

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
 Data File : VX021384.D
 Acq On : 23 Mar 2021 14:46
 Operator : JC/MD
 Sample : IBLK
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 IBLK

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\82X031621W.M
 Title : SW846 8260

Signal : TIC: VX021384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	78	87	90	rBV8	4418	9744	2.02%	0.301%
2	5.470	732	745	760	rBV	58353	164403	34.16%	5.077%
3	5.629	760	772	785	rBV	100659	281641	58.52%	8.698%
4	6.035	830	841	853	rBV	68207	175169	36.40%	5.410%
5	6.835	966	977	990	rBV	155266	360512	74.90%	11.134%
6	8.694	1285	1293	1313	rBV	298878	481295	100.00%	14.864%
7	10.094	1525	1531	1542	rBV	286038	388556	80.73%	12.000%
8	10.624	1614	1621	1625	rBV5	4457	7674	1.59%	0.237%
9	10.706	1629	1635	1638	rBV	4702	6955	1.45%	0.215%
10	10.818	1646	1654	1658	rBV	20490	26754	5.56%	0.826%
11	10.894	1658	1667	1670	rBV4	9047	18227	3.79%	0.563%
12	10.930	1670	1673	1678	rVB	11304	15937	3.31%	0.492%
13	10.988	1678	1683	1688	rVB4	4343	7274	1.51%	0.225%
14	11.041	1688	1692	1693	rBV2	4159	5285	1.10%	0.163%
15	11.065	1693	1696	1700	rVB3	7539	10814	2.25%	0.334%
