

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
 Data File : VX035572.D
 Acq On : 08 May 2023 19:54
 Operator : JC/MD
 Sample : 02648-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1635

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: VX035572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	57	63	97	rBV	1752076	4837233	22.20%	7.471%
2	5.391	693	706	719	rBV	150177	468723	2.15%	0.724%
3	5.556	719	733	754	rVB	278344	845146	3.88%	1.305%
4	5.964	788	800	818	rBV	154734	445533	2.05%	0.688%
5	6.763	922	931	944	rBV	418120	1025866	4.71%	1.584%
6	6.903	944	954	976	rBV2	288584	1081617	4.96%	1.671%
7	8.653	1235	1241	1248	rBV	883552	1442960	6.62%	2.229%
8	9.189	1325	1329	1330	rBV	429446	556585	2.55%	0.860%
9	9.415	1344	1366	1371	rBV	4032417	21786309	100.00%	33.649%
10	9.634	1393	1402	1403	rBV	1985947	4780474	21.94%	7.384%
11	11.085	1635	1640	1648	rVB	753868	970192	4.45%	1.498%
12	11.969	1780	1785	1790	rVV	5226780	6536408	30.00%	10.096%
13	12.024	1790	1794	1800	rVV	1009591	1447527	6.64%	2.236%
14	12.103	1803	1807	1817	rVB	625882	966353	4.44%	1.493%
15	12.225	1822	1827	1832	rBV	679961	889241	4.08%	1.373%
16	12.286	1832	1837	1840	rBV6	120441	245006	1.12%	0.378%
17	12.768	1912	1916	1918	rBV2	211873	308096	1.41%	0.476%
18	12.792	1918	1920	1923	rVV3	257983	340300	1.56%	0.526%
19	12.859	1927	1931	1937	rVB	660874	911915	4.19%	1.408%
20	12.975	1946	1950	1956	rBV2	399619	568073	2.61%	0.877%
21	13.073	1962	1966	1968	rBV	313216	361172	1.66%	0.558%
22	13.103	1968	1971	1974	rVV2	691901	854242	3.92%	1.319%
23	13.133	1974	1976	1985	rVB4	376027	582222	2.67%	0.899%
24	13.219	1986	1990	1994	rBV	309782	406025	1.86%	0.627%
25	13.268	1994	1998	2001	rBV	342847	389629	1.79%	0.602%
26	13.426	2019	2024	2028	rBV	645036	974780	4.47%	1.506%
27	13.511	2035	2038	2047	rVB2	454725	818103	3.76%	1.264%
28	13.707	2067	2070	2075	rVV	262286	359336	1.65%	0.555%
29	13.749	2075	2077	2083	rVB3	220980	318533	1.46%	0.492%
30	13.859	2088	2095	2098	rBV3	257249	556384	2.55%	0.859%
31	13.889	2098	2100	2105	rBV	177644	226789	1.04%	0.350%
32	14.036	2121	2124	2128	rVB	365850	414010	1.90%	0.639%
33	14.402	2181	2184	2188	rBV	392727	505988	2.32%	0.782%
34	14.615	2216	2219	2221	rBV2	207750	244741	1.12%	0.378%
35	15.542	2366	2371	2386	rVB	2064902	4366838	20.04%	6.745%
36	15.694	2393	2396	2403	rVB	240407	351821	1.61%	0.543%

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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

