

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
 Data File : VX033296.D
 Acq On : 07 Dec 2022 21:05
 Operator : JC/MD
 Sample : N5912-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FMC-TOTE-1207

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\82X120722W.M
 Title : SW846 8260

Signal : TIC: VX033296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.294	23	34	41	rBV2	8817	25895	1.04%	0.153%
2	2.142	158	173	193	rVB2	11317	61011	2.45%	0.361%
3	2.386	206	213	230	rBV	1397607	2485359	100.00%	14.725%
4	2.575	231	244	263	rBV	265754	1084678	43.64%	6.426%
5	4.227	506	515	531	rBV2	8987	26854	1.08%	0.159%
6	4.562	562	570	584	rBV	25578	74548	3.00%	0.442%
7	5.099	635	658	673	rBV	26398	93416	3.76%	0.553%
8	5.385	695	705	719	rBV	56064	162755	6.55%	0.964%
9	5.556	722	733	747	rVB	142669	405397	16.31%	2.402%
10	5.958	787	799	810	rBV2	43422	118359	4.76%	0.701%
11	6.763	921	931	950	rVB	214735	505138	20.32%	2.993%
12	7.232	1000	1008	1028	rBV2	56298	181165	7.29%	1.073%
13	7.458	1040	1045	1055	rVB	13641	27769	1.12%	0.165%
14	8.055	1136	1143	1153	rBV2	26226	47637	1.92%	0.282%
15	8.574	1222	1228	1235	rBV	44304	75149	3.02%	0.445%
16	8.647	1235	1240	1247	rVV	168167	265883	10.70%	1.575%
17	8.720	1247	1252	1257	rBV	83573	125606	5.05%	0.744%
18	9.244	1331	1338	1347	rBV	116462	189820	7.64%	1.125%
19	9.433	1363	1369	1380	rBV2	13695	27324	1.10%	0.162%
20	10.055	1460	1471	1489	rBV	444938	613066	24.67%	3.632%
21	10.195	1489	1494	1499	rBV2	33446	50883	2.05%	0.301%
22	10.299	1506	1511	1518	rVB	183053	241460	9.72%	1.431%
23	10.543	1547	1551	1556	rVB	53981	72124	2.90%	0.427%
24	10.640	1562	1567	1572	rBV	126837	164583	6.62%	0.975%
25	11.079	1634	1639	1645	rVV	316219	400403	16.11%	2.372%
26	11.286	1668	1673	1681	rBV2	82771	148537	5.98%	0.880%
27	11.378	1681	1688	1695	rVV	114711	207440	8.35%	1.229%
28	11.451	1695	1700	1704	rVV	62627	87340	3.51%	0.517%
29	11.512	1704	1710	1717	rVV6	29152	63679	2.56%	0.377%
30	11.610	1721	1726	1732	rVB	73279	108558	4.37%	0.643%
31	11.750	1744	1749	1759	rVB	183076	245597	9.88%	1.455%
32	11.975	1778	1786	1789	rBV	44908	59848	2.41%	0.355%
33	12.024	1789	1794	1800	rVB	477148	604948	24.34%	3.584%
34	12.103	1800	1807	1817	rBV2	730692	1063942	42.81%	6.303%
35	12.219	1821	1826	1828	rBV	262258	332841	13.39%	1.972%
36	12.244	1828	1830	1838	rVB2	131938	209166	8.42%	1.239%

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Integrator: RTE

Smoothing : ON

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.317	1838	1842	1849	rVB2	67701	108059	4.35%	0.640%
38	12.463	1862	1866	1872	rVB	30501	42405	1.71%	0.251%
39	12.530	1872	1877	1879	rBV	35911	50559	2.03%	0.300%
40	12.555	1879	1881	1884	rVB	33686	32900	1.32%	0.195%
41	12.615	1887	1891	1894	rVB	43367	47148	1.90%	0.279%
42	12.695	1900	1904	1912	rBV3	51718	84887	3.42%	0.503%
43	12.768	1912	1916	1918	rBV3	100078	144817	5.83%	0.858%
44	12.792	1918	1920	1926	rVB	119482	139258	5.60%	0.825%
45	12.859	1926	1931	1937	rBV2	539227	733762	29.52%	4.347%
46	12.920	1937	1941	1945	rVB4	49465	74016	2.98%	0.439%
47	12.969	1945	1949	1956	rBV2	234053	421735	16.97%	2.499%
48	13.073	1960	1966	1968	rBV2	186256	296955	11.95%	1.759%
49	13.103	1968	1971	1973	rVV2	584686	746714	30.04%	4.424%
50	13.128	1973	1975	1987	rVB4	420012	951810	38.30%	5.639%
51	13.219	1987	1990	1994	rBV3	70031	111696	4.49%	0.662%
52	13.292	1998	2002	2006	rVB2	143217	176224	7.09%	1.044%
53	13.335	2006	2009	2019	rVB3	201260	380983	15.33%	2.257%
54	13.426	2019	2024	2033	rBV2	154692	461813	18.58%	2.736%
55	13.512	2034	2038	2041	rBV	177960	249681	10.05%	1.479%
56	13.731	2071	2074	2078	rBV	210390	253865	10.21%	1.504%
57	14.231	2149	2156	2160	rBV2	126838	268792	10.82%	1.592%
58	14.371	2176	2179	2182	rVB2	23291	27209	1.09%	0.161%
59	14.408	2182	2185	2190	rVB2	21992	29060	1.17%	0.172%
60	14.481	2193	2197	2202	rBV2	65454	87924	3.54%	0.521%
61	14.633	2216	2222	2226	rVV2	58071	112741	4.54%	0.668%
62	14.780	2243	2246	2250	rVB	28395	30881	1.24%	0.183%
63	15.182	2308	2312	2315	rBV	20232	32345	1.30%	0.192%
64	15.615	2378	2383	2386	rVV	19373	33361	1.34%	0.198%
65	15.969	2435	2441	2453	rBV2	41622	89274	3.59%	0.529%