16	11.118	1700	1705	1711	rBV	217762	292252	60.72%	9.026%
17	11.259	1723	1729	1733	rBV2	14613	21472	4.46%	0.663%
18	11.377	1745	1749	1754	rBV3	6451	11740	2.44%	0.363%
19	11.430	1754	1758	1761	rVV5	6034	8762	1.82%	0.271%
20	11.471	1761	1765	1769	rVV	21396	29463	6.12%	0.910%
21	11.518	1769	1773	1779	rVB5	13676	23505	4.88%	0.726%
22	11.671	1795	1799	1803	rVB3	14511	16630	3.46%	0.514%
23	11.718	1803	1807	1810	rBV2	12823	18510	3.85%	0.572%
24	11.753	1810	1813	1816	rBV	25463	25914	5.38%	0.800%
25	11.783	1816	1818	1821	rBV3	7110	7932	1.65%	0.245%
26	11.877	1829	1834	1837	rBV2	16086	25995	5.40%	0.803%
27	11.930	1837	1843	1847	rVV5	30052	59736	12.41%	1.845%
28	11.983	1847	1852	1855	rVV3	28336	49470	10.28%	1.528%
29	12.012	1855	1857	1860	rVV4	15904	21866	4.54%	0.675%
30	12.059	1860	1865	1872	rVV	260658	348485	72.41%	10.762%
31	12.153	1878	1881	1882	rVV2	5554	6125	1.27%	0.189%
32	12.189	1884	1887	1892	rVB5	11093	17600	3.66%	0.544%
33	12.289	1898	1904	1908	rBV6	9178	19234	4.00%	0.594%
34	12.347	1910	1914	1921	rBV7	19122	40629	8.44%	1.255%
35	12.459	1921	1933	1937	rBV	18264	47549	9.88%	1.468%
36	12.506	1938	1941	1947	rVB4	21301	39569	8.22%	1.222%

