

Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX052219\
 Data File : VX009824.D
 Acq On : 23 May 2019 00:07
 Operator : JC/SP
 Sample : K2976-03 50X
 Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EP1-SB-E3-4R(14-17)

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\82X042919W.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	5.501	702	713	723	rBV2	100299	288854	5.86%	0.587%
2	5.665	726	740	755	rVV	180579	513539	10.42%	1.043%
3	6.061	793	805	817	rBV	125861	337470	6.85%	0.685%
4	6.860	923	936	951	rBV	296915	700126	14.21%	1.422%
5	8.665	1225	1232	1235	rBV	31230	56640	1.15%	0.115%
6	8.713	1235	1240	1256	rVB	637365	996612	20.22%	2.024%
7	9.043	1288	1294	1300	rVB2	35815	62026	1.26%	0.126%
8	9.445	1351	1360	1369	rBV	77464	126850	2.57%	0.258%
9	9.561	1373	1379	1385	rBV3	65588	151143	3.07%	0.307%
10	9.622	1385	1389	1393	rVB	125647	171109	3.47%	0.348%
11	9.677	1393	1398	1402	rBV	168200	253709	5.15%	0.515%
12	9.817	1415	1421	1425	rBV2	32930	50856	1.03%	0.103%
13	9.890	1425	1433	1437	rVV4	148038	365102	7.41%	0.741%
14	9.957	1440	1444	1448	rVB	142814	195293	3.96%	0.397%
15	10.061	1455	1461	1465	rBV	286386	419484	8.51%	0.852%
16	10.109	1465	1469	1474	rVB	604768	790880	16.05%	1.606%
17	10.177	1474	1480	1485	rVB5	41474	99388	2.02%	0.202%
18	10.238	1485	1490	1496	rBV2	92463	167108	3.39%	0.339%
19	10.335	1496	1506	1508	rBV2	197618	386066	7.83%	0.784%
20	10.372	1508	1512	1516	rVB2	297067	409423	8.31%	0.832%
21	10.408	1516	1518	1530	rVB	227199	382981	7.77%	0.778%
22	10.512	1530	1535	1540	rBV	148816	223069	4.53%	0.453%
23	10.585	1543	1547	1549	rBV2	57921	74919	1.52%	0.152%
24	10.640	1549	1556	1564	rBV3	597262	1049325	21.29%	2.131%
25	10.725	1564	1570	1573	rBV3	313991	494519	10.03%	1.004%
26	10.762	1574	1576	1580	rVB2	155967	190773	3.87%	0.387%
27	10.835	1580	1588	1592	rBV	1525339	2216249	44.97%	4.501%
28	10.908	1592	1600	1604	rBV	1104881	1899733	38.55%	3.858%
29	10.945	1604	1606	1611	rVB	638026	828280	16.81%	1.682%
30	11.012	1611	1617	1621	rBV3	242059	421411	8.55%	0.856%
31	11.054	1621	1624	1626	rBV2	245823	346866	7.04%	0.704%
32	11.085	1626	1629	1632	rVB	395965	484688	9.84%	0.984%
33	11.134	1632	1637	1642	rVB	1442332	1950006	39.57%	3.960%
34	11.182	1642	1645	1648	rBV3	175633	195787	3.97%	0.398%

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35	11.219	1648	1651	1653	rBV	126119	161636	3.28%	0.328%
36	11.274	1653	1660	1669	rVB4	847963	1429903	29.02%	2.904%
37	11.359	1669	1674	1676	rBV	445932	535411	10.86%	1.087%
38	11.390	1676	1679	1683	rBV2	164063	192721	3.91%	0.391%
39	11.451	1683	1689	1692	rBV2	682161	1161879	23.58%	2.360%
40	11.487	1692	1695	1696	rBV	683512	798373	16.20%	1.621%
41	11.506	1696	1698	1701	rVB	660966	610216	12.38%	1.239%
42	11.579	1707	1710	1715	rVB4	117746	162403	3.30%	0.330%
43	11.627	1715	1718	1720	rBV	121480	143341	2.91%	0.291%
44	11.682	1720	1727	1732	rVV4	411518	816042	16.56%	1.657%
45	11.737	1732	1736	1738	rVV2	336212	458007	9.29%	0.930%
46	11.768	1738	1741	1744	rVV	1603455	1886813	38.29%	3.832%
47	11.804	1744	1747	1757	rVB	3581899	4928034	100.00%	10.009%
48	11.890	1757	1761	1763	rBV2	276824	396349	8.04%	0.805%
49	11.945	1763	1770	1774	rVV3	761460	1447346	29.37%	2.939%
50	11.999	1774	1779	1781	rVV	913755	1212195	24.60%	2.462%
51	12.024	1781	1783	1786	rVV2	577152	676733	13.73%	1.374%
52	12.079	1786	1792	1797	rVV4	751456	1615416	32.78%	3.281%
53	12.140	1797	1802	1808	rVB	1292532	1765745	35.83%	3.586%
54	12.298	1823	1828	1830	rBV	535403	762407	15.47%	1.548%
55	12.322	1830	1832	1835	rVV	642052	672530	13.65%	1.366%
56	12.365	1835	1839	1846	rVV3	1328937	2345543	47.60%	4.764%
57	12.469	1846	1856	1861	rVV3	271088	769704	15.62%	1.563%
58	12.524	1861	1865	1870	rVB3	280226	507481	10.30%	1.031%
59	12.585	1870	1875	1877	rBV	495466	714178	14.49%	1.450%
60	12.609	1877	1879	1885	rVV2	590221	775802	15.74%	1.576%
61	12.664	1885	1888	1891	rVB	438336	483516	9.81%	0.982%
62	12.768	1897	1905	1911	rVV5	336734	932323	18.92%	1.893%
63	12.816	1911	1913	1914	rVV	52628	49910	1.01%	0.101%
64	12.847	1915	1918	1920	rVV2	156174	216554	4.39%	0.440%
65	12.871	1920	1922	1924	rVV2	167369	211419	4.29%	0.429%
66	12.902	1924	1927	1930	rVB2	207369	258511	5.25%	0.525%
67	12.944	1930	1934	1937	rBV3	244398	413851	8.40%	0.841%
68	12.975	1937	1939	1942	rVV	257716	265494	5.39%	0.539%
69	13.017	1942	1946	1953	rVB	391628	587706	11.93%	1.194%
70	13.078	1953	1956	1961	rBV2	107242	195213	3.96%	0.396%
71	13.121	1961	1963	1965	rVV	63533	59840	1.21%	0.122%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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72	13.146	1965	1967	1972	rVB	55811	75697	1.54%	0.154%
73	13.213	1972	1978	1983	rVB3	104354	221310	4.49%	0.449%
74	13.261	1983	1986	1989	rVB3	60888	67259	1.36%	0.137%
75	13.304	1989	1993	1995	rBV2	88861	103389	2.10%	0.210%
76	13.341	1995	1999	2006	rVB2	413233	629394	12.77%	1.278%
77	13.481	2018	2022	2031	rVB4	55055	128205	2.60%	0.260%
78	13.633	2043	2047	2052	rBV3	54043	92373	1.87%	0.188%

