

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080525\
 Data File : VX047234.D
 Acq On : 05 Aug 2025 14:02
 Operator : JC/MD
 Sample : Q2759-04 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 LIQUID-DRUMS

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\82X072125W.M
 Title : SW846 8260

Signal : TIC: VX047234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.063	153	160	188	rBV	163825	554884	2.26%	1.079%
2	5.397	693	707	724	rBV3	232634	724610	2.95%	1.409%
3	5.562	724	734	758	rVB	388139	1183459	4.82%	2.302%
4	5.964	790	800	829	rBV	240238	695053	2.83%	1.352%
5	6.769	922	932	953	rBV	661081	1700610	6.93%	3.307%
6	8.647	1234	1240	1250	rBV	1311918	2137161	8.71%	4.156%
7	10.055	1465	1471	1487	rVB	1537548	2154843	8.78%	4.191%
8	11.079	1633	1639	1650	rVB	1323135	1720273	7.01%	3.346%
9	11.476	1701	1704	1709	rVB	313931	373992	1.52%	0.727%
10	11.750	1745	1749	1759	rVB	386589	532799	2.17%	1.036%
11	12.018	1788	1793	1799	rBV	1738496	2236885	9.12%	4.350%
12	12.085	1799	1804	1810	rVB3	173465	369605	1.51%	0.719%
13	12.311	1837	1841	1848	rVB3	277058	492015	2.01%	0.957%
14	12.421	1848	1859	1863	rVV	739914	912177	3.72%	1.774%
15	12.585	1881	1886	1899	rVB	19740207	24528853	100.00%	47.705%
16	12.963	1943	1948	1954	rVB3	283758	527265	2.15%	1.025%
17	13.164	1974	1981	1985	rVB4	197473	373895	1.52%	0.727%
18	13.262	1991	1997	1999	rBV	637851	826459	3.37%	1.607%
19	13.286	1999	2001	2006	rVB3	511056	676641	2.76%	1.316%
20	13.420	2019	2023	2032	rVB3	971458	1427236	5.82%	2.776%
21	13.579	2045	2049	2055	rBV4	290871	469354	1.91%	0.913%
22	13.664	2060	2063	2070	rBV5	111084	249622	1.02%	0.485%
23	13.847	2087	2093	2098	rBV4	297675	532168	2.17%	1.035%
24	13.920	2098	2105	2110	rVB6	230086	507537	2.07%	0.987%
25	14.036	2120	2124	2127	rVB	366589	382922	1.56%	0.745%
26	14.189	2145	2149	2153	rBV	1843931	2427097	9.89%	4.720%
27	14.475	2193	2196	2205	rVB3	302801	551763	2.25%	1.073%
28	14.609	2215	2218	2220	rBV	468406	593683	2.42%	1.155%
29	14.634	2220	2222	2225	rVV	549650	584639	2.38%	1.137%
30	14.670	2225	2228	2232	rVB3	219256	279400	1.14%	0.543%
31	14.774	2243	2245	2250	rVB	231051	302911	1.23%	0.589%
32	15.475	2356	2360	2372	rVV4	177520	387515	1.58%	0.754%