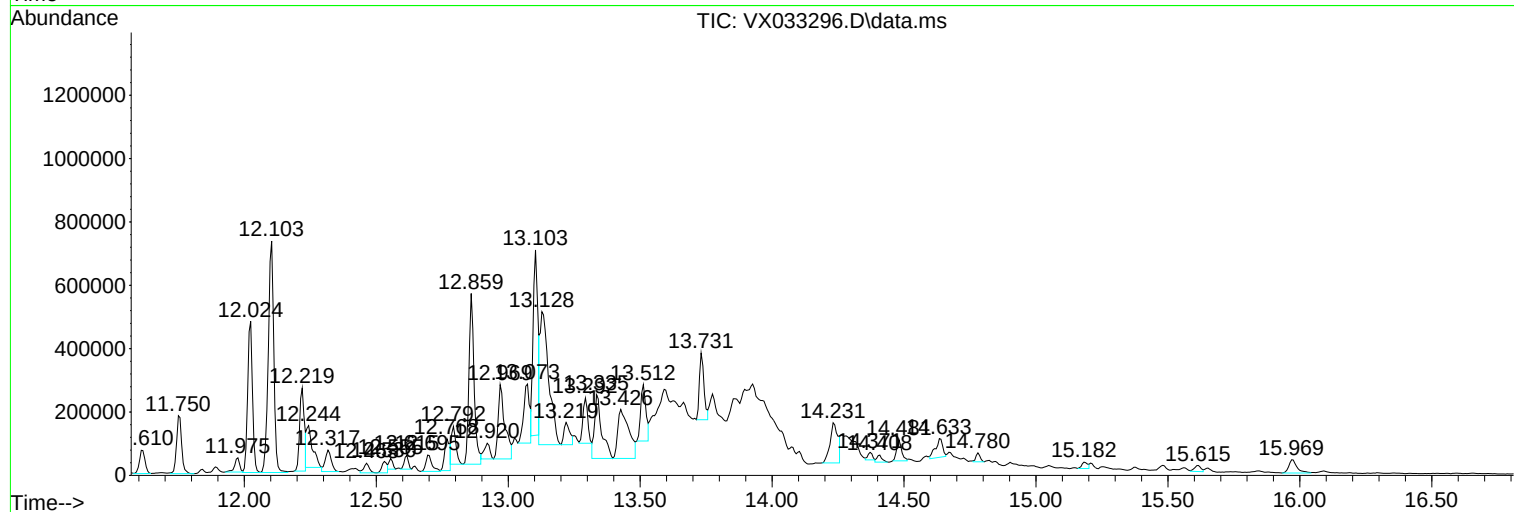
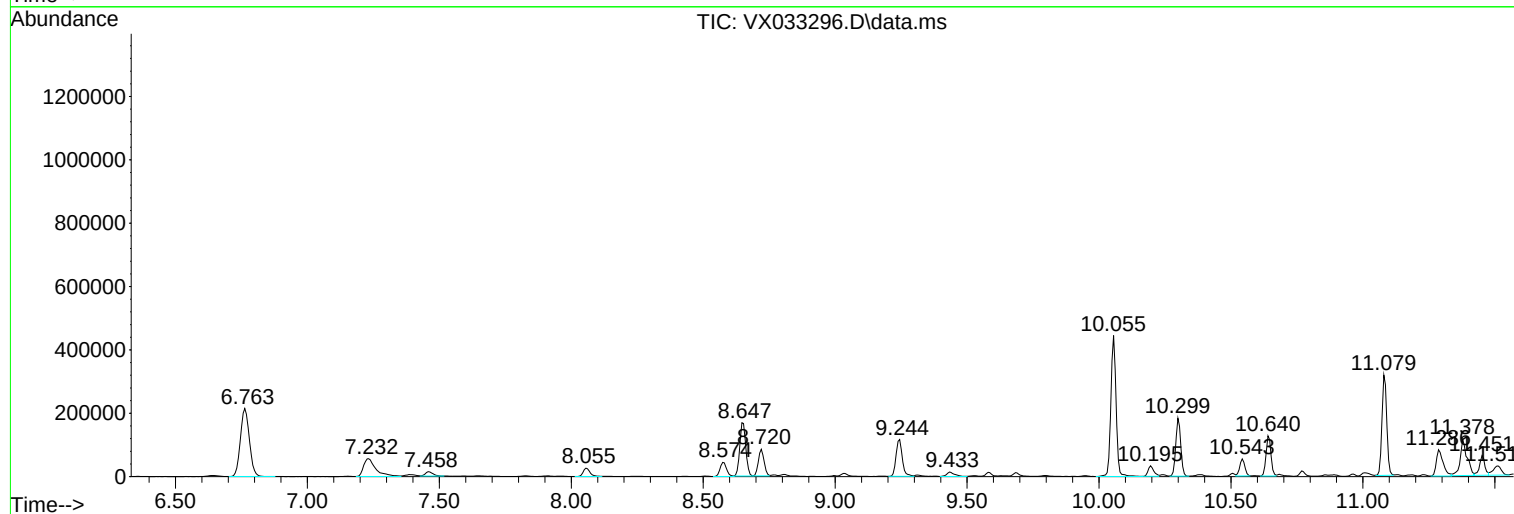
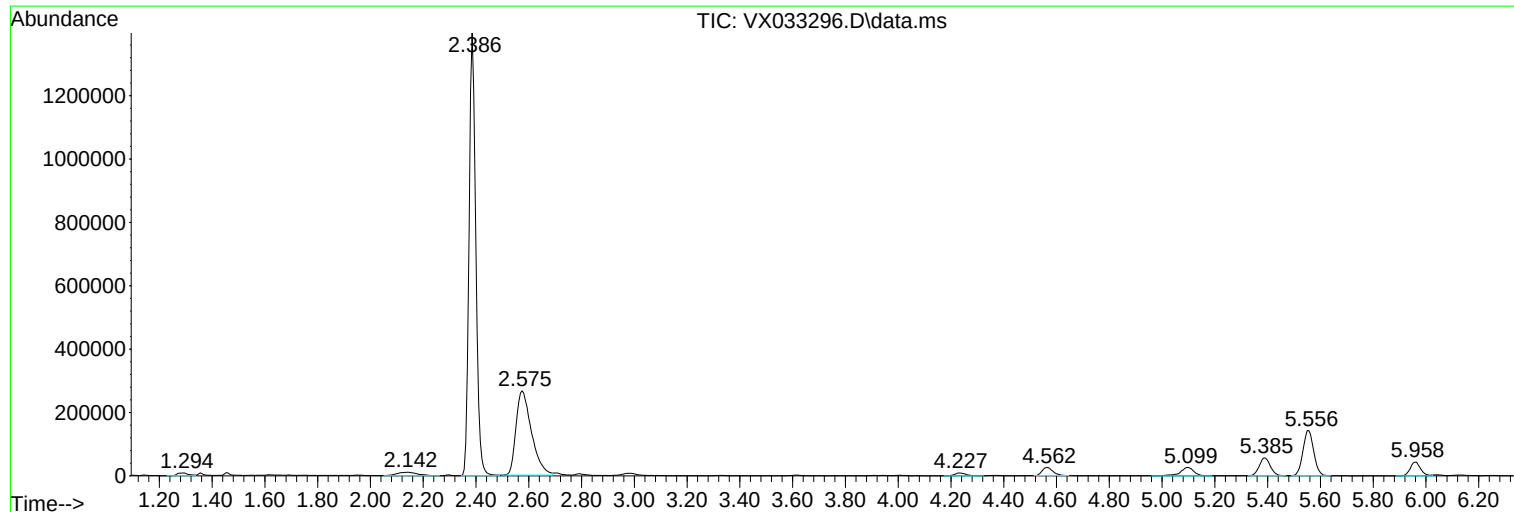
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ClientSampleId :
FMC-TOTE-1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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



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Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

