

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
 Data File : VX041704.D
 Acq On : 03 Jun 2024 15:07
 Operator : JC/MD
 Sample : P2691-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RINSATE-1

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\82X052924W.M
 Title : SW846 8260

Signal : TIC: VX041704.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	36	rBV2	16651	33177	1.45%	0.156%
2	5.385	695	705	721	rBV2	88960	258083	11.30%	1.214%
3	5.550	721	732	747	rVV	146666	418845	18.34%	1.970%
4	5.958	787	799	818	rBV	92417	243487	10.66%	1.145%
5	6.763	920	931	945	rBV	222280	532824	23.33%	2.506%
6	8.647	1234	1240	1250	rBV	465880	727290	31.85%	3.421%
7	10.055	1466	1471	1486	rVB	477940	660423	28.92%	3.106%
8	10.305	1500	1512	1517	rBV3	13484	33189	1.45%	0.156%
9	10.360	1517	1521	1532	rVB	33593	46232	2.02%	0.217%
10	10.781	1582	1590	1594	rBV	17732	25815	1.13%	0.121%
11	10.860	1594	1603	1607	rBV3	13400	27578	1.21%	0.130%
12	10.945	1612	1617	1622	rVB2	22673	32787	1.44%	0.154%
13	11.079	1634	1639	1651	rVB	429840	593255	25.98%	2.790%
14	11.189	1651	1657	1660	rBV3	21002	29378	1.29%	0.138%
15	11.378	1684	1688	1693	rVV	21695	38356	1.68%	0.180%
16	11.427	1693	1696	1701	rVV3	24586	49886	2.18%	0.235%
17	11.476	1701	1704	1711	rVB	141629	165032	7.23%	0.776%
18	11.616	1722	1727	1733	rVB4	20415	45075	1.97%	0.212%
19	11.713	1740	1743	1746	rBV	31027	33964	1.49%	0.160%
20	11.750	1746	1749	1759	rVB	39341	76684	3.36%	0.361%
21	11.890	1768	1772	1776	rVB4	19475	28056	1.23%	0.132%
22	11.945	1776	1781	1783	rBV2	26427	36127	1.58%	0.170%
23	12.018	1788	1793	1799	rBV	554231	745079	32.63%	3.504%
24	12.103	1799	1807	1815	rBV	587450	782024	34.25%	3.678%
25	12.171	1815	1818	1821	rVB	24068	24928	1.09%	0.117%
26	12.219	1821	1826	1838	rBV	1808714	2283486	100.00%	10.740%
27	12.317	1838	1842	1849	rVB4	54121	102035	4.47%	0.480%
28	12.421	1849	1859	1864	rBV	248885	323518	14.17%	1.522%
29	12.463	1864	1866	1872	rVB4	35566	56644	2.48%	0.266%
30	12.555	1872	1881	1883	rBV5	48697	105816	4.63%	0.498%
31	12.683	1898	1902	1906	rBV3	29067	49163	2.15%	0.231%
32	12.762	1912	1915	1917	rBV3	40769	50177	2.20%	0.236%
33	12.792	1917	1920	1922	rVV2	50218	58482	2.56%	0.275%
34	12.817	1922	1924	1927	rVB2	46435	46826	2.05%	0.220%
35	12.859	1927	1931	1935	rBV	255094	373741	16.37%	1.758%
36	12.969	1946	1949	1955	rBV3	135624	197904	8.67%	0.931%

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37	13.042	1956	1961	1963	rVV3	60949	86240	3.78%	0.406%
38	13.067	1963	1965	1967	rVV	104220	112577	4.93%	0.530%
39	13.103	1967	1971	1972	rVV2	364139	475617	20.83%	2.237%
40	13.128	1972	1975	1985	rVV	661961	1107644	48.51%	5.210%
41	13.213	1985	1989	1994	rVV	686707	867709	38.00%	4.081%
42	13.268	1994	1998	2001	rVV	380769	504884	22.11%	2.375%
43	13.292	2001	2002	2007	rVB3	124651	118526	5.19%	0.557%
44	13.384	2013	2017	2019	rBV2	82766	92224	4.04%	0.434%
45	13.420	2019	2023	2032	rVV	1532366	1911043	83.69%	8.989%
46	13.506	2033	2037	2041	rVV	100294	145802	6.39%	0.686%
47	13.585	2047	2050	2055	rVB6	27011	37369	1.64%	0.176%
48	13.707	2060	2070	2073	rBV	224095	433607	18.99%	2.039%
49	13.798	2083	2085	2088	rVB3	28279	24987	1.09%	0.118%
50	13.841	2088	2092	2097	rBV5	120418	262604	11.50%	1.235%
51	13.890	2097	2100	2105	rBV	107918	148067	6.48%	0.696%
52	14.036	2120	2124	2128	rVB	440201	441405	19.33%	2.076%
53	14.073	2128	2130	2133	rBV2	37076	41543	1.82%	0.195%
54	14.103	2133	2135	2138	rVV2	28663	28447	1.25%	0.134%
55	14.134	2138	2140	2143	rVB3	34835	33616	1.47%	0.158%
56	14.195	2146	2150	2164	rVV2	1248822	1803273	78.97%	8.482%
57	14.371	2176	2179	2181	rBV	33805	35532	1.56%	0.167%
58	14.402	2181	2184	2188	rBV2	203669	264638	11.59%	1.245%
59	14.475	2193	2196	2198	rBV2	96709	132158	5.79%	0.622%
60	14.573	2206	2212	2215	rBV4	137169	263690	11.55%	1.240%
61	14.615	2215	2219	2225	rVV4	232341	416761	18.25%	1.960%
62	14.670	2225	2228	2234	rVB3	64096	112342	4.92%	0.528%
63	14.755	2238	2242	2245	rBV	474560	482264	21.12%	2.268%
64	14.792	2245	2248	2251	rBV5	84460	97821	4.28%	0.460%
65	14.914	2264	2268	2283	rVB3	234704	519657	22.76%	2.444%
66	15.182	2308	2312	2314	rBV2	91696	131253	5.75%	0.617%
67	15.213	2314	2317	2320	rVV	137052	176083	7.71%	0.828%
68	15.274	2324	2327	2331	rVB3	66484	87147	3.82%	0.410%
69	15.377	2340	2344	2347	rBV3	32151	48461	2.12%	0.228%
70	15.487	2357	2362	2368	rBV	258443	375035	16.42%	1.764%
71	16.371	2503	2507	2515	rVB	61326	105540	4.62%	0.496%

