concentration range.	20
Table S8c. Mix 1 in 25% <u>DMSO</u> :75% water across the high concentration range.	21
Table S9. Mix 1 in 5% <u>methanol</u> :95% water across the high concentration range.	22
Table S10. Mix 1 in 5% <u>triacetin</u> :95% water across the high concentration range.	23

#### C. Repeatability

Table S11. Mix 1 in <u>water</u> at three levels in high concentration range.	24
Table S12a. Mix 1 in 5% <u>DMAC</u> :95% water at three levels in high concentration range.	25
Table S12b. Mix 1 in 10% <u>DMAC</u> :90% water at three levels in high concentration range.	26
Table S12c. Mix 1 in 25% <u>DMAC</u> :75% water at three levels in high concentration range.	27
Table S12d. Mix 1 in 50% <u>DMAC</u> :50% water at three levels in high concentration range.	28
Table S13. Mix 1 in 5% <u>DMF</u> :95% water at three levels in high concentration range.	29

## Contents (continued)

Table S14a. Mix 1 in 5% <u>DMAC</u> :95% water at three levels in high concentration range.	30
Table S14b. Mix 1 in 10% <u>DMAC</u> :90% water at three levels in high concentration range.	31
Table S14c. Mix 1 in 25% <u>DMAC</u> :75% water at three levels in high concentration range.	32
Table S14d. Mix 1 in 50% <u>DMAC</u> :50% water at three levels in high concentration range.	33
Table S14e. Mix 1 in 75% <u>DMAC</u> :25% water at three levels in high concentration range.	34
Table S14f. Mix 1 in 100% <u>DMAC</u> water at three levels in high concentration range.	35
Table S15. Mix 2 in 100% <u>DMAC</u> water at three levels in high concentration range.	36
Table S16a. Mix 1 in 5% <u>DMSO</u> :95% water at three levels in high concentration range.	37
Table S16b. Mix 1 in 10% <u>DMSO</u> :90% water at three levels in high concentration range.	38
Table S16c. Mix 1 in 25% <u>DMSO</u> :75% water at three levels in high concentration range.	39
Table S17. Mix 1 in 5% <u>methanol</u> :95% water at three levels in high concentration range.	40
Table S18. Mix 1 in 5% <u>triacetin</u> :95% water at three levels in high concentration range.	41
D. Limit of Quantitation	
Table S19. Mix 1 in <u>water</u> .	42
Table S20a. Mix 1 in 5% <u>DMI</u> :95% water.	43
Table S20b. Mix 1 in 10% <u>DMI</u> :90% water.	44
Table S20c. Mix 1 in 100% <u>DMI</u> .	45
Table S21a. Mix 2 in 10% <u>DMI</u> :90% water.	46
Table S21b. Mix 2 in 100% <u>DMI</u> .	47
E. Recovery	
Table S22a. Mix 1 in 5% <u>DMI</u> :95% water solution of aspirin.	48
Table S22b. Mix 1 in 100% <u>DMI</u> solution of aspirin.	49
Table S23. Mix 2 in 100% <u>DMI</u> solution of aspirin.	50
Figures	
A. Measured Headspace Concentrations Relative to Aqueous Solutions	
Figure S1. Mix 1 in water:solvent (0–10%) mixtures – <u>all solvents</u> .	51
Figure S2. Mix 1 in water:solvent (0–100%) mixtures – <u>DMAC</u> , <u>DMI</u> , and <u>DMSO</u> .	53
B. Linearity	
Figure S3. Mix 1 in 95% water:5% solvent – <u>all solvents</u> .	56
Figure S4. Mix 1 in 5, 10, 25, and 50% <u>DMAC</u> : water solutions.	58
Figure S5. Mix 1 in 5, 10, 25, 50, 75 and 100% <u>DMI</u> :water solutions in the high concentration range.	61
Figure S6. Mix 1 in 5 and 10% <u>DMI</u> : water solutions in the low concentration range.	63
Figure S7. Mix 1 in 5, 10, and 25% <u>DMSO</u> : water solutions.	66

## Tables

### A. Materials and Methods

**Table S1.** Reagent ions, primary product ion mass-to-charge ratios ( $m/z$ ), and branching ratio (in parentheses, %) for the analytes. The listed  $m/z$  are those used to quantify target compounds, not necessarily all that are available.

Compound, Molecular Formula	Reagent Ion	Product Ion Formula	Product Ion $m/z$	Ion Signal Ratios	Reference*
Acetone, C <sub>3</sub> H <sub>6</sub> O	NO <sup>+</sup>	C <sub>3</sub> H <sub>6</sub> O.NO <sup>+</sup>	88	100%	[31]
Acetonitrile, C <sub>2</sub> H <sub>3</sub> N	H <sub>3</sub> O <sup>+</sup>	C <sub>2</sub> H <sub>3</sub> N.H <sup>+</sup>	42	100%	[32]
	NO <sup>+</sup>	C <sub>2</sub> H <sub>3</sub> N.NO <sup>+</sup>	71**	100%	
Benzene, C <sub>6</sub> H <sub>6</sub>	NO <sup>+</sup>	C <sub>6</sub> H <sub>6</sub> <sup>+</sup>	78	76%	[33]
	NO <sup>+</sup>	C <sub>6</sub> H <sub>6</sub> .NO <sup>+</sup>	108	24%	
	O <sub>2</sub> <sup>+</sup>	C <sub>6</sub> H <sub>6</sub> <sup>+</sup>	78	100%	
1-Butanol, C <sub>4</sub> H <sub>10</sub> O	NO <sup>+</sup>	C <sub>4</sub> H <sub>9</sub> O <sup>+</sup>	73	95%	[29]
Chloroform, CHCl <sub>3</sub>	O <sub>2</sub> <sup>+</sup>	CH <sup>35</sup> Cl <sub>2</sub> <sup>+</sup>	83	56%	[34]
	O <sub>2</sub> <sup>+</sup>	CH <sup>35</sup> Cl <sup>37</sup> Cl <sup>+</sup>	85	38%	
Isooctane, C <sub>8</sub> H <sub>18</sub>	H <sub>3</sub> O <sup>+</sup>	C <sub>8</sub> H <sub>17</sub> <sup>+</sup>	113	22%	[35]
	NO <sup>+</sup>	C <sub>8</sub> H <sub>17</sub> <sup>+</sup>	113	93%	
Isopropyl alcohol, C <sub>3</sub> H <sub>8</sub> O	H <sub>3</sub> O <sup>+</sup>	C <sub>3</sub> H <sub>7</sub> <sup>+</sup>	43	80%	[29]
	NO <sup>+</sup>	C <sub>3</sub> H <sub>7</sub> O <sup>+</sup>	59	100%	
Methanol, CH <sub>4</sub> O	H <sub>3</sub> O <sup>+</sup>	CH <sub>4</sub> O.H <sup>+</sup>	33	100%	[29]
Methyl ethyl ketone, C <sub>4</sub> H <sub>8</sub> O	NO <sup>+</sup>	C <sub>4</sub> H <sub>8</sub> O.NO <sup>+</sup>	102	100%	[31]
	O <sub>2</sub> <sup>+</sup>	C <sub>4</sub> H <sub>8</sub> O <sup>+</sup>	72	35%	
Nitromethane, CH <sub>3</sub> NO <sub>2</sub>	H <sub>3</sub> O <sup>+</sup>	CH <sub>3</sub> NO <sub>2</sub> .H <sup>+</sup>	62	100%	[36]
	NO <sup>+</sup>	CH <sub>3</sub> NO <sub>2</sub> .NO <sup>+</sup>	91**	100%	
Propanal, C <sub>3</sub> H <sub>6</sub> O	NO <sup>+</sup>	C <sub>3</sub> H <sub>5</sub> O <sup>+</sup>	57	100%	[31]
Tetrahydrofuran, C <sub>4</sub> H <sub>8</sub> O	NO <sup>+</sup>	C <sub>4</sub> H <sub>7</sub> O <sup>+</sup>	71	100%	[37]
	O <sub>2</sub> <sup>+</sup>	C <sub>4</sub> H <sub>7</sub> O <sup>+</sup>	71	55%	
Toluene, C <sub>7</sub> H <sub>8</sub>	NO <sup>+</sup>	C <sub>7</sub> H <sub>8</sub> <sup>+</sup>	92	100%	[33]
	O <sub>2</sub> <sup>+</sup>	C <sub>7</sub> H <sub>8</sub> <sup>+</sup>	92	100%	
Trichloroethylene, C <sub>2</sub> HCl <sub>3</sub>	NO <sup>+</sup>	C <sub>2</sub> H <sup>35</sup> Cl <sub>3</sub> <sup>+</sup>	160**	42%	[34]
	NO <sup>+</sup>	C <sub>2</sub> H <sup>35</sup> Cl <sub>2</sub> <sup>37</sup> Cl <sup>+</sup>	162**	42%	
	O <sub>2</sub> <sup>+</sup>	C <sub>2</sub> H <sup>35</sup> Cl <sub>3</sub> <sup>+</sup>	130	42%	
	O <sub>2</sub> <sup>+</sup>	C <sub>2</sub> H <sup>35</sup> Cl <sub>2</sub> <sup>37</sup> Cl <sup>+</sup>	132	42%	

\* Reference numbers correspond to citations in the article itself.

\*\* The NO<sup>+</sup> product ion was only used with methanol solvent because the reaction rate coefficient ( $k$ ) is approximately 10-fold slower than the usual product ion, hence reducing sensitivity.

## B. Linearity

**Table S2.** SIFT-MS linearity data for Mix 1 in water across both low and high concentration ranges. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0051	0.0108	0.00061	0.00102	0.00101	0.00199	0.0109	0.0126	0.119	0.0135	0.00559	0.00843	0.00486	0.00027	0.00462	0.00056	0.00109	0.00149	0.00277	0.00010	0.00057	0.00058	0.00117
1	0.0107	0.0155	0.00273	0.00263	0.00315	0.00862	0.0191	0.0172	0.127	0.016	0.00881	0.0106	0.00905	0.00364	0.00988	0.00601	0.0045	0.00745	0.00735	0.00299	0.00232	0.00289	0.00244
2	0.019	0.0201	0.00509	0.00383	0.00492	0.0155	0.0245	0.0233	0.108	0.0181	0.0111	0.0128	0.0138	0.00605	0.0148	0.00991	0.00968	0.0127	0.0097	0.00504	0.00451	0.00438	0.00696
3	0.0229	0.0235	0.00668	0.00421	0.00691	0.0231	0.031	0.0288	0.116	0.0204	0.0158	0.0144	0.0175	0.00945	0.0205	0.0161	0.0135	0.0194	0.0154	0.00753	0.00636	0.00925	0.00792
5	0.0331	0.0338	0.0118	0.00813	0.0109	0.0356	0.0433	0.0414	0.132	0.0294	0.0213	0.022	0.0235	0.0167	0.0334	0.026	0.0221	0.0299	0.0207	0.0136	0.00926	0.0121	0.0146
10	0.0697	0.0599	0.0213	0.0162	0.021	0.0693	0.0751	0.0702	0.124	0.0527	0.0398	0.0401	0.0447	0.0331	0.0587	0.0514	0.0437	0.0603	0.0431	0.0266	0.0215	0.0252	0.0259
15	0.106	0.0825	0.0299	0.0225	0.0315	0.0993	0.113	0.0963	0.157	0.0799	0.0529	0.0552	0.0633	0.0485	0.0846	0.0738	0.0674	0.0893	0.0589	0.0384	0.0312	0.0397	0.0406
20	0.135	0.107	0.0423	0.0302	0.0426	0.131	0.152	0.134	0.174	0.0958	0.0694	0.0695	0.0809	0.0671	0.122	0.098	0.0927	0.123	0.0791	0.0489	0.0431	0.0554	0.0579
<b>R<sup>2</sup></b>	<b>0.9981</b>	<b>0.9995</b>	<b>0.9977</b>	<b>0.9978</b>	<b>0.9996</b>	<b>0.9996</b>	<b>0.9979</b>	<b>0.9974</b>	<b>0.8150</b>	<b>0.9928</b>	<b>0.9983</b>	<b>0.9971</b>	<b>0.9991</b>	<b>0.9993</b>	<b>0.9962</b>	<b>0.9995</b>	<b>0.9989</b>	<b>0.9993</b>	<b>0.9982</b>	<b>0.9980</b>	<b>0.9981</b>	<b>0.9963</b>	<b>0.9952</b>
0	0.0179	0.0828	0.0267	0.0049	0.019	0.00873	0.0579	0.055	0.0772	0.00246	0.102	0.0903	0.0132	0.00084	0.00619	0.00112	0.0024	0.00476	0.00152	0.00095	0.00061	0.0015	0.0015
20	0.156	0.208	0.0794	0.0381	0.0738	0.134	0.216	0.193	0.141	0.112	0.185	0.156	0.108	0.0732	0.128	0.121	0.101	0.124	0.0781	0.0663	0.0512	0.0664	0.0673
50	0.387	0.385	0.164	0.104	0.156	0.311	0.425	0.388	0.332	0.264	0.305	0.251	0.253	0.18	0.302	0.285	0.244	0.304	0.194	0.16	0.14	0.161	0.155
100	0.717	0.691	0.294	0.198	0.309	0.591	0.822	0.721	0.569	0.532	0.497	0.407	0.483	0.353	0.583	0.544	0.482	0.57	0.365	0.31	0.274	0.323	0.309
200	1.5	1.36	0.645	0.456	0.684	1.25	1.78	1.59	1.3	1.18	0.948	0.785	1.02	0.786	1.26	1.17	1.06	1.23	0.812	0.712	0.626	0.73	0.73
300	2.19	1.99	0.952	0.654	1.02	1.85	2.59	2.39	1.92	1.76	1.36	1.12	1.48	1.14	1.87	1.75	1.57	1.82	1.24	1.09	0.932	1.13	1.06
400	2.96	2.59	1.32	0.948	1.42	2.48	3.46	3.19	2.66	2.45	1.75	1.45	1.91	1.52	2.47	2.29	2.15	2.43	1.66	1.47	1.3	1.55	1.48
500	3.8	3.34	1.65	1.18	1.84	3.1	4.38	3.94	3.38	3.04	2.23	1.85	2.52	1.96	3.22	2.88	2.68	3.13	2.17	1.88	1.66	1.94	1.86
<b>R<sup>2</sup></b>	<b>0.9993</b>	<b>0.9994</b>	<b>0.9987</b>	<b>0.9978</b>	<b>0.9975</b>	<b>0.9999</b>	<b>0.9995</b>	<b>0.9993</b>	<b>0.9978</b>	<b>0.9992</b>	<b>0.9995</b>	<b>0.9993</b>	<b>0.9986</b>	<b>0.9993</b>	<b>0.9991</b>	<b>0.9997</b>	<b>0.9996</b>	<b>0.9994</b>	<b>0.9985</b>	<b>0.9989</b>	<b>0.9985</b>	<b>0.9990</b>	<b>0.9987</b>



**Table S3.** SIFT-MS linearity data for Mix 2 in water across the low concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.00328	0.0252	0.00548	0.00164	0.00458	0.00268	0.0107	0.0102	0.0721	0.00538	0.00431	0.00322	0.00344	0.00007	0.00433	0.00025	0.00091	0.00164	0.00279	0.00022	0.00033	0.00026	0.00122
1	0.0107	0.0334	0.219	0.138	0.21700	0.00659	0.143	0.14	0.132	0.0678	0.00715	0.00618	0.00519	0.00744	0.017	0.0043	0.0632	0.0142	0.0114	0.229	0.193	0.18600	0.191
2	0.0172	0.0376	0.43100	0.291	0.443	0.011	0.287	0.27	0.227	0.195	0.0104	0.00941	0.00606	0.0146	0.0304	0.0102	0.175	0.0305	0.0207	0.471	0.39700	0.38800	0.389
3	0.0256	0.0453	0.63	0.444	0.677	0.0146	0.43	0.394	0.313	0.264	0.0157	0.0142	0.00951	0.0226	0.0456	0.0137	0.252	0.0428	0.0291	0.714	0.622	0.58000	0.561
5	0.0383	0.0523	1.16	0.817	1.24	0.0228	0.783	0.715	0.56	0.511	0.0239	0.0172	0.012	0.0374	0.0681	0.0228	0.481	0.07	0.0509	1.32	1.13	1.08	1.05
10	0.0751	0.0784	2.36	1.58	2.53	0.0428	1.58	1.47	0.965	1.02	0.0427	0.0356	0.02	0.0751	0.136	0.0496	0.96	0.135	0.099	2.67	2.33	2.22	2.17
15	0.113	0.112	3.6	2.55	3.87	0.0644	2.37	2.22	1.46	1.65	0.0634	0.0498	0.0303	0.108	0.198	0.0742	1.54	0.208	0.142	4.05	3.55	3.43	3.35
20	0.152	0.131	4.71	3.22	5.04	0.0834	3.1	2.88	1.94	2.12	0.0845	0.0644	0.0374	0.146	0.266	0.0979	1.94	0.271	0.205	5.31	4.68	4.59	4.37
<b>R<sup>2</sup></b>	<b>0.9996</b>	<b>0.9955</b>	<b>0.9996</b>	<b>0.9983</b>	<b>0.9995</b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9994</b>	<b>0.9990</b>	<b>0.9984</b>	<b>0.9994</b>	<b>0.9979</b>	<b>0.9971</b>	<b>0.9996</b>	<b>0.9998</b>	<b>0.9995</b>	<b>0.9981</b>	<b>0.9997</b>	<b>0.9973</b>	<b>0.9996</b>	<b>0.9997</b>	<b>0.9995</b>	<b>0.9994</b>

**Table S4a.** SIFT-MS linearity data for Mix 1 in 5% DMAC:95% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.134	0.00704	0.00132	0.00177	0.0017	0.00679	0.0831	0.0929	0.601	0.0155	0.00408	0.00207	0.00573	0.00091	0.0325	0.00030	0.012	0.00626	0.0461	0.00067	0.00052	0.00054	0.00149
20	0.264	0.0979	0.0285	0.0189	0.0276	0.124	0.151	0.156	0.658	0.0773	0.066	0.0649	0.0755	0.0622	0.141	0.105	0.0646	0.0875	0.0895	0.0343	0.0289	0.0279	0.0307
50	0.467	0.241	0.0646	0.0436	0.0687	0.298	0.265	0.264	0.75	0.165	0.159	0.151	0.185	0.162	0.304	0.263	0.141	0.216	0.181	0.078	0.0657	0.0725	0.0654
100	0.736	0.473	0.133	0.091	0.14	0.559	0.469	0.443	0.936	0.329	0.311	0.299	0.349	0.306	0.576	0.512	0.276	0.417	0.299	0.162	0.138	0.138	0.147
200	1.32	0.904	0.382	0.248	0.399	1.11	1.14	1.04	1.45	1	0.591	0.578	0.652	0.588	1.1	1.03	0.859	0.833	0.589	0.424	0.374	0.435	0.421
300	2.05	1.47	0.608	0.397	0.653	1.77	1.83	1.68	2.12	1.55	0.976	0.941	1.1	0.971	1.77	1.59	1.35	1.35	0.932	0.709	0.615	0.654	0.675
400	2.3	1.83	0.761	0.515	0.847	2.18	2.26	2.09	2.55	2.04	1.22	1.14	1.29	1.2	2.14	2.03	1.76	1.66	1.16	0.896	0.797	0.892	0.839
500	2.85	2.2	1.02	0.643	1.08	2.57	2.82	2.65	3.31	2.69	1.43	1.37	1.58	1.45	2.65	2.38	2.28	2.03	1.42	1.21	1.07	1.21	1.15
<b>R<sup>2</sup></b>	<b>0.9912</b>	<b>0.9969</b>	<b>0.9951</b>	<b>0.9969</b>	<b>0.9962</b>	<b>0.9947</b>	<b>0.9957</b>	<b>0.9961</b>	<b>0.9911</b>	<b>0.9950</b>	<b>0.9951</b>	<b>0.9950</b>	<b>0.9936</b>	<b>0.9966</b>	<b>0.9969</b>	<b>0.9963</b>	<b>0.9952</b>	<b>0.9971</b>	<b>0.9981</b>	<b>0.9949</b>	<b>0.9950</b>	<b>0.9931</b>	<b>0.9939</b>

**Table S4b.** SIFT-MS linearity data for Mix 1 in 10% DMAC:90% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.257	0.00833	0.00131	0.00232	0.00176	0.0159	0.122	0.13	1.13	0.0359	0.00487	0.00289	0.00573	0.00235	0.0572	0.00244	0.0242	0.00843	0.0817	0.00223	0.00253	0.00255	0.0061
20	0.346	0.0995	0.024	0.017	0.0231	0.116	0.18	0.187	1.11	0.0922	0.0606	0.0571	0.0773	0.0567	0.153	0.0995	0.0844	0.0862	0.129	0.0294	0.0242	0.0278	0.0209
50	0.474	0.232	0.0535	0.0341	0.0602	0.261	0.288	0.265	1.28	0.193	0.157	0.143	0.178	0.144	0.296	0.256	0.165	0.206	0.201	0.0626	0.0512	0.0547	0.059
100	0.682	0.451	0.111	0.0737	0.124	0.492	0.447	0.42	1.38	0.383	0.276	0.279	0.332	0.268	0.536	0.487	0.321	0.389	0.318	0.136	0.113	0.122	0.123
200	1.23	0.879	0.297	0.203	0.318	0.939	0.982	0.933	2.14	1.1	0.56	0.536	0.675	0.537	1.03	0.967	0.95	0.755	0.584	0.333	0.29	0.359	0.338
300	1.75	1.31	0.469	0.328	0.504	1.41	1.49	1.36	2.69	1.69	0.808	0.789	0.99	0.805	1.47	1.42	1.43	1.14	0.846	0.518	0.449	0.562	0.537
400	2.52	1.87	0.658	0.461	0.716	1.97	2	1.87	3.32	2.23	1.16	1.13	1.39	1.15	2.13	1.99	1.92	1.62	1.18	0.706	0.633	0.745	0.751
500	3.02	2.31	0.836	0.559	0.914	2.52	2.52	2.4	4	2.94	1.49	1.42	1.68	1.43	2.57	2.56	2.5	2.01	1.45	0.92	0.827	1.02	0.963
<b>R<sup>2</sup></b>	<b>0.9947</b>	<b>0.9986</b>	<b>0.9961</b>	<b>0.9953</b>	<b>0.9958</b>	<b>0.9982</b>	<b>0.9969</b>	<b>0.9951</b>	<b>0.9921</b>	<b>0.9953</b>	<b>0.9971</b>	<b>0.9982</b>	<b>0.9992</b>	<b>0.9984</b>	<b>0.9979</b>	<b>0.9983</b>	<b>0.9955</b>	<b>0.9985</b>	<b>0.9980</b>	<b>0.9971</b>	<b>0.9953</b>	<b>0.9930</b>	<b>0.9954</b>

**Table S4c.** SIFT-MS linearity data for Mix 1 in 25% DMAC:75% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.324	0.00675	0.00038	0.00481	0.00091	0.0161	0.285	0.288	2.59	0.0318	0.00494	0.0021	0.00511	0.00302	0.0796	0.00019	0.0194	0.0158	0.168	0.0018	0.00135	0.00135	0.00193
20	0.46	0.0897	0.0136	0.00991	0.0139	0.0813	0.312	0.313	2.51	0.0926	0.0569	0.0477	0.0704	0.0466	0.148	0.0926	0.0762	0.0832	0.202	0.0153	0.0141	0.0147	0.0206
50	0.627	0.217	0.0359	0.0259	0.0363	0.192	0.371	0.37	2.5	0.183	0.135	0.126	0.184	0.112	0.273	0.226	0.153	0.175	0.266	0.0369	0.0304	0.0397	0.0427
100	0.842	0.418	0.0691	0.0436	0.0691	0.361	0.503	0.514	2.88	0.363	0.247	0.244	0.34	0.215	0.453	0.444	0.303	0.313	0.368	0.07	0.062	0.0789	0.0802
200	1.32	0.82	0.154	0.0956	0.171	0.705	0.765	0.739	3.21	0.814	0.506	0.466	0.663	0.437	0.834	0.861	0.692	0.633	0.559	0.167	0.137	0.187	0.182
300	1.63	1.21	0.241	0.16	0.258	1.05	1.04	0.987	3.73	1.24	0.756	0.695	0.968	0.647	1.24	1.34	1.05	0.921	0.771	0.244	0.204	0.292	0.304
400	2.23	1.62	0.322	0.22	0.346	1.34	1.33	1.26	4.24	1.73	0.951	0.917	1.36	0.863	1.6	1.71	1.43	1.23	0.995	0.322	0.277	0.403	0.39
500	2.65	2	0.413	0.284	0.443	1.67	1.6	1.52	4.76	2.2	1.18	1.14	1.6	1.06	2.03	2.1	1.91	1.53	1.18	0.416	0.361	0.521	0.502
<b>R<sup>2</sup></b>	<b>0.9966</b>	<b>0.9999</b>	<b>0.9989</b>	<b>0.9950</b>	<b>0.9986</b>	<b>0.9994</b>	<b>0.9986</b>	<b>0.9987</b>	<b>0.9861</b>	<b>0.9975</b>	<b>0.9986</b>	<b>0.9998</b>	<b>0.9984</b>	<b>0.9998</b>	<b>0.9997</b>	<b>0.9990</b>	<b>0.9960</b>	<b>0.9999</b>	<b>0.9996</b>	<b>0.9988</b>	<b>0.9984</b>	<b>0.9974</b>	<b>0.9975</b>

**Table S4d.** SIFT-MS linearity data for Mix 1 in 50% DMAC:50% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.429	0.0133	0.00211	0.00305	0.00346	0.019	0.0812	0.101	0.974	0.0233	0.00609	0.00356	0.00418	0.00181	0.0719	0.00030	0.0150	0.00918	0.0689	0.00156	0.00099	0.00212	0.00332
20	0.511	0.0858	0.171	0.0251	0.131	0.0579	0.0773	0.0928	0.732	0.0183	0.0492	0.046	0.0810	0.0309	0.127	0.0576	0.0172	0.0653	0.0947	0.00167	0.00103	0.00135	0.00440
50	0.690	0.197	0.123	0.0222	0.0913	0.114	0.0887	0.117	0.862	0.0296	0.115	0.107	0.209	0.0807	0.230	0.150	0.0509	0.162	0.157	0.00664	0.00304	0.00600	0.00776
100	0.939	0.373	0.103	0.0192	0.0763	0.213	0.108	0.124	0.797	0.0502	0.222	0.206	0.378	0.156	0.355	0.304	0.0782	0.319	0.256	0.0119	0.00948	0.0134	0.0143
200	1.52	0.726	0.0979	0.0259	0.0802	0.399	0.142	0.170	0.929	0.0994	0.431	0.400	0.761	0.312	0.662	0.603	0.153	0.635	0.457	0.0229	0.0175	0.0268	0.0286
300	2.08	1.11	0.136	0.0575	0.121	0.585	0.283	0.290	1.15	0.337	0.632	0.599	1.15	0.497	0.988	0.902	0.380	0.996	0.705	0.0598	0.0465	0.0680	0.0755
400	2.54	1.45	0.157	0.0724	0.152	0.763	0.337	0.354	1.26	0.442	0.841	0.784	1.48	0.645	1.28	1.21	0.521	1.34	0.916	0.0784	0.0675	0.0949	0.0936
500	3.22	1.89	0.191	0.0979	0.198	0.971	0.486	0.490	1.62	0.665	1.07	1.04	1.86	0.842	1.67	1.56	0.726	1.70	1.19	0.115	0.0914	0.128	0.121
<b>R<sup>2</sup></b>	<b>0.9987</b>	<b>0.9991</b>	<b>0.3622</b>	<b>0.9222</b>	<b>0.6102</b>	<b>0.9997</b>	<b>0.9486</b>	<b>0.9574</b>	<b>0.8288</b>	<b>0.9399</b>	<b>0.9998</b>	<b>0.9984</b>	<b>0.9996</b>	<b>0.9988</b>	<b>0.9982</b>	<b>0.9994</b>	<b>0.9679</b>	<b>0.9993</b>	<b>0.9973</b>	<b>0.9644</b>	<b>0.9668</b>	<b>0.9713</b>	<b>0.9725</b>

**Table S5.** SIFT-MS linearity data for Mix 1 in 5% DMF:95% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.00557	0.0096	0.0911	0.0144	0.0704	0.648	0.0224	0.0219	0.0905	0.00232	0.00556	0.00298	0.0134	0.00208	0.0466	0.0011	0.00608	0.00277	0.00554	0.00285	0.00456	0.00118	0.00256
20	0.132	0.12	0.104	0.0384	0.094	0.937	0.143	0.129	0.173	0.119	0.0745	0.0599	0.107	0.0641	0.154	0.114	0.108	0.107	0.0699	0.0517	0.0446	0.0532	0.0497
50	0.333	0.298	0.152	0.0843	0.149	1.01	0.329	0.308	0.362	0.288	0.194	0.15	0.241	0.163	0.32	0.284	0.245	0.255	0.17	0.124	0.104	0.141	0.125
100	0.617	0.575	0.261	0.157	0.258	1.4	0.648	0.587	0.593	0.554	0.391	0.283	0.447	0.31	0.561	0.545	0.501	0.52	0.343	0.251	0.209	0.258	0.247
200	1.22	1.15	0.505	0.342	0.524	1.83	1.36	1.24	1.42	1.14	0.761	0.593	0.864	0.605	1.08	1.15	1.07	1.03	0.68	0.531	0.455	0.559	0.551
300	1.86	1.7	0.752	0.477	0.796	2.32	1.99	1.86	2.08	1.76	1.12	0.88	1.29	0.912	1.67	1.68	1.58	1.57	1.05	0.788	0.688	0.855	0.813
400	2.4	2.24	0.98	0.653	1.02	2.63	2.59	2.36	2.74	2.35	1.49	1.12	1.62	1.18	2.13	2.21	2.11	1.96	1.37	1.01	0.915	1.13	1.08
500	3.05	2.87	1.26	0.835	1.33	3.22	3.34	3.04	3.57	3.02	1.85	1.42	2.18	1.49	2.7	2.71	2.8	2.51	1.77	1.33	1.17	1.48	1.46
<b>R<sup>2</sup></b>	<b>0.9997</b>	<b>0.9997</b>	<b>0.9971</b>	<b>0.9987</b>	<b>0.9973</b>	<b>0.9899</b>	<b>0.9994</b>	<b>0.9992</b>	<b>0.9975</b>	<b>0.9993</b>	<b>0.9999</b>	<b>0.9993</b>	<b>0.9976</b>	<b>0.9998</b>	<b>0.9995</b>	<b>0.9994</b>	<b>0.9981</b>	<b>0.9989</b>	<b>0.9995</b>	<b>0.9988</b>	<b>0.9994</b>	<b>0.9987</b>	<b>0.9970</b>

**Table S6a.** SIFT-MS linearity data for Mix 1 in 5% DMI:95% water across both low and high concentration ranges. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.00658	0.0449	0.00267	0.00653	0.00376	0.003	0.0178	0.0201	0.593	0.0254	0.00761	0.00481	0.0179	0.00128	0.0281	0.00010	0.0161	0.0267	0.0127	0.00630	0.00636	0.00199	0.00323
1	0.0126	0.0559	0.0057	0.00681	0.00521	0.00867	0.0256	0.0264	0.607	0.0381	0.0108	0.00811	0.0218	0.00456	0.0328	0.00527	0.018	0.0305	0.0181	0.00771	0.00765	0.00291	0.0057
2	0.0197	0.0629	0.00478	0.00814	0.00634	0.0134	0.0284	0.0277	0.6	0.0412	0.0152	0.00989	0.0259	0.00614	0.0408	0.0109	0.0203	0.0365	0.02	0.01	0.00829	0.00647	0.00603
3	0.0239	0.0544	0.00853	0.00897	0.00914	0.018	0.0284	0.0306	0.667	0.04	0.0153	0.0125	0.0299	0.00915	0.0406	0.0146	0.0272	0.0414	0.0236	0.0133	0.011	0.00889	0.0113
5	0.0364	0.06	0.0129	0.0119	0.0124	0.0298	0.0364	0.0383	0.596	0.0486	0.0216	0.0165	0.033	0.0142	0.0536	0.0256	0.0373	0.0495	0.0314	0.0169	0.0138	0.013	0.0138
10	0.0708	0.0874	0.0171	0.0165	0.019	0.0544	0.0597	0.0672	0.698	0.0755	0.0356	0.0309	0.0531	0.0293	0.0729	0.0471	0.0588	0.0756	0.0438	0.0263	0.0198	0.0238	0.025
15	0.0935	0.109	0.0295	0.0206	0.029	0.0831	0.0883	0.0888	0.724	0.0935	0.0516	0.0436	0.0719	0.0421	0.101	0.0751	0.0863	0.101	0.0605	0.037	0.0283	0.0368	0.036
20	0.118	0.133	0.0366	0.0266	0.0385	0.104	0.112	0.116	0.666	0.117	0.063	0.0603	0.087	0.0552	0.122	0.0994	0.104	0.126	0.0769	0.0474	0.0387	0.0517	0.0487
<b>R<sup>2</sup></b>	<b>0.9955</b>	<b>0.9733</b>	<b>0.9859</b>	<b>0.9963</b>	<b>0.9964</b>	<b>0.9987</b>	<b>0.9923</b>	<b>0.9953</b>	<b>0.5185</b>	<b>0.9909</b>	<b>0.9973</b>	<b>0.9969</b>	<b>0.9974</b>	<b>0.9993</b>	<b>0.9968</b>	<b>0.9991</b>	<b>0.9963</b>	<b>0.9996</b>	<b>0.9977</b>	<b>0.9989</b>	<b>0.9921</b>	<b>0.9962</b>	<b>0.9967</b>
0	0.0111	0.00989	0.325	0.221	0.332	0.195	0.199	0.192	0.117	0.0177	0.00657	0.00476	0.0174	0.00266	0.034	0.00106	0.0145	0.0248	0.0317	0.00631	0.00765	0.00113	0.00256
20	0.13	0.114	0.368	0.225	0.375	0.258	0.299	0.301	0.26	0.168	0.079	0.0598	0.105	0.0573	0.139	0.105	0.104	0.119	0.101	0.0489	0.0415	0.0509	0.0494
50	0.311	0.293	0.436	0.273	0.422	0.399	0.48	0.46	0.439	0.299	0.201	0.154	0.235	0.153	0.287	0.286	0.255	0.266	0.192	0.122	0.1	0.134	0.124
100	0.626	0.557	0.528	0.354	0.539	0.624	0.783	0.721	0.731	0.567	0.37	0.293	0.459	0.304	0.526	0.536	0.49	0.512	0.354	0.235	0.192	0.261	0.25
200	1.2	1.1	0.791	0.51	0.813	1.08	1.44	1.34	1.35	1.18	0.709	0.561	0.876	0.577	1.02	1.03	1.05	0.981	0.668	0.511	0.433	0.568	0.546
300	1.8	1.67	1.03	0.676	1.08	1.52	2.08	1.92	2.08	1.7	1.07	0.839	1.33	0.858	1.48	1.56	1.55	1.47	0.986	0.763	0.665	0.87	0.81
400	2.55	2.35	1.32	0.904	1.37	2.1	2.82	2.6	2.71	2.36	1.45	1.19	1.91	1.24	2.13	2.11	2.12	2.06	1.41	1.06	0.905	1.22	1.15
500	3.06	2.82	1.52	1.03	1.66	2.48	3.39	3.14	3.61	2.97	1.78	1.43	2.23	1.51	2.56	2.64	2.64	2.48	1.69	1.28	1.13	1.44	1.41
<b>R<sup>2</sup></b>	<b>0.9988</b>	<b>0.9988</b>	<b>0.9983</b>	<b>0.9955</b>	<b>0.9978</b>	<b>0.9984</b>	<b>0.9993</b>	<b>0.9992</b>	<b>0.9966</b>	<b>0.9990</b>	<b>0.9997</b>	<b>0.9988</b>	<b>0.9974</b>	<b>0.9983</b>	<b>0.9983</b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9990</b>	<b>0.9982</b>	<b>0.9991</b>	<b>0.9990</b>	<b>0.9981</b>	<b>0.9988</b>

**Table S6b.** SIFT-MS linearity data for Mix 1 in 10% DMI:10% water across both low and high concentration ranges. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.00903	0.0234	0.00996	0.0108	0.0107	0.00314	0.0163	0.0233	0.825	0.0413	0.00706	0.00806	0.0291	0.0023	0.0496	0.00038	0.0218	0.0419	0.0201	0.00953	0.00895	0.00047	0.00096
1	0.0141	0.0279	0.0142	0.0142	0.01260	0.00883	0.0235	0.0342	0.818	0.0473	0.0103	0.011	0.0359	0.00504	0.0527	0.00515	0.028	0.0465	0.0285	0.0115	0.0109	0.00252	0.00445
2	0.0171	0.0312	0.01560	0.0149	0.014	0.0134	0.0283	0.0362	0.812	0.0534	0.0129	0.0117	0.0404	0.00695	0.0545	0.0088	0.0303	0.0511	0.0293	0.0141	0.01140	0.00470	0.00427
3	0.0197	0.0396	0.0171	0.0159	0.0163	0.0172	0.0288	0.0386	0.809	0.0645	0.0148	0.0145	0.0425	0.00979	0.0586	0.0131	0.0353	0.0513	0.0321	0.0152	0.0125	0.00487	0.00568
5	0.0338	0.0458	0.0211	0.0164	0.0197	0.0256	0.0416	0.0456	0.803	0.0753	0.0208	0.0209	0.0522	0.0147	0.0661	0.0218	0.0466	0.0633	0.0373	0.0173	0.014	0.0082	0.0106
10	0.0622	0.0688	0.0259	0.0218	0.0251	0.0478	0.066	0.0676	0.851	0.102	0.0373	0.032	0.07	0.0253	0.0915	0.0458	0.0756	0.0828	0.0582	0.0276	0.0216	0.0188	0.0205
15	0.0922	0.0901	0.0312	0.0277	0.0318	0.0685	0.0916	0.089	0.868	0.122	0.0486	0.0472	0.0827	0.0379	0.115	0.0711	0.0944	0.108	0.0687	0.0342	0.0268	0.0276	0.0309
20	0.119	0.119	0.0398	0.0318	0.0378	0.0967	0.117	0.11	0.858	0.15	0.0649	0.0606	0.109	0.0494	0.132	0.0937	0.125	0.131	0.0837	0.0403	0.0324	0.0349	0.04
<b>R<sup>2</sup></b>	<b>0.9977</b>	<b>0.9970</b>	<b>0.9813</b>	<b>0.9862</b>	<b>0.9943</b>	<b>0.9976</b>	<b>0.9984</b>	<b>0.9957</b>	<b>0.7055</b>	<b>0.9927</b>	<b>0.9980</b>	<b>0.9975</b>	<b>0.9915</b>	<b>0.9996</b>	<b>0.9955</b>	<b>0.9994</b>	<b>0.9968</b>	<b>0.9972</b>	<b>0.9901</b>	<b>0.9929</b>	<b>0.9961</b>	<b>0.9964</b>	<b>0.9969</b>
0	0.0112	0.00694	0.00144	0.0202	0.00107	0.00492	0.0219	0.0343	0.431	0.0506	0.0158	0.0064	0.0545	0.0051	0.0579	0.00033	0.0106	0.0508	0.0453	0.0278	0.0249	0.00169	0.00411
20	0.125	0.12	0.0274	0.0333	0.0261	0.117	0.09	0.102	0.416	0.115	0.0859	0.064	0.141	0.0611	0.163	0.128	0.0756	0.144	0.106	0.056	0.045	0.0269	0.0241
50	0.296	0.302	0.0635	0.0572	0.0614	0.281	0.196	0.194	0.511	0.212	0.183	0.148	0.278	0.145	0.315	0.303	0.175	0.28	0.195	0.0944	0.0812	0.0605	0.061
100	0.581	0.605	0.132	0.0973	0.131	0.558	0.38	0.379	0.658	0.381	0.373	0.303	0.498	0.274	0.575	0.637	0.351	0.518	0.35	0.175	0.134	0.126	0.122
200	1.14	1.17	0.314	0.226	0.331	1.07	0.9	0.852	1.36	0.952	0.7	0.578	0.897	0.546	1.06	1.19	0.881	0.964	0.659	0.364	0.304	0.324	0.291
300	1.72	1.75	0.499	0.319	0.517	1.6	1.37	1.29	1.87	1.48	1.07	0.878	1.3	0.838	1.58	1.82	1.38	1.42	1.01	0.547	0.465	0.504	0.487
400	2.29	2.34	0.671	0.425	0.7	2.1	1.86	1.77	2.31	1.95	1.36	1.15	1.75	1.08	2.09	2.39	1.84	1.9	1.33	0.734	0.619	0.669	0.673
500	2.81	2.86	0.845	0.549	0.897	2.57	2.37	2.21	3.46	2.65	1.68	1.42	2.16	1.34	2.53	2.94	2.45	2.33	1.6	0.904	0.799	0.907	0.84
<b>R<sup>2</sup></b>	<b>0.9998</b>	<b>0.9997</b>	<b>0.9984</b>	<b>0.9974</b>	<b>0.9978</b>	<b>0.9995</b>	<b>0.9983</b>	<b>0.9986</b>	<b>0.9713</b>	<b>0.9939</b>	<b>0.9991</b>	<b>0.9998</b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9996</b>	<b>0.9996</b>	<b>0.9963</b>	<b>0.9999</b>	<b>0.9993</b>	<b>0.9991</b>	<b>0.9971</b>	<b>0.9953</b>	<b>0.9964</b>



**Table S6c.** SIFT-MS linearity data for Mix 1 in 25% DMI:75% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0336	0.0176	0.00095	0.0241	0.00134	0.00935	0.0218	0.0666	0.601	0.0818	0.0322	0.0194	0.16	0.0101	0.108	0.00116	0.0198	0.103	0.0857	0.0323	0.0275	0.00125	0.00251
20	0.144	0.132	0.0124	0.0281	0.0146	0.0852	0.0576	0.0982	0.557	0.124	0.0908	0.0696	0.25	0.0588	0.181	0.115	0.0726	0.181	0.127	0.0407	0.0333	0.011	0.0127
50	0.319	0.33	0.032	0.0399	0.0329	0.214	0.113	0.151	0.703	0.227	0.194	0.155	0.389	0.128	0.323	0.303	0.151	0.304	0.203	0.0607	0.0496	0.0337	0.0322
100	0.518	0.55	0.0604	0.0568	0.0636	0.38	0.218	0.233	0.873	0.401	0.331	0.259	0.575	0.222	0.495	0.554	0.33	0.453	0.313	0.0886	0.0748	0.0656	0.0674
200	1	1.04	0.152	0.115	0.16	0.703	0.489	0.472	1.39	0.908	0.601	0.482	0.957	0.416	0.878	1.05	0.826	0.809	0.546	0.163	0.137	0.159	0.16
300	1.54	1.59	0.246	0.174	0.257	1.05	0.734	0.728	1.93	1.45	0.881	0.73	1.42	0.627	1.27	1.54	1.3	1.18	0.794	0.251	0.205	0.245	0.259
400	2.03	2.08	0.331	0.232	0.338	1.38	1.03	0.951	2.53	1.95	1.17	0.952	1.83	0.822	1.62	2.02	1.78	1.54	1.04	0.333	0.275	0.343	0.343
500	2.44	2.58	0.407	0.271	0.433	1.69	1.22	1.16	3.31	2.5	1.39	1.14	2.13	1.01	2.02	2.56	2.31	1.88	1.28	0.397	0.336	0.444	0.411
<b>R<sup>2</sup></b>	<b>0.9990</b>	<b>0.9996</b>	<b>0.9976</b>	<b>0.9953</b>	<b>0.9976</b>	<b>0.9994</b>	<b>0.9977</b>	<b>0.9980</b>	<b>0.9857</b>	<b>0.9960</b>	<b>0.9988</b>	<b>0.9988</b>	<b>0.9981</b>	<b>0.9997</b>	<b>0.9997</b>	<b>0.9995</b>	<b>0.9963</b>	<b>0.9998</b>	<b>0.9998</b>	<b>0.9972</b>	<b>0.9977</b>	<b>0.9969</b>	<b>0.9972</b>

**Table S6d.** SIFT-MS linearity data for Mix 1 in 50% DMI:50% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0349	0.0102	0.00058	0.00757	0.00153	0.00735	0.0192	0.0393	0.241	0.0717	0.0125	0.0092	0.219	0.0125	0.111	0.00029	0.0155	0.0973	0.0599	0.0103	0.00938	0.00028	0.00142
20	0.126	0.081	0.00307	0.011	0.00306	0.0471	0.028	0.0419	0.25	0.0802	0.0518	0.0434	0.275	0.0423	0.16	0.0596	0.0236	0.142	0.0952	0.0153	0.0116	0.00139	0.00264
50	0.265	0.191	0.00819	0.0109	0.00897	0.102	0.0389	0.0557	0.307	0.11	0.108	0.101	0.398	0.0889	0.242	0.146	0.0431	0.216	0.148	0.0199	0.0161	0.00416	0.00639
100	0.488	0.365	0.0148	0.0177	0.0165	0.189	0.0621	0.0739	0.347	0.179	0.208	0.199	0.569	0.16	0.393	0.288	0.0704	0.357	0.232	0.0274	0.0196	0.0118	0.0116
200	0.946	0.71	0.0209	0.0287	0.0318	0.378	0.131	0.119	0.432	0.291	0.385	0.371	0.924	0.31	0.659	0.578	0.129	0.613	0.396	0.0427	0.0309	0.0229	0.0232
300	1.37	1.08	0.0633	0.0477	0.0665	0.568	0.217	0.234	0.611	0.403	0.578	0.55	1.25	0.463	0.952	0.884	0.3	0.946	0.6	0.0718	0.0543	0.0499	0.0495
400	1.78	1.41	0.0848	0.0668	0.0938	0.746	0.297	0.301	0.714	0.536	0.747	0.709	1.55	0.598	1.18	1.17	0.383	1.15	0.755	0.0948	0.0724	0.0702	0.0693
500	2.22	1.79	0.111	0.0816	0.124	0.936	0.364	0.359	0.877	0.624	0.915	0.895	1.9	0.75	1.48	1.43	0.5	1.44	0.931	0.113	0.0896	0.089	0.0851
<b>R<sup>2</sup></b>	<b>0.9997</b>	<b>0.9998</b>	<b>0.9660</b>	<b>0.9870</b>	<b>0.9827</b>	<b>0.9999</b>	<b>0.9935</b>	<b>0.9807</b>	<b>0.9912</b>	<b>0.9982</b>	<b>0.9994</b>	<b>0.9996</b>	<b>0.9993</b>	<b>0.9998</b>	<b>0.9994</b>	<b>0.9997</b>	<b>0.9791</b>	<b>0.9984</b>	<b>0.9994</b>	<b>0.9925</b>	<b>0.9857</b>	<b>0.9851</b>	<b>0.9846</b>