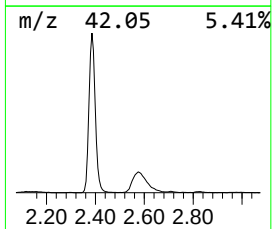
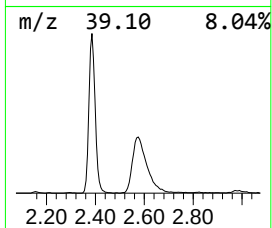
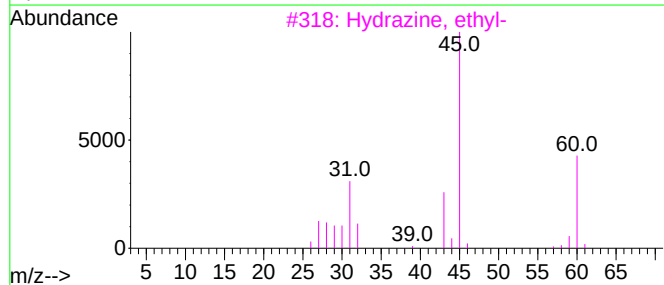
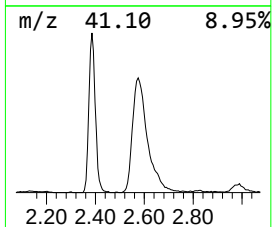
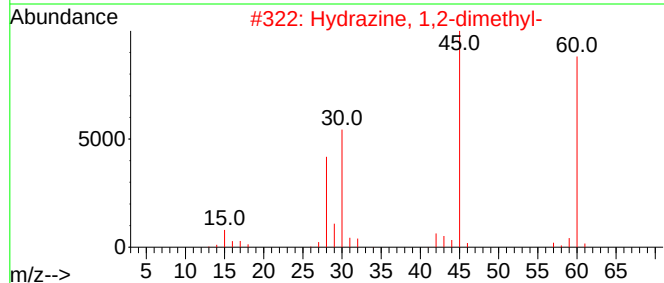
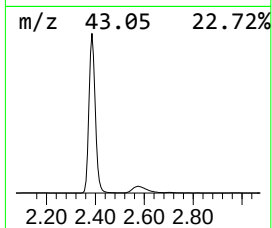
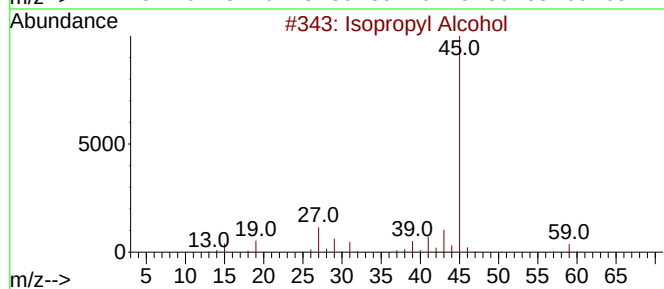
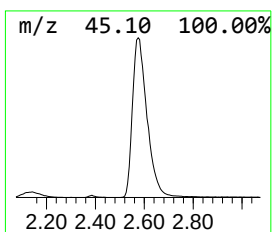
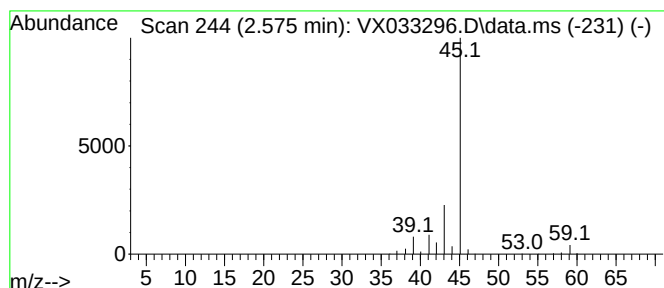
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.575	133.78 ug/l	1084680	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			Formamide	45	CH3NO	000075-12-7	4
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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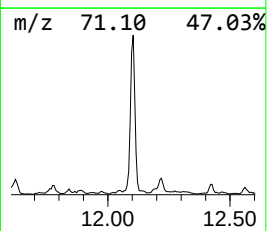
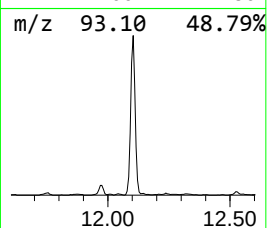
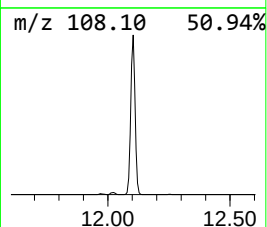
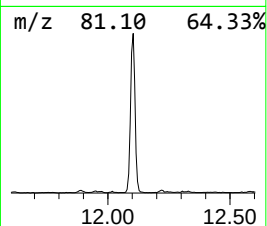
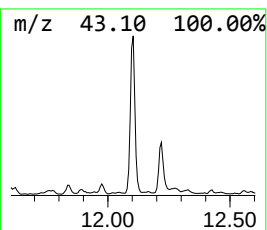
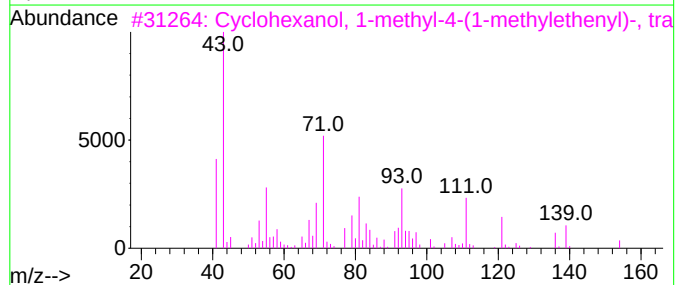
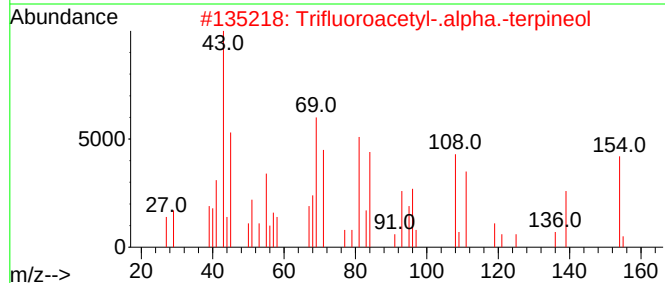
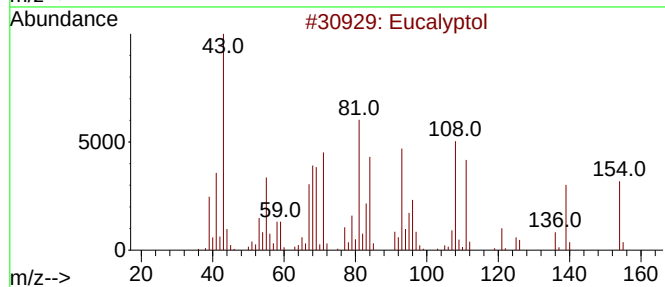
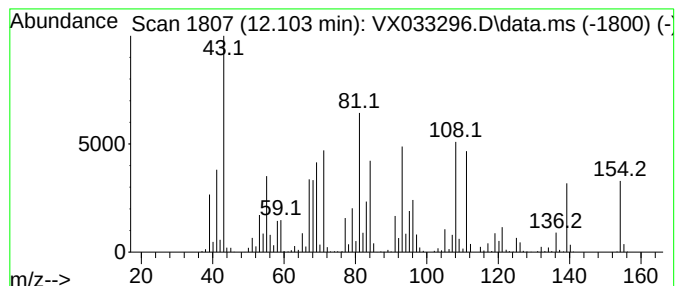
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 2 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	87.94 ug/l	1063940	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	64
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	22
4			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	22
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	15



