

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
 Data File : VX035574.D
 Acq On : 08 May 2023 20:42
 Operator : JC/MD
 Sample : 02648-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1637

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: VX035574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	56	61	83	rBV	578287	1009368	4.15%	2.072%
2	2.300	170	199	211	rBV2	249529	1471173	6.05%	3.020%
3	4.233	503	516	535	rBV	444474	1311903	5.40%	2.693%
4	5.385	693	705	719	rBV2	152584	452078	1.86%	0.928%
5	5.550	719	732	747	rBV	271785	773093	3.18%	1.587%
6	5.958	787	799	809	rBV	163883	442935	1.82%	0.909%
7	6.757	921	930	942	rBV	420379	1010662	4.16%	2.075%
8	7.281	1000	1016	1034	rBV3	62132	318306	1.31%	0.653%
9	8.647	1234	1240	1247	rBV	890937	1396347	5.75%	2.867%
10	9.646	1384	1404	1426	rBV	5082042	24302968	100.00%	49.893%
11	10.055	1466	1471	1481	rVB	896677	1331989	5.48%	2.735%
12	10.165	1485	1489	1504	rVB	158692	332143	1.37%	0.682%
13	10.756	1581	1586	1594	rVB	347028	435382	1.79%	0.894%
14	11.079	1634	1639	1644	rBV	799505	977130	4.02%	2.006%
15	11.683	1734	1738	1743	rBV	444819	502074	2.07%	1.031%
16	12.024	1790	1794	1799	rVB	949894	1185831	4.88%	2.434%
17	12.219	1821	1826	1836	rBV	4532393	5435082	22.36%	11.158%
18	14.194	2147	2150	2159	rVB	175447	246731	1.02%	0.507%
19	15.176	2304	2311	2316	rBV5	190236	486058	2.00%	0.998%
20	15.542	2366	2371	2382	rVB	1690374	2531510	10.42%	5.197%
21	15.694	2392	2396	2406	rVB2	223767	437662	1.80%	0.899%
22	16.474	2518	2524	2533	rVB	1328643	2319735	9.55%	4.762%

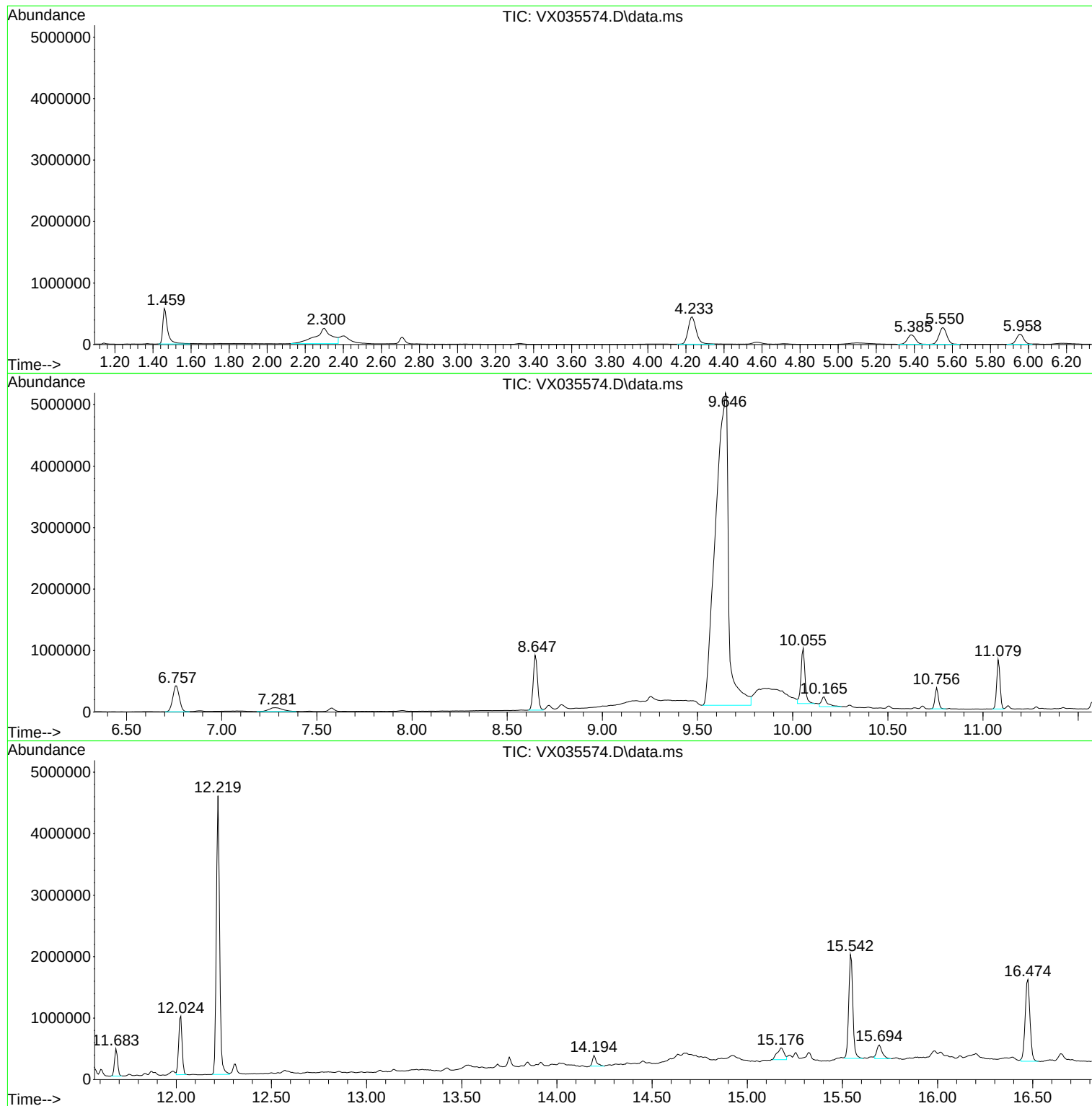
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Quant Title : SW846 8260

