

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120823\
 Data File : VN080412.D
 Acq On : 08 Dec 2023 17:33
 Operator : JC\MD
 Sample : 05729-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 STORAGE-BLANK-WATER-REF-4

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\82N111623W.M

Title : SW846 8260

Signal : TIC: VN080412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	51	60	69	rBV4	27196	86287	1.97%	0.552%
2	8.171	1047	1057	1061	rBV2	267086	632122	14.43%	4.045%
3	8.230	1061	1067	1077	rVB	377663	854920	19.52%	5.471%
4	8.582	1117	1127	1135	rBV	260528	576703	13.17%	3.691%
5	9.106	1205	1216	1226	rBV	591904	1210133	27.63%	7.744%
6	10.571	1456	1465	1473	rBV	943646	1727608	39.44%	11.056%
7	11.865	1677	1685	1693	rBV	873133	1559818	35.61%	9.982%
8	12.853	1846	1853	1860	rBV	704129	1221906	27.90%	7.820%
9	13.794	2006	2013	2021	rVB	814510	1367918	31.23%	8.754%
10	15.706	2331	2338	2341	rBV	443244	848086	19.36%	5.427%
11	15.741	2341	2344	2353	rVB	665302	1160238	26.49%	7.425%
12	15.994	2372	2387	2419	rBV6	655867	4380118	100.00%	28.031%

