

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091218\
 Data File : VX004498.D
 Acq On : 12 Sep 2018 16:49
 Operator : JC/MD
 Sample : J4724-16 50X
 Misc : 4.95g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EP1-SUT-4USTS-S

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\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	5.507	701	714	728	rBV	144841	412205	7.08%	0.385%
2	5.665	728	740	757	rVV	201699	563498	9.68%	0.526%
3	6.068	796	806	822	rBV	155838	405548	6.96%	0.379%
4	6.860	926	936	950	rBV	315775	750343	12.88%	0.701%
5	8.720	1234	1241	1255	rVB	783274	1233852	21.19%	1.153%
6	9.445	1350	1360	1369	rBV	65879	103782	1.78%	0.097%
7	9.561	1374	1379	1385	rBV2	47473	95831	1.65%	0.090%
8	9.622	1385	1389	1394	rVB	51513	74323	1.28%	0.069%
9	9.677	1394	1398	1403	rBV	120409	192957	3.31%	0.180%
10	9.878	1426	1431	1437	rVV3	114594	281744	4.84%	0.263%
11	9.957	1441	1444	1449	rVB	175468	241272	4.14%	0.225%
12	10.067	1455	1462	1466	rBV	272252	390282	6.70%	0.365%
13	10.116	1466	1470	1475	rVV	740995	992811	17.05%	0.928%
14	10.177	1475	1480	1486	rVV5	33562	80979	1.39%	0.076%
15	10.238	1486	1490	1497	rVV2	79642	151388	2.60%	0.141%
16	10.335	1497	1506	1509	rVV2	197185	384529	6.60%	0.359%
17	10.378	1509	1513	1516	rVV	311020	477737	8.20%	0.446%
18	10.414	1516	1519	1530	rVB	185467	346105	5.94%	0.323%
