

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
 Data File : VX032796.D
 Acq On : 14 Nov 2022 15:50
 Operator : JC/MD
 Sample : N5572-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31910

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032796.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.391	206	214	224	rBV	35579	70189	5.76%	1.321%
2	2.989	299	312	328	rBV3	6226	30170	2.47%	0.568%
3	4.233	503	516	527	rBV	98808	266325	21.85%	5.011%
4	4.568	562	571	590	rVB2	8580	26997	2.21%	0.508%
5	5.391	694	706	719	rBV2	63950	189482	15.54%	3.565%
6	5.556	722	733	748	rVV	104937	293984	24.12%	5.531%
7	5.958	787	799	809	rBV	70125	184826	15.16%	3.477%
8	6.763	921	931	947	rBV	157988	378258	31.03%	7.117%
9	7.256	1003	1012	1026	rBV7	4047	15339	1.26%	0.289%
10	7.580	1060	1065	1073	rVB2	8995	16221	1.33%	0.305%
11	8.579	1222	1229	1234	rBV	10295	17242	1.41%	0.324%
12	8.646	1234	1240	1247	rVV	337398	532492	43.68%	10.018%
13	8.720	1247	1252	1257	rVV	23539	35732	2.93%	0.672%
14	10.055	1462	1471	1483	rBV	335176	455330	37.35%	8.567%
15	10.305	1507	1512	1520	rVB	13284	20186	1.66%	0.380%
16	10.445	1530	1535	1541	rVB	14772	20563	1.69%	0.387%
17	10.652	1562	1569	1572	rBV2	25971	42453	3.48%	0.799%
18	10.683	1572	1574	1580	rVB	12775	14474	1.19%	0.272%
19	10.756	1582	1586	1594	rBV3	17305	29069	2.38%	0.547%
20	11.079	1634	1639	1645	rBV	330919	419092	34.38%	7.885%
21	11.426	1691	1696	1702	rVB2	8088	12881	1.06%	0.242%
22	11.573	1715	1720	1723	rBV2	9032	12534	1.03%	0.236%
23	11.756	1744	1750	1753	rBV2	10382	13984	1.15%	0.263%
24	11.890	1770	1772	1780	rVB4	11833	19600	1.61%	0.369%
25	12.024	1789	1794	1801	rVB	365625	455016	37.32%	8.561%
26	12.219	1821	1826	1838	rBV	940708	1219090	100.00%	22.936%