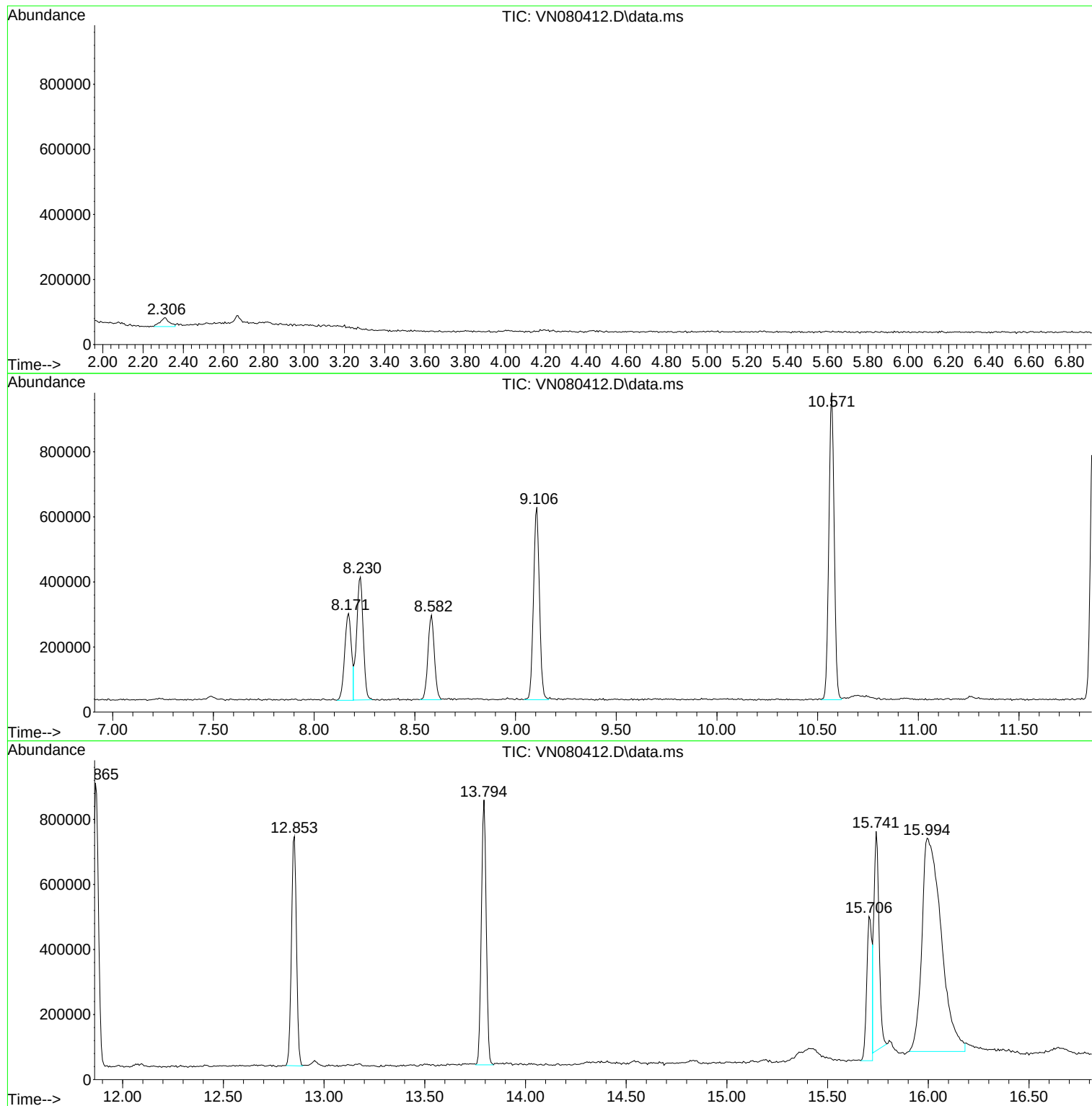
Sum of corrected areas: 15625857

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



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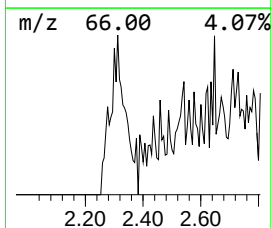
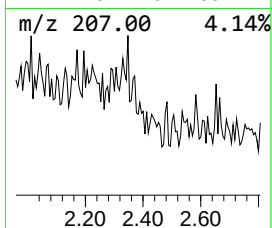
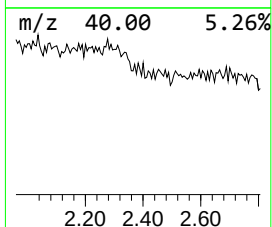
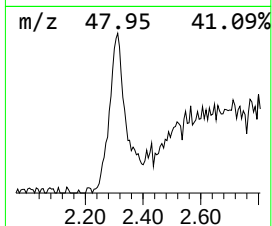
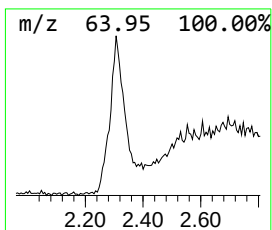
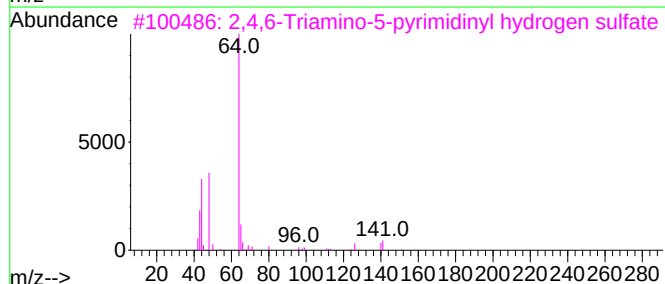
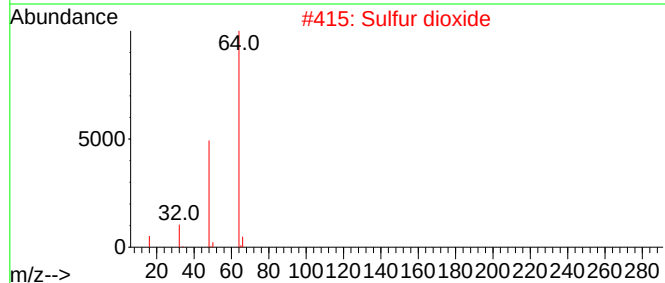
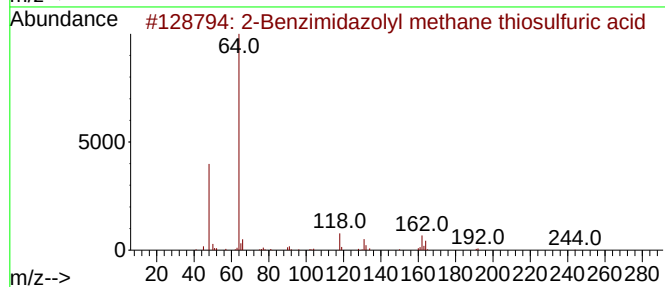
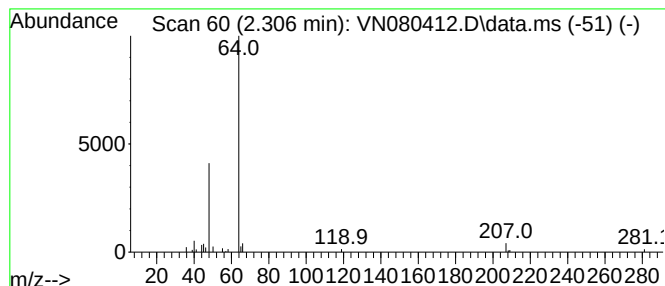
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Benzimidazolyl methane th... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	5.05 ug/l	86287	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	74
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	64
4			N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64