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ClientSampleId :
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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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Title : SW846 8260

37	12.594	1950	1956	1958	rBV4	14727	30761	6.39%	0.950%
38	12.665	1967	1968	1973	rVB5	8148	9823	2.04%	0.303%
39	12.718	1973	1977	1981	rBV3	12752	17474	3.63%	0.540%
40	12.853	1997	2000	2006	rVB4	17778	26712	5.55%	0.825%
41	12.924	2007	2012	2015	rBV2	18856	26693	5.55%	0.824%
42	13.024	2025	2029	2032	rBV2	12712	14137	2.94%	0.437%
43	13.336	2079	2082	2087	rVB5	7593	10212	2.12%	0.315%
44	13.636	2127	2133	2134	rBV4	5226	9568	1.99%	0.295%

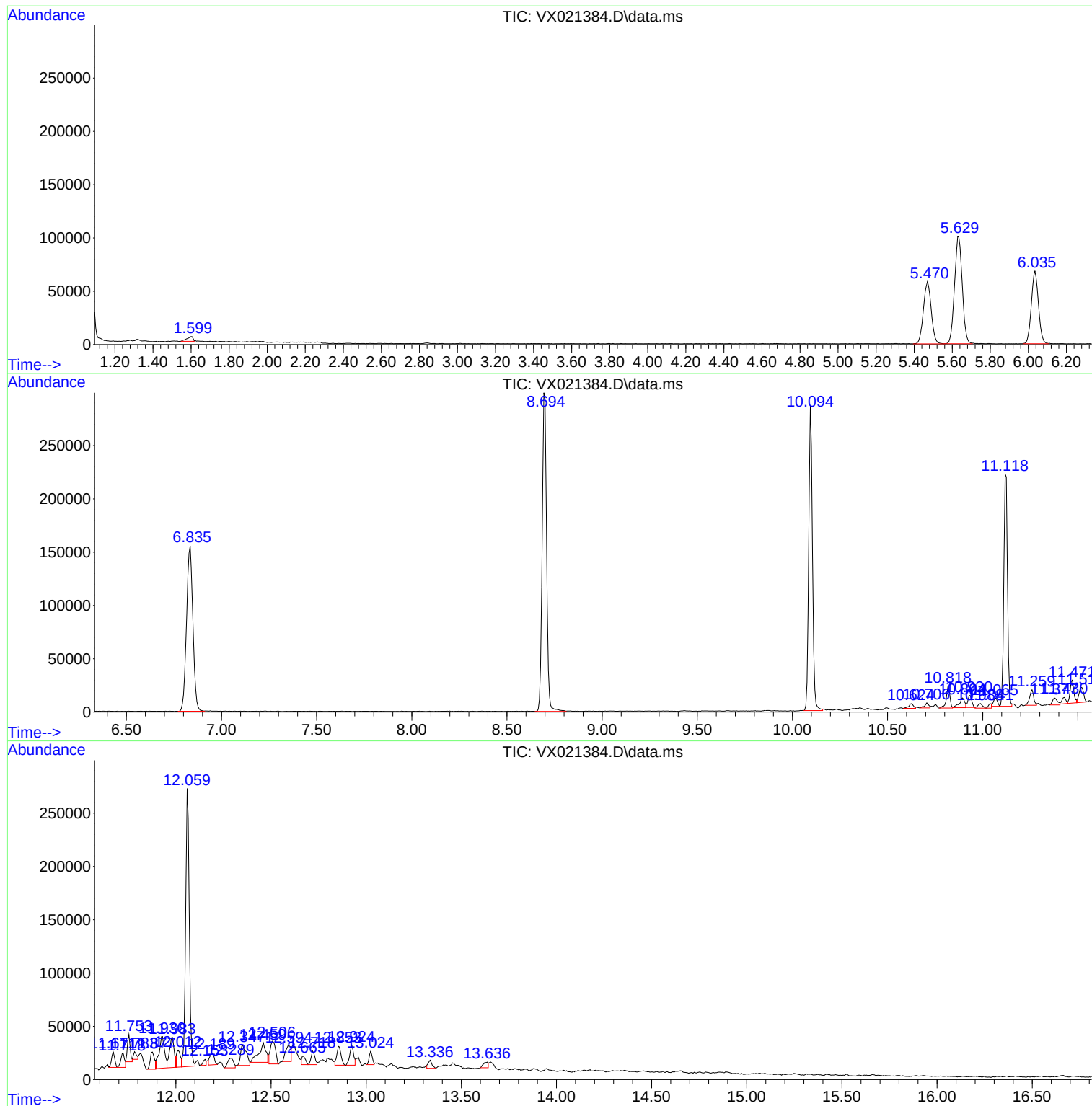
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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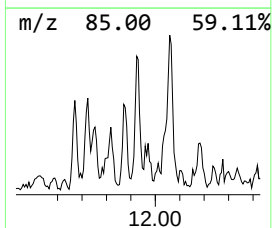
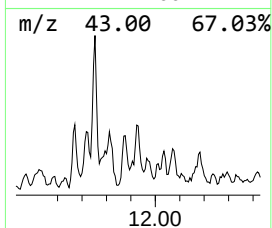
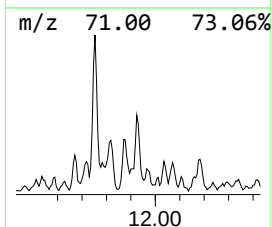
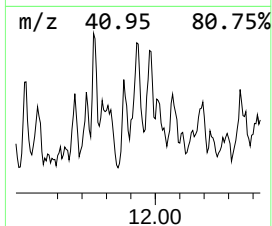
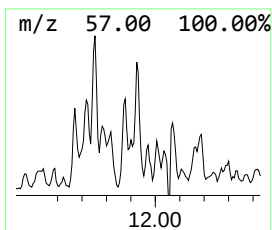
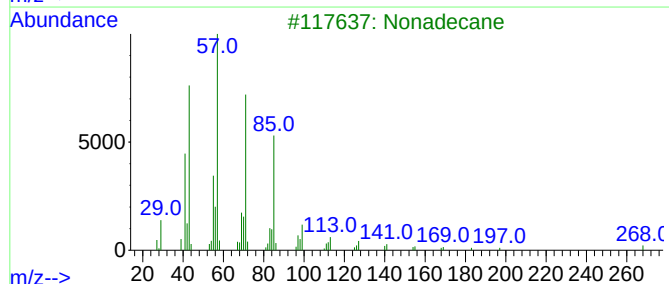
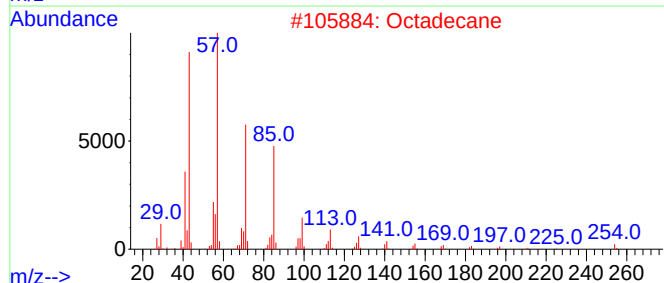
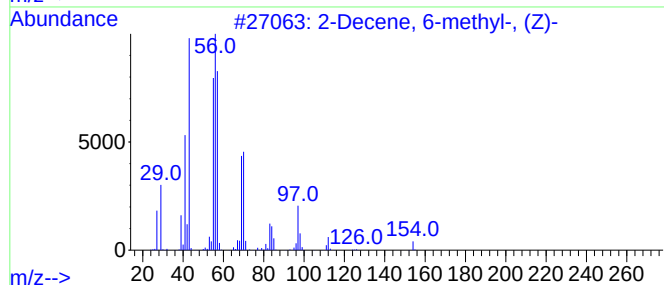