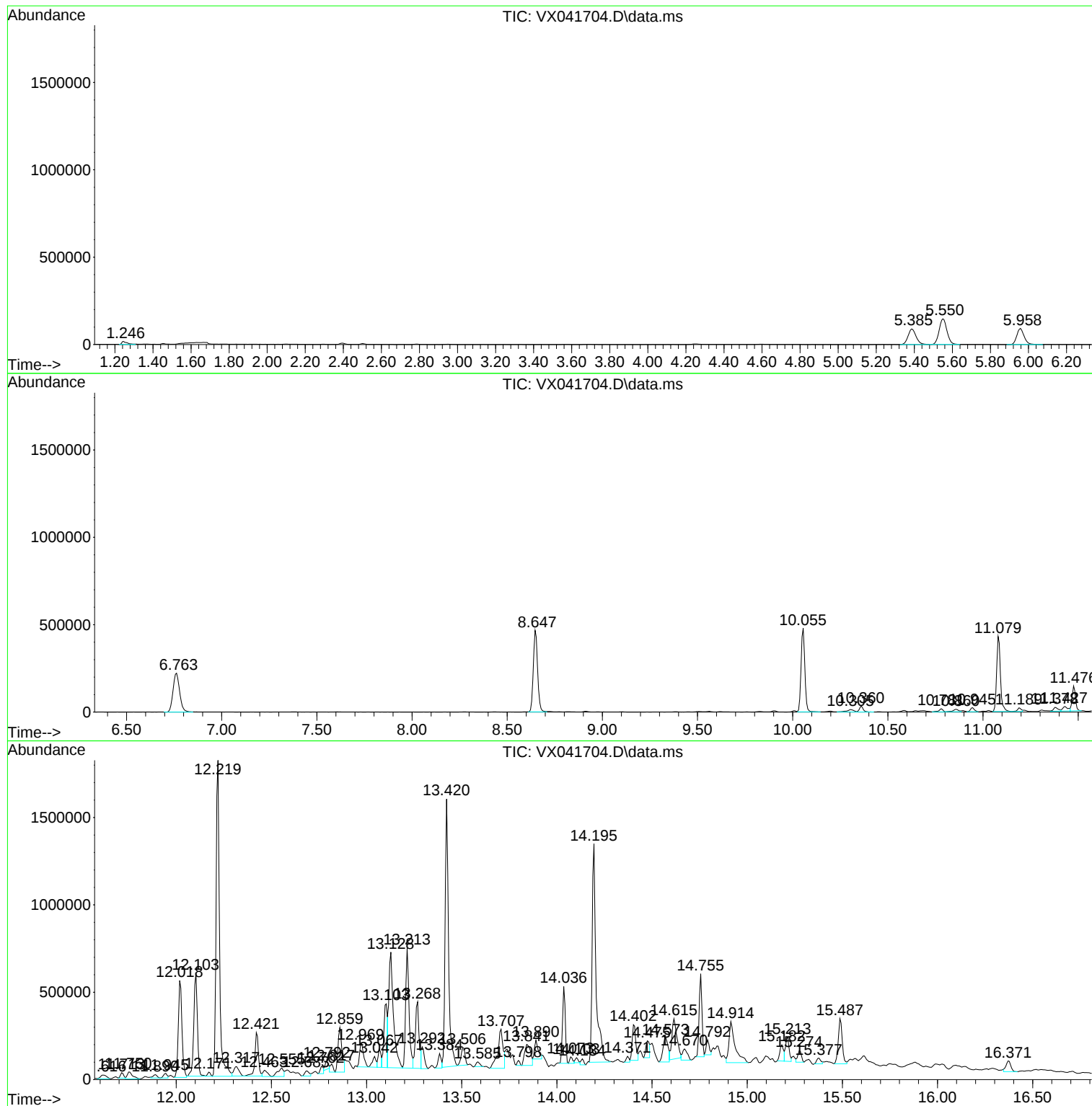
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ClientSampleId :
RINSATE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

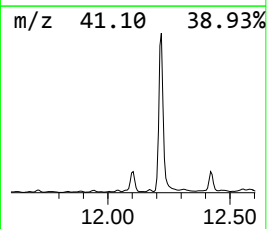
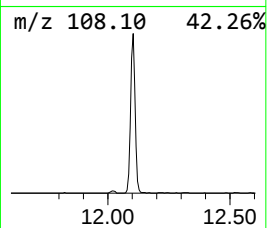
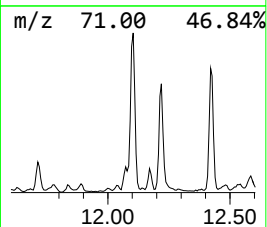
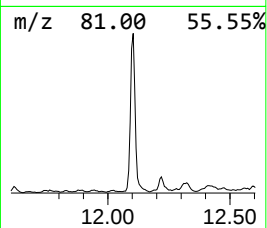
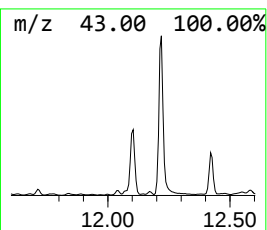
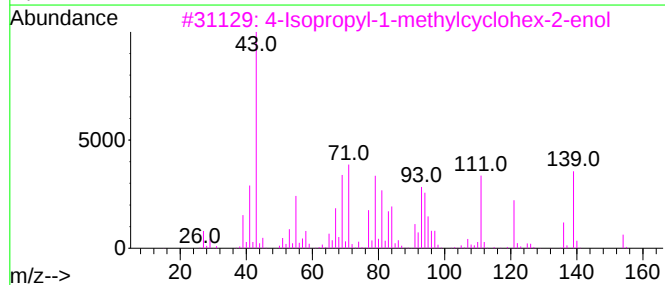
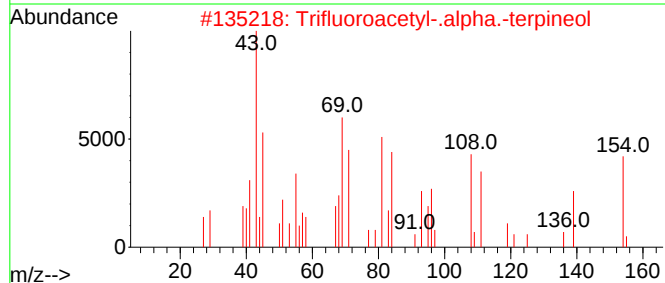
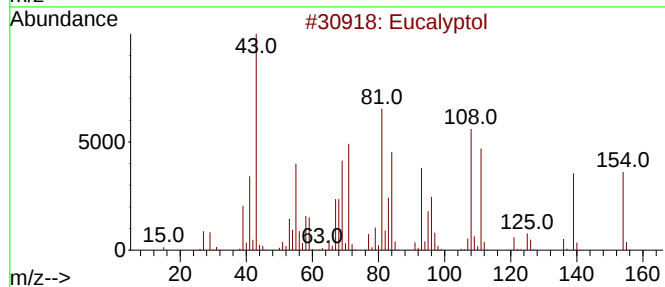
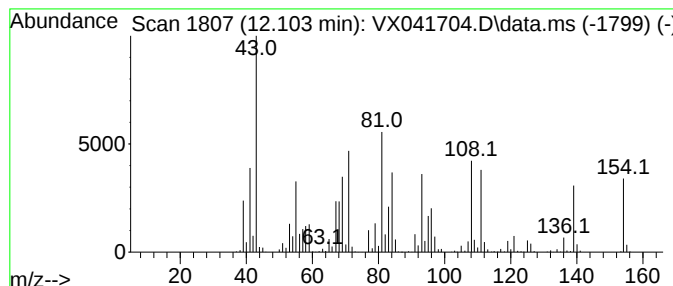
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	52.48 ug/l	782024	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	87
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	37
4			2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	35
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	25