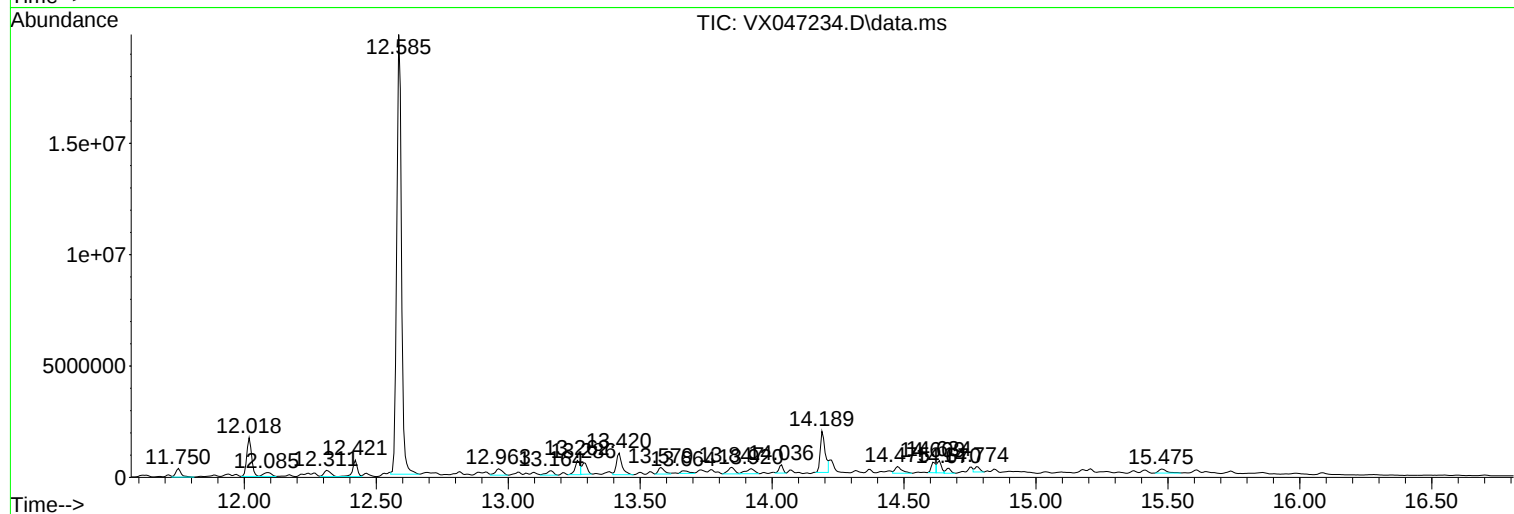
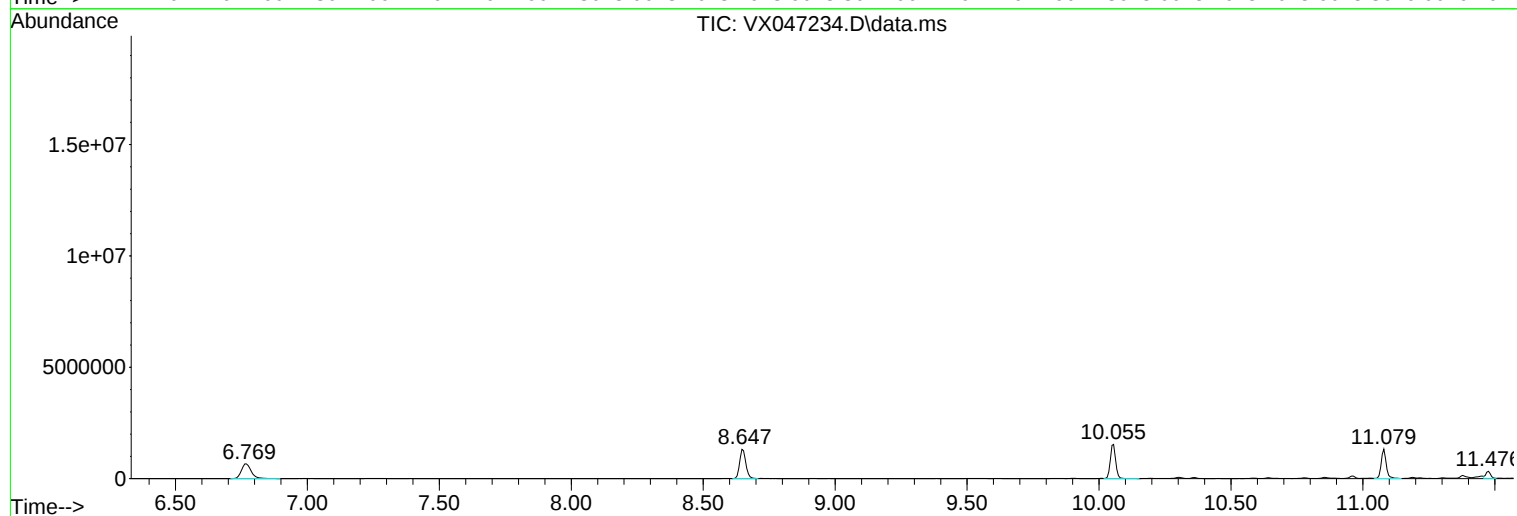
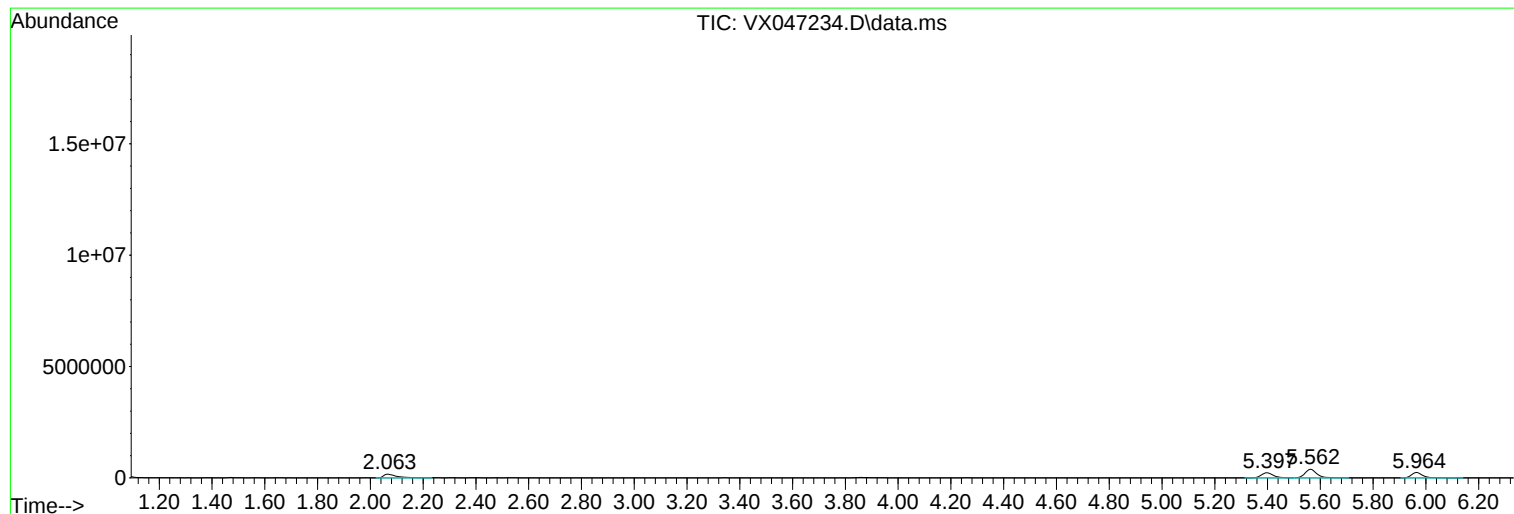
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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



