

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091218\
 Data File : VX004495.D
 Acq On : 12 Sep 2018 15:28
 Operator : JC/MD
 Sample : J4848-05 10X
 Misc : 4.45µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EP1-MW-B(4-8)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.500	702	713	727	rBV	150300	409703	1.86%	0.155%
2	5.659	728	739	755	rVB	201834	567728	2.58%	0.215%
3	6.067	795	806	819	rBV	152081	393524	1.79%	0.149%
4	6.860	925	936	956	rBV	317391	738827	3.36%	0.280%
5	8.713	1235	1240	1255	rVB	793353	1346581	6.12%	0.510%
6	9.043	1288	1294	1305	rVB	152093	250356	1.14%	0.095%
7	9.445	1350	1360	1369	rBV	629989	946028	4.30%	0.358%
8	9.561	1373	1379	1385	rBV2	417995	882383	4.01%	0.334%
9	9.622	1385	1389	1394	rVB	599287	855610	3.89%	0.324%
10	9.677	1394	1398	1403	rBV	983473	1579191	7.18%	0.598%
11	9.817	1415	1421	1426	rBV	203610	321089	1.46%	0.121%
12	9.878	1426	1431	1437	rVV3	848244	2047346	9.30%	0.775%
13	9.957	1441	1444	1449	rVB	1022389	1320529	6.00%	0.500%
14	10.067	1456	1462	1466	rBV	2027342	2735221	12.43%	1.035%
15	10.116	1466	1470	1474	rVB	767850	991856	4.51%	0.375%
16	10.176	1474	1480	1486	rVB6	182983	408317	1.86%	0.154%
17	10.237	1486	1490	1497	rBV2	448002	858610	3.90%	0.325%
18	10.335	1497	1506	1509	rBV2	1075206	2089109	9.49%	0.790%
19	10.378	1509	1513	1516	rVV	1704713	2380740	10.82%	0.901%
20	10.414	1516	1519	1530	rVB	1077381	1982388	9.01%	0.750%
21	10.512	1530	1535	1541	rBV	641840	971673	4.42%	0.368%
22	10.591	1541	1548	1550	rBV2	261917	381425	1.73%	0.144%
23	10.646	1550	1557	1561	rBV2	2696664	4415204	20.06%	1.671%
24	10.725	1565	1570	1574	rBV2	1536361	2416749	10.98%	0.914%
25	10.768	1574	1577	1581	rVB	891375	1169540	5.31%	0.443%
26	10.841	1581	1589	1593	rBV	8081558	11347607	51.57%	4.294%