27	12.304	1838	1840	1848	rVB4	27828	45561	3.74%	0.857%
28	12.414	1853	1858	1864	rVB	101994	127902	10.49%	2.406%
29	12.566	1878	1883	1886	rBV4	8438	14369	1.18%	0.270%
30	13.292	1995	2002	2007	rBV9	9258	20108	1.65%	0.378%
31	13.420	2019	2023	2033	rVB5	13573	29274	2.40%	0.551%
32	13.774	2078	2081	2084	rVV	26830	37961	3.11%	0.714%
33	13.804	2084	2086	2089	rVV	30152	34575	2.84%	0.650%
34	13.841	2089	2092	2099	rVB4	21106	34736	2.85%	0.654%
35	13.914	2100	2104	2111	rVB2	17459	25080	2.06%	0.472%
36	14.639	2214	2223	2232	rVB3	18050	43556	3.57%	0.819%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

37	14.779	2240	2246	2251	rBV	18708	26615	2.18%	0.501%
38	15.481	2354	2361	2366	rBV4	10946	19624	1.61%	0.369%
39	15.615	2378	2383	2386	rBV2	12716	19204	1.58%	0.361%
40	15.651	2386	2389	2395	rVB	9024	12881	1.06%	0.242%
41	15.974	2435	2442	2454	rBV7	14309	32170	2.64%	0.605%

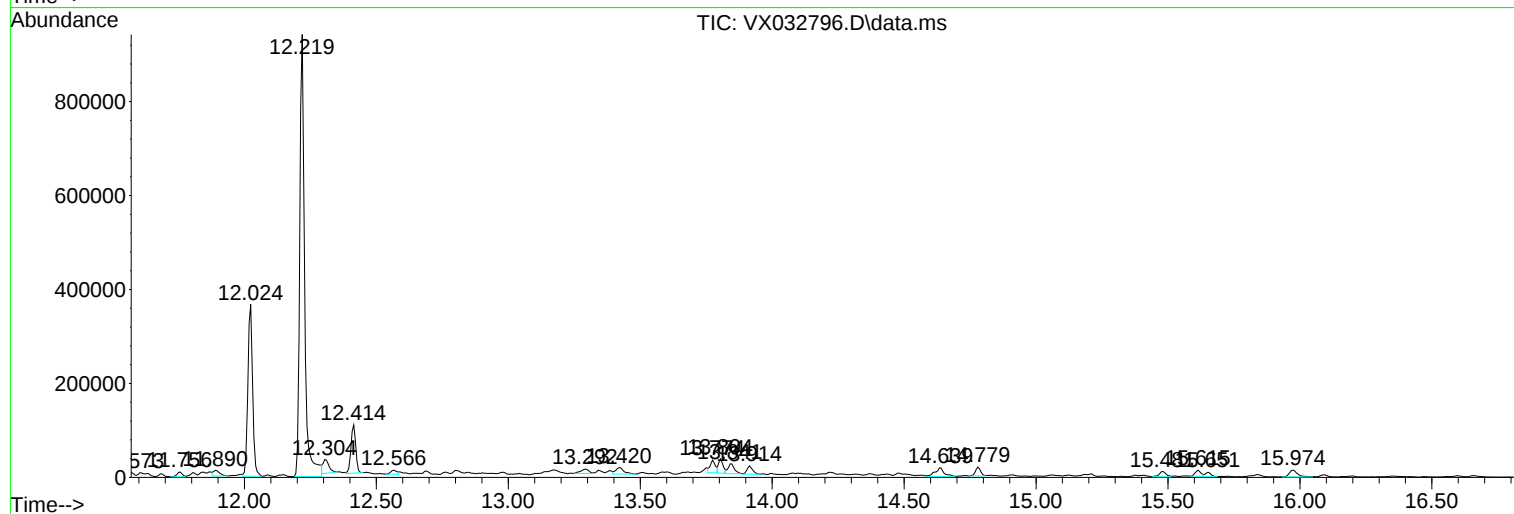
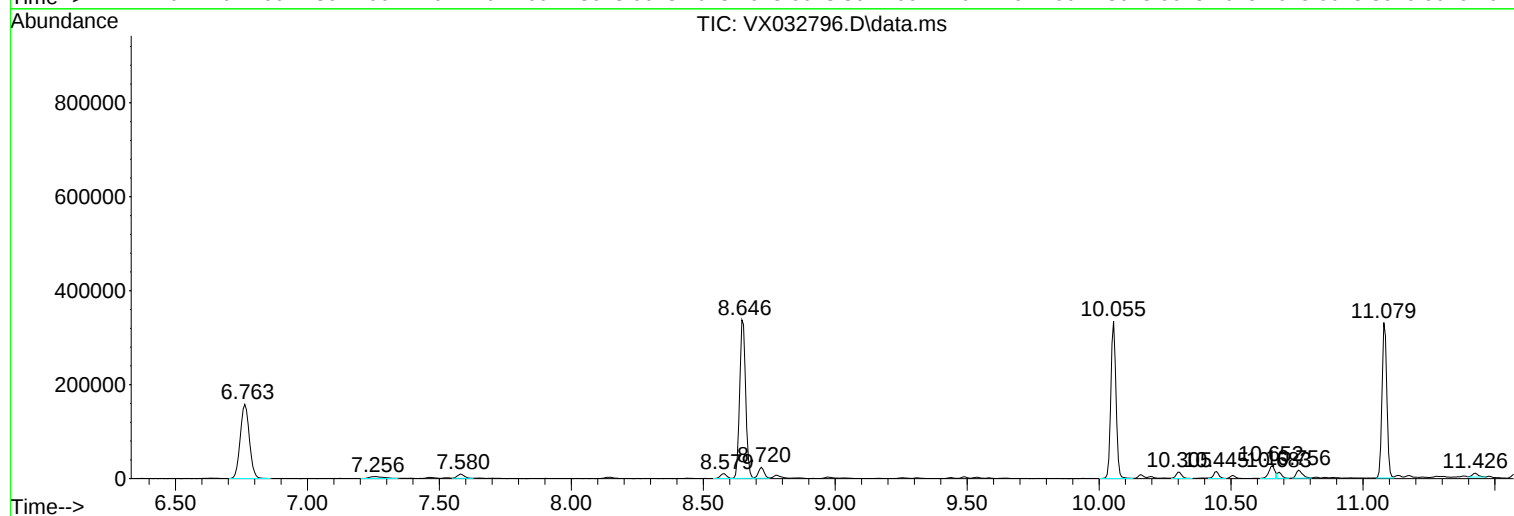
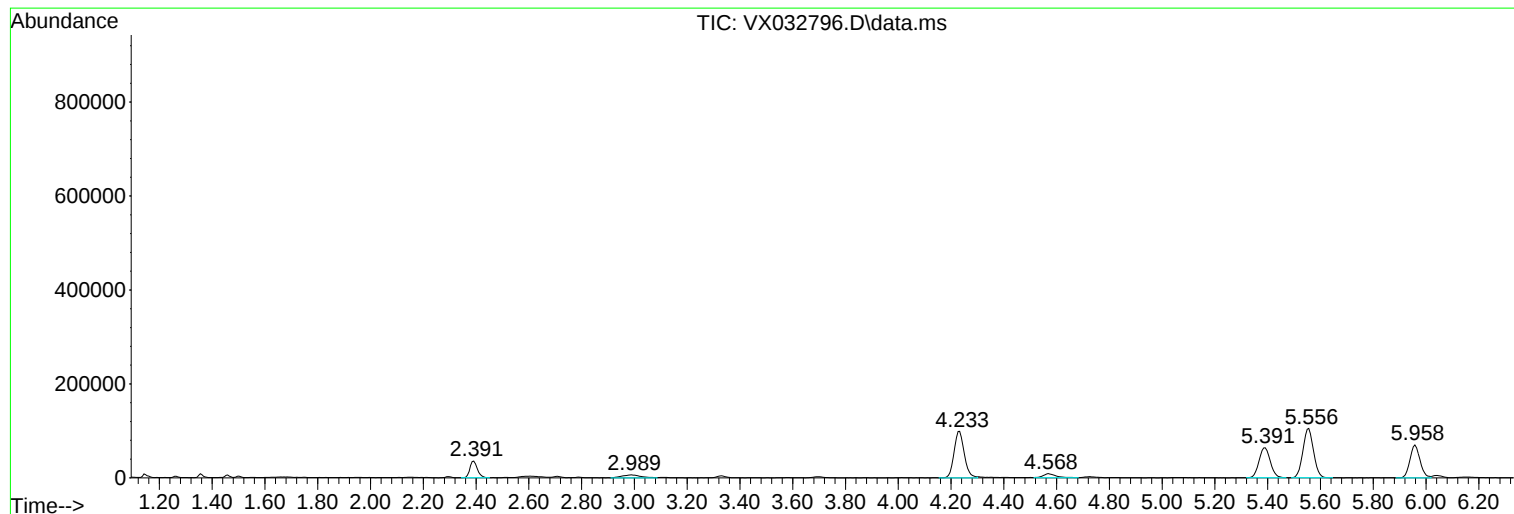
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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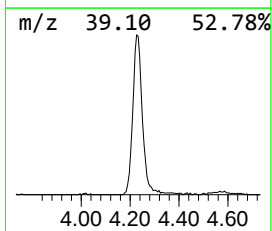
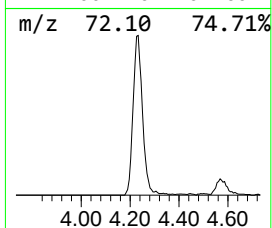
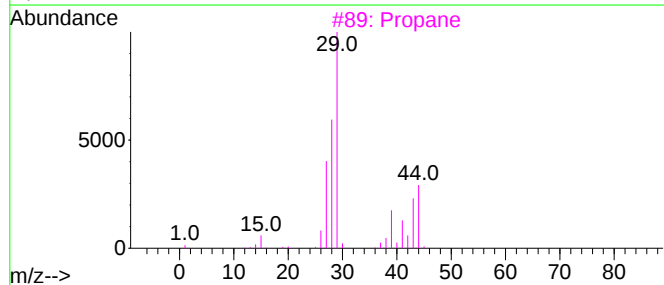
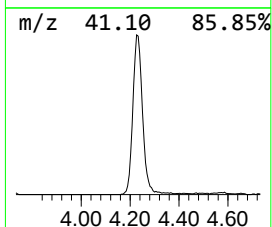
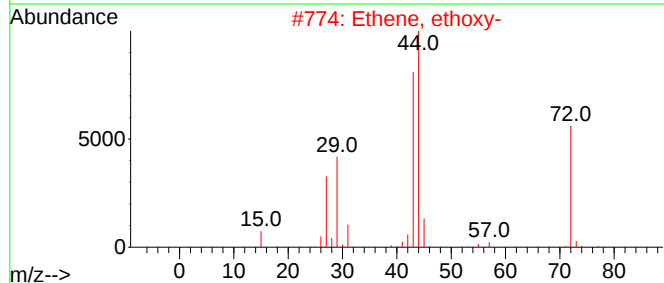
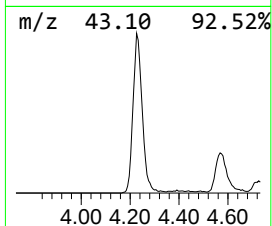
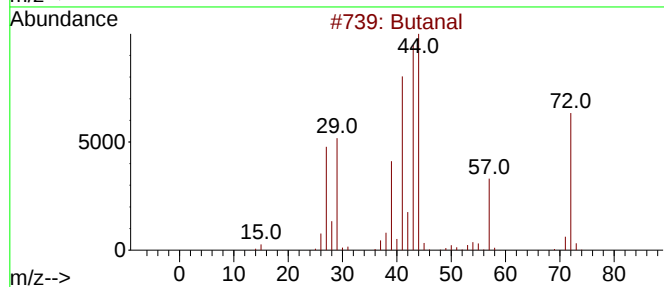
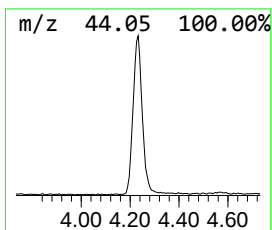
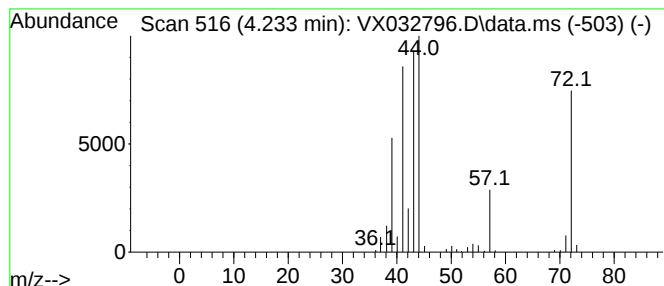
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	45.30 ug/l	266325	Pentafluorobenzene	5.556

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			Propane	44	C3H8	000074-98-6	50
