

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
 Data File : VX035573.D
 Acq On : 08 May 2023 20:17
 Operator : JC/MD
 Sample : 02648-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1636

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_X\Method\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rVV	1600867	1694730	3.74%	2.265%
2	1.752	104	109	119	rBV	492087	652771	1.44%	0.872%
3	3.111	319	332	348	rVB	181265	462741	1.02%	0.618%
4	5.385	693	705	714	rBV	175502	525943	1.16%	0.703%
5	5.550	724	732	748	rVB	308573	884234	1.95%	1.182%
6	5.958	789	799	803	rBV	181294	469050	1.04%	0.627%
7	6.038	803	812	828	rVB	2607562	7049249	15.58%	9.421%
8	6.763	921	931	943	rBV	465961	1134149	2.51%	1.516%
9	8.647	1235	1240	1246	rBV	975557	1518241	3.35%	2.029%
10	8.720	1246	1252	1259	rVV	3221127	4969352	10.98%	6.642%
11	9.689	1383	1411	1415	rBV	8130840	45259489	100.00%	60.490%
12	9.823	1427	1433	1436	rBV3	244992	632810	1.40%	0.846%
13	10.055	1466	1471	1486	rVB	1000750	1594959	3.52%	2.132%
14	10.299	1507	1511	1519	rVB	543486	748042	1.65%	1.000%
15	10.640	1563	1567	1573	rVB	457093	585775	1.29%	0.783%
16	11.079	1634	1639	1646	rVB	826008	1055406	2.33%	1.411%
17	12.024	1789	1794	1800	rBV	1048060	1318408	2.91%	1.762%
18	15.542	2366	2371	2379	rBV	1615351	2425217	5.36%	3.241%
19	16.475	2518	2524	2533	rVB	994887	1840654	4.07%	2.460%

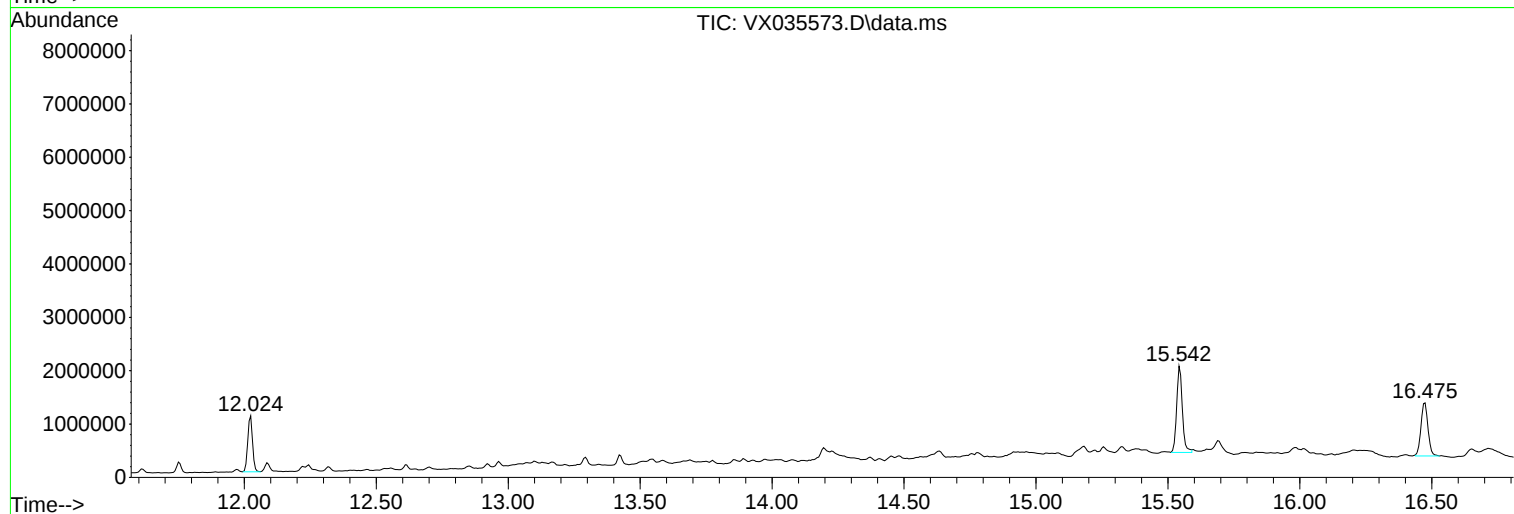
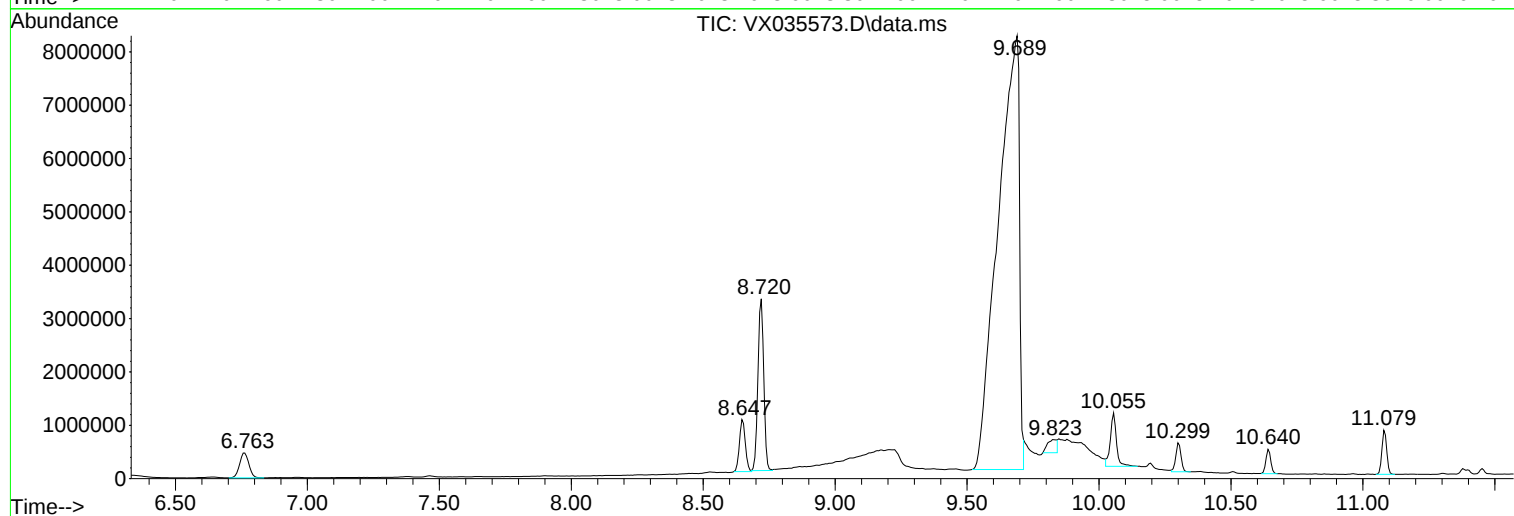
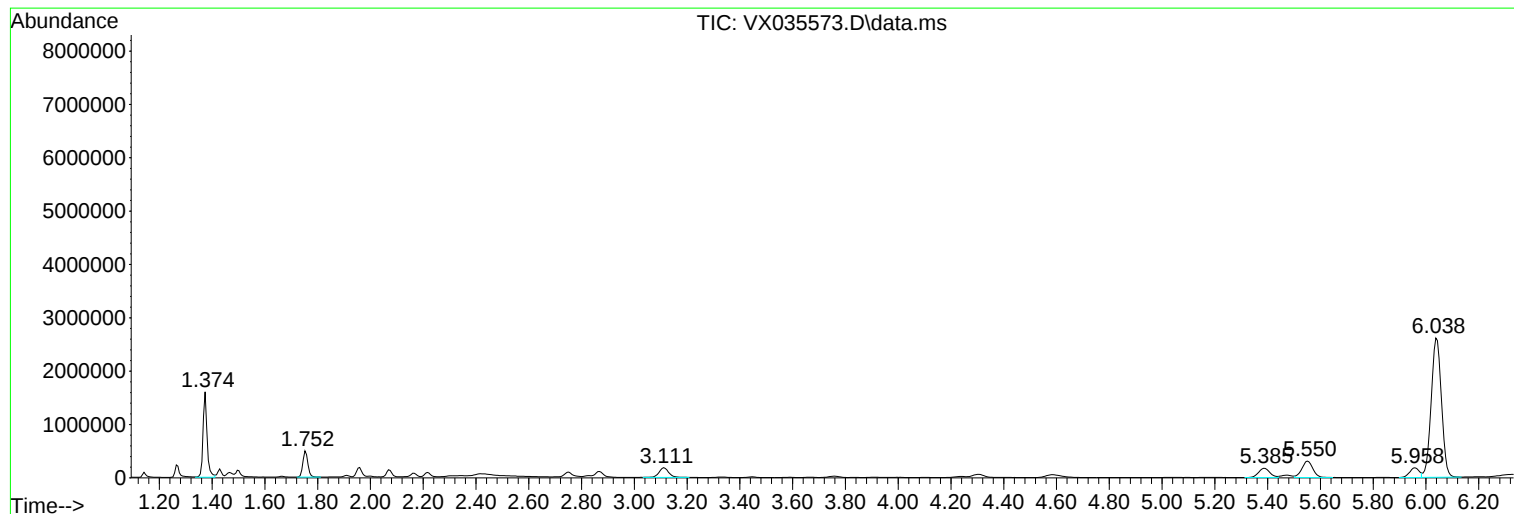
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TIC Library : C:\Database\NIST20.L
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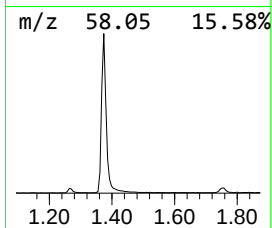