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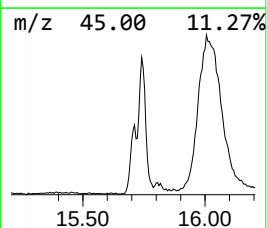
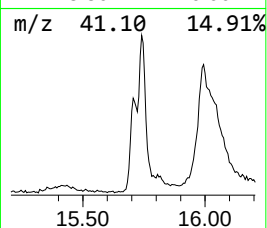
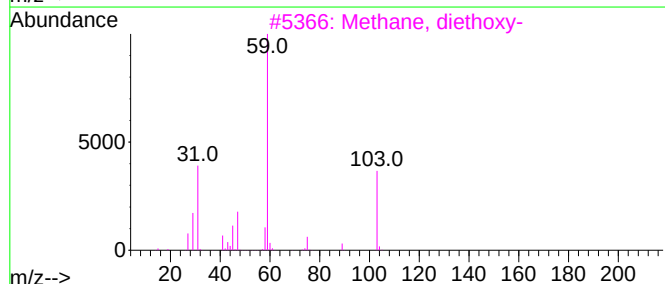
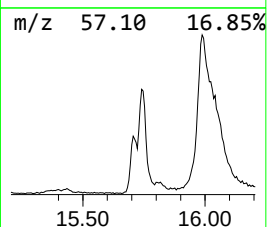
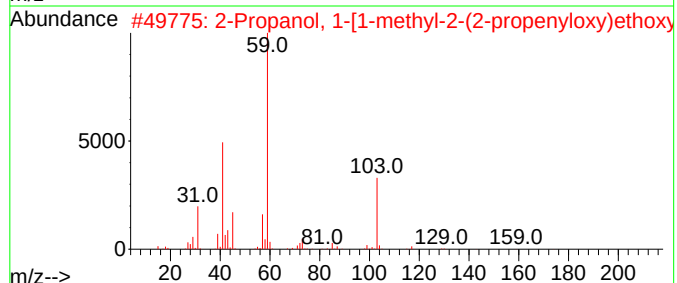
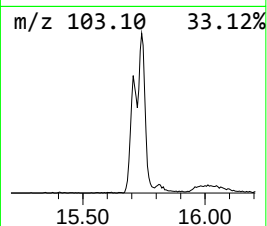
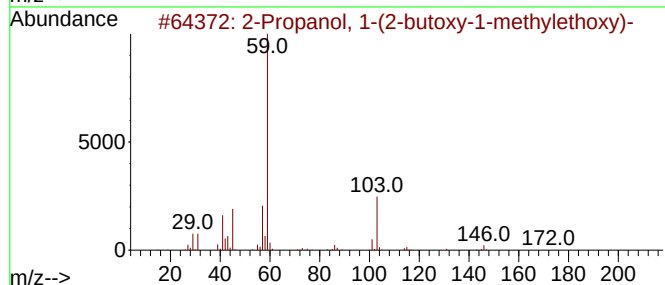
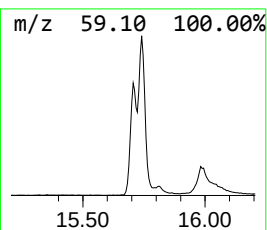
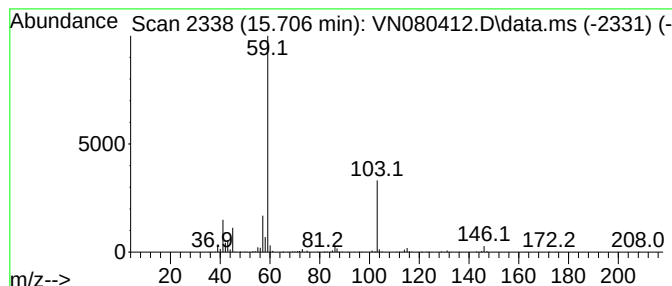
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Quant Title : SW846 8260