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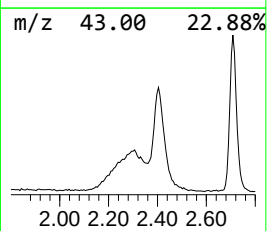
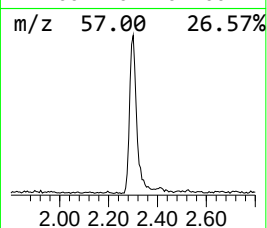
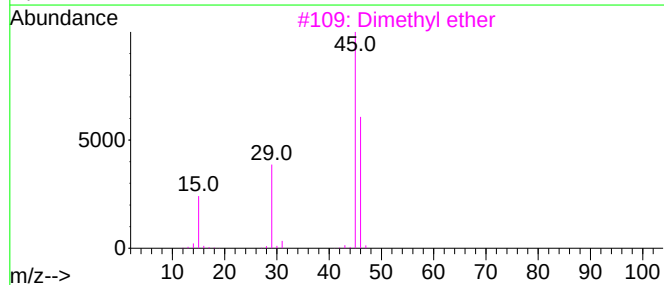
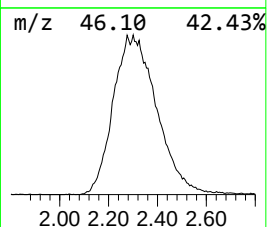
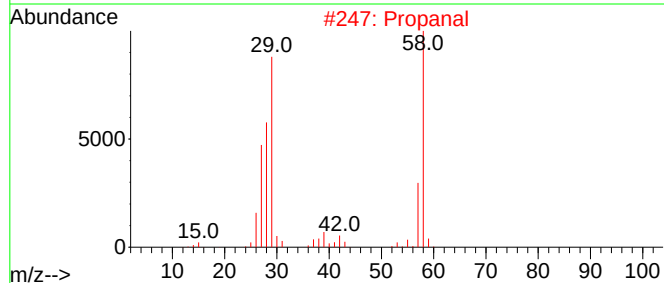
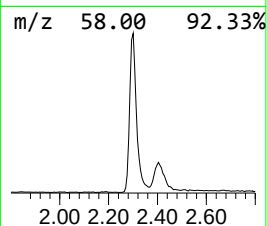
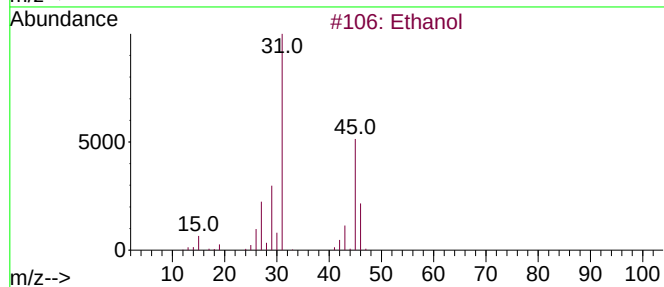
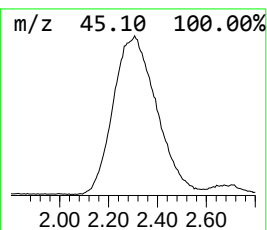
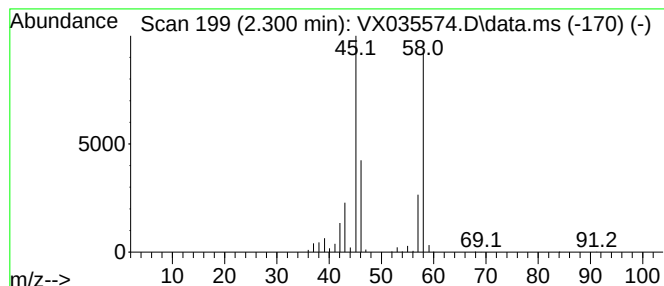
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Quant Title : SW846 8260

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

Peak Number 2 unknown2.300 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	95.15 ug/l	1471170	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	37
2			Propanal	58	C3H6O	000123-38-6	27
3			Dimethyl ether	46	C2H6O	000115-10-6	9
4			Trimethylene oxide	58	C3H6O	000503-30-0	9
5			Propylene oxide	58	C3H6O	000075-56-9	9