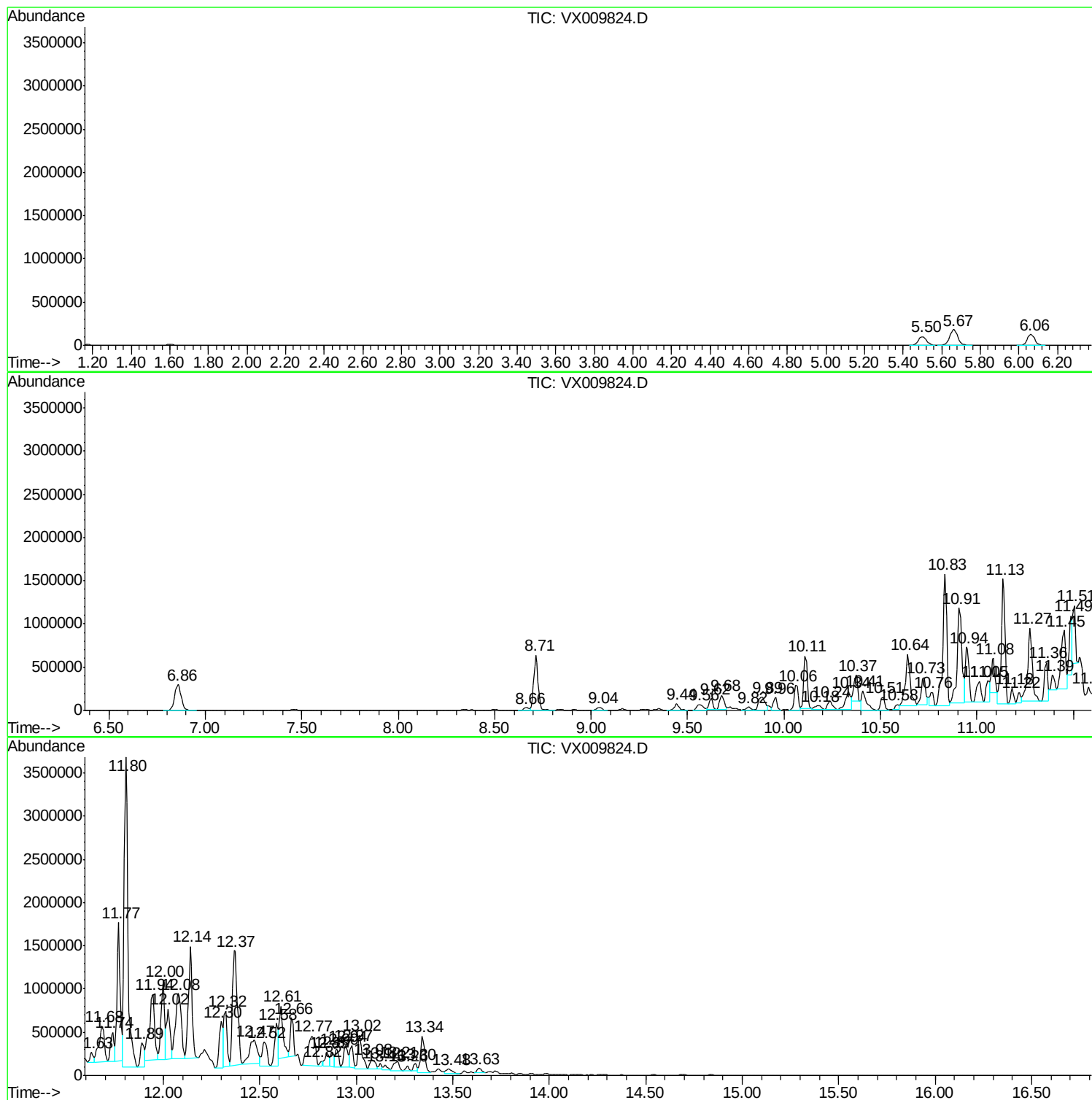
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Instrument :
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ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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



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ALS Vial : 36 Sample Multiplier: 1

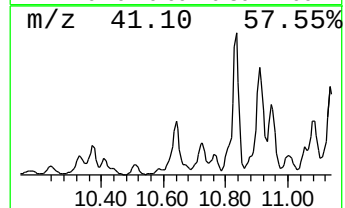
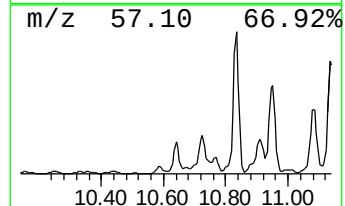
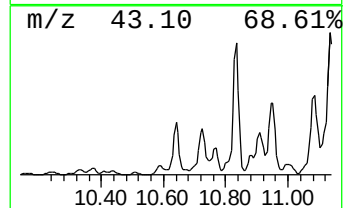
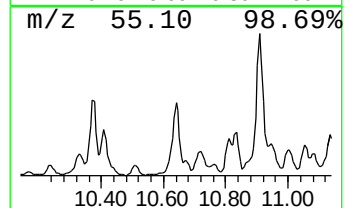
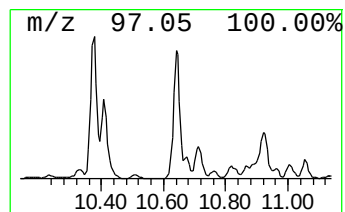
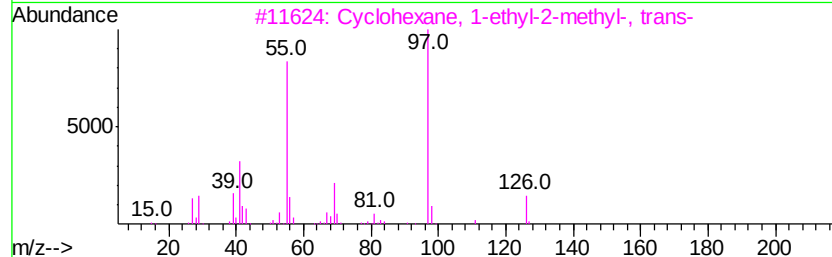
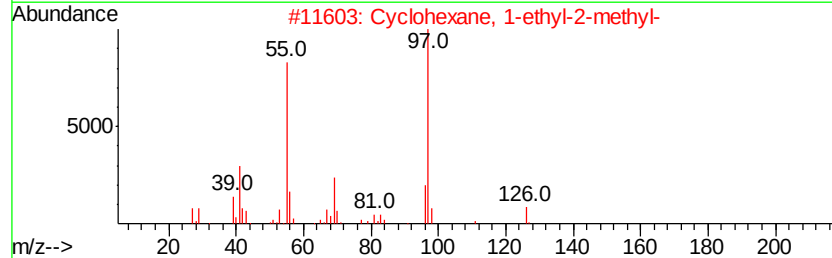
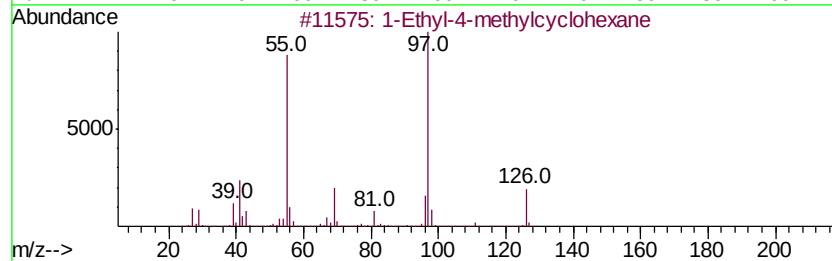
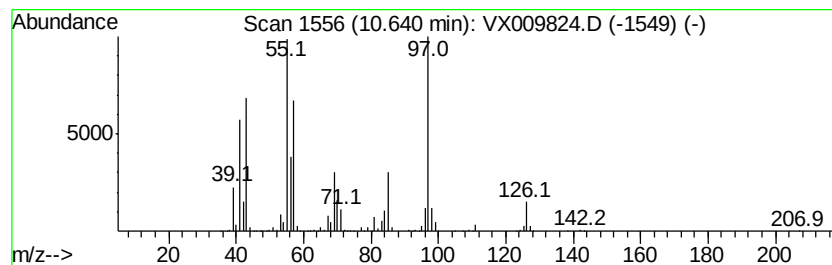
Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Ethyl-4-methylcyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.64	66.34 ug/l	1049330	Chlorobenzene-d5	10.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	60
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	60
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	60
4		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49