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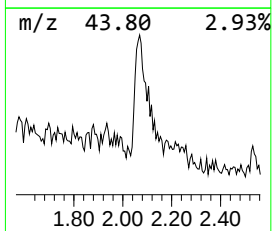
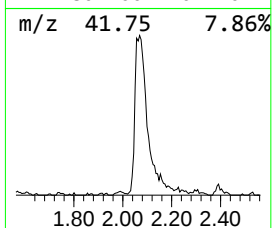
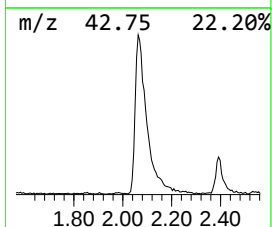
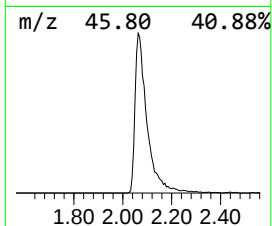
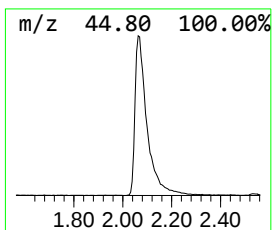
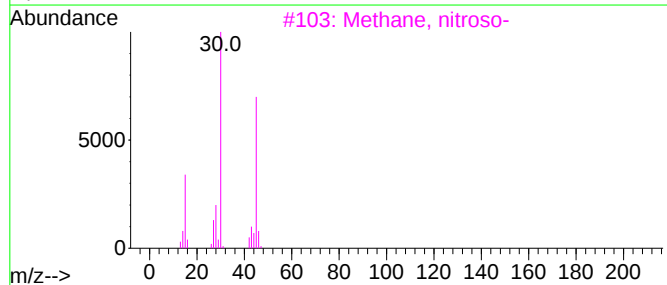
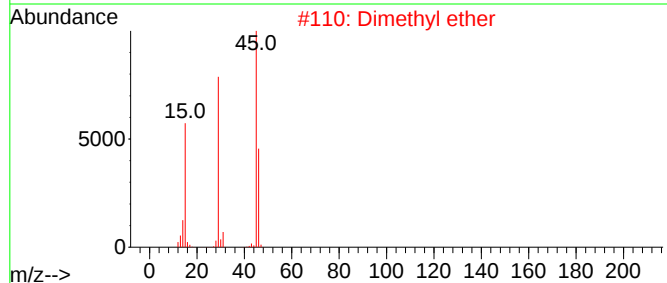
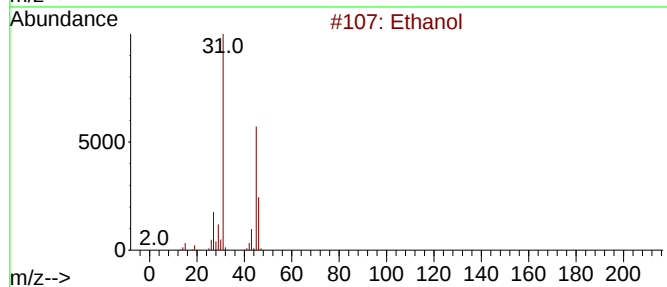
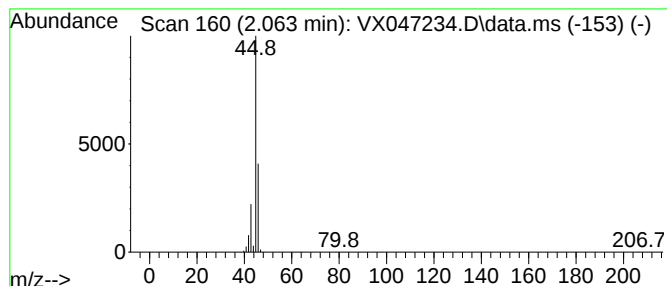
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	23.44 ug/l	554884	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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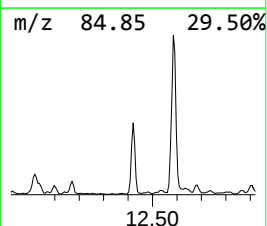
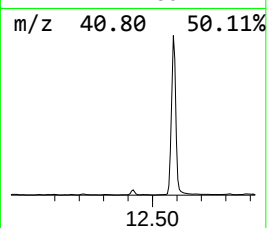
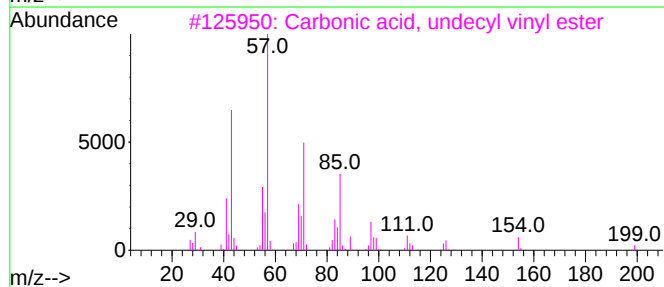
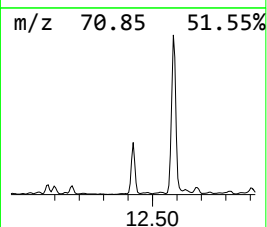
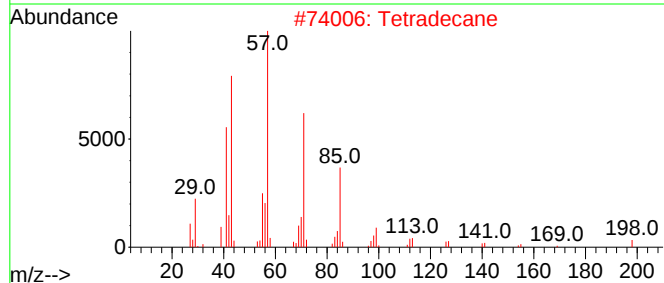
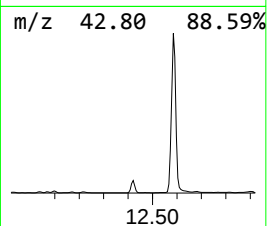
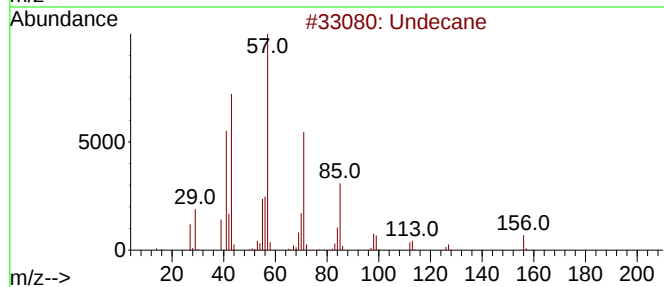
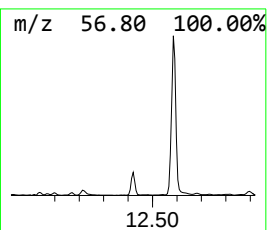
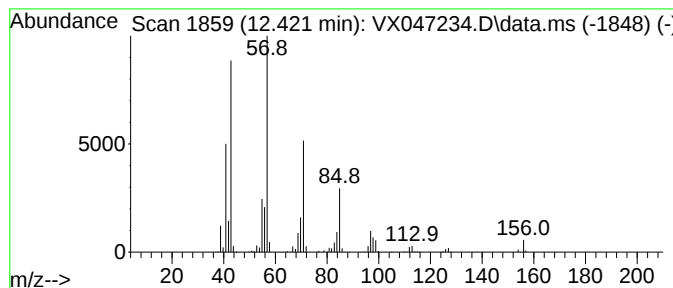
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	20.39 ug/l	912177	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Tetradecane			198	C14H30	000629-59-4	86
3	Carbonic acid, undecyl vinyl ester			242	C14H26O3	1000382-54-9	83
4	Hexadecane			226	C16H34	000544-76-3	72
5	Tridecane			184	C13H28	000629-50-5	59



