

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091222\
 Data File : VN074413.D
 Acq On : 12 Sep 2022 15:54
 Operator : JC\MD
 Sample : IBLK
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 IBLK

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
 Title : SW846 8260

Signal : TIC: VN074413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	46	52	61	rBV	77755	202305	9.83%	1.325%
2	2.663	123	132	135	rBV2	66389	153273	7.45%	1.004%
3	7.939	1018	1029	1034	rBV	259203	642426	31.21%	4.209%
4	7.998	1034	1039	1049	rVB	392237	928915	45.13%	6.086%
5	8.363	1090	1101	1111	rBV2	270294	649107	31.54%	4.253%
6	8.592	1131	1140	1145	rBV5	39484	98016	4.76%	0.642%
7	8.892	1183	1191	1203	rBV	634476	1309892	63.64%	8.582%
8	9.139	1223	1233	1239	rBV5	58319	151401	7.36%	0.992%
9	9.192	1239	1242	1250	rVB3	19044	36830	1.79%	0.241%
10	9.780	1332	1342	1348	rBV7	15032	37128	1.80%	0.243%
11	10.375	1434	1443	1451	rBV	919507	1707767	82.97%	11.189%
12	10.445	1451	1455	1462	rVB3	29521	61447	2.99%	0.403%
13	10.869	1516	1527	1538	rBV	595272	1545864	75.11%	10.128%
14	10.975	1539	1545	1546	rBV3	30547	42971	2.09%	0.282%
15	11.686	1658	1666	1677	rBV	1030067	1878815	91.28%	12.310%
16	11.904	1696	1703	1706	rBV6	22961	51266	2.49%	0.336%
17	12.233	1755	1759	1765	rVB8	10254	21768	1.06%	0.143%
18	12.674	1827	1834	1845	rVB	907053	1543784	75.01%	10.115%
19	12.833	1850	1861	1867	rBV	935679	1962416	95.34%	12.858%
20	12.992	1885	1888	1894	rVB7	32049	54419	2.64%	0.357%
21	13.563	1978	1985	1988	rBV6	16870	32949	1.60%	0.216%
22	13.616	1988	1994	2005	rVB	1187326	2058238	100.00%	13.485%
23	13.992	2052	2058	2065	rVB4	20332	39236	1.91%	0.257%