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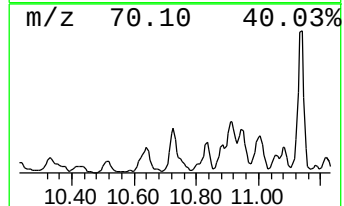
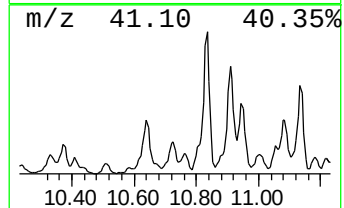
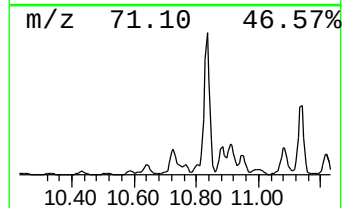
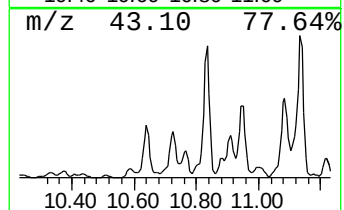
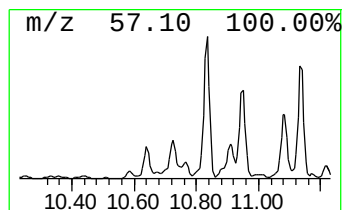
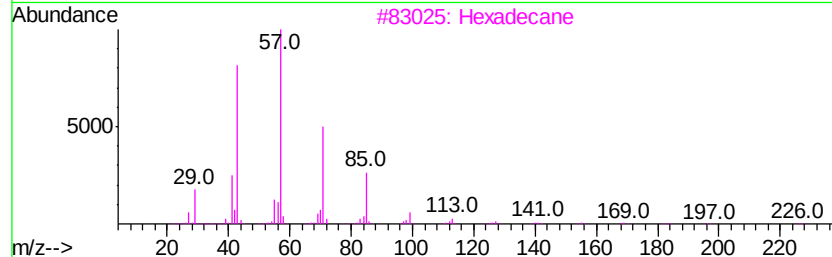
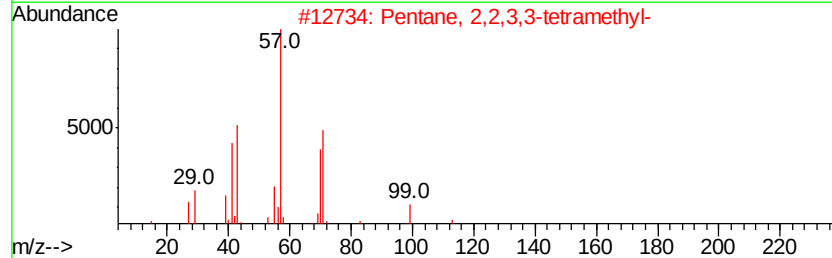
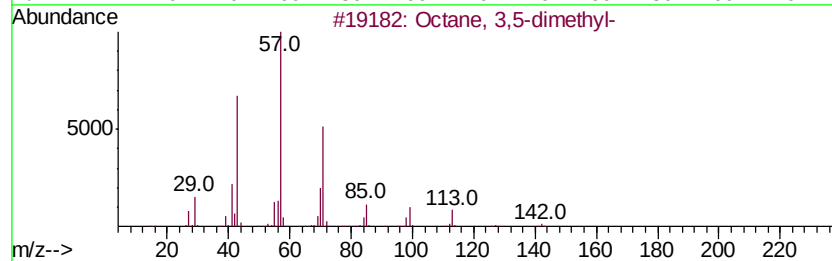
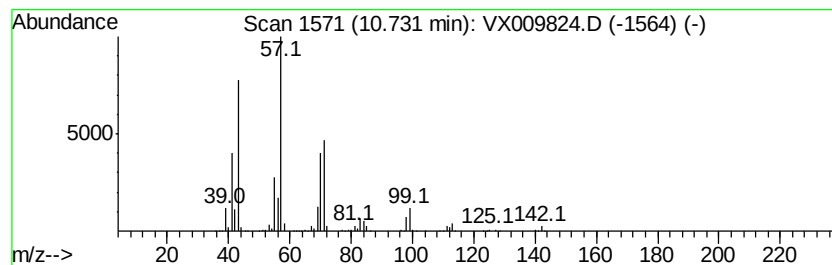
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 3,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.73	31.26 ug/l	494519	Chlorobenzene-d5	10.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	80
2		Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	72
3		Hexadecane	226	C16H34	000544-76-3	64
4		Hexane, 4-ethyl-2-methyl-	128	C9H20	003074-75-7	50
5		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50