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Instrument :
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ClientSampleId :
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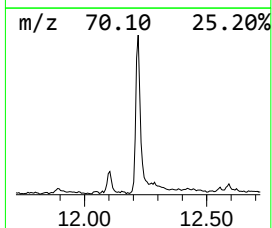
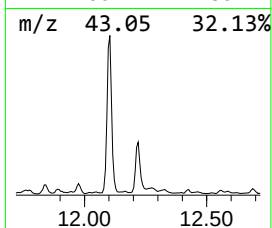
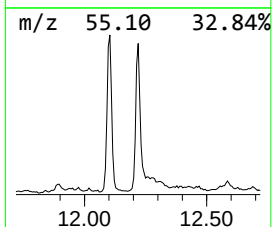
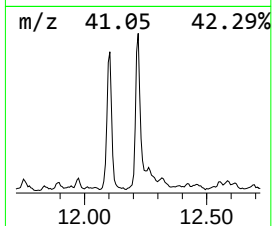
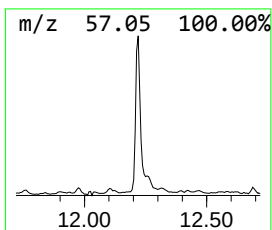
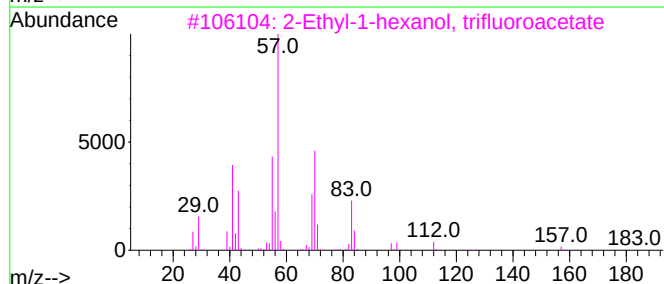
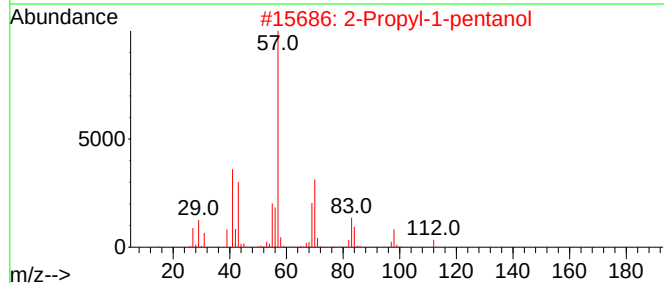
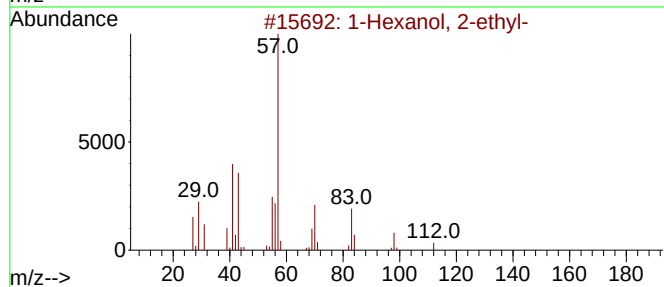
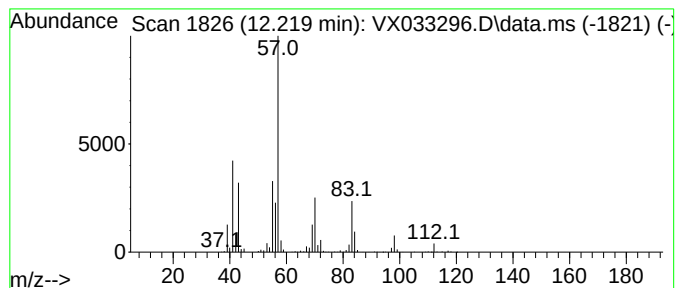
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	27.51 ug/l	332841	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	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47
4			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43



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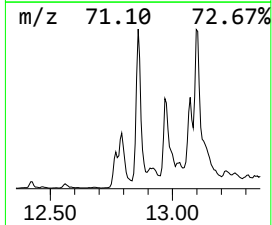
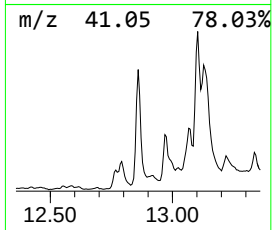
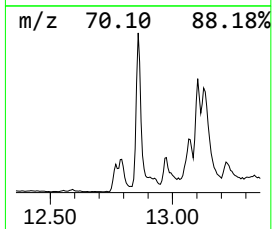
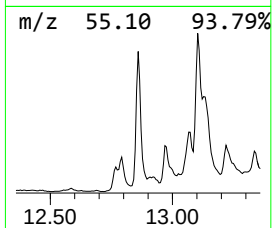
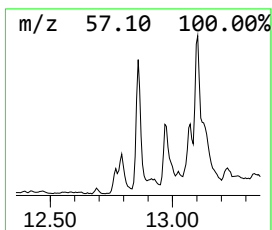
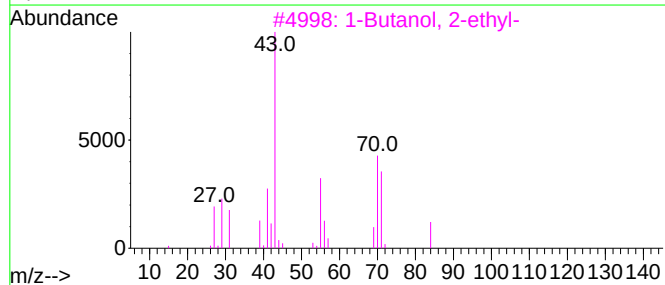
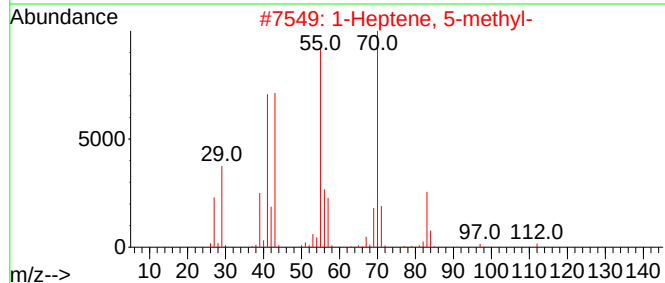
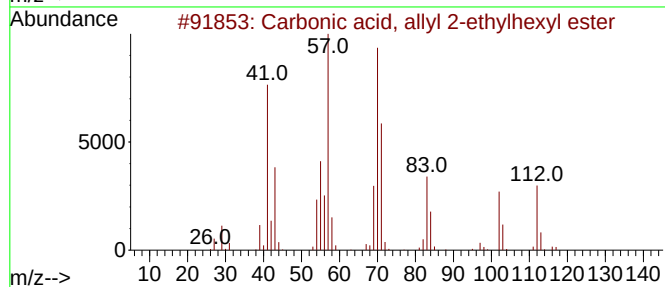
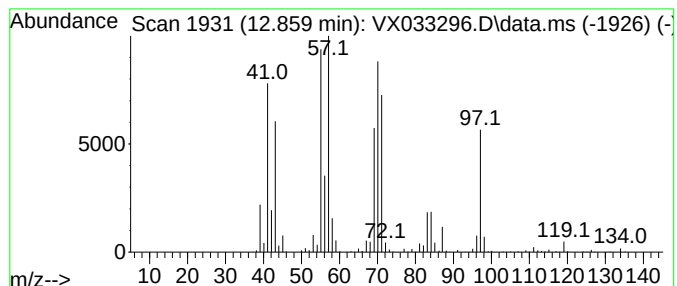
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 4 Carbonic acid, allyl 2-ethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	60.65 ug/l	733762	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, allyl 2-ethylhexy...	214	C12H22O3	1000357-80-6	53
2			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	47
3			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47
4			Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	46
5			Heptane, 3-methylene-	112	C8H16	001632-16-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