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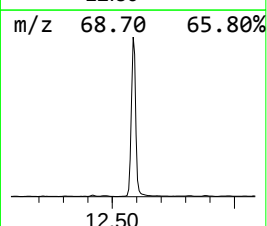
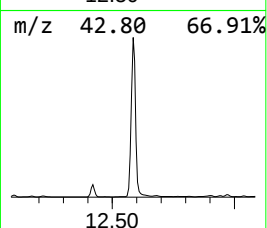
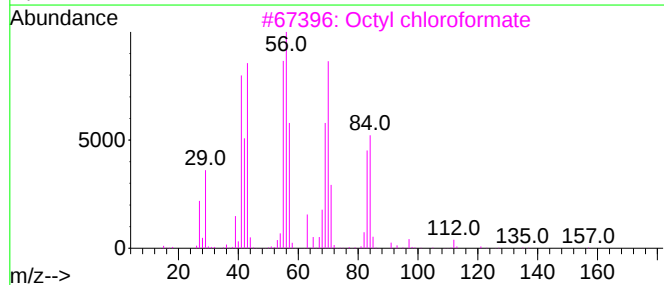
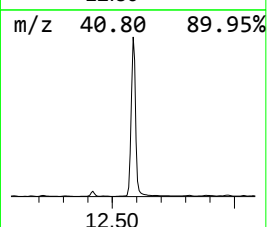
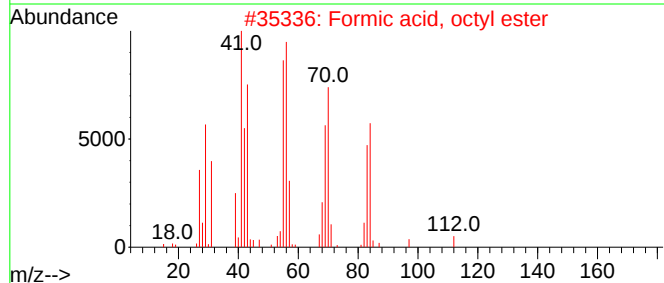
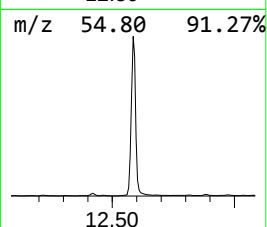
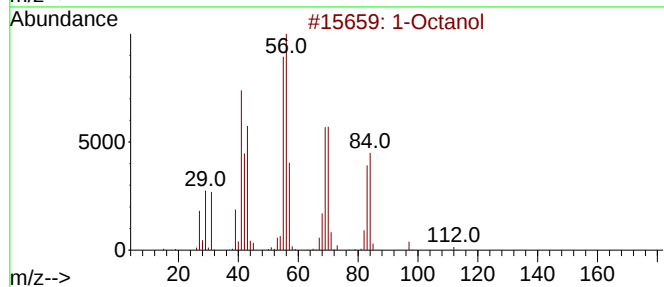
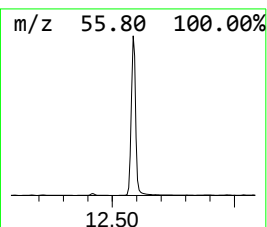
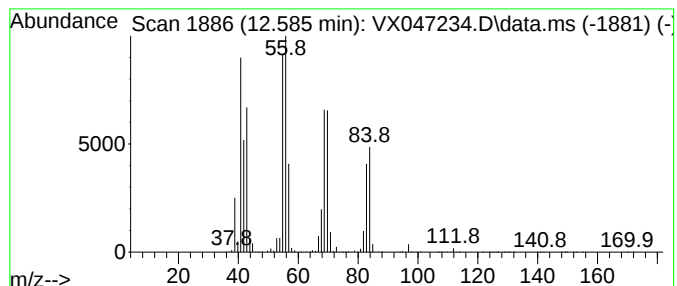
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	548.28 ug/l	24528900	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			Octyl chloroformate	192	C9H17ClO2	007452-59-7	78
4			1-Nonanol	144	C9H20O	000143-08-8	72
5			Chloromethyl octyl ether	178	C9H19ClO	024566-90-3	53