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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Instrument :
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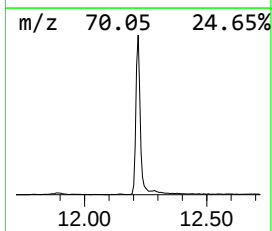
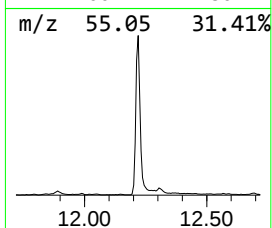
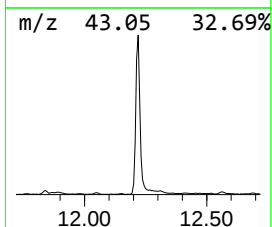
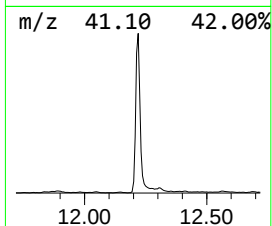
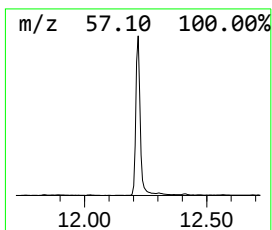
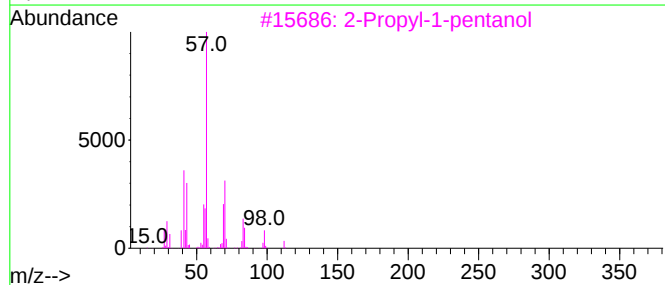
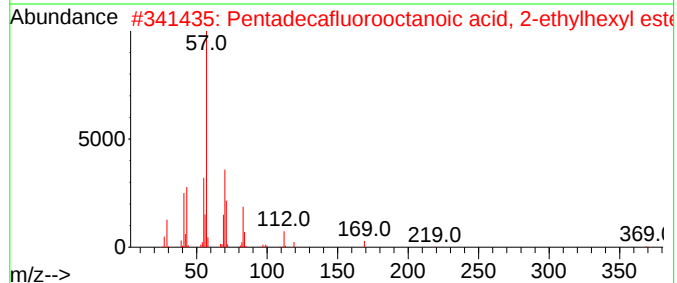
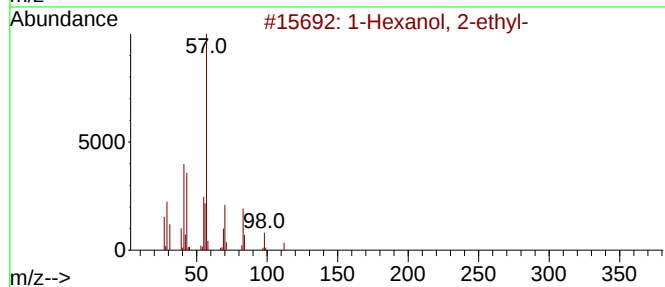
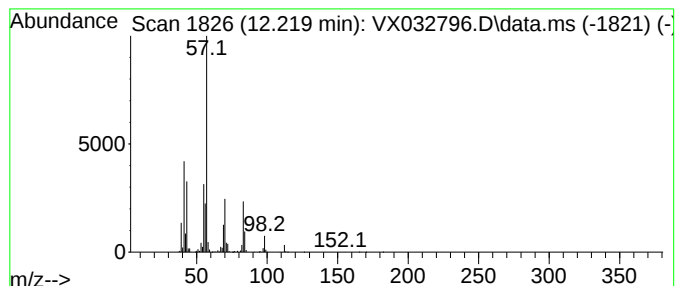
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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	133.96 ug/l	1219090	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		Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5		Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43