19	10.512	1530	1535	1541	rBV2	130137	198149	3.40%	0.185%
20	10.591	1543	1548	1550	rBV2	59112	84716	1.45%	0.079%
21	10.646	1550	1557	1561	rVV2	590733	1073658	18.44%	1.003%
22	10.725	1564	1570	1574	rVV2	443275	778955	13.38%	0.728%
23	10.768	1574	1577	1580	rVV2	265530	372203	6.39%	0.348%
24	10.835	1580	1588	1592	rVV	1938199	2846298	48.87%	2.659%
25	10.914	1592	1601	1604	rVV2	1231529	2341471	40.21%	2.188%
26	10.951	1604	1607	1612	rVV	976361	1410511	24.22%	1.318%
27	11.006	1612	1616	1621	rVV3	337953	701317	12.04%	0.655%
28	11.061	1621	1625	1626	rVV2	406101	554749	9.53%	0.518%
29	11.085	1626	1629	1632	rVV	834628	1232502	21.16%	1.151%
30	11.140	1632	1638	1648	rVV2	2368629	4663288	80.08%	4.357%
31	11.219	1648	1651	1652	rVV	276577	307257	5.28%	0.287%
32	11.243	1652	1655	1658	rVV	1106562	1639695	28.16%	1.532%
33	11.274	1658	1660	1670	rVV2	1259360	2236159	38.40%	2.089%
34	11.359	1671	1674	1676	rVV	307325	438281	7.53%	0.409%

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Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
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Filtering: 5
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35	11.396	1676	1680	1683	rVV3	577730	1089234	18.70%	1.018%
36	11.439	1683	1687	1692	rVV2	1020465	2438328	41.87%	2.278%