37	16.468	2519	2523	2543	rVB	1128958	2561006	11.76%	3.956%
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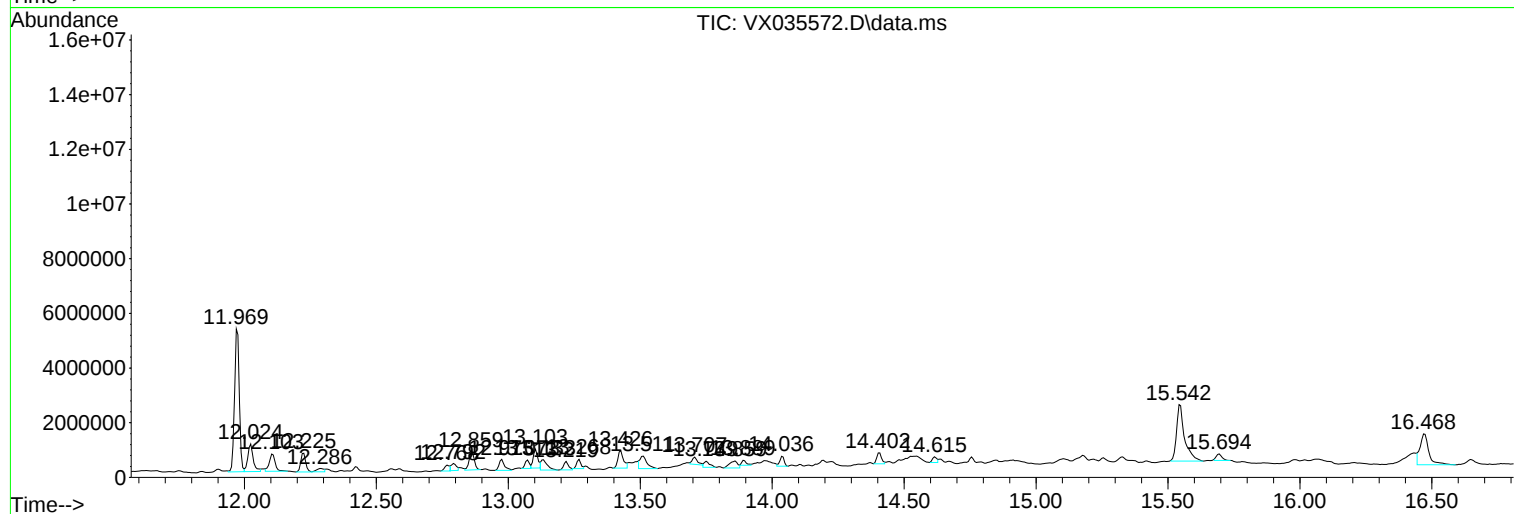
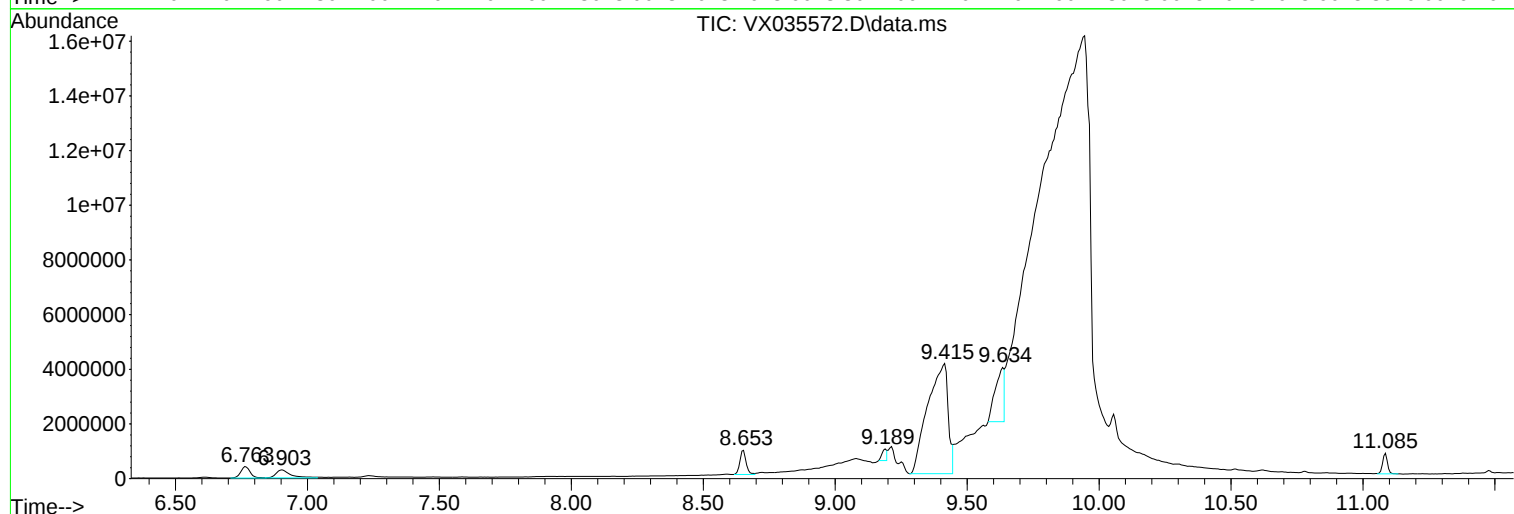
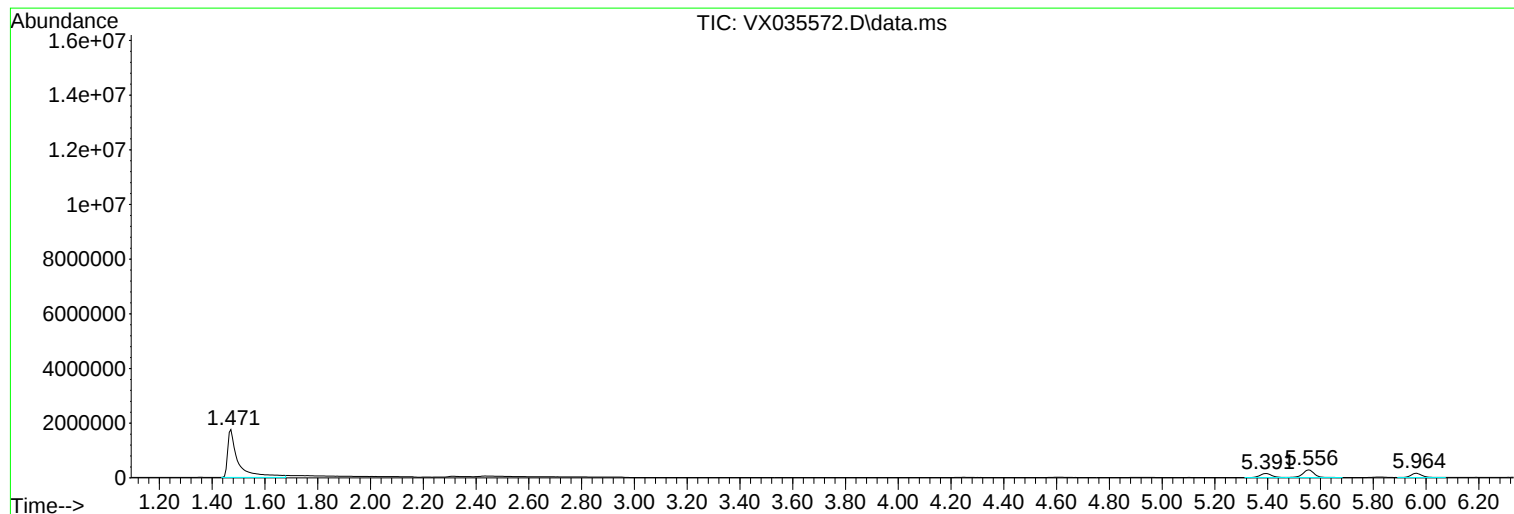
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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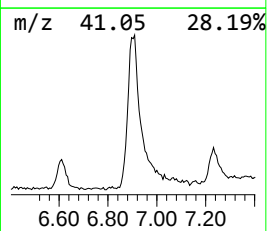
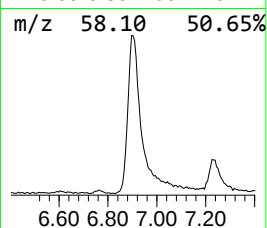
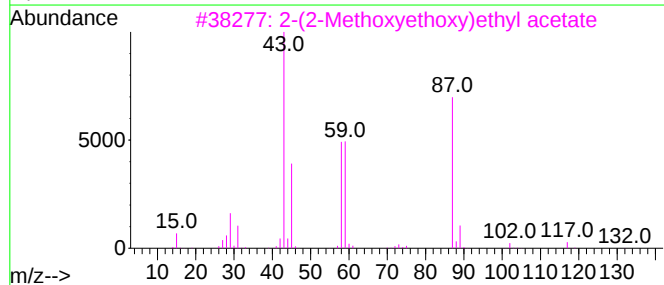
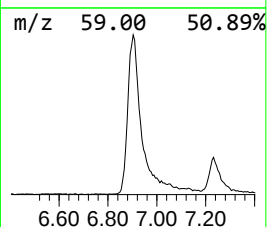
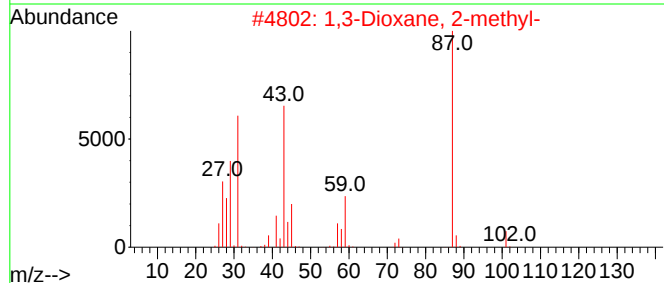
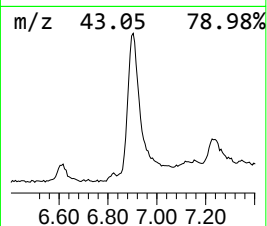
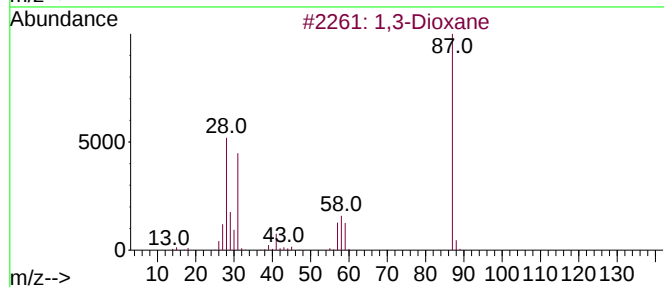
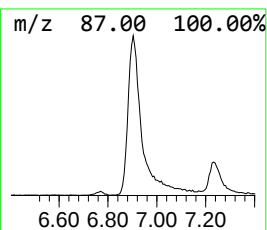
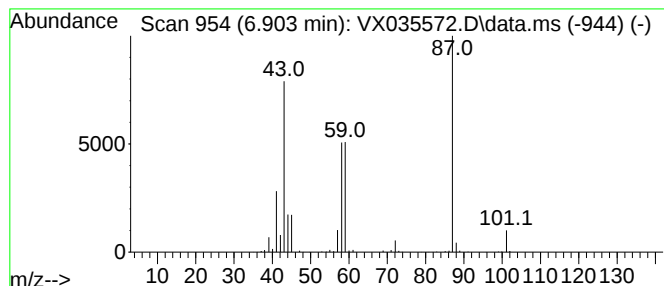
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 2 1,3-Dioxane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.903	52.72 ug/l	1081620	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane	88	C4H8O2	000505-22-6	58
2			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	42
3			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	25