24	15.198	2258	2263	2269	rVB7	14894	22692	1.10%	0.149%
25	15.557	2318	2324	2330	rBV	15676	29864	1.45%	0.196%

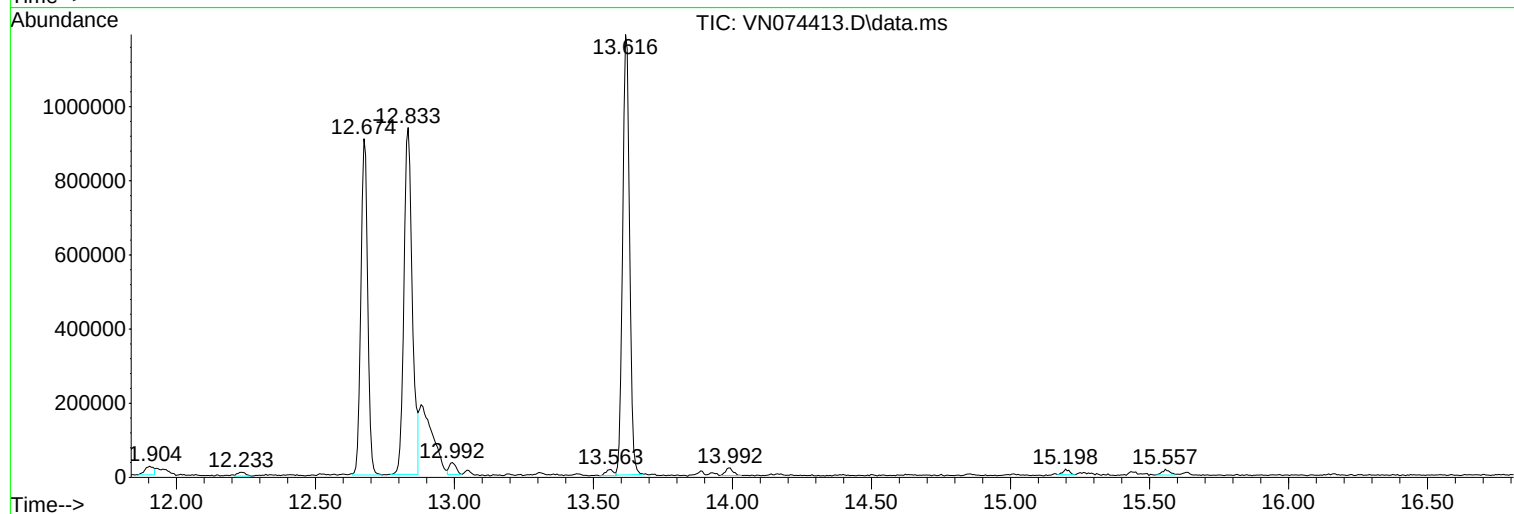
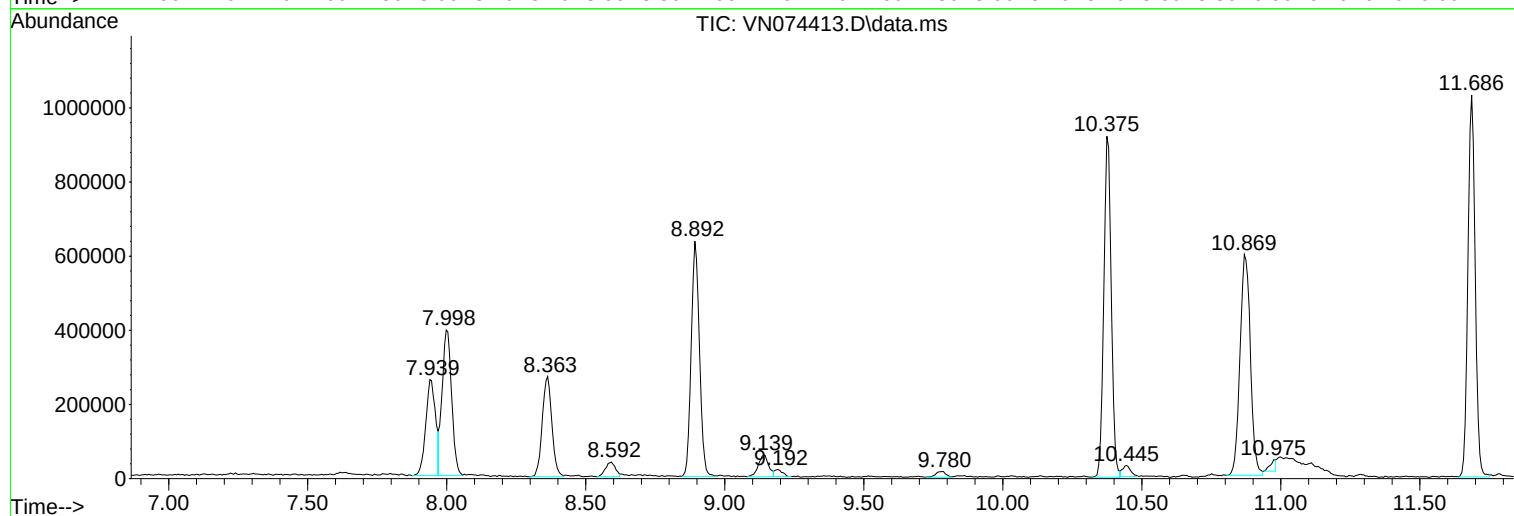
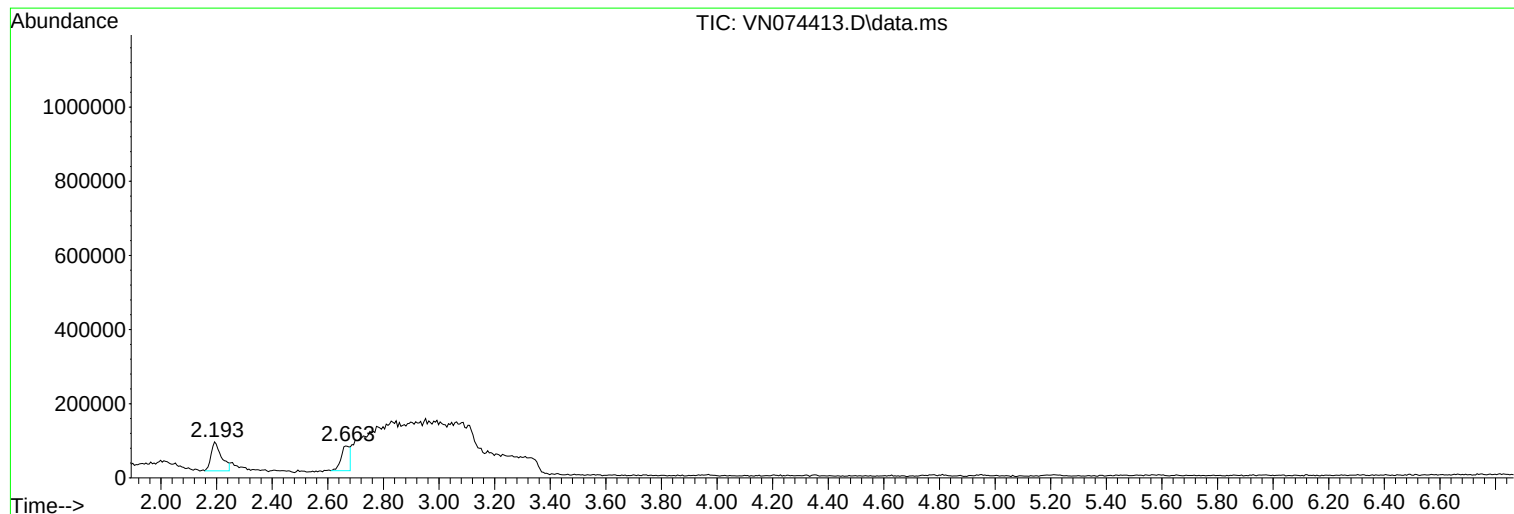
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Instrument :
MSVOA_N
ClientSampleId :
IBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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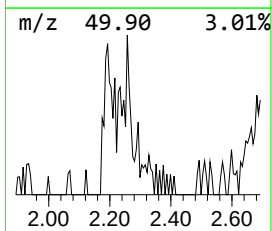
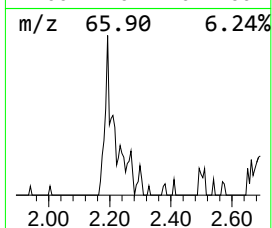
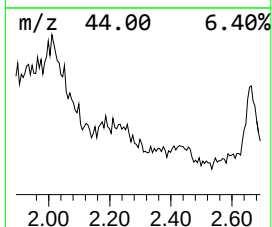
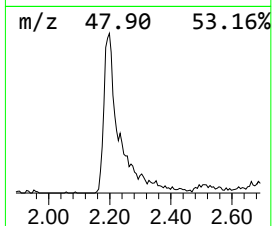
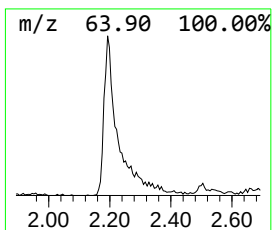
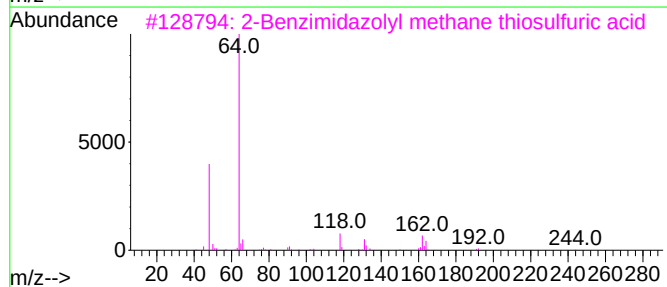
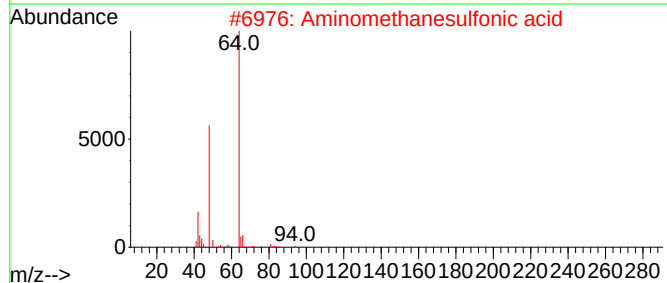
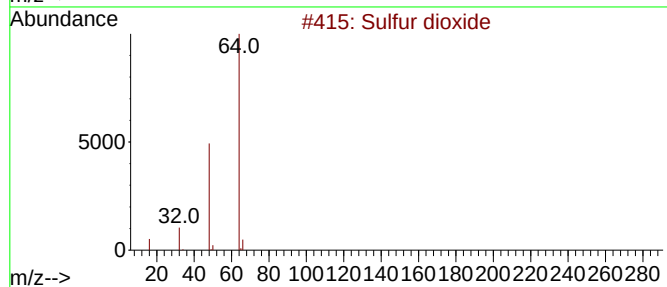