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ClientSampleId :
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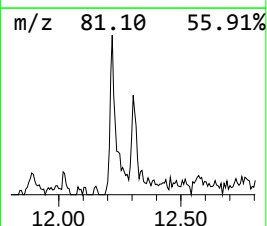
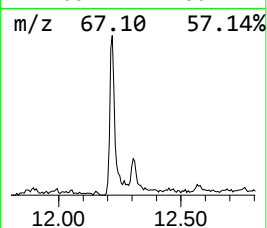
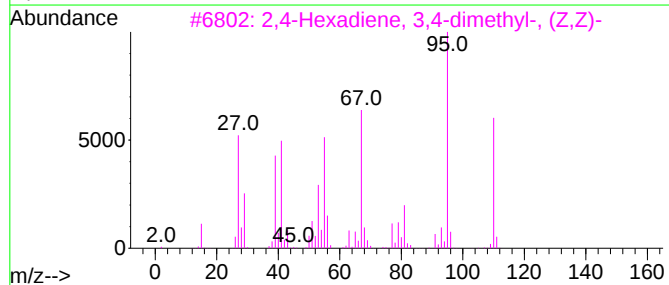
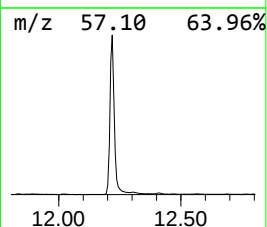
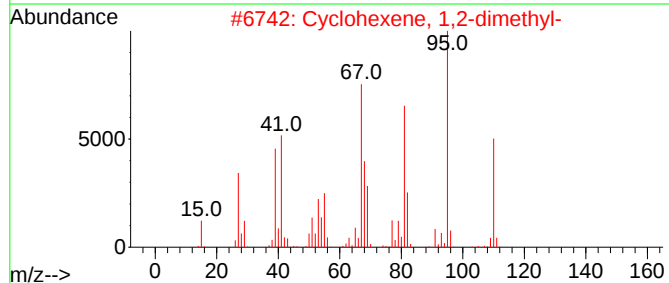
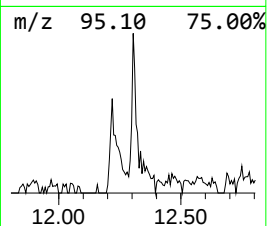
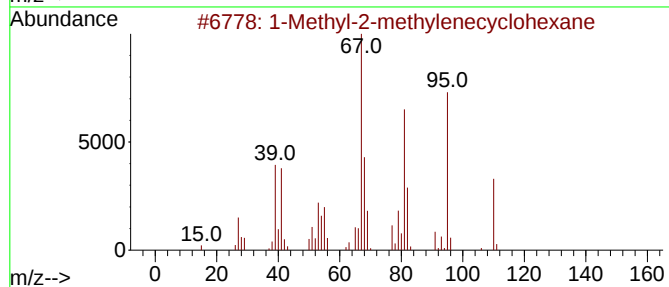
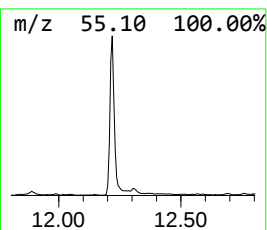
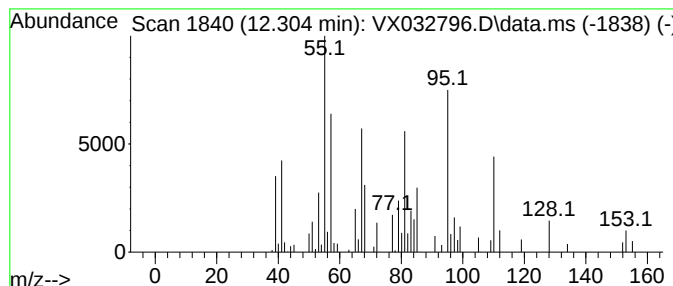
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Methyl-2-methylenecyclohe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	5.01 ug/l	45561	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	64
2			Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	64
3			2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	52
4			2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	52