**Table S6e.** SIFT-MS linearity data for Mix 1 in 75% DMI:25% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0425	0.0149	0.00056	0.00295	0.00142	0.0074	0.013	0.0216	0.34	0.106	0.0142	0.0176	0.357	0.0141	0.102	0.00106	0.0153	0.0905	0.0586	0.0043	0.00363	0.00044	0.00098
20	0.131	0.0726	0.00104	0.00292	0.00173	0.0253	0.0127	0.0266	0.283	0.111	0.0414	0.0529	0.41	0.0356	0.144	0.0306	0.0211	0.125	0.0807	0.00558	0.00536	0.00065	0.00131
50	0.253	0.155	0.00223	0.00478	0.00245	0.0585	0.0144	0.0237	0.294	0.124	0.0883	0.0998	0.552	0.0677	0.203	0.0757	0.0236	0.199	0.122	0.00711	0.00644	0.00131	0.00181
100	0.488	0.304	0.00482	0.00428	0.00443	0.111	0.0177	0.0332	0.377	0.136	0.17	0.184	0.748	0.126	0.303	0.162	0.0342	0.31	0.197	0.00925	0.00769	0.00194	0.00392
200	0.921	0.584	0.00834	0.00752	0.00717	0.221	0.0269	0.0426	0.283	0.141	0.343	0.33	1.1	0.238	0.523	0.341	0.0566	0.545	0.35	0.0125	0.0104	0.00637	0.00572
300	1.41	0.897	0.0122	0.0112	0.012	0.33	0.0373	0.0565	0.337	0.158	0.506	0.497	1.53	0.363	0.758	0.532	0.0804	0.787	0.497	0.0172	0.012	0.00707	0.00827
400	1.83	1.17	0.0267	0.0215	0.0318	0.447	0.0824	0.0879	0.451	0.318	0.659	0.643	1.81	0.478	1.01	0.701	0.161	1.01	0.668	0.0266	0.0197	0.0186	0.018
500	2.23	1.43	0.0407	0.029	0.0373	0.543	0.0931	0.108	0.536	0.361	0.783	0.797	2.19	0.597	1.18	0.83	0.216	1.26	0.819	0.0314	0.0241	0.023	0.0217
<b>R<sup>2</sup></b>	<b>0.9994</b>	<b>0.9995</b>	<b>0.9138</b>	<b>0.9196</b>	<b>0.9021</b>	<b>0.9997</b>	<b>0.9077</b>	<b>0.9573</b>	<b>0.6488</b>	<b>0.8483</b>	<b>0.9982</b>	<b>0.9998</b>	<b>0.9983</b>	<b>0.9998</b>	<b>0.9985</b>	<b>0.9980</b>	<b>0.9298</b>	<b>0.9998</b>	<b>0.9994</b>	<b>0.9791</b>	<b>0.9602</b>	<b>0.9234</b>	<b>0.9393</b>

**Table S6f.** SIFT-MS linearity data for Mix 1 in 100% DMI across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0473	0.0343	0.00008	0.00108	0.00057	0.00907	0.00909	0.152	1.38	1.11	0.0199	0.0542	0.445	0.00847	0.151	0.00091	0.025	0.0426	0.134	0.00095	0.00086	0.00118	0.00211
20	0.118	0.0729	0.0004	0.0013	0.00062	0.0182	0.00976	0.126	1.08	0.892	0.0421	0.0705	0.549	0.0219	0.168	0.0164	0.0247	0.071	0.132	0.00111	0.00111	0.00031	0.00126
50	0.216	0.132	0.00069	0.00131	0.0011	0.0266	0.00895	0.118	0.995	0.825	0.0695	0.0947	0.685	0.0375	0.197	0.0434	0.0253	0.115	0.149	0.0016	0.00070	0.00062	0.00218
100	0.397	0.246	0.002	0.00181	0.0018	0.0532	0.0102	0.111	0.912	0.902	0.13	0.15	0.9	0.0669	0.266	0.085	0.0279	0.195	0.207	0.00236	0.00182	0.00094	0.00223
200	0.761	0.441	0.00302	0.00241	0.00239	0.0994	0.0142	0.0973	0.823	0.797	0.246	0.251	1.32	0.135	0.388	0.167	0.0283	0.33	0.298	0.00317	0.00158	0.00153	0.00341
300	1.12	0.652	0.00481	0.0047	0.00404	0.148	0.0148	0.0826	0.605	0.633	0.35	0.354	1.73	0.202	0.518	0.25	0.0342	0.496	0.376	0.00366	0.0027	0.00333	0.00318
400	1.49	0.849	0.00693	0.00577	0.00572	0.196	0.0171	0.0822	0.668	0.593	0.458	0.465	2.12	0.268	0.662	0.329	0.0438	0.663	0.485	0.00511	0.00392	0.00405	0.00489
500	1.88	1.08	0.00824	0.00703	0.00716	0.244	0.0231	0.0738	0.649	0.492	0.576	0.573	2.52	0.344	0.823	0.417	0.0575	0.863	0.597	0.00613	0.00517	0.00727	0.0069
<b>R<sup>2</sup></b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9948</b>	<b>0.9744</b>	<b>0.9870</b>	<b>0.9995</b>	<b>0.9397</b>	<b>0.8459</b>	<b>0.7414</b>	<b>0.8715</b>	<b>0.9997</b>	<b>0.9994</b>	<b>0.9995</b>	<b>0.9990</b>	<b>0.9970</b>	<b>0.9999</b>	<b>0.8844</b>	<b>0.9969</b>	<b>0.9947</b>	<b>0.9877</b>	<b>0.9312</b>	<b>0.8865</b>	<b>0.8927</b>

**Table S7a.** SIFT-MS linearity data for Mix 2 in 10% DMI:90% water across the low concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.00751	0.0256	0.01680	0.0129	0.013	0.00424	0.0184	0.0271	0.854	0.0443	0.00612	0.00459	0.028	0.00266	0.047	0.00046	0.0234	0.039	0.0226	0.01950	0.01660	0.00802	0.00835
1	0.0114	0.034	0.157	0.107	0.16400	0.00763	0.115	0.117	0.845	0.129	0.00846	0.00821	0.0343	0.00805	0.06	0.00459	0.0846	0.0521	0.0319	0.154	0.132	0.14400	0.145
2	0.0184	0.0397	0.29200	0.208	0.305	0.00951	0.215	0.21	0.97	0.214	0.0139	0.011	0.0353	0.013	0.0658	0.00877	0.165	0.0593	0.0382	0.293	0.25800	0.27400	0.273
3	0.0237	0.0428	0.447	0.293	0.46	0.0133	0.323	0.309	1.06	0.32	0.0163	0.0125	0.0381	0.0188	0.0728	0.0135	0.263	0.0729	0.0474	0.445	0.384	0.43600	0.41
5	0.0358	0.0493	0.768	0.534	0.821	0.0177	0.568	0.525	1.19	0.545	0.024	0.0187	0.0413	0.0299	0.0952	0.0214	0.481	0.0912	0.0585	0.791	0.673	0.78	0.782
10	0.0678	0.0721	1.58	1.12	1.66	0.029	1.13	1.04	1.59	1.02	0.0423	0.0339	0.0507	0.0596	0.144	0.0432	0.906	0.15	0.0955	1.59	1.38	1.53	1.54
15	0.0962	0.0935	2.34	1.62	2.57	0.0477	1.7	1.56	2.35	1.78	0.061	0.0465	0.0562	0.0885	0.203	0.0635	1.58	0.197	0.146	2.41	2.09	2.4	2.33
20	0.132	0.118	3.08	2.19	3.25	0.0612	2.2	2.04	2.61	2.16	0.0764	0.0597	0.0654	0.12	0.255	0.0899	1.95	0.257	0.184	3.15	2.72	3.14	3.01
<i>R</i> <sup>2</sup>	<b>0.9989</b>	<b>0.9971</b>	<b>0.9997</b>	<b>0.9994</b>	<b>0.9987</b>	<b>0.9952</b>	<b>0.9995</b>	<b>0.9998</b>	<b>0.9836</b>	<b>0.9940</b>	<b>0.9989</b>	<b>0.9989</b>	<b>0.9800</b>	<b>0.9996</b>	<b>0.9982</b>	<b>0.9985</b>	<b>0.9950</b>	<b>0.9991</b>	<b>0.9967</b>	<b>0.9997</b>	<b>0.9996</b>	<b>0.9995</b>	<b>0.9992</b>

**Table S7b.** SIFT-MS linearity data for Mix 2 in 100% DMI across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0518	0.0442	0.00207	0.00033	0.00306	0.00632	0.012	0.134	1.41	0.964	0.0282	0.0341	0.462	0.0113	0.137	0.00022	0.0232	0.0422	0.11	0.00115	0.00080	0.00091	0.00072
20	0.111	0.0813	0.024	0.0143	0.02080	0.0123	0.0184	0.137	1.34	0.885	0.0477	0.0552	0.51	0.0363	0.194	0.0164	0.0457	0.11	0.15	0.0128	0.00916	0.00921	0.0112
50	0.232	0.143	0.06470	0.0294	0.0625	0.0195	0.029	0.122	1.19	0.776	0.0806	0.0885	0.605	0.0803	0.283	0.0435	0.0867	0.227	0.22	0.0297	0.02420	0.02170	0.0227
100	0.412	0.245	0.0934	0.059	0.0969	0.0372	0.0427	0.112	0.917	0.663	0.129	0.144	0.726	0.148	0.428	0.0863	0.141	0.402	0.324	0.0484	0.0371	0.03730	0.0375
200	0.769	0.447	0.207	0.127	0.212	0.0654	0.0857	0.149	1.06	0.787	0.25	0.242	0.927	0.29	0.738	0.175	0.264	0.755	0.573	0.0977	0.0909	0.0874	0.0863
300	1.16	0.648	0.337	0.209	0.337	0.0989	0.126	0.17	0.838	0.728	0.372	0.349	1.09	0.431	1.04	0.255	0.435	1.16	0.814	0.167	0.136	0.14	0.14
400	1.53	0.836	0.436	0.278	0.477	0.131	0.167	0.195	0.862	0.7	0.473	0.456	1.28	0.589	1.35	0.339	0.582	1.53	1.07	0.229	0.202	0.19	0.176
500	1.91	1.04	0.596	0.384	0.63	0.167	0.22	0.248	0.892	0.734	0.577	0.569	1.48	0.75	1.64	0.422	0.785	1.96	1.35	0.311	0.264	0.251	0.246
<b>R<sup>2</sup></b>	<b>0.9999</b>	<b>0.9999</b>	<b>0.9943</b>	<b>0.9932</b>	<b>0.9939</b>	<b>0.9989</b>	<b>0.9958</b>	<b>0.8495</b>	<b>0.6504</b>	<b>0.3596</b>	<b>0.9992</b>	<b>0.9997</b>	<b>0.9957</b>	<b>0.9991</b>	<b>0.9999</b>	<b>0.9998</b>	<b>0.9926</b>	<b>0.9992</b>	<b>0.9988</b>	<b>0.9912</b>	<b>0.9923</b>	<b>0.9959</b>	<b>0.9933</b>

**Table S8a.** SIFT-MS linearity data for Mix 1 in 5% DMSO:95% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0138	0.130	1.19	0.173	0.914	0.00433	0.0378	0.0336	0.187	0.00526	0.0188	0.0151	0.00937	0.00088	0.0062	0.00028	0.00384	0.00744	0.0153	0.00201	0.0016	0.00457	0.00266
20	0.145	0.192	1.14	0.168	0.880	0.135	0.126	0.105	0.224	0.0436	0.0767	0.0755	0.0848	0.0729	0.123	0.111	0.0469	0.0831	0.0635	0.0366	0.0306	0.0368	0.0354
50	0.357	0.345	1.31	0.237	1.01	0.345	0.247	0.236	0.287	0.102	0.178	0.183	0.213	0.186	0.294	0.264	0.107	0.209	0.147	0.0896	0.0777	0.0802	0.0846
100	0.701	0.586	1.37	0.288	1.10	0.686	0.462	0.422	0.405	0.199	0.359	0.349	0.408	0.364	0.630	0.537	0.226	0.412	0.263	0.186	0.151	0.153	0.166
200	1.37	1.11	1.63	0.497	1.40	1.31	1.34	1.25	0.836	0.693	0.670	0.661	0.766	0.717	1.23	1.06	0.678	0.834	0.549	0.569	0.482	0.545	0.522
300	2.09	1.61	2.29	0.766	1.96	2.03	2.04	1.86	1.27	1.02	1.03	1.01	1.17	1.10	1.90	1.64	1.03	1.26	0.862	0.862	0.717	0.818	0.789
400	2.82	2.15	2.63	0.964	2.39	2.71	2.72	2.48	1.63	1.43	1.39	1.38	1.61	1.48	2.53	2.18	1.42	1.68	1.15	1.12	0.980	1.15	1.11
500	3.39	2.66	2.73	1.23	2.61	3.27	3.50	3.26	1.90	1.75	1.63	1.65	1.95	1.76	3.16	2.63	1.82	2.12	1.39	1.37	1.23	1.40	1.36
<i>R</i> <sup>2</sup>	<b>0.9994</b>	<b>0.9996</b>	<b>0.9685</b>	<b>0.9917</b>	<b>0.9840</b>	<b>0.9993</b>	<b>0.9960</b>	<b>0.9954</b>	<b>0.9940</b>	<b>0.9943</b>	<b>0.9982</b>	<b>0.9991</b>	<b>0.9993</b>	<b>0.9989</b>	<b>0.9999</b>	<b>0.9993</b>	<b>0.9959</b>	<b>0.9999</b>	<b>0.9990</b>	<b>0.9953</b>	<b>0.9959</b>	<b>0.9937</b>	<b>0.9954</b>

**Table S8b.** SIFT-MS linearity data for Mix 1 in 10% DMSO:90% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0138	0.0366	1.39	0.193	0.991	0.00484	0.0592	0.0462	0.339	0.00795	0.0078	0.00455	0.00698	0.00187	0.00683	0.00128	0.0077	0.00494	0.0261	0.00298	0.00316	0.00509	0.00471
20	0.150	0.141	1.36	0.215	1.02	0.129	0.140	0.119	0.358	0.0468	0.0768	0.0725	0.0892	0.0735	0.131	0.107	0.0525	0.0828	0.0762	0.0331	0.0289	0.0381	0.0359
50	0.363	0.295	1.29	0.228	0.988	0.324	0.247	0.227	0.421	0.106	0.173	0.170	0.209	0.175	0.305	0.265	0.117	0.203	0.142	0.0811	0.0661	0.0823	0.0763
100	0.703	0.540	1.60	0.312	1.23	0.633	0.417	0.391	0.563	0.213	0.341	0.348	0.421	0.347	0.592	0.520	0.227	0.407	0.275	0.166	0.131	0.150	0.147
200	1.39	1.04	2.00	0.514	1.66	1.22	1.20	1.08	1.00	0.668	0.652	0.649	0.807	0.694	1.20	1.02	0.661	0.802	0.551	0.460	0.395	0.475	0.467
300	2.17	1.59	2.43	0.747	2.02	1.89	1.82	1.67	1.35	1.02	1.02	0.987	1.19	1.04	1.84	1.60	1.03	1.24	0.826	0.732	0.631	0.744	0.725
400	2.80	2.11	2.56	0.882	2.22	2.48	2.46	2.23	1.88	1.44	1.32	1.31	1.58	1.43	2.45	2.09	1.43	1.64	1.11	0.987	0.851	1.02	1.01
500	3.41	2.55	2.72	1.07	2.46	3.00	2.93	2.70	2.23	1.79	1.58	1.60	1.90	1.72	3.02	2.58	1.76	2.00	1.38	1.19	1.06	1.27	1.26
<b>R<sup>2</sup></b>	<b>0.9991</b>	<b>0.9995</b>	<b>0.9593</b>	<b>0.9943</b>	<b>0.9829</b>	<b>0.9992</b>	<b>0.9948</b>	<b>0.9960</b>	<b>0.9929</b>	<b>0.9950</b>	<b>0.9985</b>	<b>0.9996</b>	<b>0.9991</b>	<b>0.9994</b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9960</b>	<b>0.9996</b>	<b>0.9997</b>	<b>0.9963</b>	<b>0.9958</b>	<b>0.9951</b>	<b>0.9949</b>



**Table S8c.** SIFT-MS linearity data for Mix 1 in 25% DMSO:75% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0226	0.0171	2.71	0.387	2.01	0.00509	0.125	0.0948	0.785	0.0102	0.0089	0.00482	0.00819	0.00235	0.0127	0.00174	0.00959	0.00556	0.0615	0.00441	0.00438	0.00689	0.00613
20	0.167	0.121	2.75	0.394	2.01	0.109	0.184	0.149	0.798	0.0863	0.0744	0.0675	0.098	0.0671	0.128	0.102	0.0849	0.0805	0.108	0.0282	0.0247	0.0307	0.0343
50	0.400	0.275	2.48	0.385	1.85	0.262	0.273	0.237	0.855	0.202	0.174	0.170	0.222	0.170	0.299	0.254	0.208	0.204	0.176	0.0654	0.0541	0.0767	0.0698
100	0.748	0.540	7.63	1.42	6.93	0.534	0.421	0.382	1.01	0.376	0.336	0.327	0.446	0.323	0.574	0.510	0.387	0.402	0.308	0.119	0.099	0.140	0.128
200	1.49	1.05	4.76	0.828	3.59	1.03	0.87	0.800	1.73	0.903	0.672	0.656	0.889	0.659	1.13	0.968	0.884	0.785	0.573	0.287	0.238	0.330	0.309
300	2.27	1.71	2.72	0.650	2.21	1.52	1.21	1.10	1.94	1.16	1.01	1.01	1.32	1.02	1.75	1.48	1.11	1.22	0.858	0.425	0.344	0.459	0.456
400	2.80	1.96	3.90	0.906	3.04	1.91	1.60	1.45	2.38	1.84	1.21	1.22	1.63	1.25	2.21	1.87	1.65	1.52	1.07	0.571	0.484	0.690	0.644
500	3.56	2.54	3.75	1.04	3.07	2.43	2.08	1.93	2.78	2.30	1.56	1.56	2.14	1.61	2.78	2.29	2.20	1.96	1.33	0.721	0.614	0.844	0.816
<b>R<sup>2</sup></b>	<b>0.9985</b>	<b>0.9943</b>	<b>0.0028</b>	<b>0.2291</b>	<b>0.0024</b>	<b>0.9987</b>	<b>0.9971</b>	<b>0.9961</b>	<b>0.9865</b>	<b>0.9919</b>	<b>0.9969</b>	<b>0.9975</b>	<b>0.9981</b>	<b>0.9983</b>	<b>0.9993</b>	<b>0.9984</b>	<b>0.9920</b>	<b>0.9989</b>	<b>0.9991</b>	<b>0.9989</b>	<b>0.9978</b>	<b>0.9960</b>	<b>0.9974</b>

**Table S9.** SIFT-MS linearity data for Mix 1 in 5% methanol:95% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV. Note that acetonitrile and nitromethane are measured using different product ions compared to other diluent solvents, and that trichloroethylene was not measurable in methanol.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (NO <sup>+</sup> 71)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	1-Butanol (NO <sup>+</sup> 73)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Nitromethane (NO <sup>+</sup> 91)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)
0	0.0185	0.201	0.0259	0.00379	0.0356	0.00201	0.00486	0.0271	0.0195	0.00802	0.0161	0.00681
20	0.165	1.64	0.0726	0.0489	0.0871	0.114	0.0608	0.0952	0.163	0.114	0.131	0.0639
50	0.395	3.86	0.139	0.106	0.164	0.278	0.143	0.199	0.361	0.263	0.309	0.144
100	0.77	7.26	0.269	0.206	0.293	0.577	0.281	0.362	0.725	0.54	0.58	0.283
200	1.48	14.3	0.556	0.438	0.552	1.2	0.547	0.689	1.43	1.1	1.14	0.599
300	2.18	21.1	0.805	0.642	0.784	1.78	0.805	1.02	2.09	1.63	1.69	0.886
400	2.94	27.8	1.09	0.881	1.05	2.43	1.07	1.33	2.76	2.24	2.22	1.18
500	3.55	35	1.41	1.1	1.33	3.06	1.35	1.68	3.31	2.8	2.8	1.52
<b>R<sup>2</sup></b>	<b>0.9995</b>	<b>0.9999</b>	<b>0.9987</b>	<b>0.9996</b>	<b>0.9996</b>	<b>0.9997</b>	<b>0.9999</b>	<b>0.9999</b>	<b>0.9988</b>	<b>0.9997</b>	<b>0.9999</b>	<b>0.9994</b>

**Table S10.** SIFT-MS linearity data for Mix 1 in 5% triacetin:95% water across the high concentration range. SIFT-MS response is the headspace concentration in ppmV.

Concentration Level	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
0	0.0101	0.00913	0.0417	0.00816	0.0312	0.0116	0.0434	0.0399	0.321	0.00782	0.00532	0.00198	0.00996	0.00099	0.0076	0.0013	0.0029	0.00266	0.0189	0.00342	0.0051	0.0122	0.00371
20	0.139	0.12	0.0791	0.0326	0.0698	0.113	0.16	0.149	0.376	0.106	0.0808	0.057	0.0996	0.0632	0.104	0.101	0.0934	0.102	0.0814	0.0499	0.0448	0.0679	0.0528
50	0.301	0.275	0.143	0.0759	0.13	0.255	0.336	0.312	0.6	0.253	0.186	0.141	0.217	0.15	0.261	0.255	0.233	0.245	0.171	0.119	0.1	0.132	0.122
100	0.619	0.547	0.257	0.157	0.249	0.496	0.621	0.565	0.867	0.526	0.365	0.284	0.431	0.296	0.507	0.511	0.452	0.483	0.343	0.24	0.202	0.271	0.243
200	1.3	1.14	0.535	0.34	0.566	0.996	1.33	1.19	1.39	1.08	0.754	0.598	0.928	0.636	1.03	1.02	0.955	1.03	0.694	0.519	0.451	0.576	0.54
300	1.77	1.59	0.758	0.478	0.802	1.43	1.93	1.73	2.17	1.62	1.05	0.822	1.27	0.871	1.48	1.46	1.44	1.42	0.951	0.75	0.648	0.851	0.813
400	2.44	2.21	1.09	0.68	1.13	1.92	2.61	2.41	2.71	2.2	1.48	1.15	1.72	1.21	2.04	2.03	1.97	1.98	1.37	1.05	0.923	1.17	1.11
500	3.06	2.71	1.38	0.887	1.47	2.4	3.24	2.99	3.52	2.85	1.79	1.42	2.15	1.5	2.51	2.46	2.53	2.43	1.69	1.31	1.16	1.5	1.44
<b>R<sup>2</sup></b>	<b>0.9989</b>	<b>0.9992</b>	<b>0.9966</b>	<b>0.9968</b>	<b>0.9963</b>	<b>0.9998</b>	<b>0.9996</b>	<b>0.9992</b>	<b>0.9961</b>	<b>0.9989</b>	<b>0.9989</b>	<b>0.9990</b>	<b>0.9990</b>	<b>0.9990</b>	<b>0.9997</b>	<b>0.9993</b>	<b>0.9990</b>	<b>0.9990</b>	<b>0.9983</b>	<b>0.9992</b>	<b>0.9983</b>	<b>0.9987</b>	<b>0.9984</b>

## C. Repeatability

**Table S11.** SIFT-MS repeatability data for Mix 1 in water at three levels (50, 250, and 500). The replicate shown in red is an outlier and was not included in the calculation.

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.488	0.415	0.186	0.130	0.191	0.383	0.496	0.454	0.317	0.290	0.246	0.221	0.334	0.238	0.363	0.304	0.266	0.388	0.248	0.205	0.175	0.208	0.196
50–2	0.331	0.294	0.159	0.109	0.161	0.284	0.421	0.373	0.324	0.295	0.202	0.160	0.217	0.166	0.263	0.286	0.270	0.279	0.184	0.178	0.144	0.180	0.173
50–3	0.342	0.297	0.152	0.102	0.157	0.290	0.407	0.376	0.309	0.292	0.195	0.168	0.236	0.168	0.265	0.279	0.259	0.288	0.181	0.177	0.146	0.181	0.179
50–4	0.360	0.311	0.169	0.110	0.172	0.305	0.430	0.389	0.281	0.298	0.211	0.165	0.247	0.170	0.286	0.284	0.277	0.296	0.193	0.184	0.152	0.188	0.182
50–5	0.337	0.295	0.153	0.109	0.160	0.292	0.426	0.382	0.303	0.301	0.193	0.162	0.222	0.164	0.272	0.293	0.267	0.280	0.178	0.183	0.152	0.178	0.174
50–6	0.342	0.301	0.159	0.116	0.170	0.304	0.417	0.377	0.308	0.304	0.203	0.169	0.235	0.168	0.275	0.294	0.272	0.285	0.183	0.187	0.153	0.186	0.178
Mean	0.342	0.299	0.159	0.110	0.164	0.295	0.420	0.379	0.305	0.298	0.201	0.164	0.231	0.167	0.273	0.287	0.269	0.285	0.184	0.182	0.149	0.182	0.177
SD	0.0097	0.0062	0.0061	0.0044	0.0059	0.0082	0.0079	0.0056	0.0139	0.0042	0.0064	0.0034	0.0107	0.0020	0.0082	0.0056	0.0060	0.0062	0.0050	0.0038	0.0037	0.0038	0.0033
%RSD	2.8	2.1	3.8	4.1	3.6	2.8	1.9	1.5	4.6	1.4	3.2	2.1	4.6	1.2	3.0	2.0	2.2	2.2	2.7	2.1	2.5	2.1	1.9
250–1	1.868	1.675	0.793	0.556	0.834	1.615	2.071	1.892	1.481	1.468	1.113	0.925	1.318	0.979	1.575	1.499	1.318	1.549	1.028	0.880	0.761	0.909	0.902
250–2	1.618	1.445	0.696	0.489	0.757	1.425	1.861	1.702	1.481	1.298	0.975	0.777	1.108	0.829	1.375	1.399	1.238	1.349	0.911	0.789	0.683	0.803	0.804
250–3	1.718	1.545	0.768	0.523	0.813	1.505	2.011	1.822	1.511	1.398	1.023	0.830	1.198	0.894	1.455	1.449	1.308	1.439	0.959	0.863	0.741	0.865	0.838
250–4	1.748	1.575	0.764	0.518	0.806	1.525	1.981	1.802	1.501	1.438	1.023	0.840	1.208	0.888	1.445	1.399	1.308	1.459	0.968	0.846	0.711	0.871	0.849
250–5	1.798	1.575	0.747	0.528	0.820	1.495	1.981	1.812	1.411	1.398	1.013	0.836	1.258	0.918	1.475	1.379	1.298	1.459	0.979	0.841	0.737	0.862	0.841
250–6	1.548	1.425	0.734	0.495	0.757	1.405	1.881	1.712	1.551	1.398	0.948	0.759	1.078	0.807	1.385	1.349	1.278	1.339	0.890	0.803	0.694	0.841	0.789
Mean	1.716	1.540	0.751	0.519	0.798	1.495	1.965	1.790	1.489	1.399	1.016	0.827	1.194	0.885	1.452	1.412	1.291	1.432	0.956	0.837	0.721	0.858	0.837
SD	0.107	0.085	0.030	0.022	0.030	0.069	0.073	0.066	0.042	0.052	0.051	0.053	0.082	0.057	0.066	0.049	0.027	0.072	0.045	0.032	0.027	0.032	0.036
%RSD	6.2	5.5	4.1	4.3	3.8	4.6	3.7	3.7	2.8	3.7	5.1	6.4	6.9	6.4	4.5	3.5	2.1	5.0	4.7	3.8	3.8	3.7	4.3
500–1	3.298	3.005	1.571	1.118	1.733	2.885	4.191	3.782	3.381	2.998	1.943	1.609	2.288	1.726	2.915	2.689	2.738	2.869	1.978	1.749	1.569	1.870	1.838
500–2	3.208	2.935	1.511	1.068	1.693	2.785	4.091	3.682	3.371	2.898	1.913	1.549	2.188	1.686	2.875	2.709	2.618	2.749	1.898	1.749	1.599	1.880	1.818
500–3	3.288	2.935	1.561	1.068	1.693	2.755	4.071	3.732	3.231	2.948	1.893	1.559	2.238	1.696	2.825	2.669	2.638	2.739	1.858	1.729	1.559	1.850	1.788
500–4	3.218	2.925	1.601	1.068	1.733	2.855	4.111	3.762	3.421	3.008	1.903	1.559	2.218	1.706	2.885	2.799	2.728	2.769	1.908	1.749	1.579	1.840	1.848
500–5	3.158	2.885	1.551	1.078	1.673	2.815	3.991	3.702	3.231	2.828	1.923	1.529	2.138	1.646	2.865	2.789	2.658	2.709	1.848	1.699	1.529	1.840	1.768
500–6	3.198	2.885	1.551	1.078	1.683	2.745	3.991	3.662	3.191	2.858	1.893	1.559	2.178	1.676	2.785	2.709	2.618	2.729	1.888	1.699	1.539	1.820	1.788
Mean	3.228	2.928	1.558	1.080	1.701	2.807	4.075	3.720	3.304	2.923	1.912	1.560	2.208	1.689	2.859	2.727	2.666	2.760	1.896	1.729	1.562	1.850	1.808
SD	0.050	0.040	0.027	0.018	0.023	0.051	0.070	0.043	0.089	0.068	0.018	0.024	0.048	0.025	0.042	0.049	0.049	0.052	0.042	0.022	0.024	0.020	0.029
%RSD	1.5	1.4	1.7	1.6	1.4	1.8	1.7	1.1	2.7	2.3	0.93	1.5	2.2	1.5	1.5	1.8	1.8	1.9	2.2	1.3	1.5	1.1	1.6

**Table S12a.** SIFT-MS repeatability data for Mix 1 in 5% DMAC:95% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.353	0.249	0.080	0.064	0.089	0.305	0.243	0.209	0.262	0.205	0.166	0.156	0.187	0.170	0.299	0.278	0.177	0.228	0.137	0.101	0.080	0.092	0.087
50–2	0.294	0.228	0.077	0.053	0.083	0.287	0.217	0.197	0.106	0.199	0.152	0.154	0.168	0.151	0.266	0.256	0.175	0.208	0.125	0.094	0.072	0.085	0.078
50–3	0.299	0.245	0.081	0.052	0.084	0.295	0.236	0.205	0.210	0.192	0.159	0.153	0.184	0.166	0.290	0.275	0.172	0.231	0.144	0.100	0.082	0.092	0.087
50–4	0.319	0.251	0.079	0.051	0.083	0.301	0.242	0.212	0.164	0.183	0.173	0.162	0.186	0.164	0.291	0.289	0.166	0.224	0.152	0.091	0.083	0.085	0.087
50–5	0.326	0.235	0.081	0.055	0.080	0.290	0.231	0.207	0.081	0.190	0.155	0.152	0.164	0.155	0.263	0.271	0.169	0.217	0.137	0.092	0.076	0.086	0.078
50–6	0.310	0.229	0.074	0.054	0.078	0.292	0.206	0.198	0.159	0.193	0.157	0.151	0.169	0.156	0.276	0.265	0.162	0.205	0.132	0.090	0.078	0.084	0.082
<b>Mean</b>	<b>0.317</b>	<b>0.239</b>	<b>0.079</b>	<b>0.055</b>	<b>0.083</b>	<b>0.295</b>	<b>0.229</b>	<b>0.205</b>	<b>0.164</b>	<b>0.193</b>	<b>0.160</b>	<b>0.155</b>	<b>0.177</b>	<b>0.160</b>	<b>0.280</b>	<b>0.272</b>	<b>0.170</b>	<b>0.219</b>	<b>0.138</b>	<b>0.095</b>	<b>0.079</b>	<b>0.087</b>	<b>0.083</b>
<b>SD</b>	<b>0.0195</b>	<b>0.0093</b>	<b>0.0026</b>	<b>0.0041</b>	<b>0.0036</b>	<b>0.0062</b>	<b>0.0135</b>	<b>0.0055</b>	<b>0.0605</b>	<b>0.0069</b>	<b>0.0071</b>	<b>0.0036</b>	<b>0.0095</b>	<b>0.0067</b>	<b>0.0134</b>	<b>0.0103</b>	<b>0.0051</b>	<b>0.0098</b>	<b>0.0086</b>	<b>0.0045</b>	<b>0.0038</b>	<b>0.0033</b>	<b>0.0041</b>
<b>%RSD</b>	<b>6.2</b>	<b>3.9</b>	<b>3.3</b>	<b>7.6</b>	<b>4.4</b>	<b>2.1</b>	<b>5.9</b>	<b>2.7</b>	<b>37.0</b>	<b>3.6</b>	<b>4.4</b>	<b>2.4</b>	<b>5.4</b>	<b>4.2</b>	<b>4.8</b>	<b>3.8</b>	<b>3.0</b>	<b>4.5</b>	<b>6.2</b>	<b>4.8</b>	<b>4.9</b>	<b>3.7</b>	<b>4.9</b>
250–1	1.366	1.113	0.543	0.358	0.570	1.363	1.497	1.397	1.369	1.415	0.729	0.701	0.814	0.734	1.338	1.230	1.248	1.024	0.687	0.612	0.523	0.623	0.615
250–2	1.386	1.103	0.540	0.350	0.581	1.323	1.477	1.387	1.449	1.455	0.717	0.697	0.812	0.725	1.298	1.230	1.248	1.034	0.683	0.626	0.539	0.627	0.614
250–3	1.576	1.263	0.573	0.384	0.626	1.533	1.607	1.487	1.279	1.395	0.847	0.829	0.907	0.829	1.528	1.430	1.208	1.174	0.802	0.682	0.570	0.653	0.635
250–4	1.546	1.183	0.551	0.359	0.597	1.433	1.547	1.397	1.399	1.425	0.782	0.753	0.873	0.782	1.388	1.270	1.268	1.094	0.724	0.636	0.543	0.633	0.629
250–5	1.376	1.123	0.548	0.393	0.598	1.373	1.547	1.407	1.419	1.495	0.737	0.712	0.821	0.732	1.328	1.280	1.248	1.044	0.685	0.629	0.542	0.634	0.617
250–6	1.456	1.183	0.566	0.371	0.600	1.403	1.517	1.457	1.389	1.435	0.775	0.768	0.856	0.785	1.388	1.300	1.258	1.084	0.743	0.653	0.560	0.654	0.625
<b>Mean</b>	<b>1.451</b>	<b>1.161</b>	<b>0.553</b>	<b>0.369</b>	<b>0.596</b>	<b>1.405</b>	<b>1.532</b>	<b>1.422</b>	<b>1.384</b>	<b>1.436</b>	<b>0.764</b>	<b>0.743</b>	<b>0.847</b>	<b>0.765</b>	<b>1.378</b>	<b>1.290</b>	<b>1.246</b>	<b>1.075</b>	<b>0.721</b>	<b>0.640</b>	<b>0.547</b>	<b>0.638</b>	<b>0.622</b>
<b>SD</b>	<b>0.083</b>	<b>0.056</b>	<b>0.012</b>	<b>0.015</b>	<b>0.017</b>	<b>0.067</b>	<b>0.042</b>	<b>0.037</b>	<b>0.053</b>	<b>0.032</b>	<b>0.044</b>	<b>0.046</b>	<b>0.035</b>	<b>0.037</b>	<b>0.074</b>	<b>0.068</b>	<b>0.019</b>	<b>0.051</b>	<b>0.043</b>	<b>0.023</b>	<b>0.015</b>	<b>0.012</b>	<b>0.008</b>
<b>%RSD</b>	<b>5.7</b>	<b>4.8</b>	<b>2.2</b>	<b>4.1</b>	<b>2.9</b>	<b>4.7</b>	<b>2.7</b>	<b>2.6</b>	<b>3.8</b>	<b>2.2</b>	<b>5.7</b>	<b>6.3</b>	<b>4.1</b>	<b>4.9</b>	<b>5.4</b>	<b>5.2</b>	<b>1.5</b>	<b>4.7</b>	<b>5.9</b>	<b>3.5</b>	<b>2.8</b>	<b>1.9</b>	<b>1.3</b>
500–1	2.746	2.233	1.159	0.804	1.278	2.623	3.227	2.987	2.909	3.215	1.416	1.428	1.634	1.499	2.598	2.380	2.788	2.074	1.404	1.299	1.189	1.379	1.309
500–2	2.766	2.233	1.169	0.781	1.278	2.573	3.267	2.997	3.179	3.285	1.426	1.418	1.614	1.489	2.598	2.420	2.828	2.054	1.424	1.329	1.209	1.369	1.359
500–3	2.626	2.193	1.159	0.756	1.278	2.593	3.117	2.937	3.329	3.255	1.426	1.368	1.554	1.439	2.628	2.400	2.808	2.014	1.384	1.329	1.159	1.389	1.299
500–4	2.876	2.383	1.219	0.822	1.328	2.793	3.407	3.117	3.289	3.235	1.526	1.488	1.694	1.549	2.778	2.610	2.758	2.184	1.484	1.349	1.229	1.419	1.399
500–5	2.836	2.363	1.209	0.781	1.318	2.813	3.327	3.027	3.169	3.155	1.546	1.468	1.674	1.569	2.838	2.660	2.748	2.184	1.514	1.359	1.209	1.379	1.339
500–6	2.846	2.313	1.169	0.781	1.278	2.633	3.197	3.047	3.309	3.185	1.476	1.438	1.664	1.529	2.698	2.500	2.738	2.084	1.484	1.359	1.209	1.379	1.379
<b>Mean</b>	<b>2.783</b>	<b>2.286</b>	<b>1.180</b>	<b>0.788</b>	<b>1.293</b>	<b>2.672</b>	<b>3.257</b>	<b>3.019</b>	<b>3.197</b>	<b>3.221</b>	<b>1.469</b>	<b>1.435</b>	<b>1.639</b>	<b>1.512</b>	<b>2.689</b>	<b>2.495</b>	<b>2.778</b>	<b>2.099</b>	<b>1.449</b>	<b>1.338</b>	<b>1.201</b>	<b>1.386</b>	<b>1.347</b>
<b>SD</b>	<b>0.083</b>	<b>0.071</b>	<b>0.024</b>	<b>0.021</b>	<b>0.021</b>	<b>0.095</b>	<b>0.093</b>	<b>0.056</b>	<b>0.143</b>	<b>0.043</b>	<b>0.051</b>	<b>0.038</b>	<b>0.046</b>	<b>0.043</b>	<b>0.092</b>	<b>0.107</b>	<b>0.033</b>	<b>0.064</b>	<b>0.048</b>	<b>0.021</b>	<b>0.022</b>	<b>0.016</b>	<b>0.036</b>
<b>%RSD</b>	<b>3.0</b>	<b>3.1</b>	<b>2.0</b>	<b>2.6</b>	<b>1.7</b>	<b>3.6</b>	<b>2.8</b>	<b>1.8</b>	<b>4.5</b>	<b>1.3</b>	<b>3.5</b>	<b>2.7</b>	<b>2.8</b>	<b>2.8</b>	<b>3.4</b>	<b>4.3</b>	<b>1.2</b>	<b>3.0</b>	<b>3.3</b>	<b>1.6</b>	<b>1.8</b>	<b>1.2</b>	<b>2.7</b>

**Table S12b.** SIFT-MS repeatability data for Mix 1 in 10% DMAC:90% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.265	0.260	0.072	0.048	0.077	0.278	0.197	0.189	0.190	0.205	0.164	0.157	0.194	0.166	0.285	0.297	0.182	0.225	0.143	0.082	0.064	0.078	0.067
50–2	0.241	0.218	0.060	0.048	0.071	0.248	0.188	0.181	0.110	0.213	0.144	0.138	0.165	0.144	0.231	0.254	0.191	0.191	0.126	0.074	0.058	0.075	0.068
50–3	0.276	0.222	0.067	0.050	0.067	0.243	0.193	0.186	0.120	0.213	0.143	0.133	0.171	0.139	0.240	0.252	0.192	0.196	0.124	0.072	0.057	0.069	0.069
50–4	0.232	0.213	0.066	0.047	0.066	0.246	0.193	0.173	0.130	0.204	0.142	0.142	0.161	0.139	0.233	0.259	0.185	0.197	0.130	0.076	0.058	0.072	0.065
50–5	0.285	0.227	0.063	0.043	0.072	0.261	0.197	0.182	0.130	0.209	0.143	0.146	0.172	0.147	0.242	0.261	0.184	0.210	0.129	0.077	0.061	0.066	0.071
50–6	0.298	0.258	0.070	0.044	0.073	0.288	0.202	0.190	0.040	0.206	0.169	0.161	0.201	0.161	0.282	0.286	0.182	0.229	0.148	0.079	0.070	0.080	0.073
<b>Mean</b>	<b>0.266</b>	<b>0.233</b>	<b>0.066</b>	<b>0.047</b>	<b>0.071</b>	<b>0.261</b>	<b>0.195</b>	<b>0.184</b>	<b>0.120</b>	<b>0.208</b>	<b>0.151</b>	<b>0.146</b>	<b>0.178</b>	<b>0.149</b>	<b>0.252</b>	<b>0.268</b>	<b>0.186</b>	<b>0.208</b>	<b>0.134</b>	<b>0.077</b>	<b>0.061</b>	<b>0.073</b>	<b>0.069</b>
<b>SD</b>	<b>0.0233</b>	<b>0.0189</b>	<b>0.0038</b>	<b>0.0027</b>	<b>0.0038</b>	<b>0.0170</b>	<b>0.0044</b>	<b>0.0057</b>	<b>0.0440</b>	<b>0.0036</b>	<b>0.0112</b>	<b>0.0100</b>	<b>0.0149</b>	<b>0.0105</b>	<b>0.0225</b>	<b>0.0171</b>	<b>0.0040</b>	<b>0.0147</b>	<b>0.0089</b>	<b>0.0030</b>	<b>0.0045</b>	<b>0.0050</b>	<b>0.0027</b>
<b>%RSD</b>	<b>8.8</b>	<b>8.1</b>	<b>5.8</b>	<b>5.7</b>	<b>5.4</b>	<b>6.5</b>	<b>2.2</b>	<b>3.1</b>	<b>36.6</b>	<b>1.7</b>	<b>7.4</b>	<b>6.8</b>	<b>8.4</b>	<b>7.0</b>	<b>8.9</b>	<b>6.4</b>	<b>2.2</b>	<b>7.1</b>	<b>6.7</b>	<b>3.9</b>	<b>7.3</b>	<b>6.8</b>	<b>3.8</b>
250–1	1.253	1.092	0.446	0.301	0.459	1.184	1.328	1.170	1.360	1.524	0.693	0.651	0.803	0.660	1.193	1.208	1.336	0.967	0.629	0.481	0.426	0.544	0.527
250–2	1.333	1.202	0.456	0.330	0.521	1.274	1.428	1.290	1.430	1.564	0.755	0.749	0.904	0.748	1.343	1.318	1.346	1.042	0.700	0.537	0.470	0.535	0.572
250–3	1.273	1.082	0.440	0.318	0.471	1.184	1.248	1.220	1.500	1.524	0.687	0.661	0.831	0.672	1.153	1.188	1.326	0.929	0.625	0.483	0.409	0.509	0.513
250–4	1.633	1.392	0.496	0.318	0.510	1.464	1.418	1.330	0.740	1.024	0.882	0.858	0.952	0.848	1.463	1.468	0.910	1.182	0.760	0.536	0.469	0.574	0.519
250–5	1.293	1.122	0.440	0.304	0.465	1.224	1.288	1.170	1.540	1.464	0.740	0.689	0.828	0.700	1.213	1.248	1.276	0.977	0.647	0.487	0.422	0.517	0.488
250–6	1.313	1.102	0.438	0.281	0.472	1.204	1.278	1.150	1.280	1.514	0.704	0.679	0.798	0.681	1.203	1.268	1.316	0.951	0.650	0.476	0.413	0.511	0.507
<b>Mean</b>	<b>1.350</b>	<b>1.165</b>	<b>0.452</b>	<b>0.308</b>	<b>0.483</b>	<b>1.256</b>	<b>1.331</b>	<b>1.222</b>	<b>1.308</b>	<b>1.436</b>	<b>0.744</b>	<b>0.715</b>	<b>0.853</b>	<b>0.718</b>	<b>1.261</b>	<b>1.283</b>	<b>1.251</b>	<b>1.008</b>	<b>0.669</b>	<b>0.500</b>	<b>0.435</b>	<b>0.532</b>	<b>0.521</b>
<b>SD</b>	<b>0.129</b>	<b>0.109</b>	<b>0.020</b>	<b>0.016</b>	<b>0.024</b>	<b>0.098</b>	<b>0.069</b>	<b>0.067</b>	<b>0.268</b>	<b>0.186</b>	<b>0.067</b>	<b>0.071</b>	<b>0.056</b>	<b>0.065</b>	<b>0.108</b>	<b>0.093</b>	<b>0.154</b>	<b>0.085</b>	<b>0.048</b>	<b>0.026</b>	<b>0.025</b>	<b>0.023</b>	<b>0.026</b>
<b>%RSD</b>	<b>9.6</b>	<b>9.3</b>	<b>4.5</b>	<b>5.1</b>	<b>4.9</b>	<b>7.8</b>	<b>5.2</b>	<b>5.5</b>	<b>20.5</b>	<b>13.0</b>	<b>9.0</b>	<b>10.0</b>	<b>6.6</b>	<b>9.0</b>	<b>8.5</b>	<b>7.2</b>	<b>12.3</b>	<b>8.5</b>	<b>7.1</b>	<b>5.2</b>	<b>5.8</b>	<b>4.3</b>	<b>5.0</b>
500–1	2.543	2.152	0.936	0.611	1.038	2.284	2.698	2.560	3.450	3.294	1.365	1.297	1.494	1.348	2.403	2.428	2.926	1.862	1.308	1.048	0.921	1.157	1.124
500–2	3.063	2.532	0.999	0.712	1.138	2.634	2.978	2.710	3.030	3.194	1.545	1.507	1.924	1.528	2.703	2.668	2.746	2.132	1.468	1.098	0.983	1.237	1.174
500–3	2.533	2.142	0.943	0.627	1.008	2.264	2.718	2.510	3.360	3.414	1.325	1.287	1.594	1.318	2.353	2.308	2.936	1.882	1.288	1.028	0.904	1.157	1.114
500–4	2.703	2.242	0.954	0.677	1.048	2.344	2.778	2.540	2.970	3.184	1.415	1.357	1.674	1.428	2.513	2.428	2.826	1.982	1.358	1.078	0.966	1.187	1.154
500–5	2.593	2.212	0.967	0.675	1.038	2.344	2.718	2.530	3.120	3.294	1.375	1.347	1.624	1.388	2.523	2.438	2.886	1.952	1.308	1.038	0.946	1.167	1.144
500–6	2.633	2.162	0.941	0.635	1.048	2.294	2.678	2.520	3.200	3.274	1.365	1.307	1.604	1.348	2.413	2.338	2.866	1.902	1.278	1.038	0.902	1.147	1.094
<b>Mean</b>	<b>2.678</b>	<b>2.240</b>	<b>0.956</b>	<b>0.656</b>	<b>1.053</b>	<b>2.361</b>	<b>2.761</b>	<b>2.562</b>	<b>3.188</b>	<b>3.276</b>	<b>1.398</b>	<b>1.350</b>	<b>1.653</b>	<b>1.393</b>	<b>2.484</b>	<b>2.434</b>	<b>2.864</b>	<b>1.952</b>	<b>1.335</b>	<b>1.054</b>	<b>0.937</b>	<b>1.176</b>	<b>1.134</b>
<b>SD</b>	<b>0.181</b>	<b>0.135</b>	<b>0.021</b>	<b>0.035</b>	<b>0.040</b>	<b>0.126</b>	<b>0.102</b>	<b>0.068</b>	<b>0.171</b>	<b>0.076</b>	<b>0.071</b>	<b>0.075</b>	<b>0.133</b>	<b>0.070</b>	<b>0.115</b>	<b>0.115</b>	<b>0.064</b>	<b>0.090</b>	<b>0.065</b>	<b>0.025</b>	<b>0.031</b>	<b>0.030</b>	<b>0.026</b>
<b>%RSD</b>	<b>6.8</b>	<b>6.0</b>	<b>2.2</b>	<b>5.3</b>	<b>3.8</b>	<b>5.3</b>	<b>3.7</b>	<b>2.7</b>	<b>5.4</b>	<b>2.3</b>	<b>5.1</b>	<b>5.5</b>	<b>8.0</b>	<b>5.0</b>	<b>4.6</b>	<b>4.7</b>	<b>2.2</b>	<b>4.6</b>	<b>4.8</b>	<b>2.4</b>	<b>3.3</b>	<b>2.6</b>	<b>2.3</b>