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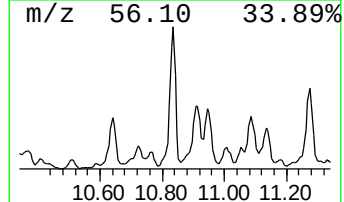
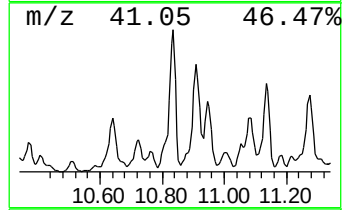
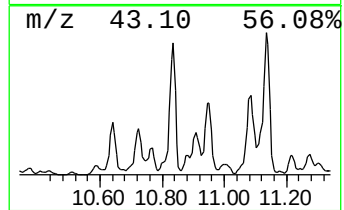
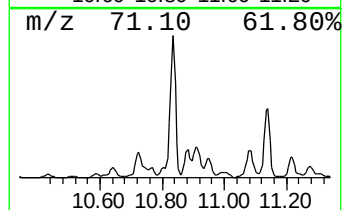
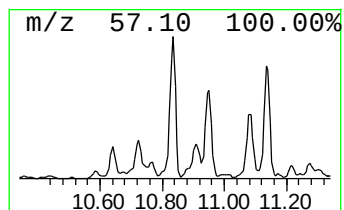
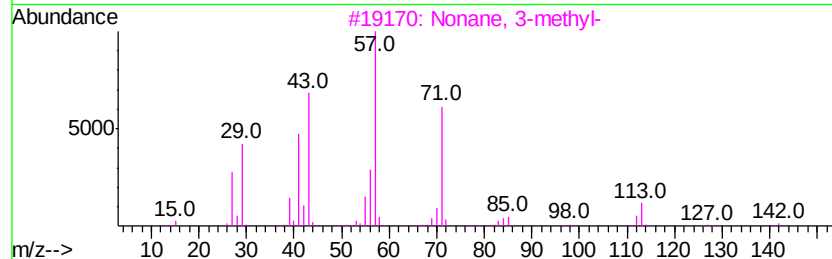
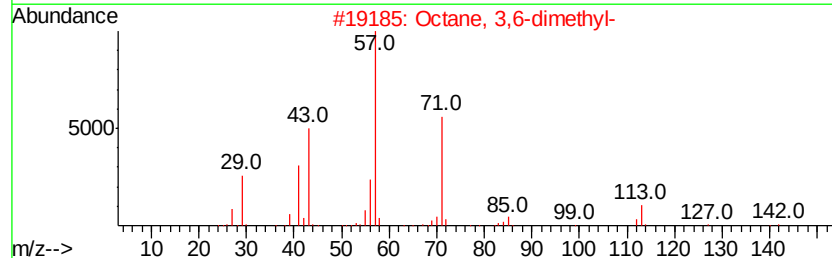
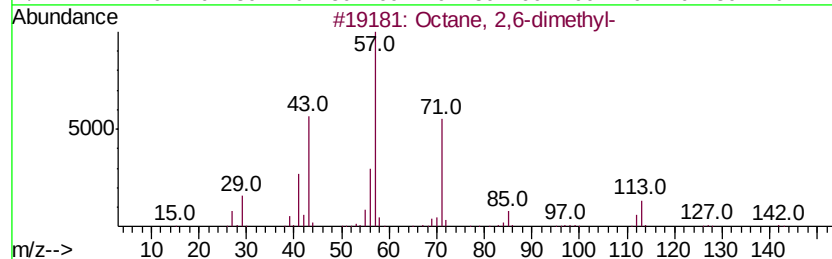
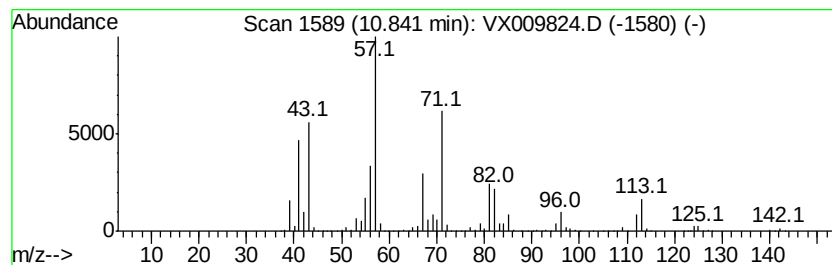
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Quant Title : SW846 8260

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

Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.84	140.11 ug/l	2216250	Chlorobenzene-d5	10.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	70
3		Nonane, 3-methyl-	142	C10H22	005911-04-6	70
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	49
5		Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	47



