

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120823\
 Data File : VN080413.D
 Acq On : 08 Dec 2023 17:57
 Operator : JC\MD
 Sample : 05729-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 STORAGE-BLANK-SAMPLE-MANAG

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: VN080413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	49	59	68	rBV	56315	171168	9.12%	1.552%
2	2.671	118	122	127	rVB	19722	32319	1.72%	0.293%
3	7.500	934	943	948	rBV3	8667	21120	1.12%	0.191%
4	8.171	1047	1057	1061	rBV	282435	655042	34.88%	5.939%
5	8.230	1061	1067	1077	rVB	407352	920407	49.01%	8.345%
6	8.582	1118	1127	1138	rBB	263294	602440	32.08%	5.462%
7	9.106	1207	1216	1224	rBV	632396	1299723	69.21%	11.784%
8	10.571	1457	1465	1472	rBV	1018382	1877830	100.00%	17.026%
9	11.865	1677	1685	1695	rBV	935667	1683912	89.67%	15.268%
10	12.076	1715	1721	1727	rBV7	9148	23450	1.25%	0.213%
11	12.853	1842	1853	1862	rBV	772774	1325002	70.56%	12.014%
12	12.959	1865	1871	1880	rVB4	18766	35951	1.91%	0.326%
13	13.794	2005	2013	2021	rVB	829788	1403182	74.72%	12.722%
14	14.306	2094	2100	2104	rBV7	8840	20535	1.09%	0.186%
15	15.706	2330	2338	2340	rBV2	158264	270336	14.40%	2.451%
16	15.741	2340	2344	2352	rVB	219051	426353	22.70%	3.866%
17	15.988	2379	2386	2400	rVB2	94597	239797	12.77%	2.174%
18	16.541	2477	2480	2489	rVB9	7595	20598	1.10%	0.187%

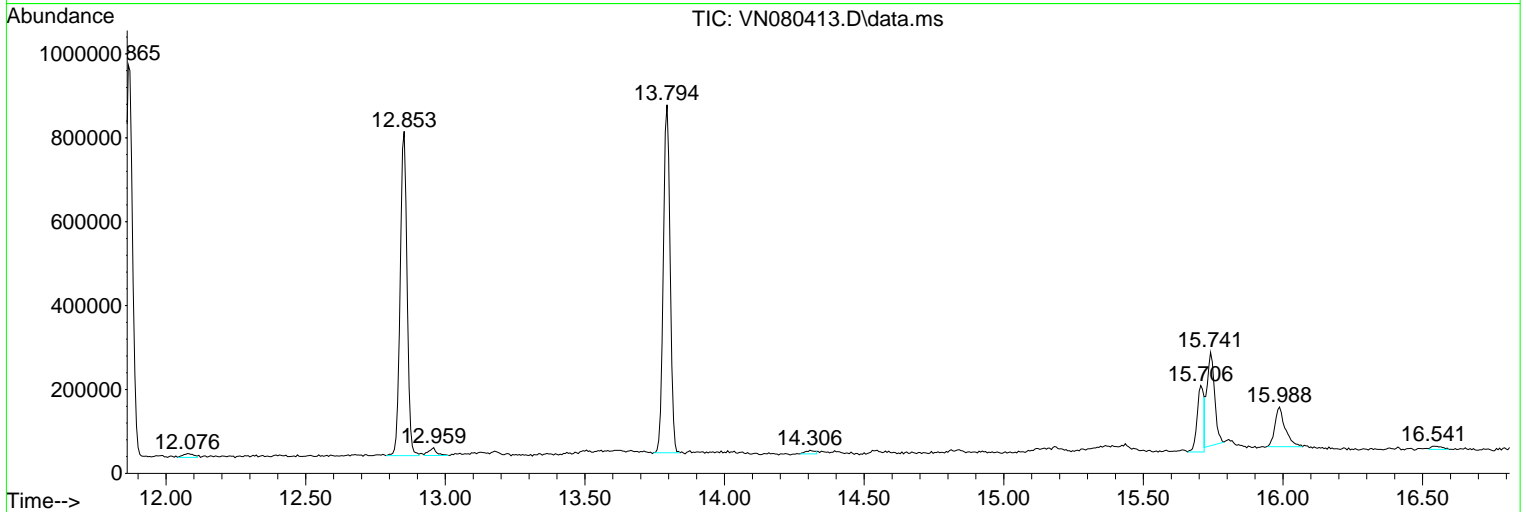
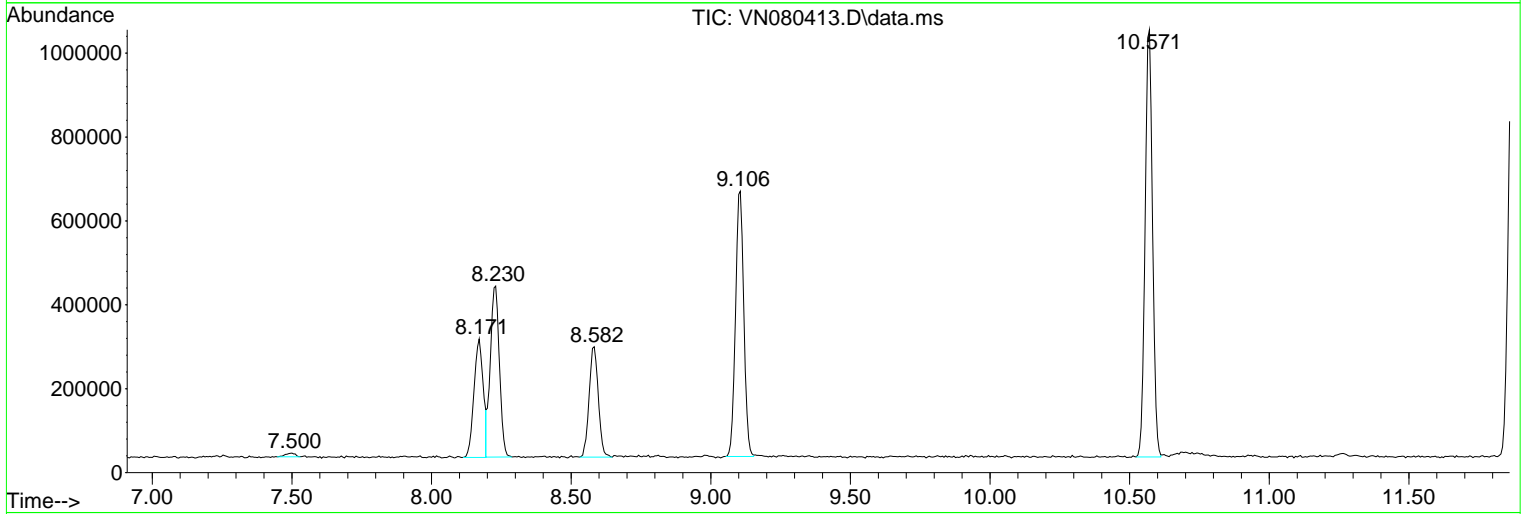
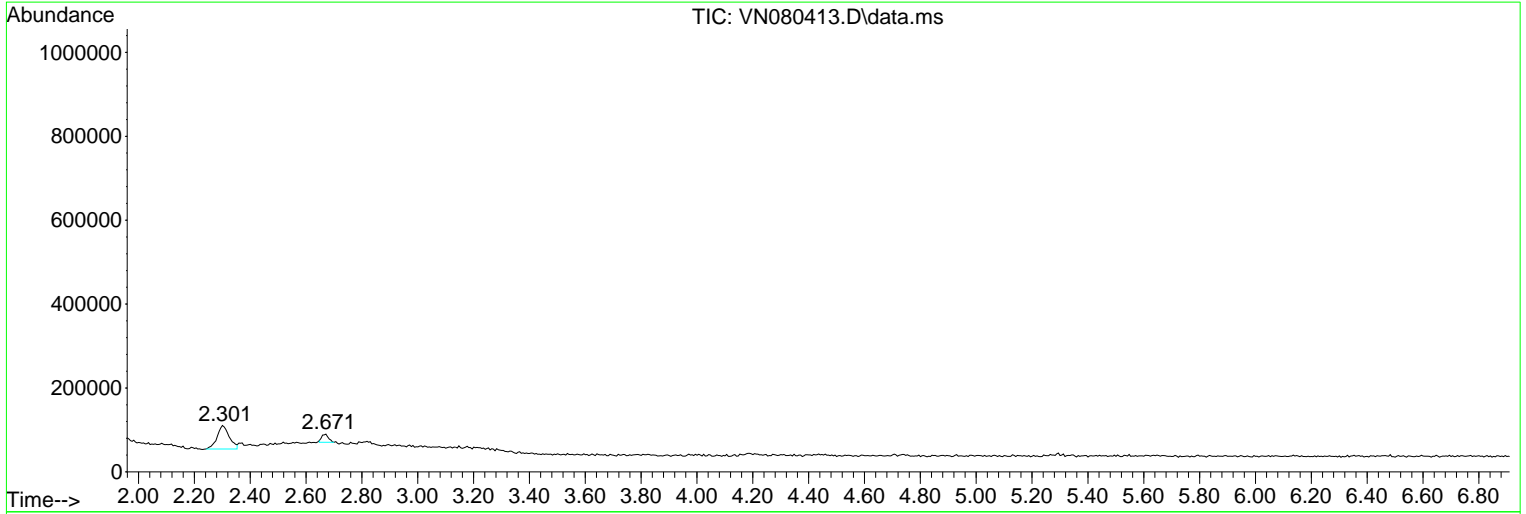
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P



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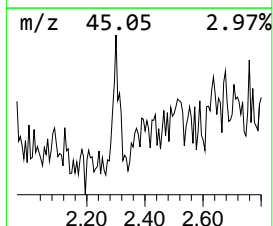
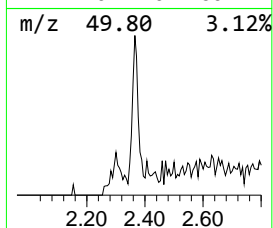
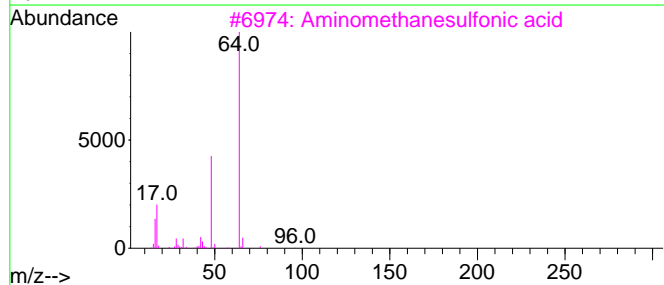
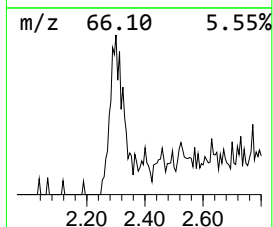