**Table S12c.** SIFT-MS repeatability data for Mix 1 in 25% DMAC:75% water at three levels (50, 250, and 500).

Level-Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50-1	0.259	0.210	0.030	0.021	0.031	0.185	0.086	0.074	-0.280	0.134	0.129	0.119	0.181	0.113	0.191	0.225	0.119	0.159	0.092	0.033	0.026	0.039	0.037
50-2	0.258	0.211	0.028	0.023	0.030	0.179	0.066	0.073	-0.050	0.140	0.129	0.123	0.183	0.115	0.182	0.222	0.122	0.151	0.081	0.033	0.025	0.037	0.038
50-3	0.285	0.200	0.033	0.020	0.029	0.180	0.087	0.074	-0.080	0.144	0.128	0.127	0.170	0.117	0.188	0.221	0.115	0.154	0.080	0.032	0.026	0.041	0.043
50-4	0.233	0.207	0.031	0.021	0.031	0.187	0.075	0.067	-0.050	0.139	0.120	0.122	0.174	0.115	0.187	0.234	0.117	0.158	0.076	0.029	0.025	0.035	0.034
50-5	0.288	0.214	0.032	0.024	0.034	0.189	0.076	0.067	-0.200	0.136	0.135	0.128	0.184	0.114	0.210	0.240	0.118	0.167	0.093	0.033	0.025	0.038	0.035
50-6	0.227	0.212	0.031	0.020	0.032	0.187	0.082	0.078	0.010	0.142	0.133	0.126	0.183	0.115	0.210	0.238	0.118	0.164	0.096	0.032	0.026	0.040	0.038
<b>Mean</b>	<b>0.258</b>	<b>0.209</b>	<b>0.031</b>	<b>0.021</b>	<b>0.031</b>	<b>0.184</b>	<b>0.079</b>	<b>0.072</b>	<b>-0.108</b>	<b>0.139</b>	<b>0.129</b>	<b>0.124</b>	<b>0.179</b>	<b>0.115</b>	<b>0.195</b>	<b>0.230</b>	<b>0.118</b>	<b>0.159</b>	<b>0.086</b>	<b>0.032</b>	<b>0.025</b>	<b>0.038</b>	<b>0.037</b>
<b>SD</b>	<b>0.0231</b>	<b>0.0045</b>	<b>0.0016</b>	<b>0.0016</b>	<b>0.0015</b>	<b>0.0037</b>	<b>0.0072</b>	<b>0.0040</b>	<b>0.0996</b>	<b>0.0034</b>	<b>0.0047</b>	<b>0.0031</b>	<b>0.0053</b>	<b>0.0012</b>	<b>0.0112</b>	<b>0.0076</b>	<b>0.0021</b>	<b>0.0055</b>	<b>0.0076</b>	<b>0.0015</b>	<b>0.0008</b>	<b>0.0020</b>	<b>0.0027</b>
<b>%RSD</b>	<b>9.0</b>	<b>2.2</b>	<b>5.1</b>	<b>7.6</b>	<b>4.7</b>	<b>2.0</b>	<b>9.2</b>	<b>5.5</b>	<b>-91.9</b>	<b>2.4</b>	<b>3.7</b>	<b>2.5</b>	<b>2.9</b>	<b>1.1</b>	<b>5.7</b>	<b>3.3</b>	<b>1.8</b>	<b>3.4</b>	<b>8.8</b>	<b>4.6</b>	<b>3.0</b>	<b>5.1</b>	<b>7.3</b>
250-1	1.216	1.043	0.229	0.151	0.250	0.868	0.745	0.661	0.810	1.228	0.617	0.602	0.839	0.580	1.000	1.130	1.061	0.787	0.518	0.233	0.194	0.299	0.282
250-2	1.216	1.033	0.239	0.164	0.245	0.869	0.725	0.649	1.170	1.218	0.618	0.611	0.860	0.566	0.990	1.130	1.041	0.797	0.499	0.233	0.197	0.297	0.282
250-3	1.296	1.093	0.247	0.158	0.264	0.914	0.775	0.732	1.290	1.258	0.645	0.636	0.884	0.592	1.030	1.160	1.061	0.828	0.549	0.235	0.206	0.294	0.301
250-4	1.306	1.053	0.228	0.151	0.250	0.871	0.735	0.722	0.920	1.188	0.623	0.609	0.872	0.570	0.990	1.110	1.011	0.799	0.499	0.239	0.199	0.285	0.273
250-5	1.266	1.043	0.236	0.150	0.250	0.898	0.715	0.632	0.990	1.198	0.630	0.620	0.866	0.570	1.000	1.120	1.011	0.780	0.509	0.240	0.195	0.300	0.288
250-6	1.256	1.023	0.234	0.151	0.237	0.861	0.688	0.614	0.870	1.128	0.626	0.600	0.852	0.554	0.950	1.110	0.978	0.787	0.492	0.223	0.190	0.289	0.268
<b>Mean</b>	<b>1.259</b>	<b>1.048</b>	<b>0.235</b>	<b>0.154</b>	<b>0.249</b>	<b>0.880</b>	<b>0.731</b>	<b>0.668</b>	<b>1.008</b>	<b>1.203</b>	<b>0.627</b>	<b>0.613</b>	<b>0.862</b>	<b>0.572</b>	<b>0.994</b>	<b>1.126</b>	<b>1.027</b>	<b>0.797</b>	<b>0.511</b>	<b>0.234</b>	<b>0.196</b>	<b>0.294</b>	<b>0.282</b>
<b>SD</b>	<b>0.035</b>	<b>0.022</b>	<b>0.006</b>	<b>0.005</b>	<b>0.008</b>	<b>0.019</b>	<b>0.027</b>	<b>0.044</b>	<b>0.169</b>	<b>0.040</b>	<b>0.009</b>	<b>0.012</b>	<b>0.014</b>	<b>0.012</b>	<b>0.024</b>	<b>0.017</b>	<b>0.030</b>	<b>0.016</b>	<b>0.019</b>	<b>0.006</b>	<b>0.005</b>	<b>0.005</b>	<b>0.011</b>
<b>%RSD</b>	<b>2.8</b>	<b>2.1</b>	<b>2.7</b>	<b>3.3</b>	<b>3.2</b>	<b>2.2</b>	<b>3.7</b>	<b>6.6</b>	<b>16.8</b>	<b>3.4</b>	<b>1.5</b>	<b>2.0</b>	<b>1.7</b>	<b>2.1</b>	<b>2.4</b>	<b>1.5</b>	<b>2.9</b>	<b>2.0</b>	<b>3.7</b>	<b>2.4</b>	<b>2.5</b>	<b>1.8</b>	<b>3.8</b>
500-1	2.416	2.043	0.493	0.335	0.549	1.674	1.545	1.452	2.680	2.738	1.215	1.168	1.685	1.107	1.920	2.150	2.321	1.564	1.042	0.497	0.443	0.640	0.641
500-2	2.416	2.023	0.501	0.351	0.547	1.654	1.545	1.432	2.420	2.628	1.205	1.198	1.655	1.087	1.940	2.120	2.231	1.564	1.052	0.505	0.435	0.631	0.620
500-3	2.416	2.033	0.502	0.346	0.528	1.674	1.545	1.442	2.560	2.608	1.205	1.208	1.685	1.077	1.950	2.160	2.281	1.564	1.022	0.502	0.435	0.635	0.610
500-4	2.346	2.023	0.507	0.337	0.546	1.704	1.575	1.452	2.640	2.608	1.225	1.158	1.645	1.077	2.010	2.230	2.251	1.544	1.032	0.491	0.428	0.624	0.613
500-5	2.176	1.993	0.495	0.317	0.535	1.704	1.555	1.472	2.550	2.568	1.245	1.158	1.615	1.077	1.980	2.230	2.221	1.534	1.052	0.479	0.411	0.630	0.599
500-6	2.446	2.113	0.502	0.325	0.546	1.744	1.565	1.502	2.700	2.578	1.245	1.198	1.665	1.117	1.990	2.320	2.201	1.594	1.112	0.484	0.432	0.642	0.610
<b>Mean</b>	<b>2.369</b>	<b>2.038</b>	<b>0.500</b>	<b>0.335</b>	<b>0.542</b>	<b>1.692</b>	<b>1.555</b>	<b>1.459</b>	<b>2.592</b>	<b>2.622</b>	<b>1.223</b>	<b>1.181</b>	<b>1.658</b>	<b>1.090</b>	<b>1.965</b>	<b>2.201</b>	<b>2.251</b>	<b>1.561</b>	<b>1.052</b>	<b>0.493</b>	<b>0.430</b>	<b>0.633</b>	<b>0.616</b>
<b>SD</b>	<b>0.092</b>	<b>0.037</b>	<b>0.005</b>	<b>0.012</b>	<b>0.008</b>	<b>0.029</b>	<b>0.012</b>	<b>0.023</b>	<b>0.095</b>	<b>0.056</b>	<b>0.017</b>	<b>0.021</b>	<b>0.024</b>	<b>0.016</b>	<b>0.031</b>	<b>0.067</b>	<b>0.040</b>	<b>0.019</b>	<b>0.029</b>	<b>0.009</b>	<b>0.010</b>	<b>0.006</b>	<b>0.013</b>
<b>%RSD</b>	<b>3.9</b>	<b>1.8</b>	<b>0.9</b>	<b>3.5</b>	<b>1.4</b>	<b>1.7</b>	<b>0.74</b>	<b>1.6</b>	<b>3.7</b>	<b>2.1</b>	<b>1.4</b>	<b>1.7</b>	<b>1.5</b>	<b>1.5</b>	<b>1.6</b>	<b>3.0</b>	<b>1.8</b>	<b>1.2</b>	<b>2.7</b>	<b>1.9</b>	<b>2.3</b>	<b>1.0</b>	<b>2.1</b>

**Table S12d.** SIFT-MS repeatability data for Mix 1 in 50% DMAC:50% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.310	0.187	0.046	0.006	0.033	0.099	0.008	0.015	-0.152	0.003	0.106	0.108	0.202	0.081	0.139	0.147	0.020	0.152	0.086	0.004	0.002	0.003	0.005
50–2	0.344	0.189	0.043	0.007	0.032	0.098	0.009	0.024	-0.136	0.004	0.108	0.104	0.211	0.081	0.145	0.152	0.022	0.159	0.083	0.003	0.003	0.003	0.003
50–3	0.384	0.186	0.035	0.006	0.024	0.100	0.007	0.009	-0.165	0.004	0.112	0.104	0.189	0.077	0.153	0.155	0.022	0.154	0.087	0.003	0.002	0.001	0.002
50–4	0.379	0.185	0.031	0.006	0.022	0.101	0.005	0.011	-0.189	0.003	0.106	0.104	0.201	0.077	0.136	0.152	0.023	0.158	0.086	0.002	0.001	0.002	0.002
50–5	0.383	0.183	0.027	0.003	0.021	0.101	0.005	0.006	-0.238	0.000	0.113	0.105	0.198	0.079	0.146	0.150	0.019	0.152	0.089	0.003	0.003	0.002	0.004
50–6	0.330	0.170	0.027	0.004	0.020	0.099	0.003	0.008	-0.208	0.000	0.108	0.100	0.196	0.076	0.142	0.147	0.019	0.146	0.081	0.002	0.003	0.002	0.004
<b>Mean</b>	<b>0.355</b>	<b>0.183</b>	<b>0.035</b>	<b>0.005</b>	<b>0.025</b>	<b>0.100</b>	<b>0.006</b>	<b>0.012</b>	<b>-0.181</b>	<b>0.002</b>	<b>0.109</b>	<b>0.105</b>	<b>0.199</b>	<b>0.078</b>	<b>0.144</b>	<b>0.150</b>	<b>0.021</b>	<b>0.153</b>	<b>0.085</b>	<b>0.003</b>	<b>0.002</b>	<b>0.002</b>	<b>0.003</b>
<b>SD</b>	<b>0.0288</b>	<b>0.0062</b>	<b>0.0074</b>	<b>0.0013</b>	<b>0.0052</b>	<b>0.0011</b>	<b>0.0022</b>	<b>0.0060</b>	<b>0.0346</b>	<b>0.0016</b>	<b>0.0027</b>	<b>0.0023</b>	<b>0.0067</b>	<b>0.0019</b>	<b>0.0054</b>	<b>0.0029</b>	<b>0.0017</b>	<b>0.0043</b>	<b>0.0026</b>	<b>0.0006</b>	<b>0.0005</b>	<b>0.0007</b>	<b>0.0011</b>
<b>%RSD</b>	<b>8.1</b>	<b>3.4</b>	<b>21.1</b>	<b>23.7</b>	<b>20.6</b>	<b>1.1</b>	<b>36.8</b>	<b>49.2</b>	<b>-19.1</b>	<b>66.2</b>	<b>2.5</b>	<b>2.2</b>	<b>3.3</b>	<b>2.5</b>	<b>3.8</b>	<b>1.9</b>	<b>8.0</b>	<b>2.8</b>	<b>3.1</b>	<b>20.7</b>	<b>20.0</b>	<b>30.3</b>	<b>36.0</b>
250–1	1.481	1.007	0.074	0.035	0.064	0.525	0.136	0.142	0.186	0.178	0.586	0.567	1.096	0.451	0.832	0.825	0.258	0.904	0.590	0.047	0.034	0.049	0.044
250–2	1.451	0.934	0.072	0.032	0.062	0.472	0.134	0.119	0.000	0.187	0.536	0.526	0.992	0.419	0.785	0.773	0.243	0.837	0.514	0.042	0.033	0.041	0.044
250–3	1.411	0.930	0.062	0.032	0.061	0.475	0.125	0.127	0.146	0.186	0.533	0.510	0.978	0.414	0.755	0.762	0.253	0.827	0.530	0.040	0.029	0.039	0.042
250–4	1.391	0.912	0.063	0.031	0.058	0.482	0.121	0.127	0.076	0.177	0.536	0.537	0.945	0.406	0.768	0.766	0.251	0.829	0.514	0.041	0.031	0.048	0.041
250–5	1.371	0.919	0.064	0.035	0.058	0.468	0.127	0.126	0.010	0.174	0.517	0.499	0.961	0.411	0.746	0.740	0.252	0.800	0.518	0.039	0.031	0.040	0.043
250–6	1.331	0.911	0.060	0.036	0.055	0.468	0.121	0.131	0.036	0.176	0.530	0.503	0.982	0.403	0.745	0.748	0.237	0.817	0.504	0.039	0.031	0.042	0.046
<b>Mean</b>	<b>1.406</b>	<b>0.935</b>	<b>0.066</b>	<b>0.034</b>	<b>0.060</b>	<b>0.482</b>	<b>0.127</b>	<b>0.129</b>	<b>0.076</b>	<b>0.179</b>	<b>0.540</b>	<b>0.524</b>	<b>0.992</b>	<b>0.418</b>	<b>0.772</b>	<b>0.769</b>	<b>0.249</b>	<b>0.835</b>	<b>0.528</b>	<b>0.041</b>	<b>0.031</b>	<b>0.043</b>	<b>0.043</b>
<b>SD</b>	<b>0.050</b>	<b>0.033</b>	<b>0.005</b>	<b>0.002</b>	<b>0.003</b>	<b>0.020</b>	<b>0.006</b>	<b>0.007</b>	<b>0.069</b>	<b>0.005</b>	<b>0.022</b>	<b>0.023</b>	<b>0.049</b>	<b>0.016</b>	<b>0.030</b>	<b>0.027</b>	<b>0.007</b>	<b>0.033</b>	<b>0.029</b>	<b>0.003</b>	<b>0.002</b>	<b>0.004</b>	<b>0.002</b>
<b>%RSD</b>	<b>3.5</b>	<b>3.5</b>	<b>7.7</b>	<b>5.8</b>	<b>5.1</b>	<b>4.1</b>	<b>4.6</b>	<b>5.4</b>	<b>91.5</b>	<b>2.8</b>	<b>4.0</b>	<b>4.5</b>	<b>4.9</b>	<b>3.8</b>	<b>3.9</b>	<b>3.6</b>	<b>2.8</b>	<b>3.9</b>	<b>5.4</b>	<b>6.6</b>	<b>5.6</b>	<b>9.1</b>	<b>3.6</b>
500–1	2.771	1.757	0.145	0.092	0.152	0.899	0.363	0.358	0.576	0.605	1.004	0.946	1.846	0.781	1.438	1.420	0.688	1.621	1.021	0.109	0.089	0.137	0.126
500–2	2.821	1.787	0.153	0.097	0.157	0.928	0.373	0.359	0.466	0.610	0.994	0.996	1.846	0.808	1.488	1.460	0.703	1.611	1.071	0.114	0.092	0.148	0.134
500–3	2.501	1.737	0.146	0.096	0.143	0.905	0.374	0.364	0.556	0.602	0.987	0.953	1.726	0.784	1.488	1.480	0.718	1.571	1.031	0.108	0.090	0.144	0.127
500–4	2.611	1.797	0.146	0.095	0.153	0.934	0.384	0.368	0.576	0.603	1.014	0.958	1.776	0.793	1.518	1.500	0.716	1.621	1.071	0.117	0.091	0.140	0.130
500–5	2.691	1.797	0.151	0.086	0.160	0.906	0.383	0.389	0.586	0.627	1.024	0.968	1.796	0.800	1.528	1.500	0.727	1.631	1.051	0.114	0.090	0.136	0.131
500–6	2.971	1.867	0.223	0.110	0.210	0.952	0.405	0.398	0.596	0.665	1.044	1.036	1.916	0.864	1.598	1.480	0.741	1.681	1.121	0.126	0.101	0.148	0.148
<b>Mean</b>	<b>2.728</b>	<b>1.790</b>	<b>0.161</b>	<b>0.096</b>	<b>0.162</b>	<b>0.921</b>	<b>0.380</b>	<b>0.373</b>	<b>0.559</b>	<b>0.618</b>	<b>1.011</b>	<b>0.977</b>	<b>1.817</b>	<b>0.805</b>	<b>1.510</b>	<b>1.473</b>	<b>0.716</b>	<b>1.622</b>	<b>1.061</b>	<b>0.115</b>	<b>0.092</b>	<b>0.142</b>	<b>0.132</b>
<b>SD</b>	<b>0.151</b>	<b>0.041</b>	<b>0.028</b>	<b>0.007</b>	<b>0.022</b>	<b>0.019</b>	<b>0.013</b>	<b>0.015</b>	<b>0.043</b>	<b>0.022</b>	<b>0.019</b>	<b>0.031</b>	<b>0.060</b>	<b>0.028</b>	<b>0.049</b>	<b>0.027</b>	<b>0.017</b>	<b>0.032</b>	<b>0.033</b>	<b>0.006</b>	<b>0.004</b>	<b>0.005</b>	<b>0.007</b>
<b>%RSD</b>	<b>5.5</b>	<b>2.3</b>	<b>17.5</b>	<b>7.5</b>	<b>13.5</b>	<b>2.1</b>	<b>3.4</b>	<b>4.1</b>	<b>7.8</b>	<b>3.6</b>	<b>1.9</b>	<b>3.2</b>	<b>3.3</b>	<b>3.5</b>	<b>3.2</b>	<b>1.9</b>	<b>2.4</b>	<b>2.0</b>	<b>3.1</b>	<b>5.2</b>	<b>4.5</b>	<b>3.4</b>	<b>5.5</b>



**Table S13.** SIFT-MS repeatability data for the Mix 1 in 5% DMF:95% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.342	0.296	0.049	0.081	0.077	0.070	0.375	0.321	0.322	0.340	0.191	0.151	0.222	0.159	0.247	0.289	0.316	0.271	0.176	0.152	0.130	0.176	0.170
50–2	0.325	0.290	0.031	0.073	0.066	0.152	0.375	0.341	0.337	0.351	0.192	0.151	0.224	0.155	0.257	0.288	0.302	0.255	0.172	0.158	0.130	0.166	0.165
50–3	0.327	0.283	0.024	0.076	0.062	0.189	0.366	0.331	0.285	0.351	0.194	0.155	0.226	0.163	0.256	0.272	0.318	0.259	0.169	0.154	0.123	0.166	0.169
50–4	0.315	0.295	0.004	0.065	0.048	0.194	0.364	0.341	0.307	0.341	0.185	0.151	0.215	0.155	0.253	0.282	0.313	0.263	0.172	0.149	0.127	0.164	0.174
50–5	0.340	0.305	0.013	0.079	0.054	0.230	0.387	0.340	0.350	0.339	0.211	0.166	0.245	0.175	0.277	0.302	0.325	0.273	0.181	0.156	0.136	0.177	0.167
50–6	0.320	0.299	-0.001	0.081	0.054	0.182	0.376	0.339	0.317	0.347	0.193	0.154	0.222	0.163	0.258	0.287	0.310	0.263	0.180	0.151	0.129	0.174	0.169
<b>Mean</b>	<b>0.328</b>	<b>0.295</b>	<b>0.020</b>	<b>0.076</b>	<b>0.060</b>	<b>0.170</b>	<b>0.373</b>	<b>0.336</b>	<b>0.320</b>	<b>0.345</b>	<b>0.195</b>	<b>0.155</b>	<b>0.226</b>	<b>0.162</b>	<b>0.258</b>	<b>0.286</b>	<b>0.314</b>	<b>0.264</b>	<b>0.175</b>	<b>0.154</b>	<b>0.129</b>	<b>0.171</b>	<b>0.169</b>
<b>SD</b>	<b>0.0099</b>	<b>0.0069</b>	<b>0.0170</b>	<b>0.0055</b>	<b>0.0095</b>	<b>0.0500</b>	<b>0.0075</b>	<b>0.0073</b>	<b>0.0208</b>	<b>0.0050</b>	<b>0.0080</b>	<b>0.0053</b>	<b>0.0093</b>	<b>0.0068</b>	<b>0.0092</b>	<b>0.0089</b>	<b>0.0071</b>	<b>0.0063</b>	<b>0.0044</b>	<b>0.0030</b>	<b>0.0039</b>	<b>0.0053</b>	<b>0.0028</b>
<b>%RSD</b>	<b>3.0</b>	<b>2.3</b>	<b>84.8</b>	<b>7.3</b>	<b>15.8</b>	<b>29.5</b>	<b>2.0</b>	<b>2.2</b>	<b>6.5</b>	<b>1.5</b>	<b>4.1</b>	<b>3.4</b>	<b>4.1</b>	<b>4.2</b>	<b>3.6</b>	<b>3.1</b>	<b>2.3</b>	<b>2.4</b>	<b>2.5</b>	<b>2.0</b>	<b>3.0</b>	<b>3.1</b>	<b>1.6</b>
250–1	1.552	1.420	0.507	0.413	0.589	1.480	1.670	1.527	1.686	1.598	0.943	0.757	1.094	0.783	1.324	1.389	1.445	1.286	0.867	0.700	0.599	0.782	0.765
250–2	1.592	1.430	0.492	0.407	0.572	1.420	1.730	1.527	1.706	1.578	0.932	0.730	1.124	0.784	1.314	1.339	1.445	1.296	0.866	0.695	0.600	0.753	0.747
250–3	1.592	1.460	0.536	0.413	0.588	1.550	1.760	1.577	1.726	1.608	0.956	0.748	1.144	0.794	1.364	1.399	1.455	1.296	0.891	0.714	0.618	0.787	0.751
250–4	1.612	1.480	0.500	0.411	0.589	1.430	1.740	1.577	1.676	1.608	0.958	0.761	1.134	0.777	1.354	1.419	1.465	1.316	0.866	0.701	0.606	0.761	0.744
250–5	1.622	1.480	0.557	0.411	0.605	1.720	1.760	1.597	1.676	1.598	0.986	0.768	1.164	0.823	1.364	1.419	1.455	1.326	0.910	0.702	0.617	0.776	0.737
250–6	1.622	1.470	0.512	0.417	0.588	1.440	1.730	1.557	1.766	1.548	0.959	0.764	1.144	0.803	1.354	1.409	1.435	1.346	0.874	0.703	0.603	0.774	0.752
<b>Mean</b>	<b>1.599</b>	<b>1.457</b>	<b>0.517</b>	<b>0.412</b>	<b>0.589</b>	<b>1.507</b>	<b>1.731</b>	<b>1.560</b>	<b>1.706</b>	<b>1.590</b>	<b>0.956</b>	<b>0.755</b>	<b>1.134</b>	<b>0.794</b>	<b>1.345</b>	<b>1.395</b>	<b>1.450</b>	<b>1.311</b>	<b>0.879</b>	<b>0.703</b>	<b>0.607</b>	<b>0.772</b>	<b>0.750</b>
<b>SD</b>	<b>0.024</b>	<b>0.024</b>	<b>0.022</b>	<b>0.003</b>	<b>0.010</b>	<b>0.105</b>	<b>0.030</b>	<b>0.026</b>	<b>0.032</b>	<b>0.021</b>	<b>0.017</b>	<b>0.013</b>	<b>0.022</b>	<b>0.015</b>	<b>0.020</b>	<b>0.027</b>	<b>0.010</b>	<b>0.021</b>	<b>0.016</b>	<b>0.006</b>	<b>0.008</b>	<b>0.012</b>	<b>0.009</b>
<b>%RSD</b>	<b>1.5</b>	<b>1.6</b>	<b>4.3</b>	<b>0.73</b>	<b>1.6</b>	<b>7.0</b>	<b>1.7</b>	<b>1.7</b>	<b>1.9</b>	<b>1.3</b>	<b>1.7</b>	<b>1.7</b>	<b>1.9</b>	<b>1.9</b>	<b>1.4</b>	<b>2.0</b>	<b>0.66</b>	<b>1.6</b>	<b>1.9</b>	<b>0.82</b>	<b>1.3</b>	<b>1.5</b>	<b>1.1</b>
500–1	3.272	2.940	1.246	0.924	1.420	2.810	3.650	3.317	3.776	3.368	1.914	1.556	2.284	1.605	2.714	2.709	2.995	2.616	1.805	1.507	1.297	1.688	1.638
500–2	3.212	3.040	1.266	0.968	1.400	2.770	3.780	3.397	3.736	3.428	1.944	1.566	2.324	1.635	2.774	2.809	3.045	2.716	1.835	1.527	1.337	1.708	1.648
500–3	3.222	3.000	1.226	0.959	1.420	2.740	3.670	3.467	3.906	3.308	1.934	1.536	2.274	1.615	2.724	2.799	3.015	2.646	1.865	1.517	1.357	1.718	1.658
500–4	3.182	2.880	1.236	0.932	1.390	2.690	3.640	3.297	3.776	3.408	1.874	1.496	2.194	1.575	2.664	2.739	3.055	2.576	1.795	1.477	1.317	1.728	1.638
500–5	3.222	2.930	1.236	0.917	1.380	2.950	3.740	3.387	3.626	3.308	1.944	1.536	2.234	1.635	2.764	2.759	2.965	2.596	1.895	1.477	1.337	1.688	1.658
500–6	3.112	2.850	1.206	0.908	1.340	2.530	3.670	3.257	3.666	3.208	1.864	1.446	2.064	1.525	2.674	2.729	2.965	2.546	1.765	1.467	1.337	1.638	1.638
<b>Mean</b>	<b>3.204</b>	<b>2.940</b>	<b>1.236</b>	<b>0.934</b>	<b>1.392</b>	<b>2.748</b>	<b>3.691</b>	<b>3.354</b>	<b>3.748</b>	<b>3.338</b>	<b>1.913</b>	<b>1.523</b>	<b>2.229</b>	<b>1.598</b>	<b>2.719</b>	<b>2.757</b>	<b>3.006</b>	<b>2.616</b>	<b>1.827</b>	<b>1.496</b>	<b>1.331</b>	<b>1.695</b>	<b>1.647</b>
<b>SD</b>	<b>0.049</b>	<b>0.065</b>	<b>0.018</b>	<b>0.022</b>	<b>0.027</b>	<b>0.127</b>	<b>0.051</b>	<b>0.070</b>	<b>0.090</b>	<b>0.074</b>	<b>0.032</b>	<b>0.041</b>	<b>0.084</b>	<b>0.039</b>	<b>0.041</b>	<b>0.036</b>	<b>0.035</b>	<b>0.054</b>	<b>0.044</b>	<b>0.023</b>	<b>0.019</b>	<b>0.029</b>	<b>0.009</b>
<b>%RSD</b>	<b>1.5</b>	<b>2.2</b>	<b>1.5</b>	<b>2.3</b>	<b>2.0</b>	<b>4.6</b>	<b>1.4</b>	<b>2.1</b>	<b>2.4</b>	<b>2.2</b>	<b>1.7</b>	<b>2.7</b>	<b>3.8</b>	<b>2.4</b>	<b>1.5</b>	<b>1.3</b>	<b>1.2</b>	<b>2.1</b>	<b>2.4</b>	<b>1.5</b>	<b>1.4</b>	<b>1.7</b>	<b>0.55</b>

**Table S14a.** SIFT-MS repeatability data for the Mix 1 in 5% DMI:95% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.338	0.291	0.152	0.109	0.174	0.264	0.373	0.357	0.282	0.304	0.192	0.155	0.244	0.173	0.275	0.257	0.288	0.268	0.178	0.161	0.133	0.180	0.162
50–2	0.322	0.295	0.156	0.108	0.168	0.271	0.389	0.354	0.256	0.286	0.193	0.155	0.225	0.164	0.273	0.272	0.291	0.272	0.173	0.160	0.140	0.176	0.171
50–3	0.362	0.302	0.165	0.108	0.171	0.277	0.398	0.366	0.268	0.297	0.181	0.161	0.251	0.177	0.273	0.263	0.278	0.286	0.182	0.159	0.139	0.172	0.182
50–4	0.326	0.285	0.152	0.093	0.156	0.263	0.390	0.350	0.298	0.286	0.191	0.150	0.224	0.162	0.272	0.283	0.293	0.261	0.163	0.154	0.134	0.171	0.164
50–5	0.334	0.284	0.162	0.108	0.164	0.256	0.402	0.353	0.327	0.303	0.187	0.155	0.241	0.163	0.266	0.265	0.298	0.271	0.175	0.148	0.133	0.173	0.169
50–6	0.336	0.293	0.170	0.104	0.179	0.275	0.400	0.345	0.280	0.310	0.191	0.155	0.238	0.169	0.278	0.267	0.292	0.283	0.176	0.151	0.139	0.164	0.178
<b>Mean</b>	<b>0.336</b>	<b>0.292</b>	<b>0.160</b>	<b>0.105</b>	<b>0.169</b>	<b>0.268</b>	<b>0.392</b>	<b>0.354</b>	<b>0.285</b>	<b>0.298</b>	<b>0.189</b>	<b>0.156</b>	<b>0.237</b>	<b>0.168</b>	<b>0.272</b>	<b>0.268</b>	<b>0.290</b>	<b>0.273</b>	<b>0.174</b>	<b>0.155</b>	<b>0.136</b>	<b>0.172</b>	<b>0.171</b>
<b>SD</b>	<b>0.0128</b>	<b>0.0061</b>	<b>0.0067</b>	<b>0.0056</b>	<b>0.0073</b>	<b>0.0073</b>	<b>0.0098</b>	<b>0.0065</b>	<b>0.0227</b>	<b>0.0091</b>	<b>0.0041</b>	<b>0.0032</b>	<b>0.0098</b>	<b>0.0055</b>	<b>0.0036</b>	<b>0.0081</b>	<b>0.0061</b>	<b>0.0086</b>	<b>0.0059</b>	<b>0.0049</b>	<b>0.0030</b>	<b>0.0049</b>	<b>0.0071</b>
<b>%RSD</b>	<b>3.8</b>	<b>2.1</b>	<b>4.2</b>	<b>5.3</b>	<b>4.4</b>	<b>2.7</b>	<b>2.5</b>	<b>1.8</b>	<b>8.0</b>	<b>3.0</b>	<b>2.2</b>	<b>2.0</b>	<b>4.1</b>	<b>3.3</b>	<b>1.3</b>	<b>3.0</b>	<b>2.1</b>	<b>3.1</b>	<b>3.4</b>	<b>3.1</b>	<b>2.2</b>	<b>2.8</b>	<b>4.2</b>
250–1	1.710	1.457	0.765	0.456	0.783	1.282	1.801	1.629	1.547	1.501	0.917	0.772	1.209	0.825	1.318	1.229	1.350	1.313	0.875	0.735	0.638	0.800	0.795
250–2	1.570	1.417	0.697	0.470	0.735	1.242	1.741	1.579	1.547	1.411	0.912	0.741	1.129	0.785	1.288	1.289	1.320	1.263	0.854	0.714	0.611	0.759	0.766
250–3	1.640	1.397	0.710	0.445	0.757	1.252	1.751	1.569	1.507	1.421	0.893	0.748	1.159	0.804	1.288	1.249	1.330	1.263	0.834	0.706	0.611	0.784	0.770
250–4	1.710	1.497	0.774	0.493	0.790	1.312	1.781	1.659	1.477	1.501	0.916	0.780	1.259	0.842	1.298	1.229	1.340	1.333	0.881	0.727	0.631	0.785	0.758
250–5	1.640	1.427	0.712	0.448	0.743	1.242	1.751	1.589	1.487	1.471	0.912	0.736	1.169	0.810	1.258	1.209	1.340	1.273	0.865	0.697	0.605	0.777	0.752
250–6	1.630	1.447	0.789	0.452	0.800	1.222	1.721	1.609	1.467	1.491	0.903	0.747	1.159	0.789	1.298	1.239	1.320	1.283	0.864	0.704	0.625	0.786	0.781
<b>Mean</b>	<b>1.650</b>	<b>1.441</b>	<b>0.741</b>	<b>0.461</b>	<b>0.768</b>	<b>1.259</b>	<b>1.758</b>	<b>1.606</b>	<b>1.505</b>	<b>1.466</b>	<b>0.908</b>	<b>0.754</b>	<b>1.181</b>	<b>0.809</b>	<b>1.291</b>	<b>1.241</b>	<b>1.333</b>	<b>1.288</b>	<b>0.862</b>	<b>0.713</b>	<b>0.620</b>	<b>0.781</b>	<b>0.770</b>
<b>SD</b>	<b>0.049</b>	<b>0.032</b>	<b>0.036</b>	<b>0.017</b>	<b>0.024</b>	<b>0.030</b>	<b>0.026</b>	<b>0.031</b>	<b>0.032</b>	<b>0.037</b>	<b>0.008</b>	<b>0.016</b>	<b>0.042</b>	<b>0.020</b>	<b>0.018</b>	<b>0.025</b>	<b>0.011</b>	<b>0.026</b>	<b>0.015</b>	<b>0.013</b>	<b>0.012</b>	<b>0.012</b>	<b>0.014</b>
<b>%RSD</b>	<b>2.9</b>	<b>2.2</b>	<b>4.8</b>	<b>3.6</b>	<b>3.2</b>	<b>2.4</b>	<b>1.5</b>	<b>1.9</b>	<b>2.1</b>	<b>2.5</b>	<b>0.92</b>	<b>2.1</b>	<b>3.6</b>	<b>2.4</b>	<b>1.4</b>	<b>2.0</b>	<b>0.83</b>	<b>2.0</b>	<b>1.8</b>	<b>1.9</b>	<b>1.9</b>	<b>1.6</b>	<b>1.9</b>
500–1	3.470	3.087	1.615	1.041	1.702	2.592	3.831	3.559	3.397	3.081	1.874	1.604	2.519	1.718	2.778	2.499	2.800	2.763	1.855	1.550	1.397	1.810	1.708
500–2	3.180	2.867	1.465	0.971	1.622	2.462	3.661	3.349	3.197	3.071	1.794	1.464	2.289	1.608	2.608	2.489	2.800	2.553	1.775	1.500	1.337	1.690	1.688
500–3	3.150	2.917	1.425	1.021	1.592	2.552	3.661	3.429	3.327	2.991	1.854	1.524	2.269	1.578	2.688	2.689	2.780	2.603	1.785	1.480	1.357	1.660	1.658
500–4	3.650	3.277	1.595	1.061	1.742	2.752	3.981	3.619	3.407	3.061	1.974	1.694	2.669	1.818	2.928	2.709	2.840	2.943	1.985	1.600	1.437	1.750	1.758
500–5	3.190	2.867	1.455	1.011	1.582	2.392	3.651	3.379	3.227	3.061	1.714	1.474	2.319	1.608	2.638	2.369	2.770	2.573	1.735	1.480	1.367	1.690	1.668
500–6	3.190	2.927	1.535	0.991	1.652	2.402	3.651	3.369	3.137	2.971	1.754	1.504	2.379	1.608	2.588	2.339	2.700	2.603	1.775	1.450	1.307	1.640	1.588
<b>Mean</b>	<b>3.305</b>	<b>2.991</b>	<b>1.515</b>	<b>1.016</b>	<b>1.649</b>	<b>2.525</b>	<b>3.739</b>	<b>3.451</b>	<b>3.282</b>	<b>3.039</b>	<b>1.827</b>	<b>1.544</b>	<b>2.408</b>	<b>1.657</b>	<b>2.704</b>	<b>2.516</b>	<b>2.781</b>	<b>2.673</b>	<b>1.818</b>	<b>1.510</b>	<b>1.367</b>	<b>1.706</b>	<b>1.678</b>
<b>SD</b>	<b>0.188</b>	<b>0.148</b>	<b>0.072</b>	<b>0.030</b>	<b>0.058</b>	<b>0.125</b>	<b>0.126</b>	<b>0.102</b>	<b>0.102</b>	<b>0.042</b>	<b>0.085</b>	<b>0.081</b>	<b>0.143</b>	<b>0.085</b>	<b>0.118</b>	<b>0.142</b>	<b>0.043</b>	<b>0.139</b>	<b>0.083</b>	<b>0.050</b>	<b>0.042</b>	<b>0.057</b>	<b>0.052</b>
<b>%RSD</b>	<b>5.7</b>	<b>4.9</b>	<b>4.7</b>	<b>2.9</b>	<b>3.5</b>	<b>4.9</b>	<b>3.4</b>	<b>3.0</b>	<b>3.1</b>	<b>1.4</b>	<b>4.7</b>	<b>5.2</b>	<b>5.9</b>	<b>5.1</b>	<b>4.3</b>	<b>5.6</b>	<b>1.5</b>	<b>5.2</b>	<b>4.5</b>	<b>3.3</b>	<b>3.0</b>	<b>3.4</b>	<b>3.1</b>

**Table S14b.** SIFT-MS repeatability data for Mix 1 in 10% DMI:90% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.265	0.276	0.071	0.065	0.077	0.250	0.215	0.221	0.621	0.328	0.161	0.134	0.249	0.131	0.280	0.280	0.264	0.260	0.184	0.108	0.086	0.088	0.075
50–2	0.261	0.280	0.081	0.071	0.076	0.258	0.215	0.226	0.591	0.329	0.172	0.136	0.253	0.135	0.274	0.286	0.257	0.267	0.184	0.109	0.089	0.082	0.079
50–3	0.272	0.277	0.075	0.066	0.080	0.251	0.225	0.221	0.562	0.333	0.164	0.131	0.251	0.135	0.279	0.287	0.262	0.264	0.180	0.106	0.087	0.083	0.082
50–4	0.272	0.279	0.078	0.057	0.086	0.250	0.211	0.223	0.540	0.332	0.171	0.139	0.256	0.131	0.283	0.284	0.262	0.267	0.179	0.110	0.089	0.091	0.083
50–5	0.263	0.274	0.075	0.066	0.078	0.261	0.218	0.215	0.459	0.343	0.167	0.135	0.245	0.136	0.288	0.299	0.258	0.261	0.184	0.103	0.089	0.087	0.075
50–6	0.270	0.283	0.076	0.060	0.077	0.263	0.218	0.221	0.619	0.358	0.174	0.138	0.259	0.133	0.296	0.282	0.259	0.270	0.190	0.107	0.088	0.081	0.078
<b>Mean</b>	<b>0.267</b>	<b>0.278</b>	<b>0.076</b>	<b>0.064</b>	<b>0.079</b>	<b>0.256</b>	<b>0.217</b>	<b>0.222</b>	<b>0.565</b>	<b>0.337</b>	<b>0.168</b>	<b>0.135</b>	<b>0.252</b>	<b>0.133</b>	<b>0.283</b>	<b>0.286</b>	<b>0.261</b>	<b>0.265</b>	<b>0.184</b>	<b>0.108</b>	<b>0.088</b>	<b>0.085</b>	<b>0.078</b>
<b>SD</b>	<b>0.0044</b>	<b>0.0029</b>	<b>0.0031</b>	<b>0.0046</b>	<b>0.0033</b>	<b>0.0054</b>	<b>0.0043</b>	<b>0.0033</b>	<b>0.0557</b>	<b>0.0105</b>	<b>0.0046</b>	<b>0.0026</b>	<b>0.0046</b>	<b>0.0020</b>	<b>0.0071</b>	<b>0.0061</b>	<b>0.0025</b>	<b>0.0035</b>	<b>0.0035</b>	<b>0.0023</b>	<b>0.0010</b>	<b>0.0036</b>	<b>0.0030</b>
<b>%RSD</b>	<b>1.6</b>	<b>1.0</b>	<b>4.0</b>	<b>7.1</b>	<b>4.2</b>	<b>2.1</b>	<b>2.0</b>	<b>1.5</b>	<b>9.8</b>	<b>3.1</b>	<b>2.7</b>	<b>1.9</b>	<b>1.8</b>	<b>1.5</b>	<b>2.5</b>	<b>2.1</b>	<b>0.96</b>	<b>1.3</b>	<b>1.9</b>	<b>2.1</b>	<b>1.1</b>	<b>4.2</b>	<b>3.9</b>
250–1	1.318	1.361	0.442	0.302	0.461	1.198	1.230	1.136	2.012	1.665	0.780	0.672	1.088	0.649	1.245	1.340	1.507	1.148	0.757	0.493	0.422	0.471	0.462
250–2	1.298	1.361	0.431	0.308	0.465	1.218	1.210	1.146	2.172	1.705	0.808	0.669	1.068	0.648	1.225	1.390	1.537	1.138	0.743	0.486	0.412	0.466	0.469
250–3	1.308	1.381	0.426	0.302	0.448	1.218	1.180	1.116	2.132	1.645	0.800	0.666	1.058	0.643	1.215	1.400	1.417	1.138	0.739	0.472	0.401	0.462	0.455
250–4	1.278	1.301	0.420	0.288	0.450	1.178	1.160	1.096	2.012	1.575	0.764	0.638	1.008	0.611	1.205	1.380	1.437	1.088	0.717	0.461	0.385	0.436	0.454
250–5	1.358	1.401	0.433	0.282	0.448	1.258	1.210	1.126	2.112	1.635	0.810	0.692	1.098	0.660	1.265	1.370	1.407	1.148	0.774	0.481	0.407	0.460	0.464
250–6	2.988	3.141	1.169	0.764	1.219	2.798	3.130	2.816	5.082	4.205	1.767	1.519	2.238	1.510	2.825	3.270	3.757	2.608	1.766	1.199	1.039	1.230	1.208
<b>Mean</b>	<b>1.312</b>	<b>1.361</b>	<b>0.430</b>	<b>0.296</b>	<b>0.454</b>	<b>1.214</b>	<b>1.198</b>	<b>1.124</b>	<b>2.088</b>	<b>1.645</b>	<b>0.793</b>	<b>0.667</b>	<b>1.064</b>	<b>0.642</b>	<b>1.231</b>	<b>1.376</b>	<b>1.461</b>	<b>1.132</b>	<b>0.746</b>	<b>0.479</b>	<b>0.406</b>	<b>0.459</b>	<b>0.461</b>
<b>SD</b>	<b>0.027</b>	<b>0.033</b>	<b>0.007</b>	<b>0.010</b>	<b>0.007</b>	<b>0.027</b>	<b>0.025</b>	<b>0.017</b>	<b>0.065</b>	<b>0.042</b>	<b>0.018</b>	<b>0.017</b>	<b>0.031</b>	<b>0.017</b>	<b>0.022</b>	<b>0.021</b>	<b>0.052</b>	<b>0.022</b>	<b>0.019</b>	<b>0.011</b>	<b>0.012</b>	<b>0.012</b>	<b>0.006</b>
<b>%RSD</b>	<b>2.0</b>	<b>2.5</b>	<b>1.7</b>	<b>3.3</b>	<b>1.6</b>	<b>2.2</b>	<b>2.1</b>	<b>1.5</b>	<b>3.1</b>	<b>2.6</b>	<b>2.2</b>	<b>2.6</b>	<b>2.9</b>	<b>2.6</b>	<b>1.7</b>	<b>1.5</b>	<b>3.5</b>	<b>2.0</b>	<b>2.5</b>	<b>2.3</b>	<b>3.0</b>	<b>2.6</b>	<b>1.2</b>
500–1	3.008	3.171	1.029	0.674	1.099	2.728	2.850	2.666	4.112	3.465	1.767	1.499	2.378	1.450	2.735	3.060	3.167	2.488	1.696	1.089	0.938	1.090	1.068
500–2	2.778	2.951	1.009	0.653	1.069	2.558	2.710	2.566	4.412	3.685	1.647	1.389	2.248	1.370	2.555	2.830	3.357	2.358	1.616	1.059	0.922	1.090	1.058
500–3	2.518	2.591	0.922	0.596	0.967	2.298	2.510	2.316	4.052	3.325	1.497	1.259	2.018	1.230	2.325	2.660	2.977	2.128	1.446	0.958	0.839	0.969	0.948
500–4	2.538	2.591	0.922	0.621	0.999	2.318	2.540	2.376	4.152	3.595	1.507	1.269	1.928	1.250	2.345	2.660	3.187	2.128	1.486	0.984	0.861	1.020	0.997
500–5	2.578	2.751	0.928	0.618	1.009	2.388	2.570	2.456	4.452	3.625	1.567	1.299	2.108	1.280	2.425	2.670	3.227	2.228	1.496	1.009	0.872	1.020	0.993
500–6	2.548	2.681	0.930	0.596	0.970	2.408	2.510	2.286	4.202	3.405	1.557	1.289	1.968	1.260	2.365	2.800	3.057	2.178	1.476	0.980	0.838	0.997	0.984
<b>Mean</b>	<b>2.661</b>	<b>2.789</b>	<b>0.956</b>	<b>0.626</b>	<b>1.019</b>	<b>2.450</b>	<b>2.615</b>	<b>2.445</b>	<b>4.230</b>	<b>3.516</b>	<b>1.590</b>	<b>1.334</b>	<b>2.108</b>	<b>1.306</b>	<b>2.458</b>	<b>2.780</b>	<b>3.162</b>	<b>2.251</b>	<b>1.536</b>	<b>1.014</b>	<b>0.879</b>	<b>1.031</b>	<b>1.008</b>
<b>SD</b>	<b>0.178</b>	<b>0.210</b>	<b>0.045</b>	<b>0.029</b>	<b>0.049</b>	<b>0.150</b>	<b>0.125</b>	<b>0.136</b>	<b>0.150</b>	<b>0.128</b>	<b>0.093</b>	<b>0.085</b>	<b>0.159</b>	<b>0.078</b>	<b>0.145</b>	<b>0.143</b>	<b>0.121</b>	<b>0.131</b>	<b>0.089</b>	<b>0.046</b>	<b>0.039</b>	<b>0.045</b>	<b>0.042</b>
<b>%RSD</b>	<b>6.7</b>	<b>7.5</b>	<b>4.7</b>	<b>4.6</b>	<b>4.8</b>	<b>6.1</b>	<b>4.8</b>	<b>5.5</b>	<b>3.5</b>	<b>3.6</b>	<b>5.8</b>	<b>6.4</b>	<b>7.6</b>	<b>6.0</b>	<b>5.9</b>	<b>5.1</b>	<b>3.8</b>	<b>5.8</b>	<b>5.8</b>	<b>4.6</b>	<b>4.4</b>	<b>4.4</b>	<b>4.2</b>