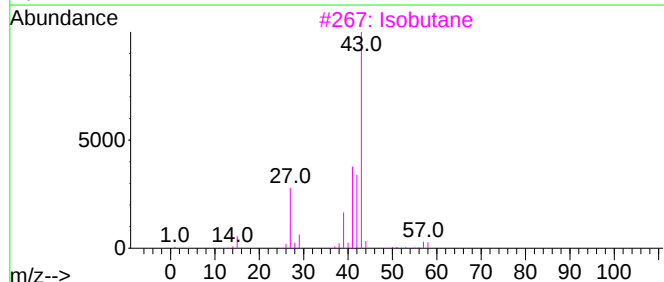
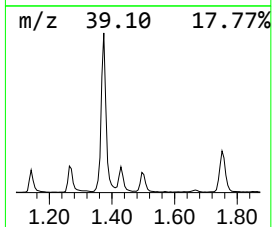
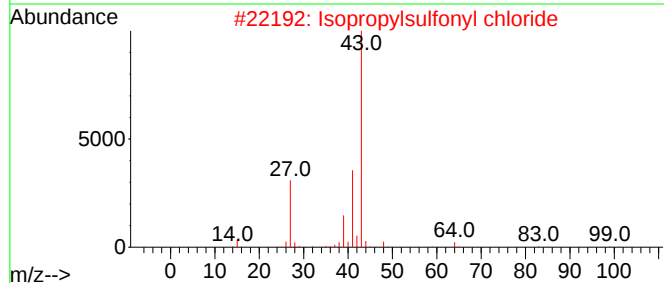
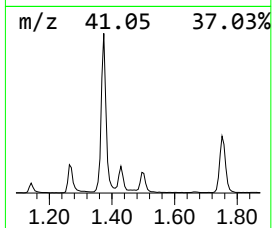
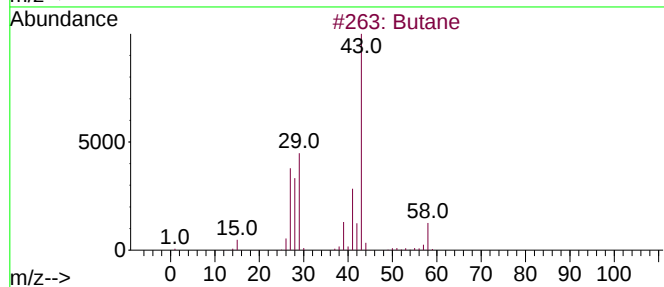
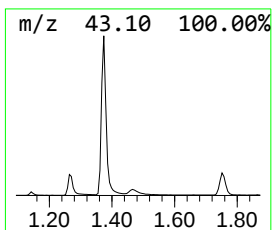
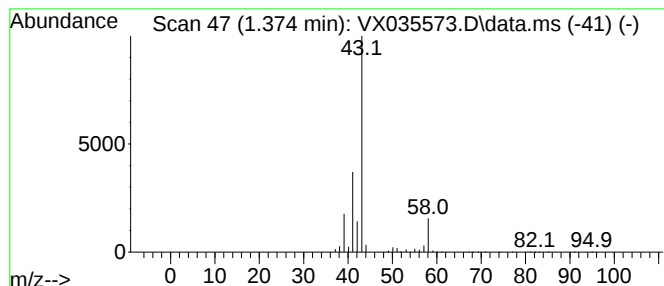
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Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	95.83 ug/l	1694730	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Acetone	58	C3H6O	000067-64-1	4



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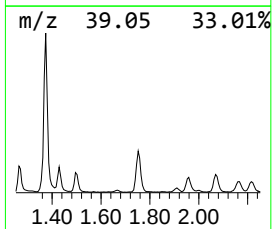
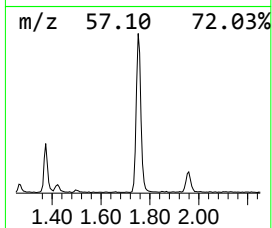
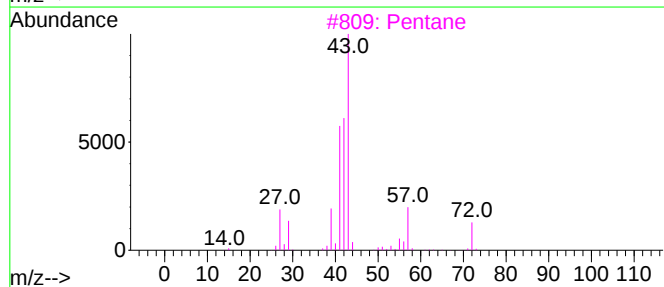
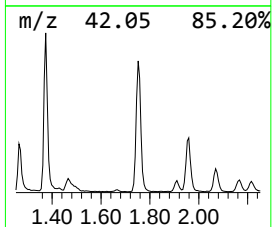
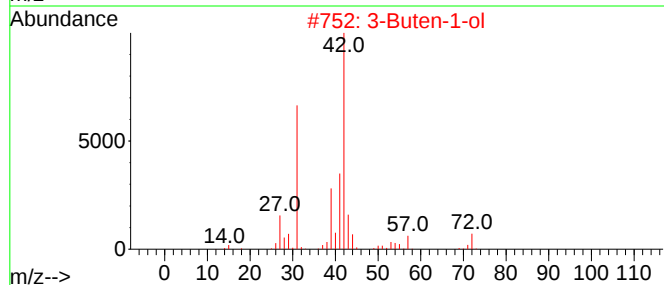
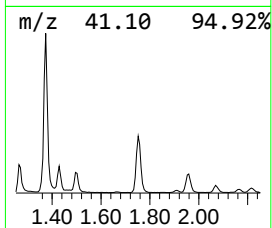