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

Peak Number 2 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.706	31.00 ug/l	848086	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83		
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78		
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	64		
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	59		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	56		



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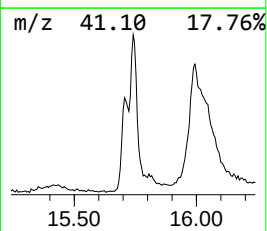
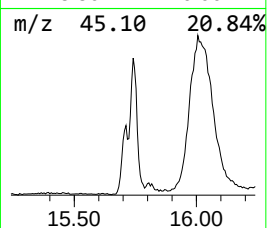
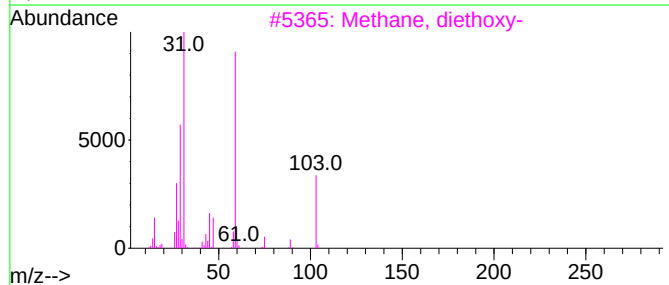
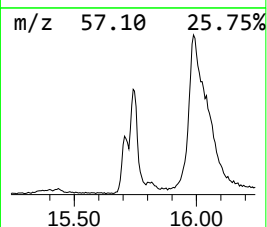
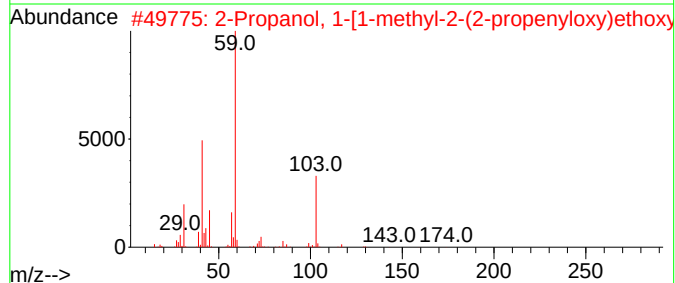
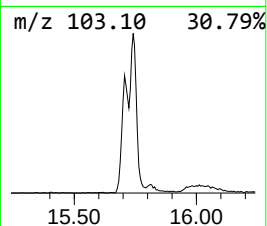
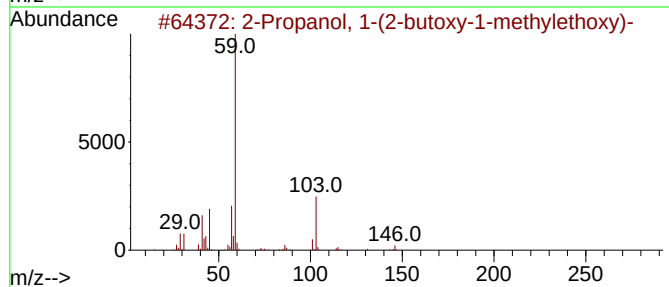
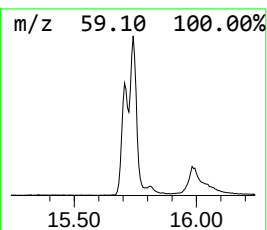
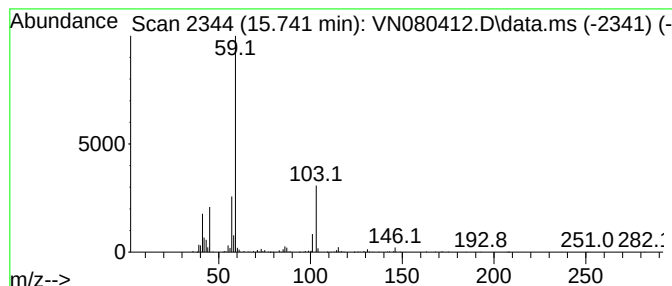
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Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.741	42.41 ug/l	1160240	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90		
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78		
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72		
4	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	64		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	56		