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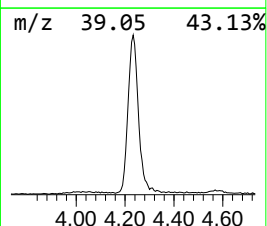
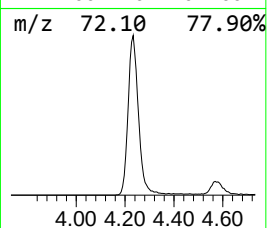
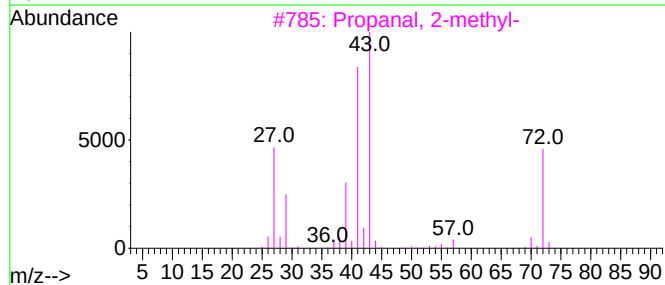
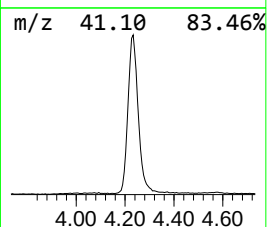
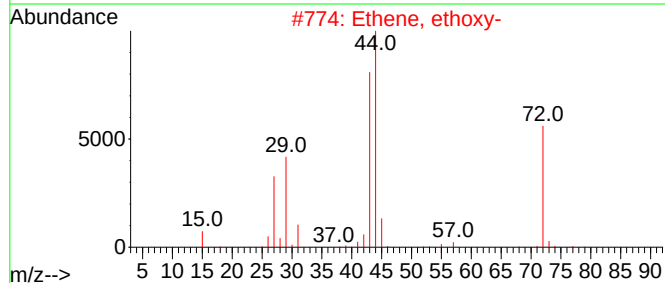
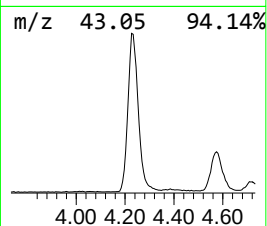
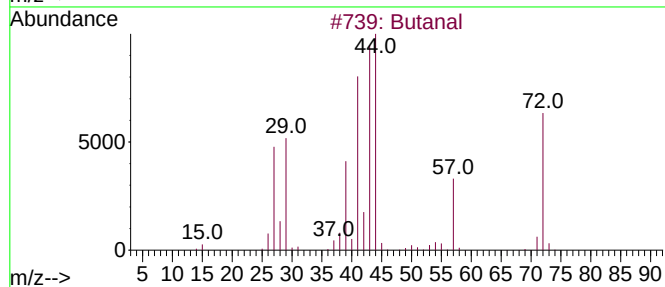
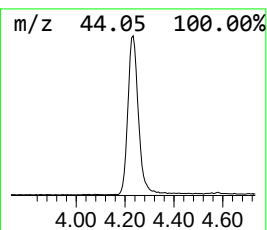
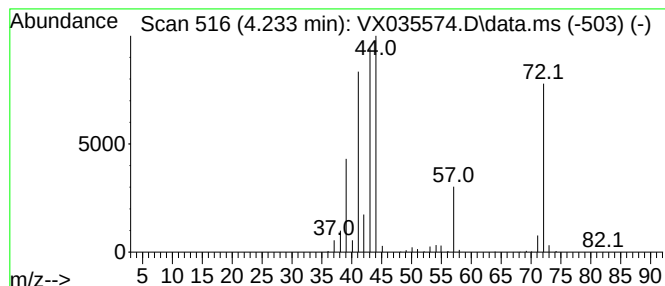
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	84.85 ug/l	1311900	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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Instrument :
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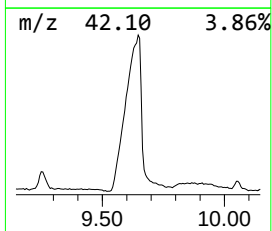
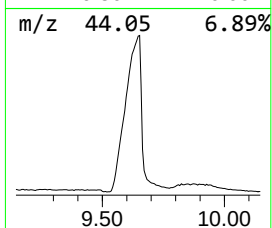
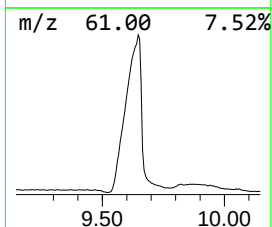
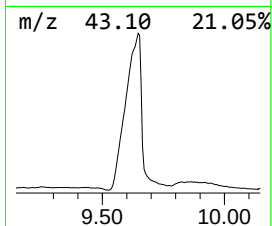
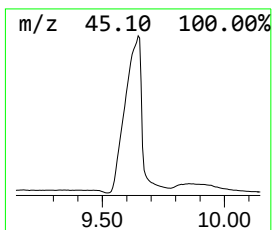
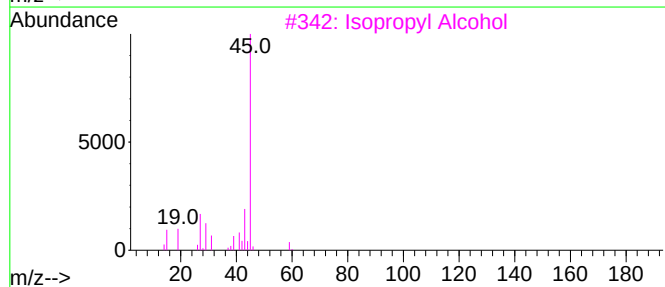