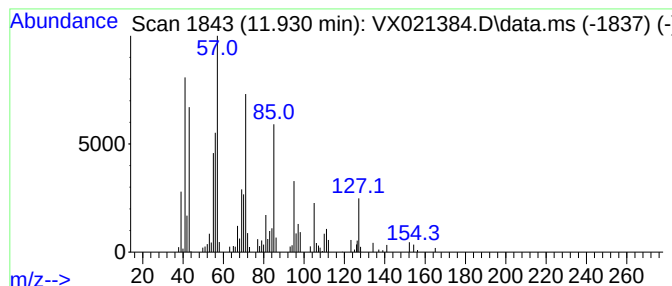
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Decene, 6-methyl-, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.930	8.57 ug/l	59736	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Decene, 6-methyl-, (Z)-	154	C11H22	074630-31-2	60
2		Octadecane	254	C18H38	000593-45-3	43
3		Nonadecane	268	C19H40	000629-92-5	43
4		Heneicosane	296	C21H44	000629-94-7	43
5		5,5-Dimethyl-3-oxo-1-pyrroline, ...	127	C6H9NO2	1000305-98-3	41



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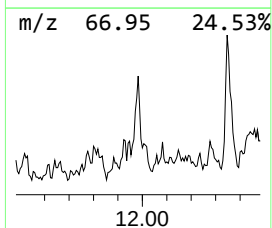
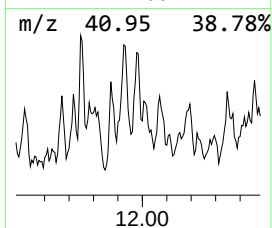
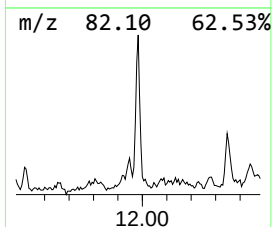
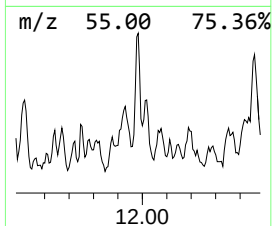
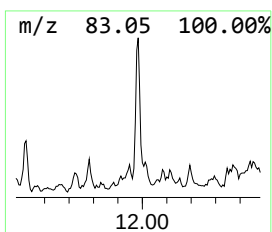
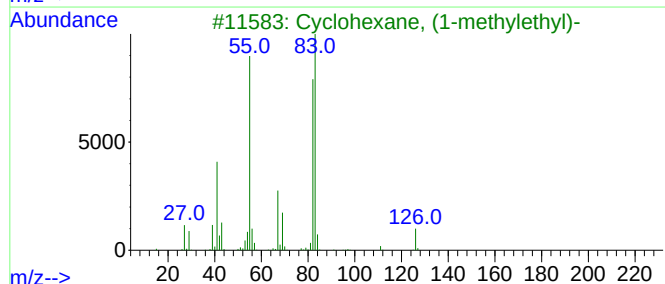
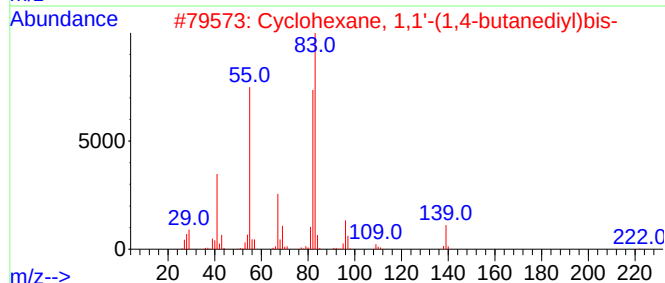
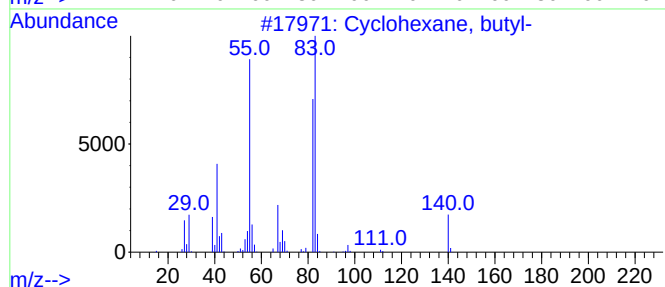
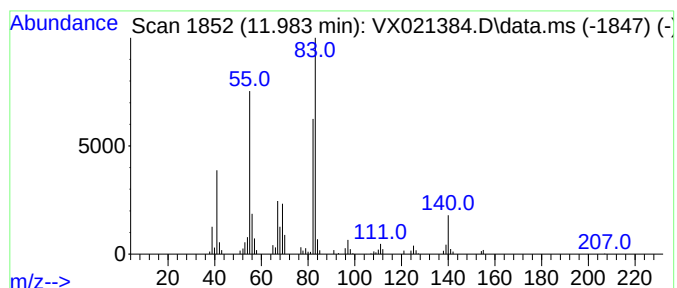
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Cyclohexane, butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.983	7.10 ug/l	49470	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	87
2			Cyclohexane, 1,1'-(1,4-butanediyl)-	222	C16H30	006165-44-2	78