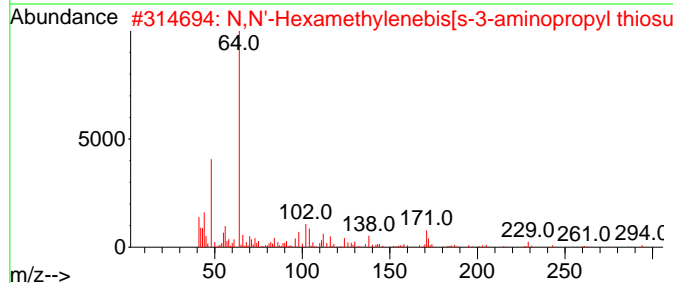
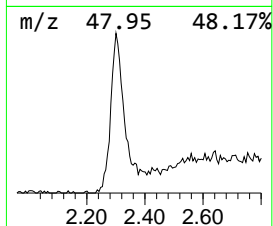
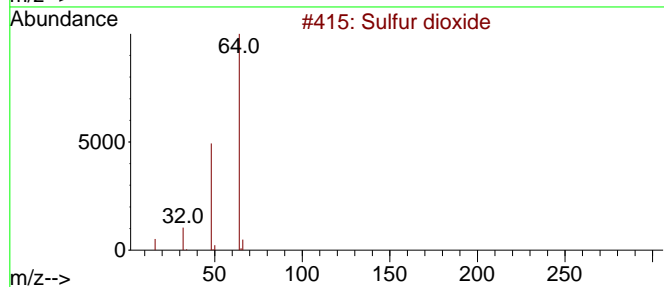
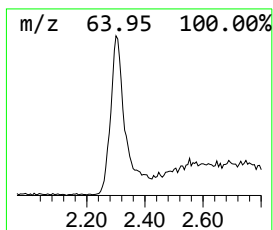
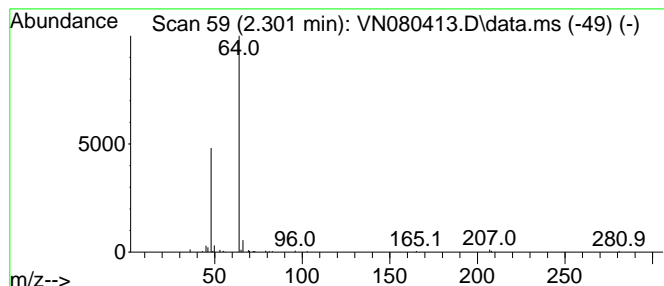
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
 Quant Title : SW846 8260

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

 Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.301	9.30 ug/l	171168	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	74
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74



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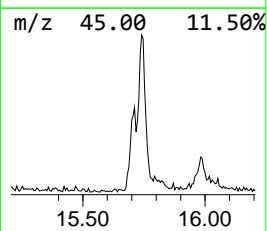
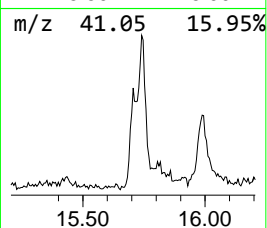
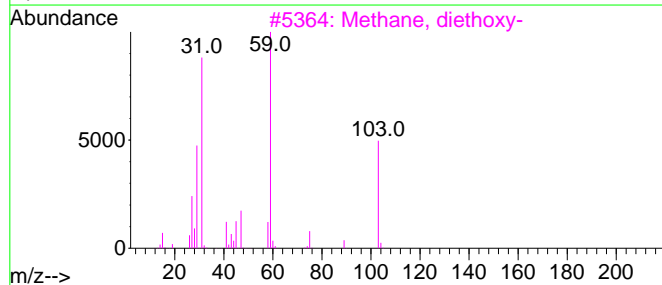
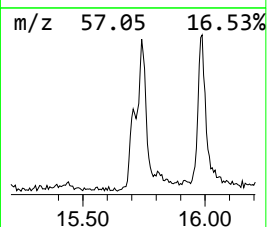
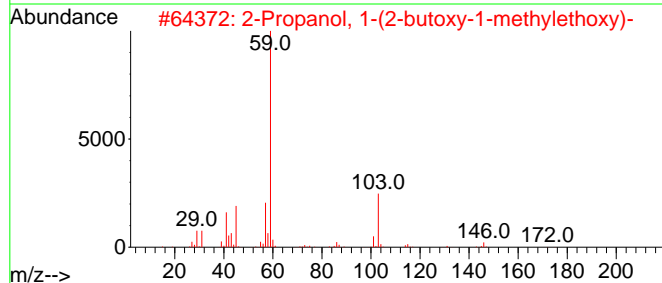
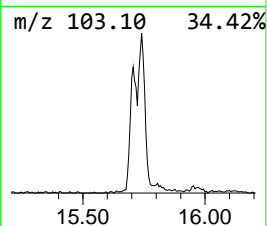
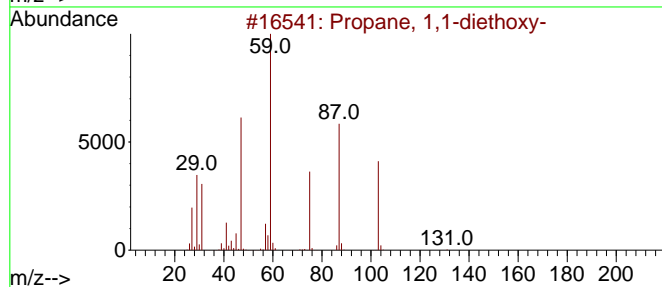