**Table S14c.** SIFT-MS repeatability data for Mix 1 in 25% DMI:75% water at three levels (50, 250, and 500).

Level-Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50-1	0.337	0.321	0.073	0.062	0.081	0.308	0.206	0.212	0.586	0.319	0.197	0.172	0.303	0.161	0.344	0.339	0.240	0.329	0.220	0.109	0.093	0.081	0.069
50-2	0.300	0.296	0.071	0.057	0.078	0.284	0.213	0.209	0.546	0.320	0.184	0.144	0.260	0.141	0.316	0.327	0.263	0.289	0.188	0.104	0.087	0.080	0.069
50-3	0.296	0.299	0.066	0.063	0.071	0.278	0.193	0.186	0.502	0.305	0.180	0.150	0.279	0.145	0.306	0.312	0.248	0.286	0.197	0.102	0.087	0.074	0.071
50-4	0.321	0.315	0.072	0.067	0.074	0.306	0.200	0.205	0.541	0.308	0.190	0.160	0.281	0.162	0.333	0.334	0.234	0.312	0.204	0.106	0.084	0.073	0.068
50-5	0.302	0.304	0.068	0.060	0.069	0.292	0.205	0.194	0.539	0.293	0.188	0.151	0.271	0.150	0.317	0.327	0.231	0.288	0.193	0.099	0.083	0.070	0.062
50-6	0.331	0.315	0.074	0.068	0.075	0.313	0.198	0.209	0.536	0.320	0.198	0.165	0.291	0.155	0.329	0.337	0.247	0.311	0.207	0.109	0.089	0.070	0.080
<b>Mean</b>	<b>0.314</b>	<b>0.308</b>	<b>0.071</b>	<b>0.063</b>	<b>0.075</b>	<b>0.297</b>	<b>0.202</b>	<b>0.203</b>	<b>0.542</b>	<b>0.311</b>	<b>0.190</b>	<b>0.157</b>	<b>0.281</b>	<b>0.152</b>	<b>0.324</b>	<b>0.329</b>	<b>0.244</b>	<b>0.303</b>	<b>0.201</b>	<b>0.104</b>	<b>0.087</b>	<b>0.075</b>	<b>0.070</b>
<b>SD</b>	<b>0.0160</b>	<b>0.0092</b>	<b>0.0030</b>	<b>0.0036</b>	<b>0.0038</b>	<b>0.0130</b>	<b>0.0064</b>	<b>0.0094</b>	<b>0.0245</b>	<b>0.0100</b>	<b>0.0065</b>	<b>0.0096</b>	<b>0.0137</b>	<b>0.0078</b>	<b>0.0125</b>	<b>0.0090</b>	<b>0.0106</b>	<b>0.0160</b>	<b>0.0104</b>	<b>0.0037</b>	<b>0.0035</b>	<b>0.0043</b>	<b>0.0053</b>
<b>%RSD</b>	<b>5.1</b>	<b>3.0</b>	<b>4.3</b>	<b>5.8</b>	<b>5.0</b>	<b>4.4</b>	<b>3.2</b>	<b>4.6</b>	<b>4.5</b>	<b>3.2</b>	<b>3.4</b>	<b>6.1</b>	<b>4.9</b>	<b>5.1</b>	<b>3.9</b>	<b>2.7</b>	<b>4.3</b>	<b>5.3</b>	<b>5.2</b>	<b>3.5</b>	<b>4.1</b>	<b>5.8</b>	<b>7.7</b>
250-1	1.465	1.487	0.454	0.307	0.476	1.408	1.262	1.184	2.198	1.806	0.889	0.746	1.146	0.719	1.365	1.580	1.618	1.268	0.826	0.508	0.428	0.501	0.473
250-2	1.495	1.547	0.484	0.330	0.511	1.408	1.332	1.274	2.238	1.896	0.923	0.769	1.186	0.759	1.435	1.650	1.688	1.328	0.877	0.538	0.456	0.521	0.512
250-3	1.405	1.457	0.469	0.326	0.496	1.328	1.292	1.194	2.108	1.856	0.851	0.720	1.116	0.680	1.305	1.480	1.678	1.218	0.816	0.519	0.439	0.506	0.513
250-4	1.465	1.467	0.488	0.343	0.510	1.378	1.322	1.234	2.248	1.956	0.887	0.735	1.156	0.706	1.315	1.520	1.728	1.238	0.838	0.528	0.449	0.523	0.511
250-5	1.435	1.457	0.480	0.351	0.513	1.338	1.352	1.234	2.398	1.946	0.833	0.726	1.136	0.723	1.335	1.480	1.718	1.228	0.826	0.538	0.451	0.515	0.530
250-6	1.405	1.477	0.495	0.340	0.517	1.348	1.372	1.274	2.258	1.956	0.860	0.714	1.126	0.706	1.345	1.530	1.758	1.238	0.819	0.533	0.450	0.533	0.517
<b>Mean</b>	<b>1.445</b>	<b>1.482</b>	<b>0.478</b>	<b>0.332</b>	<b>0.504</b>	<b>1.368</b>	<b>1.322</b>	<b>1.233</b>	<b>2.241</b>	<b>1.902</b>	<b>0.874</b>	<b>0.735</b>	<b>1.145</b>	<b>0.715</b>	<b>1.350</b>	<b>1.540</b>	<b>1.698</b>	<b>1.253</b>	<b>0.833</b>	<b>0.527</b>	<b>0.446</b>	<b>0.517</b>	<b>0.510</b>
<b>SD</b>	<b>0.033</b>	<b>0.031</b>	<b>0.013</b>	<b>0.014</b>	<b>0.014</b>	<b>0.032</b>	<b>0.037</b>	<b>0.035</b>	<b>0.086</b>	<b>0.056</b>	<b>0.029</b>	<b>0.018</b>	<b>0.023</b>	<b>0.024</b>	<b>0.043</b>	<b>0.060</b>	<b>0.044</b>	<b>0.037</b>	<b>0.021</b>	<b>0.011</b>	<b>0.009</b>	<b>0.011</b>	<b>0.017</b>
<b>%RSD</b>	<b>2.3</b>	<b>2.1</b>	<b>2.8</b>	<b>4.3</b>	<b>2.8</b>	<b>2.3</b>	<b>2.8</b>	<b>2.8</b>	<b>3.8</b>	<b>3.0</b>	<b>3.4</b>	<b>2.5</b>	<b>2.0</b>	<b>3.3</b>	<b>3.2</b>	<b>3.9</b>	<b>2.6</b>	<b>2.9</b>	<b>2.5</b>	<b>2.1</b>	<b>2.1</b>	<b>2.1</b>	<b>3.4</b>
500-1	2.875	2.987	1.109	0.726	1.159	2.698	3.052	2.714	5.088	4.296	1.776	1.490	2.186	1.430	2.695	3.080	3.768	2.488	1.657	1.160	1.009	1.189	1.168
500-2	2.775	2.857	1.089	0.706	1.139	2.648	2.962	2.764	5.078	4.236	1.706	1.450	2.076	1.350	2.655	3.050	3.738	2.438	1.677	1.150	1.029	1.199	1.148
500-3	2.875	2.957	1.089	0.725	1.169	2.668	2.952	2.764	5.198	4.236	1.696	1.400	2.196	1.390	2.705	3.030	3.928	2.448	1.647	1.150	1.009	1.239	1.198
500-4	2.905	2.947	1.069	0.709	1.159	2.598	2.912	2.704	4.938	4.216	1.666	1.410	2.186	1.380	2.645	2.940	3.908	2.428	1.617	1.130	0.982	1.199	1.188
500-5	3.035	3.087	1.099	0.750	1.219	2.758	3.062	2.844	5.098	4.266	1.726	1.490	2.326	1.480	2.725	3.110	3.818	2.558	1.707	1.180	1.019	1.259	1.198
500-6	2.985	3.137	1.169	0.763	1.219	2.798	3.132	2.814	5.098	4.206	1.766	1.520	2.236	1.510	2.825	3.270	3.758	2.608	1.767	1.200	1.039	1.229	1.208
<b>Mean</b>	<b>2.908</b>	<b>2.995</b>	<b>1.104</b>	<b>0.729</b>	<b>1.177</b>	<b>2.695</b>	<b>3.012</b>	<b>2.768</b>	<b>5.083</b>	<b>4.242</b>	<b>1.723</b>	<b>1.460</b>	<b>2.201</b>	<b>1.423</b>	<b>2.708</b>	<b>3.080</b>	<b>3.820</b>	<b>2.495</b>	<b>1.678</b>	<b>1.161</b>	<b>1.015</b>	<b>1.219</b>	<b>1.185</b>
<b>SD</b>	<b>0.084</b>	<b>0.093</b>	<b>0.031</b>	<b>0.021</b>	<b>0.031</b>	<b>0.067</b>	<b>0.076</b>	<b>0.050</b>	<b>0.076</b>	<b>0.030</b>	<b>0.039</b>	<b>0.044</b>	<b>0.074</b>	<b>0.056</b>	<b>0.059</b>	<b>0.100</b>	<b>0.074</b>	<b>0.067</b>	<b>0.048</b>	<b>0.023</b>	<b>0.018</b>	<b>0.025</b>	<b>0.021</b>
<b>%RSD</b>	<b>2.9</b>	<b>3.1</b>	<b>2.9</b>	<b>2.8</b>	<b>2.6</b>	<b>2.5</b>	<b>2.5</b>	<b>1.8</b>	<b>1.5</b>	<b>0.72</b>	<b>2.2</b>	<b>3.0</b>	<b>3.4</b>	<b>4.0</b>	<b>2.2</b>	<b>3.2</b>	<b>1.9</b>	<b>2.7</b>	<b>2.9</b>	<b>2.0</b>	<b>1.8</b>	<b>2.1</b>	<b>1.7</b>

**Table S14d.** SIFT-MS repeatability data for Mix 1 in 50% DMI:50% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.262	0.238	0.009	0.014	0.009	0.120	0.019	0.048	0.357	0.110	0.127	0.102	0.501	0.094	0.261	0.206	0.063	0.264	0.163	0.023	0.019	0.006	0.010
50–2	0.252	0.229	0.009	0.016	0.009	0.119	0.017	0.044	0.354	0.101	0.135	0.099	0.478	0.087	0.274	0.198	0.062	0.252	0.162	0.022	0.020	0.005	0.007
50–3	0.259	0.229	0.008	0.014	0.009	0.115	0.015	0.044	0.286	0.115	0.124	0.109	0.494	0.094	0.261	0.193	0.062	0.250	0.149	0.023	0.017	0.007	0.006
50–4	0.264	0.231	0.007	0.015	0.009	0.114	0.019	0.045	0.374	0.110	0.127	0.109	0.498	0.093	0.275	0.197	0.063	0.258	0.158	0.021	0.017	0.009	0.006
50–5	0.253	0.229	0.008	0.017	0.008	0.117	0.019	0.049	0.395	0.103	0.129	0.107	0.483	0.095	0.252	0.198	0.063	0.246	0.156	0.020	0.017	0.007	0.007
50–6	0.256	0.227	0.008	0.014	0.009	0.120	0.016	0.051	0.339	0.112	0.133	0.105	0.473	0.091	0.280	0.206	0.062	0.250	0.151	0.023	0.018	0.007	0.009
<b>Mean</b>	<b>0.257</b>	<b>0.230</b>	<b>0.008</b>	<b>0.015</b>	<b>0.009</b>	<b>0.117</b>	<b>0.018</b>	<b>0.047</b>	<b>0.350</b>	<b>0.109</b>	<b>0.129</b>	<b>0.105</b>	<b>0.488</b>	<b>0.092</b>	<b>0.267</b>	<b>0.199</b>	<b>0.062</b>	<b>0.253</b>	<b>0.156</b>	<b>0.022</b>	<b>0.018</b>	<b>0.007</b>	<b>0.007</b>
<b>SD</b>	<b>0.0044</b>	<b>0.0035</b>	<b>0.0007</b>	<b>0.0012</b>	<b>0.0004</b>	<b>0.0024</b>	<b>0.0015</b>	<b>0.0025</b>	<b>0.0339</b>	<b>0.0049</b>	<b>0.0038</b>	<b>0.0037</b>	<b>0.0104</b>	<b>0.0027</b>	<b>0.0098</b>	<b>0.0048</b>	<b>0.0006</b>	<b>0.0060</b>	<b>0.0052</b>	<b>0.0011</b>	<b>0.0010</b>	<b>0.0014</b>	<b>0.0017</b>
<b>%RSD</b>	<b>1.7</b>	<b>1.5</b>	<b>8.4</b>	<b>7.8</b>	<b>4.7</b>	<b>2.0</b>	<b>8.3</b>	<b>5.3</b>	<b>9.7</b>	<b>4.5</b>	<b>2.9</b>	<b>3.5</b>	<b>2.1</b>	<b>2.9</b>	<b>3.7</b>	<b>2.4</b>	<b>0.93</b>	<b>2.4</b>	<b>3.3</b>	<b>4.8</b>	<b>5.5</b>	<b>20.7</b>	<b>23.6</b>
250–1	1.195	1.146	0.075	0.057	0.080	0.536	0.225	0.223	0.764	0.468	0.605	0.502	1.346	0.413	0.878	0.980	0.401	0.868	0.539	0.074	0.063	0.071	0.077
250–2	1.195	1.146	0.076	0.054	0.081	0.524	0.225	0.237	0.621	0.465	0.602	0.502	1.376	0.411	0.860	0.960	0.409	0.853	0.555	0.079	0.064	0.071	0.069
250–3	1.215	1.126	0.077	0.069	0.080	0.525	0.216	0.243	0.659	0.474	0.593	0.500	1.386	0.417	0.868	0.948	0.417	0.858	0.543	0.079	0.065	0.069	0.069
250–4	1.215	1.156	0.080	0.057	0.078	0.540	0.222	0.222	0.746	0.480	0.613	0.511	1.406	0.417	0.850	0.975	0.405	0.853	0.539	0.078	0.063	0.078	0.065
250–5	1.165	1.126	0.076	0.055	0.077	0.524	0.207	0.216	0.716	0.443	0.591	0.505	1.396	0.409	0.833	0.937	0.389	0.840	0.523	0.072	0.066	0.066	0.069
250–6	1.145	1.106	0.077	0.051	0.077	0.495	0.225	0.229	0.752	0.460	0.603	0.485	1.316	0.397	0.825	0.924	0.396	0.814	0.526	0.076	0.059	0.073	0.065
<b>Mean</b>	<b>1.188</b>	<b>1.134</b>	<b>0.077</b>	<b>0.057</b>	<b>0.079</b>	<b>0.524</b>	<b>0.220</b>	<b>0.228</b>	<b>0.709</b>	<b>0.465</b>	<b>0.601</b>	<b>0.501</b>	<b>1.371</b>	<b>0.410</b>	<b>0.852</b>	<b>0.954</b>	<b>0.403</b>	<b>0.848</b>	<b>0.537</b>	<b>0.076</b>	<b>0.063</b>	<b>0.071</b>	<b>0.069</b>
<b>SD</b>	<b>0.026</b>	<b>0.017</b>	<b>0.002</b>	<b>0.006</b>	<b>0.002</b>	<b>0.014</b>	<b>0.007</b>	<b>0.009</b>	<b>0.052</b>	<b>0.012</b>	<b>0.007</b>	<b>0.008</b>	<b>0.031</b>	<b>0.007</b>	<b>0.019</b>	<b>0.020</b>	<b>0.009</b>	<b>0.017</b>	<b>0.011</b>	<b>0.003</b>	<b>0.002</b>	<b>0.003</b>	<b>0.004</b>
<b>%RSD</b>	<b>2.2</b>	<b>1.5</b>	<b>2.0</b>	<b>9.9</b>	<b>2.0</b>	<b>2.7</b>	<b>3.0</b>	<b>4.1</b>	<b>7.4</b>	<b>2.5</b>	<b>1.2</b>	<b>1.6</b>	<b>2.3</b>	<b>1.7</b>	<b>2.2</b>	<b>2.1</b>	<b>2.2</b>	<b>2.0</b>	<b>2.0</b>	<b>3.6</b>	<b>3.4</b>	<b>4.8</b>	<b>6.0</b>
500–1	2.205	2.176	0.160	0.108	0.164	1.047	0.446	0.447	1.190	0.846	1.185	0.974	2.326	0.772	1.583	1.890	0.787	1.547	1.017	0.142	0.109	0.150	0.144
500–2	2.245	2.266	0.163	0.107	0.170	1.047	0.448	0.462	1.170	0.855	1.165	0.954	2.326	0.796	1.613	1.950	0.781	1.577	0.997	0.145	0.113	0.156	0.145
500–3	2.285	2.246	0.164	0.114	0.170	1.057	0.475	0.441	1.240	0.852	1.175	0.950	2.426	0.819	1.563	1.890	0.776	1.587	0.997	0.153	0.120	0.160	0.142
500–4	2.355	2.336	0.163	0.116	0.175	1.097	0.468	0.471	1.130	0.793	1.225	1.028	2.506	0.824	1.573	1.950	0.732	1.617	1.047	0.149	0.119	0.152	0.144
500–5	2.285	2.246	0.158	0.106	0.176	1.047	0.473	0.480	1.240	0.819	1.155	0.986	2.366	0.801	1.623	1.920	0.775	1.617	1.017	0.148	0.120	0.160	0.148
500–6	2.155	2.156	0.163	0.102	0.159	1.027	0.463	0.442	1.140	0.775	1.175	0.958	2.296	0.769	1.543	1.870	0.733	1.517	0.972	0.143	0.115	0.148	0.141
<b>Mean</b>	<b>2.255</b>	<b>2.237</b>	<b>0.162</b>	<b>0.109</b>	<b>0.169</b>	<b>1.053</b>	<b>0.462</b>	<b>0.457</b>	<b>1.185</b>	<b>0.823</b>	<b>1.180</b>	<b>0.975</b>	<b>2.375</b>	<b>0.797</b>	<b>1.583</b>	<b>1.911</b>	<b>0.764</b>	<b>1.577</b>	<b>1.007</b>	<b>0.147</b>	<b>0.116</b>	<b>0.154</b>	<b>0.144</b>
<b>SD</b>	<b>0.064</b>	<b>0.059</b>	<b>0.002</b>	<b>0.005</b>	<b>0.006</b>	<b>0.021</b>	<b>0.011</b>	<b>0.015</b>	<b>0.043</b>	<b>0.031</b>	<b>0.022</b>	<b>0.027</b>	<b>0.072</b>	<b>0.021</b>	<b>0.028</b>	<b>0.031</b>	<b>0.023</b>	<b>0.036</b>	<b>0.023</b>	<b>0.004</b>	<b>0.004</b>	<b>0.005</b>	<b>0.002</b>
<b>%RSD</b>	<b>2.8</b>	<b>2.6</b>	<b>1.3</b>	<b>4.4</b>	<b>3.5</b>	<b>2.0</b>	<b>2.5</b>	<b>3.3</b>	<b>3.7</b>	<b>3.7</b>	<b>1.9</b>	<b>2.7</b>	<b>3.0</b>	<b>2.6</b>	<b>1.7</b>	<b>1.6</b>	<b>3.0</b>	<b>2.3</b>	<b>2.3</b>	<b>2.6</b>	<b>3.5</b>	<b>3.0</b>	<b>1.6</b>

**Table S14e.** SIFT-MS repeatability data for Mix 1 in 75% DMI:25% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.277	0.192	0.003	0.006	0.003	0.062	-0.004	0.012	0.340	0.130	0.116	0.115	0.707	0.076	0.215	0.108	0.044	0.227	0.132	0.007	0.006	0.001	0.003
50–2	0.270	0.192	0.002	0.007	0.003	0.060	-0.007	0.011	0.339	0.119	0.113	0.115	0.696	0.078	0.216	0.109	0.042	0.215	0.136	0.008	0.005	0.002	0.002
50–3	0.268	0.190	0.001	0.004	0.003	0.066	-0.006	0.012	0.242	0.150	0.108	0.120	0.682	0.076	0.212	0.104	0.044	0.222	0.131	0.009	0.005	0.002	0.003
50–4	0.266	0.195	0.002	0.005	0.002	0.061	-0.009	0.014	0.290	0.122	0.110	0.113	0.672	0.071	0.234	0.111	0.042	0.222	0.134	0.007	0.005	0.002	0.002
50–5	0.259	0.190	0.003	0.005	0.002	0.066	-0.004	0.007	0.206	0.128	0.112	0.111	0.660	0.075	0.226	0.107	0.044	0.208	0.127	0.007	0.004	0.003	0.003
50–6	0.267	0.195	0.002	0.005	0.003	0.062	-0.007	0.010	0.252	0.115	0.107	0.106	0.652	0.071	0.225	0.112	0.041	0.221	0.132	0.008	0.004	0.002	0.003
<b>Mean</b>	<b>0.268</b>	<b>0.192</b>	<b>0.002</b>	<b>0.005</b>	<b>0.003</b>	<b>0.063</b>	<b>-0.006</b>	<b>0.011</b>	<b>0.278</b>	<b>0.128</b>	<b>0.111</b>	<b>0.113</b>	<b>0.678</b>	<b>0.074</b>	<b>0.221</b>	<b>0.108</b>	<b>0.043</b>	<b>0.220</b>	<b>0.132</b>	<b>0.008</b>	<b>0.005</b>	<b>0.002</b>	<b>0.003</b>
<b>SD</b>	<b>0.0053</b>	<b>0.0021</b>	<b>0.0008</b>	<b>0.0008</b>	<b>0.0005</b>	<b>0.0024</b>	<b>0.0017</b>	<b>0.0022</b>	<b>0.0498</b>	<b>0.0113</b>	<b>0.0031</b>	<b>0.0043</b>	<b>0.0192</b>	<b>0.0027</b>	<b>0.0077</b>	<b>0.0026</b>	<b>0.0012</b>	<b>0.0061</b>	<b>0.0028</b>	<b>0.0009</b>	<b>0.0007</b>	<b>0.0006</b>	<b>0.0004</b>
<b>%RSD</b>	<b>2.0</b>	<b>1.1</b>	<b>37.5</b>	<b>15.6</b>	<b>19.7</b>	<b>3.8</b>	<b>-28.0</b>	<b>19.7</b>	<b>17.9</b>	<b>8.9</b>	<b>2.7</b>	<b>3.8</b>	<b>2.8</b>	<b>3.6</b>	<b>3.5</b>	<b>2.4</b>	<b>2.7</b>	<b>2.8</b>	<b>2.1</b>	<b>12.0</b>	<b>13.6</b>	<b>30.2</b>	<b>15.9</b>
250–1	1.177	0.934	0.021	0.017	0.020	0.302	0.029	0.130	1.486	1.162	0.501	0.432	1.607	0.313	0.738	0.555	0.181	0.734	0.515	0.020	0.015	0.018	0.013
250–2	1.227	0.954	0.020	0.018	0.019	0.304	0.036	0.058	0.450	0.286	0.525	0.465	1.707	0.315	0.688	0.533	0.182	0.729	0.471	0.019	0.016	0.016	0.013
250–3	1.177	0.927	0.021	0.018	0.021	0.298	0.030	0.055	0.562	0.287	0.509	0.442	1.657	0.307	0.683	0.543	0.194	0.739	0.449	0.021	0.014	0.016	0.019
250–4	1.177	0.929	0.020	0.016	0.018	0.295	0.035	0.057	0.576	0.305	0.520	0.459	1.687	0.310	0.698	0.553	0.184	0.728	0.476	0.020	0.014	0.016	0.013
250–5	1.147	0.906	0.020	0.015	0.021	0.296	0.031	0.045	0.476	0.258	0.516	0.455	1.657	0.300	0.671	0.540	0.168	0.695	0.444	0.019	0.015	0.015	0.014
250–6	1.217	0.937	0.021	0.013	0.019	0.298	0.030	0.049	0.395	0.271	0.510	0.457	1.677	0.308	0.691	0.555	0.187	0.727	0.465	0.023	0.014	0.015	0.018
<b>Mean</b>	<b>1.187</b>	<b>0.931</b>	<b>0.020</b>	<b>0.016</b>	<b>0.020</b>	<b>0.299</b>	<b>0.032</b>	<b>0.066</b>	<b>0.657</b>	<b>0.428</b>	<b>0.514</b>	<b>0.451</b>	<b>1.665</b>	<b>0.309</b>	<b>0.695</b>	<b>0.546</b>	<b>0.183</b>	<b>0.726</b>	<b>0.470</b>	<b>0.020</b>	<b>0.015</b>	<b>0.016</b>	<b>0.015</b>
<b>SD</b>	<b>0.027</b>	<b>0.014</b>	<b>0.001</b>	<b>0.002</b>	<b>0.001</b>	<b>0.003</b>	<b>0.003</b>	<b>0.029</b>	<b>0.376</b>	<b>0.329</b>	<b>0.008</b>	<b>0.011</b>	<b>0.031</b>	<b>0.005</b>	<b>0.021</b>	<b>0.008</b>	<b>0.008</b>	<b>0.014</b>	<b>0.023</b>	<b>0.001</b>	<b>0.001</b>	<b>0.001</b>	<b>0.002</b>
<b>%RSD</b>	<b>2.3</b>	<b>1.5</b>	<b>2.7</b>	<b>10.7</b>	<b>5.8</b>	<b>1.1</b>	<b>8.3</b>	<b>44.5</b>	<b>57.2</b>	<b>76.7</b>	<b>1.5</b>	<b>2.5</b>	<b>1.9</b>	<b>1.6</b>	<b>3.0</b>	<b>1.5</b>	<b>4.3</b>	<b>2.0</b>	<b>4.9</b>	<b>6.8</b>	<b>3.9</b>	<b>5.5</b>	<b>16.3</b>
500–1	2.217	1.805	0.043	0.034	0.044	0.594	0.097	0.107	0.637	0.420	0.984	0.861	2.827	0.607	1.273	1.099	0.367	1.327	0.841	0.038	0.028	0.036	0.032
500–2	2.327	1.875	0.044	0.030	0.050	0.595	0.098	0.111	0.641	0.456	1.006	0.868	2.917	0.615	1.273	1.099	0.381	1.347	0.872	0.040	0.028	0.040	0.035
500–3	2.297	1.835	0.050	0.035	0.046	0.609	0.099	0.102	0.585	0.430	1.006	0.864	2.867	0.600	1.293	1.089	0.376	1.367	0.854	0.039	0.029	0.033	0.035
500–4	2.317	1.865	0.044	0.031	0.044	0.589	0.094	0.108	0.618	0.451	0.996	0.824	2.817	0.612	1.293	1.119	0.385	1.357	0.868	0.041	0.028	0.036	0.035
500–5	2.277	1.845	0.047	0.031	0.049	0.598	0.090	0.116	0.699	0.459	1.006	0.864	2.757	0.608	1.303	1.099	0.377	1.367	0.877	0.037	0.030	0.039	0.032
500–6	2.257	1.815	0.046	0.029	0.048	0.617	0.093	0.116	0.722	0.469	1.026	0.863	2.737	0.610	1.293	1.139	0.383	1.347	0.894	0.041	0.028	0.034	0.034
<b>Mean</b>	<b>2.282</b>	<b>1.840</b>	<b>0.046</b>	<b>0.032</b>	<b>0.047</b>	<b>0.600</b>	<b>0.095</b>	<b>0.110</b>	<b>0.650</b>	<b>0.448</b>	<b>1.004</b>	<b>0.857</b>	<b>2.820</b>	<b>0.609</b>	<b>1.288</b>	<b>1.107</b>	<b>0.378</b>	<b>1.352</b>	<b>0.868</b>	<b>0.039</b>	<b>0.028</b>	<b>0.036</b>	<b>0.034</b>
<b>SD</b>	<b>0.037</b>	<b>0.025</b>	<b>0.002</b>	<b>0.002</b>	<b>0.002</b>	<b>0.010</b>	<b>0.003</b>	<b>0.005</b>	<b>0.047</b>	<b>0.017</b>	<b>0.013</b>	<b>0.015</b>	<b>0.061</b>	<b>0.005</b>	<b>0.011</b>	<b>0.017</b>	<b>0.006</b>	<b>0.014</b>	<b>0.017</b>	<b>0.001</b>	<b>0.001</b>	<b>0.003</b>	<b>0.001</b>
<b>%RSD</b>	<b>1.6</b>	<b>1.4</b>	<b>5.1</b>	<b>6.2</b>	<b>5.3</b>	<b>1.6</b>	<b>3.3</b>	<b>4.5</b>	<b>7.2</b>	<b>3.8</b>	<b>1.3</b>	<b>1.8</b>	<b>2.2</b>	<b>0.8</b>	<b>0.9</b>	<b>1.5</b>	<b>1.6</b>	<b>1.0</b>	<b>1.9</b>	<b>3.8</b>	<b>2.4</b>	<b>7.2</b>	<b>4.4</b>

**Table S14f.** SIFT-MS repeatability data for Mix 1 in 100% DMI at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.190	0.159	0.002	0.001	0.000	0.029	-0.008	0.170	2.463	1.069	0.099	0.112	0.846	0.038	0.237	0.053	0.033	0.125	0.165	0.001	0.001	0.001	0.002
50–2	0.207	0.167	0.002	0.001	0.000	0.029	-0.002	0.190	2.503	1.189	0.093	0.112	0.859	0.037	0.248	0.051	0.034	0.125	0.164	0.001	0.001	0.000	-0.001
50–3	0.193	0.169	0.000	0.001	0.001	0.031	-0.004	0.182	2.683	1.159	0.104	0.118	0.858	0.039	0.270	0.057	0.035	0.124	0.167	0.001	0.001	0.001	0.000
50–4	0.196	0.168	0.001	0.004	0.000	0.029	-0.005	0.180	2.473	1.139	0.101	0.111	0.846	0.038	0.260	0.057	0.037	0.118	0.161	0.001	0.000	0.001	-0.001
50–5	0.210	0.158	0.000	0.001	0.000	0.031	-0.003	0.181	2.503	1.169	0.102	0.114	0.856	0.037	0.258	0.054	0.035	0.119	0.169	0.002	0.000	0.001	0.001
50–6	0.190	0.168	0.001	0.000	0.000	0.031	-0.004	0.189	2.493	1.289	0.096	0.111	0.863	0.034	0.271	0.060	0.036	0.124	0.179	0.001	0.001	0.001	0.000
<b>Mean</b>	<b>0.198</b>	<b>0.165</b>	<b>0.001</b>	<b>0.001</b>	<b>0.000</b>	<b>0.030</b>	<b>-0.004</b>	<b>0.182</b>	<b>2.520</b>	<b>1.169</b>	<b>0.099</b>	<b>0.113</b>	<b>0.855</b>	<b>0.037</b>	<b>0.258</b>	<b>0.055</b>	<b>0.035</b>	<b>0.122</b>	<b>0.167</b>	<b>0.001</b>	<b>0.001</b>	<b>0.001</b>	<b>0.000</b>
<b>SD</b>	<b>0.0080</b>	<b>0.0045</b>	<b>0.0006</b>	<b>0.0012</b>	<b>0.0003</b>	<b>0.0010</b>	<b>0.0018</b>	<b>0.0066</b>	<b>0.0745</b>	<b>0.0656</b>	<b>0.0037</b>	<b>0.0024</b>	<b>0.0065</b>	<b>0.0015</b>	<b>0.0119</b>	<b>0.0030</b>	<b>0.0013</b>	<b>0.0029</b>	<b>0.0057</b>	<b>0.0003</b>	<b>0.0004</b>	<b>0.0003</b>	<b>0.0010</b>
<b>%RSD</b>	<b>4.0</b>	<b>2.7</b>	<b>55.0</b>	<b>101.6</b>	<b>196.8</b>	<b>3.5</b>	<b>-43.3</b>	<b>3.6</b>	<b>3.0</b>	<b>5.6</b>	<b>3.7</b>	<b>2.2</b>	<b>0.76</b>	<b>4.1</b>	<b>4.6</b>	<b>5.3</b>	<b>3.6</b>	<b>2.4</b>	<b>3.4</b>	<b>29.2</b>	<b>61.1</b>	<b>30.2</b>	<b>868.1</b>
250–1	0.939	0.694	0.004	0.006	0.004	0.134	0.002	0.096	1.263	0.782	0.373	0.326	1.905	0.167	0.483	0.274	0.051	0.441	0.355	0.003	0.002	0.004	0.002
250–2	0.871	0.679	0.004	0.005	0.003	0.126	-0.002	0.086	1.273	0.700	0.375	0.321	1.885	0.168	0.469	0.261	0.047	0.451	0.343	0.003	0.001	0.002	0.002
250–3	0.935	0.685	0.004	0.002	0.003	0.131	-0.003	0.084	1.213	0.706	0.382	0.324	1.915	0.167	0.479	0.262	0.049	0.450	0.339	0.003	0.002	0.002	0.001
250–4	0.931	0.704	0.005	0.004	0.004	0.135	0.000	0.084	1.293	0.736	0.370	0.322	1.905	0.161	0.473	0.269	0.047	0.444	0.330	0.003	0.002	0.003	0.001
250–5	0.921	0.703	0.005	0.004	0.004	0.136	-0.001	0.087	1.193	0.736	0.374	0.323	1.905	0.167	0.487	0.261	0.051	0.446	0.343	0.003	0.002	0.003	0.001
250–6	0.908	0.689	0.005	0.004	0.004	0.132	-0.001	0.085	1.193	0.770	0.372	0.321	1.895	0.169	0.487	0.270	0.048	0.440	0.326	0.004	0.002	0.003	0.002
<b>Mean</b>	<b>0.918</b>	<b>0.692</b>	<b>0.005</b>	<b>0.004</b>	<b>0.004</b>	<b>0.132</b>	<b>-0.001</b>	<b>0.087</b>	<b>1.238</b>	<b>0.738</b>	<b>0.374</b>	<b>0.323</b>	<b>1.902</b>	<b>0.167</b>	<b>0.480</b>	<b>0.266</b>	<b>0.049</b>	<b>0.445</b>	<b>0.339</b>	<b>0.003</b>	<b>0.002</b>	<b>0.003</b>	<b>0.001</b>
<b>SD</b>	<b>0.023</b>	<b>0.009</b>	<b>0.001</b>	<b>0.001</b>	<b>0.000</b>	<b>0.003</b>	<b>0.001</b>	<b>0.004</b>	<b>0.040</b>	<b>0.030</b>	<b>0.004</b>	<b>0.002</b>	<b>0.009</b>	<b>0.003</b>	<b>0.007</b>	<b>0.005</b>	<b>0.002</b>	<b>0.004</b>	<b>0.009</b>	<b>0.000</b>	<b>0.000</b>	<b>0.001</b>	<b>0.000</b>
<b>%RSD</b>	<b>2.5</b>	<b>1.3</b>	<b>11.9</b>	<b>34.3</b>	<b>11.4</b>	<b>2.5</b>	<b>-204.5</b>	<b>4.9</b>	<b>3.2</b>	<b>4.1</b>	<b>1.0</b>	<b>0.55</b>	<b>0.50</b>	<b>1.5</b>	<b>1.4</b>	<b>1.9</b>	<b>3.3</b>	<b>0.93</b>	<b>2.8</b>	<b>11.9</b>	<b>16.3</b>	<b>24.1</b>	<b>30.4</b>
500–1	1.914	1.393	0.012	0.007	0.013	0.270	0.008	0.049	0.569	0.424	0.745	0.643	3.235	0.355	0.864	0.539	0.102	0.917	0.633	0.008	0.006	0.006	0.006
500–2	1.864	1.383	0.013	0.009	0.012	0.266	0.007	0.063	0.631	0.462	0.727	0.635	3.145	0.353	0.868	0.544	0.104	0.941	0.619	0.009	0.007	0.009	0.005
500–3	1.884	1.363	0.013	0.009	0.012	0.274	0.012	0.067	0.816	0.507	0.763	0.636	3.165	0.349	0.844	0.543	0.107	0.918	0.645	0.009	0.006	0.006	0.006
500–4	1.904	1.363	0.011	0.008	0.011	0.271	0.008	0.060	0.835	0.497	0.729	0.625	3.155	0.357	0.839	0.551	0.107	0.912	0.625	0.008	0.005	0.007	0.004
500–5	1.934	1.373	0.013	0.011	0.013	0.269	0.008	0.059	0.799	0.508	0.722	0.618	3.165	0.343	0.851	0.547	0.108	0.912	0.625	0.009	0.006	0.007	0.003
500–6	1.904	1.373	0.010	0.009	0.011	0.280	0.009	0.070	0.674	0.576	0.691	0.615	3.125	0.358	0.847	0.542	0.102	0.917	0.621	0.008	0.006	0.006	0.005
<b>Mean</b>	<b>1.901</b>	<b>1.375</b>	<b>0.012</b>	<b>0.009</b>	<b>0.012</b>	<b>0.272</b>	<b>0.009</b>	<b>0.061</b>	<b>0.721</b>	<b>0.495</b>	<b>0.730</b>	<b>0.629</b>	<b>3.165</b>	<b>0.353</b>	<b>0.853</b>	<b>0.544</b>	<b>0.105</b>	<b>0.919</b>	<b>0.628</b>	<b>0.008</b>	<b>0.006</b>	<b>0.007</b>	<b>0.005</b>
<b>SD</b>	<b>0.022</b>	<b>0.011</b>	<b>0.001</b>	<b>0.001</b>	<b>0.001</b>	<b>0.004</b>	<b>0.002</b>	<b>0.007</b>	<b>0.101</b>	<b>0.047</b>	<b>0.022</b>	<b>0.010</b>	<b>0.034</b>	<b>0.005</b>	<b>0.010</b>	<b>0.004</b>	<b>0.002</b>	<b>0.010</b>	<b>0.009</b>	<b>0.000</b>	<b>0.001</b>	<b>0.001</b>	<b>0.001</b>
<b>%RSD</b>	<b>1.2</b>	<b>0.78</b>	<b>8.1</b>	<b>14.5</b>	<b>6.7</b>	<b>1.6</b>	<b>20.6</b>	<b>10.7</b>	<b>14.1</b>	<b>9.4</b>	<b>3.0</b>	<b>1.6</b>	<b>1.1</b>	<b>1.5</b>	<b>1.2</b>	<b>0.70</b>	<b>2.3</b>	<b>1.1</b>	<b>1.4</b>	<b>5.6</b>	<b>9.1</b>	<b>15.3</b>	<b>18.3</b>

**Table S15.** SIFT-MS repeatability data for Mix 2 in 100% DMI at three levels (50, 250, and 500).

Level-Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50-1	0.180	0.109	0.070	0.041	0.072	0.014	0.021	0.009	-0.110	0.110	0.054	0.049	0.128	0.068	0.161	0.042	0.085	0.177	0.113	0.034	0.026	0.031	0.030
50-2	0.180	0.110	0.064	0.043	0.073	0.016	0.020	-0.008	-0.040	0.110	0.055	0.061	0.135	0.067	0.153	0.043	0.083	0.192	0.117	0.034	0.028	0.028	0.029
50-3	0.175	0.108	0.068	0.043	0.076	0.019	0.021	0.010	0.270	0.240	0.058	0.063	0.131	0.068	0.170	0.043	0.084	0.191	0.133	0.033	0.026	0.030	0.023
50-4	0.174	0.113	0.067	0.047	0.069	0.017	0.019	-0.015	-0.020	0.000	0.051	0.058	0.129	0.066	0.151	0.043	0.084	0.177	0.113	0.032	0.025	0.027	0.029
50-5	0.176	0.113	0.069	0.049	0.069	0.015	0.024	0.014	0.150	0.180	0.057	0.062	0.135	0.066	0.161	0.042	0.083	0.180	0.126	0.031	0.026	0.024	0.026
50-6	0.174	0.117	0.071	0.038	0.070	0.018	0.017	-0.014	-0.140	0.020	0.062	0.057	0.131	0.063	0.150	0.044	0.081	0.181	0.107	0.033	0.027	0.028	0.026
<b>Mean</b>	<b>0.177</b>	<b>0.112</b>	<b>0.068</b>	<b>0.043</b>	<b>0.071</b>	<b>0.017</b>	<b>0.020</b>	<b>-0.001</b>	<b>0.018</b>	<b>0.110</b>	<b>0.056</b>	<b>0.058</b>	<b>0.132</b>	<b>0.066</b>	<b>0.158</b>	<b>0.043</b>	<b>0.084</b>	<b>0.183</b>	<b>0.118</b>	<b>0.033</b>	<b>0.026</b>	<b>0.028</b>	<b>0.027</b>
<b>SD</b>	<b>0.0026</b>	<b>0.0030</b>	<b>0.0023</b>	<b>0.0036</b>	<b>0.0025</b>	<b>0.0018</b>	<b>0.0021</b>	<b>0.0120</b>	<b>0.1455</b>	<b>0.0837</b>	<b>0.0035</b>	<b>0.0047</b>	<b>0.0027</b>	<b>0.0015</b>	<b>0.0071</b>	<b>0.0006</b>	<b>0.0012</b>	<b>0.0062</b>	<b>0.0088</b>	<b>0.0010</b>	<b>0.0007</b>	<b>0.0024</b>	<b>0.0021</b>
<b>%RSD</b>	<b>1.5</b>	<b>2.7</b>	<b>3.3</b>	<b>8.2</b>	<b>3.5</b>	<b>11.1</b>	<b>10.3</b>	<b>-1795.1</b>	<b>793.8</b>	<b>76.1</b>	<b>6.3</b>	<b>8.0</b>	<b>2.1</b>	<b>2.3</b>	<b>4.5</b>	<b>1.5</b>	<b>1.5</b>	<b>3.4</b>	<b>7.4</b>	<b>3.2</b>	<b>2.8</b>	<b>8.5</b>	<b>7.9</b>
250-1	0.920	0.553	0.401	0.270	0.434	0.076	0.133	0.033	1.120	0.100	0.286	0.253	0.557	0.359	0.748	0.217	0.578	0.950	0.578	0.194	0.169	0.186	0.165
250-2	0.949	0.571	0.422	0.270	0.418	0.078	0.131	0.019	0.310	-0.066	0.298	0.260	0.553	0.372	0.739	0.218	0.578	0.952	0.585	0.195	0.172	0.178	0.165
250-3	0.941	0.563	0.396	0.268	0.429	0.074	0.126	0.030	0.290	0.070	0.290	0.259	0.553	0.362	0.753	0.209	0.603	0.929	0.603	0.204	0.166	0.183	0.182
250-4	0.890	0.529	0.411	0.263	0.423	0.073	0.131	0.028	-0.070	0.210	0.285	0.249	0.519	0.345	0.742	0.212	0.512	0.903	0.604	0.193	0.166	0.179	0.180
250-5	0.929	0.575	0.422	0.258	0.423	0.075	0.125	0.031	0.120	0.090	0.290	0.254	0.551	0.362	0.736	0.211	0.617	0.932	0.594	0.200	0.168	0.182	0.179
250-6	0.919	0.564	0.414	0.270	0.414	0.074	0.134	0.031	0.110	0.060	0.294	0.256	0.553	0.362	0.768	0.220	0.647	0.966	0.581	0.199	0.167	0.181	0.172
<b>Mean</b>	<b>0.925</b>	<b>0.559</b>	<b>0.411</b>	<b>0.266</b>	<b>0.424</b>	<b>0.075</b>	<b>0.130</b>	<b>0.029</b>	<b>0.313</b>	<b>0.077</b>	<b>0.290</b>	<b>0.255</b>	<b>0.548</b>	<b>0.361</b>	<b>0.748</b>	<b>0.214</b>	<b>0.590</b>	<b>0.938</b>	<b>0.591</b>	<b>0.198</b>	<b>0.168</b>	<b>0.181</b>	<b>0.173</b>
<b>SD</b>	<b>0.019</b>	<b>0.015</b>	<b>0.010</b>	<b>0.005</b>	<b>0.007</b>	<b>0.002</b>	<b>0.003</b>	<b>0.005</b>	<b>0.382</b>	<b>0.081</b>	<b>0.004</b>	<b>0.004</b>	<b>0.013</b>	<b>0.008</b>	<b>0.011</b>	<b>0.004</b>	<b>0.042</b>	<b>0.020</b>	<b>0.010</b>	<b>0.004</b>	<b>0.002</b>	<b>0.003</b>	<b>0.007</b>
<b>%RSD</b>	<b>2.0</b>	<b>2.7</b>	<b>2.4</b>	<b>1.7</b>	<b>1.6</b>	<b>2.2</b>	<b>2.6</b>	<b>15.9</b>	<b>122.0</b>	<b>104.5</b>	<b>1.5</b>	<b>1.5</b>	<b>2.4</b>	<b>2.2</b>	<b>1.4</b>	<b>1.9</b>	<b>7.1</b>	<b>2.2</b>	<b>1.7</b>	<b>2.0</b>	<b>1.2</b>	<b>1.5</b>	<b>4.0</b>
500-1	1.882	1.226	0.956	0.627	1.003	0.160	0.357	0.202	18.840	0.640	0.584	0.590	1.035	0.773	1.557	0.430	1.450	1.976	1.269	0.473	0.414	0.514	0.447
500-2	1.892	1.136	0.970	0.602	1.023	0.165	0.342	0.208	8.740	0.640	0.567	0.536	1.025	0.755	1.547	0.430	1.440	2.016	1.279	0.474	0.427	0.479	0.447
500-3	1.892	1.106	0.963	0.646	1.023	0.169	0.334	0.198	4.970	0.630	0.599	0.528	1.065	0.778	1.597	0.435	1.450	2.026	1.289	0.470	0.412	0.460	0.470
500-4	1.882	1.096	0.970	0.622	1.023	0.166	0.338	0.201	2.940	0.520	0.584	0.535	1.065	0.758	1.567	0.431	1.430	2.026	1.299	0.470	0.417	0.465	0.454
500-5	1.902	1.096	0.976	0.620	1.003	0.168	0.327	0.184	2.120	0.520	0.580	0.526	1.035	0.758	1.537	0.438	1.450	1.956	1.309	0.488	0.413	0.487	0.472
500-6	1.822	1.076	0.955	0.625	1.023	0.161	0.328	0.185	1.620	0.450	0.582	0.522	1.035	0.751	1.537	0.431	1.410	1.926	1.259	0.478	0.415	0.458	0.445
<b>Mean</b>	<b>1.879</b>	<b>1.123</b>	<b>0.965</b>	<b>0.623</b>	<b>1.017</b>	<b>0.165</b>	<b>0.338</b>	<b>0.196</b>	<b>6.538</b>	<b>0.567</b>	<b>0.583</b>	<b>0.540</b>	<b>1.043</b>	<b>0.763</b>	<b>1.557</b>	<b>0.432</b>	<b>1.439</b>	<b>1.987</b>	<b>1.284</b>	<b>0.476</b>	<b>0.417</b>	<b>0.477</b>	<b>0.455</b>
<b>SD</b>	<b>0.026</b>	<b>0.050</b>	<b>0.008</b>	<b>0.013</b>	<b>0.009</b>	<b>0.003</b>	<b>0.010</b>	<b>0.009</b>	<b>5.990</b>	<b>0.074</b>	<b>0.009</b>	<b>0.023</b>	<b>0.016</b>	<b>0.010</b>	<b>0.021</b>	<b>0.003</b>	<b>0.015</b>	<b>0.038</b>	<b>0.017</b>	<b>0.006</b>	<b>0.005</b>	<b>0.019</b>	<b>0.011</b>
<b>%RSD</b>	<b>1.4</b>	<b>4.4</b>	<b>0.80</b>	<b>2.1</b>	<b>0.93</b>	<b>2.0</b>	<b>3.0</b>	<b>4.5</b>	<b>91.6</b>	<b>13.0</b>	<b>1.6</b>	<b>4.3</b>	<b>1.5</b>	<b>1.3</b>	<b>1.3</b>	<b>0.69</b>	<b>1.0</b>	<b>1.9</b>	<b>1.3</b>	<b>1.3</b>	<b>1.2</b>	<b>4.1</b>	<b>2.4</b>