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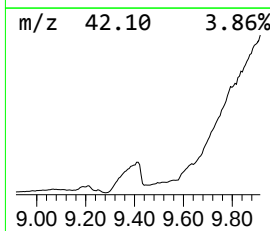
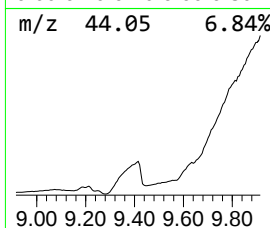
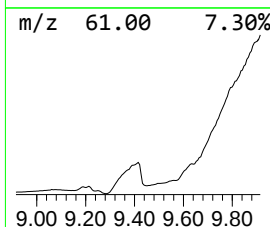
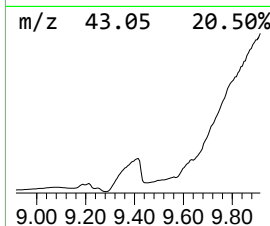
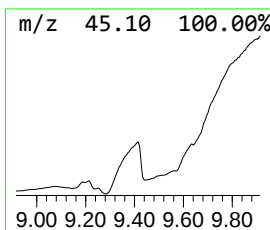
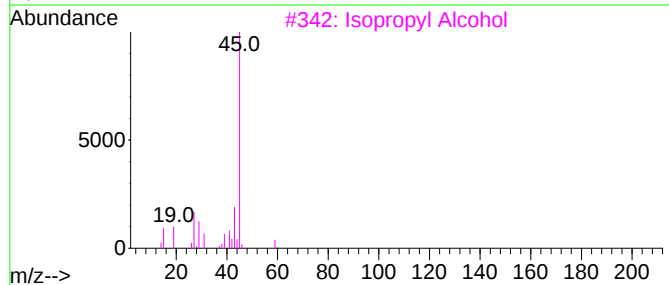
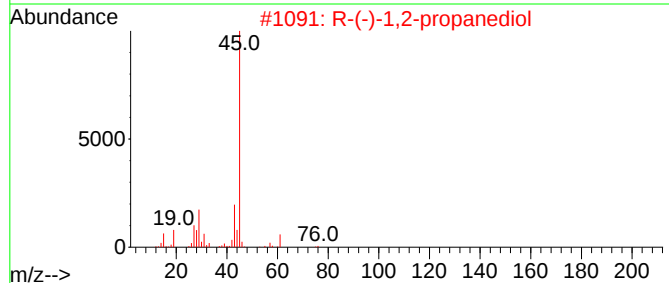
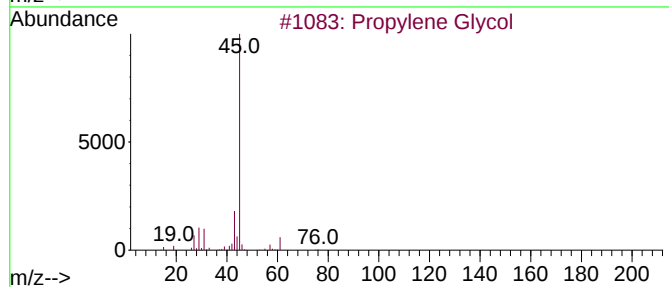
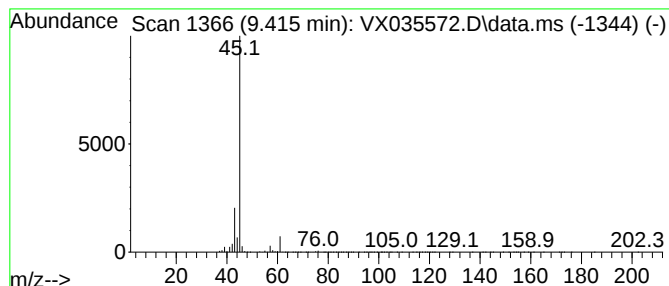
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.415	227.87 ug/l	21786300	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			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40