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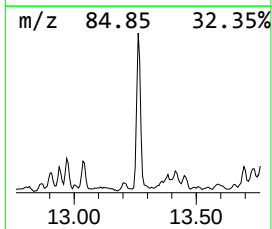
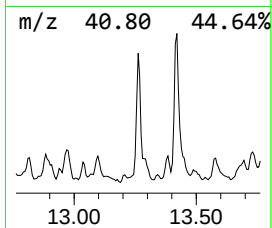
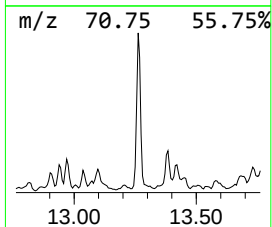
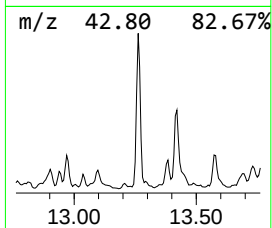
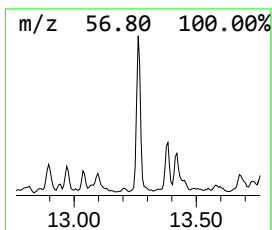
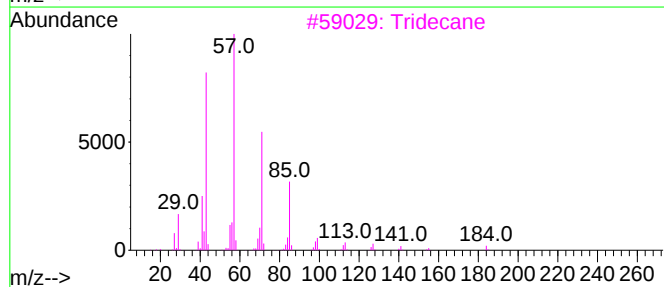
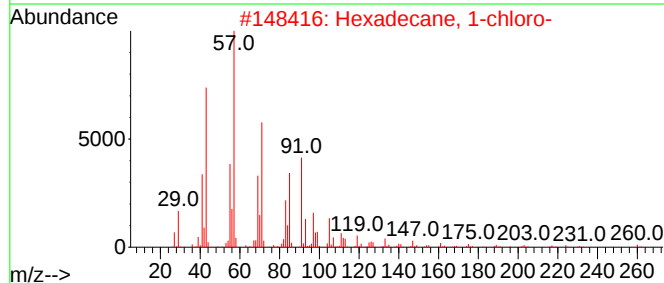
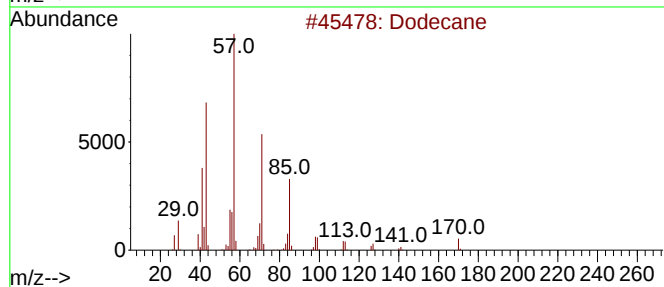
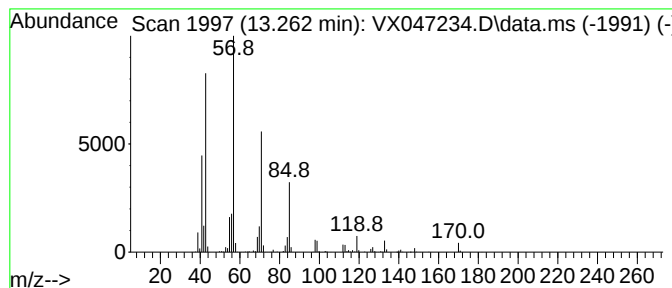
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Quant Title : SW846 8260

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

Peak Number 4 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.262	18.47 ug/l	826459	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	83
3			Tridecane	184	C13H28	000629-50-5	80
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	80
5			Tetradecane	198	C14H30	000629-59-4	80



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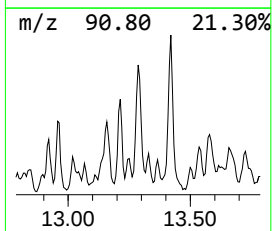
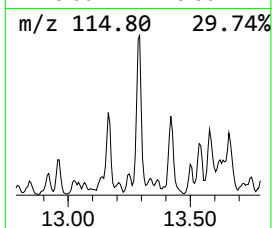
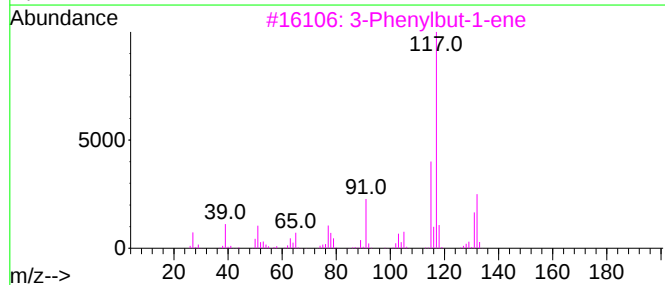
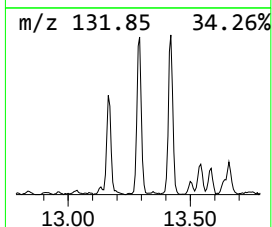
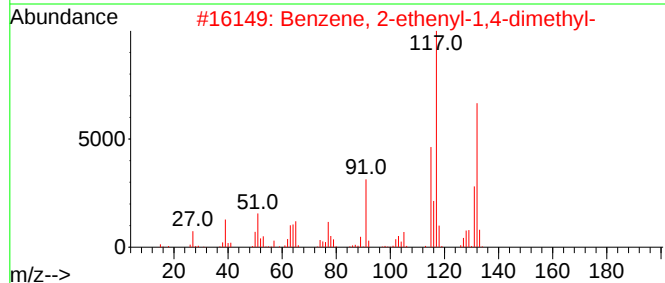
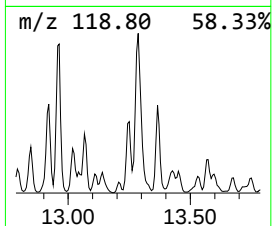
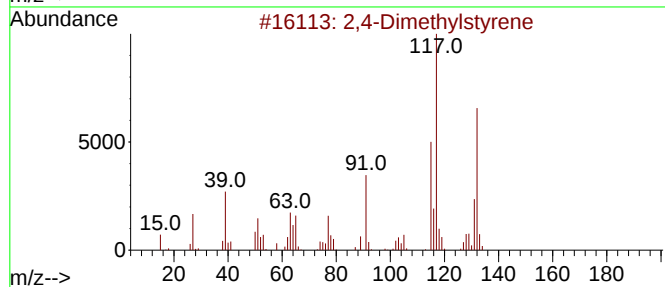
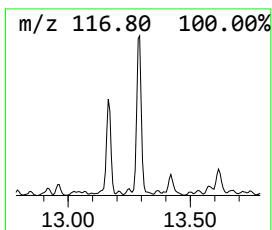
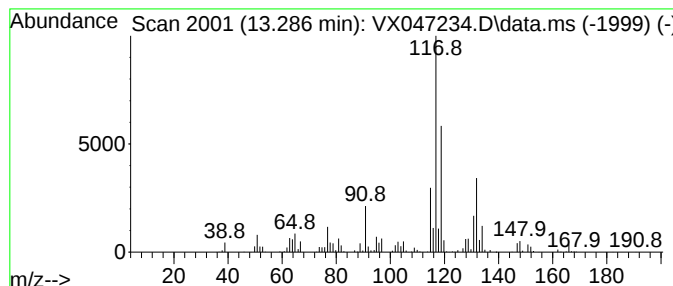
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 5 2,4-Dimethylstyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	15.12 ug/l	676641	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	93
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	86
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86