**Table S16a.** SIFT-MS repeatability data for Mix 1 in 5% DMSO:95% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.341	0.216	0.070	0.052	0.027	0.352	0.204	0.177	0.121	0.087	0.165	0.171	0.201	0.182	0.313	0.279	0.099	0.207	0.133	0.085	0.070	0.074	0.077
50–2	0.353	0.225	0.160	0.015	0.106	0.350	0.198	0.175	0.138	0.084	0.170	0.178	0.227	0.183	0.315	0.275	0.099	0.205	0.127	0.084	0.065	0.073	0.068
50–3	0.344	0.214	-0.060	0.022	-0.050	0.355	0.186	0.168	0.123	0.084	0.161	0.161	0.204	0.175	0.301	0.263	0.097	0.205	0.129	0.083	0.065	0.067	0.069
50–4	0.377	0.244	0.380	0.078	0.276	0.369	0.209	0.191	0.106	0.084	0.184	0.182	0.219	0.193	0.323	0.296	0.097	0.221	0.135	0.088	0.068	0.073	0.067
50–5	0.345	0.220	-0.030	0.048	-0.035	0.352	0.202	0.174	0.097	0.083	0.173	0.169	0.207	0.176	0.314	0.279	0.100	0.207	0.133	0.079	0.066	0.067	0.069
50–6	0.331	0.206	-0.120	0.021	-0.099	0.344	0.186	0.170	0.090	0.086	0.164	0.164	0.195	0.174	0.307	0.271	0.100	0.197	0.126	0.082	0.066	0.066	0.064
<b>Mean</b>	<b>0.349</b>	<b>0.221</b>	<b>0.067</b>	<b>0.039</b>	<b>0.037</b>	<b>0.353</b>	<b>0.198</b>	<b>0.176</b>	<b>0.113</b>	<b>0.085</b>	<b>0.170</b>	<b>0.171</b>	<b>0.208</b>	<b>0.181</b>	<b>0.312</b>	<b>0.277</b>	<b>0.099</b>	<b>0.207</b>	<b>0.130</b>	<b>0.084</b>	<b>0.067</b>	<b>0.070</b>	<b>0.069</b>
<b>SD</b>	<b>0.0143</b>	<b>0.0119</b>	<b>0.1669</b>	<b>0.0222</b>	<b>0.1247</b>	<b>0.0076</b>	<b>0.0088</b>	<b>0.0074</b>	<b>0.0164</b>	<b>0.0015</b>	<b>0.0076</b>	<b>0.0073</b>	<b>0.0109</b>	<b>0.0066</b>	<b>0.0068</b>	<b>0.0100</b>	<b>0.0012</b>	<b>0.0071</b>	<b>0.0034</b>	<b>0.0028</b>	<b>0.0016</b>	<b>0.0034</b>	<b>0.0042</b>
<b>%RSD</b>	<b>4.1</b>	<b>5.4</b>	<b>250.3</b>	<b>56.5</b>	<b>332.4</b>	<b>2.2</b>	<b>4.4</b>	<b>4.2</b>	<b>14.6</b>	<b>1.7</b>	<b>4.5</b>	<b>4.3</b>	<b>5.2</b>	<b>3.6</b>	<b>2.2</b>	<b>3.6</b>	<b>1.3</b>	<b>3.4</b>	<b>2.6</b>	<b>3.3</b>	<b>2.4</b>	<b>4.9</b>	<b>6.1</b>
250–1	1.69	1.19	0.350	0.390	0.446	1.59	1.42	1.34	0.737	0.741	0.809	0.820	0.956	0.871	1.48	1.29	0.755	0.986	0.632	0.614	0.507	0.599	0.554
250–2	1.68	1.21	0.550	0.377	0.566	1.64	1.50	1.39	0.794	0.799	0.807	0.828	0.967	0.890	1.53	1.29	0.802	1.02	0.663	0.642	0.543	0.643	0.590
250–3	1.76	1.24	0.340	0.367	0.416	1.67	1.50	1.43	0.760	0.755	0.820	0.822	0.991	0.913	1.56	1.33	0.789	1.03	0.664	0.652	0.551	0.638	0.606
250–4	1.70	1.19	1.06	0.405	0.956	1.69	1.50	1.42	0.782	0.755	0.827	0.819	0.952	0.886	1.54	1.35	0.786	1.01	0.659	0.621	0.548	0.598	0.598
250–5	1.95	1.47	2.37	0.475	1.98	1.86	1.66	1.52	0.714	0.668	0.822	0.957	1.161	0.993	1.65	1.52	0.738	1.12	0.722	0.695	0.596	0.634	0.620
250–6	1.88	1.42	0.940	0.408	0.826	1.93	1.63	1.56	0.666	0.706	0.788	0.899	1.101	0.933	1.60	1.49	0.742	1.08	0.683	0.692	0.589	0.645	0.618
<b>Mean</b>	<b>1.77</b>	<b>1.29</b>	<b>0.935</b>	<b>0.404</b>	<b>0.864</b>	<b>1.73</b>	<b>1.54</b>	<b>1.44</b>	<b>0.742</b>	<b>0.737</b>	<b>0.812</b>	<b>0.857</b>	<b>1.021</b>	<b>0.914</b>	<b>1.56</b>	<b>1.38</b>	<b>0.769</b>	<b>1.04</b>	<b>0.670</b>	<b>0.653</b>	<b>0.556</b>	<b>0.627</b>	<b>0.598</b>
<b>SD</b>	<b>0.103</b>	<b>0.114</b>	<b>0.698</b>	<b>0.035</b>	<b>0.534</b>	<b>0.122</b>	<b>0.083</b>	<b>0.075</b>	<b>0.043</b>	<b>0.041</b>	<b>0.013</b>	<b>0.053</b>	<b>0.080</b>	<b>0.040</b>	<b>0.054</b>	<b>0.092</b>	<b>0.025</b>	<b>0.046</b>	<b>0.027</b>	<b>0.031</b>	<b>0.030</b>	<b>0.020</b>	<b>0.022</b>
<b>%RSD</b>	<b>5.8</b>	<b>8.9</b>	<b>74.6</b>	<b>8.7</b>	<b>61.8</b>	<b>7.1</b>	<b>5.4</b>	<b>5.2</b>	<b>5.8</b>	<b>5.6</b>	<b>1.6</b>	<b>6.1</b>	<b>7.9</b>	<b>4.4</b>	<b>3.4</b>	<b>6.7</b>	<b>3.2</b>	<b>4.4</b>	<b>4.1</b>	<b>4.8</b>	<b>5.4</b>	<b>3.2</b>	<b>3.7</b>
500–1	3.37	2.52	1.38	1.03	1.56	3.20	3.67	3.48	2.25	2.20	1.63	1.63	1.95	1.82	3.12	2.61	2.14	2.05	1.40	1.60	1.42	1.63	1.59
500–2	3.48	2.52	1.24	1.02	1.48	3.20	3.73	3.38	2.17	2.08	1.61	1.66	1.96	1.82	3.09	2.54	2.03	2.03	1.36	1.56	1.41	1.60	1.58
500–3	3.40	2.49	1.48	0.997	1.64	3.19	3.69	3.44	2.22	2.07	1.59	1.62	1.93	1.81	3.13	2.53	2.06	2.05	1.39	1.58	1.40	1.63	1.60
500–4	3.41	2.52	1.36	0.987	1.49	3.25	3.70	3.52	2.13	2.06	1.65	1.64	1.94	1.83	3.20	2.65	2.05	2.07	1.42	1.59	1.41	1.67	1.55
500–5	3.93	2.84	1.28	1.06	1.50	3.57	4.05	3.74	2.08	2.04	1.80	1.80	2.14	1.97	3.48	2.91	2.04	2.27	1.58	1.70	1.50	1.75	1.69
500–6	3.40	2.48	1.10	1.03	1.33	3.23	3.66	3.51	2.02	2.08	1.62	1.60	1.89	1.80	3.17	2.62	2.04	2.06	1.38	1.61	1.41	1.67	1.63
<b>Mean</b>	<b>3.49</b>	<b>2.56</b>	<b>1.31</b>	<b>1.02</b>	<b>1.50</b>	<b>3.27</b>	<b>3.75</b>	<b>3.51</b>	<b>2.15</b>	<b>2.09</b>	<b>1.65</b>	<b>1.66</b>	<b>1.97</b>	<b>1.84</b>	<b>3.20</b>	<b>2.64</b>	<b>2.06</b>	<b>2.09</b>	<b>1.43</b>	<b>1.60</b>	<b>1.42</b>	<b>1.65</b>	<b>1.60</b>
<b>SD</b>	<b>0.196</b>	<b>0.125</b>	<b>0.120</b>	<b>0.023</b>	<b>0.094</b>	<b>0.134</b>	<b>0.136</b>	<b>0.112</b>	<b>0.079</b>	<b>0.052</b>	<b>0.070</b>	<b>0.066</b>	<b>0.080</b>	<b>0.058</b>	<b>0.131</b>	<b>0.127</b>	<b>0.037</b>	<b>0.082</b>	<b>0.073</b>	<b>0.045</b>	<b>0.034</b>	<b>0.048</b>	<b>0.044</b>
<b>%RSD</b>	<b>5.6</b>	<b>4.9</b>	<b>9.2</b>	<b>2.2</b>	<b>6.3</b>	<b>4.1</b>	<b>3.6</b>	<b>3.2</b>	<b>3.7</b>	<b>2.5</b>	<b>4.2</b>	<b>4.0</b>	<b>4.1</b>	<b>3.2</b>	<b>4.1</b>	<b>4.8</b>	<b>1.8</b>	<b>3.9</b>	<b>5.1</b>	<b>2.8</b>	<b>2.4</b>	<b>2.9</b>	<b>2.8</b>

**Table S16b.** SIFT-MS repeatability data for Mix 1 in 10% DMSO:90% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.388	0.289	0.520	0.113	0.419	0.358	0.162	0.152	0.071	0.077	0.184	0.184	0.240	0.192	0.317	0.291	0.093	0.217	0.144	0.070	0.054	0.064	0.059
50–2	0.343	0.251	0.340	0.076	0.299	0.315	0.142	0.138	0.004	0.068	0.167	0.162	0.204	0.169	0.277	0.253	0.086	0.194	0.116	0.066	0.047	0.057	0.050
50–3	0.341	0.247	0.200	0.073	0.219	0.310	0.143	0.127	0.064	0.064	0.160	0.160	0.201	0.164	0.291	0.250	0.082	0.186	0.122	0.061	0.048	0.053	0.054
50–4	0.355	0.256	1.010	0.167	0.759	0.325	0.136	0.140	0.046	0.069	0.166	0.161	0.204	0.169	0.297	0.267	0.089	0.194	0.129	0.058	0.046	0.053	0.052
50–5	0.357	0.263	1.400	0.234	1.049	0.343	0.150	0.131	0.077	0.074	0.184	0.179	0.219	0.176	0.309	0.270	0.092	0.208	0.124	0.063	0.047	0.053	0.051
50–6	0.323	0.243	0.430	0.075	0.359	0.304	0.139	0.131	0.095	0.066	0.156	0.156	0.196	0.157	0.273	0.248	0.080	0.187	0.116	0.054	0.043	0.049	0.046
<b>Mean</b>	<b>0.351</b>	<b>0.259</b>	<b>0.650</b>	<b>0.123</b>	<b>0.517</b>	<b>0.326</b>	<b>0.145</b>	<b>0.136</b>	<b>0.060</b>	<b>0.070</b>	<b>0.170</b>	<b>0.167</b>	<b>0.211</b>	<b>0.171</b>	<b>0.294</b>	<b>0.263</b>	<b>0.087</b>	<b>0.198</b>	<b>0.125</b>	<b>0.062</b>	<b>0.047</b>	<b>0.055</b>	<b>0.052</b>
<b>SD</b>	<b>0.0199</b>	<b>0.0152</b>	<b>0.4195</b>	<b>0.0597</b>	<b>0.2923</b>	<b>0.0190</b>	<b>0.0086</b>	<b>0.0082</b>	<b>0.0288</b>	<b>0.0046</b>	<b>0.0109</b>	<b>0.0105</b>	<b>0.0149</b>	<b>0.0109</b>	<b>0.0158</b>	<b>0.0150</b>	<b>0.0049</b>	<b>0.0112</b>	<b>0.0096</b>	<b>0.0051</b>	<b>0.0033</b>	<b>0.0048</b>	<b>0.0040</b>
<b>%RSD</b>	<b>5.7</b>	<b>5.9</b>	<b>64.5</b>	<b>48.5</b>	<b>56.5</b>	<b>5.8</b>	<b>5.9</b>	<b>6.0</b>	<b>48.4</b>	<b>6.5</b>	<b>6.4</b>	<b>6.3</b>	<b>7.1</b>	<b>6.4</b>	<b>5.4</b>	<b>5.7</b>	<b>5.6</b>	<b>5.7</b>	<b>7.6</b>	<b>8.1</b>	<b>6.9</b>	<b>8.7</b>	<b>7.6</b>
250–1	1.706	1.243	0.460	0.316	0.519	1.515	1.171	1.074	0.691	0.675	0.824	0.806	0.993	0.837	1.463	1.299	0.681	0.967	0.630	0.495	0.406	0.479	0.469
250–2	1.686	1.253	0.310	0.333	0.459	1.545	1.181	1.074	0.602	0.655	0.790	0.797	1.003	0.845	1.463	1.269	0.717	0.994	0.638	0.477	0.402	0.479	0.477
250–3	1.676	1.263	0.340	0.309	0.469	1.515	1.171	1.094	0.624	0.682	0.803	0.817	0.984	0.835	1.463	1.279	0.708	0.993	0.647	0.496	0.423	0.507	0.480
250–4	1.756	1.253	0.980	0.347	0.939	1.535	1.211	1.114	0.605	0.681	0.808	0.811	0.993	0.855	1.463	1.279	0.708	0.979	0.622	0.501	0.418	0.495	0.495
250–5	1.696	1.253	0.270	0.316	0.409	1.535	1.231	1.144	0.644	0.664	0.808	0.808	1.003	0.829	1.473	1.319	0.717	0.976	0.639	0.500	0.426	0.491	0.485
250–6	1.616	1.243	0.100	0.296	0.299	1.525	1.191	1.074	0.711	0.672	0.789	0.774	0.933	0.822	1.443	1.289	0.691	0.986	0.640	0.490	0.417	0.489	0.484
<b>Mean</b>	<b>1.690</b>	<b>1.252</b>	<b>0.410</b>	<b>0.320</b>	<b>0.516</b>	<b>1.528</b>	<b>1.192</b>	<b>1.095</b>	<b>0.646</b>	<b>0.672</b>	<b>0.804</b>	<b>0.803</b>	<b>0.985</b>	<b>0.837</b>	<b>1.462</b>	<b>1.289</b>	<b>0.704</b>	<b>0.983</b>	<b>0.636</b>	<b>0.493</b>	<b>0.415</b>	<b>0.490</b>	<b>0.482</b>
<b>SD</b>	<b>0.041</b>	<b>0.007</b>	<b>0.276</b>	<b>0.016</b>	<b>0.201</b>	<b>0.011</b>	<b>0.022</b>	<b>0.026</b>	<b>0.042</b>	<b>0.009</b>	<b>0.012</b>	<b>0.014</b>	<b>0.024</b>	<b>0.011</b>	<b>0.009</b>	<b>0.016</b>	<b>0.013</b>	<b>0.010</b>	<b>0.008</b>	<b>0.008</b>	<b>0.009</b>	<b>0.010</b>	<b>0.008</b>
<b>%RSD</b>	<b>2.5</b>	<b>0.55</b>	<b>67.4</b>	<b>5.2</b>	<b>39.0</b>	<b>0.72</b>	<b>1.8</b>	<b>2.4</b>	<b>6.4</b>	<b>1.4</b>	<b>1.5</b>	<b>1.7</b>	<b>2.4</b>	<b>1.3</b>	<b>0.61</b>	<b>1.3</b>	<b>1.9</b>	<b>1.0</b>	<b>1.3</b>	<b>1.6</b>	<b>2.1</b>	<b>2.0</b>	<b>1.6</b>
500–1	3.316	2.523	1.250	0.897	1.419	3.005	3.161	2.924	1.941	2.022	1.582	1.585	1.923	1.698	2.993	2.539	1.922	2.015	1.354	1.297	1.157	1.435	1.345
500–2	3.436	2.523	1.530	0.947	1.629	2.945	3.201	2.924	1.821	1.982	1.572	1.605	1.973	1.738	2.963	2.469	1.952	2.015	1.334	1.337	1.157	1.405	1.395
500–3	3.446	2.543	0.960	0.867	1.229	3.025	3.201	2.864	1.891	1.922	1.592	1.595	1.933	1.718	3.043	2.589	1.952	1.985	1.324	1.317	1.157	1.365	1.345
500–4	3.426	2.573	1.180	0.857	1.359	3.005	3.191	2.974	1.961	1.992	1.572	1.605	1.963	1.718	3.003	2.549	1.972	2.015	1.374	1.327	1.137	1.435	1.345
500–5	3.396	2.553	1.130	0.817	1.329	2.995	3.221	2.914	1.971	1.942	1.592	1.625	1.953	1.718	3.033	2.529	1.952	2.025	1.374	1.327	1.167	1.375	1.385
500–6	3.396	2.533	1.170	0.877	1.379	2.975	3.221	2.934	1.861	1.982	1.572	1.595	1.923	1.718	3.023	2.509	1.962	1.985	1.334	1.337	1.187	1.435	1.405
<b>Mean</b>	<b>3.403</b>	<b>2.542</b>	<b>1.203</b>	<b>0.877</b>	<b>1.391</b>	<b>2.992</b>	<b>3.199</b>	<b>2.922</b>	<b>1.908</b>	<b>1.974</b>	<b>1.581</b>	<b>1.602</b>	<b>1.945</b>	<b>1.718</b>	<b>3.010</b>	<b>2.530</b>	<b>1.952</b>	<b>2.007</b>	<b>1.349</b>	<b>1.324</b>	<b>1.160</b>	<b>1.408</b>	<b>1.370</b>
<b>SD</b>	<b>0.043</b>	<b>0.018</b>	<b>0.171</b>	<b>0.040</b>	<b>0.122</b>	<b>0.026</b>	<b>0.020</b>	<b>0.032</b>	<b>0.055</b>	<b>0.033</b>	<b>0.009</b>	<b>0.012</b>	<b>0.020</b>	<b>0.012</b>	<b>0.027</b>	<b>0.037</b>	<b>0.015</b>	<b>0.016</b>	<b>0.020</b>	<b>0.014</b>	<b>0.015</b>	<b>0.029</b>	<b>0.026</b>
<b>%RSD</b>	<b>1.3</b>	<b>0.70</b>	<b>14.2</b>	<b>4.5</b>	<b>8.7</b>	<b>0.86</b>	<b>0.64</b>	<b>1.1</b>	<b>2.9</b>	<b>1.7</b>	<b>0.57</b>	<b>0.78</b>	<b>1.0</b>	<b>0.67</b>	<b>0.89</b>	<b>1.5</b>	<b>0.78</b>	<b>0.78</b>	<b>1.5</b>	<b>1.0</b>	<b>1.3</b>	<b>2.1</b>	<b>1.9</b>

**Table S16c.** SIFT-MS repeatability data for Mix 1 in 25% DMSO:75% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.362	0.259	0.410	0.096	0.290	0.262	0.132	0.137	0.087	0.195	0.158	0.169	0.228	0.165	0.283	0.244	0.187	0.195	0.120	0.060	0.049	0.069	0.061
50–2	0.343	0.258	-0.140	0.071	-0.100	0.265	0.157	0.150	0.072	0.196	0.159	0.153	0.212	0.162	0.283	0.259	0.204	0.195	0.123	0.060	0.052	0.068	0.064
50–3	0.368	0.270	0.100	0.099	0.070	0.270	0.151	0.144	0.089	0.185	0.160	0.167	0.226	0.167	0.297	0.255	0.195	0.205	0.124	0.065	0.049	0.074	0.067
50–4	0.359	0.256	0.100	0.102	0.030	0.259	0.153	0.139	0.089	0.184	0.155	0.159	0.216	0.163	0.274	0.255	0.192	0.192	0.114	0.061	0.050	0.069	0.067
50–5	0.360	0.254	-0.140	0.089	-0.060	0.256	0.151	0.129	0.071	0.193	0.160	0.154	0.216	0.163	0.279	0.255	0.194	0.192	0.116	0.063	0.048	0.068	0.058
50–6	0.374	0.257	0.040	0.089	0.050	0.262	0.145	0.131	0.077	0.184	0.169	0.164	0.214	0.165	0.276	0.245	0.180	0.194	0.120	0.064	0.046	0.059	0.064
<b>Mean</b>	<b>0.361</b>	<b>0.259</b>	<b>0.047</b>	<b>0.091</b>	<b>0.047</b>	<b>0.262</b>	<b>0.148</b>	<b>0.139</b>	<b>0.081</b>	<b>0.189</b>	<b>0.160</b>	<b>0.161</b>	<b>0.218</b>	<b>0.164</b>	<b>0.282</b>	<b>0.252</b>	<b>0.192</b>	<b>0.196</b>	<b>0.119</b>	<b>0.062</b>	<b>0.049</b>	<b>0.068</b>	<b>0.064</b>
<b>SD</b>	<b>0.0096</b>	<b>0.0052</b>	<b>0.1853</b>	<b>0.0101</b>	<b>0.1245</b>	<b>0.0044</b>	<b>0.0081</b>	<b>0.0072</b>	<b>0.0078</b>	<b>0.0053</b>	<b>0.0043</b>	<b>0.0061</b>	<b>0.0061</b>	<b>0.0017</b>	<b>0.0075</b>	<b>0.0056</b>	<b>0.0074</b>	<b>0.0044</b>	<b>0.0035</b>	<b>0.0018</b>	<b>0.0020</b>	<b>0.0047</b>	<b>0.0034</b>
<b>%RSD</b>	<b>2.6</b>	<b>2.0</b>	<b>397.0</b>	<b>11.2</b>	<b>266.7</b>	<b>1.7</b>	<b>5.4</b>	<b>5.2</b>	<b>9.6</b>	<b>2.8</b>	<b>2.7</b>	<b>3.8</b>	<b>2.8</b>	<b>1.0</b>	<b>2.7</b>	<b>2.2</b>	<b>3.8</b>	<b>2.3</b>	<b>3.0</b>	<b>2.9</b>	<b>4.1</b>	<b>6.9</b>	<b>5.3</b>
250–1	1.707	1.223	0.160	0.265	0.290	1.205	1.045	0.955	1.265	1.240	0.779	0.766	0.992	0.761	1.357	1.188	1.230	0.954	0.612	0.389	0.327	0.465	0.476
250–2	1.777	1.293	0.510	0.277	0.570	1.235	1.065	0.975	1.175	1.250	0.807	0.786	1.042	0.805	1.407	1.228	1.250	0.975	0.638	0.408	0.346	0.485	0.475
250–3	1.817	1.273	0.590	0.304	1.010	1.265	1.085	0.975	1.095	1.310	0.819	0.795	1.092	0.798	1.427	1.228	1.260	0.994	0.657	0.413	0.351	0.477	0.479
250–4	1.707	1.243	0.570	0.291	0.540	1.205	1.025	0.965	1.145	1.260	0.782	0.765	1.052	0.813	1.387	1.168	1.250	0.961	0.638	0.392	0.334	0.487	0.464
250–5	1.797	1.253	0.570	0.276	0.570	1.205	1.075	0.955	1.305	1.290	0.785	0.776	1.062	0.812	1.387	1.198	1.260	0.972	0.627	0.411	0.344	0.483	0.479
250–6	1.767	1.263	0.240	0.220	0.310	1.215	0.995	0.925	1.145	1.260	0.781	0.789	1.052	0.811	1.387	1.188	1.230	0.987	0.625	0.394	0.329	0.469	0.437
<b>Mean</b>	<b>1.762</b>	<b>1.258</b>	<b>0.440</b>	<b>0.272</b>	<b>0.548</b>	<b>1.222</b>	<b>1.048</b>	<b>0.959</b>	<b>1.188</b>	<b>1.268</b>	<b>0.792</b>	<b>0.780</b>	<b>1.048</b>	<b>0.800</b>	<b>1.392</b>	<b>1.200</b>	<b>1.247</b>	<b>0.974</b>	<b>0.632</b>	<b>0.401</b>	<b>0.338</b>	<b>0.478</b>	<b>0.468</b>
<b>SD</b>	<b>0.042</b>	<b>0.022</b>	<b>0.173</b>	<b>0.026</b>	<b>0.237</b>	<b>0.022</b>	<b>0.031</b>	<b>0.017</b>	<b>0.073</b>	<b>0.024</b>	<b>0.015</b>	<b>0.011</b>	<b>0.030</b>	<b>0.018</b>	<b>0.021</b>	<b>0.022</b>	<b>0.012</b>	<b>0.014</b>	<b>0.014</b>	<b>0.010</b>	<b>0.009</b>	<b>0.008</b>	<b>0.015</b>
<b>%RSD</b>	<b>2.4</b>	<b>1.8</b>	<b>39.3</b>	<b>9.7</b>	<b>43.3</b>	<b>1.8</b>	<b>2.9</b>	<b>1.8</b>	<b>6.2</b>	<b>1.9</b>	<b>1.9</b>	<b>1.5</b>	<b>2.8</b>	<b>2.3</b>	<b>1.5</b>	<b>1.8</b>	<b>1.0</b>	<b>1.4</b>	<b>2.2</b>	<b>2.4</b>	<b>2.7</b>	<b>1.7</b>	<b>3.2</b>
500–1	3.647	2.733	0.710	0.813	1.230	2.515	2.225	2.045	2.275	2.280	1.701	1.655	2.452	1.688	2.857	2.478	2.270	1.984	1.439	0.849	0.731	1.013	0.979
500–2	3.447	2.483	0.820	0.549	0.950	2.445	2.035	1.885	2.695	2.620	1.581	1.525	1.972	1.558	2.757	2.398	2.500	1.914	1.309	0.781	0.668	0.958	0.949
500–3	3.537	2.573	0.970	0.633	1.060	2.525	2.045	1.935	2.405	2.510	1.621	1.575	2.102	1.638	2.847	2.438	2.430	1.964	1.349	0.773	0.680	0.955	0.913
500–4	3.417	2.483	2.910	1.553	2.990	2.415	1.985	1.875	2.495	2.500	1.561	1.505	2.042	1.588	2.737	2.358	2.450	1.894	1.289	0.769	0.671	0.933	0.890
500–5	3.437	2.483	1.160	0.653	1.180	2.435	1.955	1.855	2.425	2.410	1.531	1.515	1.992	1.568	2.787	2.368	2.380	1.914	1.289	0.772	0.659	0.925	0.899
500–6	3.517	2.523	0.940	0.601	1.060	2.375	1.975	1.835	2.335	2.460	1.531	1.535	2.052	1.568	2.717	2.328	2.410	1.874	1.249	0.769	0.654	0.898	0.880
<b>Mean</b>	<b>3.501</b>	<b>2.546</b>	<b>1.252</b>	<b>0.800</b>	<b>1.412</b>	<b>2.452</b>	<b>2.037</b>	<b>1.905</b>	<b>2.438</b>	<b>2.463</b>	<b>1.588</b>	<b>1.552</b>	<b>2.102</b>	<b>1.601</b>	<b>2.784</b>	<b>2.395</b>	<b>2.407</b>	<b>1.924</b>	<b>1.320</b>	<b>0.785</b>	<b>0.677</b>	<b>0.947</b>	<b>0.918</b>
<b>SD</b>	<b>0.078</b>	<b>0.090</b>	<b>0.754</b>	<b>0.346</b>	<b>0.712</b>	<b>0.053</b>	<b>0.090</b>	<b>0.070</b>	<b>0.134</b>	<b>0.104</b>	<b>0.059</b>	<b>0.051</b>	<b>0.162</b>	<b>0.047</b>	<b>0.053</b>	<b>0.051</b>	<b>0.071</b>	<b>0.038</b>	<b>0.061</b>	<b>0.029</b>	<b>0.025</b>	<b>0.036</b>	<b>0.035</b>
<b>%RSD</b>	<b>2.2</b>	<b>3.5</b>	<b>60.3</b>	<b>43.3</b>	<b>50.4</b>	<b>2.2</b>	<b>4.4</b>	<b>3.7</b>	<b>5.5</b>	<b>4.2</b>	<b>3.7</b>	<b>3.3</b>	<b>7.7</b>	<b>2.9</b>	<b>1.9</b>	<b>2.1</b>	<b>3.0</b>	<b>2.0</b>	<b>4.6</b>	<b>3.7</b>	<b>3.8</b>	<b>3.8</b>	<b>3.8</b>

**Table S17.** SIFT-MS repeatability data for Mix 1 in 5% methanol:95% water at three levels (50, 250, and 500). The replicate shown in red is an outlier and was not included in the calculation. Note that acetonitrile and nitromethane are measured using different product ions compared to other diluent solvents, and that trichloroethylene was not measurable in methanol.

Level–Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (NO <sup>+</sup> 71)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	1-Butanol (NO <sup>+</sup> 73)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Nitromethane (NO <sup>+</sup> 91)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)
50–1	0.416	3.705	0.149	0.132	0.087	0.380	0.123	0.162	0.534	0.336	0.296	0.171
50–2	0.393	3.525	0.143	0.136	0.082	0.368	0.122	0.155	0.464	0.326	0.282	0.168
50–3	0.404	3.545	0.145	0.138	0.082	0.366	0.120	0.160	0.490	0.331	0.283	0.169
50–4	0.429	3.845	0.152	0.147	0.096	0.379	0.132	0.172	0.529	0.342	0.307	0.174
50–5	0.404	3.615	0.149	0.144	0.087	0.370	0.120	0.159	0.491	0.331	0.289	0.171
50–6	0.408	3.605	0.144	0.139	0.091	0.372	0.126	0.159	0.497	0.335	0.288	0.168
<b>Mean</b>	<b>0.409</b>	<b>3.640</b>	<b>0.147</b>	<b>0.140</b>	<b>0.087</b>	<b>0.372</b>	<b>0.124</b>	<b>0.161</b>	<b>0.500</b>	<b>0.334</b>	<b>0.291</b>	<b>0.170</b>
<b>SD</b>	<b>0.011</b>	<b>0.108</b>	<b>0.003</b>	<b>0.005</b>	<b>0.005</b>	<b>0.005</b>	<b>0.004</b>	<b>0.005</b>	<b>0.024</b>	<b>0.005</b>	<b>0.009</b>	<b>0.002</b>
<b>%RSD</b>	<b>2.7</b>	<b>3.0</b>	<b>2.2</b>	<b>3.6</b>	<b>5.6</b>	<b>1.4</b>	<b>3.4</b>	<b>3.3</b>	<b>4.8</b>	<b>1.5</b>	<b>2.9</b>	<b>1.2</b>
250–1	2.030	18.255	0.725	0.636	0.497	1.717	0.622	0.828	2.566	1.534	1.454	0.786
250–2	2.040	18.155	0.728	0.641	0.498	1.667	0.606	0.840	2.536	1.514	1.454	0.776
250–3	2.060	18.455	0.737	0.661	0.503	1.687	0.616	0.853	2.536	1.534	1.474	0.787
250–4	2.010	17.655	0.716	0.647	0.483	1.747	0.608	0.819	2.596	1.564	1.414	0.767
250–5	2.000	17.655	0.698	0.625	0.485	1.667	0.595	0.816	2.396	1.494	1.414	0.750
250–6	1.920	17.255	0.692	0.604	0.477	1.717	0.573	0.789	2.236	1.564	1.384	0.739
<b>Mean</b>	<b>2.010</b>	<b>17.905</b>	<b>0.716</b>	<b>0.636</b>	<b>0.490</b>	<b>1.700</b>	<b>0.604</b>	<b>0.824</b>	<b>2.477</b>	<b>1.534</b>	<b>1.433</b>	<b>0.767</b>
<b>SD</b>	<b>0.045</b>	<b>0.415</b>	<b>0.016</b>	<b>0.018</b>	<b>0.009</b>	<b>0.029</b>	<b>0.016</b>	<b>0.020</b>	<b>0.125</b>	<b>0.025</b>	<b>0.031</b>	<b>0.018</b>
<b>%RSD</b>	<b>2.2</b>	<b>2.3</b>	<b>2.3</b>	<b>2.8</b>	<b>1.9</b>	<b>1.7</b>	<b>2.6</b>	<b>2.4</b>	<b>5.0</b>	<b>1.6</b>	<b>2.1</b>	<b>2.3</b>
500–1	3.980	35.955	1.488	1.365	1.030	3.567	1.233	1.662	4.806	3.194	2.884	1.617
500–2	3.200	27.855	2.368	1.325	0.776	2.807	0.939	1.312	3.506	2.604	2.224	1.287
500–3	3.920	35.855	2.158	1.405	1.010	3.547	1.213	1.672	4.716	3.204	2.864	1.607
500–4	3.980	35.755	1.808	1.365	1.010	3.427	1.213	1.652	4.846	3.124	2.864	1.587
500–5	3.960	35.255	1.658	1.325	1.010	3.547	1.193	1.662	4.446	3.174	2.824	1.597
500–6	3.810	34.755	1.598	1.325	1.000	3.507	1.173	1.612	4.376	3.204	2.784	1.587
<b>Mean</b>	<b>3.930</b>	<b>35.515</b>	<b>1.742</b>	<b>1.357</b>	<b>1.012</b>	<b>3.519</b>	<b>1.205</b>	<b>1.652</b>	<b>4.638</b>	<b>3.180</b>	<b>2.844</b>	<b>1.599</b>
<b>SD</b>	<b>0.064</b>	<b>0.450</b>	<b>0.232</b>	<b>0.030</b>	<b>0.010</b>	<b>0.050</b>	<b>0.020</b>	<b>0.021</b>	<b>0.191</b>	<b>0.030</b>	<b>0.036</b>	<b>0.012</b>
<b>%RSD</b>	<b>1.6</b>	<b>1.3</b>	<b>13.3</b>	<b>2.2</b>	<b>1.0</b>	<b>1.4</b>	<b>1.7</b>	<b>1.3</b>	<b>4.1</b>	<b>0.95</b>	<b>1.3</b>	<b>0.73</b>

**Table S18.** SIFT-MS repeatability data for Mix 1 in 5% triacetin:95% water at three levels (50, 250, and 500).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
50–1	0.317	0.280	0.149	0.103	0.154	0.269	0.372	0.338	0.210	0.298	0.194	0.161	0.229	0.165	0.259	0.265	0.257	0.269	0.169	0.158	0.130	0.157	0.166
50–2	0.346	0.292	0.158	0.099	0.160	0.273	0.395	0.357	0.260	0.301	0.200	0.160	0.234	0.170	0.270	0.277	0.267	0.274	0.167	0.167	0.135	0.178	0.171
50–3	0.315	0.275	0.158	0.101	0.160	0.260	0.372	0.336	0.261	0.290	0.193	0.154	0.226	0.163	0.264	0.267	0.260	0.260	0.171	0.152	0.130	0.168	0.163
50–4	0.332	0.284	0.156	0.114	0.165	0.274	0.382	0.346	0.269	0.294	0.196	0.160	0.246	0.170	0.268	0.266	0.253	0.269	0.175	0.158	0.137	0.173	0.170
50–5	0.311	0.279	0.148	0.099	0.159	0.264	0.373	0.346	0.215	0.294	0.199	0.156	0.222	0.165	0.269	0.265	0.260	0.263	0.164	0.147	0.132	0.161	0.160
50–6	0.315	0.280	0.161	0.096	0.163	0.270	0.390	0.333	0.233	0.291	0.202	0.155	0.213	0.158	0.273	0.285	0.262	0.264	0.171	0.148	0.131	0.160	0.161
<b>Mean</b>	<b>0.323</b>	<b>0.281</b>	<b>0.155</b>	<b>0.102</b>	<b>0.161</b>	<b>0.268</b>	<b>0.380</b>	<b>0.343</b>	<b>0.241</b>	<b>0.295</b>	<b>0.198</b>	<b>0.157</b>	<b>0.229</b>	<b>0.165</b>	<b>0.267</b>	<b>0.271</b>	<b>0.260</b>	<b>0.266</b>	<b>0.170</b>	<b>0.155</b>	<b>0.132</b>	<b>0.166</b>	<b>0.165</b>
<b>SD</b>	<b>0.0124</b>	<b>0.0053</b>	<b>0.0048</b>	<b>0.0058</b>	<b>0.0034</b>	<b>0.0049</b>	<b>0.0092</b>	<b>0.0080</b>	<b>0.0233</b>	<b>0.0038</b>	<b>0.0032</b>	<b>0.0027</b>	<b>0.0102</b>	<b>0.0041</b>	<b>0.0045</b>	<b>0.0076</b>	<b>0.0043</b>	<b>0.0046</b>	<b>0.0035</b>	<b>0.0069</b>	<b>0.0026</b>	<b>0.0075</b>	<b>0.0042</b>
<b>%RSD</b>	<b>3.8</b>	<b>1.9</b>	<b>3.1</b>	<b>5.6</b>	<b>2.1</b>	<b>1.8</b>	<b>2.4</b>	<b>2.3</b>	<b>9.6</b>	<b>1.3</b>	<b>1.6</b>	<b>1.7</b>	<b>4.5</b>	<b>2.5</b>	<b>1.7</b>	<b>2.8</b>	<b>1.7</b>	<b>1.7</b>	<b>2.0</b>	<b>4.4</b>	<b>2.0</b>	<b>4.5</b>	<b>2.6</b>
250–1	1.579	1.428	0.738	0.492	0.781	1.327	1.784	1.609	1.516	1.377	0.954	0.764	1.175	0.822	1.354	1.239	1.228	1.319	0.868	0.735	0.615	0.782	0.738
250–2	1.619	1.408	0.729	0.484	0.734	1.287	1.744	1.569	1.466	1.387	0.925	0.762	1.135	0.808	1.294	1.259	1.238	1.289	0.844	0.721	0.624	0.791	0.758
250–3	1.589	1.378	0.785	0.485	0.789	1.267	1.724	1.589	1.466	1.377	0.919	0.759	1.135	0.794	1.294	1.209	1.208	1.289	0.835	0.696	0.606	0.784	0.747
250–4	1.609	1.418	0.780	0.499	0.809	1.287	1.744	1.599	1.436	1.417	0.960	0.768	1.155	0.811	1.294	1.259	1.218	1.289	0.859	0.734	0.619	0.759	0.783
250–5	1.719	1.478	0.802	0.505	0.816	1.337	1.774	1.629	1.346	1.377	0.965	0.798	1.245	0.856	1.334	1.269	1.208	1.349	0.883	0.737	0.641	0.772	0.768
250–6	1.579	1.388	0.847	0.465	0.816	1.267	1.694	1.549	1.376	1.377	0.930	0.748	1.155	0.785	1.254	1.249	1.228	1.269	0.837	0.711	0.612	0.769	0.742
<b>Mean</b>	<b>1.616</b>	<b>1.416</b>	<b>0.780</b>	<b>0.488</b>	<b>0.791</b>	<b>1.295</b>	<b>1.744</b>	<b>1.591</b>	<b>1.434</b>	<b>1.385</b>	<b>0.943</b>	<b>0.766</b>	<b>1.167</b>	<b>0.812</b>	<b>1.304</b>	<b>1.248</b>	<b>1.221</b>	<b>1.300</b>	<b>0.854</b>	<b>0.722</b>	<b>0.619</b>	<b>0.776</b>	<b>0.756</b>
<b>SD</b>	<b>0.049</b>	<b>0.032</b>	<b>0.040</b>	<b>0.013</b>	<b>0.029</b>	<b>0.027</b>	<b>0.030</b>	<b>0.026</b>	<b>0.058</b>	<b>0.015</b>	<b>0.018</b>	<b>0.015</b>	<b>0.038</b>	<b>0.023</b>	<b>0.032</b>	<b>0.020</b>	<b>0.011</b>	<b>0.026</b>	<b>0.017</b>	<b>0.015</b>	<b>0.011</b>	<b>0.011</b>	<b>0.016</b>
<b>%RSD</b>	<b>3.0</b>	<b>2.3</b>	<b>5.1</b>	<b>2.6</b>	<b>3.6</b>	<b>2.1</b>	<b>1.7</b>	<b>1.6</b>	<b>4.0</b>	<b>1.1</b>	<b>1.9</b>	<b>2.0</b>	<b>3.2</b>	<b>2.8</b>	<b>2.5</b>	<b>1.6</b>	<b>0.91</b>	<b>2.0</b>	<b>2.0</b>	<b>2.1</b>	<b>1.8</b>	<b>1.4</b>	<b>2.1</b>
500–1	3.239	2.938	1.716	1.049	1.766	2.627	3.654	3.439	3.226	2.897	1.934	1.558	2.335	1.650	2.724	2.599	2.508	2.659	1.834	1.547	1.387	1.719	1.667
500–2	3.219	2.868	1.676	1.029	1.706	2.527	3.634	3.269	3.106	2.867	1.874	1.518	2.305	1.600	2.674	2.529	2.518	2.579	1.764	1.507	1.327	1.689	1.647
500–3	3.259	2.858	1.606	1.029	1.716	2.547	3.594	3.369	3.016	2.827	1.894	1.518	2.325	1.620	2.634	2.509	2.538	2.609	1.764	1.497	1.347	1.619	1.617
500–4	3.119	2.808	1.596	0.999	1.676	2.537	3.634	3.269	3.136	2.887	1.904	1.488	2.195	1.580	2.614	2.559	2.478	2.579	1.744	1.457	1.337	1.649	1.627
500–5	3.169	2.818	1.636	1.049	1.686	2.537	3.594	3.269	3.136	2.767	1.854	1.478	2.175	1.560	2.614	2.569	2.508	2.559	1.754	1.487	1.327	1.639	1.617
500–6	3.259	2.628	1.626	1.069	1.726	2.497	3.604	3.299	2.876	2.817	1.664	1.378	2.115	1.600	2.614	2.199	2.318	2.529	1.774	1.497	1.347	1.649	1.637
<b>Mean</b>	<b>3.211</b>	<b>2.819</b>	<b>1.642</b>	<b>1.037</b>	<b>1.713</b>	<b>2.545</b>	<b>3.619</b>	<b>3.319</b>	<b>3.083</b>	<b>2.844</b>	<b>1.854</b>	<b>1.489</b>	<b>2.242</b>	<b>1.601</b>	<b>2.646</b>	<b>2.494</b>	<b>2.478</b>	<b>2.585</b>	<b>1.772</b>	<b>1.498</b>	<b>1.345</b>	<b>1.660</b>	<b>1.635</b>
<b>SD</b>	<b>0.051</b>	<b>0.095</b>	<b>0.041</b>	<b>0.022</b>	<b>0.029</b>	<b>0.040</b>	<b>0.023</b>	<b>0.064</b>	<b>0.111</b>	<b>0.045</b>	<b>0.089</b>	<b>0.056</b>	<b>0.084</b>	<b>0.029</b>	<b>0.041</b>	<b>0.135</b>	<b>0.074</b>	<b>0.041</b>	<b>0.029</b>	<b>0.027</b>	<b>0.020</b>	<b>0.033</b>	<b>0.018</b>
<b>%RSD</b>	<b>1.6</b>	<b>3.4</b>	<b>2.5</b>	<b>2.1</b>	<b>1.7</b>	<b>1.6</b>	<b>0.63</b>	<b>1.9</b>	<b>3.6</b>	<b>1.6</b>	<b>4.8</b>	<b>3.8</b>	<b>3.7</b>	<b>1.8</b>	<b>1.5</b>	<b>5.4</b>	<b>3.0</b>	<b>1.6</b>	<b>1.6</b>	<b>1.8</b>	<b>1.5</b>	<b>2.0</b>	<b>1.1</b>

## D. Limit of Quantitation (LOQ)

**Table S19.** SIFT-MS LOQ data for Mix 1 in water at three levels (1, 2, and 5).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	7.9	5.1	2.3	1.4	1.9	6.0	4.7	6.8	23.1	2.7	3.7	3.6	4.4	3.0	4.7	4.0	3.5	5.7	4.3	2.6	1.6	1.2	1.7
1–2	7.1	4.3	2.0	0.5	2.1	6.2	5.3	6.9	20.1	4.9	3.6	3.3	4.3	3.5	4.8	4.2	3.4	6.2	3.8	2.3	2.0	2.0	3.4
1–3	6.2	4.7	1.8	0.9	2.1	5.9	5.4	8.1	22.1	3.0	4.1	3.8	4.8	3.4	5.8	4.4	3.2	5.6	4.6	2.5	2.1	2.4	3.1
<b>Mean</b>	<b>7.1</b>	<b>4.7</b>	<b>2.0</b>	<b>1.0</b>	<b>2.0</b>	<b>6.1</b>	<b>5.1</b>	<b>7.3</b>	<b>21.8</b>	<b>3.5</b>	<b>3.8</b>	<b>3.6</b>	<b>4.5</b>	<b>3.3</b>	<b>5.1</b>	<b>4.2</b>	<b>3.3</b>	<b>5.8</b>	<b>4.2</b>	<b>2.5</b>	<b>1.9</b>	<b>1.9</b>	<b>2.7</b>
<b>SD</b>	<b>0.67</b>	<b>0.33</b>	<b>0.20</b>	<b>0.37</b>	<b>0.08</b>	<b>0.12</b>	<b>0.31</b>	<b>0.59</b>	<b>1.25</b>	<b>1.00</b>	<b>0.23</b>	<b>0.17</b>	<b>0.19</b>	<b>0.20</b>	<b>0.50</b>	<b>0.18</b>	<b>0.10</b>	<b>0.26</b>	<b>0.34</b>	<b>0.14</b>	<b>0.21</b>	<b>0.48</b>	<b>0.72</b>
<b>%RSD</b>	<b>9.4</b>	<b>7.0</b>	<b>9.8</b>	<b>38.6</b>	<b>4.1</b>	<b>2.0</b>	<b>6.0</b>	<b>8.1</b>	<b>5.7</b>	<b>28.2</b>	<b>6.0</b>	<b>4.9</b>	<b>4.2</b>	<b>6.1</b>	<b>9.8</b>	<b>4.3</b>	<b>3.1</b>	<b>4.5</b>	<b>8.1</b>	<b>5.9</b>	<b>11.0</b>	<b>25.6</b>	<b>26.3</b>
2–1	16.6	9.0	4.0	3.0	3.9	12.8	10.4	13.0	6.2	6.9	7.5	7.5	7.8	6.8	9.9	9.2	8.3	11.2	8.7	5.1	4.8	4.7	5.5
2–2	14.9	10.0	4.6	2.7	4.1	12.0	11.6	14.4	5.9	8.4	8.1	6.4	9.3	6.9	10.3	9.8	8.1	11.4	8.6	5.4	4.0	5.7	6.0
2–3	15.2	10.0	4.5	2.7	3.8	13.1	11.4	12.4	6.0	7.6	7.7	6.3	7.8	6.1	10.1	8.8	7.3	11.5	7.5	5.2	4.1	4.8	4.8
<b>Mean</b>	<b>15.5</b>	<b>9.6</b>	<b>4.4</b>	<b>2.8</b>	<b>3.9</b>	<b>12.6</b>	<b>11.1</b>	<b>13.3</b>	<b>6.0</b>	<b>7.7</b>	<b>7.7</b>	<b>6.7</b>	<b>8.3</b>	<b>6.6</b>	<b>10.1</b>	<b>9.2</b>	<b>7.9</b>	<b>11.4</b>	<b>8.2</b>	<b>5.2</b>	<b>4.3</b>	<b>5.1</b>	<b>5.4</b>
<b>SD</b>	<b>0.74</b>	<b>0.47</b>	<b>0.28</b>	<b>0.17</b>	<b>0.12</b>	<b>0.46</b>	<b>0.52</b>	<b>0.84</b>	<b>0.12</b>	<b>0.61</b>	<b>0.25</b>	<b>0.54</b>	<b>0.71</b>	<b>0.37</b>	<b>0.16</b>	<b>0.42</b>	<b>0.44</b>	<b>0.12</b>	<b>0.56</b>	<b>0.11</b>	<b>0.35</b>	<b>0.42</b>	<b>0.48</b>
<b>%RSD</b>	<b>4.8</b>	<b>4.9</b>	<b>6.4</b>	<b>6.0</b>	<b>3.1</b>	<b>3.7</b>	<b>4.7</b>	<b>6.3</b>	<b>2.1</b>	<b>8.0</b>	<b>3.2</b>	<b>8.1</b>	<b>8.5</b>	<b>5.5</b>	<b>1.6</b>	<b>4.6</b>	<b>5.5</b>	<b>1.1</b>	<b>6.8</b>	<b>2.2</b>	<b>8.3</b>	<b>8.4</b>	<b>8.9</b>
5–1	34.2	25.4	9.0	5.5	11.7	31.4	34.3	29.9	34.1	22.7	16.3	17.1	20.6	16.6	27.3	23.0	20.1	28.2	20.9	12.5	9.9	10.6	12.4
5–2	35.1	24.8	10.7	6.6	12.2	32.4	31.1	28.5	41.1	21.3	17.0	16.2	21.2	17.3	28.8	24.2	23.0	31.3	20.0	12.5	12.0	12.6	13.2
5–3	32.6	26.4	10.3	8.2	10.8	32.2	34.6	34.7	38.1	24.9	19.5	16.8	22.7	16.7	26.4	24.7	20.4	31.2	19.9	12.0	10.0	11.5	13.0
<b>Mean</b>	<b>33.9</b>	<b>25.5</b>	<b>10.0</b>	<b>6.7</b>	<b>11.5</b>	<b>32.0</b>	<b>33.3</b>	<b>31.0</b>	<b>37.8</b>	<b>23.0</b>	<b>17.6</b>	<b>16.7</b>	<b>21.5</b>	<b>16.9</b>	<b>27.5</b>	<b>23.9</b>	<b>21.2</b>	<b>30.3</b>	<b>20.2</b>	<b>12.3</b>	<b>10.6</b>	<b>11.5</b>	<b>12.8</b>
<b>SD</b>	<b>1.03</b>	<b>0.66</b>	<b>0.73</b>	<b>1.10</b>	<b>0.58</b>	<b>0.43</b>	<b>1.58</b>	<b>2.65</b>	<b>2.87</b>	<b>1.48</b>	<b>1.37</b>	<b>0.37</b>	<b>0.88</b>	<b>0.31</b>	<b>0.99</b>	<b>0.71</b>	<b>1.30</b>	<b>1.44</b>	<b>0.45</b>	<b>0.24</b>	<b>0.97</b>	<b>0.82</b>	<b>0.34</b>
<b>%RSD</b>	<b>3.0</b>	<b>2.6</b>	<b>7.2</b>	<b>16.4</b>	<b>5.0</b>	<b>1.4</b>	<b>4.8</b>	<b>8.6</b>	<b>7.6</b>	<b>6.4</b>	<b>7.8</b>	<b>2.2</b>	<b>4.1</b>	<b>1.8</b>	<b>3.6</b>	<b>3.0</b>	<b>6.1</b>	<b>4.8</b>	<b>2.2</b>	<b>1.9</b>	<b>9.1</b>	<b>7.1</b>	<b>2.7</b>