37	11.487	1692	1695	1697	rVV	1684644	2402967	41.26%	2.245%
38	11.536	1701	1703	1708	rVV4	1050200	1706875	29.31%	1.595%
39	11.579	1708	1710	1716	rVV4	381045	897861	15.42%	0.839%
40	11.634	1716	1719	1721	rVV	418453	669821	11.50%	0.626%
41	11.689	1721	1728	1732	rVV7	1030392	2523881	43.34%	2.358%
42	11.737	1732	1736	1738	rVV2	1010720	1508822	25.91%	1.410%
43	11.774	1738	1742	1745	rVV	3668956	5060095	86.89%	4.728%
44	11.810	1745	1748	1757	rVV	3390810	5823628	100.00%	5.441%
45	11.896	1757	1762	1764	rVV2	747594	1292765	22.20%	1.208%
46	11.945	1764	1770	1775	rVV5	1574103	3570232	61.31%	3.336%
47	11.999	1775	1779	1782	rVV	1980106	3160798	54.28%	2.953%
48	12.030	1782	1784	1787	rVV3	1285009	1734567	29.78%	1.621%
49	12.091	1787	1794	1798	rVV3	1709147	4436899	76.19%	4.145%
50	12.146	1798	1803	1809	rVV2	1671565	4478962	76.91%	4.185%
51	12.225	1809	1816	1824	rVV3	1337382	3228753	55.44%	3.017%
52	12.323	1824	1832	1836	rVV2	1218196	2870973	49.30%	2.682%
53	12.371	1836	1840	1846	rVV4	2259185	4173151	71.66%	3.899%
54	12.475	1846	1857	1861	rVV3	910174	3156932	54.21%	2.949%
55	12.524	1861	1865	1871	rVV4	1216952	2570719	44.14%	2.402%
56	12.591	1871	1876	1877	rVV	966768	1417606	24.34%	1.324%
57	12.609	1877	1879	1882	rVV2	1313796	1996775	34.29%	1.866%
58	12.670	1886	1889	1897	rVV	1012332	2168725	37.24%	2.026%
59	12.737	1897	1900	1903	rVV2	711069	1181984	20.30%	1.104%