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LIQUID-DRUMS

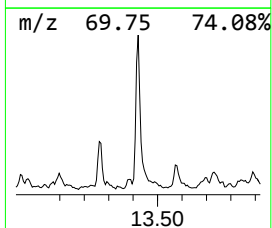
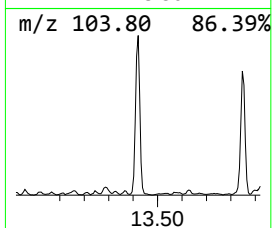
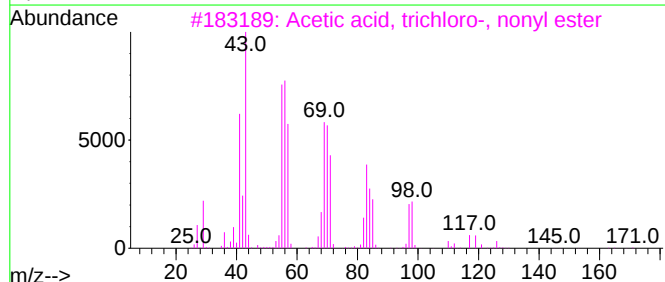
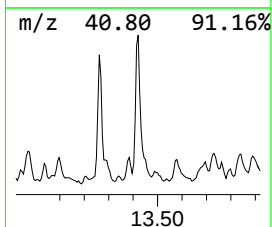
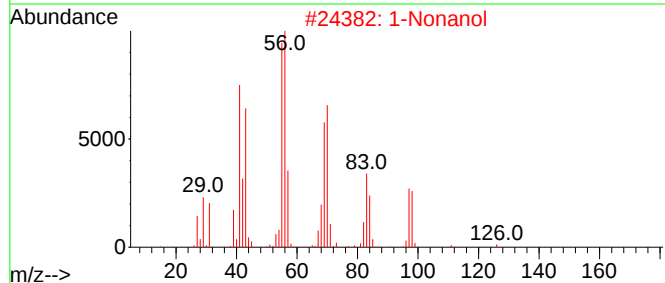
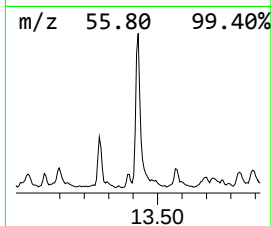
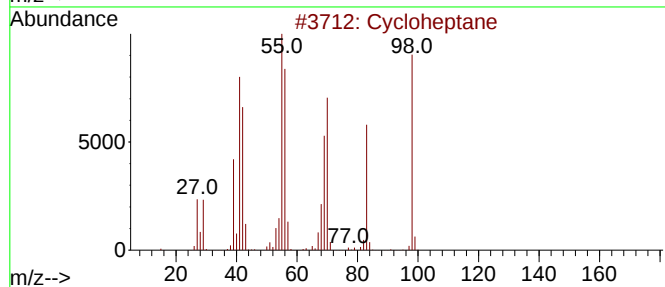
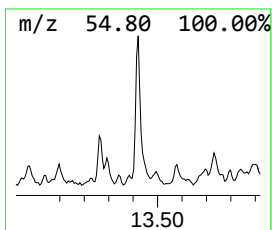
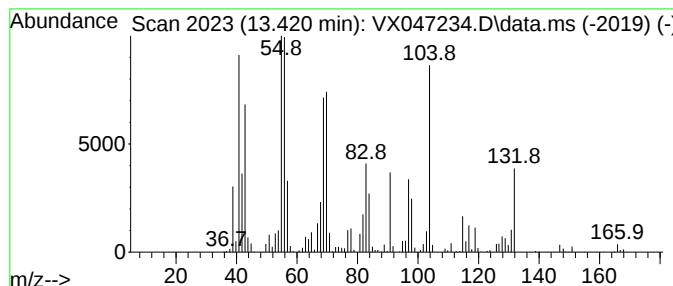
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Quant Title : SW846 8260

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

Peak Number 6 Cycloheptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	31.90 ug/l	1427240	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane	98	C7H14	000291-64-5	70
2			1-Nonanol	144	C9H20O	000143-08-8	58
3			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	52
4			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	50
5			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080525\
Data File : VX047234.D
Acq On : 05 Aug 2025 14:02
Operator : JC/MD
Sample : Q2759-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LIQUID-DRUMS