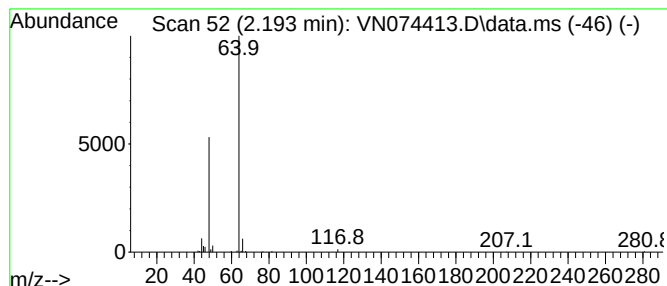
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	10.89 ug/l	202305	Pentafluorobenzene	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	64
4			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64



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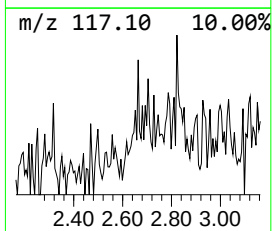
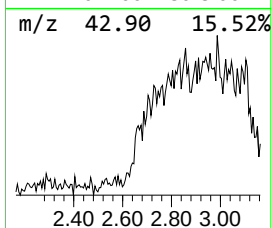
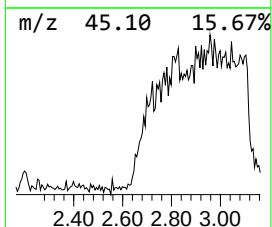
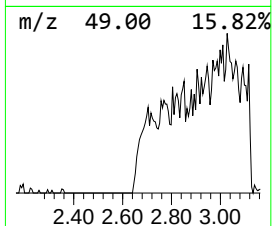
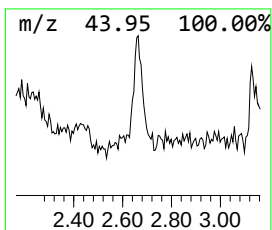
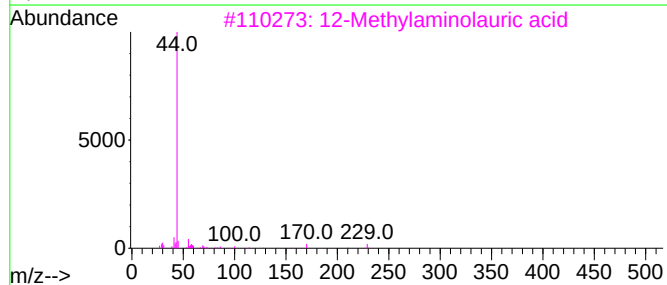
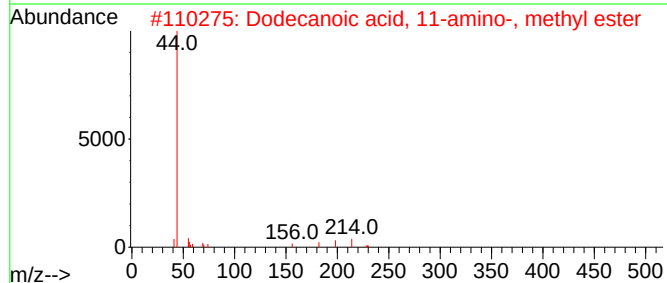
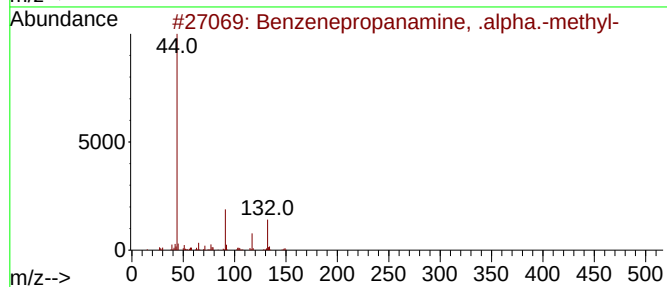
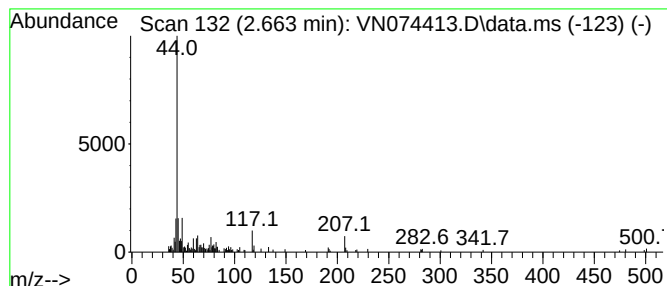
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Peak Number 2 Benzenepropanamine, .alpha.... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.663	8.25 ug/l	153273	Pentafluorobenzene	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanamine, .alpha.-methyl-	149	C10H15N	022374-89-6	53
2			Dodecanoic acid, 11-amino-, meth...	229	C13H27NO2	056817-92-6	47
3			12-Methylaminolauric acid	229	C13H27NO2	007408-81-3	47
4			(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	47
5			N-Methyl-2-phenyl-1-propylamine	149	C10H15N	000093-88-9	47



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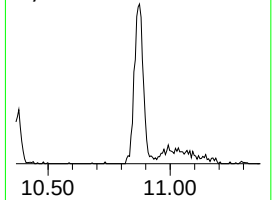
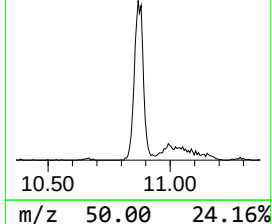
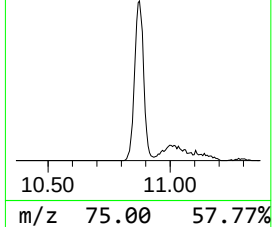
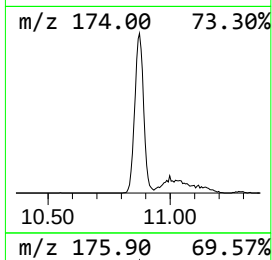
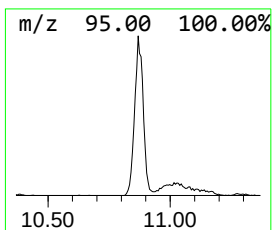
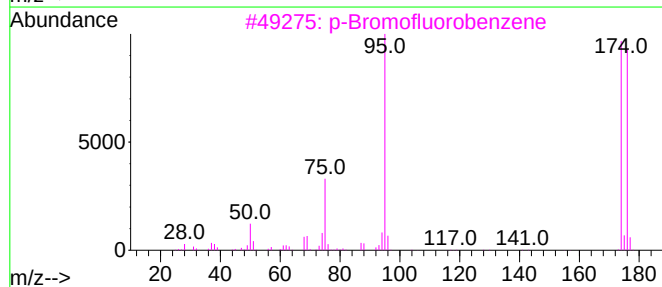
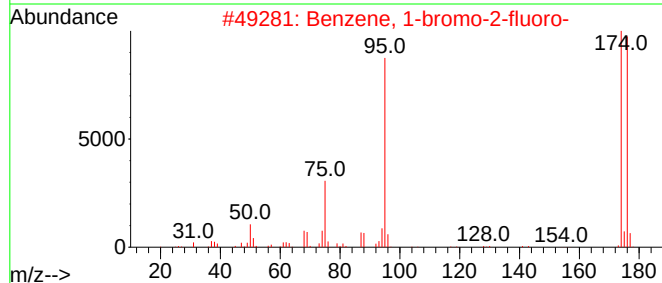
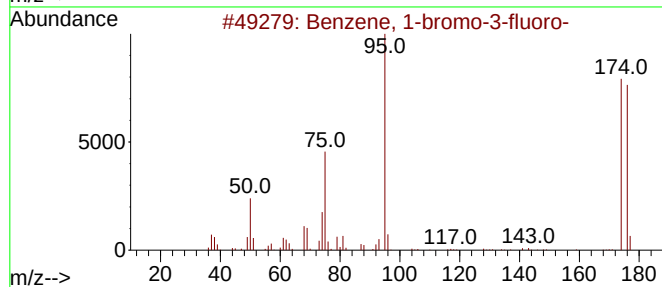