5			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	52



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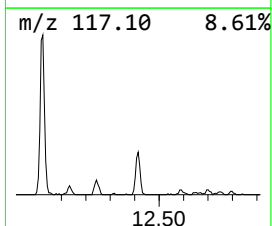
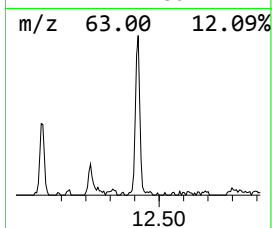
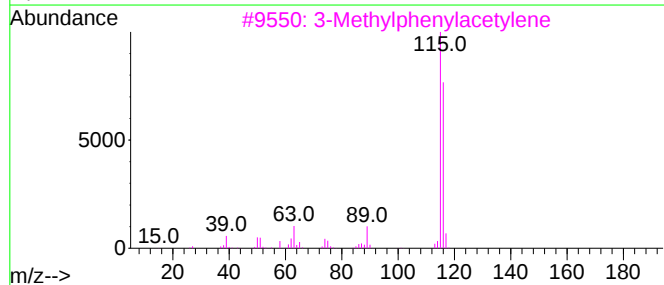
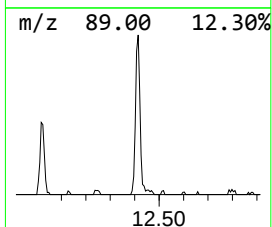
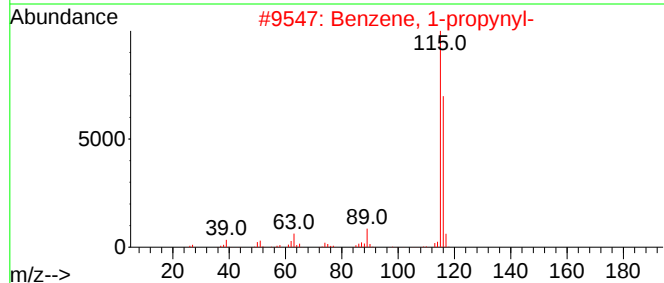
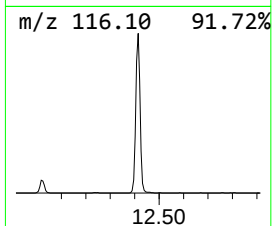
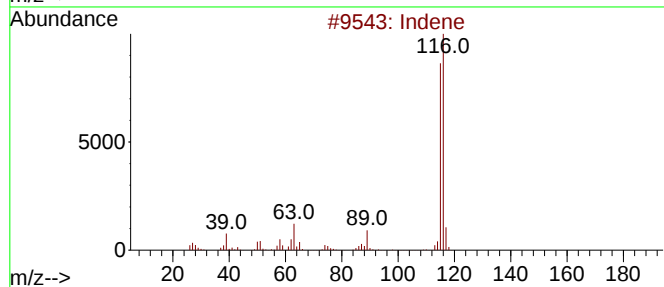
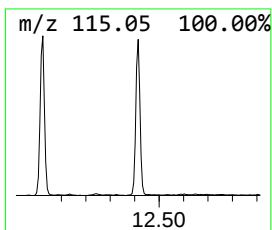
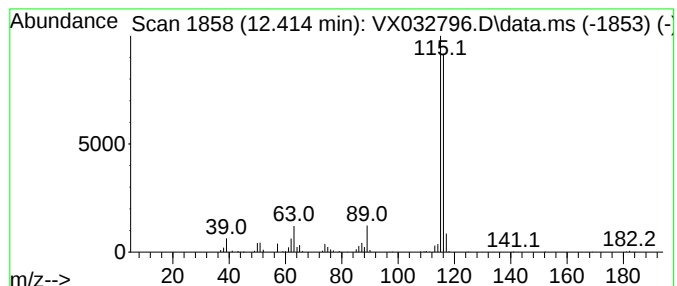
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	14.05 ug/l	127902	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.233	45.3	ug/l	266325	1	5.556	293984	50.0
1-Hexanol, 2-et...	12.219	134.0	ug/l	1219090	4	12.024	455016	50.0
1-Methyl-2-meth...	12.304	5.0	ug/l	45561	4	12.024	455016	50.0
Indene	12.414	14.1	ug/l	127902	4	12.024	455016	50.0