**Table S20a.** SIFT-MS LOQ data for Mix 1 in 5% DMI:95% water at three levels (1, 2, and 5).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	4.2	7.6	1.3	-1.1	0.1	5.1	2.9	8.2	16.0	3.9	3.8	3.0	4.1	3.0	7.1	5.2	4.5	7.1	4.1	2.4	3.2	2.4	2.3
1–2	7.5	17.2	1.8	-1.3	1.1	6.2	5.3	8.7	42.0	10.6	6.8	3.5	5.1	2.6	7.7	4.9	4.8	8.9	7.1	2.0	1.3	1.7	0.0
1–3	6.1	17.7	3.0	-0.1	1.4	5.6	8.4	6.1	14.0	12.3	3.9	2.9	3.8	3.2	5.4	5.1	4.1	6.8	6.4	2.3	2.4	0.9	1.7
<b>Mean</b>	<b>6.0</b>	<b>14.2</b>	<b>2.0</b>	<b>-0.8</b>	<b>0.9</b>	<b>5.6</b>	<b>5.5</b>	<b>7.7</b>	<b>24.0</b>	<b>8.9</b>	<b>4.8</b>	<b>3.1</b>	<b>4.3</b>	<b>2.9</b>	<b>6.7</b>	<b>5.1</b>	<b>4.5</b>	<b>7.6</b>	<b>5.9</b>	<b>2.2</b>	<b>2.3</b>	<b>1.7</b>	<b>1.3</b>
<b>SD</b>	<b>1.35</b>	<b>4.65</b>	<b>0.75</b>	<b>0.52</b>	<b>0.54</b>	<b>0.45</b>	<b>2.25</b>	<b>1.13</b>	<b>12.75</b>	<b>3.63</b>	<b>1.39</b>	<b>0.28</b>	<b>0.56</b>	<b>0.25</b>	<b>0.97</b>	<b>0.11</b>	<b>0.29</b>	<b>0.93</b>	<b>1.28</b>	<b>0.18</b>	<b>0.76</b>	<b>0.59</b>	<b>0.96</b>
<b>%RSD</b>	<b>22.7</b>	<b>32.8</b>	<b>36.8</b>	<b>-63.2</b>	<b>63.5</b>	<b>8.0</b>	<b>40.7</b>	<b>14.7</b>	<b>53.1</b>	<b>40.6</b>	<b>29.1</b>	<b>8.9</b>	<b>12.8</b>	<b>8.5</b>	<b>14.5</b>	<b>2.2</b>	<b>6.4</b>	<b>12.2</b>	<b>21.8</b>	<b>8.3</b>	<b>32.6</b>	<b>35.5</b>	<b>72.1</b>
2–1	12.1	18.5	3.2	2.5	2.1	11.3	8.5	14.1	-1.0	11.9	8.0	6.9	9.1	6.1	8.8	10.0	7.5	13.0	8.5	4.4	2.3	2.4	3.2
2–2	10.5	17.5	2.7	2.4	3.0	12.8	10.3	12.5	3.0	13.5	6.7	6.2	9.4	5.3	8.7	9.2	8.1	12.6	11.4	4.0	3.5	2.9	3.3
2–3	12.9	21.5	3.2	2.2	2.5	11.2	10.6	13.6	3.0	18.8	8.5	5.6	9.0	5.1	10.5	10.7	7.0	12.3	8.1	4.8	3.3	4.2	3.6
<b>Mean</b>	<b>11.9</b>	<b>19.2</b>	<b>3.0</b>	<b>2.3</b>	<b>2.5</b>	<b>11.8</b>	<b>9.8</b>	<b>13.4</b>	<b>1.7</b>	<b>14.7</b>	<b>7.7</b>	<b>6.2</b>	<b>9.2</b>	<b>5.5</b>	<b>9.3</b>	<b>10.0</b>	<b>7.5</b>	<b>12.6</b>	<b>9.3</b>	<b>4.4</b>	<b>3.0</b>	<b>3.2</b>	<b>3.4</b>
<b>SD</b>	<b>1.00</b>	<b>1.70</b>	<b>0.23</b>	<b>0.10</b>	<b>0.35</b>	<b>0.73</b>	<b>0.93</b>	<b>0.67</b>	<b>1.89</b>	<b>2.95</b>	<b>0.76</b>	<b>0.53</b>	<b>0.17</b>	<b>0.43</b>	<b>0.83</b>	<b>0.61</b>	<b>0.45</b>	<b>0.29</b>	<b>1.47</b>	<b>0.31</b>	<b>0.54</b>	<b>0.79</b>	<b>0.16</b>
<b>%RSD</b>	<b>8.4</b>	<b>8.9</b>	<b>7.6</b>	<b>4.2</b>	<b>14.0</b>	<b>6.2</b>	<b>9.5</b>	<b>5.0</b>	<b>113.1</b>	<b>20.0</b>	<b>9.9</b>	<b>8.6</b>	<b>1.9</b>	<b>7.9</b>	<b>8.8</b>	<b>6.1</b>	<b>6.0</b>	<b>2.3</b>	<b>15.8</b>	<b>7.1</b>	<b>17.9</b>	<b>25.0</b>	<b>4.8</b>
5–1	32.9	11.8	8.5	6.1	7.5	26.7	17.4	19.1	48.0	34.3	14.1	13.0	14.3	13.6	27.4	24.9	19.6	26.6	18.2	10.5	7.3	12.1	9.1
5–2	27.4	11.6	9.3	4.9	6.6	26.6	17.0	20.3	18.0	19.0	13.5	11.5	17.8	13.2	23.2	24.4	20.4	25.9	18.4	11.5	7.1	9.6	9.8
5–3	29.2	9.7	10.3	5.2	8.2	26.8	18.5	19.9	35.0	23.3	14.5	11.8	16.3	13.0	26.8	24.6	23.8	26.0	19.7	11.5	8.4	11.5	11.0
<b>Mean</b>	<b>29.9</b>	<b>11.0</b>	<b>9.3</b>	<b>5.4</b>	<b>7.4</b>	<b>26.7</b>	<b>17.6</b>	<b>19.8</b>	<b>33.7</b>	<b>25.5</b>	<b>14.0</b>	<b>12.1</b>	<b>16.1</b>	<b>13.3</b>	<b>25.8</b>	<b>24.6</b>	<b>21.3</b>	<b>26.2</b>	<b>18.8</b>	<b>11.2</b>	<b>7.6</b>	<b>11.0</b>	<b>9.9</b>
<b>SD</b>	<b>2.29</b>	<b>0.95</b>	<b>0.74</b>	<b>0.51</b>	<b>0.65</b>	<b>0.08</b>	<b>0.63</b>	<b>0.50</b>	<b>12.28</b>	<b>6.44</b>	<b>0.41</b>	<b>0.65</b>	<b>1.43</b>	<b>0.25</b>	<b>1.85</b>	<b>0.21</b>	<b>1.82</b>	<b>0.31</b>	<b>0.66</b>	<b>0.47</b>	<b>0.57</b>	<b>1.07</b>	<b>0.78</b>
<b>%RSD</b>	<b>7.7</b>	<b>8.6</b>	<b>7.9</b>	<b>9.5</b>	<b>8.8</b>	<b>0.31</b>	<b>3.6</b>	<b>2.5</b>	<b>36.5</b>	<b>25.2</b>	<b>2.9</b>	<b>5.4</b>	<b>8.9</b>	<b>1.9</b>	<b>7.2</b>	<b>0.83</b>	<b>8.6</b>	<b>1.2</b>	<b>3.5</b>	<b>4.2</b>	<b>7.5</b>	<b>9.7</b>	<b>7.9</b>

**Table S20b.** SIFT-MS LOQ data for Mix 1 in 10% DMI:90% water at three levels (1, 2, and 5).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	6.4	11.9	-0.3	2.5	1.0	5.5	2.0	0.7	-48.0	-1.8	3.2	2.6	4.2	2.5	1.4	5.0	3.3	3.9	1.4	0.3	2.7	2.2	1.3
1–2	4.8	11.8	-0.2	-0.7	0.7	5.6	1.8	-0.7	-62.0	2.1	2.9	2.7	3.8	2.0	1.8	4.8	0.8	4.0	1.8	-0.7	3.4	1.2	-1.2
1–3	6.8	14.4	1.6	-2.8	1.2	4.6	2.8	-0.4	-88.0	3.3	4.1	4.6	5.8	2.1	-0.5	5.0	2.4	5.4	4.7	1.8	2.7	2.4	3.7
<b>Mean</b>	<b>6.0</b>	<b>12.7</b>	<b>0.4</b>	<b>-0.3</b>	<b>1.0</b>	<b>5.2</b>	<b>2.2</b>	<b>-0.1</b>	<b>-66.0</b>	<b>1.2</b>	<b>3.4</b>	<b>3.3</b>	<b>4.6</b>	<b>2.2</b>	<b>0.9</b>	<b>4.9</b>	<b>2.2</b>	<b>4.4</b>	<b>2.6</b>	<b>0.5</b>	<b>2.9</b>	<b>1.9</b>	<b>1.3</b>
<b>SD</b>	<b>0.86</b>	<b>1.20</b>	<b>0.89</b>	<b>2.18</b>	<b>0.20</b>	<b>0.47</b>	<b>0.43</b>	<b>0.60</b>	<b>16.57</b>	<b>2.18</b>	<b>0.51</b>	<b>0.93</b>	<b>0.86</b>	<b>0.19</b>	<b>1.00</b>	<b>0.10</b>	<b>1.03</b>	<b>0.68</b>	<b>1.47</b>	<b>1.02</b>	<b>0.34</b>	<b>0.53</b>	<b>1.99</b>
<b>%RSD</b>	<b>14.4</b>	<b>9.5</b>	<b>227.2</b>	<b>-653.8</b>	<b>20.6</b>	<b>9.1</b>	<b>19.6</b>	<b>-451.4</b>	<b>-25.1</b>	<b>181.4</b>	<b>15.0</b>	<b>28.0</b>	<b>18.8</b>	<b>8.8</b>	<b>111.5</b>	<b>2.0</b>	<b>47.7</b>	<b>15.4</b>	<b>55.8</b>	<b>208.8</b>	<b>11.6</b>	<b>27.3</b>	<b>154.5</b>
2–1	11.7	16.8	1.1	1.8	2.8	10.4	6.1	5.0	-49.0	7.7	7.5	6.9	12.4	4.5	6.5	8.8	6.8	11.9	7.8	2.3	2.9	2.9	3.3
2–2	12.0	23.4	2.8	2.5	2.6	11.6	12.2	3.7	31.0	2.9	8.1	6.6	15.6	5.3	7.3	10.9	9.0	14.2	7.2	4.8	4.6	6.0	6.8
2–3	10.4	15.3	1.6	3.7	2.6	9.4	6.3	3.5	-13.0	3.1	7.1	5.8	14.4	4.4	7.2	9.3	4.8	9.0	7.5	0.9	0.7	1.8	2.5
<b>Mean</b>	<b>11.4</b>	<b>18.5</b>	<b>1.8</b>	<b>2.7</b>	<b>2.7</b>	<b>10.5</b>	<b>8.2</b>	<b>4.1</b>	<b>-10.3</b>	<b>4.6</b>	<b>7.6</b>	<b>6.5</b>	<b>14.1</b>	<b>4.8</b>	<b>7.0</b>	<b>9.7</b>	<b>6.9</b>	<b>11.7</b>	<b>7.5</b>	<b>2.7</b>	<b>2.7</b>	<b>3.6</b>	<b>4.2</b>
<b>SD</b>	<b>0.69</b>	<b>3.52</b>	<b>0.73</b>	<b>0.78</b>	<b>0.07</b>	<b>0.90</b>	<b>2.83</b>	<b>0.66</b>	<b>32.71</b>	<b>2.22</b>	<b>0.41</b>	<b>0.46</b>	<b>1.32</b>	<b>0.38</b>	<b>0.36</b>	<b>0.86</b>	<b>1.72</b>	<b>2.13</b>	<b>0.24</b>	<b>1.61</b>	<b>1.61</b>	<b>1.75</b>	<b>1.87</b>
<b>%RSD</b>	<b>6.1</b>	<b>19.0</b>	<b>39.5</b>	<b>29.4</b>	<b>2.7</b>	<b>8.6</b>	<b>34.5</b>	<b>16.4</b>	<b>-316.6</b>	<b>48.5</b>	<b>5.4</b>	<b>7.2</b>	<b>9.3</b>	<b>8.1</b>	<b>5.1</b>	<b>8.9</b>	<b>25.0</b>	<b>18.2</b>	<b>3.3</b>	<b>60.3</b>	<b>58.4</b>	<b>49.3</b>	<b>44.9</b>
5–1	27.2	27.0	6.6	3.7	5.2	21.2	23.4	18.0	-45.0	16.6	12.5	14.6	17.0	12.0	24.9	23.7	19.9	22.3	14.3	7.5	6.2	10.5	7.5
5–2	27.6	30.2	5.9	2.7	4.5	22.5	21.4	15.6	-43.0	16.2	13.5	12.2	19.2	11.4	18.9	23.1	17.8	19.8	16.4	6.5	5.7	10.1	7.5
5–3	23.9	27.9	3.6	3.9	4.6	21.1	21.4	15.4	-38.0	13.4	14.1	13.4	17.2	10.4	22.6	24.1	17.3	21.5	15.0	6.4	7.1	8.5	6.2
<b>Mean</b>	<b>26.2</b>	<b>28.4</b>	<b>5.4</b>	<b>3.4</b>	<b>4.8</b>	<b>21.6</b>	<b>22.1</b>	<b>16.3</b>	<b>-42.0</b>	<b>15.4</b>	<b>13.4</b>	<b>13.4</b>	<b>17.8</b>	<b>11.3</b>	<b>22.1</b>	<b>23.6</b>	<b>18.3</b>	<b>21.2</b>	<b>15.2</b>	<b>6.8</b>	<b>6.4</b>	<b>9.7</b>	<b>7.0</b>
<b>SD</b>	<b>1.66</b>	<b>1.35</b>	<b>1.26</b>	<b>0.52</b>	<b>0.31</b>	<b>0.64</b>	<b>0.94</b>	<b>1.18</b>	<b>2.94</b>	<b>1.42</b>	<b>0.66</b>	<b>0.98</b>	<b>0.99</b>	<b>0.66</b>	<b>2.47</b>	<b>0.41</b>	<b>1.13</b>	<b>1.04</b>	<b>0.87</b>	<b>0.50</b>	<b>0.58</b>	<b>0.86</b>	<b>0.61</b>
<b>%RSD</b>	<b>6.3</b>	<b>4.8</b>	<b>23.5</b>	<b>15.3</b>	<b>6.6</b>	<b>2.9</b>	<b>4.3</b>	<b>7.2</b>	<b>-7.0</b>	<b>9.2</b>	<b>4.9</b>	<b>7.3</b>	<b>5.6</b>	<b>5.9</b>	<b>11.2</b>	<b>1.7</b>	<b>6.1</b>	<b>4.9</b>	<b>5.7</b>	<b>7.3</b>	<b>9.1</b>	<b>9.0</b>	<b>8.7</b>



**Table S20c.** SIFT-MS LOQ data for Mix 1 in 100% DMI at five levels (1, 2, 5, 10, and 20). The replicate indicated in red is an outlier and was not included in the calculation.

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	18.0	-53.0	0.2	0.0	-0.2	1.9	1.3	-19.9	-375.0	-162.0	3.9	-210.0	38.0	3.9	15.0	5.0	3.5	4.5	21.7	0.1	0.3	-0.1	0.5
1–2	20.9	-63.0	-0.2	-0.1	-0.3	2.0	2.0	-2.9	-220.0	-55.0	4.6	-220.0	37.0	3.3	13.0	4.5	3.9	11.0	26.4	-0.4	0.2	-0.3	-0.7
<b>1–3</b>																							
<b>Mean</b>	<b>19.5</b>	<b>-58.0</b>	<b>0.0</b>	<b>-0.1</b>	<b>-0.2</b>	<b>1.9</b>	<b>1.7</b>	<b>-11.4</b>	<b>-297.5</b>	<b>-108.5</b>	<b>4.3</b>	<b>-215.0</b>	<b>37.5</b>	<b>3.6</b>	<b>14.0</b>	<b>4.7</b>	<b>3.7</b>	<b>7.8</b>	<b>24.1</b>	<b>-0.1</b>	<b>0.3</b>	<b>-0.2</b>	<b>-0.1</b>
<b>SD</b>	<b>1.45</b>	<b>5.00</b>	<b>0.17</b>	<b>0.04</b>	<b>0.03</b>	<b>0.09</b>	<b>0.35</b>	<b>8.50</b>	<b>77.5</b>	<b>53.5</b>	<b>0.35</b>	<b>5.00</b>	<b>0.50</b>	<b>0.33</b>	<b>1.00</b>	<b>0.27</b>	<b>0.20</b>	<b>3.25</b>	<b>2.35</b>	<b>0.22</b>	<b>0.03</b>	<b>0.09</b>	<b>0.60</b>
<b>%RSD</b>	<b>7.5</b>	<b>-8.6</b>	<b>4350.0</b>	<b>-41.2</b>	<b>-12.2</b>	<b>4.4</b>	<b>21.2</b>	<b>-74.6</b>	<b>-26.1</b>	<b>-49.3</b>	<b>8.2</b>	<b>-2.3</b>	<b>1.3</b>	<b>9.1</b>	<b>7.1</b>	<b>5.6</b>	<b>5.4</b>	<b>41.9</b>	<b>9.8</b>	<b>-163.4</b>	<b>11.2</b>	<b>-42.3</b>	<b>-545.5</b>
2–1	42.2	-51.0	0.4	-1.0	0.4	5.1	4.1	43.0	1090.0	367.0	12.8	-199.0	60.0	6.8	43.0	9.8	7.9	13.7	50.6	0.1	0.4	1.1	-1.4
2–2	48.9	-59.0	-0.2	-1.0	-0.2	4.9	1.0	20.0	290.0	133.0	12.2	-212.0	61.0	7.5	39.0	8.8	2.7	17.2	47.6	-0.2	0.3	0.6	-0.3
2–3	40.5	-50.0	-0.3	-1.0	0.0	4.8	2.6	14.0	-60.0	50.0	11.2	-190.0	54.0	6.0	35.0	8.0	7.7	16.1	41.3	-0.3	0.7	-0.5	-0.5
<b>Mean</b>	<b>43.9</b>	<b>-53.3</b>	<b>0.0</b>	<b>-1.0</b>	<b>0.1</b>	<b>4.9</b>	<b>2.6</b>	<b>25.7</b>	<b>440.0</b>	<b>183.3</b>	<b>12.1</b>	<b>-200.3</b>	<b>58.3</b>	<b>6.7</b>	<b>39.0</b>	<b>8.8</b>	<b>6.1</b>	<b>15.7</b>	<b>46.5</b>	<b>-0.1</b>	<b>0.5</b>	<b>0.4</b>	<b>-0.7</b>
<b>SD</b>	<b>3.63</b>	<b>4.03</b>	<b>0.28</b>	<b>0.01</b>	<b>0.26</b>	<b>0.12</b>	<b>1.27</b>	<b>12.50</b>	<b>481.3</b>	<b>134.2</b>	<b>0.66</b>	<b>9.03</b>	<b>3.09</b>	<b>0.61</b>	<b>3.27</b>	<b>0.72</b>	<b>2.41</b>	<b>1.46</b>	<b>3.88</b>	<b>0.14</b>	<b>0.19</b>	<b>0.66</b>	<b>0.48</b>
<b>%RSD</b>	<b>8.3</b>	<b>-7.6</b>	<b>-1715.5</b>	<b>-0.7</b>	<b>304.4</b>	<b>2.6</b>	<b>49.3</b>	<b>48.7</b>	<b>109.4</b>	<b>73.2</b>	<b>5.5</b>	<b>-4.5</b>	<b>5.3</b>	<b>9.1</b>	<b>8.4</b>	<b>8.1</b>	<b>39.4</b>	<b>9.3</b>	<b>8.3</b>	<b>-114.0</b>	<b>38.9</b>	<b>159.5</b>	<b>-66.7</b>
5–1	106.3	-25.0	0.7	-0.4	-0.1	10.9	0.9	-22.4	-490.0	-168.0	24.5	-176.0	110.0	16.2	33.0	22.7	7.5	43.4	40.8	-0.2	0.3	0.2	-0.7
5–2	96.3	47.0	0.5	-1.0	0.8	10.7	0.9	-0.6	-80.0	67.0	23.2	-19.0	101.0	15.1	41.0	20.4	7.3	42.4	38.5	-0.4	0.4	0.6	-1.2
5–3	93.3	59.0	0.6	0.2	0.5	12.6	-1.7	-11.6	-389.0	-81.0	25.3	-17.0	113.0	15.2	36.0	19.8	6.6	43.6	39.8	0.0	0.4	0.0	-0.3
<b>Mean</b>	<b>98.6</b>	<b>27.0</b>	<b>0.6</b>	<b>-0.4</b>	<b>0.4</b>	<b>11.4</b>	<b>0.0</b>	<b>-11.5</b>	<b>-319.7</b>	<b>-60.7</b>	<b>24.3</b>	<b>-70.7</b>	<b>108.0</b>	<b>15.5</b>	<b>36.7</b>	<b>20.9</b>	<b>7.1</b>	<b>43.1</b>	<b>39.7</b>	<b>-0.2</b>	<b>0.4</b>	<b>0.3</b>	<b>-0.7</b>
<b>SD</b>	<b>5.56</b>	<b>37.09</b>	<b>0.11</b>	<b>0.49</b>	<b>0.38</b>	<b>0.85</b>	<b>1.20</b>	<b>8.90</b>	<b>174.4</b>	<b>97.01</b>	<b>0.87</b>	<b>74.49</b>	<b>5.10</b>	<b>0.50</b>	<b>3.30</b>	<b>1.25</b>	<b>0.39</b>	<b>0.52</b>	<b>0.94</b>	<b>0.14</b>	<b>0.06</b>	<b>0.25</b>	<b>0.39</b>
<b>%RSD</b>	<b>5.6</b>	<b>137.4</b>	<b>18.5</b>	<b>-127.0</b>	<b>89.14</b>	<b>7.5</b>	<b>2404.2</b>	<b>-77.2</b>	<b>-54.6</b>	<b>-159.9</b>	<b>3.6</b>	<b>-105.4</b>	<b>4.7</b>	<b>3.2</b>	<b>9.0</b>	<b>6.0</b>	<b>5.4</b>	<b>1.2</b>	<b>2.4</b>	<b>-68.2</b>	<b>16.3</b>	<b>88.8</b>	<b>-53.2</b>
10–1	191.3	103.0	1.1	-0.4	1.3	24.6	-2.1	-42.2	-724.0	-351.0	51.9	2.0	231.0	32.9	51.0	41.6	18.1	94.0	51.6	0.6	1.0	1.0	-0.3
10–2	201.3	109.0	2.1	0.7	0.7	23.3	-0.5	-40.0	-704.0	-298.0	53.2	32.0	209.0	32.7	46.0	43.8	16.8	95.0	54.6	0.7	1.1	0.5	0.5
10–3	196.3	115.0	0.2	0.2	1.4	24.4	-1.8	-43.5	-661.0	-347.0	57.4	14.0	224.0	33.5	50.0	42.5	18.4	95.0	47.6	0.7	1.0	0.5	-1.1
<b>Mean</b>	<b>196.3</b>	<b>109.0</b>	<b>1.1</b>	<b>0.2</b>	<b>1.1</b>	<b>24.1</b>	<b>-1.5</b>	<b>-41.9</b>	<b>-696.3</b>	<b>-332.0</b>	<b>54.2</b>	<b>16.0</b>	<b>221.3</b>	<b>33.0</b>	<b>49.0</b>	<b>42.6</b>	<b>17.8</b>	<b>94.7</b>	<b>51.3</b>	<b>0.7</b>	<b>1.0</b>	<b>0.7</b>	<b>-0.3</b>
<b>SD</b>	<b>4.08</b>	<b>4.90</b>	<b>0.76</b>	<b>0.45</b>	<b>0.29</b>	<b>0.57</b>	<b>0.69</b>	<b>1.44</b>	<b>26.28</b>	<b>24.10</b>	<b>2.35</b>	<b>12.33</b>	<b>9.18</b>	<b>0.34</b>	<b>2.16</b>	<b>0.90</b>	<b>0.69</b>	<b>0.47</b>	<b>2.87</b>	<b>0.03</b>	<b>0.06</b>	<b>0.24</b>	<b>0.63</b>
<b>%RSD</b>	<b>2.1</b>	<b>4.5</b>	<b>66.3</b>	<b>286.7</b>	<b>26.23</b>	<b>2.4</b>	<b>-47.2</b>	<b>-3.4</b>	<b>-3.8</b>	<b>-7.3</b>	<b>4.3</b>	<b>77.1</b>	<b>4.1</b>	<b>1.0</b>	<b>4.4</b>	<b>2.1</b>	<b>3.9</b>	<b>0.50</b>	<b>5.6</b>	<b>5.0</b>	<b>6.2</b>	<b>34.3</b>	<b>-218.3</b>
20–1	427.3	180.0	2.1	0.5	2.4	51.9	3.4	-53.0	-836.0	-449.0	120.7	1.0	416.0	76.4	120.0	97.5	37.8	208.0	105.6	1.7	2.0	1.7	0.7
20–2	415.3	201.0	2.2	1.0	2.1	54.4	1.9	-56.4	-899.0	-506.0	124.7	-12.0	420.0	76.6	131.0	96.1	39.9	208.0	104.6	1.8	2.1	1.3	0.9
20–3	400.3	179.0	2.1	0.2	2.2	51.4	2.2	-53.9	-764.0	-449.0	115.7	0.0	396.0	71.3	121.0	92.3	35.8	201.0	98.6	2.0	1.8	3.1	0.8
<b>Mean</b>	<b>414.3</b>	<b>186.7</b>	<b>2.2</b>	<b>0.5</b>	<b>2.3</b>	<b>52.5</b>	<b>2.5</b>	<b>-54.4</b>	<b>-833.0</b>	<b>-468.0</b>	<b>120.4</b>	<b>-3.7</b>	<b>410.7</b>	<b>74.7</b>	<b>124.0</b>	<b>95.3</b>	<b>37.8</b>	<b>205.7</b>	<b>102.9</b>	<b>1.9</b>	<b>2.0</b>	<b>2.0</b>	<b>0.8</b>
<b>SD</b>	<b>11.05</b>	<b>10.14</b>	<b>0.03</b>	<b>0.35</b>	<b>0.11</b>	<b>1.31</b>	<b>0.65</b>	<b>1.44</b>	<b>55.15</b>	<b>26.87</b>	<b>3.68</b>	<b>5.91</b>	<b>10.50</b>	<b>2.45</b>	<b>4.97</b>	<b>2.20</b>	<b>1.67</b>	<b>3.30</b>	<b>3.09</b>	<b>0.11</b>	<b>0.15</b>	<b>0.79</b>	<b>0.07</b>
<b>%RSD</b>	<b>2.7</b>	<b>5.4</b>	<b>1.2</b>	<b>63.8</b>	<b>4.94</b>	<b>2.5</b>	<b>25.9</b>	<b>-2.6</b>	<b>-6.6</b>	<b>-5.7</b>	<b>3.1</b>	<b>-161.1</b>	<b>2.6</b>	<b>3.3</b>	<b>4.0</b>	<b>2.3</b>	<b>4.4</b>	<b>1.6</b>	<b>3.0</b>	<b>5.7</b>	<b>7.4</b>	<b>38.9</b>	<b>8.6</b>

**Table S21a.** SIFT-MS LOQ data for Mix 2 in 10% DMI:90% water at three levels (1, 2, and 5).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	6.8	8.5	123.7	89.6	133.6	2.8	93.0	87.6	28.0	77.2	4.1	3.0	5.3	5.4	15.5	3.9	74.4	7.4	9.2	126.6	104.5	125.0	119.4
1–2	6.6	10.0	128.7	80.0	126.6	3.9	92.0	82.7	64.0	95.2	3.2	2.8	4.5	5.3	16.8	4.6	85.4	9.2	10.7	124.6	108.5	134.0	121.4
1–3	7.8	10.7	121.7	88.8	132.6	3.2	87.9	84.6	50.0	82.2	4.8	2.7	5.5	4.9	16.8	3.8	76.4	8.7	9.2	126.6	110.5	121.0	124.4
<b>Mean</b>	<b>7.1</b>	<b>9.7</b>	<b>124.7</b>	<b>86.1</b>	<b>130.9</b>	<b>3.3</b>	<b>91.0</b>	<b>85.0</b>	<b>47.3</b>	<b>84.9</b>	<b>4.0</b>	<b>2.8</b>	<b>5.1</b>	<b>5.2</b>	<b>16.4</b>	<b>4.1</b>	<b>78.7</b>	<b>8.4</b>	<b>9.7</b>	<b>126.0</b>	<b>107.8</b>	<b>126.7</b>	<b>121.8</b>
<b>SD</b>	<b>0.52</b>	<b>0.92</b>	<b>2.94</b>	<b>4.35</b>	<b>3.09</b>	<b>0.45</b>	<b>2.21</b>	<b>2.02</b>	<b>14.82</b>	<b>7.59</b>	<b>0.65</b>	<b>0.10</b>	<b>0.43</b>	<b>0.21</b>	<b>0.61</b>	<b>0.36</b>	<b>4.78</b>	<b>0.76</b>	<b>0.71</b>	<b>0.94</b>	<b>2.49</b>	<b>5.44</b>	<b>2.05</b>
<b>%RSD</b>	<b>7.4</b>	<b>9.4</b>	<b>2.4</b>	<b>5.0</b>	<b>2.4</b>	<b>13.6</b>	<b>2.4</b>	<b>2.4</b>	<b>31.3</b>	<b>8.9</b>	<b>16.4</b>	<b>3.5</b>	<b>8.5</b>	<b>4.0</b>	<b>3.7</b>	<b>8.7</b>	<b>6.1</b>	<b>9.0</b>	<b>7.3</b>	<b>0.75</b>	<b>2.3</b>	<b>4.3</b>	<b>1.7</b>
2–1	12.0	14.8	277.7	191.7	285.6	6.7	194.0	169.6	191.0	183.2	8.5	5.6	5.3	10.7	25.6	10.1	187.4	21.2	15.5	280.6	240.5	275.0	256.4
2–2	12.9	15.4	291.7	201.7	291.6	5.4	200.0	187.6	141.0	181.2	9.7	5.4	4.7	12.1	28.3	9.1	194.4	20.5	18.5	289.6	236.5	284.0	276.4
2–3	14.0	18.4	280.7	175.7	295.6	6.0	200.0	178.6	124.0	178.2	10.1	4.7	6.5	11.0	23.1	9.9	170.4	21.6	18.9	278.6	238.5	276.0	265.4
<b>Mean</b>	<b>13.0</b>	<b>16.2</b>	<b>283.4</b>	<b>189.7</b>	<b>290.9</b>	<b>6.1</b>	<b>198.0</b>	<b>178.6</b>	<b>152.0</b>	<b>180.9</b>	<b>9.4</b>	<b>5.2</b>	<b>5.5</b>	<b>11.2</b>	<b>25.7</b>	<b>9.7</b>	<b>184.1</b>	<b>21.1</b>	<b>17.6</b>	<b>283.0</b>	<b>238.5</b>	<b>278.3</b>	<b>266.1</b>
<b>SD</b>	<b>0.82</b>	<b>1.57</b>	<b>6.02</b>	<b>10.71</b>	<b>4.11</b>	<b>0.52</b>	<b>2.83</b>	<b>7.35</b>	<b>28.44</b>	<b>2.05</b>	<b>0.68</b>	<b>0.39</b>	<b>0.75</b>	<b>0.60</b>	<b>2.12</b>	<b>0.45</b>	<b>10.08</b>	<b>0.45</b>	<b>1.52</b>	<b>4.78</b>	<b>1.63</b>	<b>4.03</b>	<b>8.18</b>
<b>%RSD</b>	<b>6.3</b>	<b>9.7</b>	<b>2.1</b>	<b>5.6</b>	<b>1.4</b>	<b>8.6</b>	<b>1.4</b>	<b>4.1</b>	<b>18.7</b>	<b>1.1</b>	<b>7.2</b>	<b>7.4</b>	<b>13.6</b>	<b>5.4</b>	<b>8.3</b>	<b>4.6</b>	<b>5.5</b>	<b>2.2</b>	<b>8.6</b>	<b>1.7</b>	<b>0.68</b>	<b>1.4</b>	<b>3.1</b>
5–1	31.5	23.0	751.7	503.7	787.6	13.7	523.0	480.6	381.0	412.2	16.9	13.5	11.0	27.7	54.0	21.7	398.4	50.3	38.2	769.6	650.5	764.0	723.4
5–2	26.5	20.5	748.7	512.7	779.6	16.4	513.0	461.6	441.0	495.2	18.3	12.8	11.4	30.0	60.1	25.6	463.4	55.8	38.5	771.6	652.5	773.0	767.4
5–3	31.9	23.6	736.7	484.7	762.6	14.2	535.0	463.6	431.0	456.2	17.1	12.8	12.1	27.4	55.7	24.3	426.4	50.8	41.9	757.6	640.5	774.0	730.4
<b>Mean</b>	<b>30.0</b>	<b>22.4</b>	<b>745.7</b>	<b>500.4</b>	<b>776.6</b>	<b>14.8</b>	<b>523.7</b>	<b>468.6</b>	<b>417.7</b>	<b>454.5</b>	<b>17.4</b>	<b>13.0</b>	<b>11.5</b>	<b>28.3</b>	<b>56.6</b>	<b>23.9</b>	<b>429.4</b>	<b>52.3</b>	<b>39.5</b>	<b>766.3</b>	<b>647.8</b>	<b>770.3</b>	<b>740.4</b>
<b>SD</b>	<b>2.46</b>	<b>1.34</b>	<b>6.48</b>	<b>11.67</b>	<b>10.42</b>	<b>1.17</b>	<b>8.99</b>	<b>8.52</b>	<b>26.25</b>	<b>33.91</b>	<b>0.62</b>	<b>0.33</b>	<b>0.45</b>	<b>1.16</b>	<b>2.57</b>	<b>1.62</b>	<b>26.62</b>	<b>2.48</b>	<b>1.68</b>	<b>6.18</b>	<b>5.25</b>	<b>4.50</b>	<b>19.30</b>
<b>%RSD</b>	<b>8.2</b>	<b>6.0</b>	<b>0.87</b>	<b>2.3</b>	<b>1.3</b>	<b>7.9</b>	<b>1.7</b>	<b>1.8</b>	<b>6.3</b>	<b>7.5</b>	<b>3.6</b>	<b>2.5</b>	<b>4.0</b>	<b>4.1</b>	<b>4.5</b>	<b>6.8</b>	<b>6.2</b>	<b>4.7</b>	<b>4.2</b>	<b>0.81</b>	<b>0.81</b>	<b>0.58</b>	<b>2.6</b>

**Table S21b.** SIFT-MS LOQ data for Mix 2 in 100% DMI at three levels (1, 2, and 5).

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
1–1	17.4	10.0	6.2	3.0	8.8	1.3	5.9	5.5	-449.0	-176.0	6.2	-7.0	30.0	6.4	15.0	4.1	16.9	21.1	26.9	3.0	2.7	2.9	2.6
1–2	15.1	2.0	6.4	2.3	6.7	1.7	4.7	7.8	-340.0	-112.0	5.6	0.0	31.0	6.0	17.0	4.0	16.7	19.9	23.9	2.9	2.8	2.4	3.6
1–3	15.4	4.0	7.1	2.9	8.2	1.8	4.8	21.7	-310.0	-78.0	5.2	-6.0	35.0	5.2	19.0	4.5	16.7	21.5	22.0	3.6	2.6	3.3	3.5
<b>Mean</b>	<b>16.0</b>	<b>5.3</b>	<b>6.6</b>	<b>2.7</b>	<b>7.9</b>	<b>1.6</b>	<b>5.1</b>	<b>11.7</b>	<b>-366.3</b>	<b>-122.0</b>	<b>5.7</b>	<b>-4.3</b>	<b>32.0</b>	<b>5.8</b>	<b>17.0</b>	<b>4.2</b>	<b>16.8</b>	<b>20.8</b>	<b>24.3</b>	<b>3.2</b>	<b>2.7</b>	<b>2.9</b>	<b>3.2</b>
<b>SD</b>	<b>1.02</b>	<b>3.40</b>	<b>0.38</b>	<b>0.32</b>	<b>0.86</b>	<b>0.21</b>	<b>0.57</b>	<b>7.16</b>	<b>59.72</b>	<b>40.63</b>	<b>0.41</b>	<b>3.09</b>	<b>2.16</b>	<b>0.52</b>	<b>1.63</b>	<b>0.23</b>	<b>0.09</b>	<b>0.68</b>	<b>2.02</b>	<b>0.28</b>	<b>0.11</b>	<b>0.38</b>	<b>0.46</b>
<b>%RSD</b>	<b>6.4</b>	<b>63.7</b>	<b>5.8</b>	<b>11.8</b>	<b>10.9</b>	<b>12.9</b>	<b>11.2</b>	<b>61.3</b>	<b>-16.3</b>	<b>-33.3</b>	<b>7.3</b>	<b>-71.3</b>	<b>6.8</b>	<b>8.8</b>	<b>9.6</b>	<b>5.6</b>	<b>0.6</b>	<b>3.3</b>	<b>8.3</b>	<b>8.8</b>	<b>3.9</b>	<b>13.0</b>	<b>14.3</b>
2–1	34.7	17.0	15.3	10.8	16.1	2.9	8.6	-6.4	-605.0	-178.0	9.4	4.0	46.0	12.6	37.0	8.9	29.5	35.5	31.9	8.6	6.4	7.7	5.5
2–2	37.9	14.0	15.4	10.0	16.6	3.4	4.2	2.3	-469.0	-134.0	9.7	18.0	47.0	14.6	38.0	9.7	33.7	35.7	36.9	7.6	6.3	6.1	6.4
2–3	38.9	21.0	18.6	12.5	15.6	2.4	6.0	31.1	-210.0	43.0	8.6	31.0	43.0	12.1	36.0	8.4	30.3	39.1	33.9	7.8	6.0	5.7	6.0
<b>Mean</b>	<b>37.2</b>	<b>17.3</b>	<b>16.5</b>	<b>11.1</b>	<b>16.1</b>	<b>2.9</b>	<b>6.3</b>	<b>9.0</b>	<b>-428.0</b>	<b>-89.7</b>	<b>9.2</b>	<b>17.7</b>	<b>45.3</b>	<b>13.1</b>	<b>37.0</b>	<b>9.0</b>	<b>31.2</b>	<b>36.8</b>	<b>34.2</b>	<b>8.0</b>	<b>6.2</b>	<b>6.5</b>	<b>6.0</b>
<b>SD</b>	<b>1.79</b>	<b>2.87</b>	<b>1.53</b>	<b>1.04</b>	<b>0.41</b>	<b>0.41</b>	<b>1.83</b>	<b>16.03</b>	<b>163.84</b>	<b>95.51</b>	<b>0.46</b>	<b>11.03</b>	<b>1.70</b>	<b>1.08</b>	<b>0.82</b>	<b>0.53</b>	<b>1.82</b>	<b>1.65</b>	<b>2.05</b>	<b>0.41</b>	<b>0.16</b>	<b>0.85</b>	<b>0.36</b>
<b>%RSD</b>	<b>4.8</b>	<b>16.5</b>	<b>9.3</b>	<b>9.4</b>	<b>2.5</b>	<b>14.2</b>	<b>29.1</b>	<b>178.1</b>	<b>-38.3</b>	<b>-106.5</b>	<b>5.0</b>	<b>62.4</b>	<b>3.7</b>	<b>8.3</b>	<b>2.2</b>	<b>5.9</b>	<b>5.8</b>	<b>4.5</b>	<b>6.0</b>	<b>5.1</b>	<b>2.6</b>	<b>13.2</b>	<b>6.1</b>
5–1	89.4	38.0	46.6	29.0	48.5	6.1	14.3	-8.0	-702.0	-246.0	23.9	8.0	74.0	34.9	58.0	21.6	82.2	93.3	47.9	20.3	19.1	19.4	21.8
5–2	83.4	48.0	43.4	31.2	48.3	5.9	14.1	-1.3	-655.0	-165.0	21.2	20.0	64.0	36.7	58.0	20.2	83.2	92.3	47.9	22.1	16.2	21.8	20.8
5–3	90.4	42.0	47.2	30.0	48.5	5.5	12.6	-6.8	-700.0	-221.0	20.0	11.0	62.0	34.4	68.0	21.2	78.2	96.3	44.9	19.6	18.1	21.6	20.0
<b>Mean</b>	<b>87.7</b>	<b>42.7</b>	<b>45.8</b>	<b>30.0</b>	<b>48.4</b>	<b>5.8</b>	<b>13.7</b>	<b>-5.4</b>	<b>-685.7</b>	<b>-210.7</b>	<b>21.7</b>	<b>13.0</b>	<b>66.7</b>	<b>35.3</b>	<b>61.3</b>	<b>21.0</b>	<b>81.2</b>	<b>94.0</b>	<b>46.9</b>	<b>20.7</b>	<b>17.8</b>	<b>20.9</b>	<b>20.8</b>
<b>SD</b>	<b>3.09</b>	<b>4.11</b>	<b>1.67</b>	<b>0.90</b>	<b>0.09</b>	<b>0.25</b>	<b>0.76</b>	<b>2.92</b>	<b>21.70</b>	<b>33.87</b>	<b>1.63</b>	<b>5.10</b>	<b>5.25</b>	<b>0.99</b>	<b>4.71</b>	<b>0.59</b>	<b>2.16</b>	<b>1.70</b>	<b>1.41</b>	<b>1.05</b>	<b>1.20</b>	<b>1.09</b>	<b>0.74</b>
<b>%RSD</b>	<b>3.5</b>	<b>9.6</b>	<b>3.6</b>	<b>3.0</b>	<b>0.19</b>	<b>4.3</b>	<b>5.5</b>	<b>-54.4</b>	<b>-3.2</b>	<b>-16.1</b>	<b>7.5</b>	<b>39.2</b>	<b>7.9</b>	<b>2.8</b>	<b>7.7</b>	<b>2.8</b>	<b>2.7</b>	<b>1.8</b>	<b>3.0</b>	<b>5.1</b>	<b>6.8</b>	<b>5.2</b>	<b>3.5</b>

## E. Recovery

**Table S22a.** SIFT-MS recovery data for Mix 1 spiked into aspirin dissolved in 5% DMI:95% water at 25, 50, and 100% of 500 level.