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72
4			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	72
5			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	72



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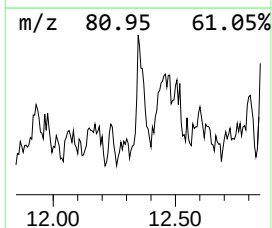
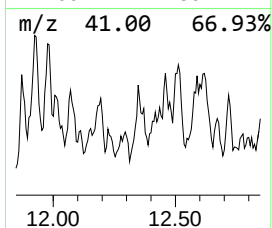
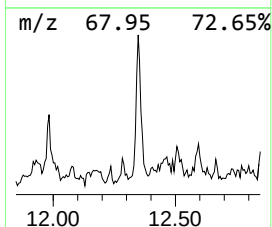
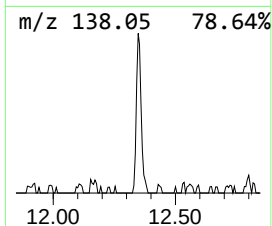
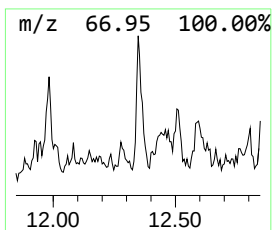
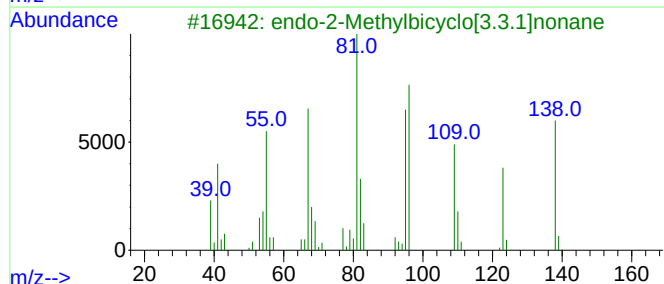
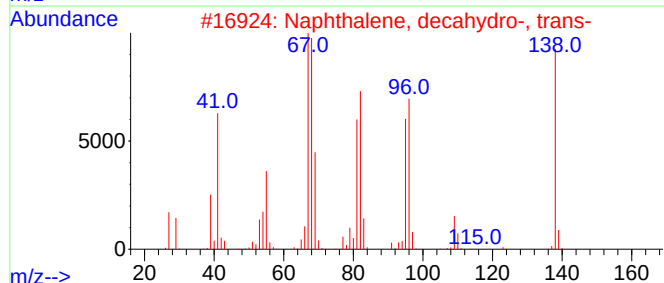
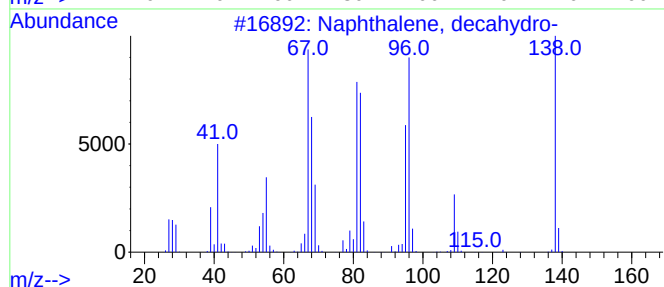
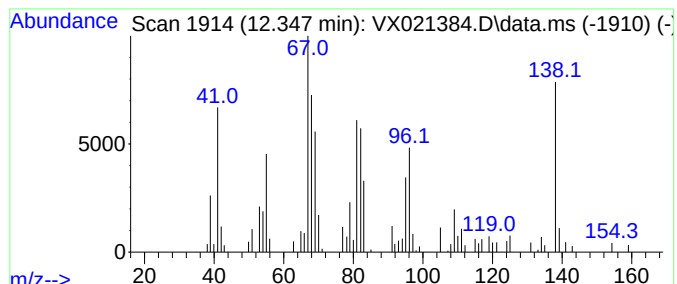
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, decahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.347	5.83 ug/l	40629	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	94
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
3			endo-2-Methylbicyclo[3.3.1]nonane	138	C10H18	042558-37-2	83
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	76
5			Cyclopentanone, 2-(2-methylpropyl)-	138	C9H14O	016856-72-7	64



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Instrument :