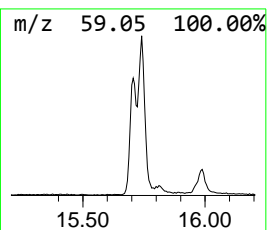
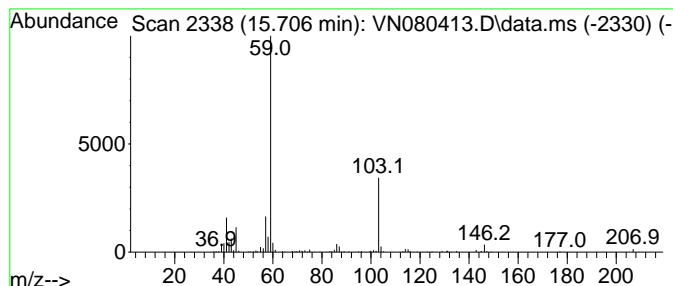
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 Peak Number 2 Propane, 1,1-diethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.706	9.63 ug/l	270336	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	78
2		2-Propanol, 1-(2-butoxy-1-methyl...)	190	C10H22O3	029911-28-2	74
3		Methane, diethoxy-	104	C5H12O2	000462-95-3	64
4		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5		2-Propanol, 1-[1-methyl-2-(2-pro...]	174	C9H18O3	055956-25-7	56



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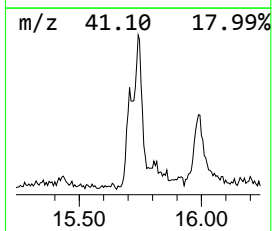
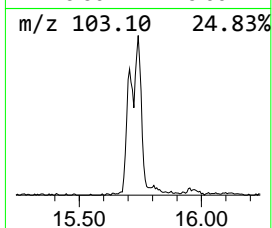
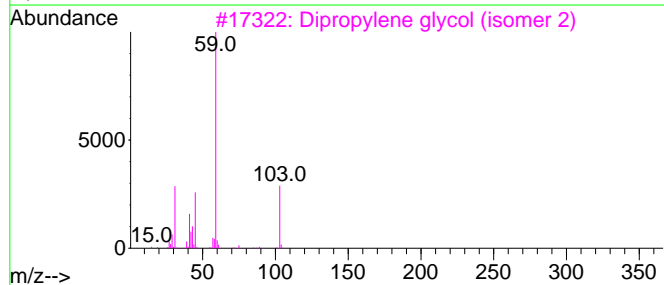
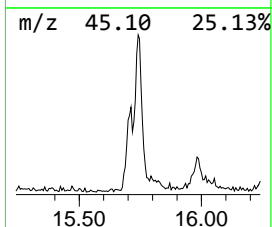
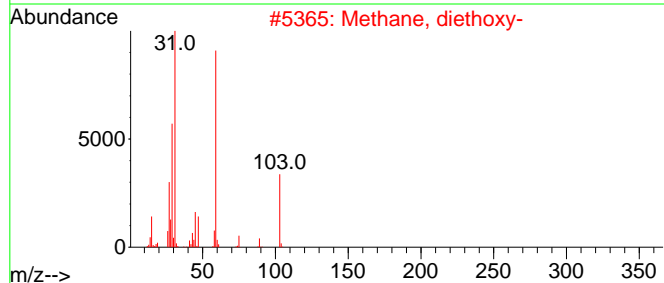
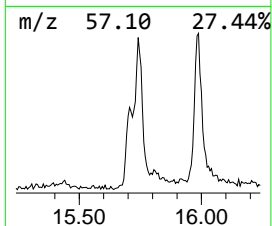