27	10.914	1593	1601	1605	rBV2	5533762	9472091	43.04%	3.584%
28	10.951	1605	1607	1612	rVB	3427612	4162749	18.92%	1.575%
29	11.012	1612	1617	1621	rVB3	1041415	1891089	8.59%	0.716%
30	11.060	1621	1625	1626	rBV	1373891	1537939	6.99%	0.582%
31	11.085	1626	1629	1633	rVV2	2578366	3949940	17.95%	1.495%
32	11.140	1633	1638	1643	rVB	6095750	8166028	37.11%	3.090%
33	11.188	1643	1646	1649	rVB2	703479	792623	3.60%	0.300%
34	11.219	1649	1651	1653	rBV	699725	817866	3.72%	0.309%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
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35	11.249	1653	1656	1657	rVV	1138645	1322232	6.01%	0.500%
36	11.280	1657	1661	1669	rVB4	4659928	7098370	32.26%	2.686%
37	11.365	1671	1675	1677	rBV	1213290	1567743	7.12%	0.593%
38	11.396	1677	1680	1684	rVV2	1576645	2658395	12.08%	1.006%
39	11.451	1684	1689	1692	rVV2	2585929	4799602	21.81%	1.816%
40	11.493	1692	1696	1698	rVV	5705958	9295242	42.24%	3.517%
41	11.542	1701	1704	1708	rVV3	3095227	4653111	21.15%	1.761%
42	11.585	1708	1711	1716	rVV4	664120	1014810	4.61%	0.384%
43	11.634	1716	1719	1721	rVV	822790	1014660	4.61%	0.384%
44	11.664	1721	1724	1725	rVV	1098063	1340351	6.09%	0.507%
45	11.688	1725	1728	1733	rVV5	2646002	3970082	18.04%	1.502%
46	11.743	1733	1737	1739	rVV2	2377945	3290582	14.95%	1.245%
47	11.774	1739	1742	1745	rVV	11379035	13298417	60.43%	5.032%
48	11.810	1745	1748	1758	rVB	14548199	22005643	100.00%	8.326%
49	11.896	1758	1762	1764	rBV	1986460	2673361	12.15%	1.012%
50	11.951	1764	1771	1775	rVV4	4840622	9151950	41.59%	3.463%
51	12.005	1775	1780	1782	rVV	6458769	8635909	39.24%	3.268%
52	12.030	1782	1784	1788	rVV3	3673610	4880446	22.18%	1.847%
53	12.097	1788	1795	1798	rVV3	3005280	6308690	28.67%	2.387%
54	12.146	1798	1803	1809	rVV2	3402897	6189294	28.13%	2.342%