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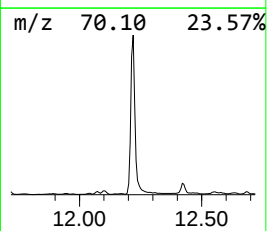
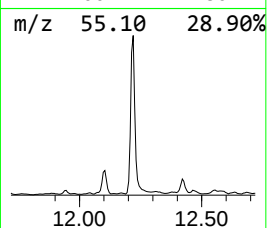
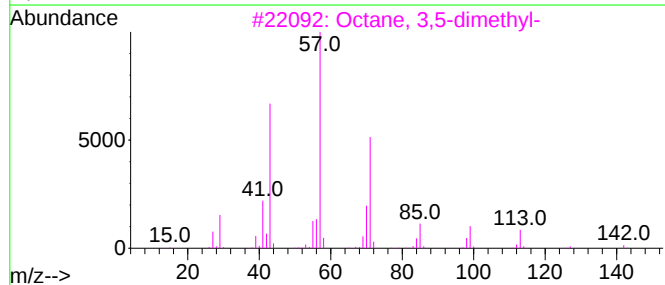
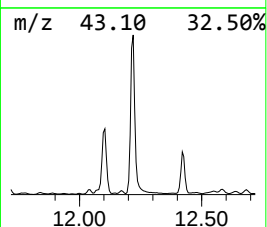
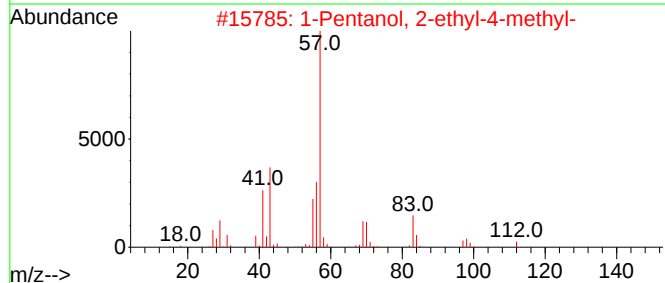
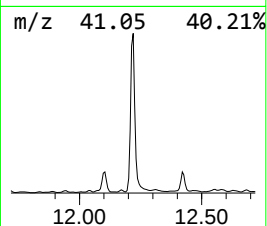
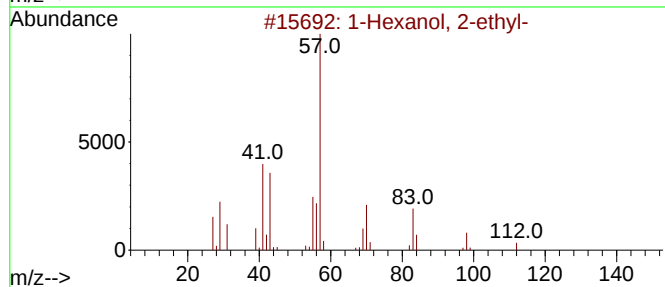
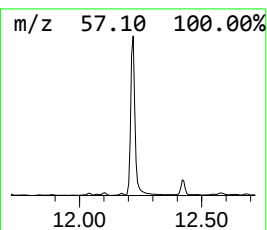
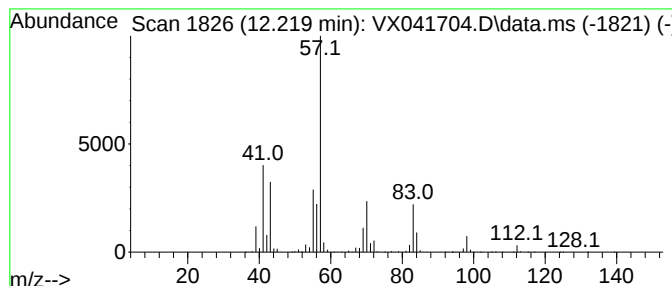
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	153.24 ug/l	2283490	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			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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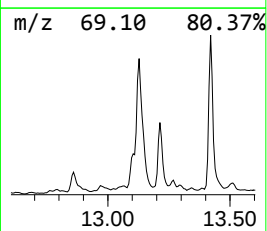
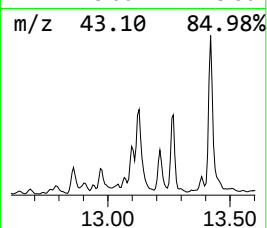
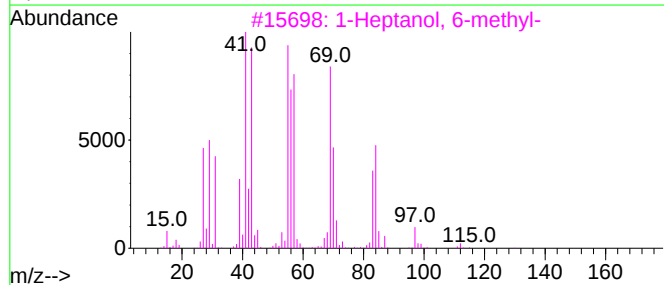
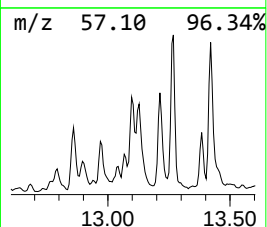
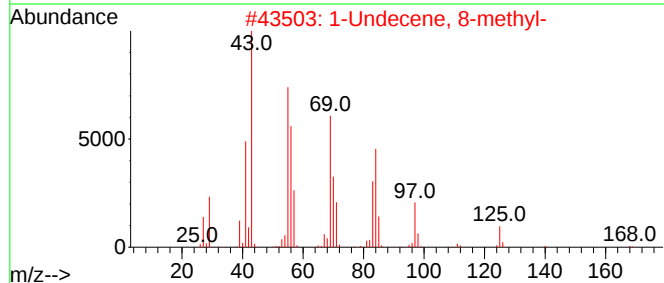
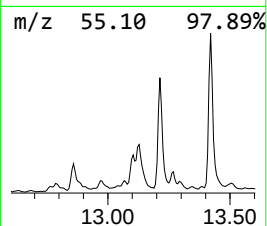
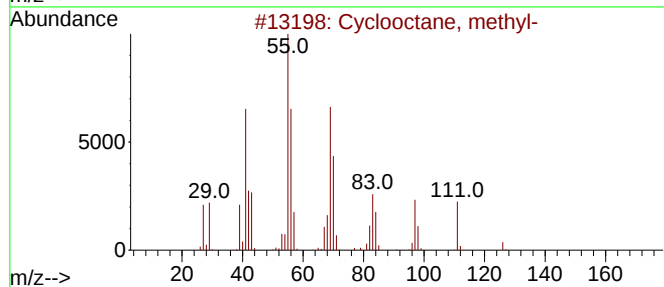
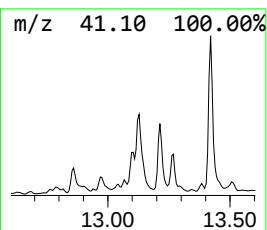
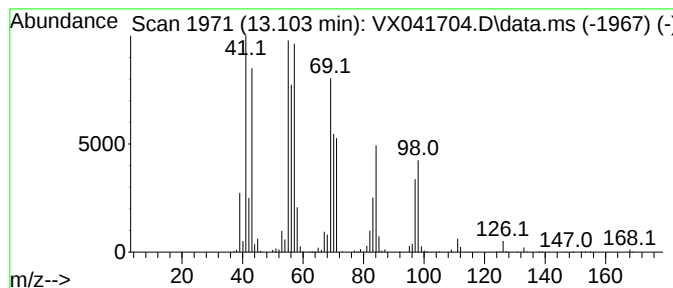
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclooctane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	31.92 ug/l	475617	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, methyl-	126	C9H18	001502-38-1	64
2			1-Undecene, 8-methyl-	168	C12H24	074630-40-3	52
3			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	50
4			3-Heptene	98	C7H14	000592-78-9	46
5			3-Heptene, (E)-	98	C7H14	014686-14-7	46