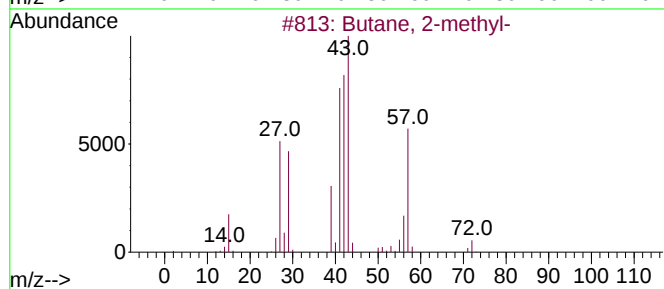
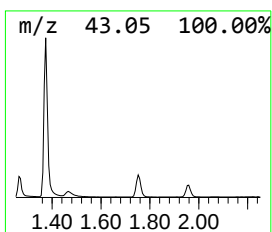
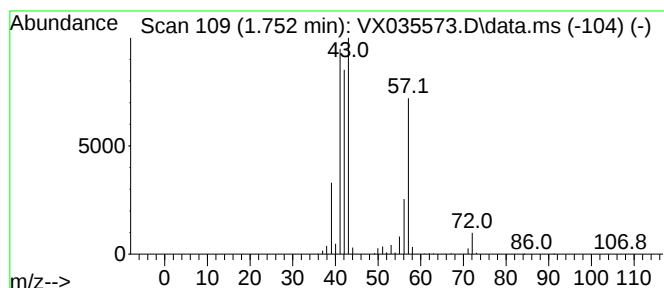
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Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	36.91 ug/l	652771	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	80
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	33
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	28
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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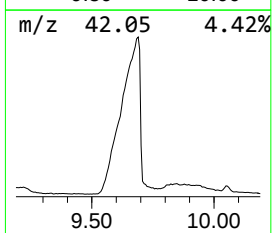
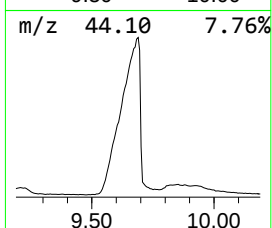
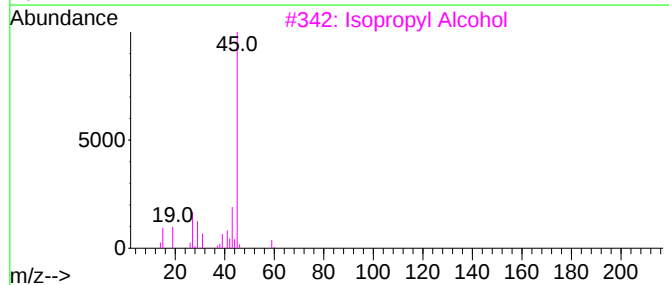
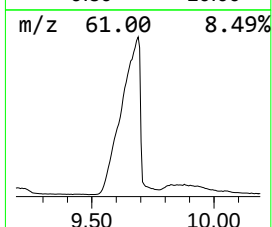
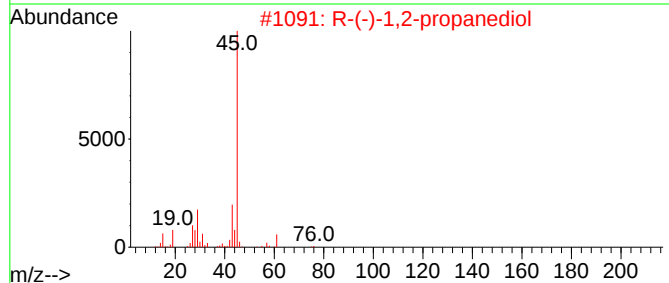
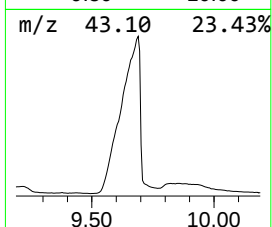
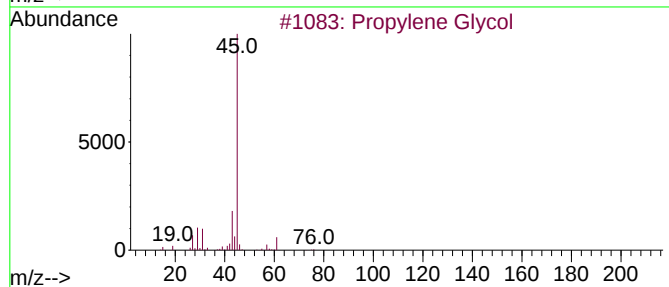