55	12.225	1809	1816	1824	rVB6	1712171	4968474	22.58%	1.880%
56	12.304	1824	1829	1830	rBV3	2448528	2918526	13.26%	1.104%
57	12.329	1830	1833	1836	rVB	4054381	4766180	21.66%	1.803%
58	12.377	1836	1841	1847	rVB3	7293439	12611760	57.31%	4.772%
59	12.481	1847	1858	1862	rBV3	1948623	5552693	25.23%	2.101%
60	12.530	1862	1866	1871	rVB3	2036931	3731055	16.95%	1.412%
61	12.591	1871	1876	1877	rBV	2619434	3045144	13.84%	1.152%
62	12.615	1877	1880	1883	rVV	3534911	4853582	22.06%	1.836%
63	12.670	1886	1889	1893	rVV	2214639	2566120	11.66%	0.971%
64	12.743	1897	1901	1902	rBV2	1202349	1426619	6.48%	0.540%
65	12.774	1903	1906	1912	rVB4	1745222	3515092	15.97%	1.330%
66	12.822	1912	1914	1915	rBV	276570	257097	1.17%	0.097%
67	12.853	1916	1919	1921	rBV2	564310	648462	2.95%	0.245%
68	12.877	1921	1923	1926	rBV	666252	657422	2.99%	0.249%
69	12.944	1931	1934	1937	rBV3	1861604	2594999	11.79%	0.982%
70	12.981	1937	1940	1943	rVB	1288587	1538516	6.99%	0.582%
71	13.024	1943	1947	1949	rBV	1806271	2207453	10.03%	0.835%

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72	13.084	1954	1957	1962	rVV3	981977	2261554	10.28%	0.856%
73	13.127	1962	1964	1966	rVV	782435	915497	4.16%	0.346%
74	13.152	1966	1968	1973	rVV	659038	1129672	5.13%	0.427%
75	13.213	1973	1978	1983	rVV4	867240	1997866	9.08%	0.756%
76	13.267	1984	1987	1990	rVV3	597546	815346	3.71%	0.309%
77	13.310	1990	1994	1996	rVV2	699765	1008431	4.58%	0.382%
78	13.347	1996	2000	2007	rVV2	2323332	3790648	17.23%	1.434%
79	13.426	2011	2013	2018	rVV2	341203	572984	2.60%	0.217%
80	13.481	2018	2022	2031	rVB	1514682	2376702	10.80%	0.899%
81	13.566	2031	2036	2039	rBV2	202926	324120	1.47%	0.123%
82	13.639	2044	2048	2053	rBV3	341824	616292	2.80%	0.233%
83	13.725	2059	2062	2067	rVB2	209244	311445	1.42%	0.118%