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
125–1	97.7	100.2	109.1	109.6	109.0	98.4	106.6	107.2	130.9	109.6	102.2	97.1	96.4	98.2	97.1	102.7	104.9	96.9	99.0	109.6	104.1	111.8	108.6
125–2	99.4	104.0	111.2	118.3	111.4	106.5	108.6	106.7	116.5	104.7	106.4	103.5	103.6	102.6	105.4	107.2	103.8	104.0	99.6	106.5	109.8	111.5	110.0
125–3	101.3	101.9	112.0	107.7	109.8	103.1	109.9	107.9	117.9	101.7	105.1	99.4	100.0	97.9	104.0	103.8	106.4	101.5	97.0	109.9	109.0	113.8	107.7
<b>Mean</b>	<b>99.5</b>	<b>102.0</b>	<b>110.8</b>	<b>111.9</b>	<b>110.1</b>	<b>102.6</b>	<b>108.4</b>	<b>107.3</b>	<b>121.8</b>	<b>105.3</b>	<b>104.5</b>	<b>100.0</b>	<b>100.0</b>	<b>99.6</b>	<b>102.2</b>	<b>104.6</b>	<b>105.1</b>	<b>100.8</b>	<b>98.5</b>	<b>108.7</b>	<b>107.7</b>	<b>112.4</b>	<b>108.8</b>
<b>SD</b>	<b>1.48</b>	<b>1.53</b>	<b>1.24</b>	<b>4.62</b>	<b>0.98</b>	<b>3.31</b>	<b>1.37</b>	<b>0.51</b>	<b>6.50</b>	<b>3.25</b>	<b>1.74</b>	<b>2.65</b>	<b>2.96</b>	<b>2.17</b>	<b>3.64</b>	<b>1.93</b>	<b>1.04</b>	<b>2.92</b>	<b>1.13</b>	<b>1.55</b>	<b>2.54</b>	<b>1.05</b>	<b>0.98</b>
<b>%RSD</b>	<b>1.5</b>	<b>1.5</b>	<b>1.1</b>	<b>4.1</b>	<b>0.89</b>	<b>3.2</b>	<b>1.3</b>	<b>0.47</b>	<b>5.3</b>	<b>3.1</b>	<b>1.7</b>	<b>2.7</b>	<b>3.0</b>	<b>2.2</b>	<b>3.6</b>	<b>1.8</b>	<b>0.99</b>	<b>2.9</b>	<b>1.1</b>	<b>1.4</b>	<b>2.4</b>	<b>0.93</b>	<b>0.90</b>
250–1	99.8	103.1	109.8	106.5	111.7	100.1	108.9	107.3	126.2	107.8	103.3	100.6	102.7	99.6	100.8	102.5	107.0	103.0	101.6	107.6	110.6	112.8	108.5
250–2	99.8	101.5	108.7	111.2	108.1	102.3	106.3	107.3	121.1	103.6	106.0	100.8	98.0	101.4	99.3	106.7	104.3	101.5	101.2	106.6	110.2	111.6	107.1
250–3	101.7	102.3	109.1	109.4	107.9	99.3	106.9	108.7	116.0	103.6	100.6	98.1	99.7	100.8	100.0	99.1	105.7	100.0	101.1	106.6	108.6	111.9	107.5
<b>Mean</b>	<b>100.4</b>	<b>102.3</b>	<b>109.2</b>	<b>109.0</b>	<b>109.2</b>	<b>100.5</b>	<b>107.4</b>	<b>107.7</b>	<b>121.1</b>	<b>105.0</b>	<b>103.3</b>	<b>99.8</b>	<b>100.1</b>	<b>100.6</b>	<b>100.0</b>	<b>102.8</b>	<b>105.7</b>	<b>101.5</b>	<b>101.3</b>	<b>106.9</b>	<b>109.8</b>	<b>112.1</b>	<b>107.7</b>
<b>SD</b>	<b>0.88</b>	<b>0.66</b>	<b>0.43</b>	<b>1.92</b>	<b>1.72</b>	<b>1.25</b>	<b>1.09</b>	<b>0.65</b>	<b>4.13</b>	<b>1.97</b>	<b>2.24</b>	<b>1.24</b>	<b>1.96</b>	<b>0.76</b>	<b>0.63</b>	<b>3.10</b>	<b>1.09</b>	<b>1.20</b>	<b>0.19</b>	<b>0.49</b>	<b>0.89</b>	<b>0.50</b>	<b>0.62</b>
<b>%RSD</b>	<b>0.88</b>	<b>0.65</b>	<b>0.40</b>	<b>1.8</b>	<b>1.6</b>	<b>1.2</b>	<b>1.0</b>	<b>0.60</b>	<b>3.4</b>	<b>1.9</b>	<b>2.2</b>	<b>1.2</b>	<b>2.0</b>	<b>0.75</b>	<b>0.63</b>	<b>3.0</b>	<b>1.0</b>	<b>1.2</b>	<b>0.19</b>	<b>0.46</b>	<b>0.81</b>	<b>0.45</b>	<b>0.58</b>
500–1	97.3	100.7	105.2	107.4	105.2	98.0	103.0	103.4	121.6	95.4	101.4	98.5	95.2	97.9	101.2	101.8	98.4	98.8	102.1	102.9	105.3	105.7	104.3
500–2	99.5	101.9	103.9	102.1	105.2	98.8	103.0	104.4	115.5	98.7	100.1	99.8	97.7	98.6	99.7	100.5	99.1	100.3	103.8	101.2	108.4	103.5	105.0
500–3	98.2	101.5	104.2	100.5	103.2	98.0	103.3	103.0	118.7	95.4	102.0	97.8	95.7	98.6	98.5	103.4	96.7	98.8	99.9	102.1	108.4	102.8	102.1
<b>Mean</b>	<b>98.3</b>	<b>101.4</b>	<b>104.4</b>	<b>103.3</b>	<b>104.5</b>	<b>98.3</b>	<b>103.1</b>	<b>103.6</b>	<b>118.6</b>	<b>96.5</b>	<b>101.2</b>	<b>98.7</b>	<b>96.2</b>	<b>98.4</b>	<b>99.8</b>	<b>101.9</b>	<b>98.1</b>	<b>99.3</b>	<b>101.9</b>	<b>102.1</b>	<b>107.3</b>	<b>104.0</b>	<b>103.8</b>
<b>SD</b>	<b>0.89</b>	<b>0.51</b>	<b>0.54</b>	<b>2.94</b>	<b>0.93</b>	<b>0.35</b>	<b>0.15</b>	<b>0.59</b>	<b>2.51</b>	<b>1.55</b>	<b>0.81</b>	<b>0.80</b>	<b>1.09</b>	<b>0.33</b>	<b>1.10</b>	<b>1.21</b>	<b>0.99</b>	<b>0.69</b>	<b>1.59</b>	<b>0.70</b>	<b>1.45</b>	<b>1.25</b>	<b>1.26</b>
<b>%RSD</b>	<b>0.91</b>	<b>0.50</b>	<b>0.51</b>	<b>2.8</b>	<b>0.89</b>	<b>0.35</b>	<b>0.15</b>	<b>0.57</b>	<b>2.1</b>	<b>1.6</b>	<b>0.80</b>	<b>0.81</b>	<b>1.1</b>	<b>0.33</b>	<b>1.1</b>	<b>1.2</b>	<b>1.0</b>	<b>0.70</b>	<b>1.6</b>	<b>0.69</b>	<b>1.4</b>	<b>1.2</b>	<b>1.2</b>

**Table S22b.** SIFT-MS recovery data for Mix 1 spiked into aspirin dissolved in 100% DMI at 25, 50, and 100% of 500 level.

Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
125–1	105.1	110.6	134.3	53.9	134.7	112.5	112.9	100.1	-12.5	64.9	159.0	142.8	99.3	103.6	107.1	117.7	113.1	100.1	111.4	131.0	232.3	106.8	115.1
125–2	94.0	201.9	87.0	-33.2	71.2	98.1	85.7	220.2	243.5	330.1	92.4	789.2	92.9	93.2	98.1	102.8	108.0	91.4	80.9	52.4	84.3	75.7	5.7
125–3	107.9	102.4	100.3	-12.6	148.2	110.4	80.6	54.4	20.4	112.7	185.9	94.1	93.5	104.1	103.9	111.2	116.9	103.3	104.0	157.2	178.5	183.1	105.2
<b>Mean</b>	<b>102.3</b>	<b>138.3</b>	<b>107.2</b>	<b>2.7</b>	<b>118.1</b>	<b>107.0</b>	<b>93.0</b>	<b>124.9</b>	<b>83.8</b>	<b>169.2</b>	<b>145.8</b>	<b>342.0</b>	<b>95.2</b>	<b>100.3</b>	<b>103.0</b>	<b>110.6</b>	<b>112.6</b>	<b>98.3</b>	<b>98.8</b>	<b>113.5</b>	<b>165.0</b>	<b>121.9</b>	<b>75.3</b>
<b>SD</b>	<b>6.0</b>	<b>45.1</b>	<b>19.9</b>	<b>37.2</b>	<b>33.6</b>	<b>6.3</b>	<b>14.2</b>	<b>69.9</b>	<b>113.8</b>	<b>115.4</b>	<b>39.3</b>	<b>316.8</b>	<b>2.9</b>	<b>5.0</b>	<b>3.7</b>	<b>6.1</b>	<b>3.7</b>	<b>5.0</b>	<b>13.0</b>	<b>44.5</b>	<b>61.2</b>	<b>45.1</b>	<b>49.4</b>
<b>%RSD</b>	<b>5.9</b>	<b>32.6</b>	<b>18.6</b>	<b>1358.1</b>	<b>28.4</b>	<b>5.9</b>	<b>15.3</b>	<b>56.0</b>	<b>135.8</b>	<b>68.2</b>	<b>27.0</b>	<b>92.6</b>	<b>3.0</b>	<b>5.0</b>	<b>3.6</b>	<b>5.5</b>	<b>3.3</b>	<b>5.1</b>	<b>13.1</b>	<b>39.2</b>	<b>37.1</b>	<b>37.0</b>	<b>65.5</b>
250–1	104.3	109.7	93.9	68.0	171.8	108.9	205.0	94.1	134.5	171.9	119.9	134.2	102.8	105.0	101.4	111.8	115.6	105.6	100.0	153.0	214.6	88.4	129.8
250–2	106.4	110.0	182.2	63.9	132.9	111.6	209.2	116.2	178.6	209.6	110.6	133.7	103.6	103.7	100.2	110.4	119.8	105.1	97.4	127.2	175.9	144.2	112.2
250–3	102.3	110.0	88.9	106.3	158.2	107.1	162.4	128.3	164.1	194.6	109.6	134.2	106.0	105.7	104.9	108.5	113.4	102.6	93.3	121.2	186.0	78.5	74.8
<b>Mean</b>	<b>104.3</b>	<b>109.9</b>	<b>121.7</b>	<b>79.4</b>	<b>154.3</b>	<b>109.2</b>	<b>192.2</b>	<b>112.9</b>	<b>159.0</b>	<b>192.0</b>	<b>113.4</b>	<b>134.0</b>	<b>104.1</b>	<b>104.8</b>	<b>102.2</b>	<b>110.2</b>	<b>116.3</b>	<b>104.4</b>	<b>96.9</b>	<b>133.8</b>	<b>192.1</b>	<b>103.7</b>	<b>105.6</b>
<b>SD</b>	<b>1.7</b>	<b>0.19</b>	<b>42.8</b>	<b>19.1</b>	<b>16.1</b>	<b>1.9</b>	<b>21.1</b>	<b>14.1</b>	<b>18.4</b>	<b>15.5</b>	<b>4.6</b>	<b>0.27</b>	<b>1.4</b>	<b>0.82</b>	<b>2.0</b>	<b>1.3</b>	<b>2.7</b>	<b>1.3</b>	<b>2.8</b>	<b>13.8</b>	<b>16.4</b>	<b>28.9</b>	<b>23.0</b>
<b>%RSD</b>	<b>1.6</b>	<b>0.17</b>	<b>35.2</b>	<b>24.1</b>	<b>10.4</b>	<b>1.7</b>	<b>11.0</b>	<b>12.5</b>	<b>11.6</b>	<b>8.1</b>	<b>4.1</b>	<b>0.20</b>	<b>1.3</b>	<b>0.78</b>	<b>2.0</b>	<b>1.2</b>	<b>2.3</b>	<b>1.3</b>	<b>2.8</b>	<b>10.3</b>	<b>8.5</b>	<b>27.9</b>	<b>21.7</b>
500–1	103.2	111.6	140.5	82.9	150.7	110.2	257.8	58.9	105.5	131.2	106.7	154.3	97.3	111.4	103.9	109.5	115.3	105.5	103.2	148.0	198.9	105.3	131.6
500–2	102.7	111.6	146.8	92.0	158.2	111.6	321.6	62.6	101.5	124.3	107.7	156.5	98.9	111.8	103.4	108.6	115.3	105.0	102.6	161.4	145.5	111.5	96.5
500–3	102.7	112.6	97.2	67.5	152.4	112.9	353.5	54.2	93.0	102.6	104.2	157.4	99.7	108.8	105.0	108.6	116.4	104.2	102.8	184.5	206.1	140.1	111.4
<b>Mean</b>	<b>102.8</b>	<b>112.0</b>	<b>128.2</b>	<b>80.8</b>	<b>153.8</b>	<b>111.6</b>	<b>311.0</b>	<b>58.6</b>	<b>100.0</b>	<b>119.4</b>	<b>106.2</b>	<b>156.1</b>	<b>98.6</b>	<b>110.7</b>	<b>104.1</b>	<b>108.9</b>	<b>115.7</b>	<b>104.9</b>	<b>102.9</b>	<b>164.6</b>	<b>183.5</b>	<b>119.0</b>	<b>113.2</b>
<b>SD</b>	<b>0.24</b>	<b>0.47</b>	<b>22.1</b>	<b>10.1</b>	<b>3.2</b>	<b>1.1</b>	<b>39.8</b>	<b>3.4</b>	<b>5.2</b>	<b>12.2</b>	<b>1.5</b>	<b>1.3</b>	<b>1.0</b>	<b>1.3</b>	<b>0.67</b>	<b>0.44</b>	<b>0.50</b>	<b>0.52</b>	<b>0.23</b>	<b>15.1</b>	<b>27.0</b>	<b>15.2</b>	<b>14.4</b>
<b>%RSD</b>	<b>0.23</b>	<b>0.42</b>	<b>17.2</b>	<b>12.5</b>	<b>2.1</b>	<b>0.99</b>	<b>12.8</b>	<b>5.9</b>	<b>5.2</b>	<b>10.2</b>	<b>1.4</b>	<b>0.84</b>	<b>1.0</b>	<b>1.2</b>	<b>0.64</b>	<b>0.41</b>	<b>0.43</b>	<b>0.50</b>	<b>0.23</b>	<b>9.2</b>	<b>14.7</b>	<b>12.7</b>	<b>12.7</b>

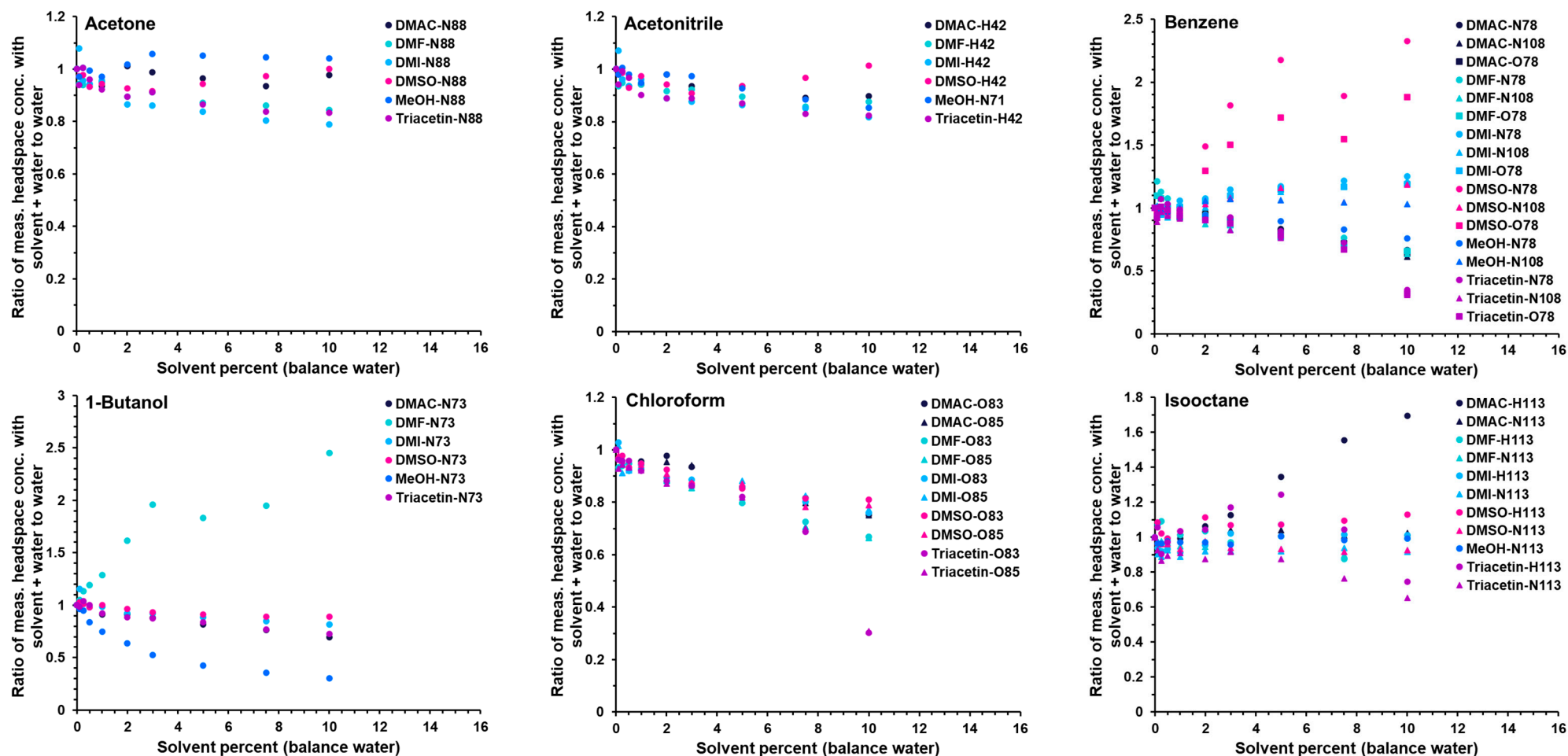
**Table S23.** SIFT-MS recovery data for Mix 2 spiked into aspirin dissolved in 100% DMI at 25, 50, and 100% of 500 level.

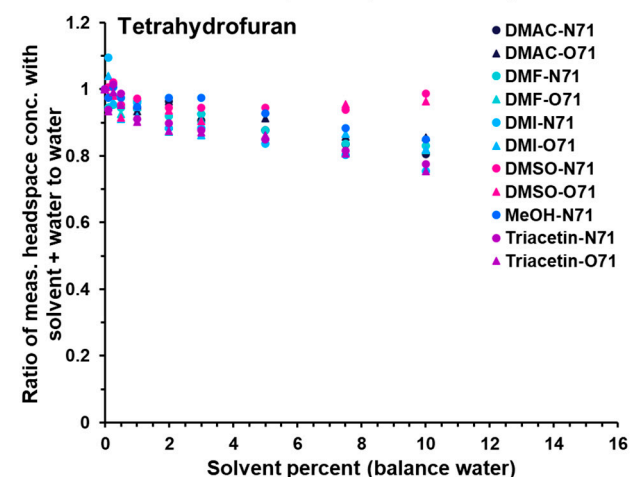
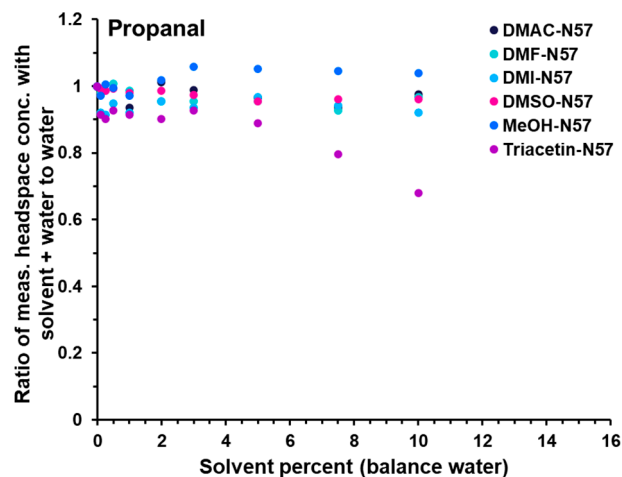
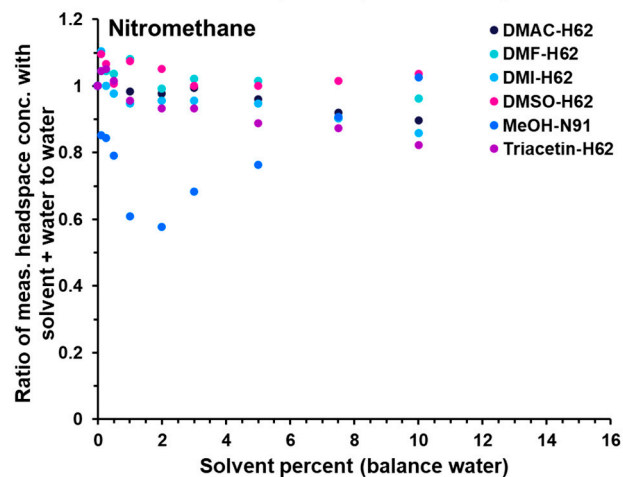
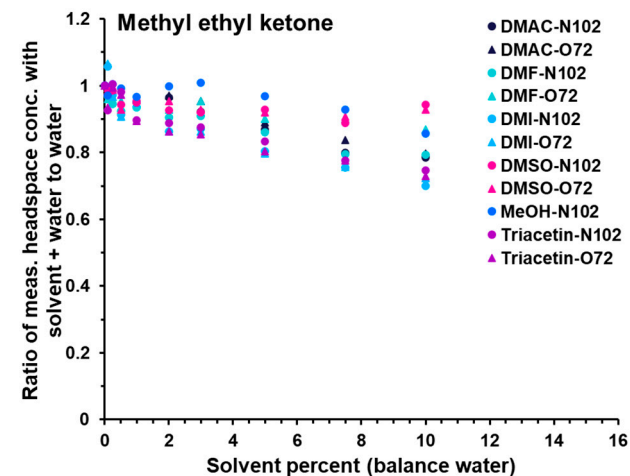
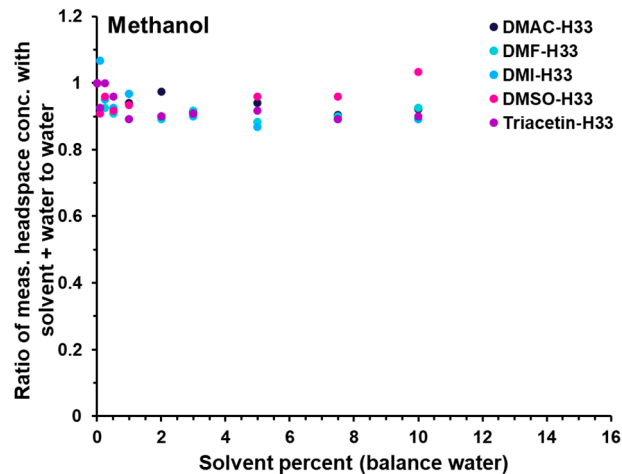
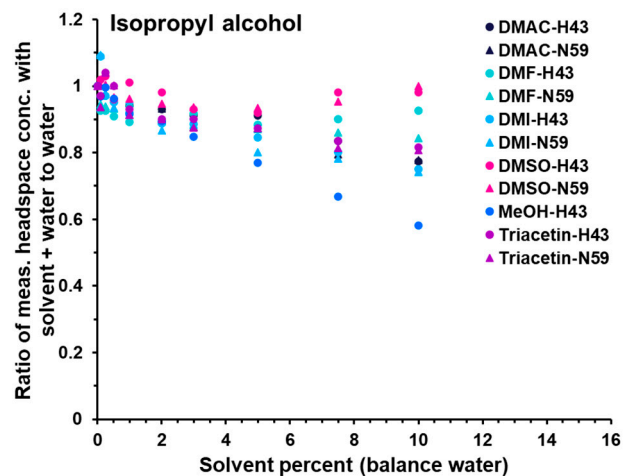
Level—Replicate Number; Statistics	Acetone (NO <sup>+</sup> 88)	Acetonitrile (H <sub>3</sub> O <sup>+</sup> 42)	Benzene (NO <sup>+</sup> 78)	Benzene (NO <sup>+</sup> 108)	Benzene (O <sub>2</sub> <sup>+</sup> 78)	1-Butanol (NO <sup>+</sup> 73)	Chloroform (O <sub>2</sub> <sup>+</sup> 83)	Chloroform (O <sub>2</sub> <sup>+</sup> 85)	Isooctane (H <sub>3</sub> O <sup>+</sup> 113)	Isooctane (NO <sup>+</sup> 113)	Isopropyl alcohol (H <sub>3</sub> O <sup>+</sup> 43)	Isopropyl alcohol (NO <sup>+</sup> 59)	Methanol (H <sub>3</sub> O <sup>+</sup> 33)	Methyl ethyl ketone (NO <sup>+</sup> 102)	Methyl ethyl ketone (O <sub>2</sub> <sup>+</sup> 72)	Nitromethane (H <sub>3</sub> O <sup>+</sup> 62)	Propanal (NO <sup>+</sup> 57)	Tetrahydrofuran (NO <sup>+</sup> 71)	Tetrahydrofuran (O <sub>2</sub> <sup>+</sup> 71)	Toluene (NO <sup>+</sup> 92)	Toluene (O <sub>2</sub> <sup>+</sup> 92)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 130)	Trichloroethylene (O <sub>2</sub> <sup>+</sup> 132)
125–1	98.8	99.5	100.0	99.3	102.0	95.4	109.0	97.1	226.9	107.4	101.8	67.5	98.4	100.1	106.4	101.0	107.1	95.7	105.9	98.0	105.6	108.9	111.7
125–2	98.0	98.3	98.7	114.4	103.2	97.7	110.7	100.6	209.6	100.1	95.6	64.5	100.0	102.0	105.3	101.0	106.6	96.6	104.8	101.7	103.8	117.7	109.6
125–3	97.1	99.1	101.2	92.4	101.2	103.5	95.3	104.0	284.6	129.1	97.0	64.5	97.2	102.0	103.1	102.0	107.9	96.1	103.4	101.7	104.7	102.0	104.5
<b>Mean</b>	<b>98.0</b>	<b>99.0</b>	<b>100.0</b>	<b>102.1</b>	<b>102.1</b>	<b>98.9</b>	<b>105.0</b>	<b>100.6</b>	<b>240.4</b>	<b>112.2</b>	<b>98.1</b>	<b>65.5</b>	<b>98.5</b>	<b>101.4</b>	<b>105.0</b>	<b>101.4</b>	<b>107.2</b>	<b>96.1</b>	<b>104.7</b>	<b>100.5</b>	<b>104.7</b>	<b>109.5</b>	<b>108.6</b>
<b>SD</b>	<b>0.70</b>	<b>0.52</b>	<b>1.03</b>	<b>9.18</b>	<b>0.85</b>	<b>3.43</b>	<b>6.91</b>	<b>2.82</b>	<b>32.06</b>	<b>12.33</b>	<b>2.64</b>	<b>1.44</b>	<b>1.14</b>	<b>0.91</b>	<b>1.37</b>	<b>0.46</b>	<b>0.57</b>	<b>0.39</b>	<b>1.04</b>	<b>1.73</b>	<b>0.75</b>	<b>6.39</b>	<b>3.01</b>
<b>%RSD</b>	<b>0.71</b>	<b>0.53</b>	<b>1.0</b>	<b>9.0</b>	<b>0.83</b>	<b>3.5</b>	<b>6.6</b>	<b>2.8</b>	<b>13.3</b>	<b>11.0</b>	<b>2.7</b>	<b>2.2</b>	<b>1.2</b>	<b>0.90</b>	<b>1.3</b>	<b>0.45</b>	<b>0.53</b>	<b>0.41</b>	<b>1.0</b>	<b>1.7</b>	<b>0.72</b>	<b>5.8</b>	<b>2.8</b>
250–1	103.1	104.7	107.1	108.7	105.1	102.4	109.2	115.8	240.4	104.5	104.2	68.5	102.0	104.3	104.0	104.2	110.8	100.9	104.7	107.1	104.6	100.8	110.0
250–2	105.3	103.6	104.8	102.2	108.5	99.7	111.5	119.3	312.5	144.4	101.4	69.4	100.8	107.6	113.2	104.7	110.2	99.8	112.0	108.5	110.1	116.9	116.7
250–3	103.2	108.7	108.8	115.6	110.7	107.5	110.7	109.8	234.6	128.1	106.9	75.2	111.9	107.2	114.2	105.7	115.5	104.0	109.6	109.9	110.1	112.5	112.6
<b>Mean</b>	<b>103.9</b>	<b>105.7</b>	<b>106.9</b>	<b>108.8</b>	<b>108.1</b>	<b>103.2</b>	<b>110.5</b>	<b>114.9</b>	<b>262.5</b>	<b>125.6</b>	<b>104.2</b>	<b>71.0</b>	<b>104.9</b>	<b>106.4</b>	<b>110.5</b>	<b>104.9</b>	<b>112.2</b>	<b>101.6</b>	<b>108.8</b>	<b>108.5</b>	<b>108.2</b>	<b>110.1</b>	<b>113.1</b>
<b>SD</b>	<b>1.00</b>	<b>2.18</b>	<b>1.63</b>	<b>5.47</b>	<b>2.30</b>	<b>3.21</b>	<b>0.95</b>	<b>3.92</b>	<b>35.43</b>	<b>16.38</b>	<b>2.23</b>	<b>2.97</b>	<b>4.98</b>	<b>1.44</b>	<b>4.59</b>	<b>0.61</b>	<b>2.35</b>	<b>1.77</b>	<b>3.03</b>	<b>1.12</b>	<b>2.56</b>	<b>6.80</b>	<b>2.74</b>
<b>%RSD</b>	<b>1.0</b>	<b>2.1</b>	<b>1.5</b>	<b>5.0</b>	<b>2.1</b>	<b>3.1</b>	<b>0.86</b>	<b>3.4</b>	<b>13.5</b>	<b>13.0</b>	<b>2.1</b>	<b>4.2</b>	<b>4.7</b>	<b>1.4</b>	<b>4.2</b>	<b>0.58</b>	<b>2.1</b>	<b>1.7</b>	<b>2.8</b>	<b>1.0</b>	<b>2.4</b>	<b>6.2</b>	<b>2.4</b>
500–1	100.0	100.5	102.7	103.1	107.7	100.6	105.0	119.5	237.0	128.4	99.1	72.2	97.9	100.2	103.7	100.9	106.9	99.0	106.4	100.0	102.5	107.5	108.2
500–2	101.2	104.7	102.3	105.9	107.7	99.9	103.8	101.0	228.4	116.6	99.4	72.8	100.9	102.1	105.8	97.2	108.3	98.4	105.5	103.7	87.0	91.2	86.2
500–3	96.9	102.6	100.5	105.7	104.6	99.2	105.4	106.2	206.7	122.1	100.1	69.5	95.9	101.2	106.5	99.2	108.3	100.8	104.6	102.1	102.7	106.5	106.4
<b>Mean</b>	<b>99.4</b>	<b>102.6</b>	<b>101.9</b>	<b>104.9</b>	<b>106.7</b>	<b>99.9</b>	<b>104.7</b>	<b>108.9</b>	<b>224.0</b>	<b>122.4</b>	<b>99.5</b>	<b>71.5</b>	<b>98.2</b>	<b>101.2</b>	<b>105.3</b>	<b>99.1</b>	<b>107.8</b>	<b>99.4</b>	<b>105.5</b>	<b>101.9</b>	<b>97.4</b>	<b>101.7</b>	<b>100.2</b>
<b>SD</b>	<b>1.79</b>	<b>1.72</b>	<b>0.95</b>	<b>1.26</b>	<b>1.47</b>	<b>0.60</b>	<b>0.65</b>	<b>7.81</b>	<b>12.74</b>	<b>4.82</b>	<b>0.43</b>	<b>1.46</b>	<b>2.04</b>	<b>0.79</b>	<b>1.17</b>	<b>1.50</b>	<b>0.65</b>	<b>1.02</b>	<b>0.74</b>	<b>1.50</b>	<b>7.35</b>	<b>7.49</b>	<b>9.97</b>
<b>%RSD</b>	<b>1.8</b>	<b>1.7</b>	<b>0.94</b>	<b>1.2</b>	<b>1.4</b>	<b>0.60</b>	<b>0.62</b>	<b>7.2</b>	<b>5.7</b>	<b>3.9</b>	<b>0.43</b>	<b>2.0</b>	<b>2.1</b>	<b>0.78</b>	<b>1.1</b>	<b>1.5</b>	<b>0.60</b>	<b>1.0</b>	<b>0.70</b>	<b>1.5</b>	<b>7.5</b>	<b>7.4</b>	<b>9.9</b>

## Figures

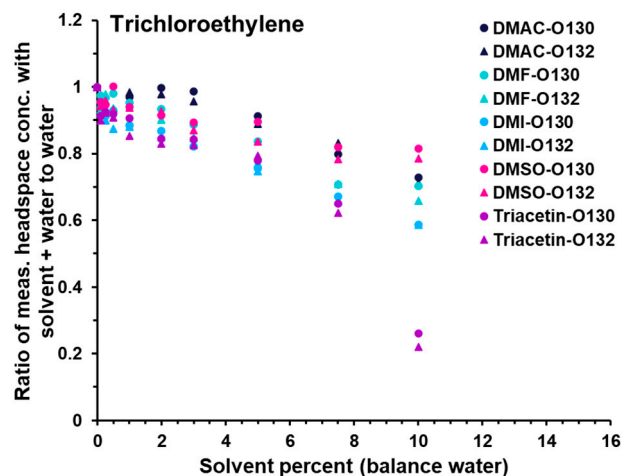
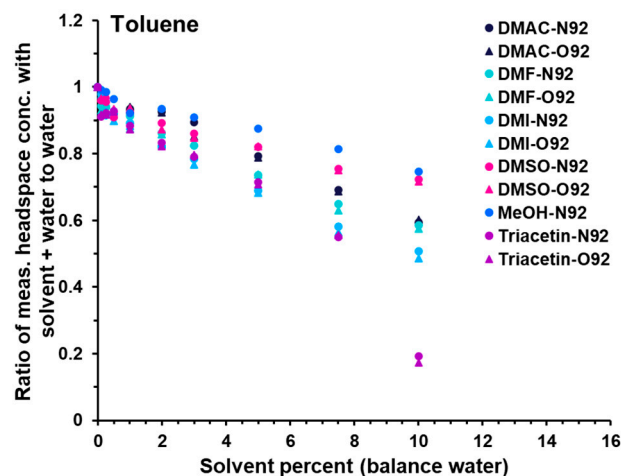
### A. Measured Headspace Concentrations Relative to Aqueous Solutions

**Figure S1.** Ratio of measured headspace concentration of analytes (Mix 1) in the solvent-water mixes (0 to 10% solvent) to that obtained in aqueous solution. All measurements have the blank subtracted. The legend indicates first the matrix, then the reagent ion (first letter), and finally the product ion  $m/z$ . All product ions are shown.

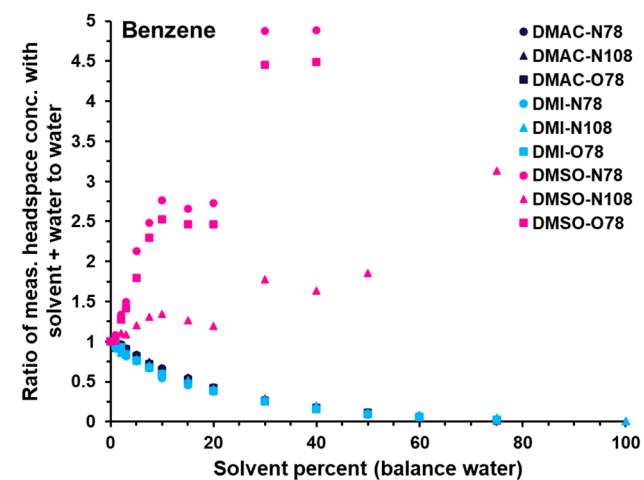
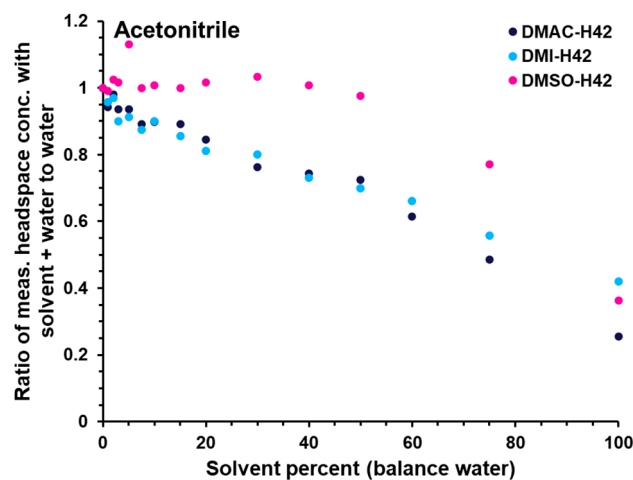
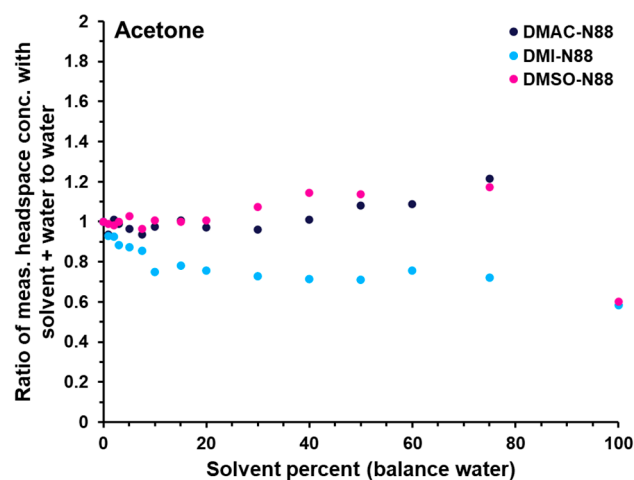


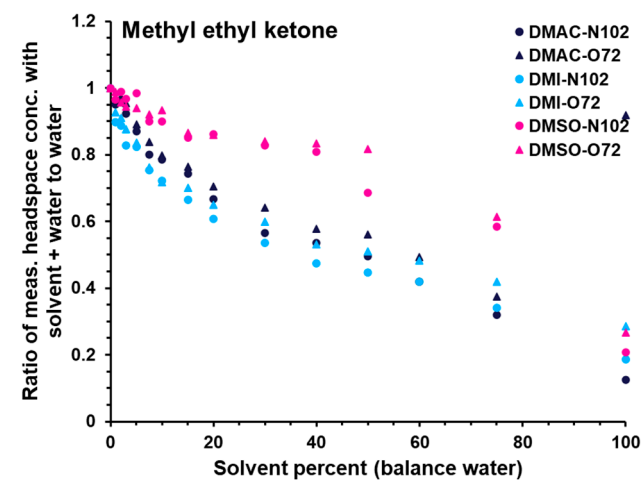
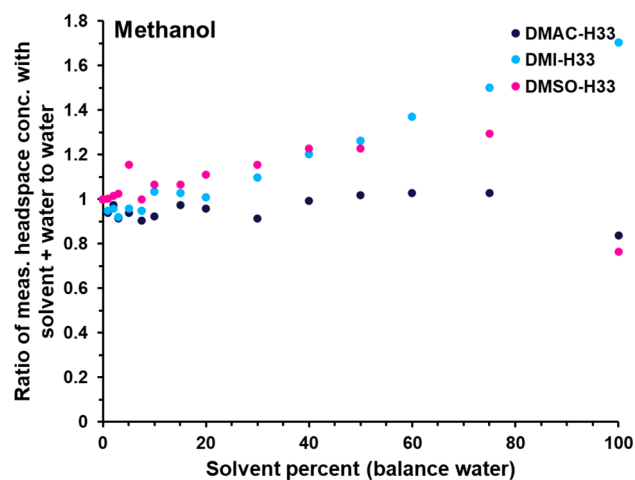
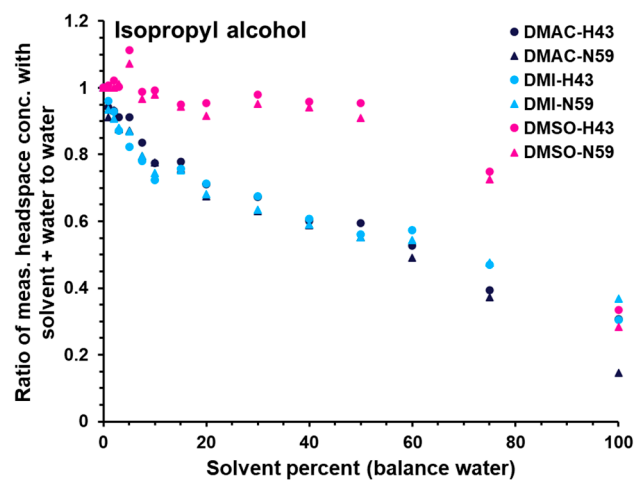
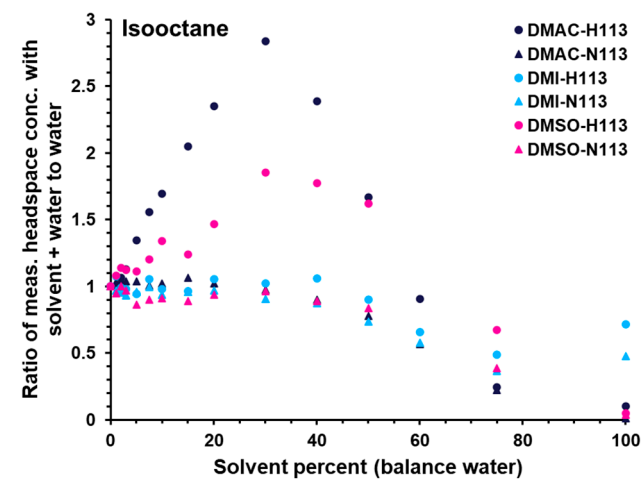
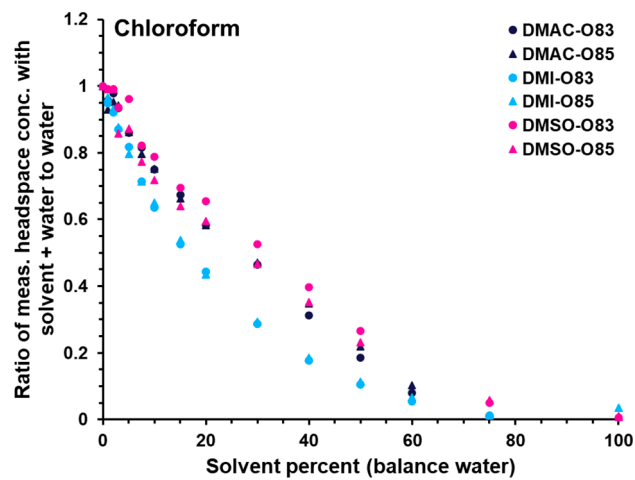
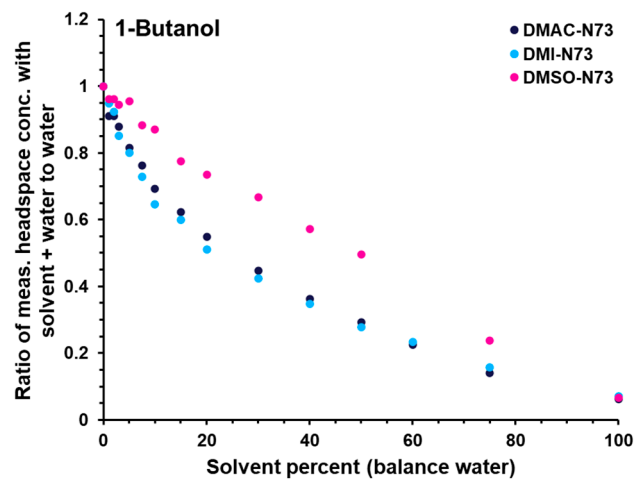


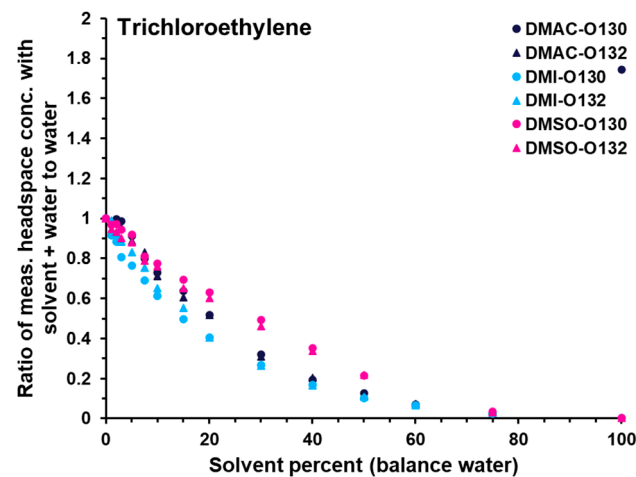
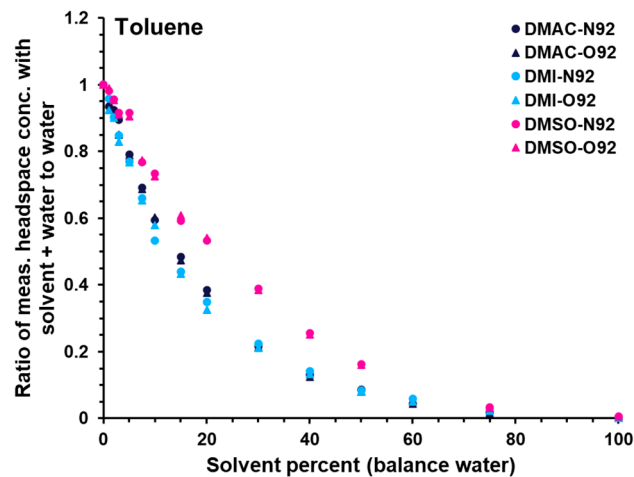
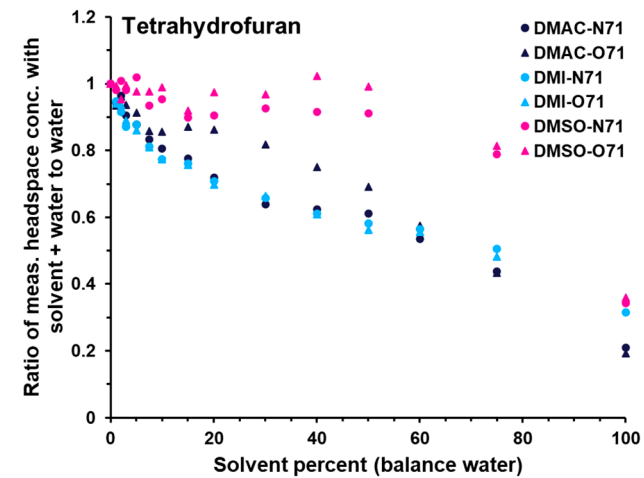
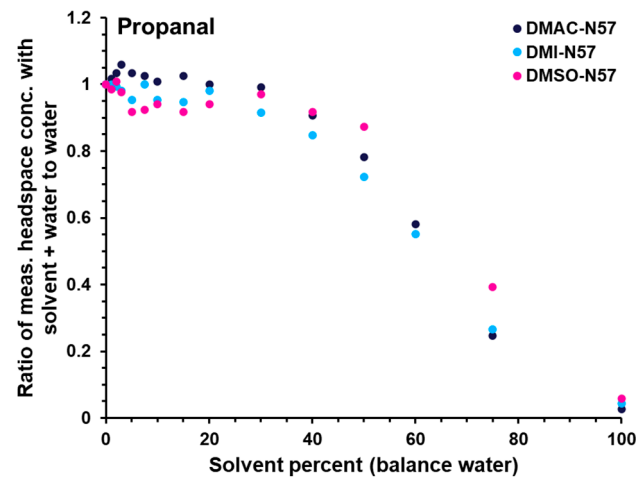
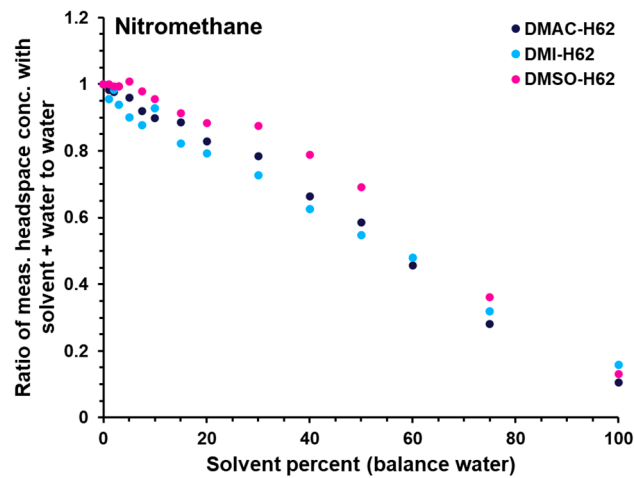




**Figure S2.** Ratio of measured headspace concentration of all analytes (Mix 1) in DMAC-water, DMI-water, or DMAC-water mixtures (0 to 100% solvent) to that obtained in pure aqueous solution. All measurements have the blank subtracted. The legend indicates first the matrix, then the reagent ion (first letter), and finally the product ion  $m/z$ . All product ions are shown.