60	12.774	1903	1906	1912	rVV4	721514	1736341	29.82%	1.622%
61	12.822	1912	1914	1915	rVV2	316987	336618	5.78%	0.314%
62	12.853	1916	1919	1921	rVV2	498086	804577	13.82%	0.752%
63	12.877	1921	1923	1925	rVV	607649	752550	12.92%	0.703%
64	12.902	1925	1927	1930	rVV2	466639	656543	11.27%	0.613%
65	12.944	1930	1934	1937	rVV3	908141	1524901	26.18%	1.425%
66	12.975	1937	1939	1942	rVV	562303	834710	14.33%	0.780%
67	13.024	1943	1947	1949	rVV	689283	1106967	19.01%	1.034%
68	13.097	1953	1959	1962	rVV4	351569	865407	14.86%	0.809%
69	13.127	1962	1964	1966	rVV	254277	307344	5.28%	0.287%
70	13.152	1966	1968	1973	rVV	215663	384765	6.61%	0.359%
71	13.213	1973	1978	1983	rVV4	254012	616758	10.59%	0.576%

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72	13.268	1983	1987	1990	rVV3	200603	316464	5.43%	0.296%
73	13.310	1990	1994	1996	rVV2	215551	331565	5.69%	0.310%
74	13.347	1996	2000	2005	rVV2	679489	1150946	19.76%	1.075%
75	13.389	2005	2007	2011	rVV	117239	190339	3.27%	0.178%
76	13.438	2011	2015	2018	rVV2	136684	249297	4.28%	0.233%
77	13.481	2018	2022	2031	rVB2	461534	740405	12.71%	0.692%
78	13.566	2031	2036	2039	rBV4	56370	93668	1.61%	0.088%
79	13.639	2044	2048	2053	rBV3	100887	172176	2.96%	0.161%
80	13.725	2059	2062	2067	rVB2	60247	87254	1.50%	0.082%