84	13.834	2077	2080	2087	rVB	341383	543844	2.47%	0.206%

Sum of corrected areas: 264290144

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ClientSampled :
EP1-MW-B(4-8)

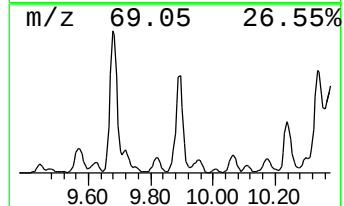
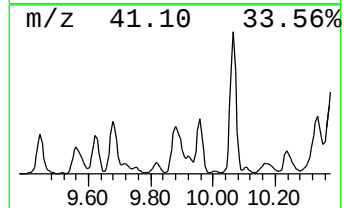
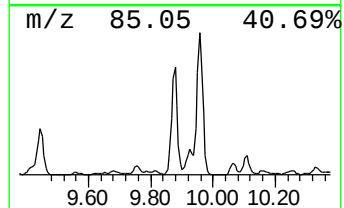
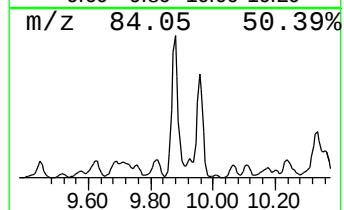
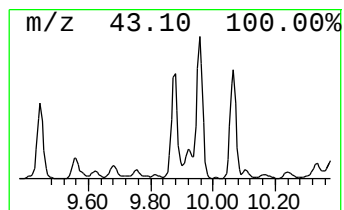
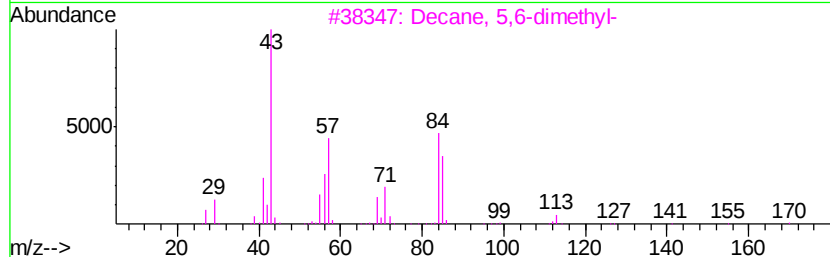
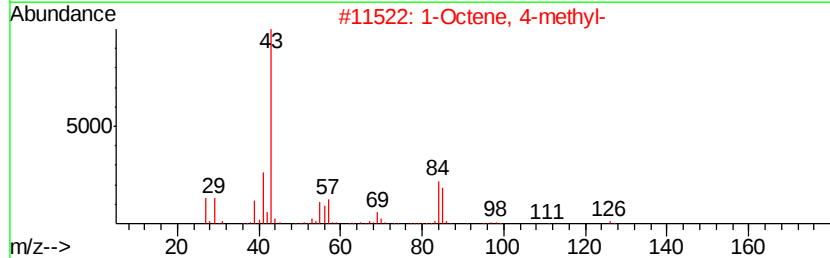
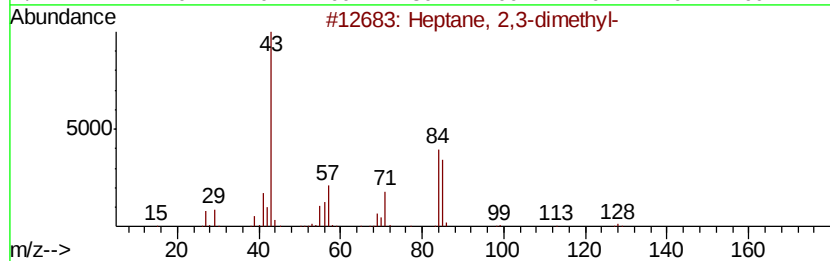
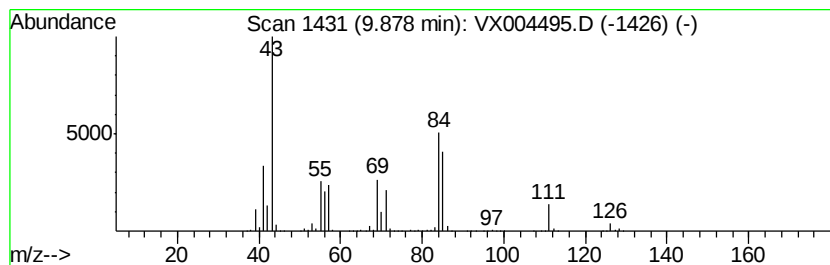
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	103.21 ug/l	2047350	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	83
2		1-Octene, 4-methyl-	126	C9H18	013151-12-7	62
3		Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	59
4		Nonane	128	C9H20	000111-84-2	50
5		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50



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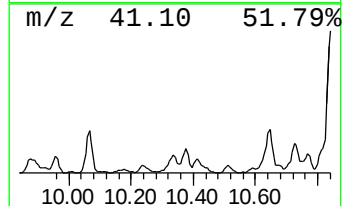
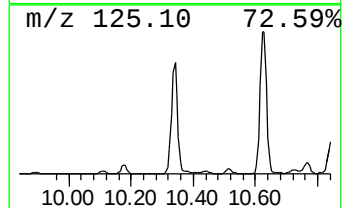
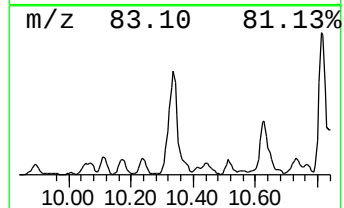
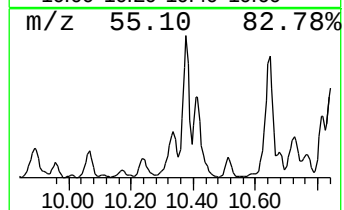
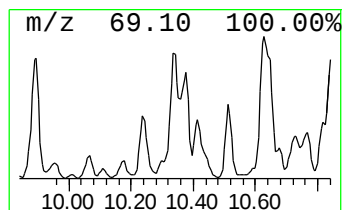
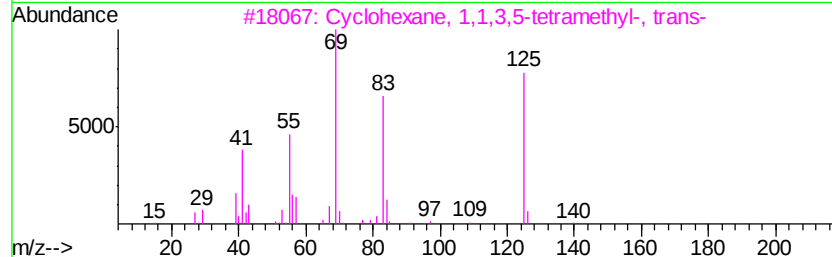
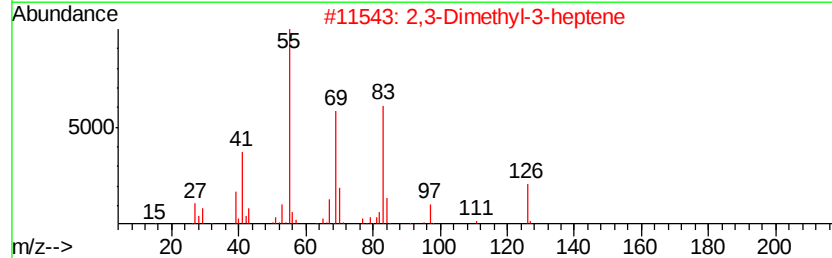
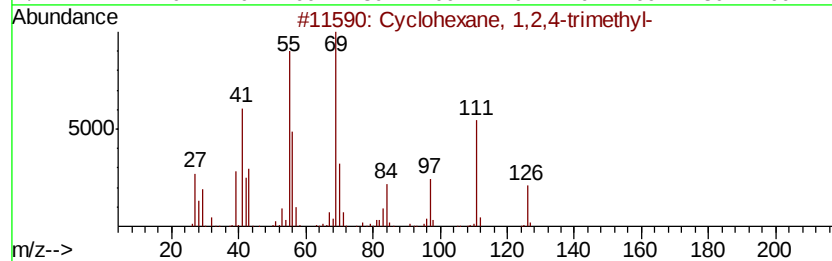
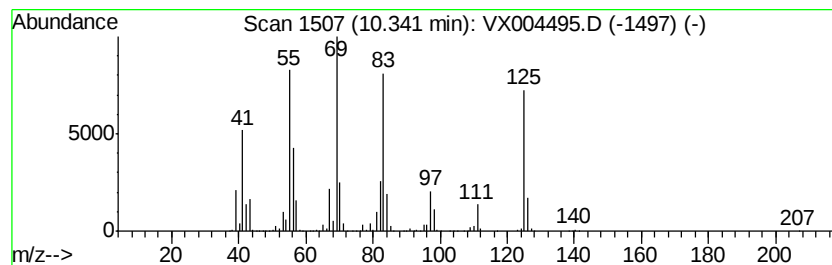
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	105.31 ug/l	2089110	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	70
2		2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	64
3		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	43
4		Cyclopentanone, 2,4,4-trimethyl-	126	C8H14O	004694-12-6	38
5		2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	38



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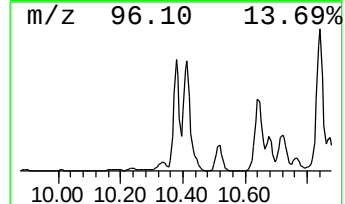