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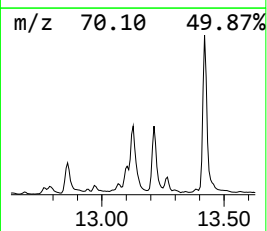
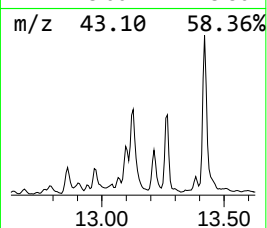
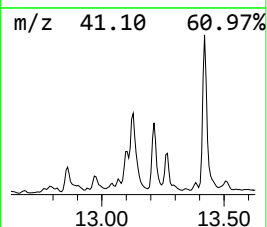
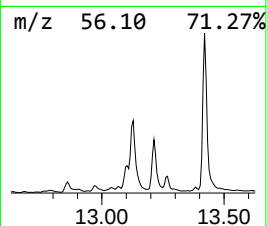
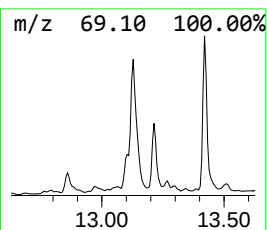
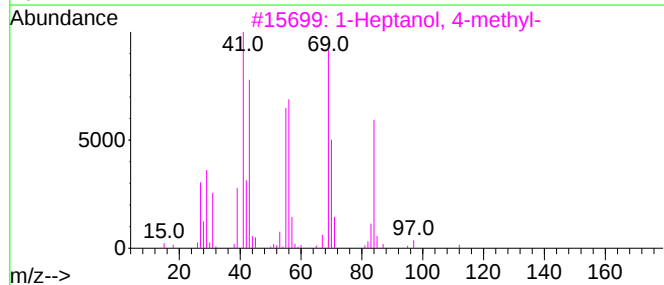
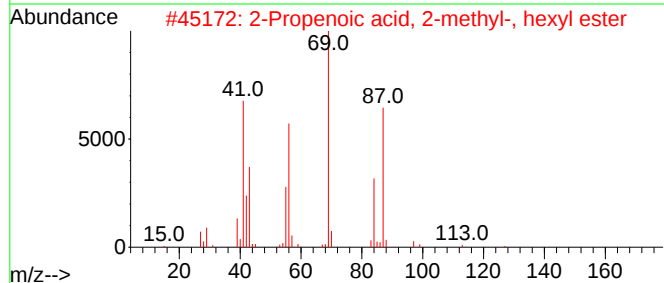
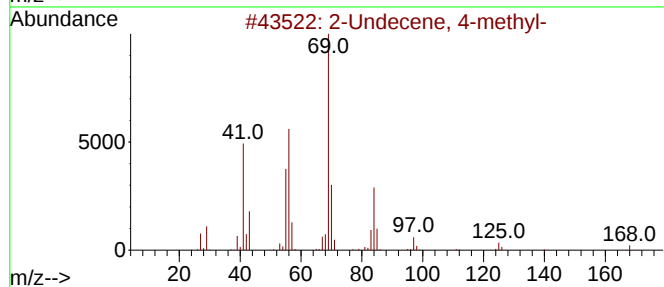
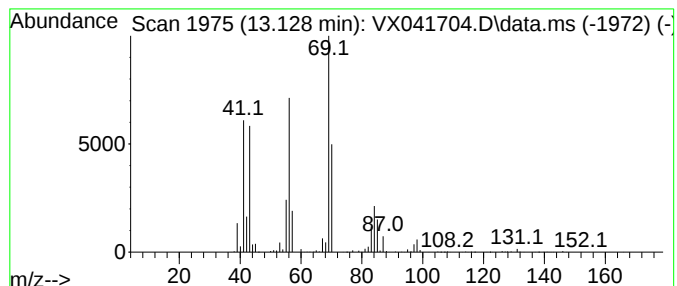
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Undecene, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	74.33 ug/l	1107640	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecene, 4-methyl-	168	C12H24	091695-32-8	64		
2	2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	53		
3	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	45		
4	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	43		
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