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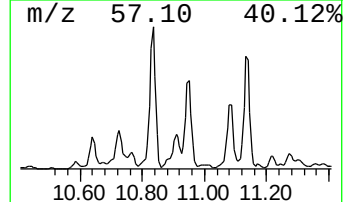
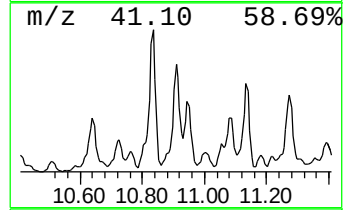
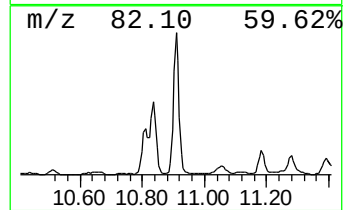
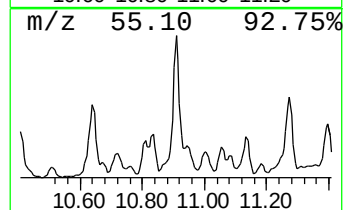
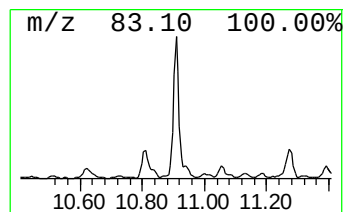
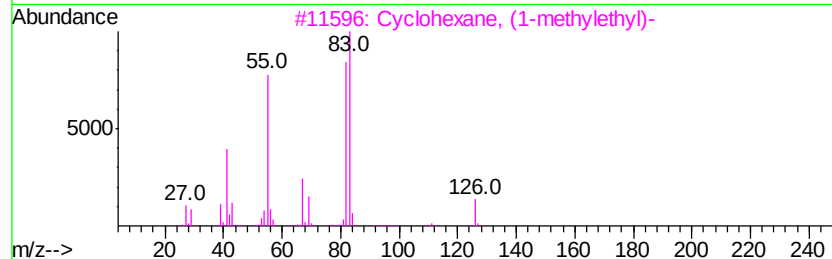
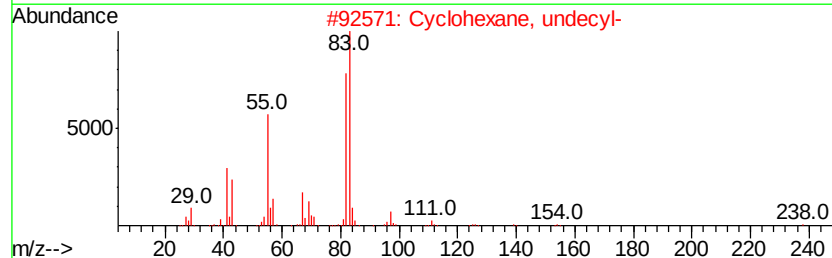
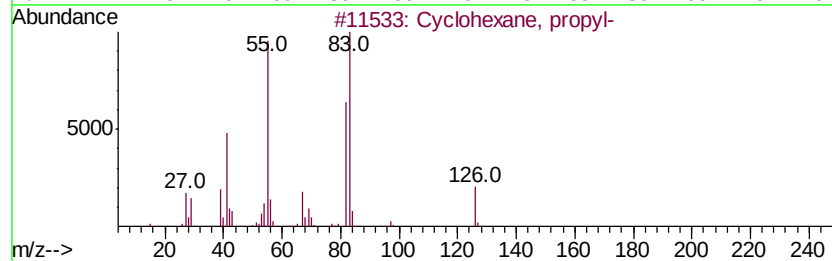
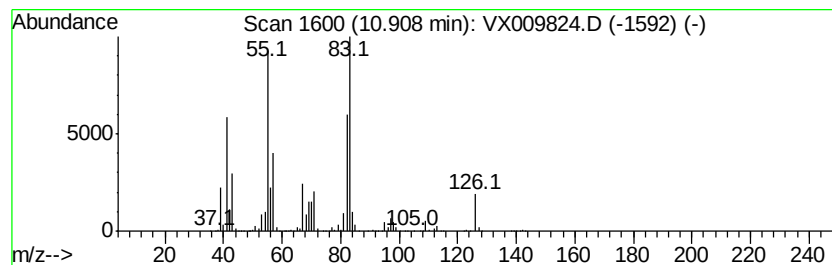
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	120.10 ug/l	1899730	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	76
2		Cyclohexane, undecyl-	238	C17H34	054105-66-7	64
3		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	60
4		Cyclohexane, butyl-	140	C10H20	001678-93-9	59
5		Cyclohexane, octyl-	196	C14H28	001795-15-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX052219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

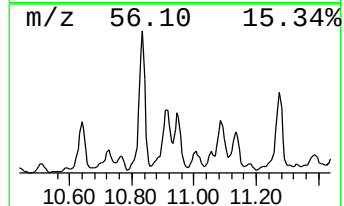
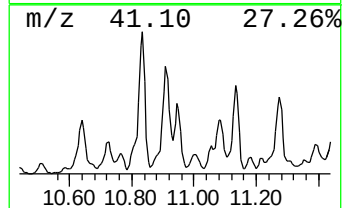
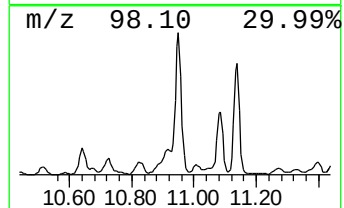
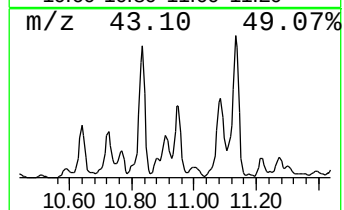
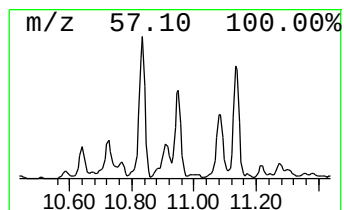
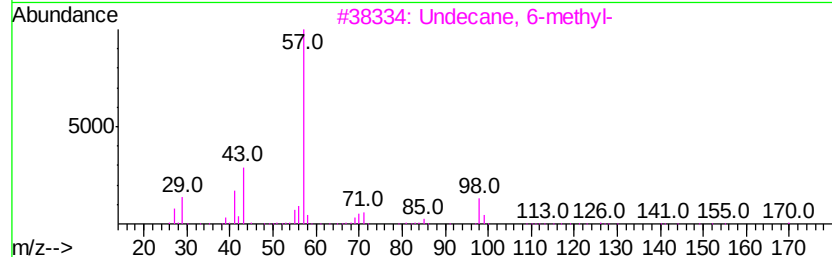
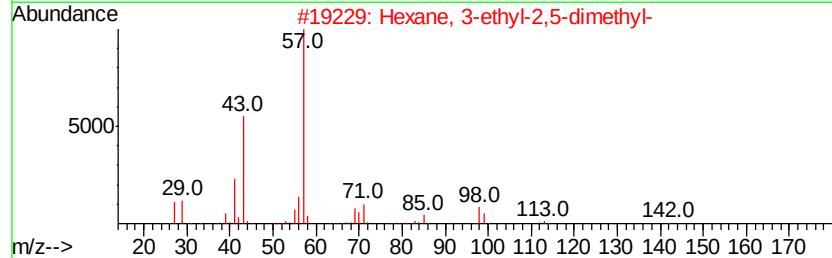
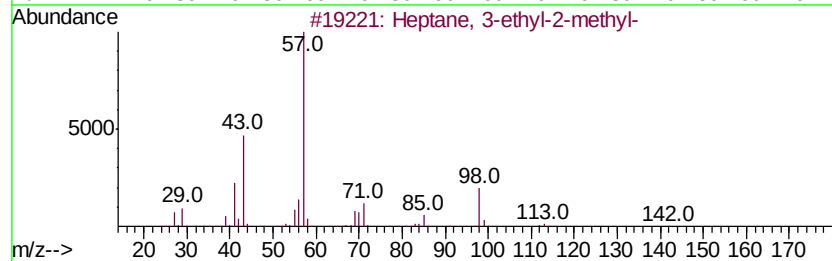
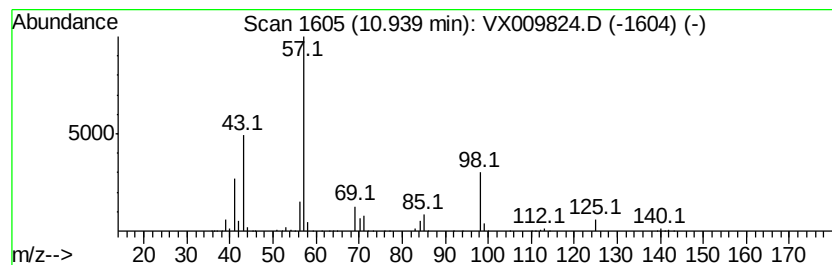
Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 5 Heptane, 3-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.94	52.36 ug/l	828280	Chlorobenzene-d5	10.11		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	72
2		Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	59
3		Undecane, 6-methyl-	170	C12H26	017302-33-9	50
4		1,3,2-Dioxaborolane, 4,4-dimethy...	142	C6H11B03	1000063-89-2	43
5		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX052219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