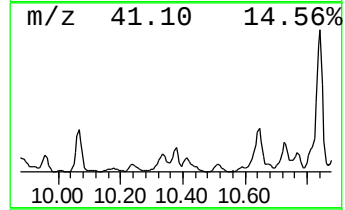
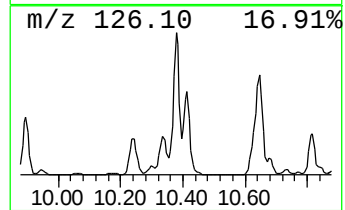
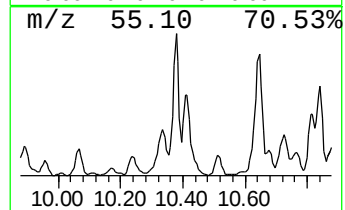
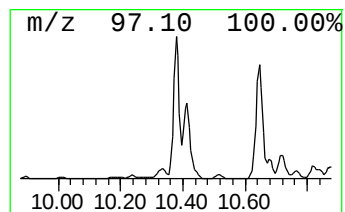
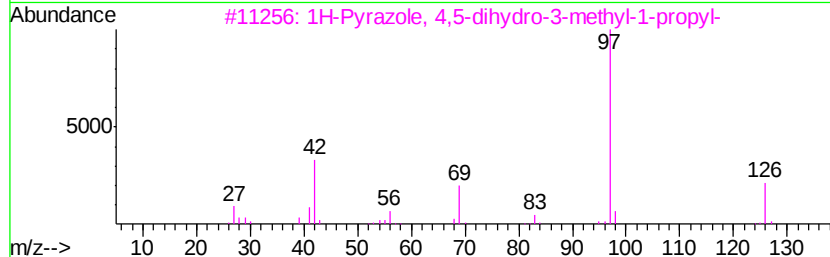
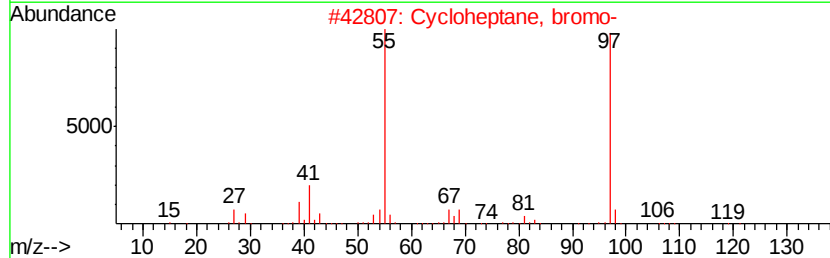
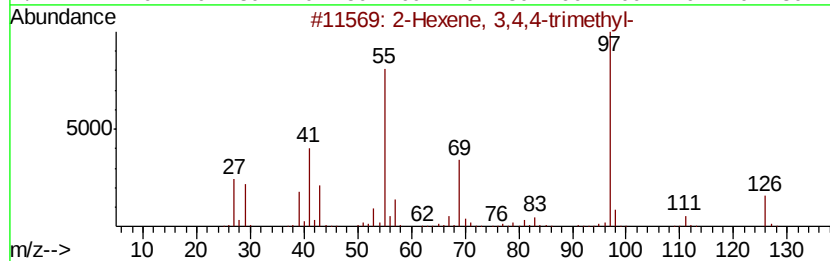
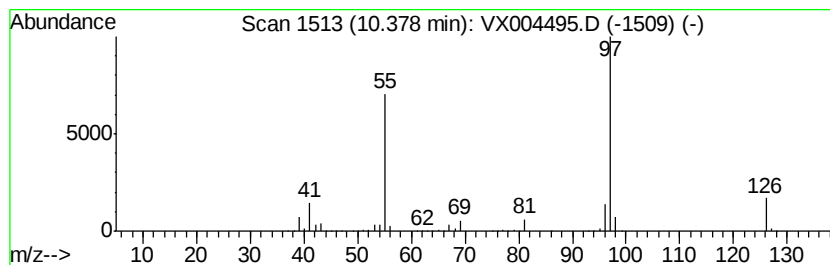
Instrument :
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EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Hexene, 3,4,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.38	120.01 ug/l	2380740	Chlorobenzene-d5	10.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	72
2	Cycloheptane, bromo-	176	C7H13Br	002404-35-5	64
3	1H-Pyrazole, 4,5-dihydro-3-methyl...	126	C7H14N2	026964-49-8	59
4	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	58
5	4-Octen-3-one	126	C8H14O	014129-48-7	56



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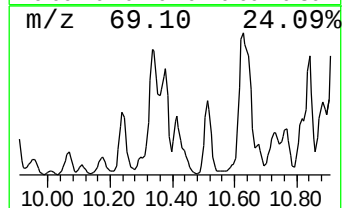
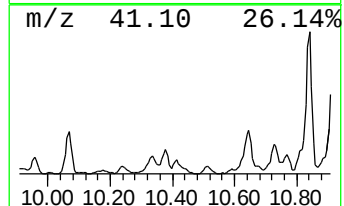
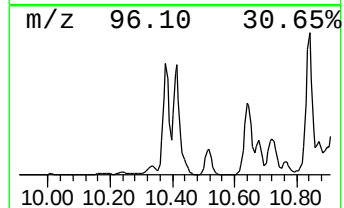
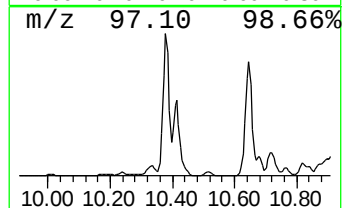
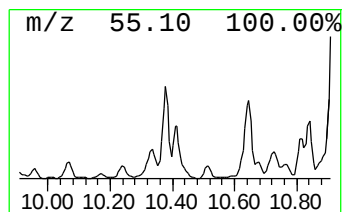
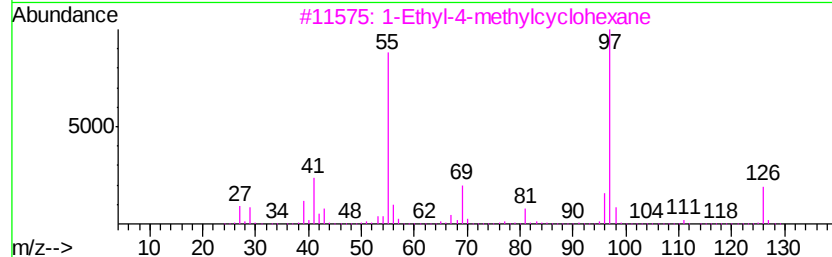
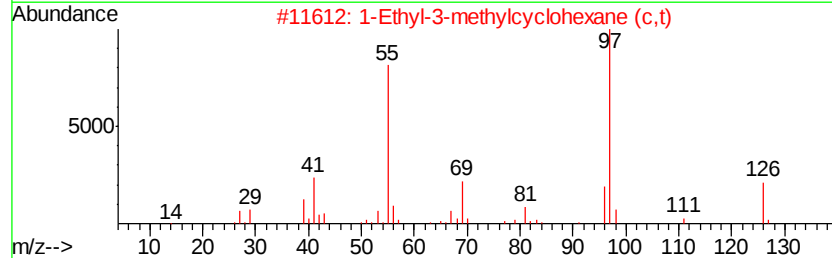
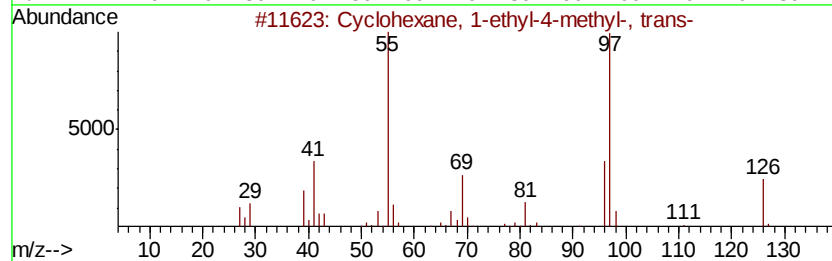
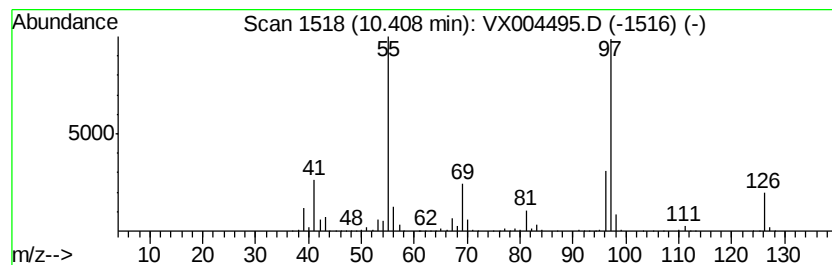
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	99.93 ug/l	1982390	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	94
2		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	90
3		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	90
4		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45u/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

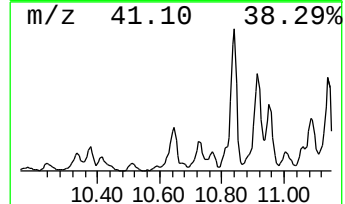
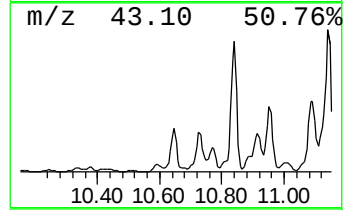
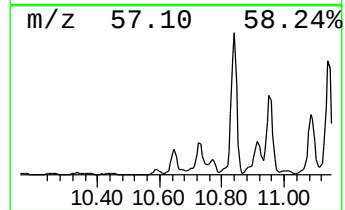