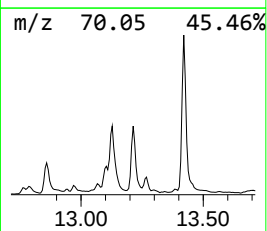
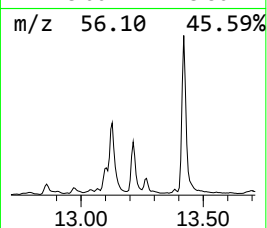
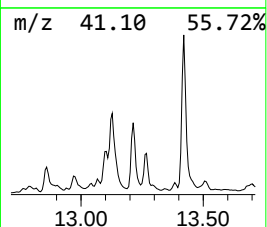
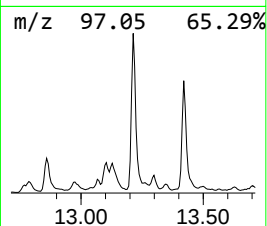
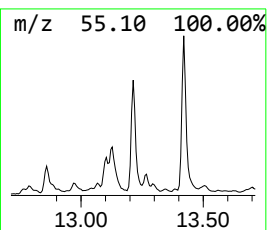
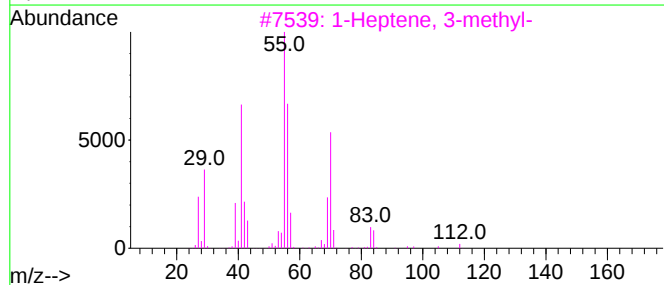
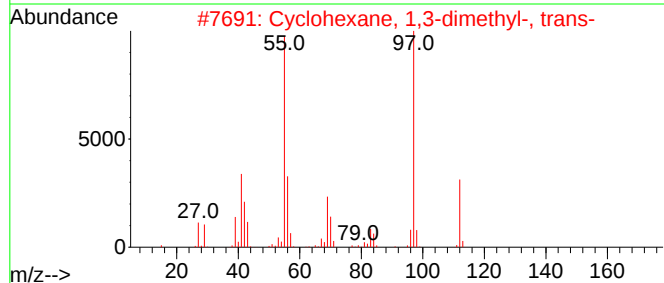
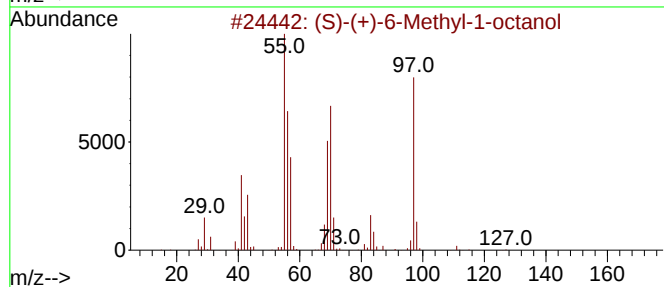
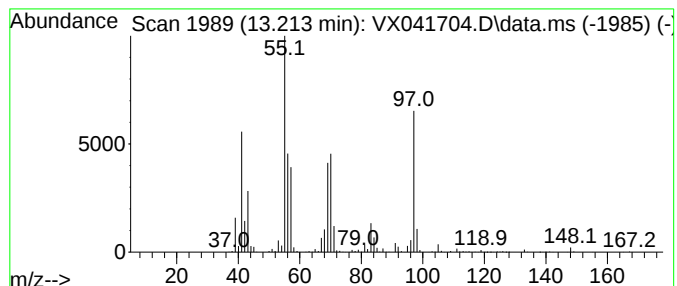
Instrument :
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ClientSampleId :
RINSATE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 5 (S)-(+)-6-Methyl-1-octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.213	58.23 ug/l	867709	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	59
3	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	53
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50
5	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

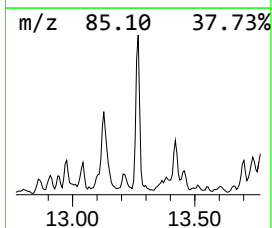
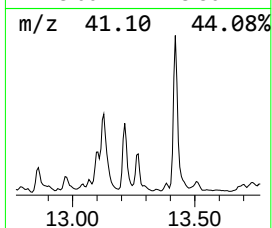
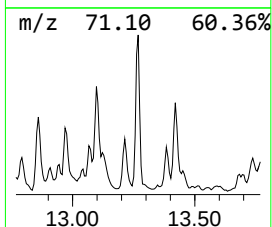
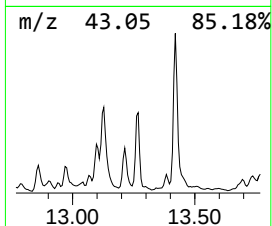
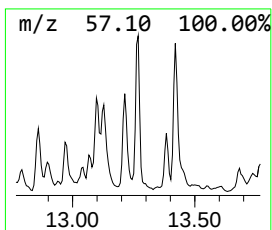
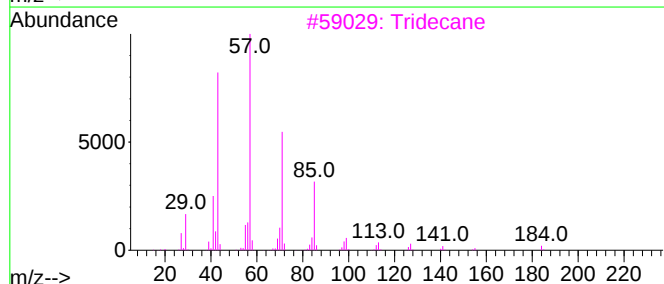
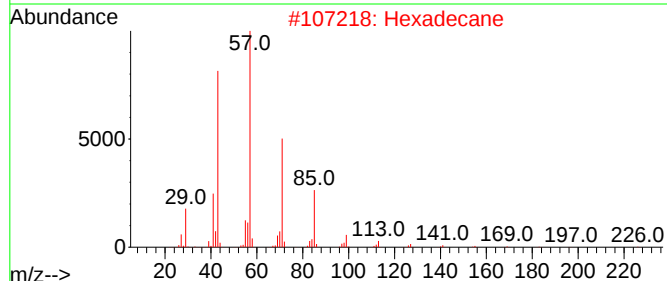
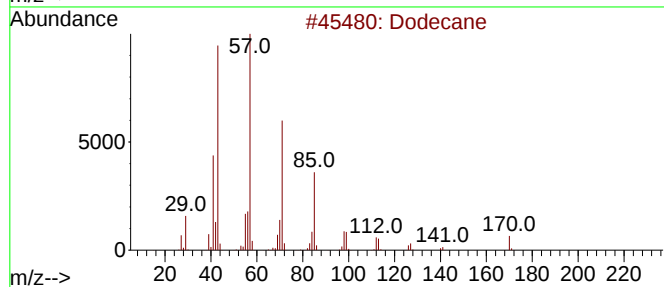
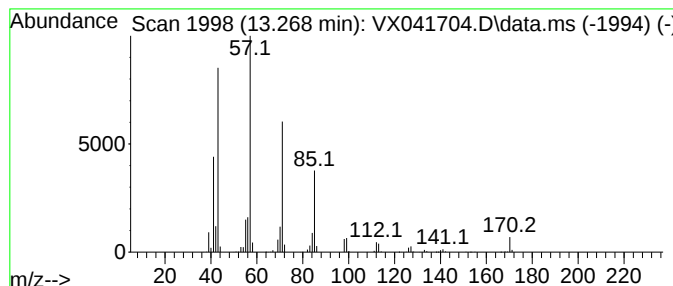
Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.268	33.88 ug/l	504884	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	80
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