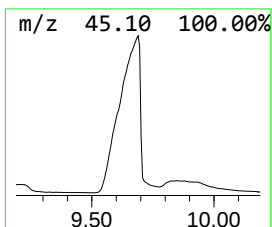
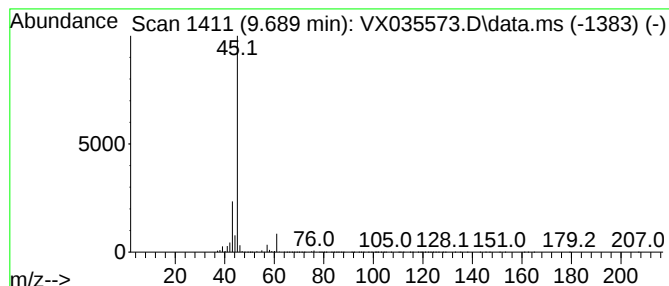
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Peak Number 3 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.689	1418.83 ug/l	45259500	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	40



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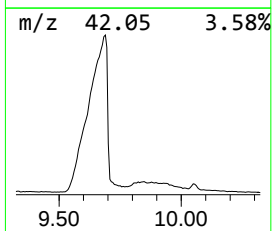
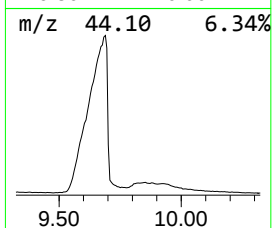
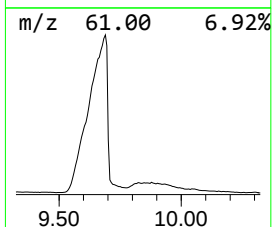
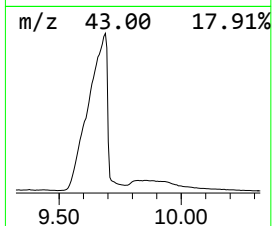
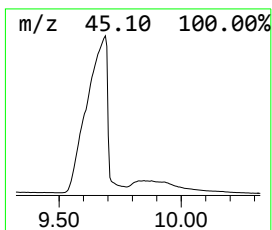
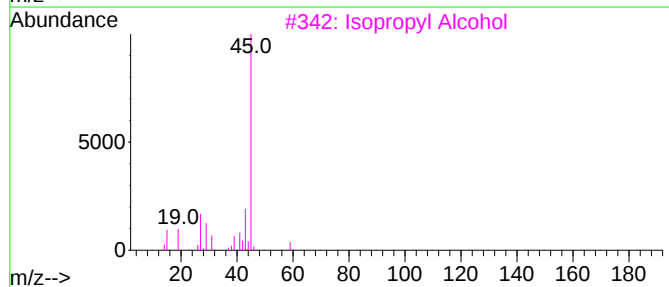
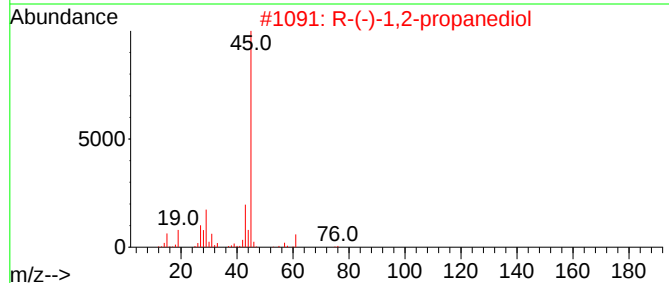
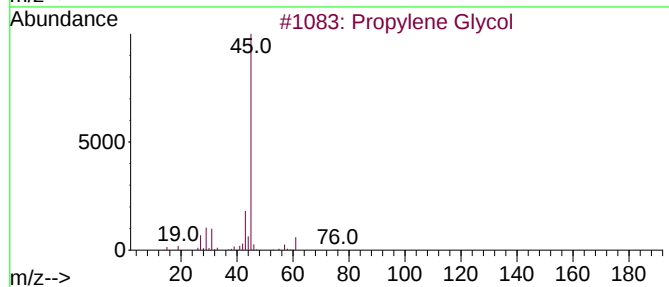
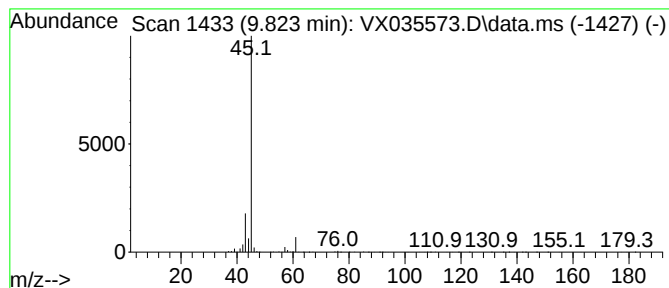
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TIC Integration Parameters: LSCINT.P