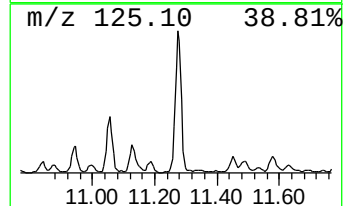
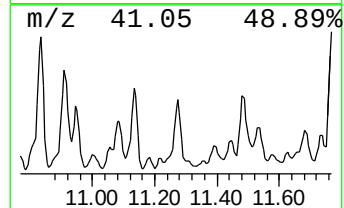
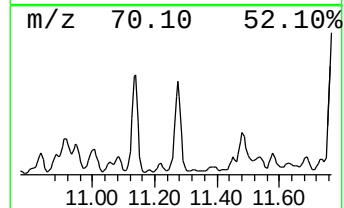
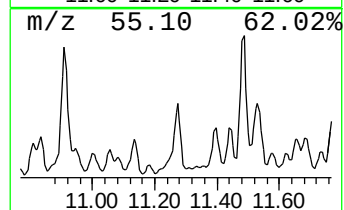
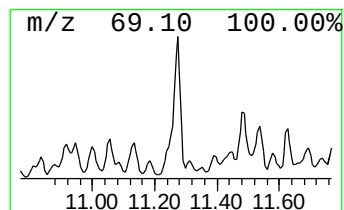
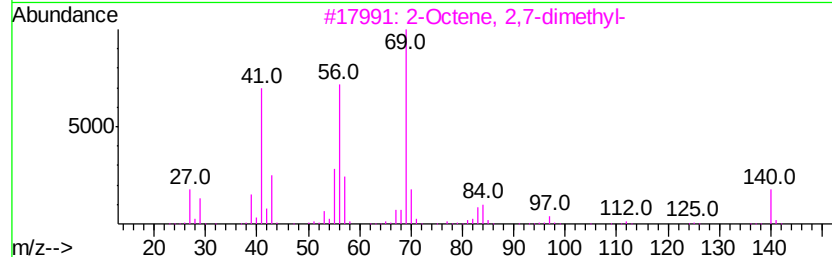
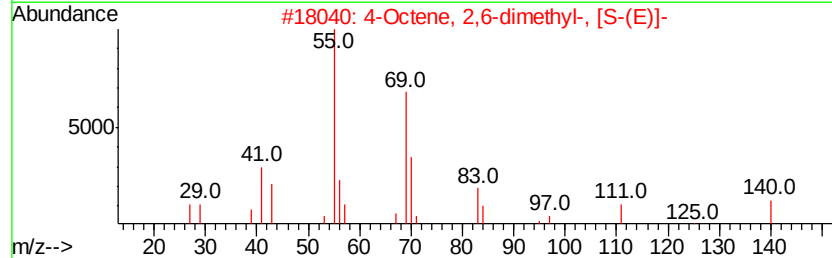
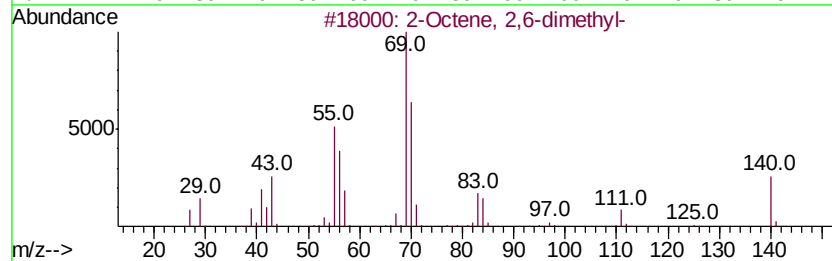
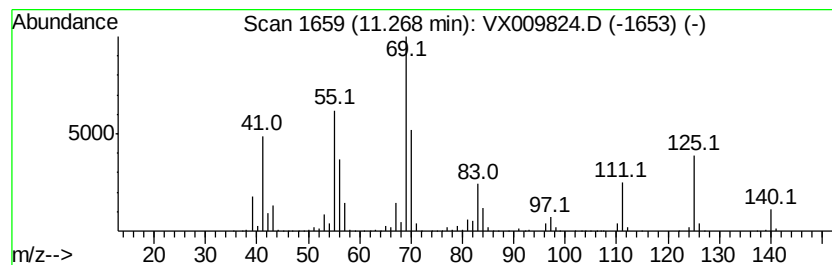
Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Octene, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	44.26 ug/l	1429900	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Octene, 2,6-dimethyl-	140 C10H20	004057-42-5	58
2	4-Octene, 2,6-dimethyl-, [S-(E)]-	140 C10H20	062960-76-3	58
3	2-Octene, 2,7-dimethyl-	140 C10H20	002050-81-9	49
4	1,1,4-Trimethylcyclohexane	126 C9H18	007094-27-1	47
5	Cyclohexane, 1,1,2,3-tetramethyl-	140 C10H20	006783-92-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX052219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55u/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