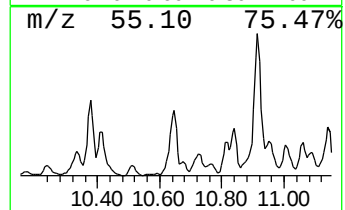
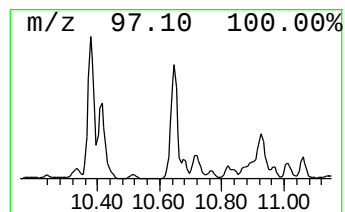
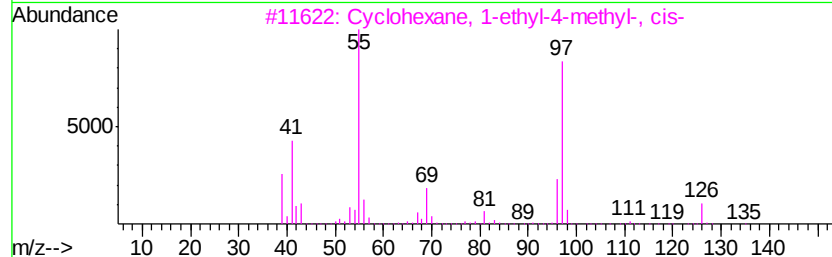
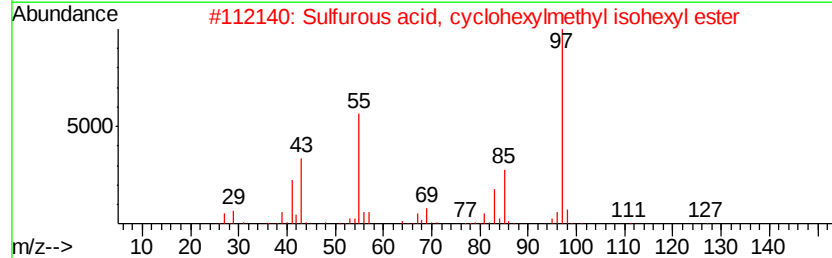
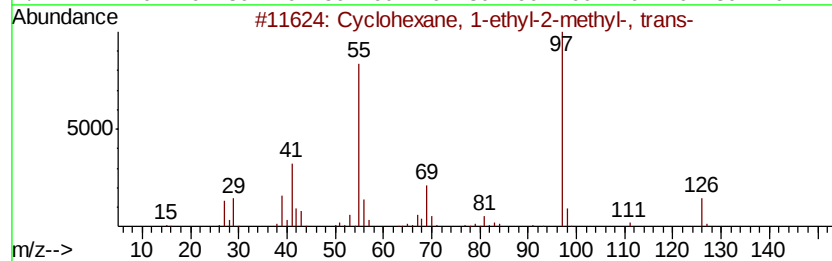
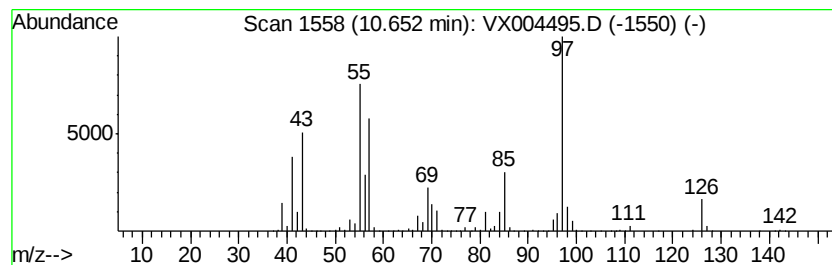
Instrument :
MSVOA_X
ClientSampled :
EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	222.57 ug/l	4415200	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126 C9H18	004923-78-8 64
2		Sulfurous acid, cyclohexylmethyl...	262 C13H26O3S	1000309-21-5 59
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	004926-78-7 58
4		1-Ethyl-4-methylcyclohexane	126 C9H18	003728-56-1 58
5		3-Heptene, 3-ethyl-	126 C9H18	074764-46-8 58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45u/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

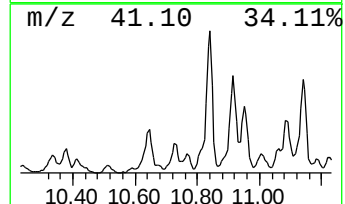
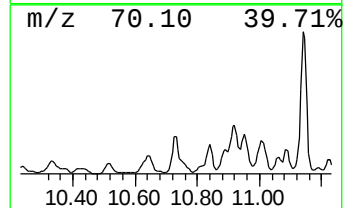
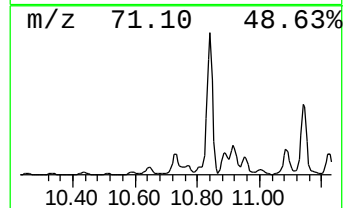
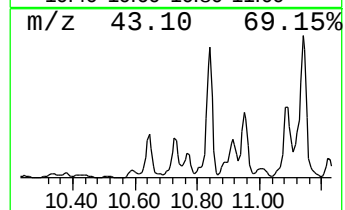
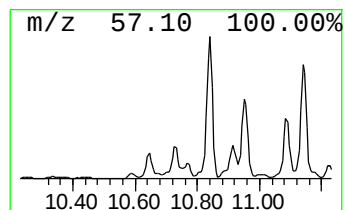
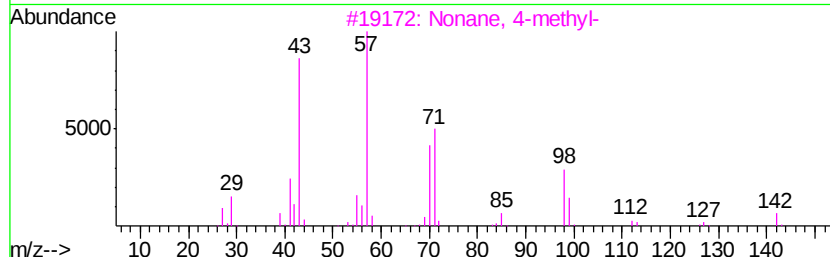
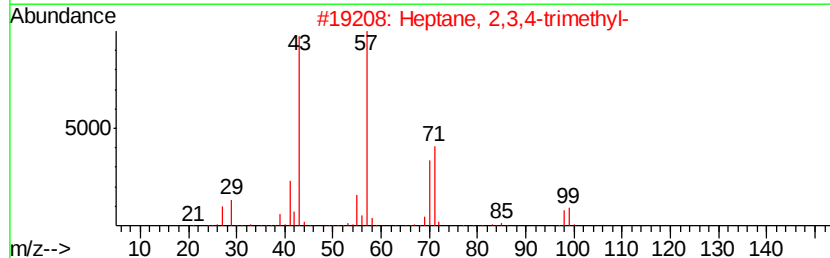
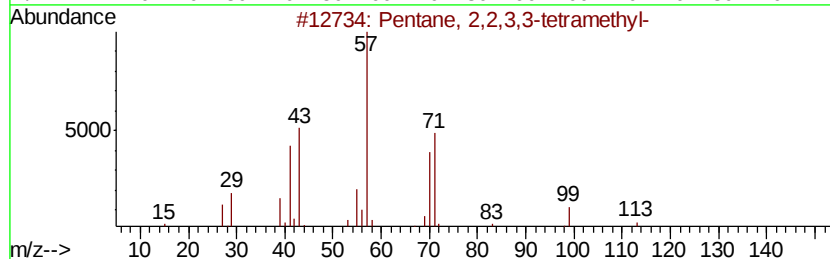
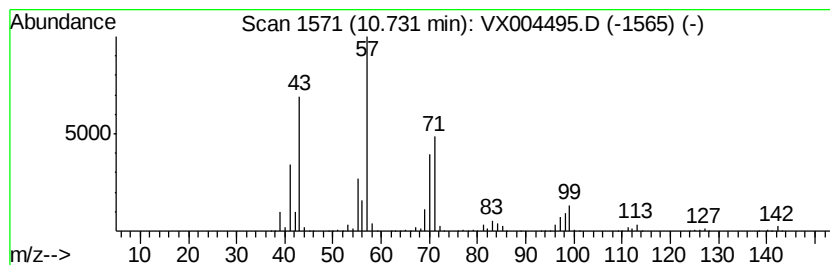
Instrument :
MSVOA_X
ClientSampleId :
EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,3,3-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.73	121.83 ug/l	2416750	Chlorobenzene-d5	10.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	72
2	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	72
3	Nonane, 4-methyl-	142	C10H22	017301-94-9	64
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	52
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45uL/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

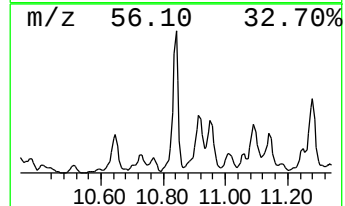