Peak Number 4 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.823	19.84 ug/l	632810	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Butanol	74	C4H10O	000078-92-2	40



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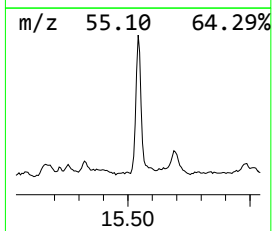
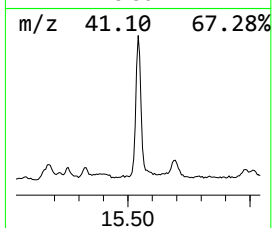
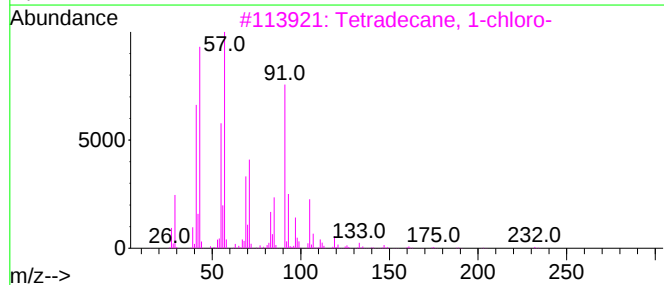
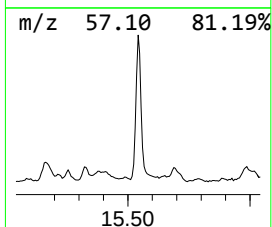
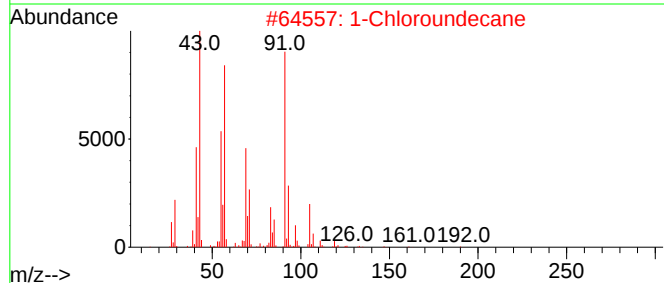
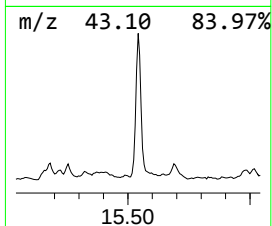
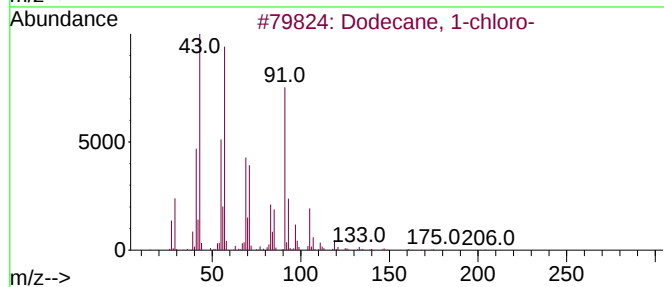
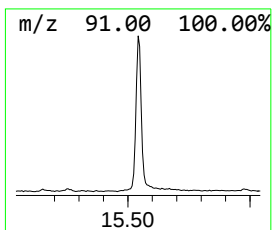
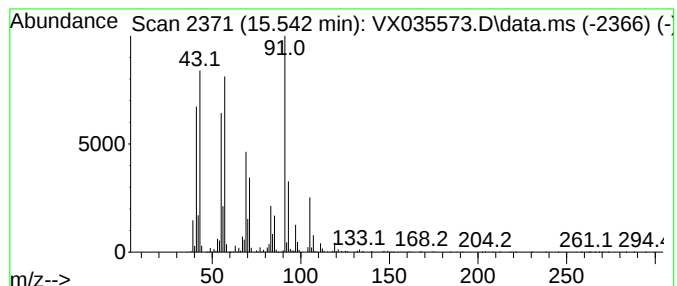
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Peak Number 5 Dodecane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	91.98 ug/l	2425220	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	96
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	91