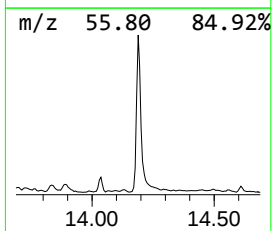
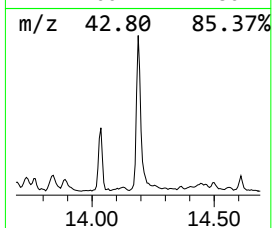
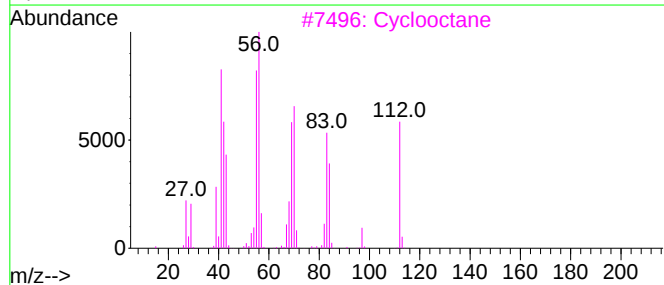
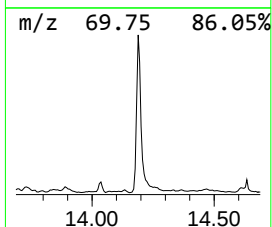
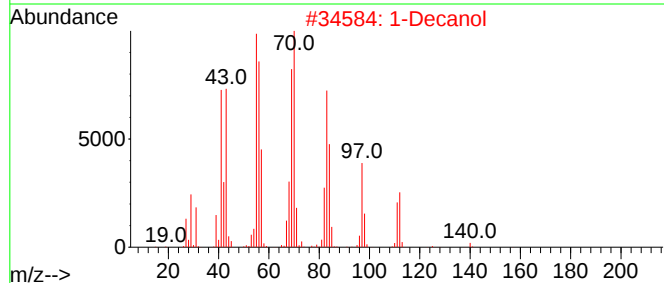
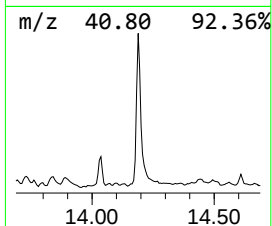
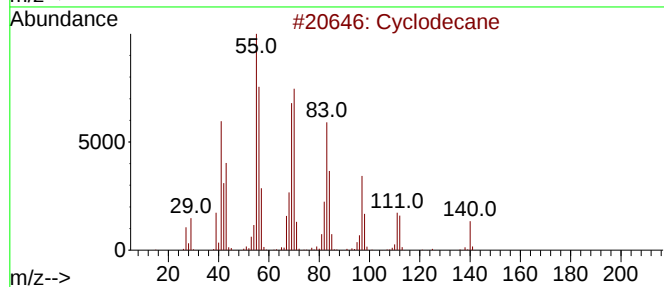
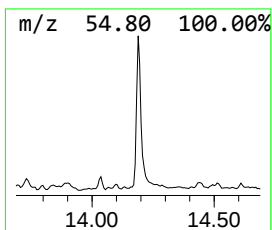
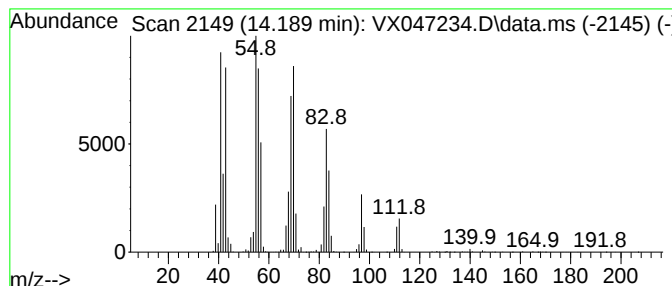
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Quant Title : SW846 8260

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

Peak Number 7 Cyclodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.189	54.25 ug/l	2427100	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecane	140	C10H20	000293-96-9	94
2			1-Decanol	158	C10H22O	000112-30-1	91
3			Cyclooctane	112	C8H16	000292-64-8	87
4			Formic acid, decyl ester	186	C11H22O2	005451-52-5	86
5			1-Dodecanol	186	C12H26O	000112-53-8	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080525\
Data File : VX047234.D
Acq On : 05 Aug 2025 14:02
Operator : JC/MD
Sample : Q2759-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

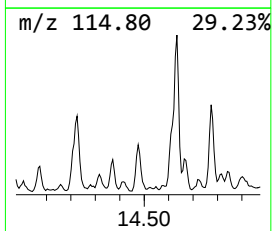
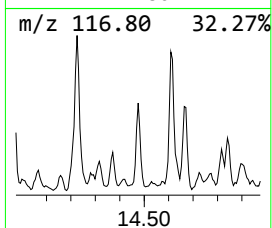
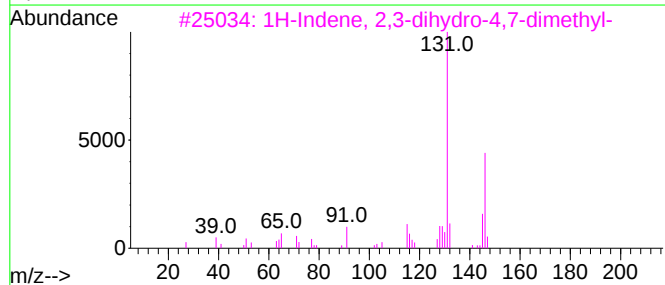
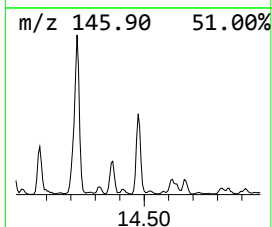
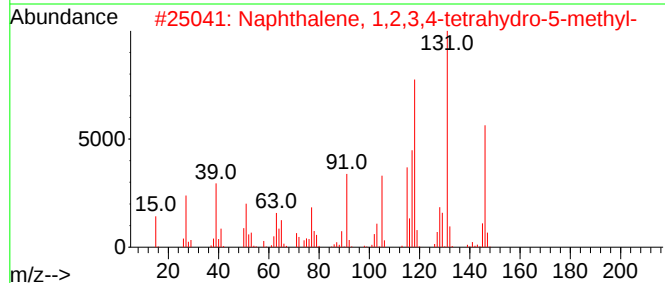
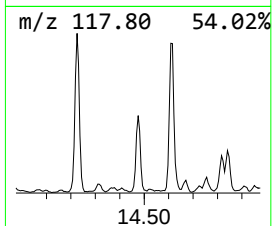
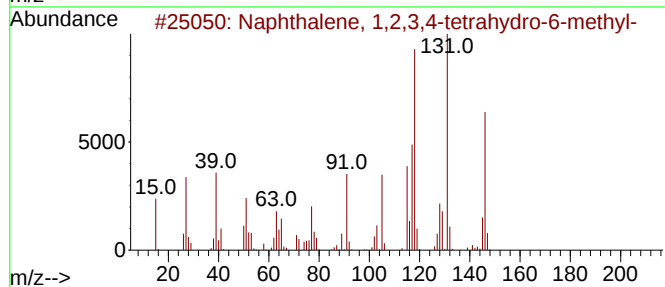
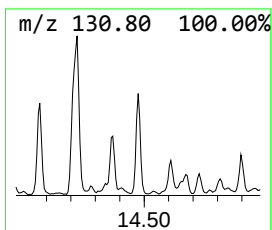
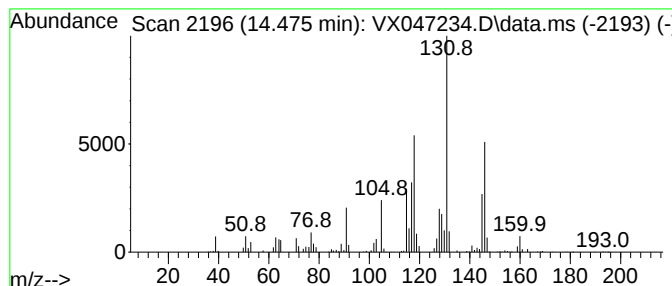
Instrument :
MSVOA_X
ClientSampleId :
LIQUID-DRUMS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.475	12.33 ug/l	551763	1,4-Dichlorobenzene-d4		12.018	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001680-51-9	94
2	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	002809-64-5	94
3	1H-Indene, 2,3-dihydro-4,7-dimet...		146	C11H14	006682-71-9	64
4	1H-1,3,2-Benzodiazaborole, 2-eth...		146	C8H11BN2	074663-81-3	62
5	2-Propenal, 3-(4-methylphenyl)-		146	C10H10O	001504-75-2	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080525\
Data File : VX047234.D
Acq On : 05 Aug 2025 14:02
Operator : JC/MD
Sample : Q2759-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LIQUID-DRUMS