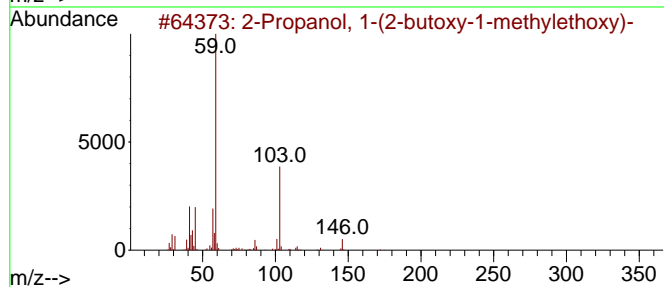
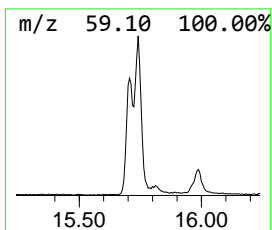
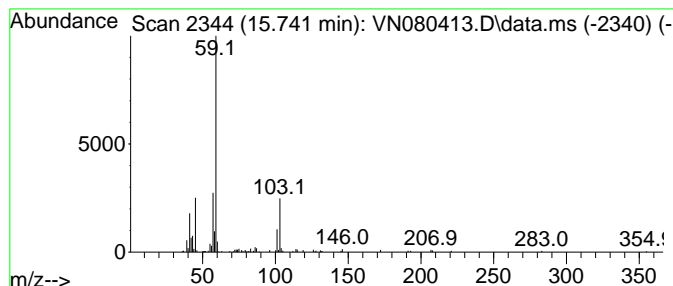
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 Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.741	15.19 ug/l	426353	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	78
2			Methane, diethoxy-	104	C5H12O2	000462-95-3	72
3			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
4			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
5			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64



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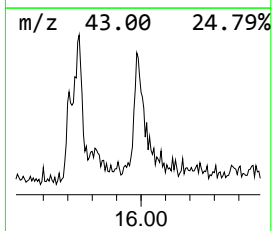
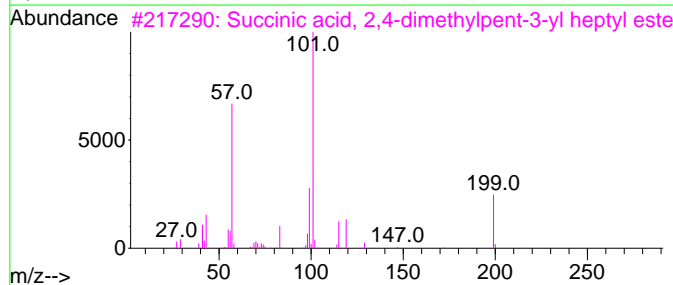
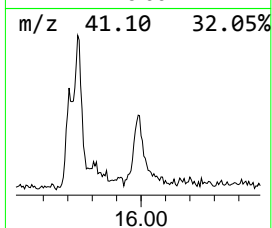
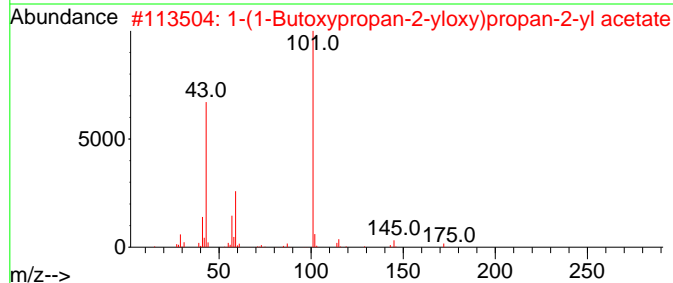
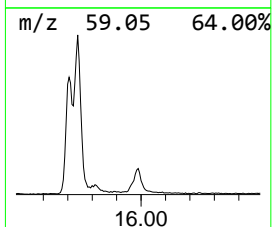
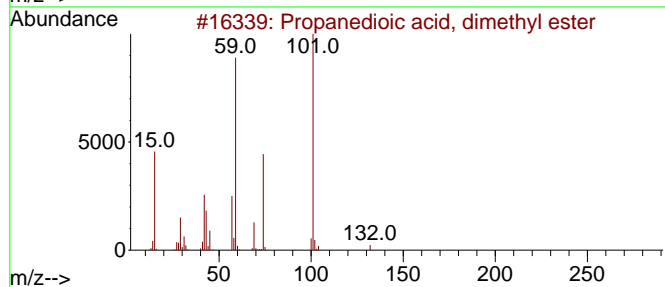
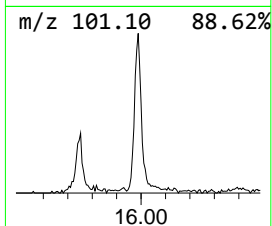