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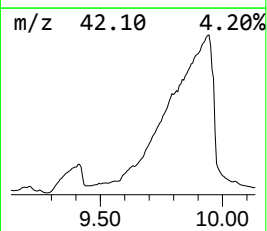
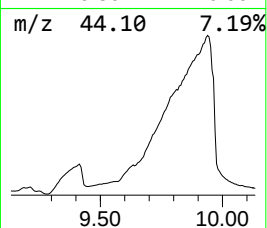
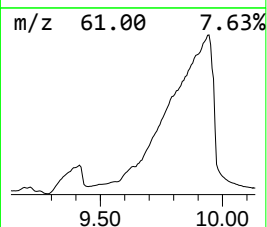
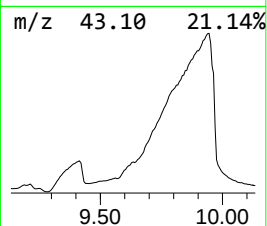
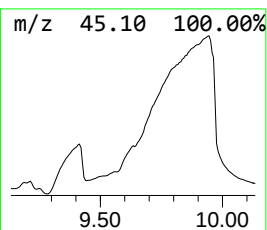
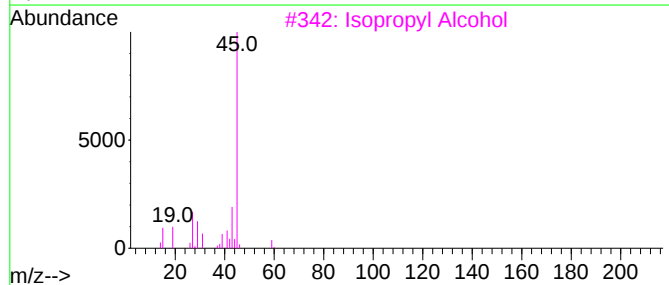
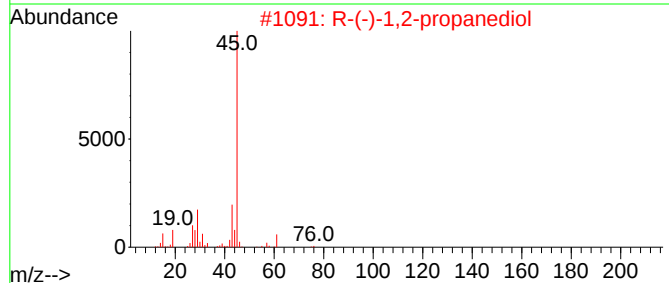
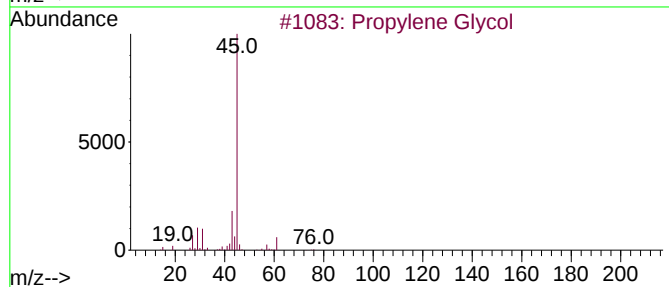
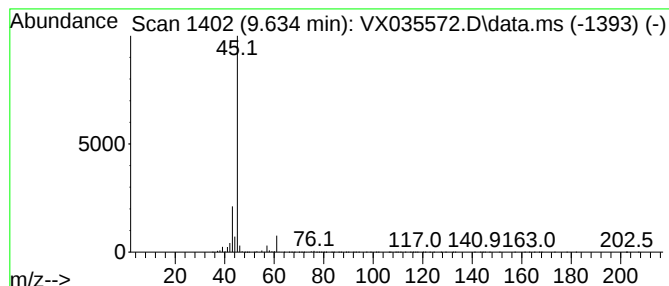
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 R-(-)-1,2-propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.634	50.00 ug/l	4780470	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			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12