81	13.835	2077	2080	2087	rVB	96550	155853	2.68%	0.146%

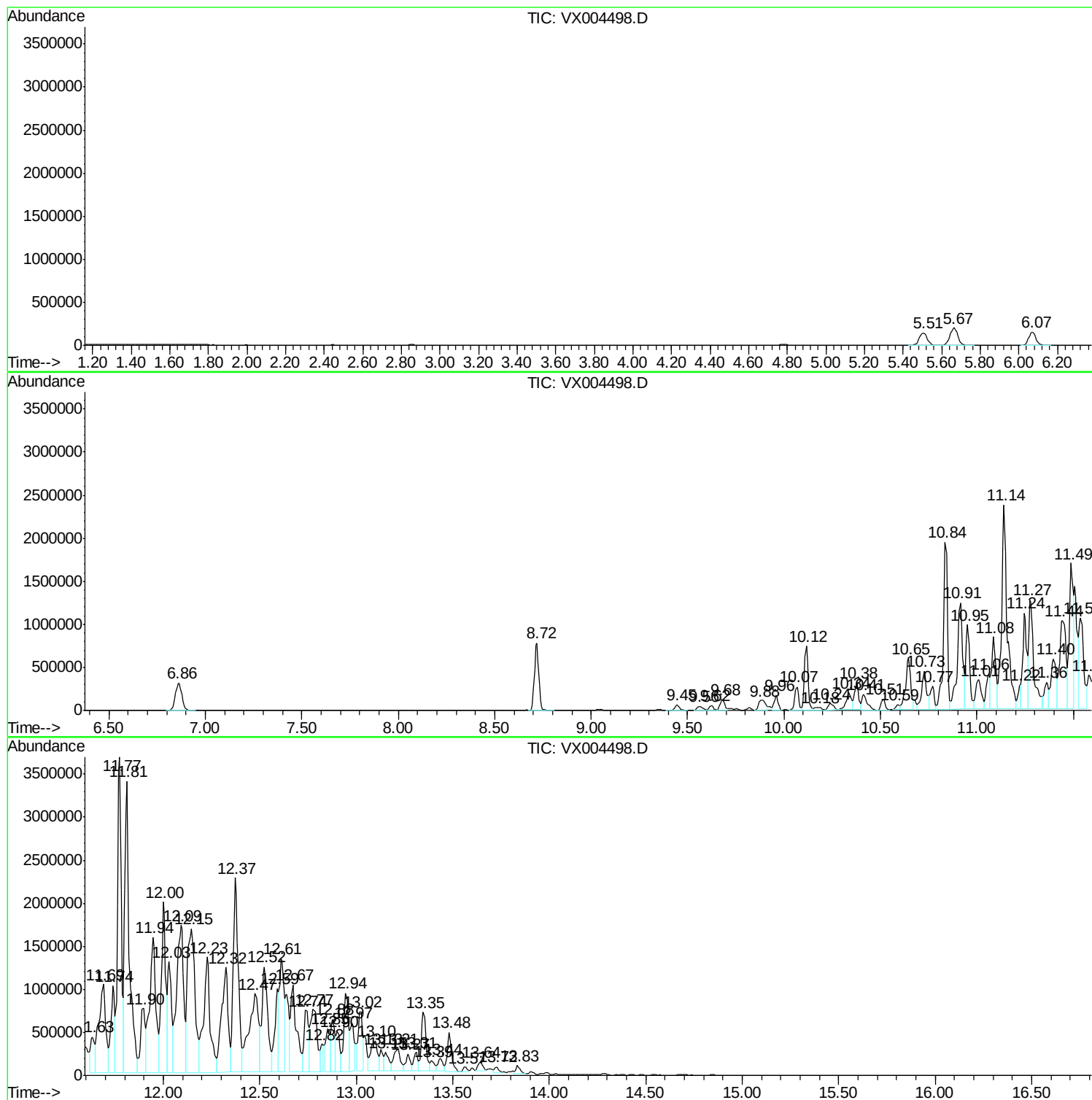
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ClientSampleId :
EP1-SUT-4USTS-S

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



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ALS Vial : 16 Sample Multiplier: 1

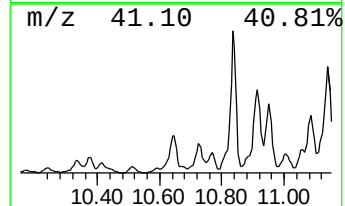
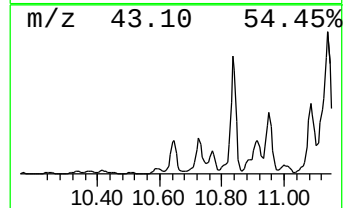
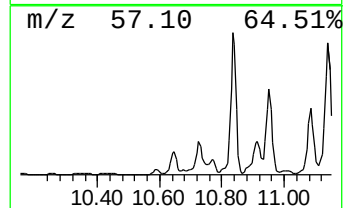
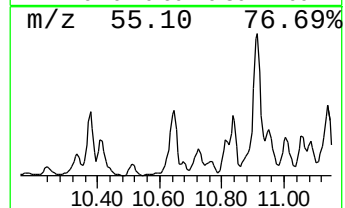
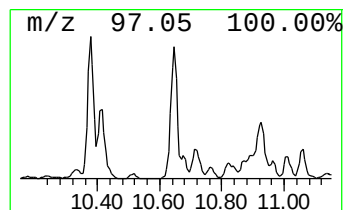
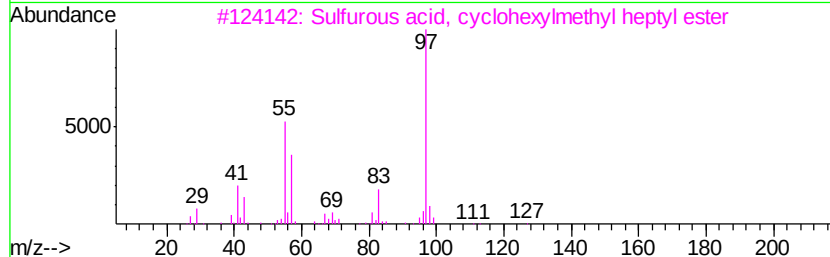
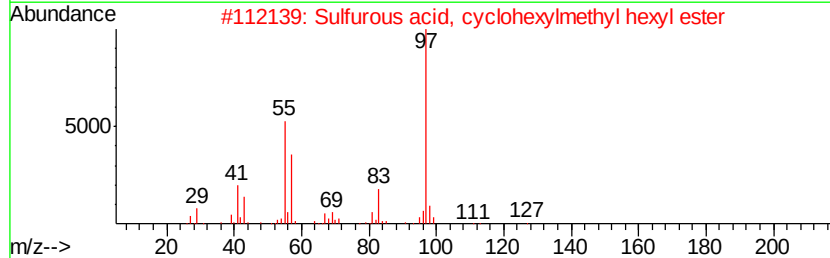
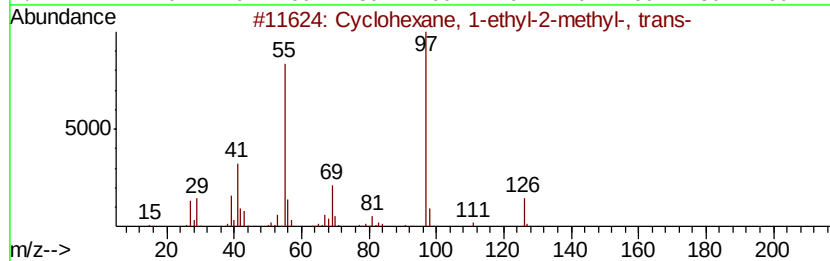
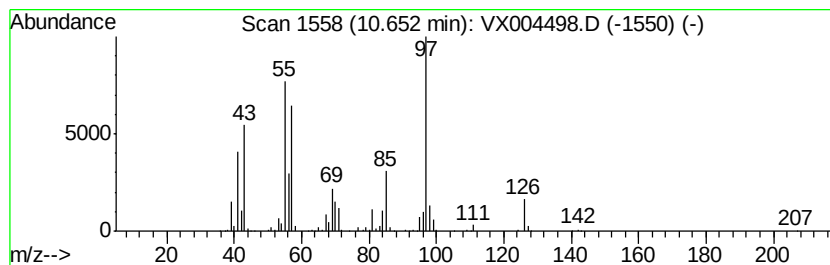
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.65	54.07 ug/l	1073660	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	55
2		Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	53
3		Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	50
4		3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	49
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49



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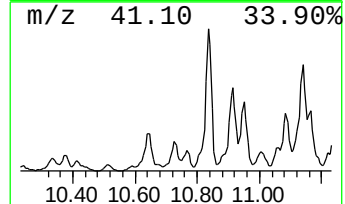
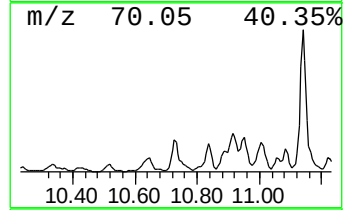
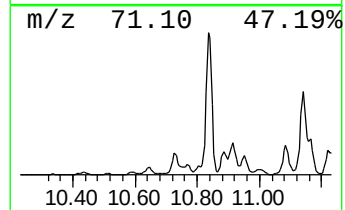
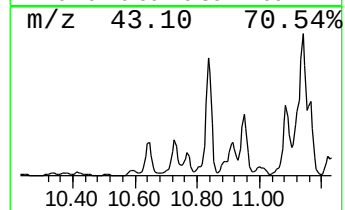
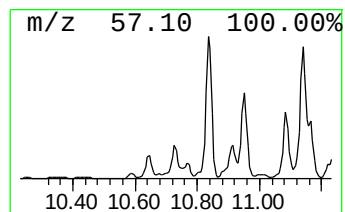