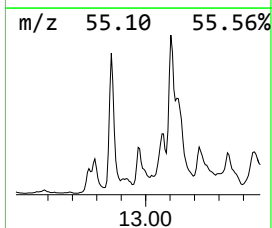
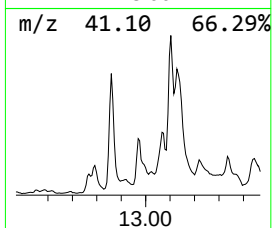
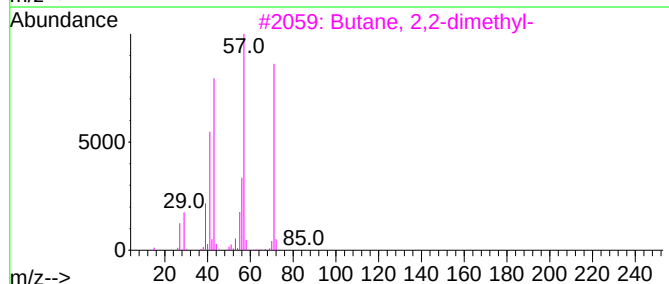
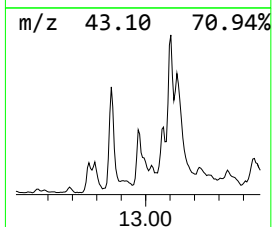
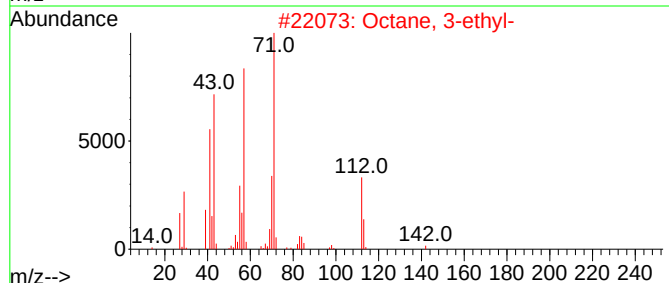
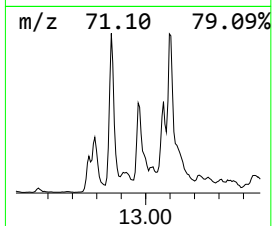
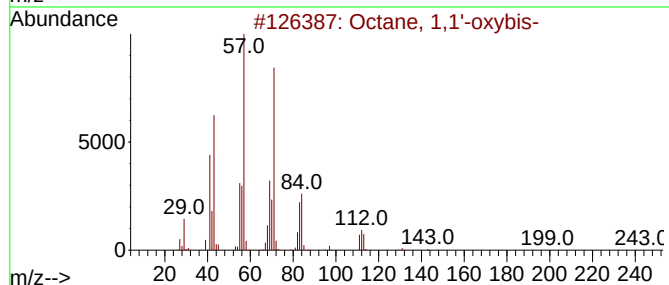
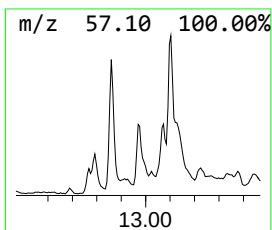
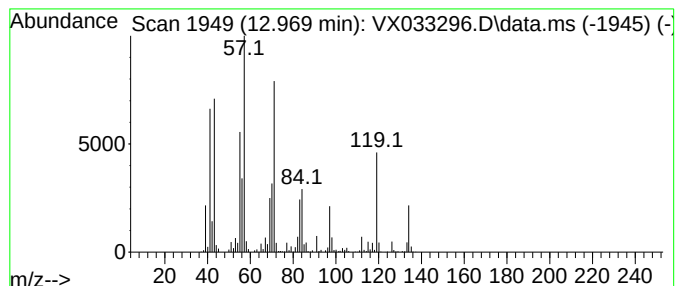
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Quant Title : SW846 8260

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

Peak Number 5 Octane, 1,1'-oxybis- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	34.86 ug/l	421735	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	52
2			Octane, 3-ethyl-	142	C10H22	005881-17-4	38
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	35
4			Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	35
5			1-Decene, 4-methyl-	154	C11H22	013151-29-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