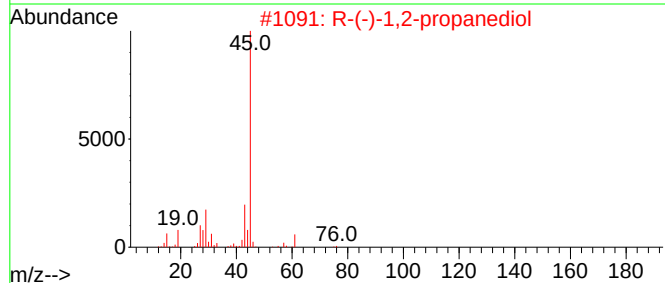
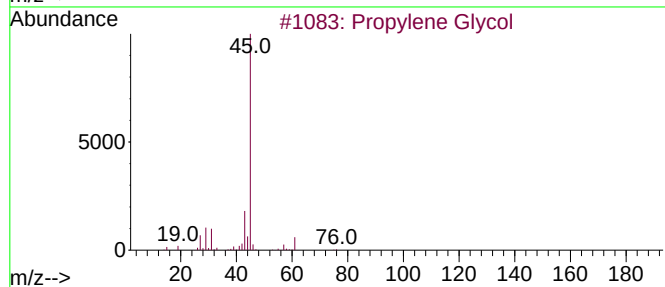
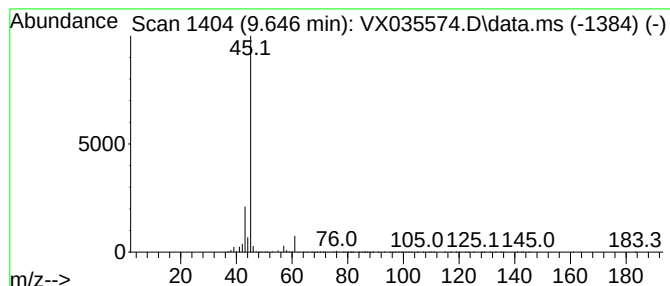
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Peak Number 4 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.646	912.28 ug/l	24303000	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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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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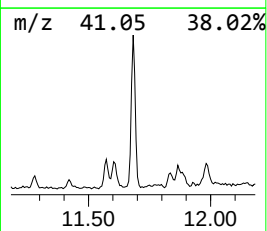
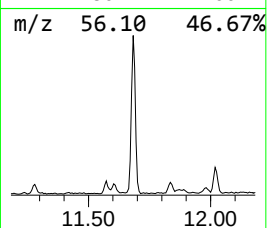
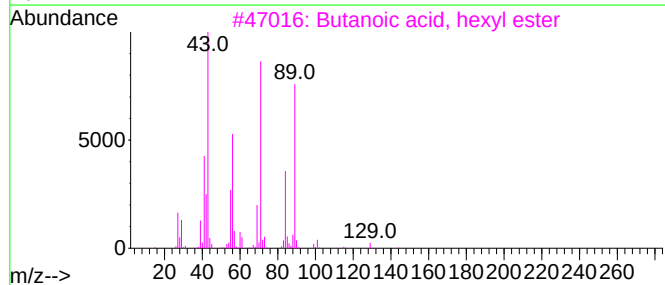
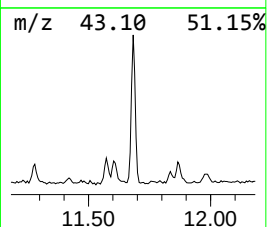
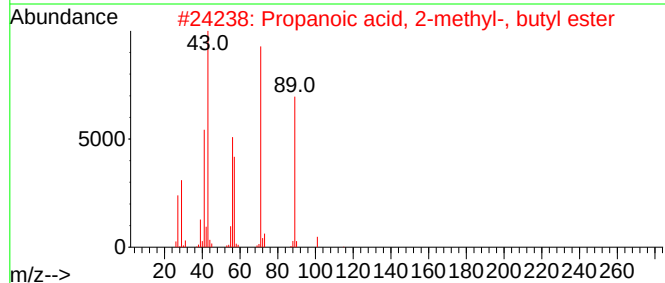
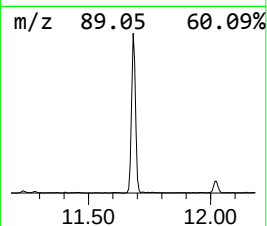
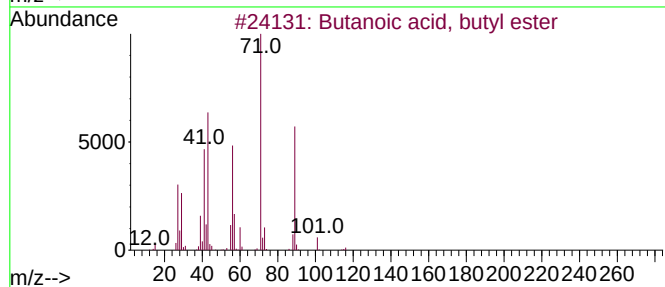
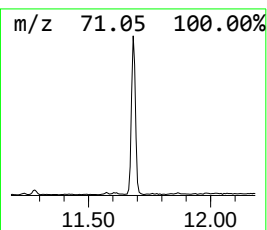
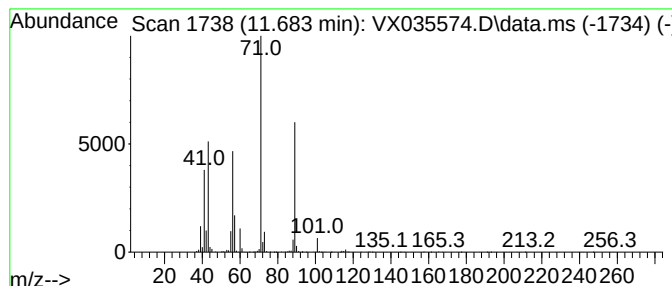
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Quant Title : SW846 8260