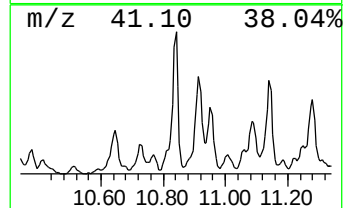
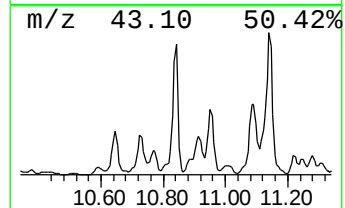
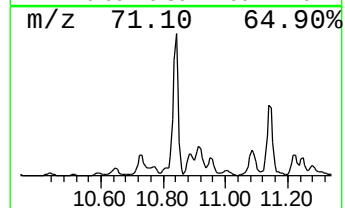
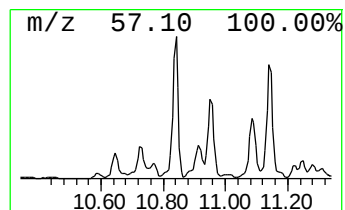
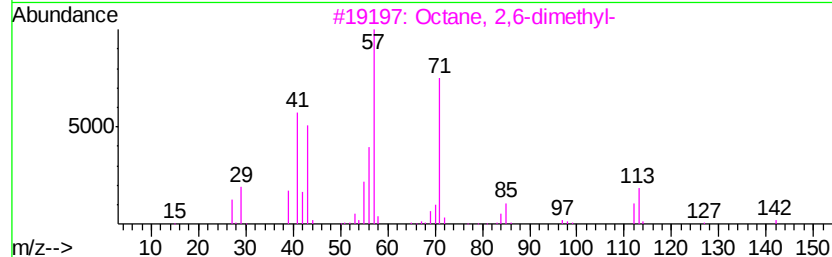
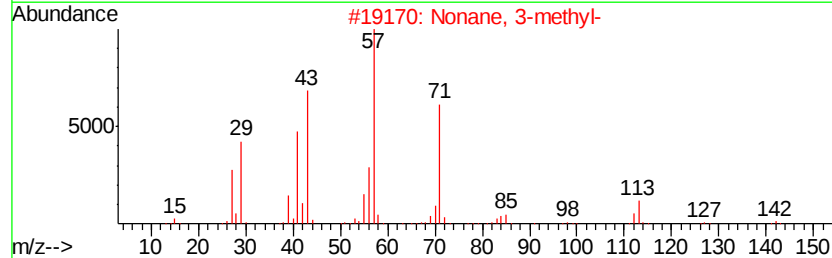
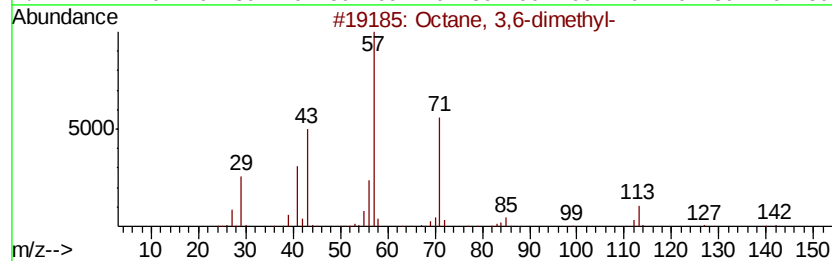
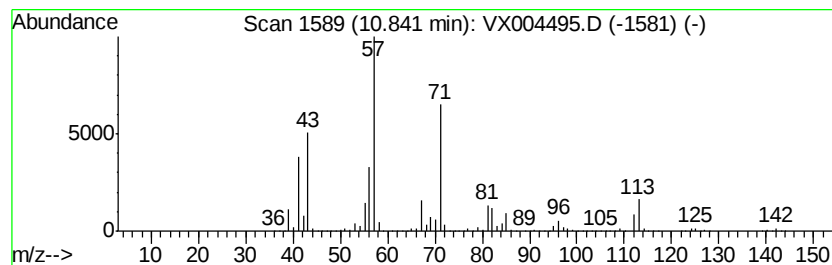
Instrument :
MSVOA_X
ClientSampled :
EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 7 Octane, 3,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	572.04 ug/l	11347600	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octane, 3,6-dimethyl-	142 C10H22	015869-94-0 87
2		Nonane, 3-methyl-	142 C10H22	005911-04-6 87
3		Octane, 2,6-dimethyl-	142 C10H22	002051-30-1 83
4		Sulfurous acid, butyl 2-ethylhex...	250 C12H26O3S	1000309-18-8 59
5		Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2 50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45u/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-MW-B(4-8)

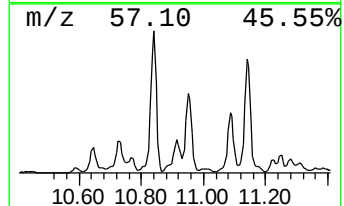
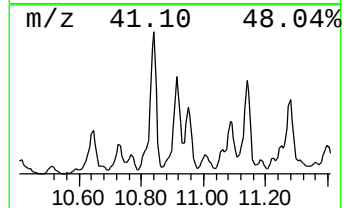
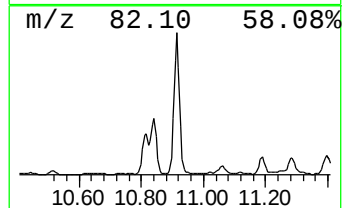
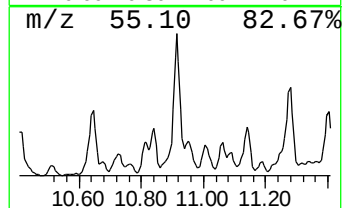
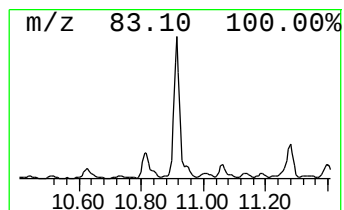
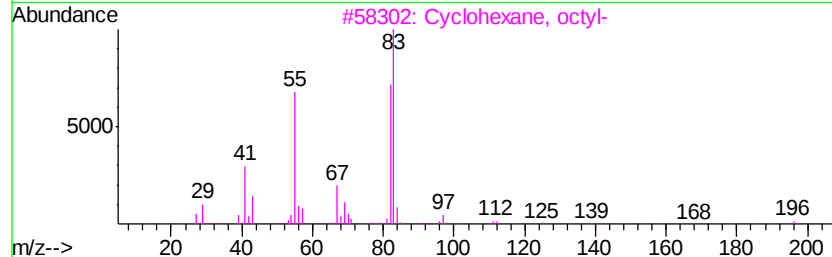
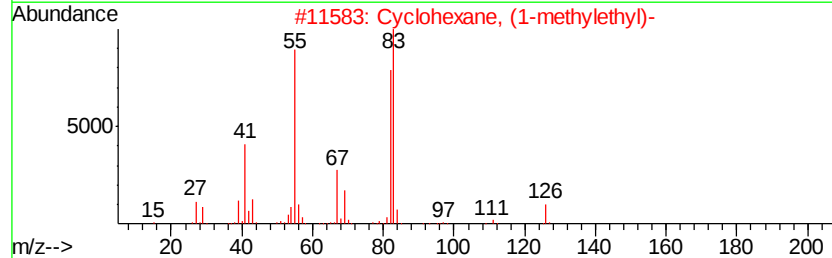
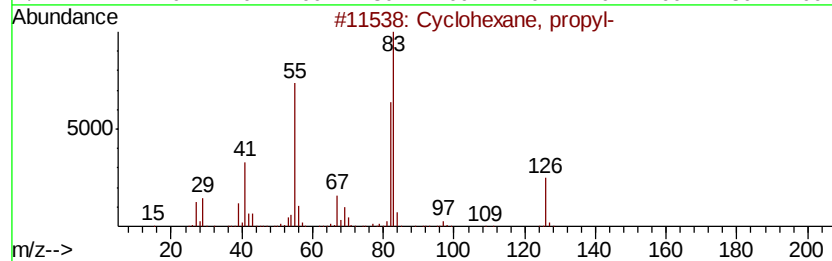
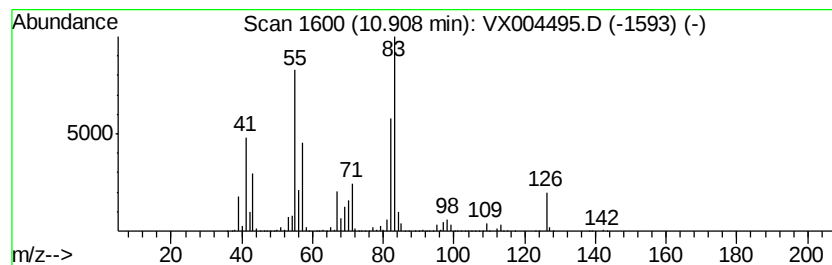
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	477.49 ug/l	9472090	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	81
2		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	64
3		Cyclohexane, octyl-	196	C14H28	001795-15-9	59
4		Cyclohexane, 1,1'-(1,4-butanediol-...)	222	C16H30	006165-44-2	53
5		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45u/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