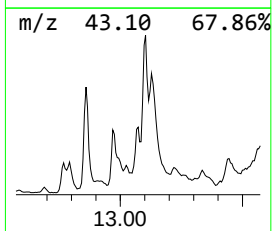
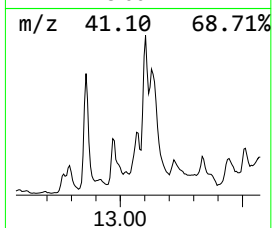
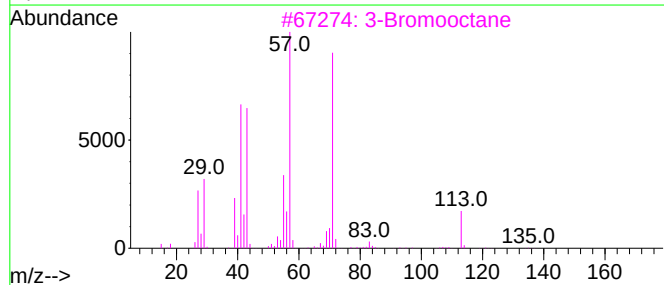
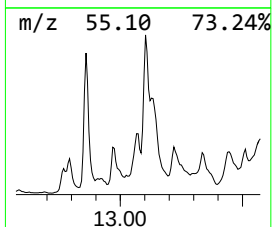
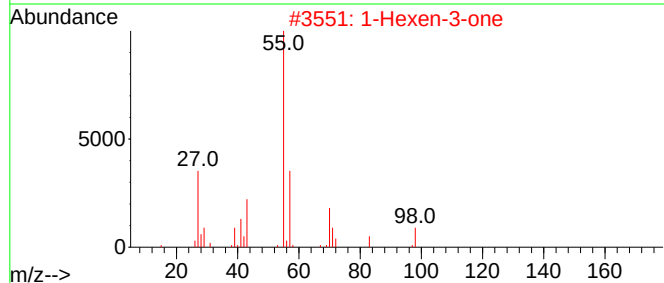
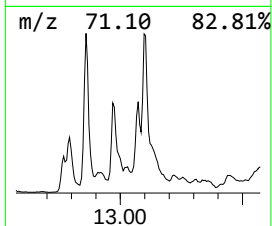
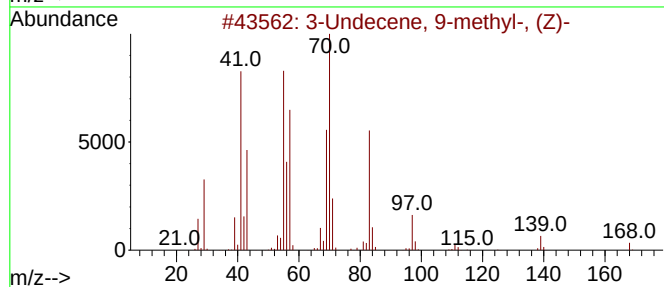
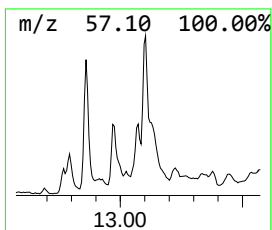
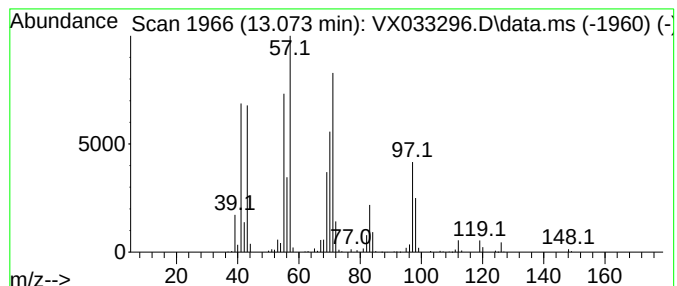
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.073 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.073	24.54 ug/l	296955	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Undecene, 9-methyl-, (Z)-	168	C12H24	074630-50-5	35
2		1-Hexen-3-one	98	C6H10O	001629-60-3	35
3		3-Bromooctane	192	C8H17Br	000999-64-4	35
4		2-Octene	112	C8H16	000111-67-1	30
5		2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

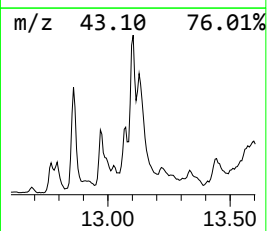
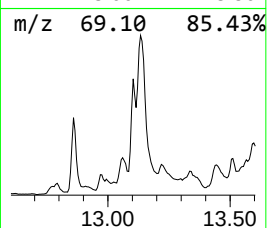
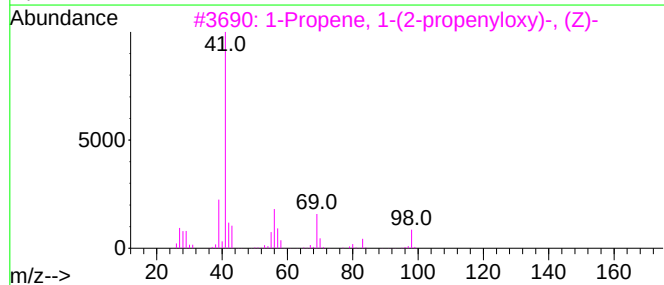
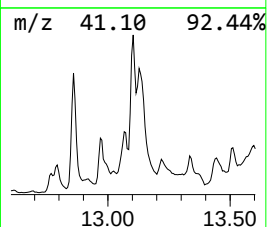
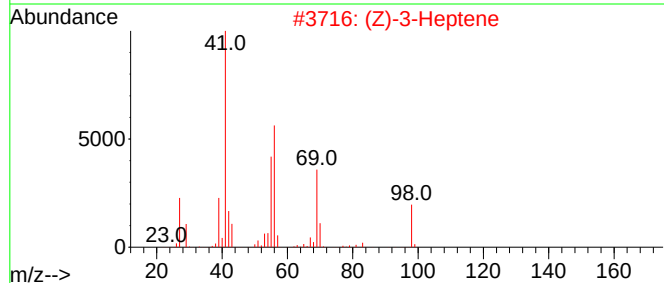
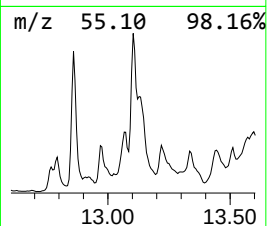
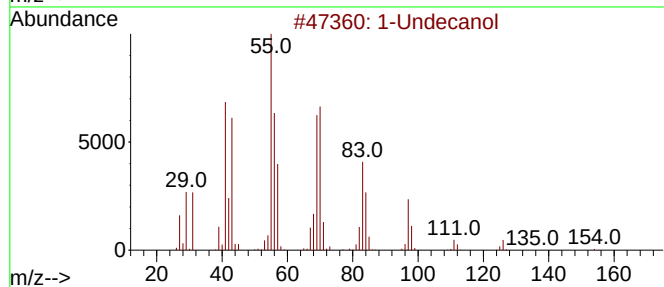
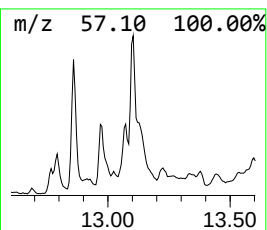
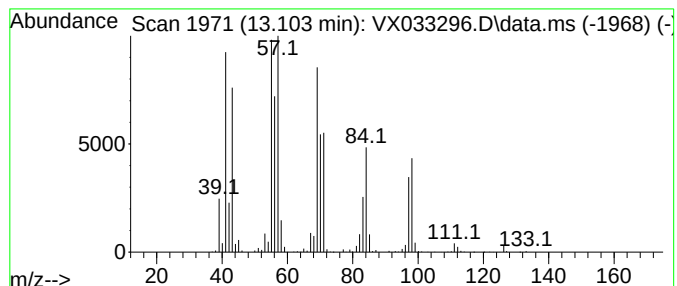
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.103 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	61.72 ug/l	746714	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Undecanol	172	C11H24O	000112-42-5	47
2			(Z)-3-Heptene	98	C7H14	007642-10-6	43
3			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	43
4			3-Methyl-3-hexene	98	C7H14	003404-65-7	38
5			3-Heptene, (E)-	98	C7H14	014686-14-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