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Peak Number 5 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	21.17 ug/l	502074	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	78
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64



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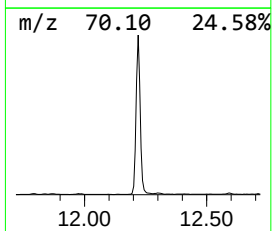
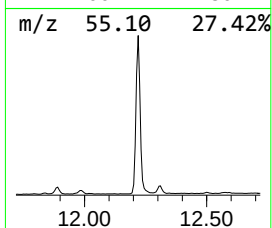
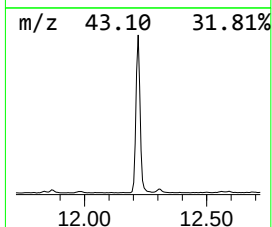
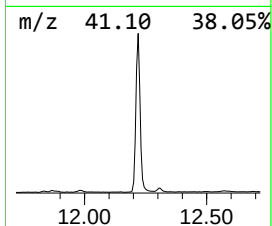
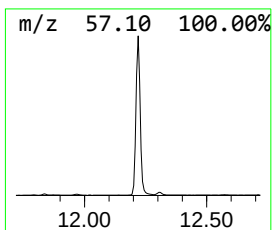
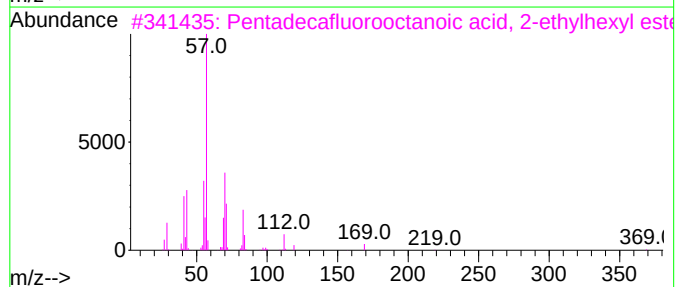
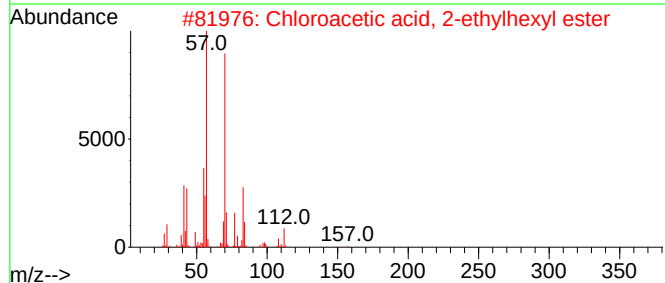
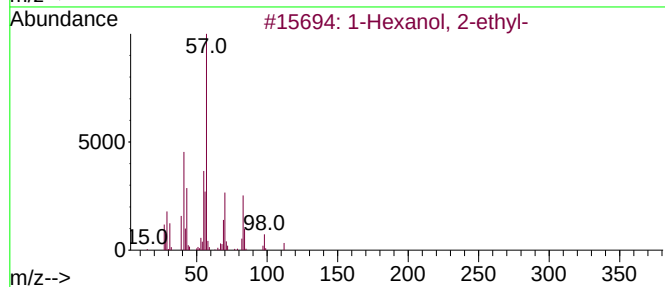
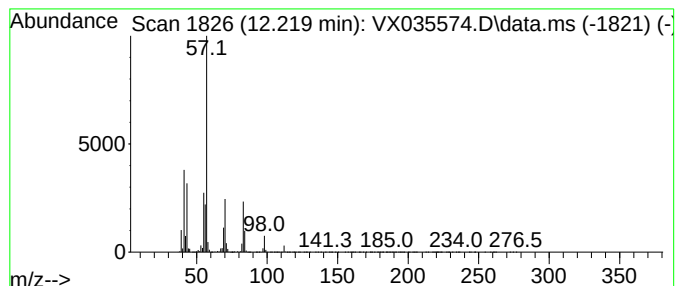
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	229.17 ug/l	5435080	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	Chloroacetic acid, 2-ethylhexyl ...			206	C10H19ClO2	005345-58-4	59
3	Pentadecafluorooctanoic acid, 2-...			526	C16H17F15O2	1000406-80-9	59
4	1-Decene, 2,4-dimethyl-			168	C12H24	055170-80-4	53
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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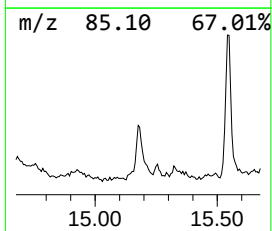
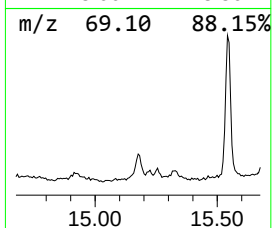
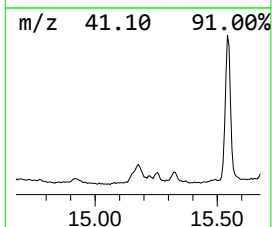
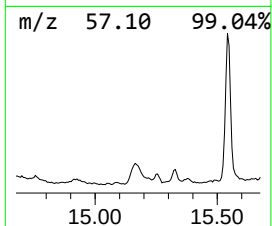
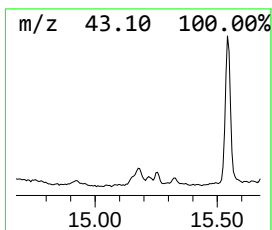
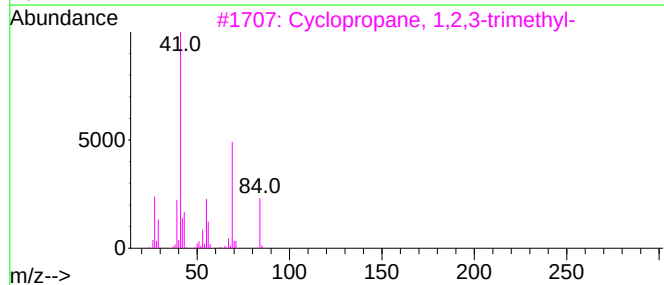
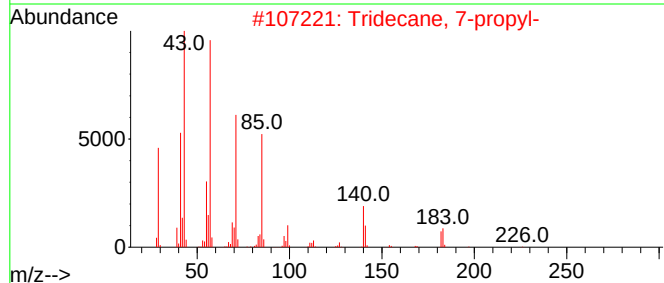
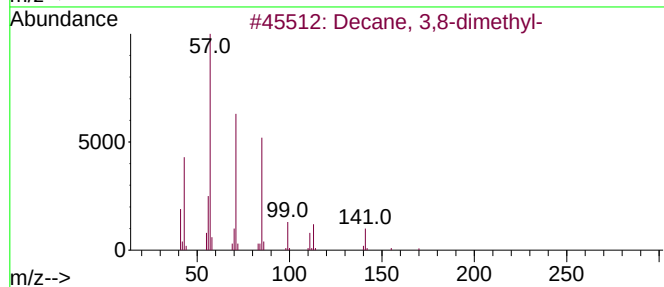
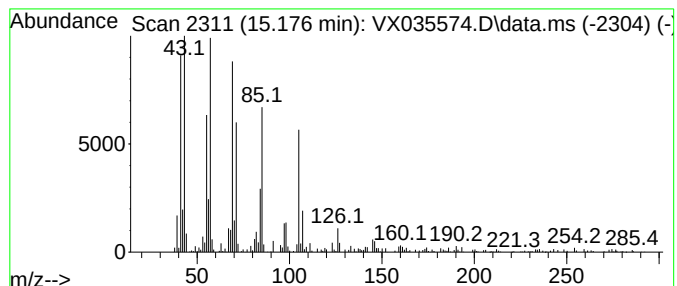
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.176 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.176	20.49 ug/l	486058	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	41
2			Tridecane, 7-propyl-	226	C16H34	055045-09-5	41
3			Cyclopropane, 1,2,3-trimethyl-	84	C6H12	042984-19-0	38
4			2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	38
5			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035574.D
Acq On : 08 May 2023 20:42
Operator : JC/MD
Sample : 02648-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1637