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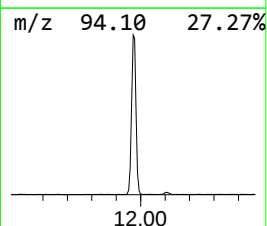
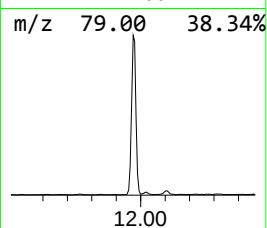
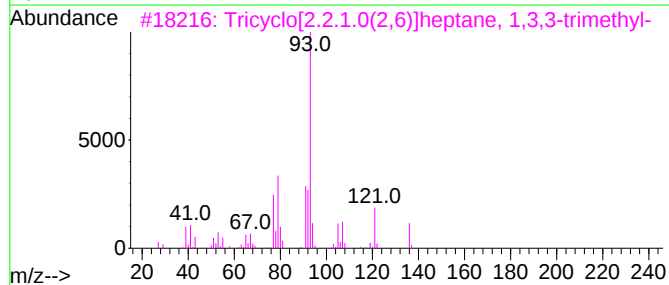
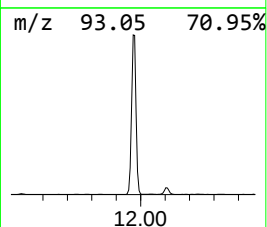
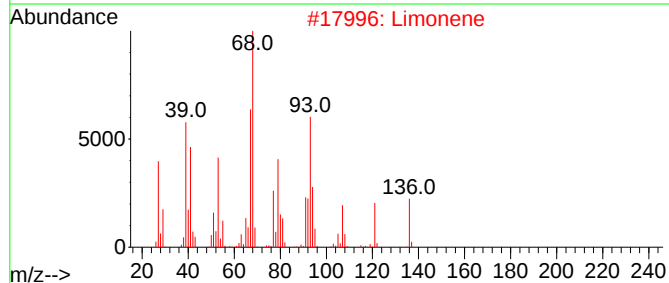
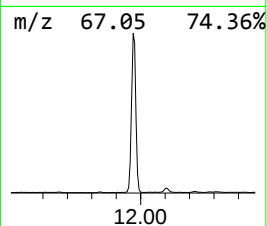
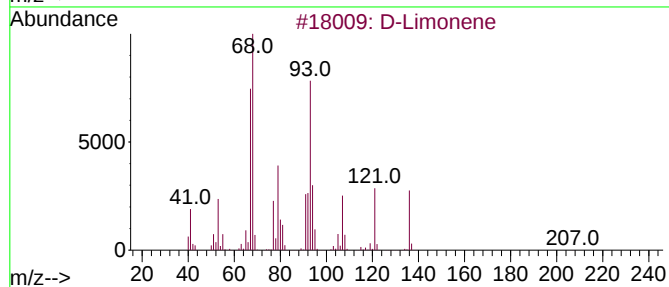
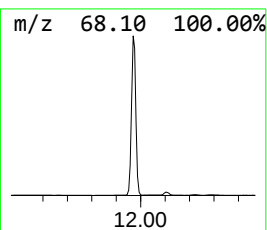
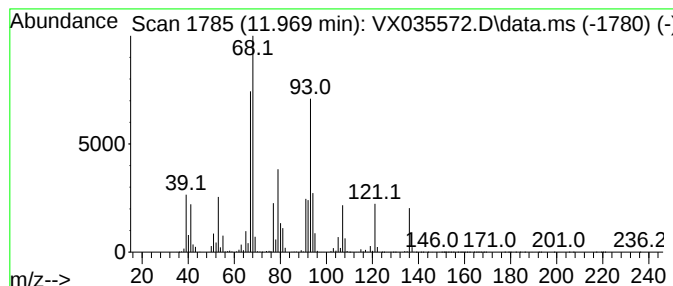
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 D-Limonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	225.78 ug/l	6536410	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Limonene	136	C10H16	000138-86-3	91
3			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	86
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	68
5			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	58



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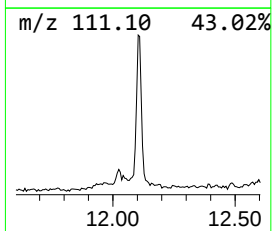
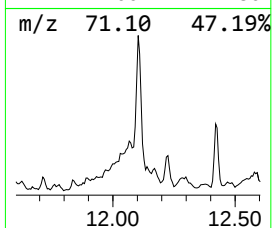
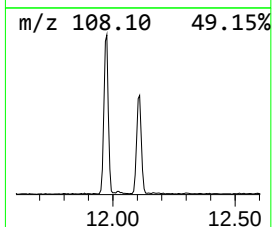
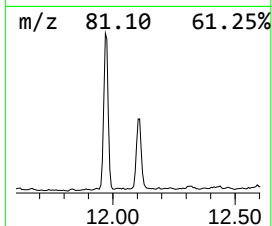
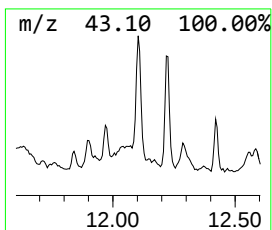
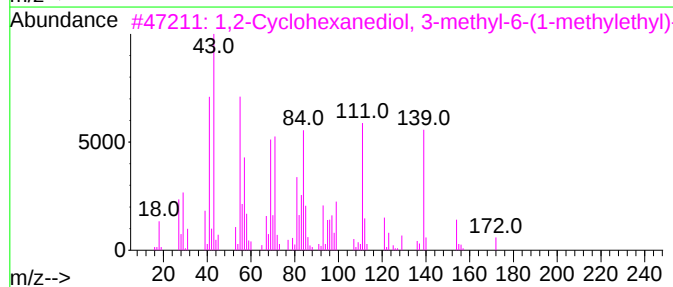
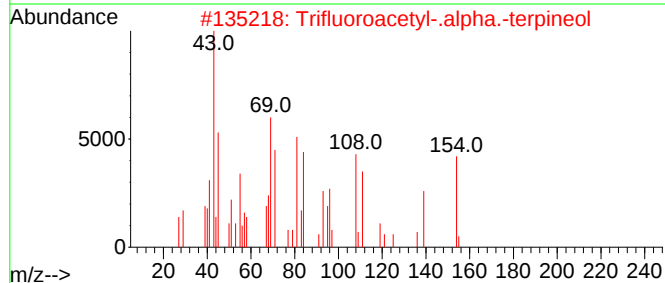
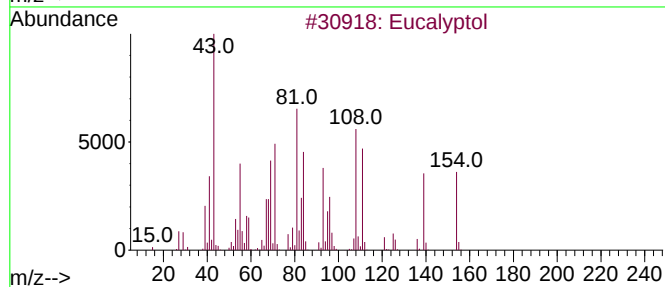
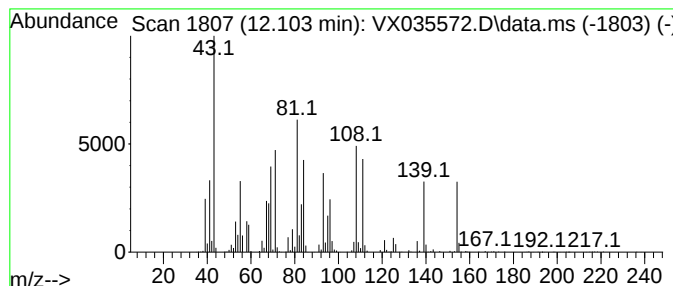
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 6 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	33.38 ug/l	966353	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	43
3			1,2-Cyclohexanediol, 3-methyl-6-...	172	C10H20O2	042962-93-6	42
4			2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	35
5			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035572.D
Acq On : 08 May 2023 19:54
Operator : JC/MD
Sample : 02648-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1635