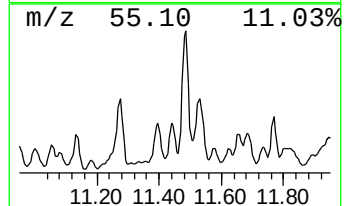
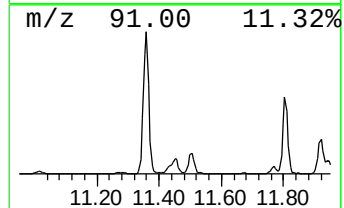
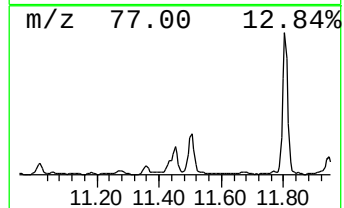
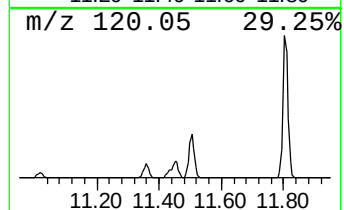
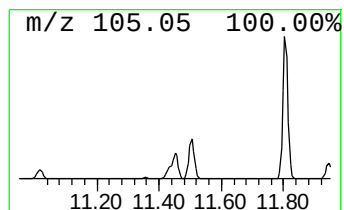
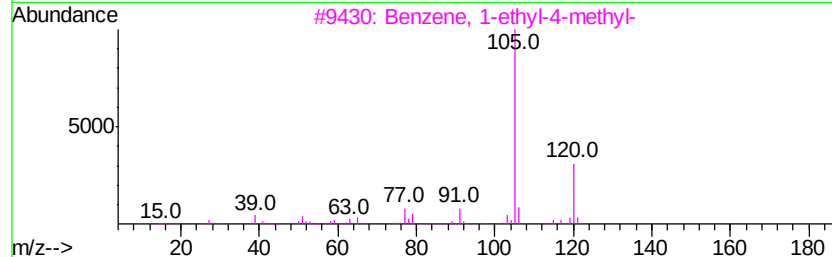
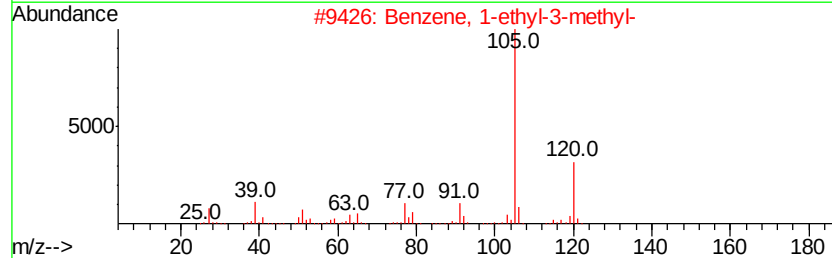
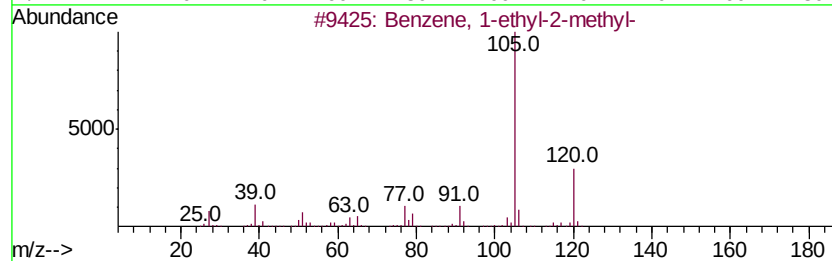
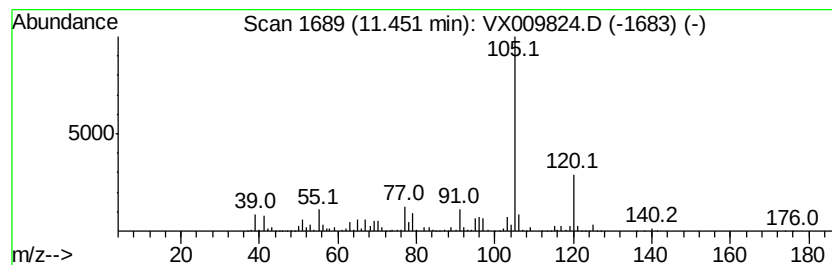
Instrument :
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ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	35.96 ug/l	1161880	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 94
2		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 76
3		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 76
4		Mesitylene	120 C9H12	000108-67-8 76
5		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 76



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VO52219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55a/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

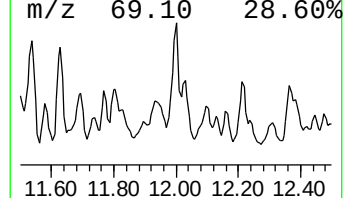
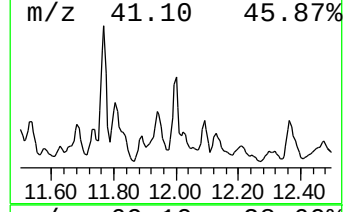
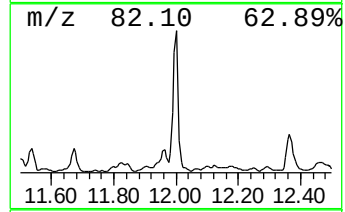
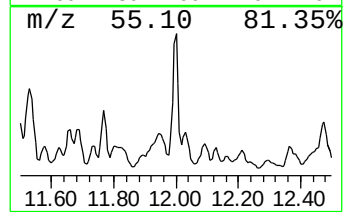
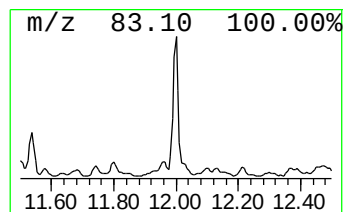
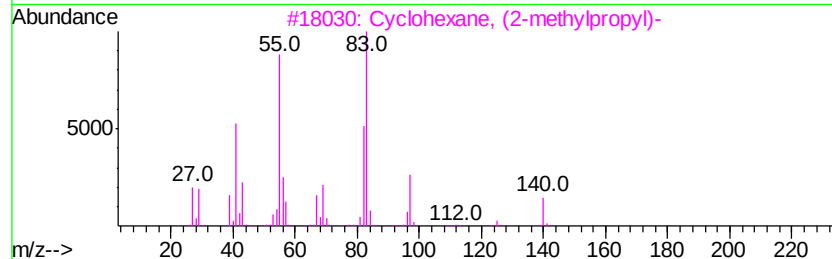
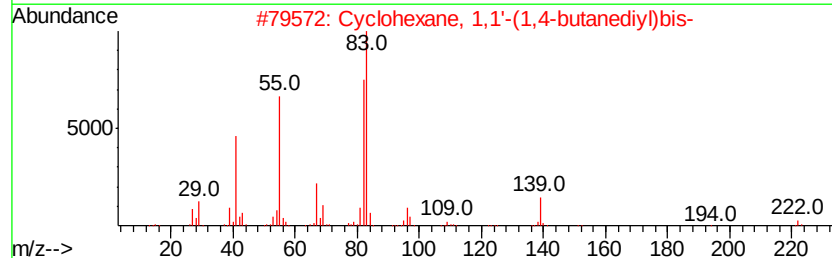
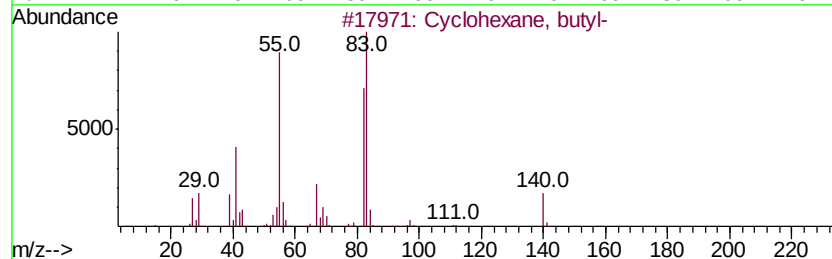
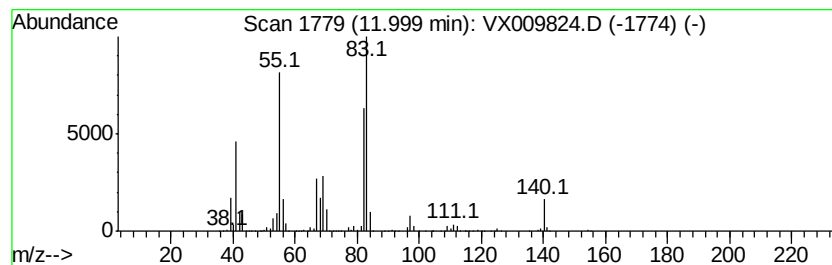
Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	37.52 ug/l	1212200	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, butyl-	140 C10H20	001678-93-9 91
2		Cyclohexane, 1,1'-(1,4-butanediyl)...	222 C16H30	006165-44-2 72
3		Cyclohexane, (2-methylpropyl)-	140 C10H20	001678-98-4 72
4		Cyclohexane, propyl-	126 C9H18	001678-92-8 72
5		Cyclohexane, (1-methylethyl)-	126 C9H18	000696-29-7 64