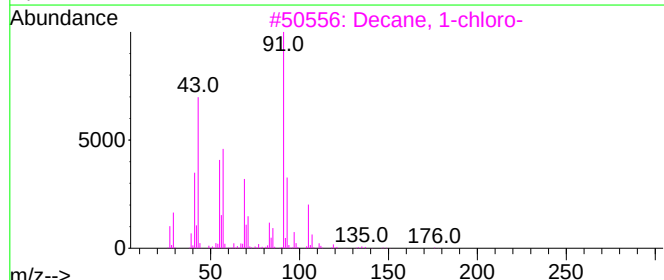
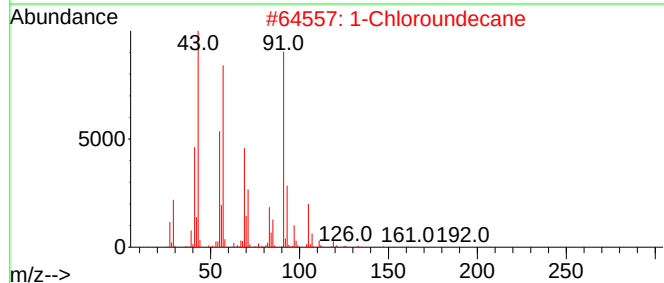
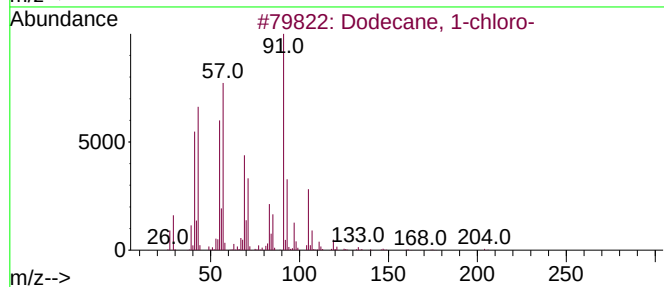
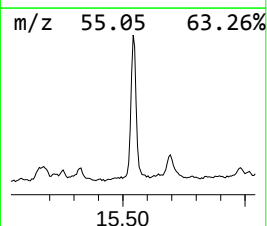
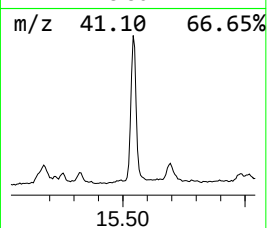
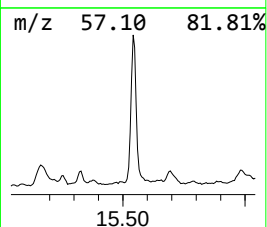
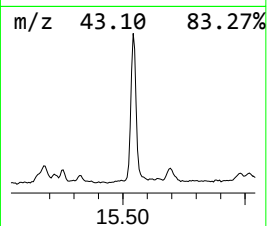
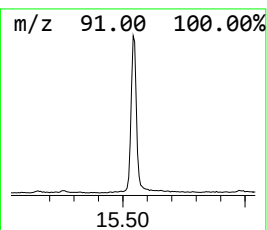
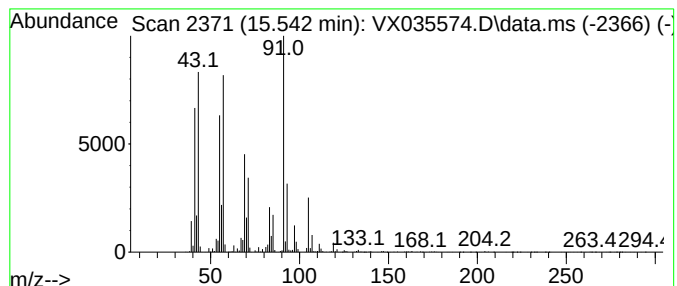
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	106.74 ug/l	2531510	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	97
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	91
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	76
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	58
5			Nonane, 1-chloro-	162	C9H19Cl	002473-01-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035574.D
Acq On : 08 May 2023 20:42
Operator : JC/MD
Sample : 02648-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1637