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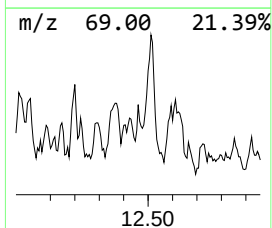
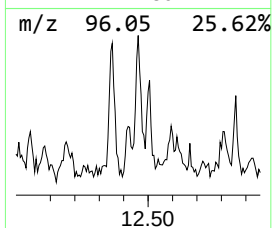
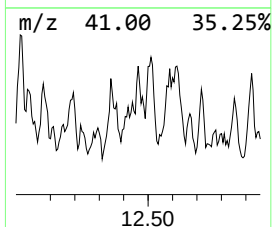
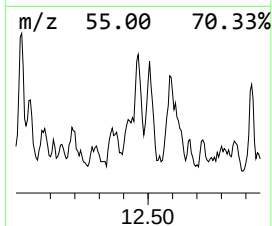
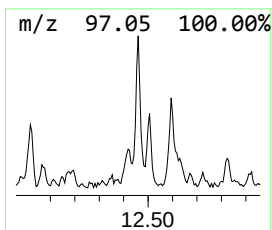
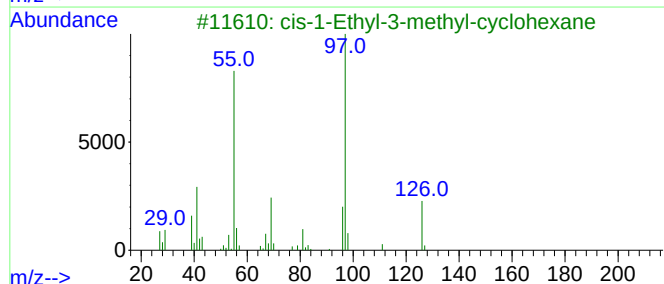
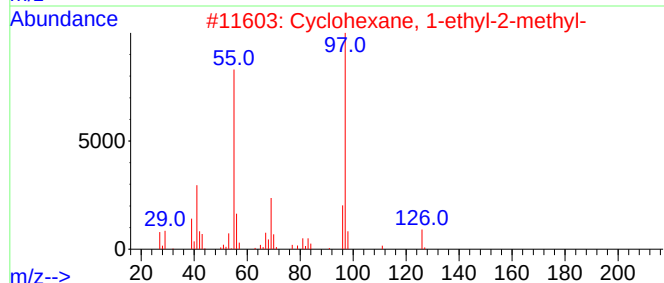
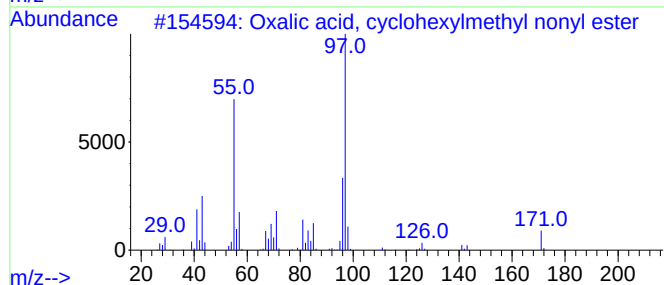
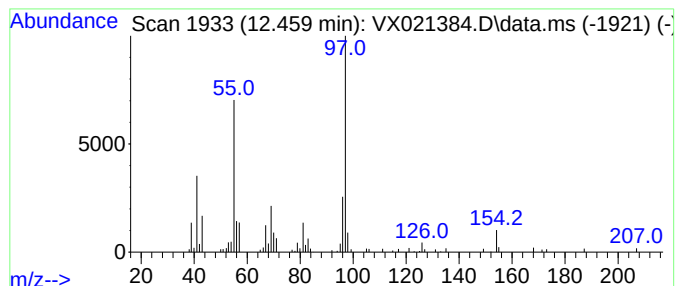
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxalic acid, cyclohexylmeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.459	6.82 ug/l	47549	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclohexylmethyl no...	312	C18H32O4	1000309-68-6	90
2			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	81
3			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	74
4			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	64
5			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	59



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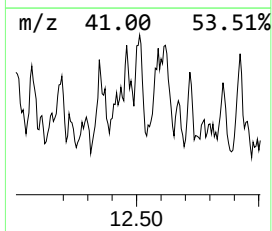
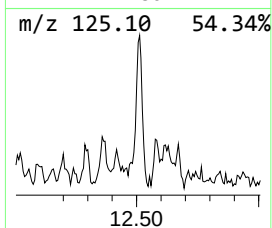
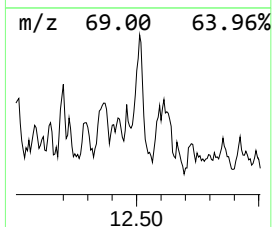
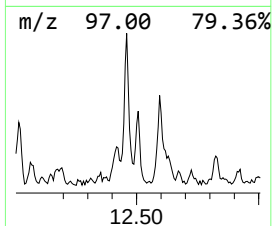
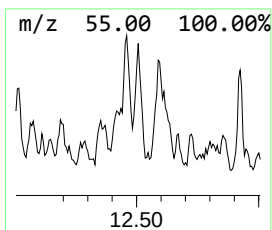