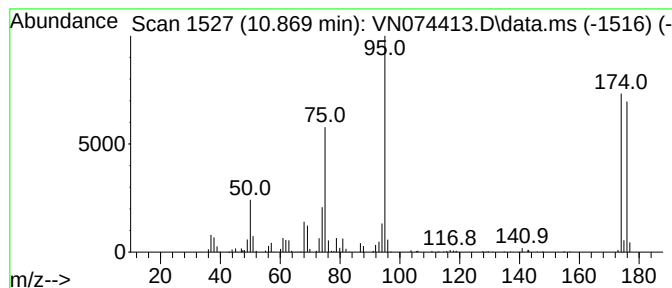
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ClientSampleId :
IBLK

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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-bromo-3-fluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.869	41.14 ug/l	1545860	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	96
2	Benzene, 1-bromo-2-fluoro-	174	C6H4BrF	001072-85-1	93
3	p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	91
4	Spiro[4,2]hept-1-ene, 1,2-diaza-...	174	C5H7BrN2	211738-70-4	50
5	Methane, dibromo-	172	CH2Br2	000074-95-3	35



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.193	10.9	ug/l	202305	1	7.998	928915	50.0
Benzenepropanam...	2.663	8.3	ug/l	153273	1	7.998	928915	50.0
Benzene, 1-brom...	10.869	41.1	ug/l	1545860	3	11.686	1878820	50.0