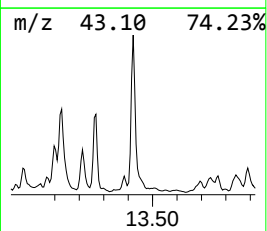
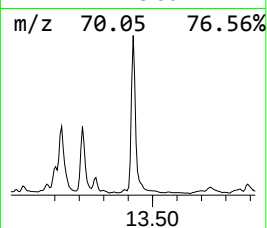
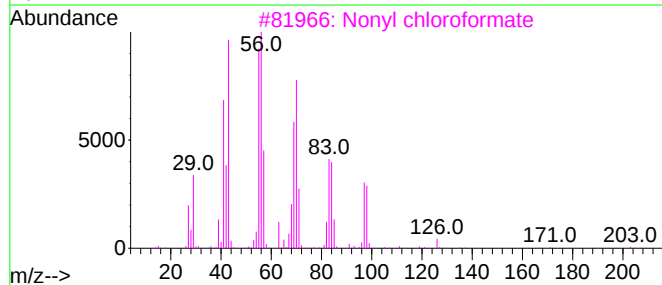
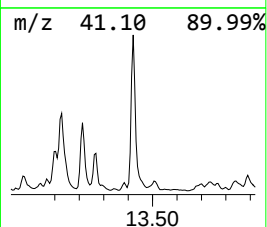
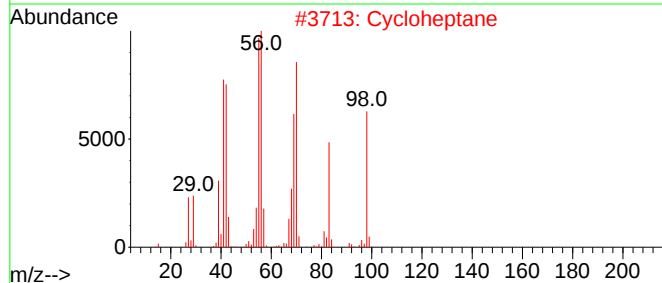
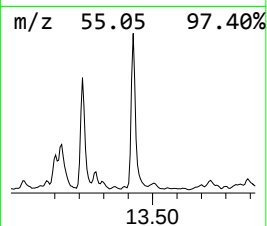
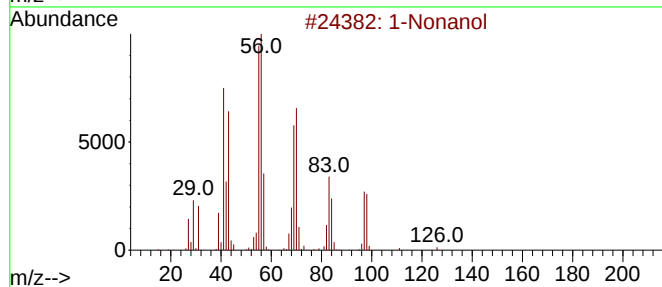
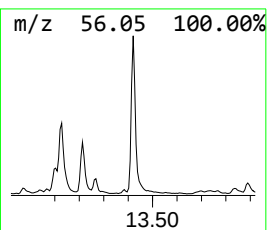
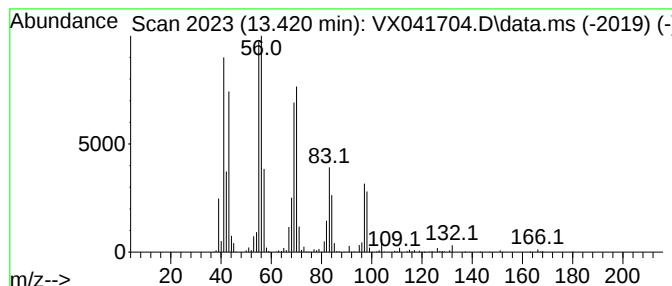
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Quant Title : SW846 8260

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

Peak Number 7 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	128.24 ug/l	1911040	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol			144	C9H20O	000143-08-8	91
2	Cycloheptane			98	C7H14	000291-64-5	87
3	Nonyl chloroformate			206	C10H19ClO2	057045-82-6	86
4	Cyclopropane, 1-ethyl-2-heptyl-			168	C12H24	074663-86-8	72
5	Isopropylcyclobutane			98	C7H14	000872-56-0	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