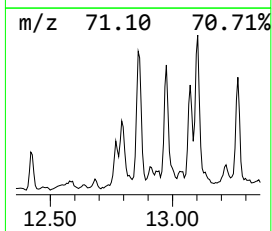
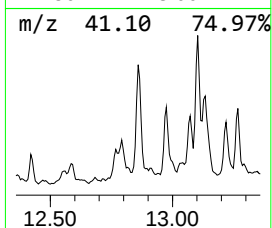
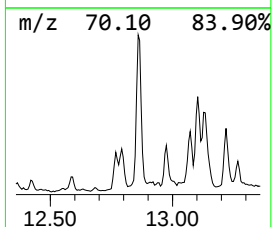
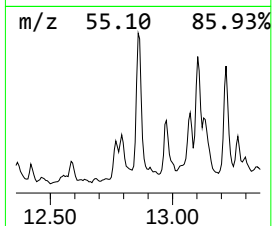
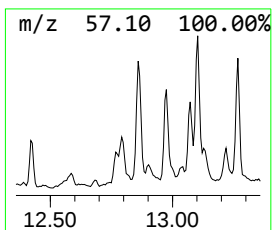
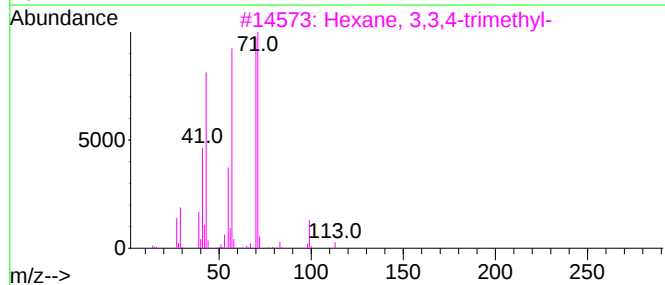
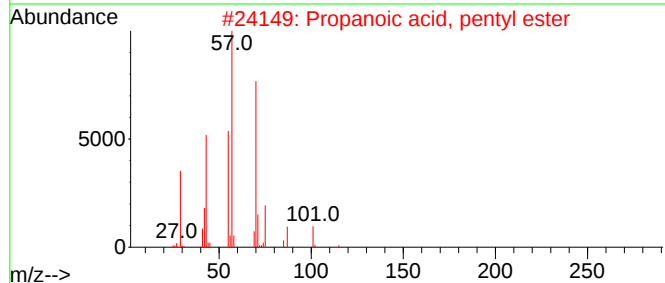
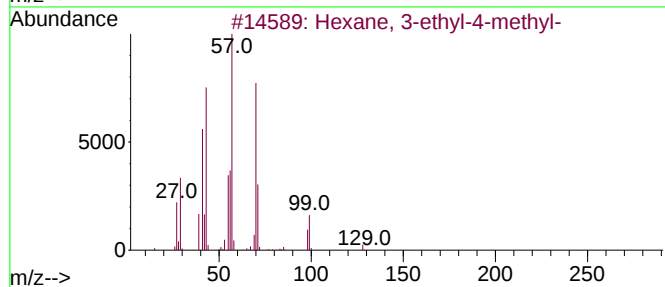
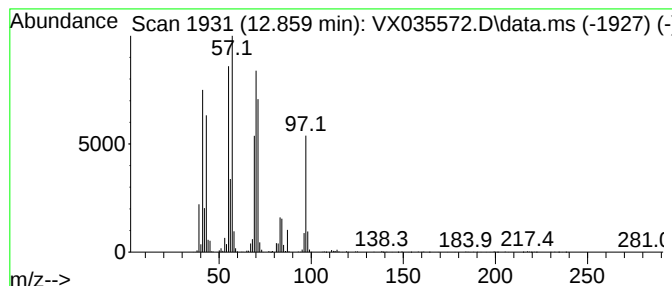
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 3-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	31.50 ug/l	911915	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	50
2			Propanoic acid, pentyl ester	144	C8H16O2	000624-54-4	43
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	43
4			Oxalic acid, 2-ethylhexyl isohex...	286	C16H30O4	1000309-38-8	35
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035572.D
Acq On : 08 May 2023 19:54
Operator : JC/MD
Sample : 02648-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1635