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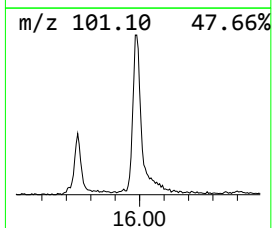
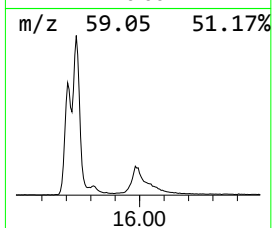
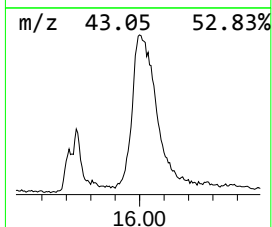
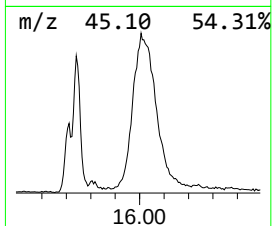
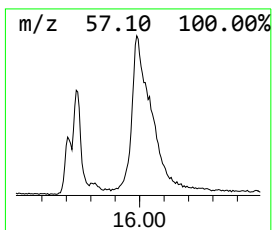
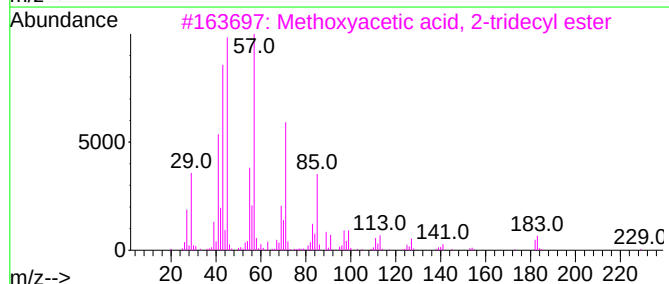
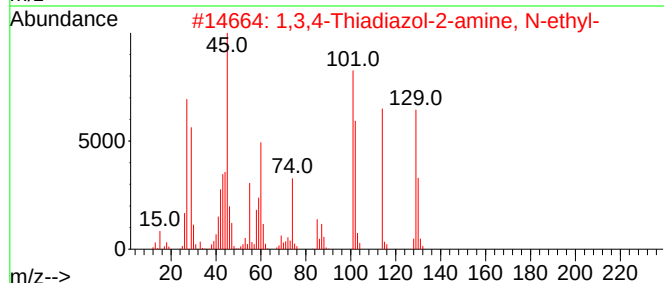
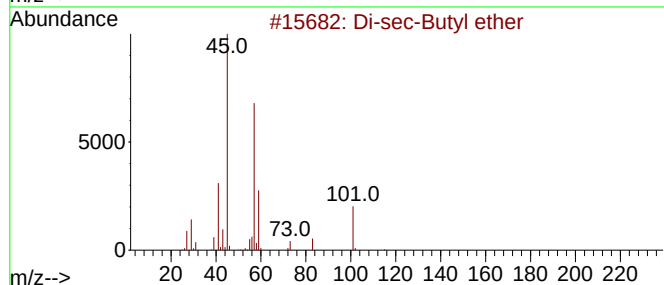
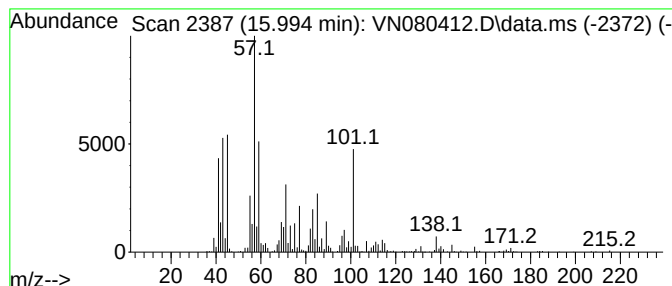
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Peak Number 4 Di-sec-Butyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.994	160.10 ug/l	4380120	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
2			1,3,4-Thiadiazol-2-amine, N-ethyl-	129	C4H7N3S	013275-68-8	35
3			Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	30
4			Methoxyacetic acid, 2-pentadecyl...	300	C18H36O3	1000282-05-1	27
5			Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Benzimidazoly...	2.306	5.0	ug/l	86287	1	8.230	854920	50.0
2-Propanol, 1-(...	15.706	31.0	ug/l	848086	4	13.794	1367920	50.0
2-Propanol, 1-[...	15.741	42.4	ug/l	1160240	4	13.794	1367920	50.0
Di-sec-Butyl ether	15.994	160.1	ug/l	4380120	4	13.794	1367920	50.0