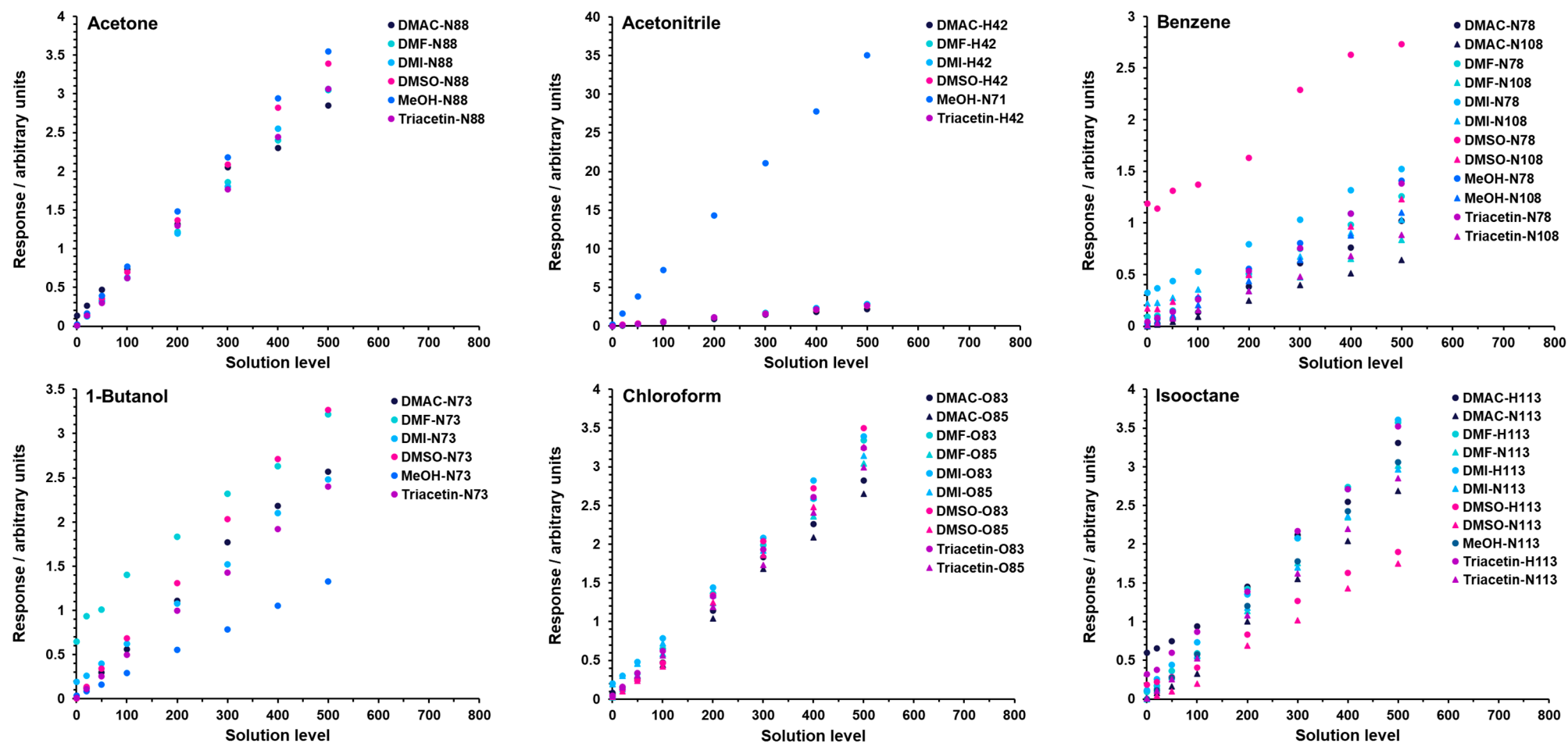


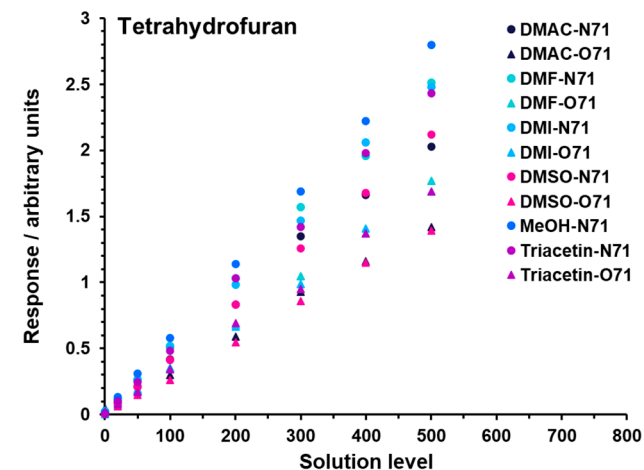
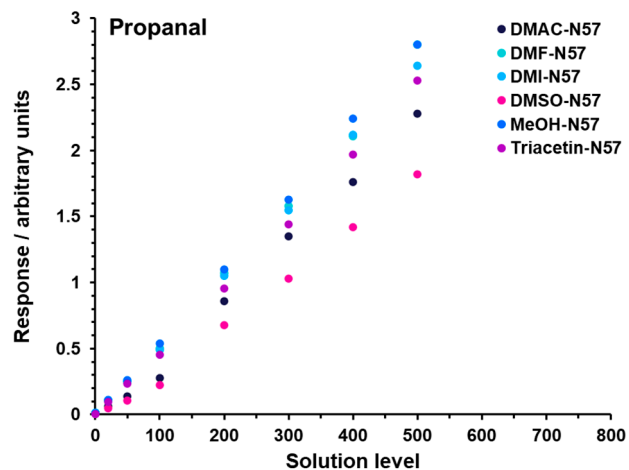
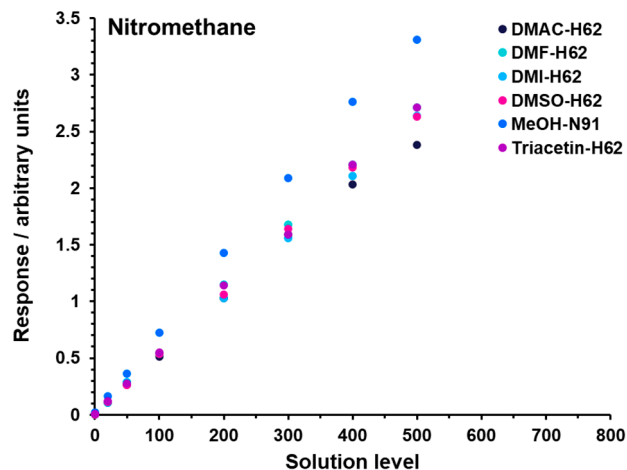
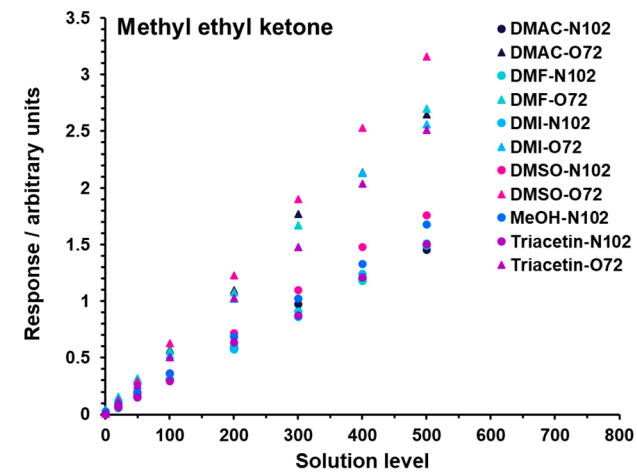
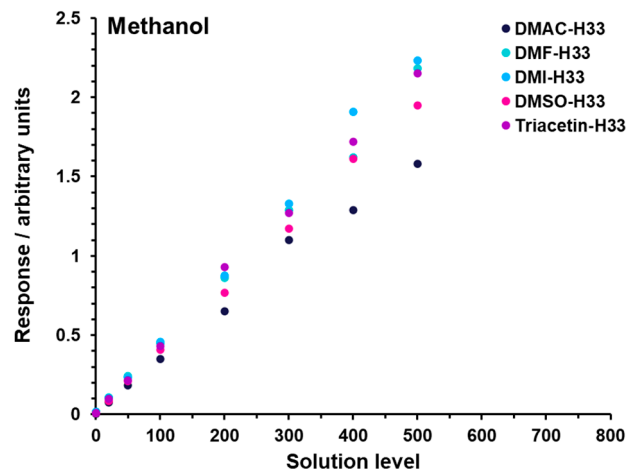
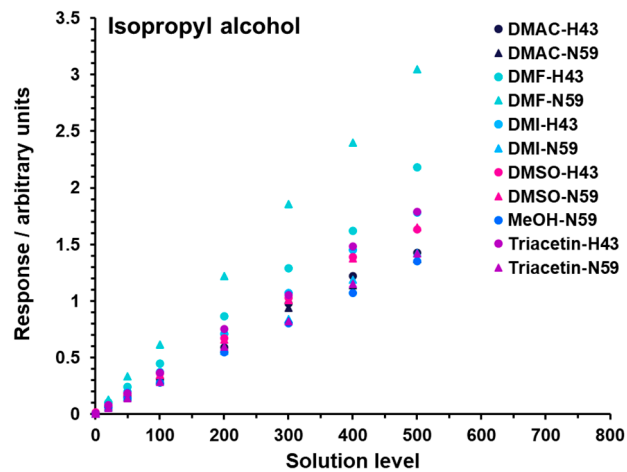


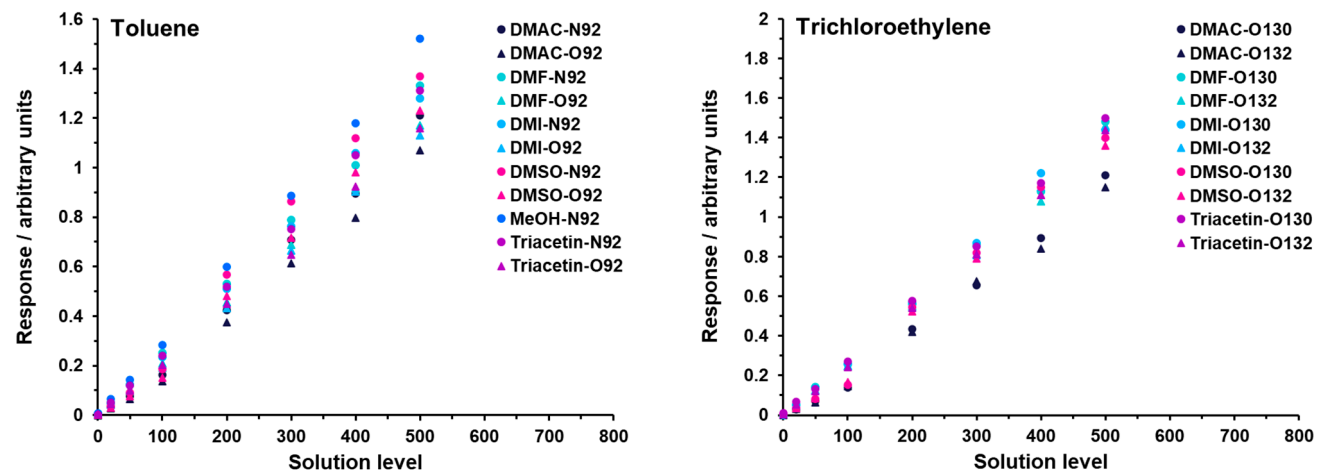


## B. Linearity

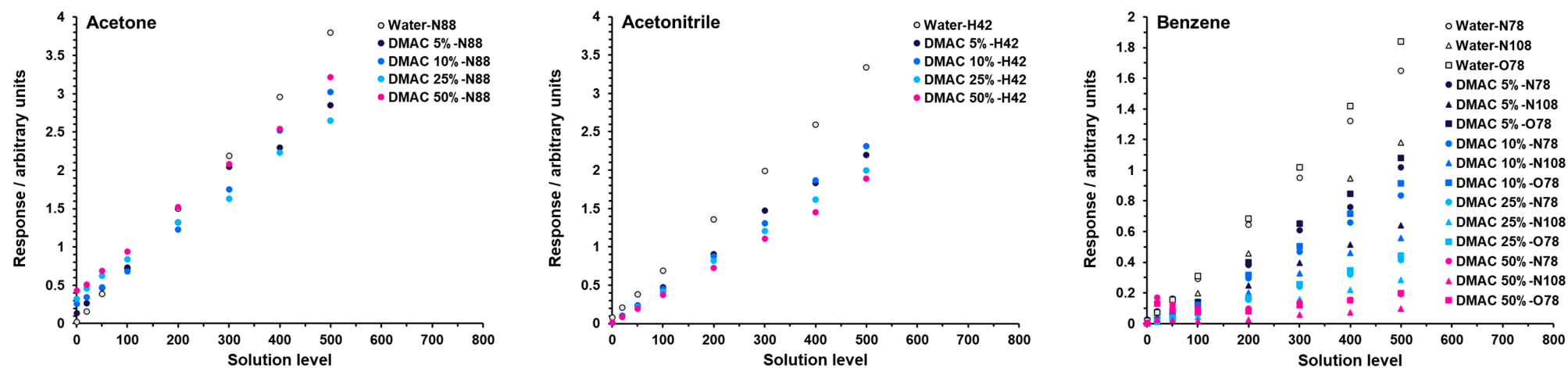
**Figure S3.** SIFT-MS linearity data for Mix 1 in 5% solvent:95% water for all six solvents evaluated.

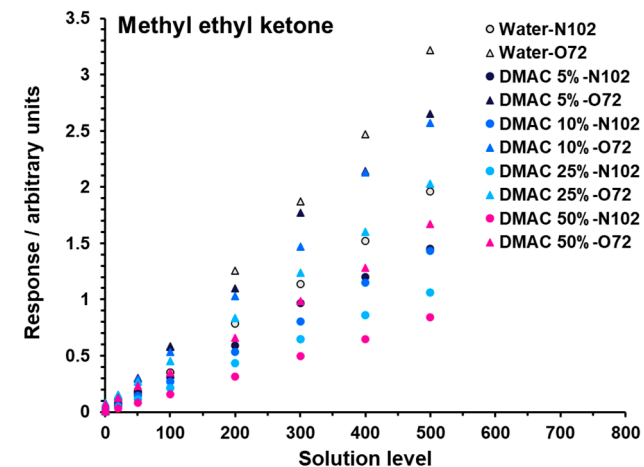
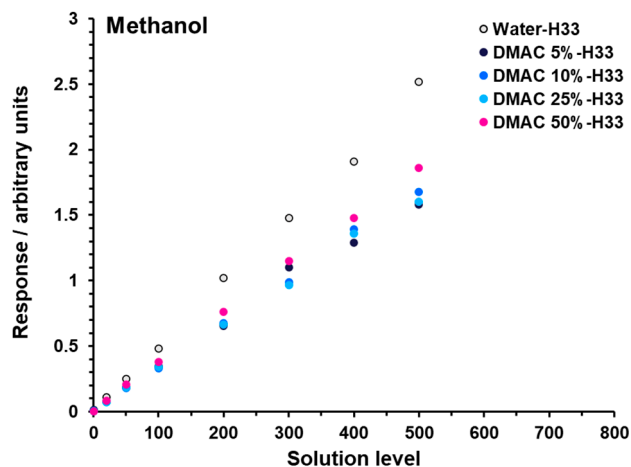
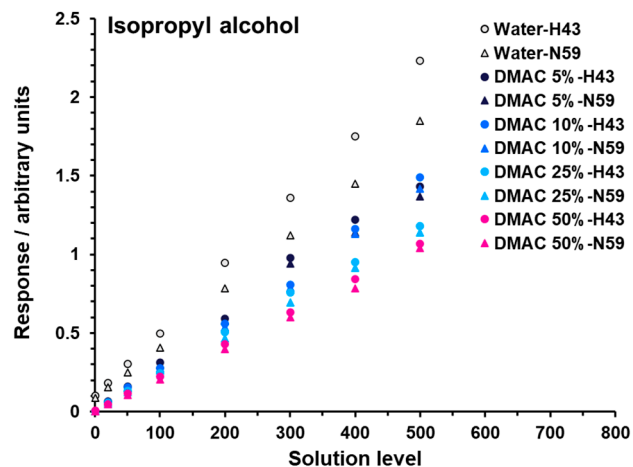
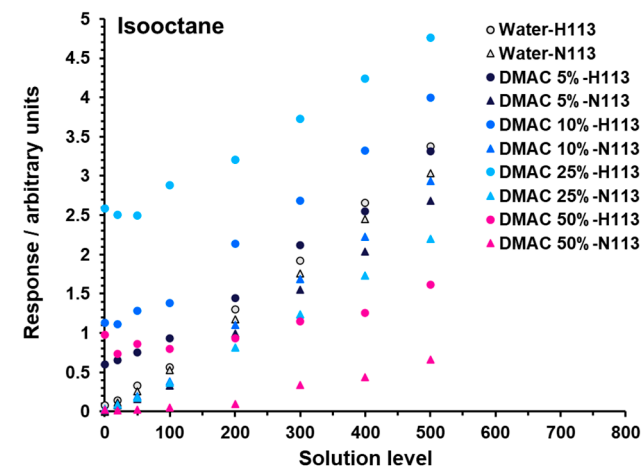
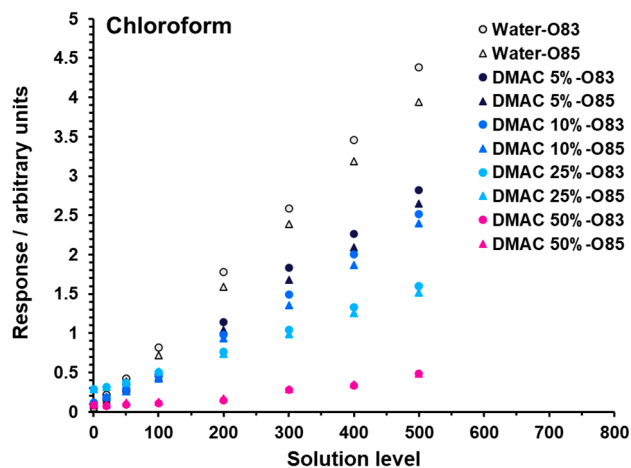
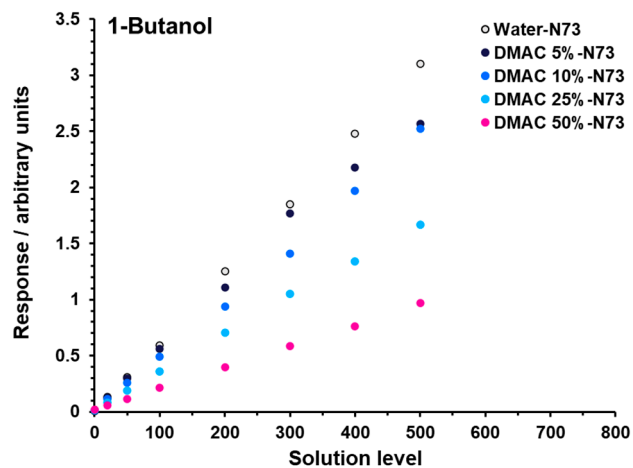


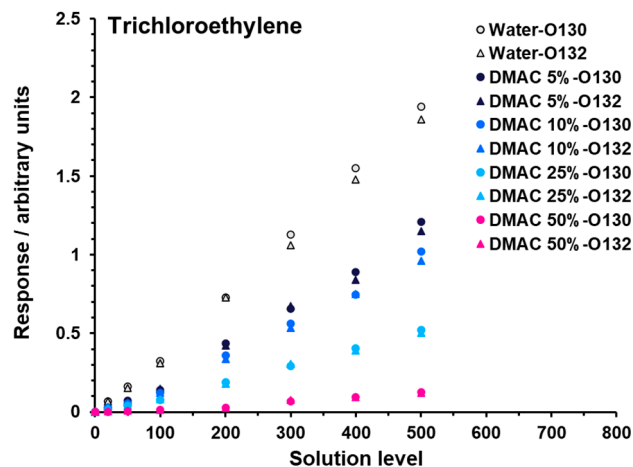
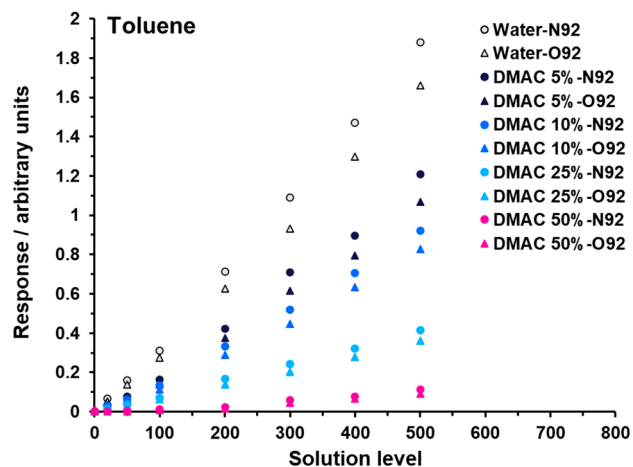
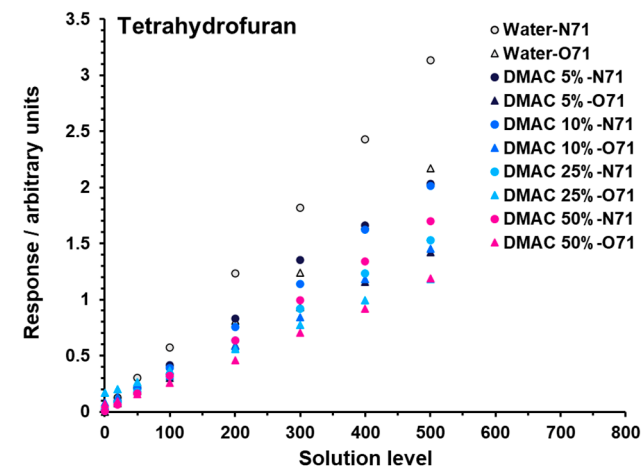
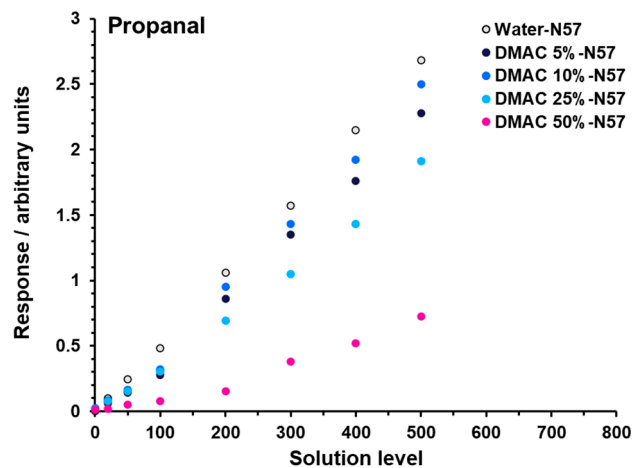
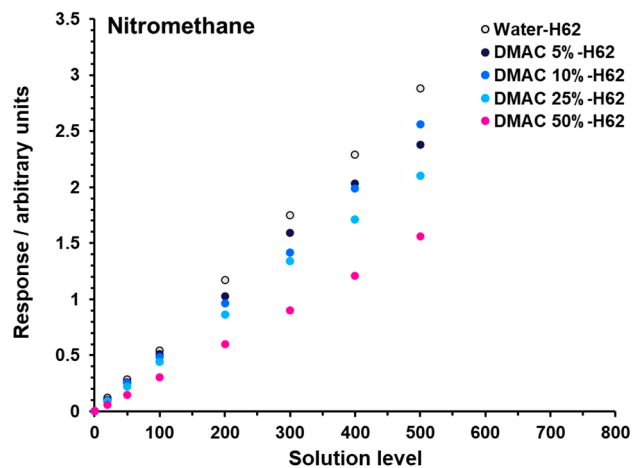




**Figure S4.** SIFT-MS linearity data for Mix 1 in 5, 10, 25%, and 50% DMAC (balance water) across the high concentration range.

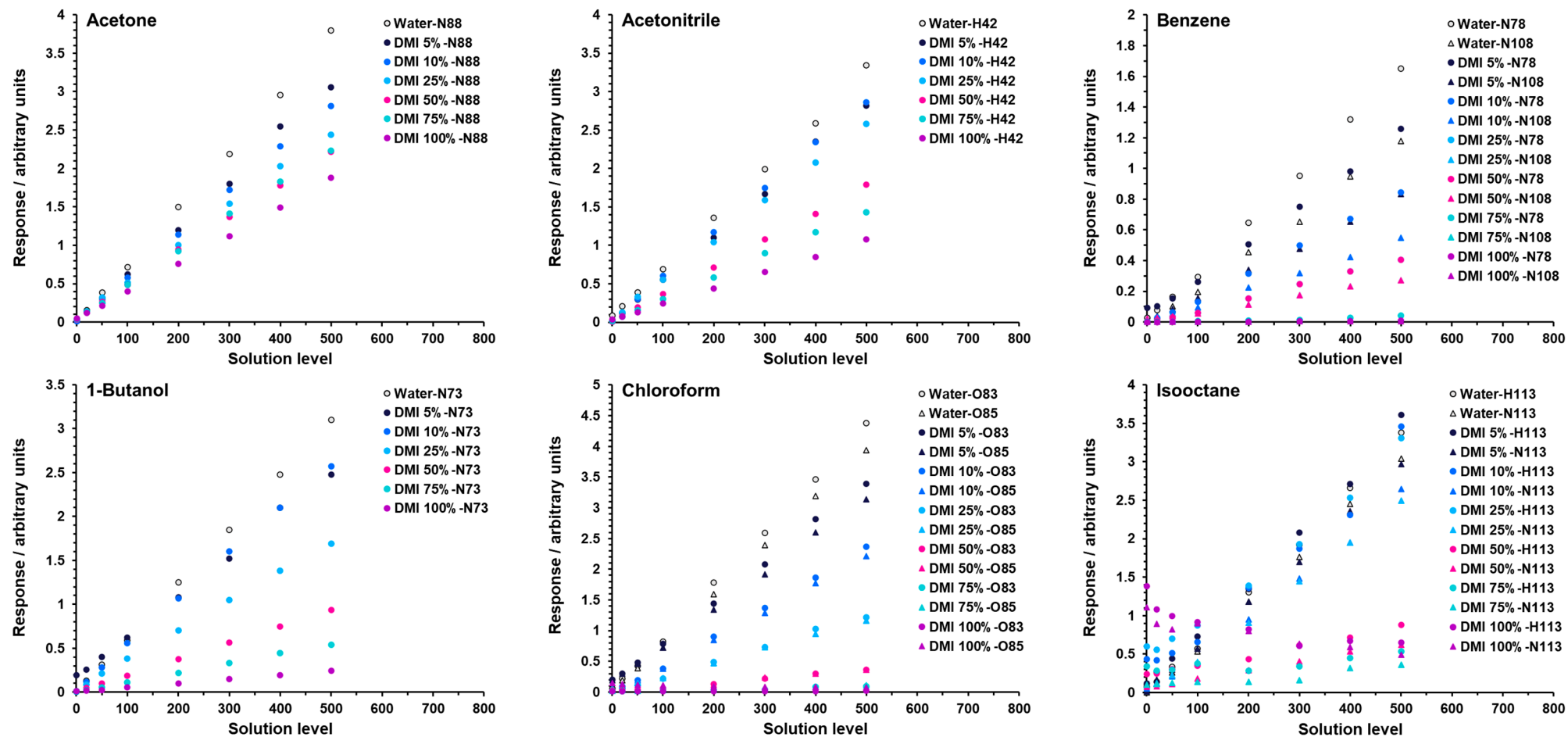


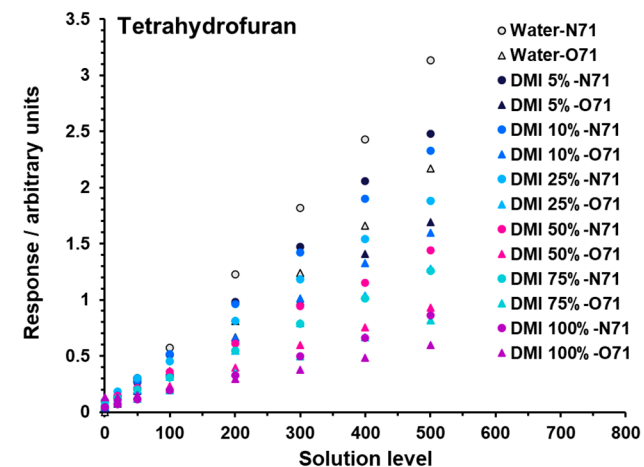
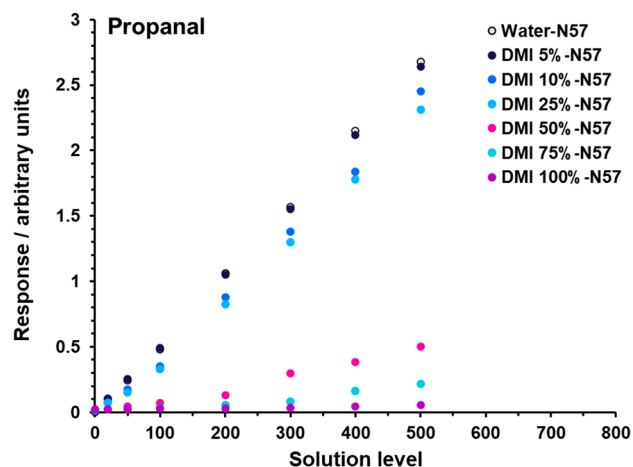
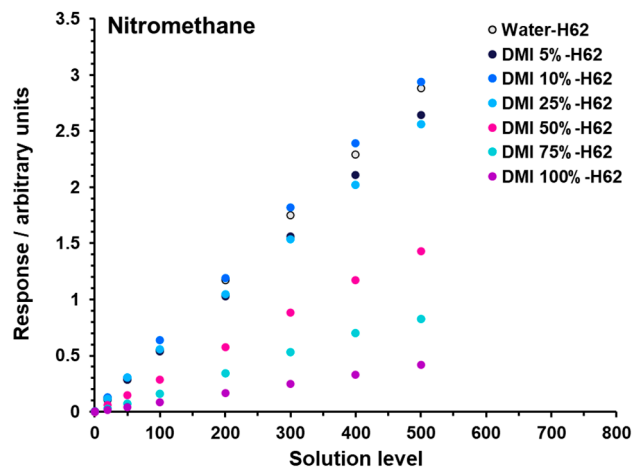
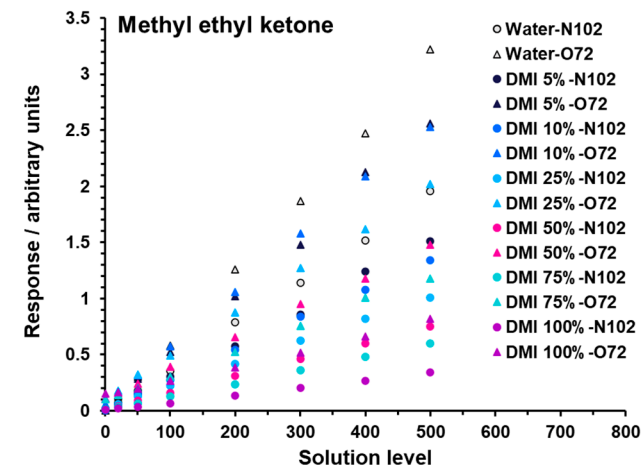
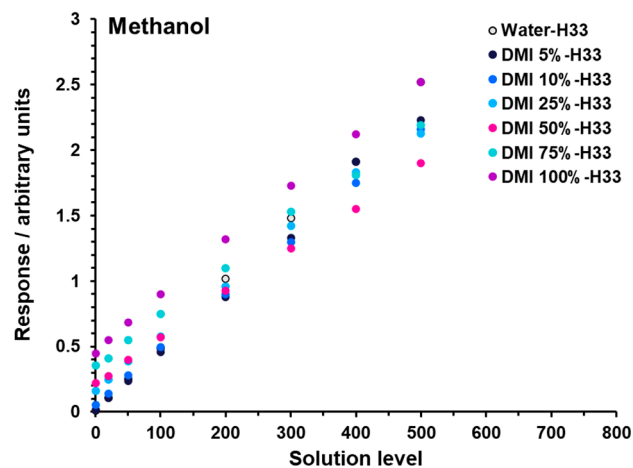
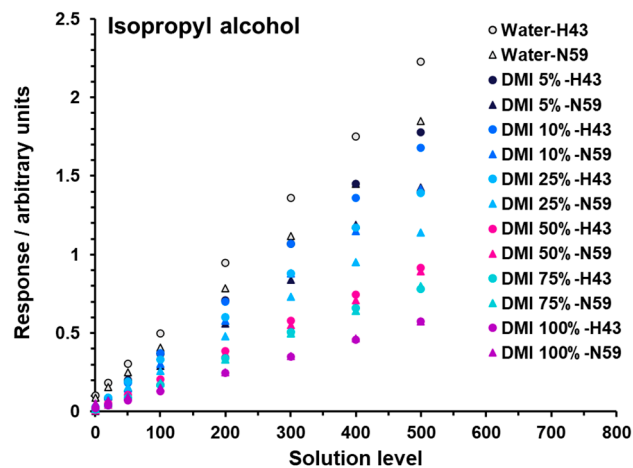


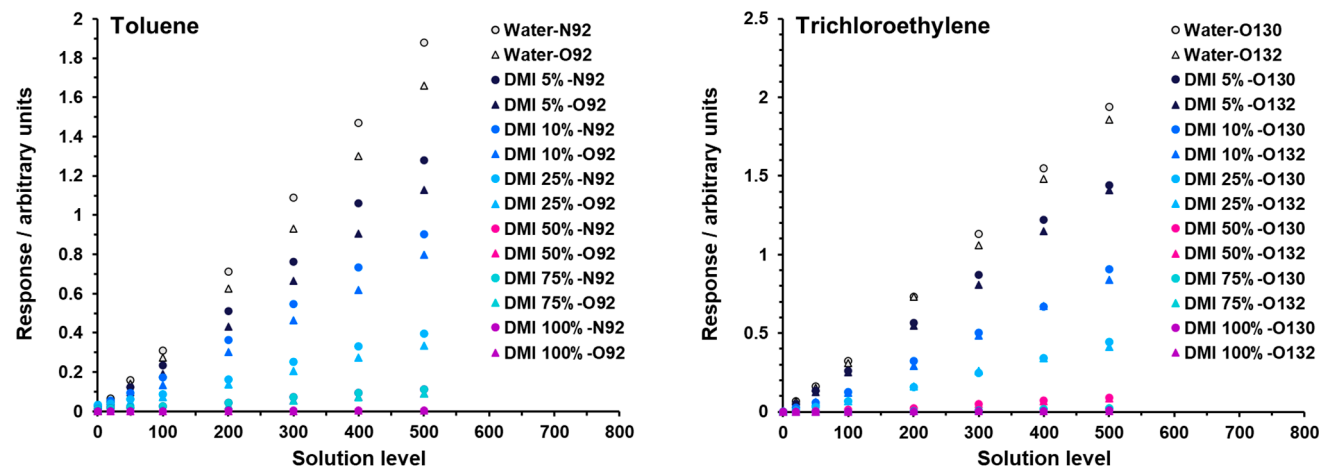




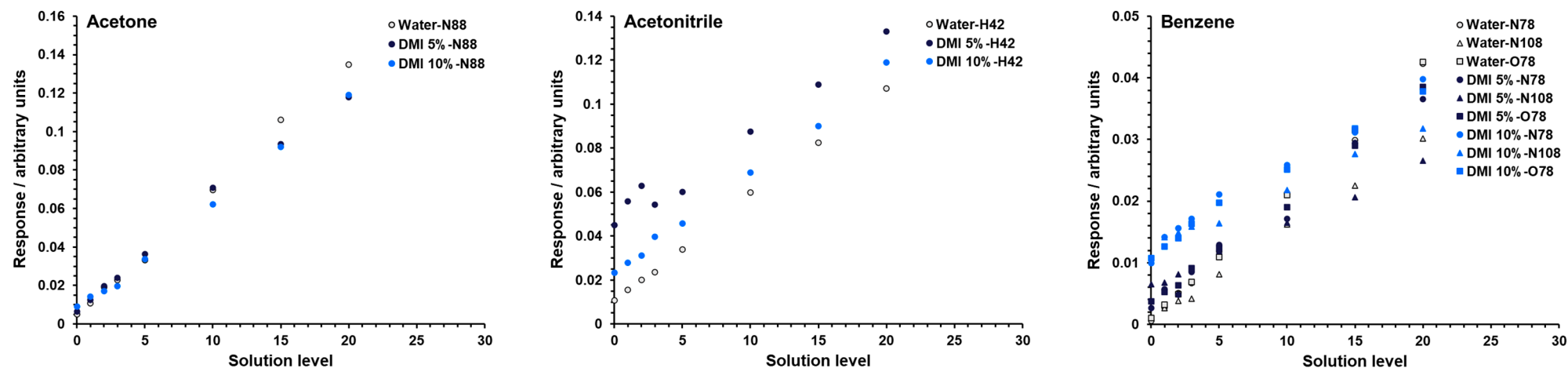
**Figure S5.** SIFT-MS linearity data for Mix 1 in 5, 10, 25, 50, 75 and 100% DMI (balance water) across the high concentration range.

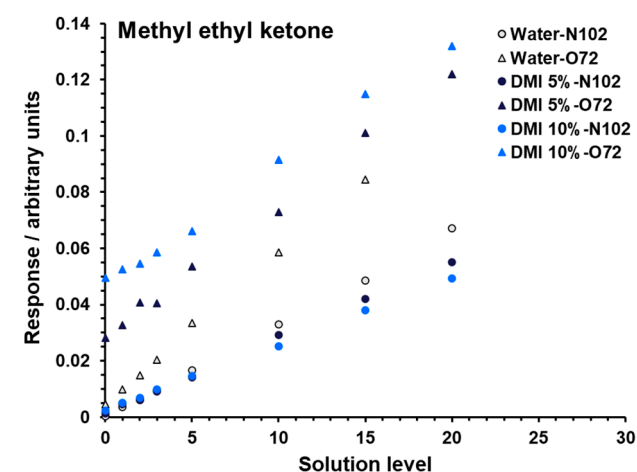
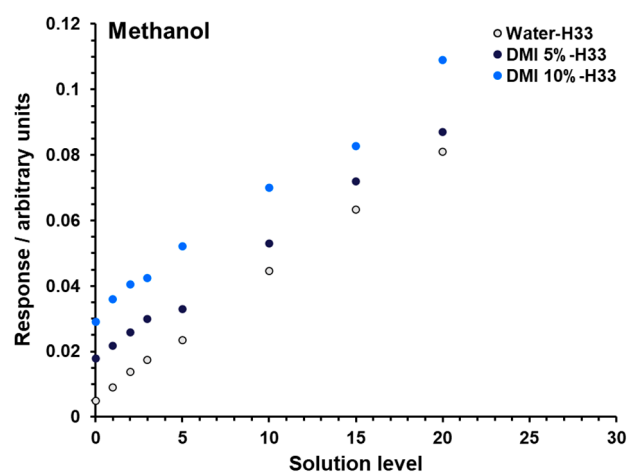
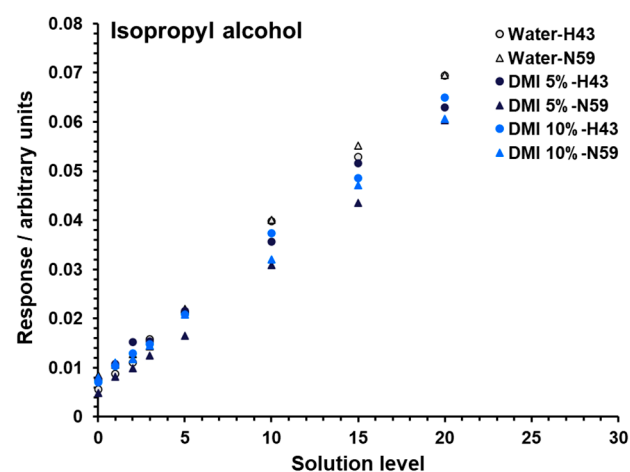
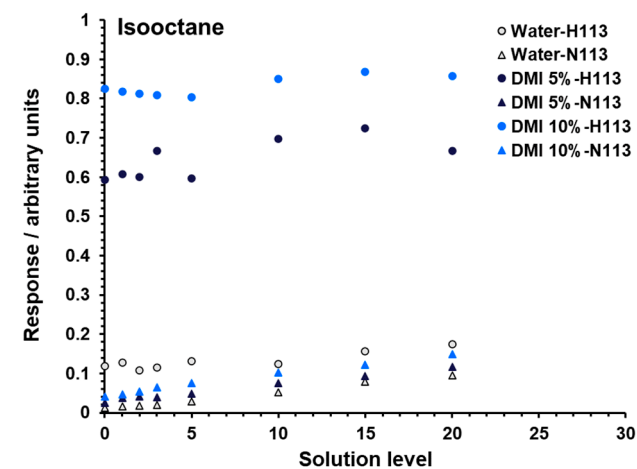
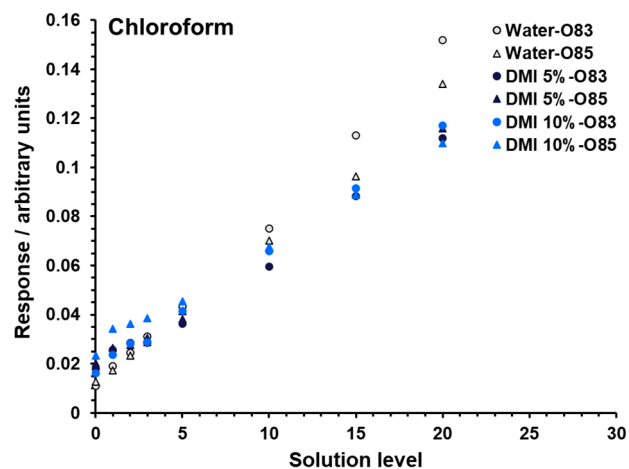
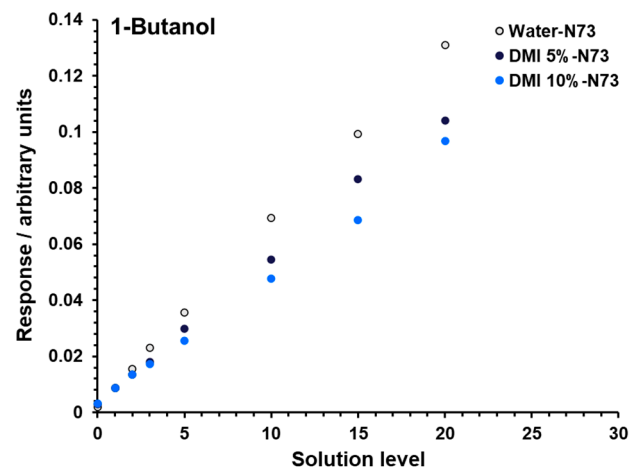


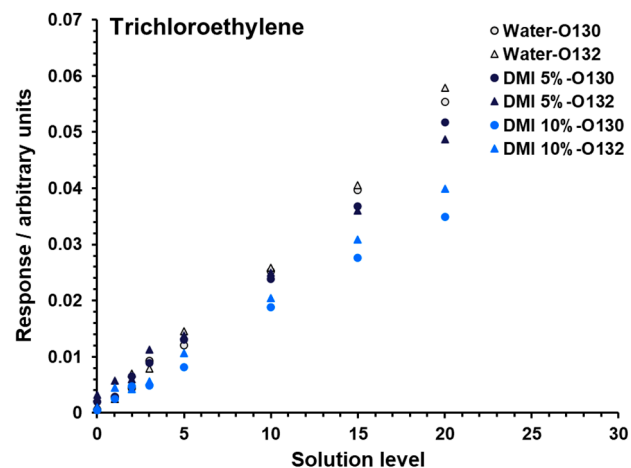
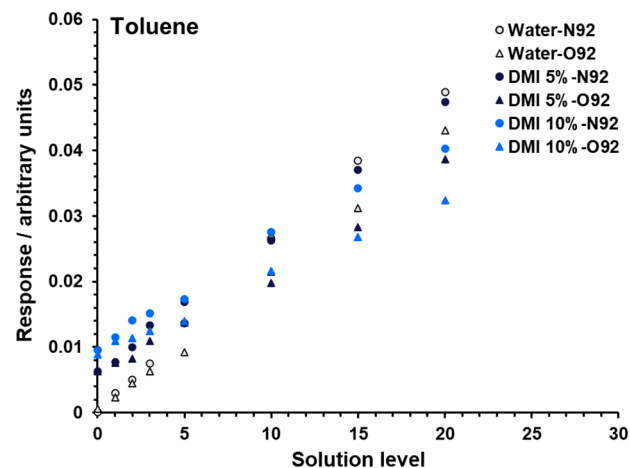
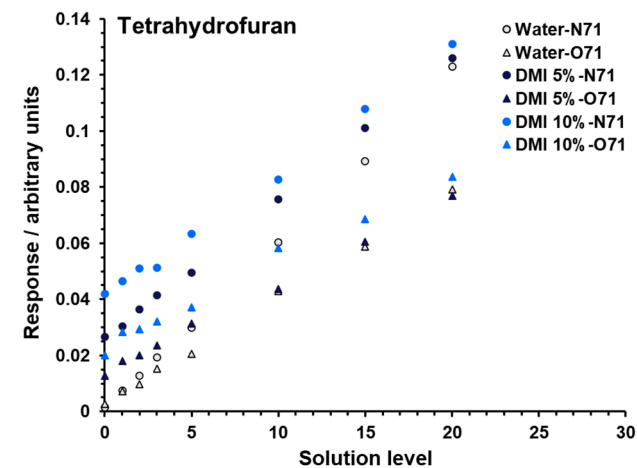
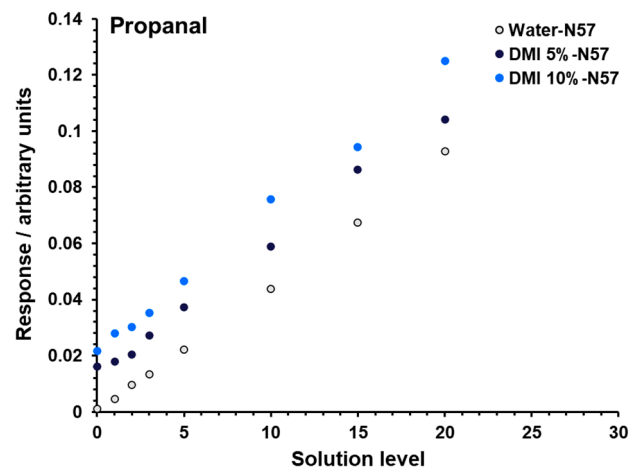
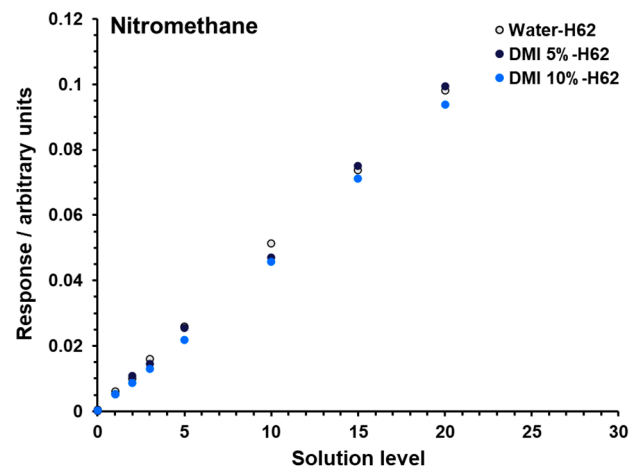




**Figure S6.** SIFT-MS linearity data for Mix 1 in 5 and 10% DMI (balance water) across the low concentration range.







**Figure S7.** SIFT-MS linearity data for the analyte mix in 5, 10, and 25% DMSO (balance water) across the high concentration range.