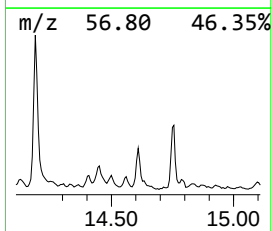
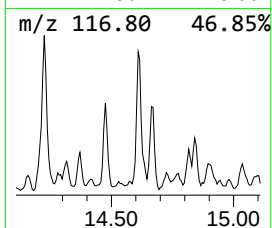
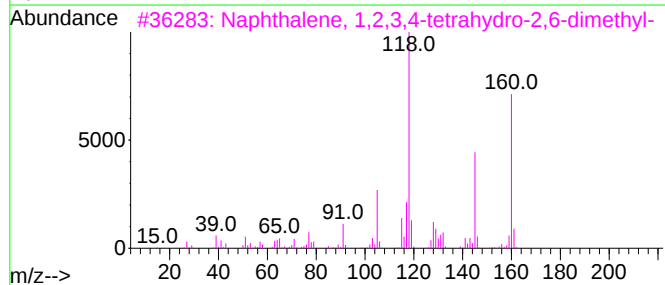
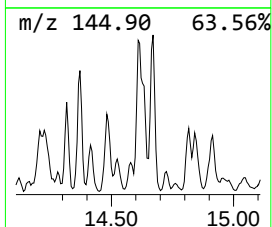
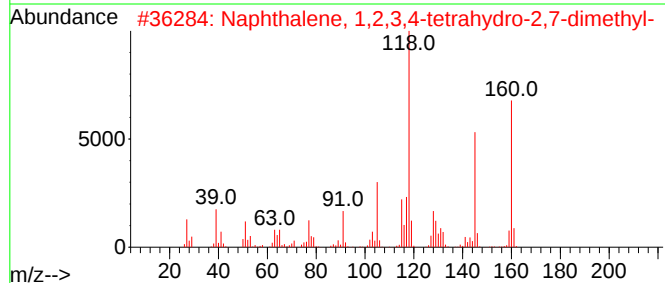
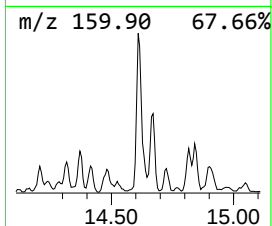
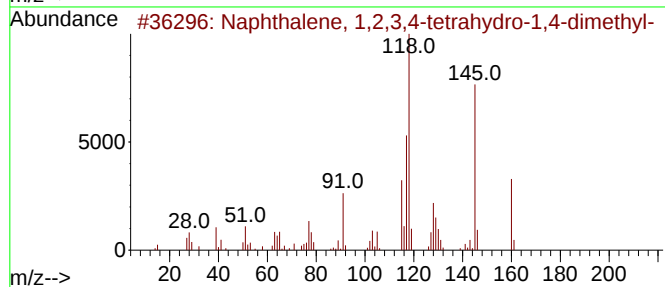
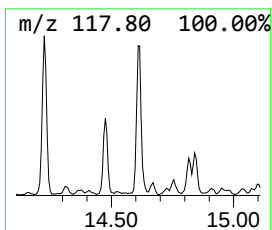
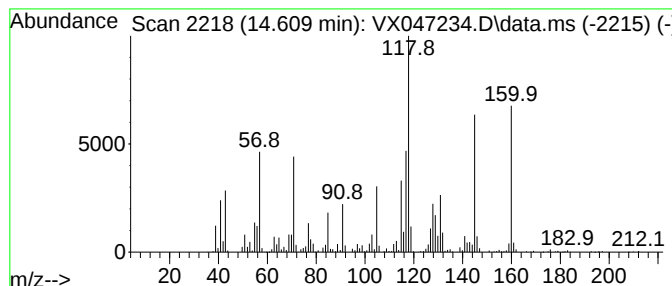
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.609	13.27 ug/l	593683	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	86
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	83
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	58
4			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	46
5			Azetidine, 3-methyl-3-phenyl-	147	C10H13N	005961-33-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080525\
Data File : VX047234.D
Acq On : 05 Aug 2025 14:02
Operator : JC/MD
Sample : Q2759-04 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LIQUID-DRUMS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.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
Ethanol	2.063	23.4	ug/l	554884	1	5.562	1183460	50.0
Undecane	12.421	20.4	ug/l	912177	4	12.018	2236890	50.0
1-Octanol	12.585	548.3	ug/l	24528900	4	12.018	2236890	50.0
Dodecane	13.262	18.5	ug/l	826459	4	12.018	2236890	50.0
2,4-Dimethylsty...	13.286	15.1	ug/l	676641	4	12.018	2236890	50.0
Cycloheptane	13.420	31.9	ug/l	1427240	4	12.018	2236890	50.0
Cyclodecane	14.189	54.3	ug/l	2427100	4	12.018	2236890	50.0
Naphthalene, 1,...	14.475	12.3	ug/l	551763	4	12.018	2236890	50.0
Naphthalene, 1,...	14.609	13.3	ug/l	593683	4	12.018	2236890	50.0