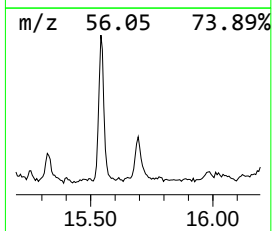
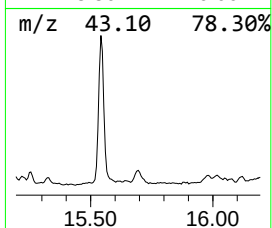
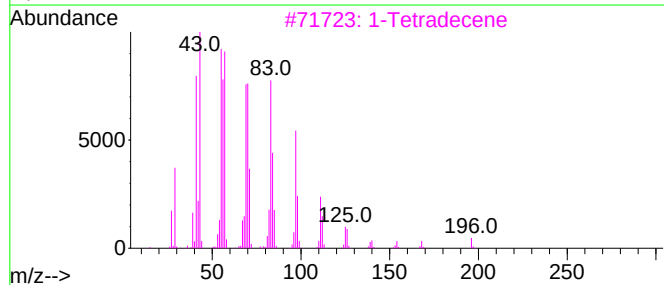
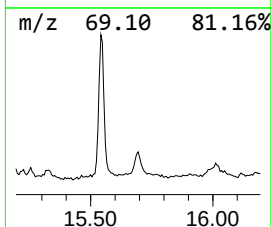
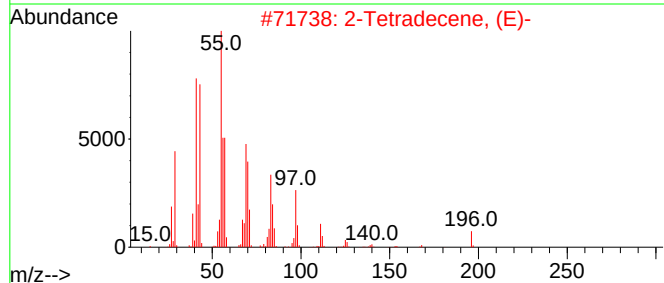
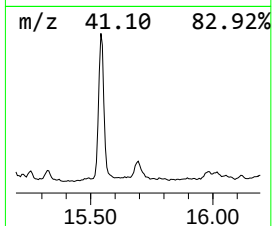
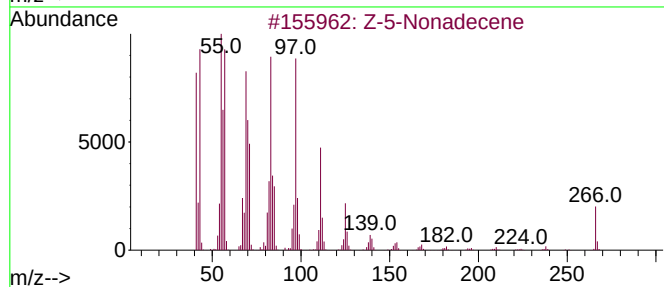
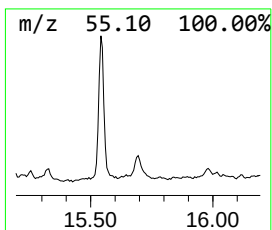
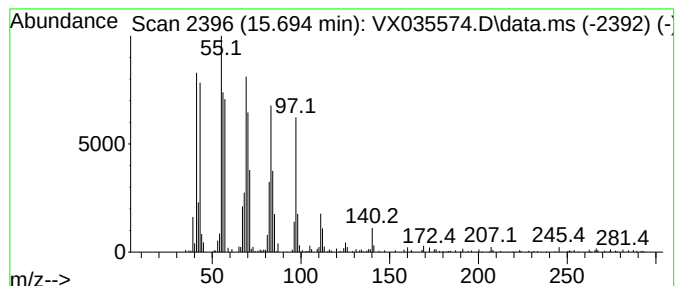
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Quant Title : SW846 8260