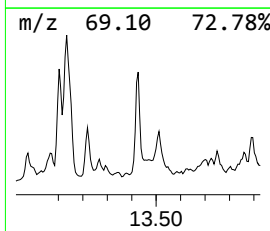
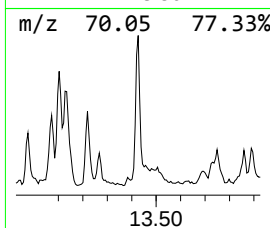
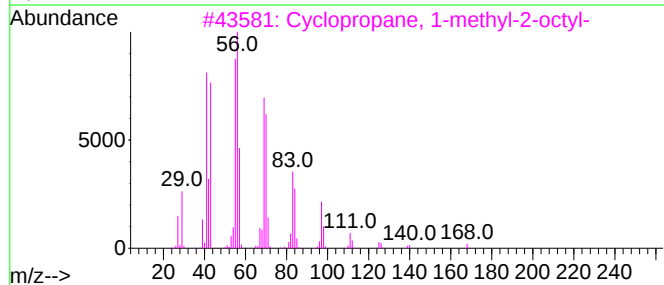
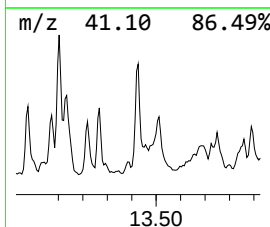
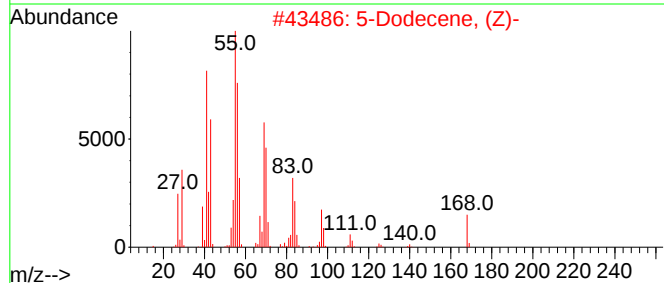
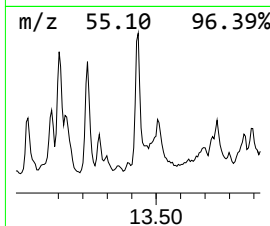
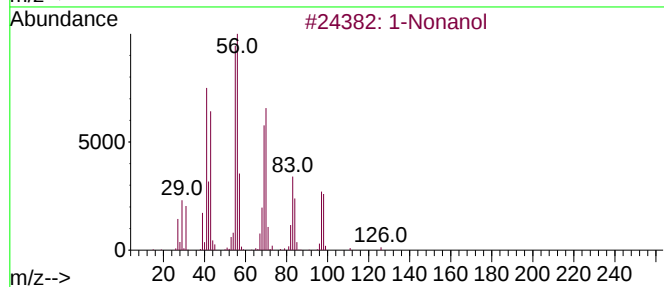
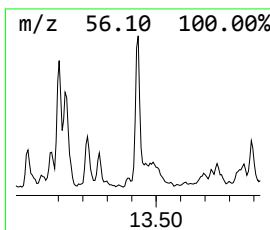
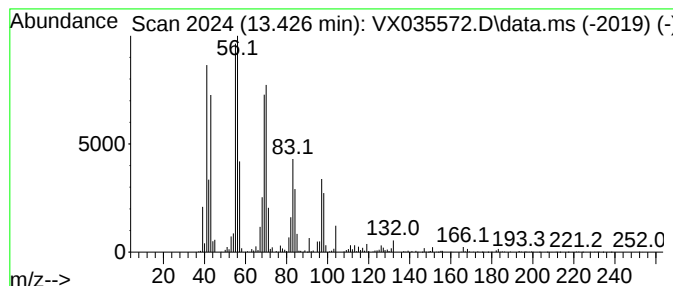
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Quant Title : SW846 8260

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

Peak Number 8 1-Nonanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	33.67 ug/l	974780	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	87
2			5-Dodecene, (Z)-	168	C12H24	007206-28-2	83
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
4			1-Nonene	126	C9H18	000124-11-8	76
5			Cycloheptane	98	C7H14	000291-64-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035572.D
Acq On : 08 May 2023 19:54
Operator : JC/MD
Sample : 02648-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1635

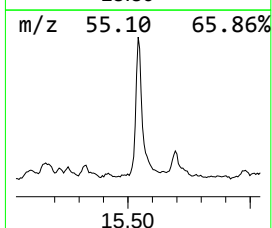
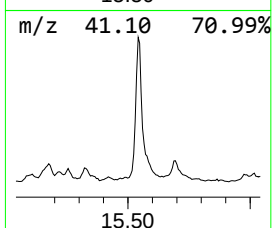
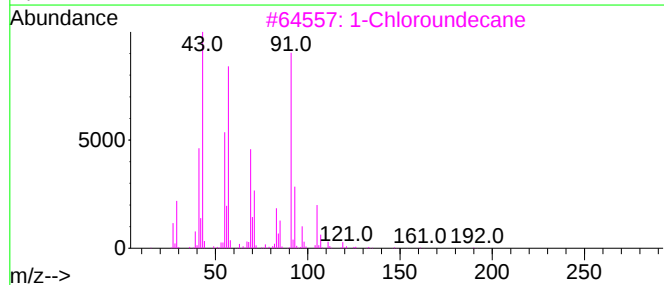
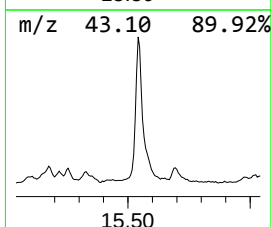
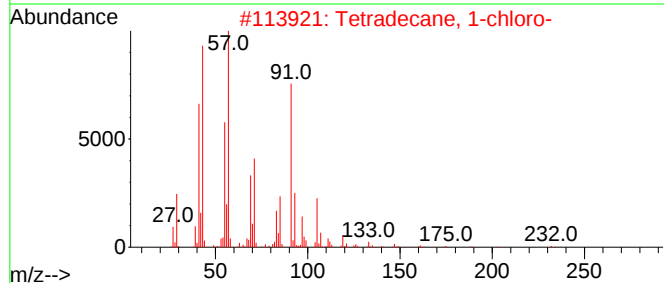
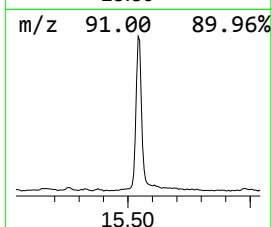
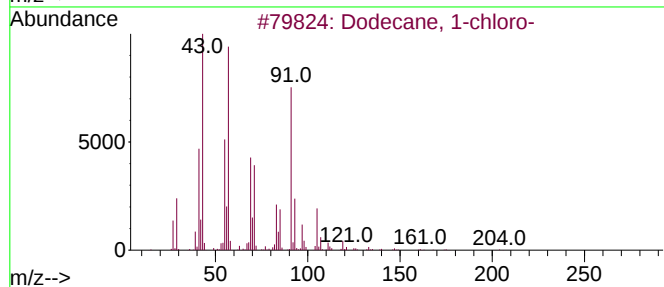
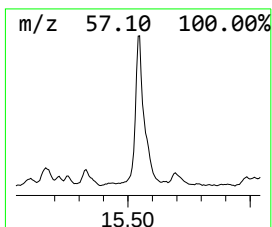
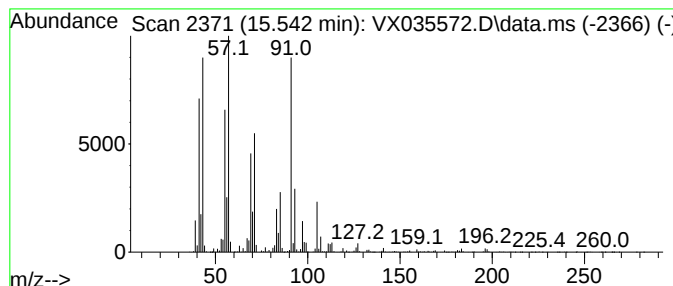
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	150.84 ug/l	4366840	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	93
2			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	91
3			1-Chloroundecane	190	C11H23Cl	002473-03-2	64
4			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	46
5			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035572.D
Acq On : 08 May 2023 19:54
Operator : JC/MD
Sample : 02648-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1635