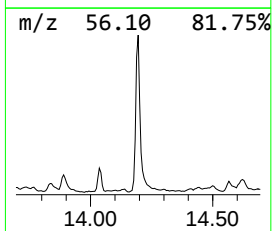
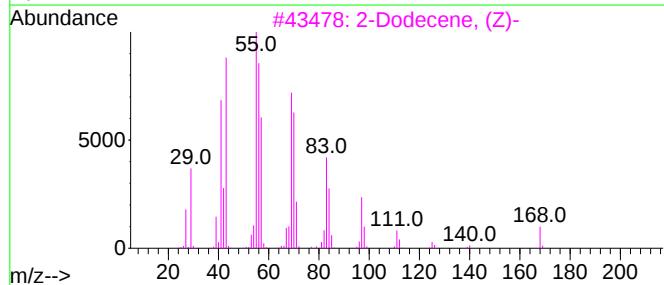
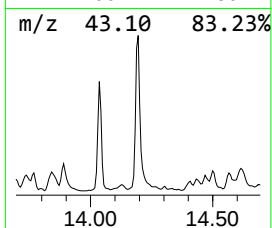
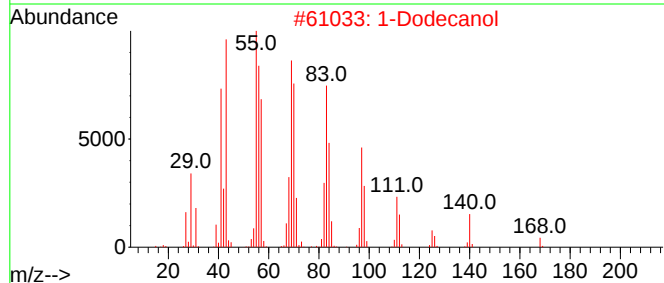
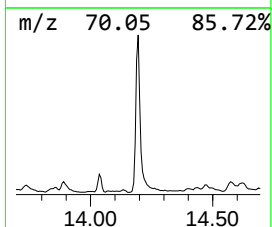
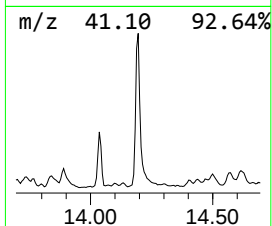
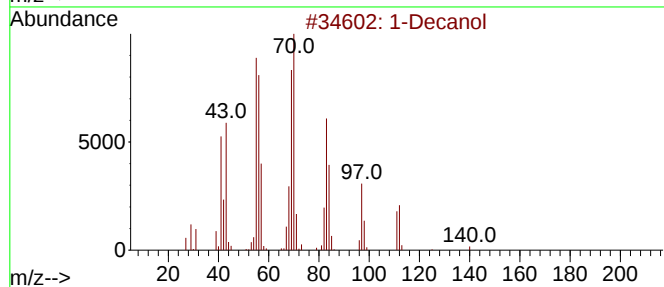
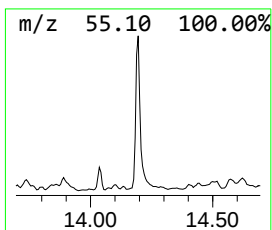
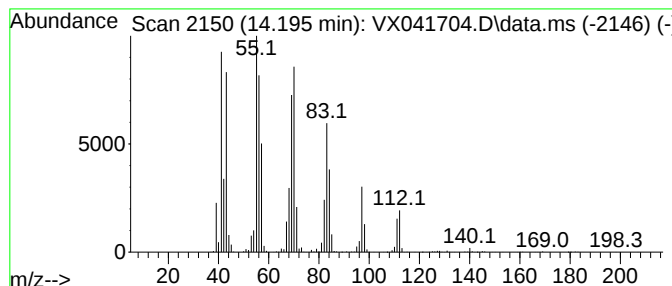
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Quant Title : SW846 8260

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

Peak Number 8 1-Decanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	121.01 ug/l	1803270	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol		158	C10H22O	000112-30-1	91
2	1-Dodecanol		186	C12H26O	000112-53-8	87
3	2-Dodecene, (Z)-		168	C12H24	007206-26-0	87
4	1-Undecene		154	C11H22	000821-95-4	86
5	Dichloroacetic acid, decyl ester		268	C12H22Cl2O2	083005-00-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

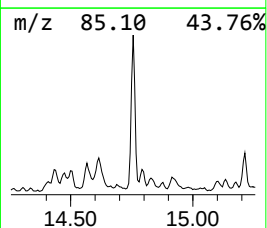
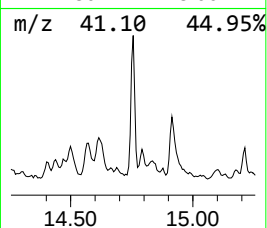
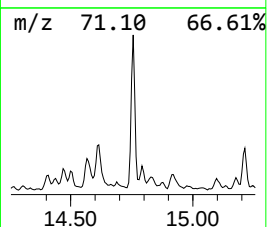
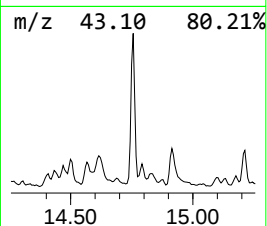
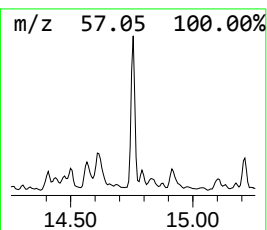
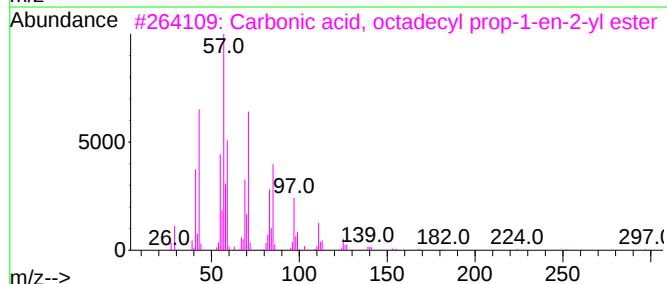
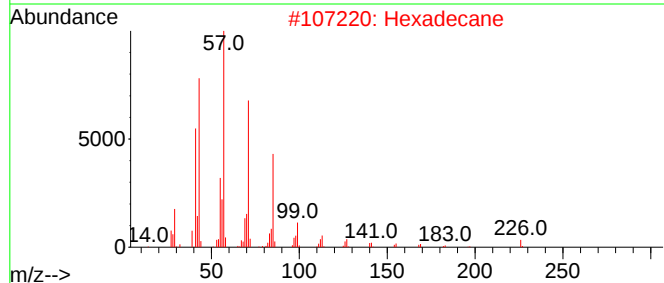
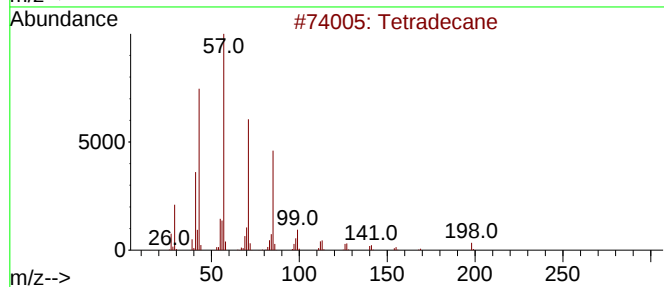
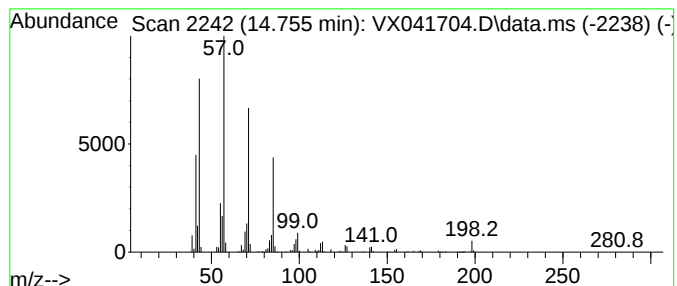
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Quant Title : SW846 8260