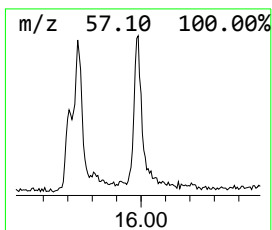
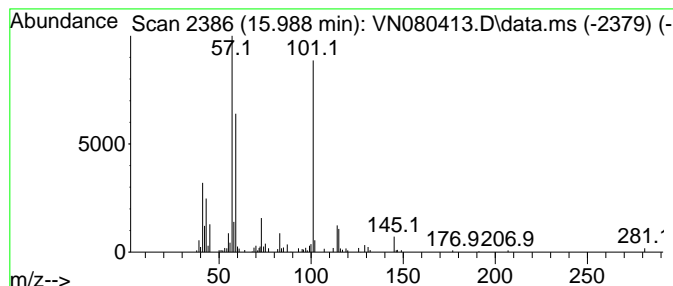
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 Peak Number 4 Propanedioic acid, dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.988	8.54 ug/l	239797	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	59
2			1-(1-Butoxypropan-2-yloxy)propan...	232	C12H24O4	1000367-08-4	53
3			Succinic acid, 2,4-dimethylpent-...	314	C18H34O4	1000349-36-0	47
4			Silane, ethenylmethoxydimethyl-	116	C5H12OSi	016546-47-7	43
5			Ethanol, 2,2'-oxybis-, dipropanoate	218	C10H18O5	006942-59-2	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.301	9.3	ug/l	171168	1	8.230	920407	50.0
Propane, 1,1-di...	15.706	9.6	ug/l	270336	4	13.794	1403180	50.0
2-Propanol, 1-(...	15.741	15.2	ug/l	426353	4	13.794	1403180	50.0
Propanedioic ac...	15.988	8.5	ug/l	239797	4	13.794	1403180	50.0