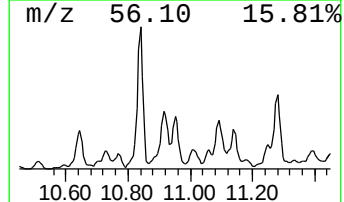
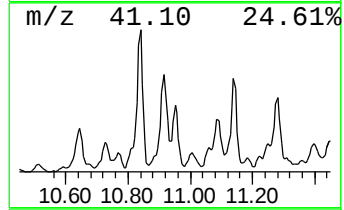
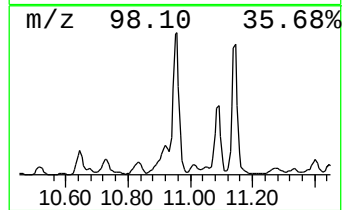
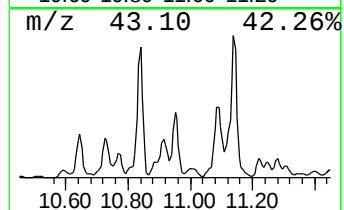
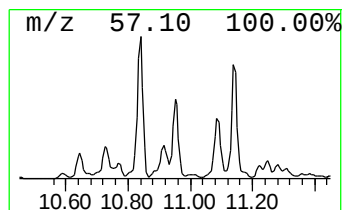
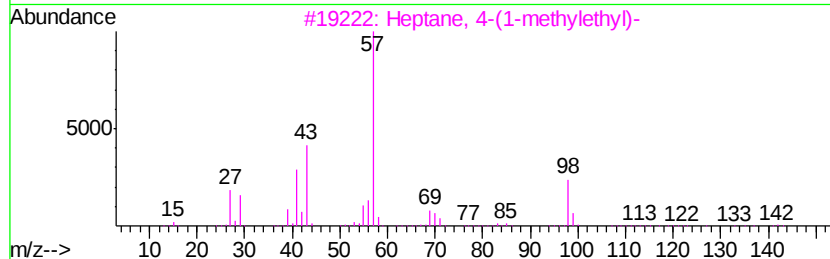
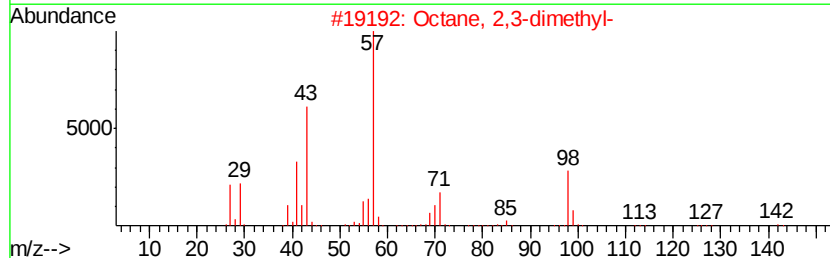
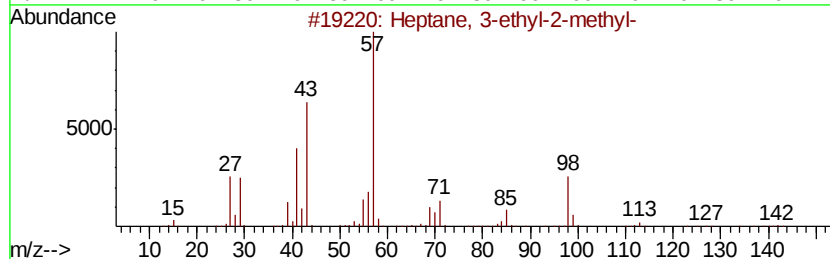
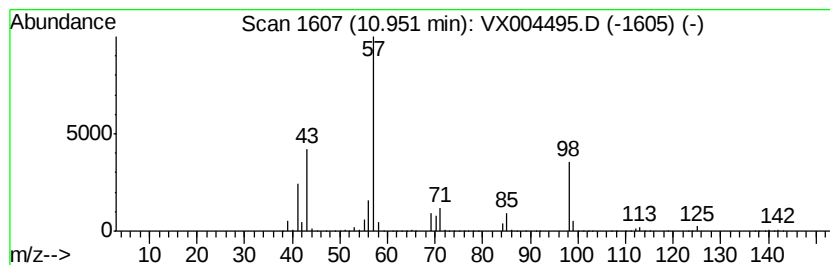
Instrument :
MSVOA_X
ClientSampleId :
EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 9 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	209.85 ug/l	4162750	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptane, 3-ethyl-2-methyl-	142 C10H22	014676-29-0	91
2	Octane, 2,3-dimethyl-	142 C10H22	007146-60-3	64
3	Heptane, 4-(1-methylethyl)-	142 C10H22	052896-87-4	53
4	Undecane, 6-methyl-	170 C12H26	017302-33-9	50
5	Undecane, 2,6-dimethyl-	184 C13H28	017301-23-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091218\
Data File : VX004495.D
Acq On : 12 Sep 2018 15:28
Operator : JC/MD
Sample : J4848-05 10X
Misc : 4.45g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-MW-B(4-8)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.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
Heptane, 2,3-dime...	9.88	103.2	ug/l	2047350	3	10.12	991856	50.0
Cyclohexane, 1,2,...	10.34	105.3	ug/l	2089110	3	10.12	991856	50.0
2-Hexene, 3,4,4-t...	10.38	120.0	ug/l	2380740	3	10.12	991856	50.0
Cyclohexane, 1-et...	10.41	99.9	ug/l	1982390	3	10.12	991856	50.0
Cyclohexane, 1-et...	10.65	222.6	ug/l	4415200	3	10.12	991856	50.0
Pentane, 2,2,3,3-...	10.73	121.8	ug/l	2416750	3	10.12	991856	50.0
Octane, 3,6-dimet...	10.84	572.0	ug/l	11347600	3	10.12	991856	50.0
Cyclohexane, propyl-	10.91	477.5	ug/l	9472090	3	10.12	991856	50.0
Heptane, 3-ethyl-...	10.95	209.8	ug/l	4162750	3	10.12	991856	50.0