3			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	64
4			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	59
5			1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	47



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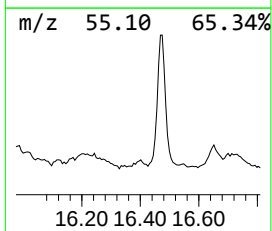
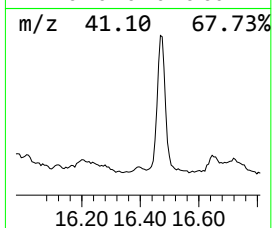
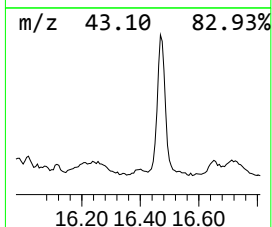
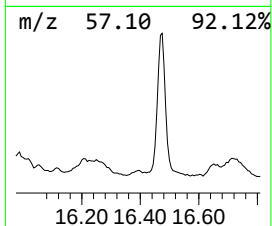
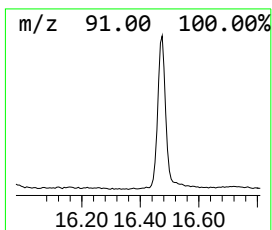
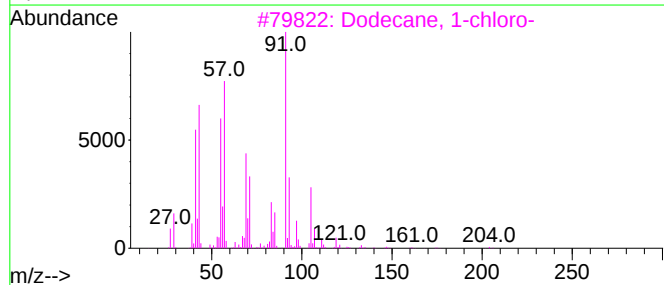
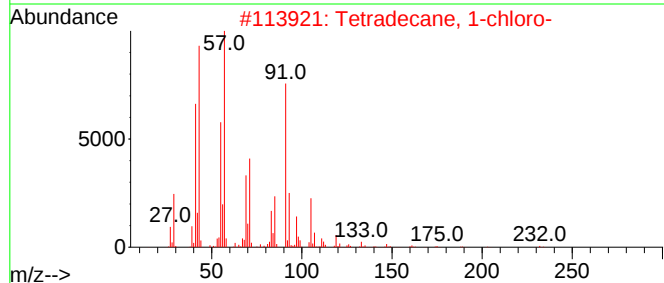
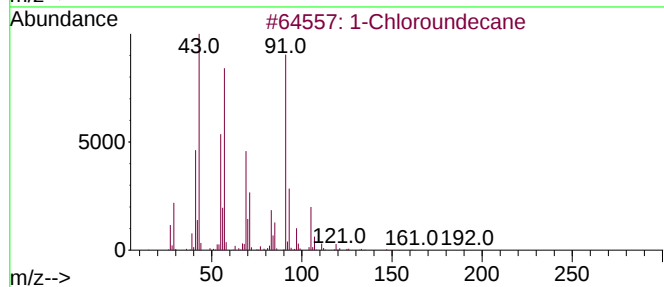
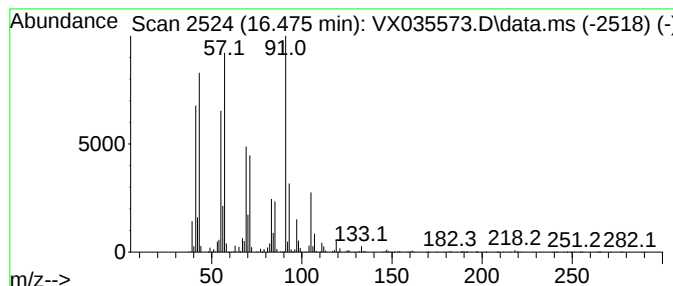
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 6 Tetradecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.475	69.81 ug/l	1840650	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Chloroundecane	190	C11H23Cl	002473-03-2	93
2			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	91
3			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
4			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	53
5			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035573.D
Acq On : 08 May 2023 20:17
Operator : JC/MD
Sample : 02648-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1636

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.374	95.8	ug/l	1694730	1	5.550	884234	50.0
Butane, 2-methyl-	1.752	36.9	ug/l	652771	1	5.550	884234	50.0
Propylene Glycol	9.689	1418.8	ug/l	45259500	3	10.055	1594960	50.0
R-(-)-1,2-propa...	9.823	19.8	ug/l	632810	3	10.055	1594960	50.0
Dodecane, 1-chl...	15.542	92.0	ug/l	2425220	4	12.024	1318410	50.0
Tetradecane, 1-...	16.475	69.8	ug/l	1840650	4	12.024	1318410	50.0