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

Peak Number 9 Z-5-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.694	18.45 ug/l	437662	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Z-5-Nonadecene	266	C19H38	1000131-11-8	94
2		2-Tetradecene, (E)-	196	C14H28	035953-54-9	93
3		1-Tetradecene	196	C14H28	001120-36-1	91
4		3-Hexadecene, (Z)-	224	C16H32	034303-81-6	91
5		7-Hexadecene, (Z)-	224	C16H32	035507-09-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035574.D
Acq On : 08 May 2023 20:42
Operator : JC/MD
Sample : 02648-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1637

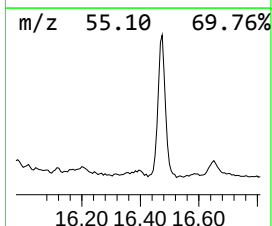
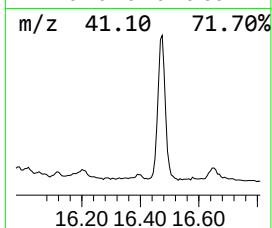
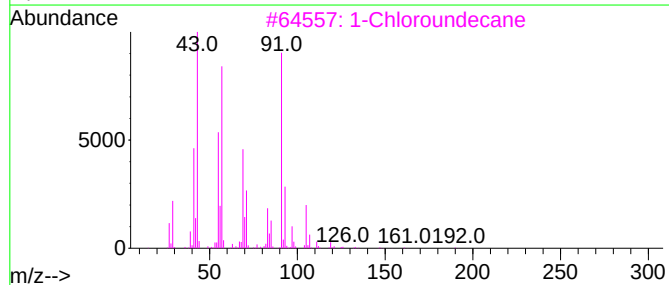
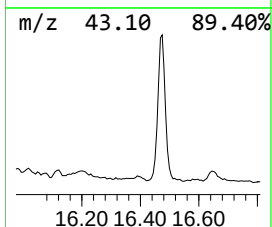
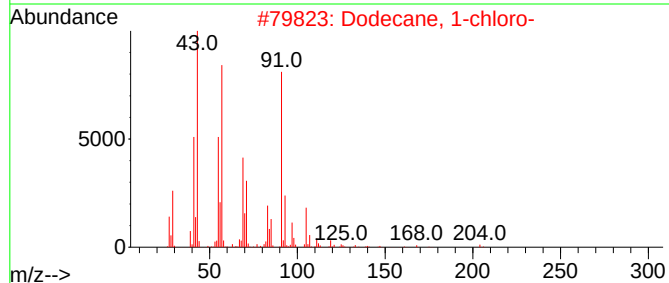
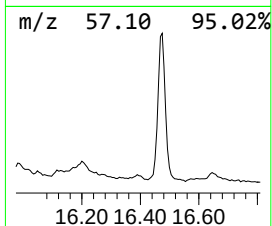
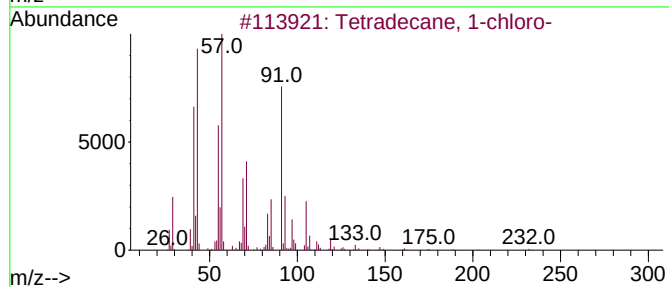
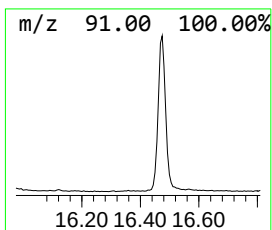
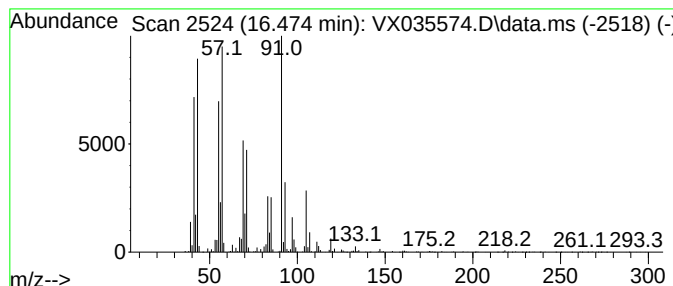
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.474	97.81 ug/l	2319740	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	91
2			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
3			1-Chloroundecane	190	C11H23Cl	002473-03-2	80
4			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	55
5			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035574.D
Acq On : 08 May 2023 20:42
Operator : JC/MD
Sample : 02648-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1637

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
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Butanal	4.233	84.8	ug/l	1311900	1	5.550	773093	50.0
Propylene Glycol	9.646	912.3	ug/l	24303000	3	10.055	1331990	50.0
Butanoic acid, ...	11.683	21.2	ug/l	502074	4	12.024	1185830	50.0
1-Hexanol, 2-et...	12.219	229.2	ug/l	5435080	4	12.024	1185830	50.0
unknown15.176	15.176	20.5	ug/l	486058	4	12.024	1185830	50.0
Dodecane, 1-chl...	15.542	106.7	ug/l	2531510	4	12.024	1185830	50.0
Z-5-Nonadecene	15.694	18.4	ug/l	437662	4	12.024	1185830	50.0
Tetradecane, 1-...	16.474	97.8	ug/l	2319740	4	12.024	1185830	50.0