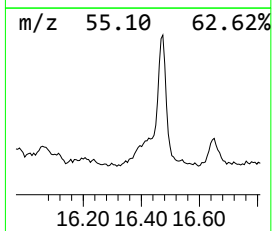
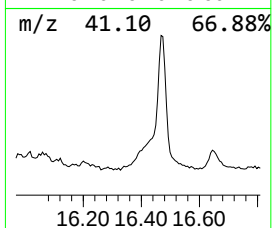
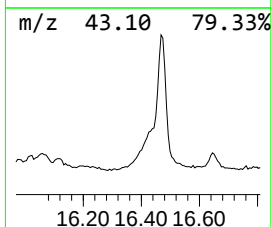
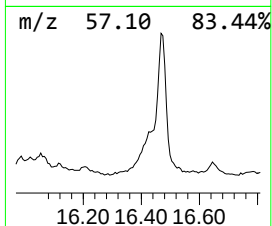
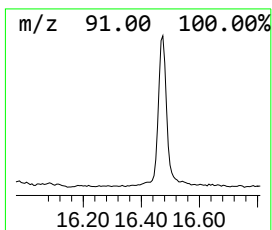
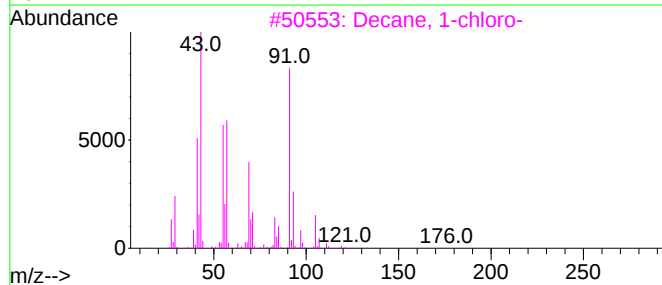
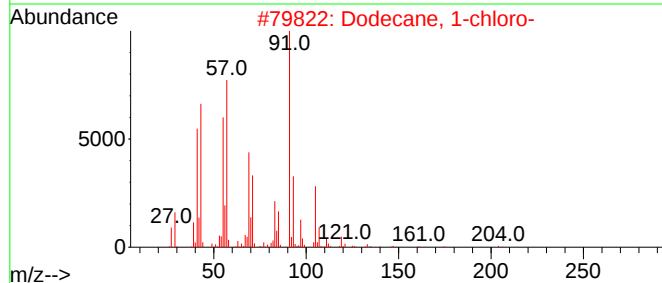
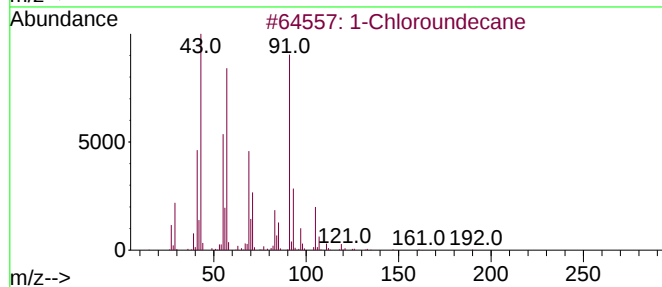
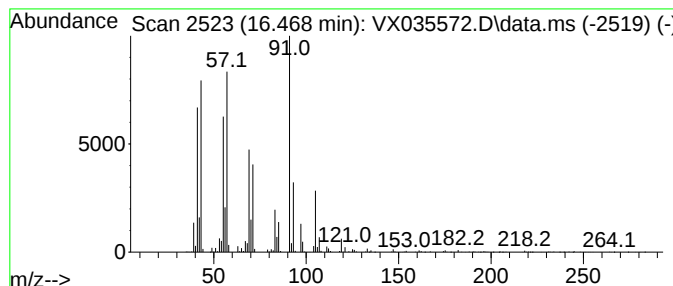
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Quant Title : SW846 8260

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

Peak Number 10 1-Chloroundecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	88.46 ug/l	2561010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Chloroundecane	190	C11H23Cl	002473-03-2	96
2			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	87
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	64
4			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	52
5			Nonane, 1-chloro-	162	C9H19Cl	002473-01-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035572.D
Acq On : 08 May 2023 19:54
Operator : JC/MD
Sample : 02648-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1635

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
1,3-Dioxane	6.903	52.7	ug/l	1081620	2	6.763	1025870	50.0
Propylene Glycol	9.415	227.9	ug/l	21786300	3	10.055	4780470	50.0
R-(-)-1,2-propa...	9.634	50.0	ug/l	4780470	3	10.055	4780470	50.0
D-Limonene	11.969	225.8	ug/l	6536410	4	12.024	1447530	50.0
Eucalyptol	12.103	33.4	ug/l	966353	4	12.024	1447530	50.0
Hexane, 3-ethyl...	12.859	31.5	ug/l	911915	4	12.024	1447530	50.0
1-Nonanol	13.426	33.7	ug/l	974780	4	12.024	1447530	50.0
Dodecane, 1-chl...	15.542	150.8	ug/l	4366840	4	12.024	1447530	50.0
1-Chloroundecane	16.468	88.5	ug/l	2561010	4	12.024	1447530	50.0