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX052219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55q/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

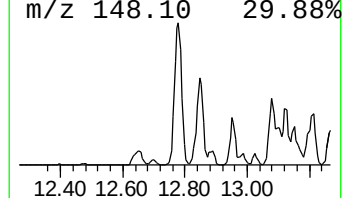
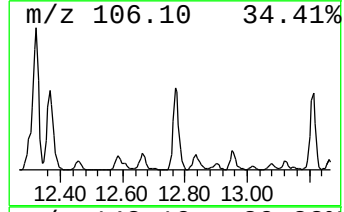
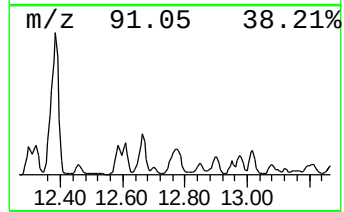
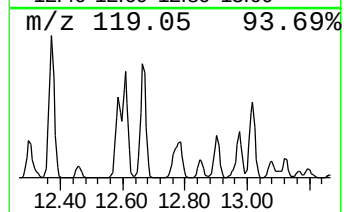
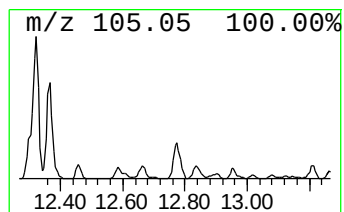
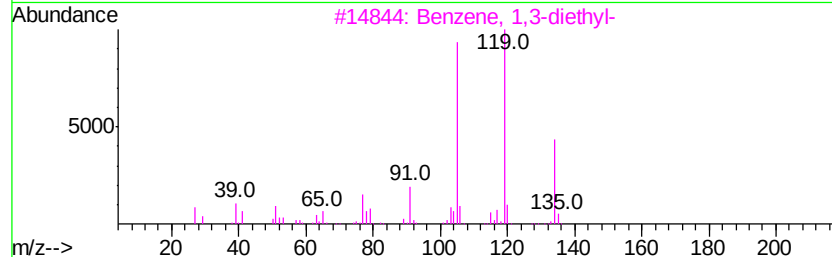
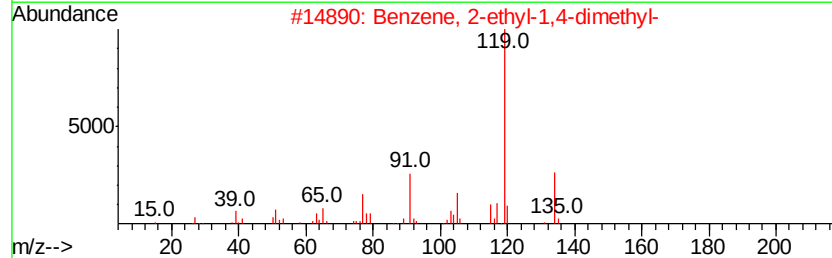
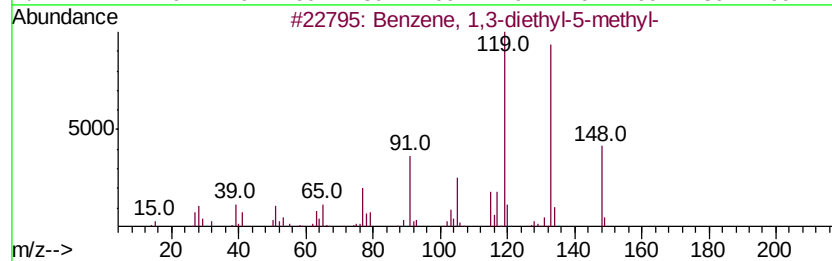
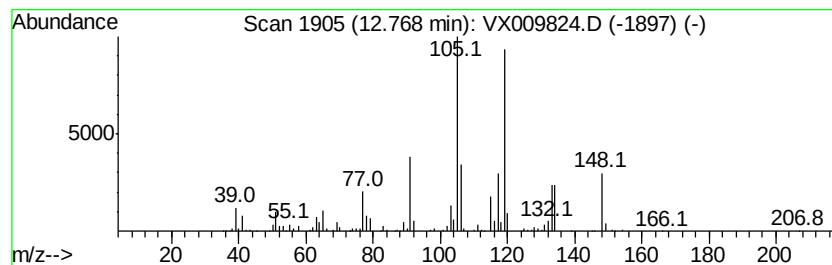
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,3-diethyl-5-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	28.86 ug/l	932323	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	64
2		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	58
3		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	58
4		Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	52
5		1-Methyl-1-silabenzocyclobutene	134	C8H10Si	160841-06-5	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052219\
Data File : VX009824.D
Acq On : 23 May 2019 00:07
Operator : JC/SP
Sample : K2976-03 50X
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-E3-4R(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.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
1-Ethyl-4-methylc...	10.64	66.3	ug/l	1049330	3	10.11	790880	50.0
Octane, 3,5-dimet...	10.73	31.3	ug/l	494519	3	10.11	790880	50.0
Octane, 2,6-dimet...	10.84	140.1	ug/l	2216250	3	10.11	790880	50.0
Cyclohexane, propyl-	10.91	120.1	ug/l	1899730	3	10.11	790880	50.0
Heptane, 3-ethyl-...	10.94	52.4	ug/l	828280	3	10.11	790880	50.0
2-Octene, 2,6-dim...	11.27	44.3	ug/l	1429900	4	12.08	1615420	50.0
Benzene, 1-ethyl-...	11.45	36.0	ug/l	1161880	4	12.08	1615420	50.0
Cyclohexane, butyl-	12.00	37.5	ug/l	1212200	4	12.08	1615420	50.0
Benzene, 1,3-diet...	12.77	28.9	ug/l	932323	4	12.08	1615420	50.0