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

Peak Number 9 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	32.36 ug/l	482264	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	98
2			Hexadecane	226	C16H34	000544-76-3	91
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
4			Tridecane	184	C13H28	000629-50-5	86
5			Tridecane, 7-propyl-	226	C16H34	055045-09-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

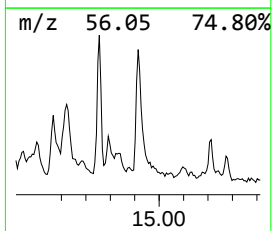
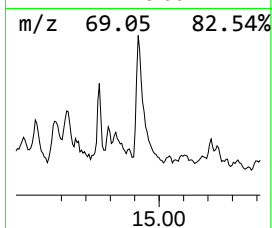
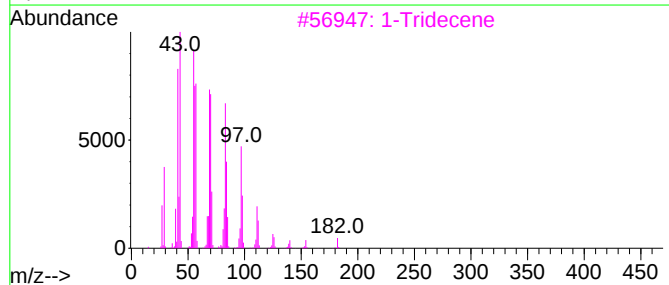
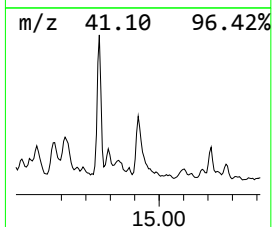
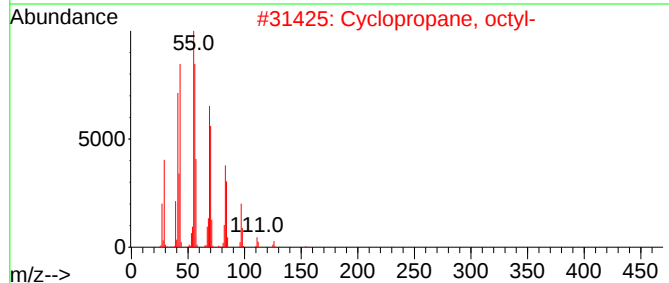
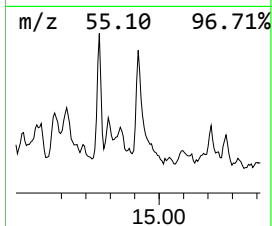
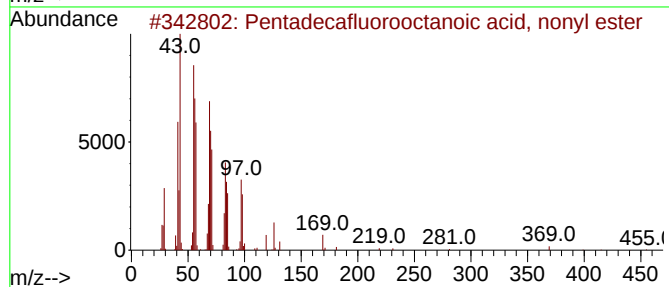
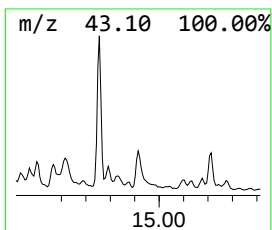
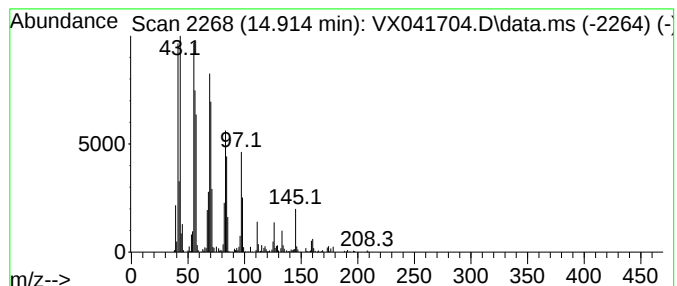
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Quant Title : SW846 8260

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

Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.914	34.87 ug/l	519657	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, no...	540	C17H19F15O2	1000406-03-9	87
2			Cyclopropane, octyl-	154	C11H22	001472-09-9	87
3			1-Tridecene	182	C13H26	002437-56-1	87
4			1-Undecanol	172	C11H24O	000112-42-5	87
5			Chloroacetic acid, undecyl ester	248	C13H25ClO2	005458-29-7	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041704.D
Acq On : 03 Jun 2024 15:07
Operator : JC/MD
Sample : P2691-02 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RINSATE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.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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1-Hexanol, 2-et...	12.219	153.2	ug/l	2283490	4	12.024	745079	50.0
Cyclooctane, me...	13.103	31.9	ug/l	475617	4	12.024	745079	50.0
2-Undecene, 4-m...	13.128	74.3	ug/l	1107640	4	12.024	745079	50.0
(S)-(+)-6-Methy...	13.213	58.2	ug/l	867709	4	12.024	745079	50.0
Dodecane	13.268	33.9	ug/l	504884	4	12.024	745079	50.0
1-Nonanol	13.420	128.2	ug/l	1911040	4	12.024	745079	50.0
1-Decanol	14.195	121.0	ug/l	1803270	4	12.024	745079	50.0
Tetradecane	14.756	32.4	ug/l	482264	4	12.024	745079	50.0
Pentadecafluoro...	14.914	34.9	ug/l	519657	4	12.024	745079	50.0