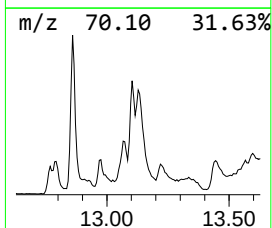
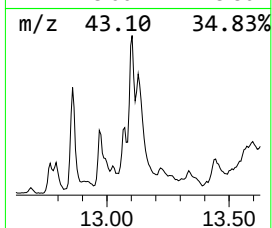
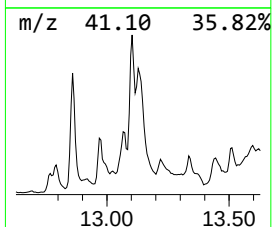
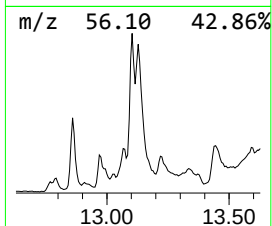
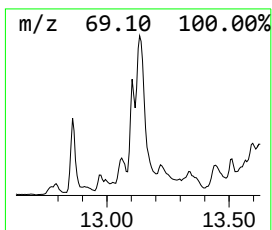
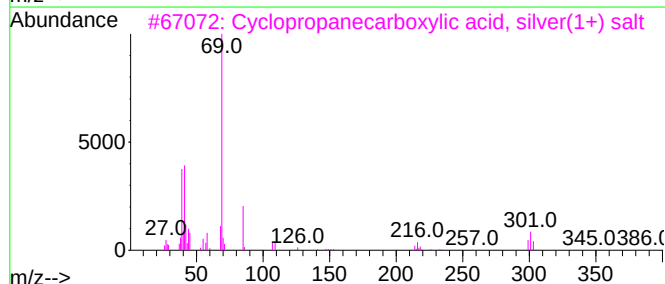
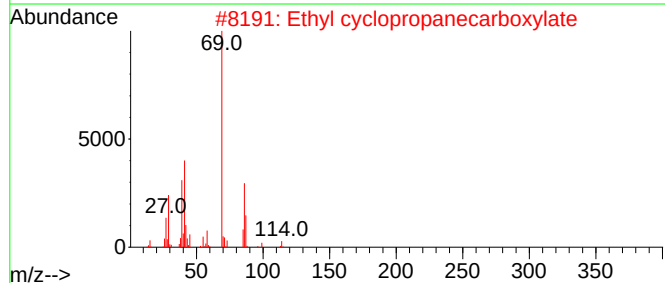
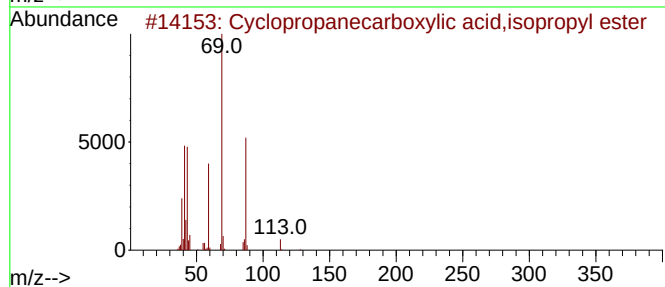
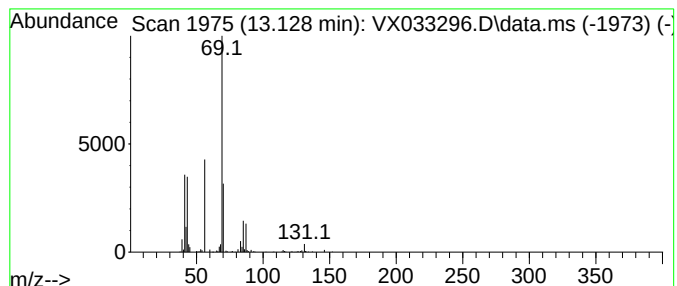
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.128 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	78.67 ug/l	951810	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, isopropyl ester	128	C7H12O2	006887-83-8	38
2			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	28
3			Cyclopropanecarboxylic acid, silver(1+) salt	192	C4H5AgO2	075112-77-5	25
4			2-Propenoic acid, 2-methyl-, 3-methyl-	156	C9H16O2	007336-27-8	25
5			Trifluoroacetic acid, heptyl ester	212	C9H15F3O2	002710-89-6	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

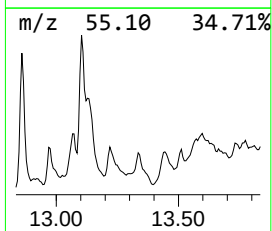
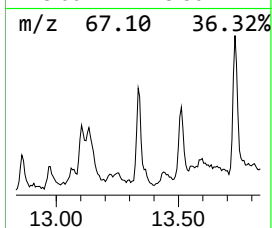
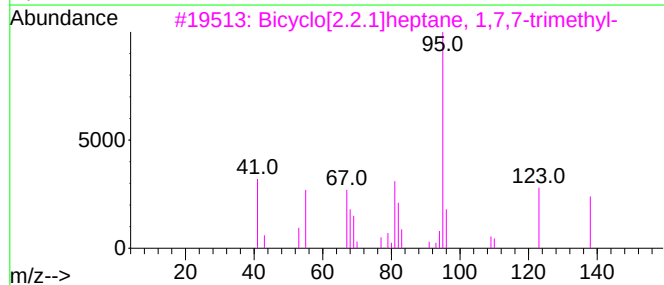
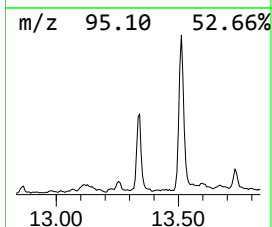
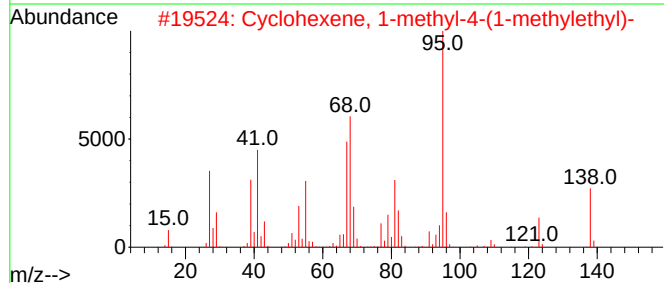
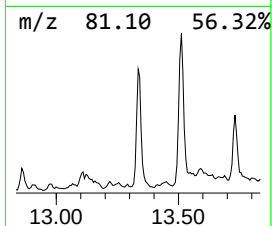
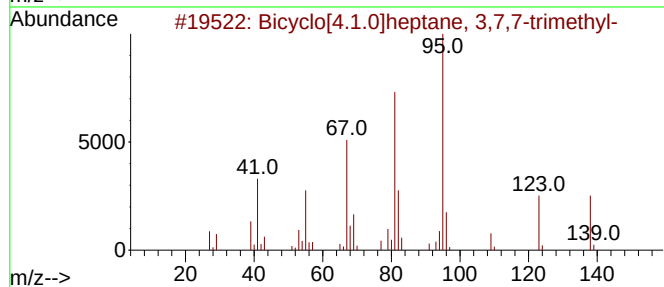
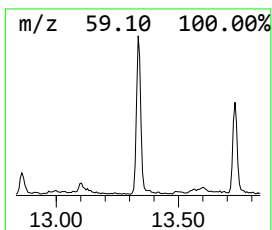
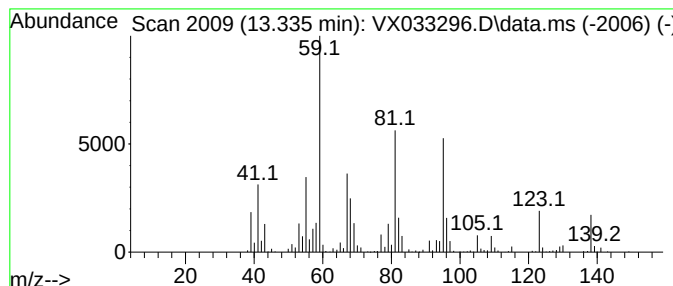
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Quant Title : SW846 8260