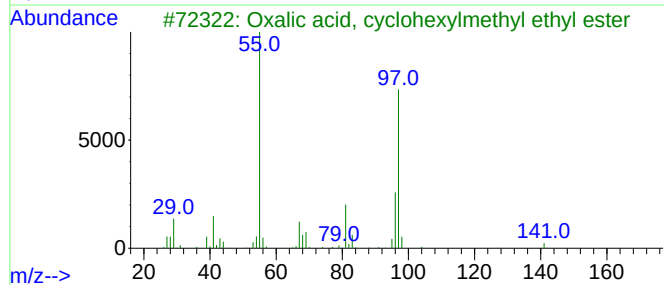
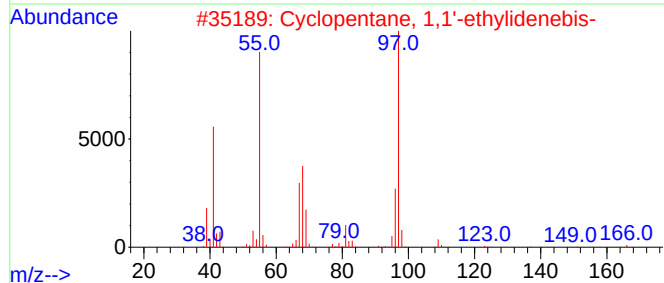
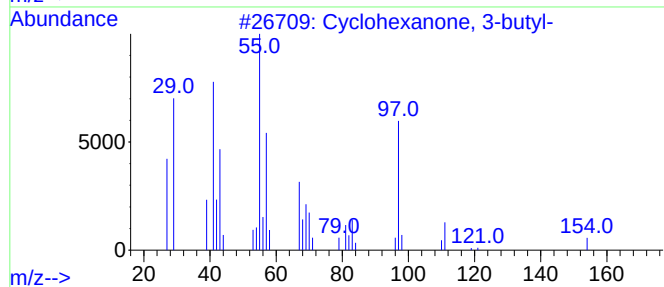
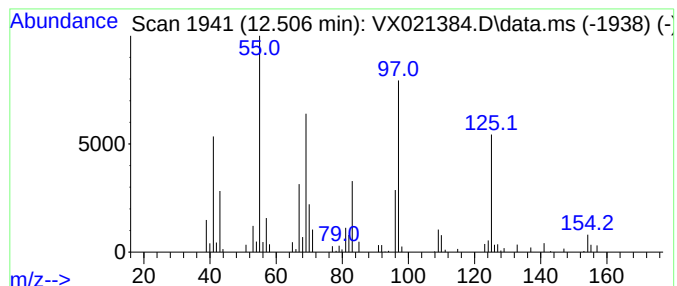
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexanone, 3-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.506	5.68 ug/l	39569	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	50
2			Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	47
3			Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	43
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	43
5			Oxalic acid, di(cyclohexylmethyl...	282	C16H26O4	1000309-68-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021384.D
Acq On : 23 Mar 2021 14:46
Operator : JC/MD
Sample : IBLK
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
IBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Decene, 6-met...	11.930	8.6	ug/l	59736	4	12.059	348485	50.0
Cyclohexane, bu...	11.983	7.1	ug/l	49470	4	12.059	348485	50.0
Naphthalene, de...	12.347	5.8	ug/l	40629	4	12.059	348485	50.0
Oxalic acid, cy...	12.459	6.8	ug/l	47549	4	12.059	348485	50.0
Cyclohexanone, ...	12.506	5.7	ug/l	39569	4	12.059	348485	50.0