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

Peak Number 9 Bicyclo[4.1.0]heptane, 3,7,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	31.49 ug/l	380983	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	86
2			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	005502-88-5	55
3			Bicyclo[2.2.1]heptane, 1,7,7-tri...	138	C10H18	000464-15-3	55
4			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	50
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

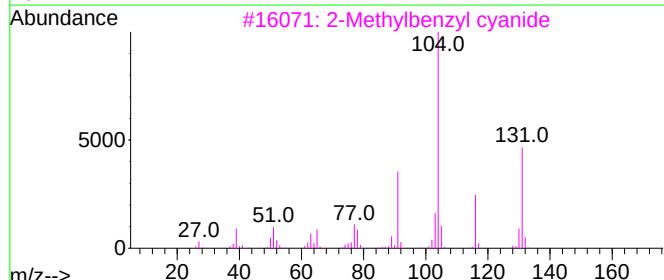
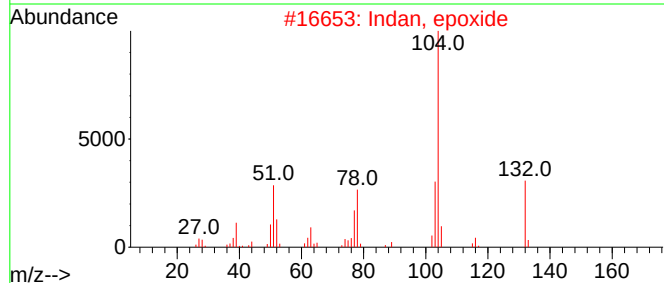
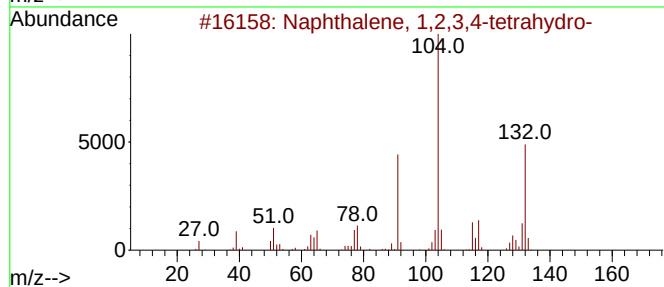
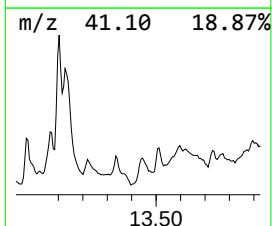
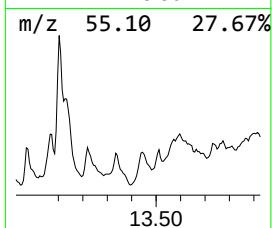
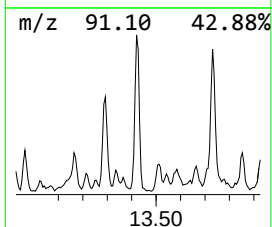
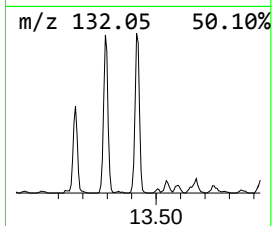
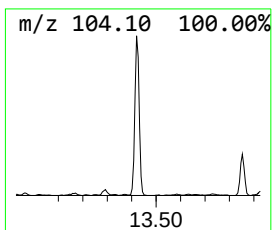
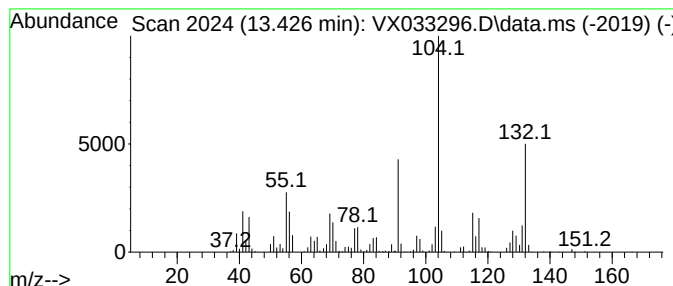
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	38.17 ug/l	461813	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	93
2		Indan, epoxide	132	C9H8O	000768-22-9	52
3		2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
4		Glutaric acid, isobutyl 2-methyl...	292	C17H24O4	1000371-32-5	43
5		2-Furanone, 4-phenyltetrahydro	162	C10H10O2	1000197-38-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
Data File : VX033296.D
Acq On : 07 Dec 2022 21:05
Operator : JC/MD
Sample : N5912-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-TOTE-1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.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
Isopropyl Alcohol	2.575	133.8	ug/l	1084680	1	5.556	405397	50.0
Eucalyptol	12.103	87.9	ug/l	1063940	4	12.024	604948	50.0
1-Hexanol, 2-et...	12.219	27.5	ug/l	332841	4	12.024	604948	50.0
Carbonic acid, ...	12.859	60.6	ug/l	733762	4	12.024	604948	50.0
Octane, 1,1'-ox...	12.969	34.9	ug/l	421735	4	12.024	604948	50.0
unknown13.073	13.073	24.5	ug/l	296955	4	12.024	604948	50.0
unknown13.103	13.103	61.7	ug/l	746714	4	12.024	604948	50.0
unknown13.128	13.128	78.7	ug/l	951810	4	12.024	604948	50.0
Bicyclo[4.1.0]h...	13.335	31.5	ug/l	380983	4	12.024	604948	50.0
Naphthalene, 1,...	13.426	38.2	ug/l	461813	4	12.024	604948	50.0