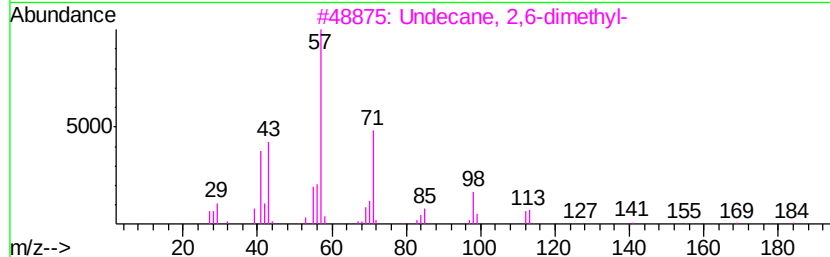
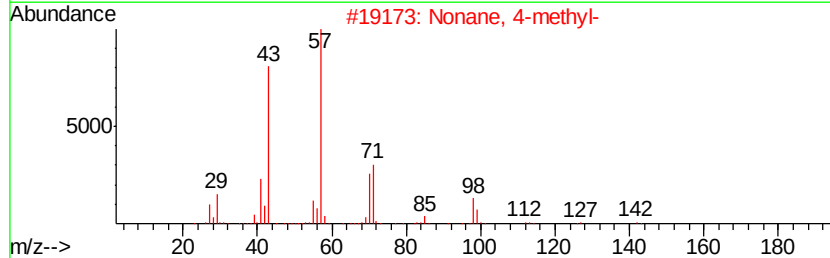
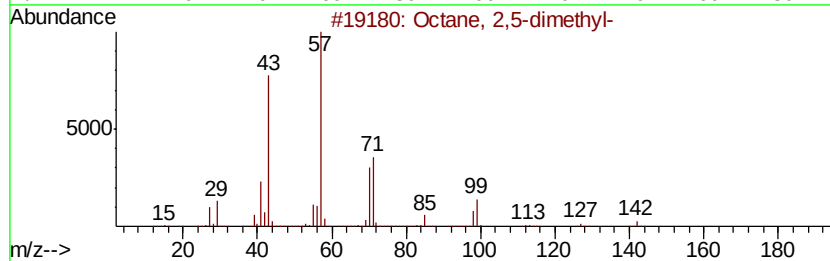
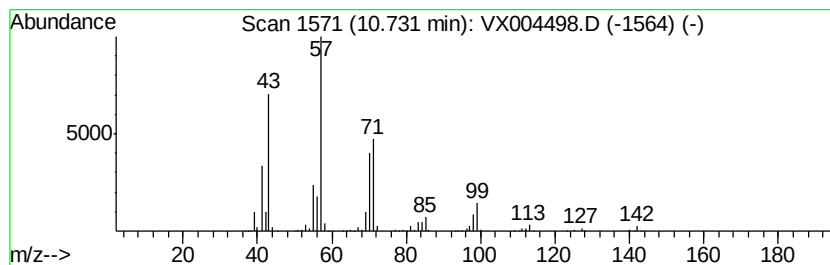
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.73	39.23 ug/l	778955	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	90
2		Nonane, 4-methyl-	142	C10H22	017301-94-9	83
3		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
4		Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	59
5		Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	59



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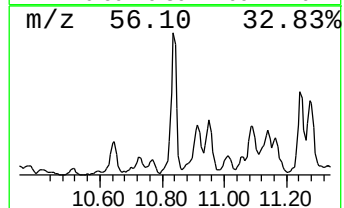
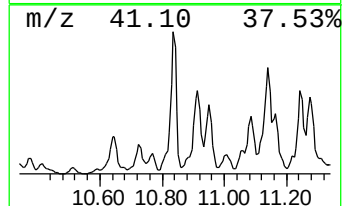
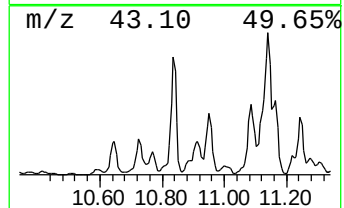
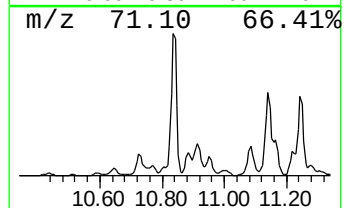
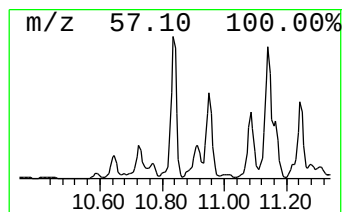
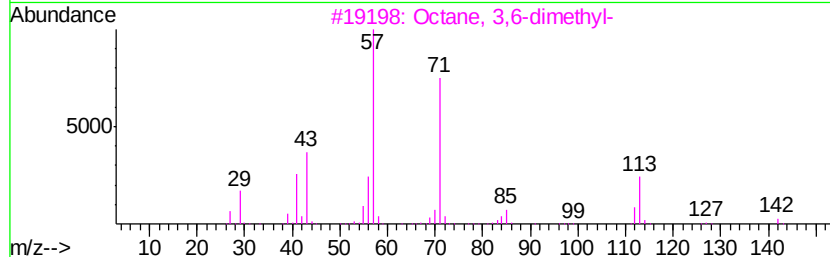
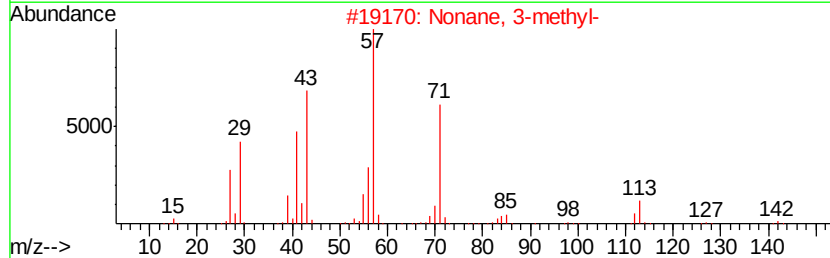
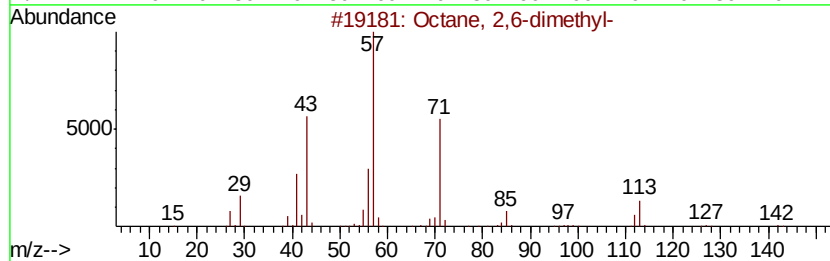
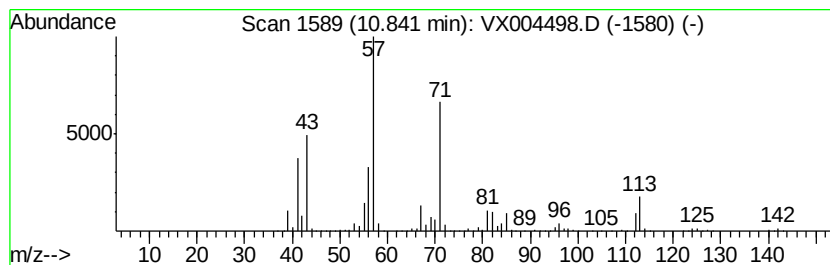
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	143.35 ug/l	2846300	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octane, 2,6-dimethyl-	142 C10H22	002051-30-1 94
2		Nonane, 3-methyl-	142 C10H22	005911-04-6 87
3		Octane, 3,6-dimethyl-	142 C10H22	015869-94-0 87
4		Sulfurous acid, di(2-ethylhexyl)...	306 C16H34O3S	1000309-19-1 53
5		Sulfurous acid, decyl 2-ethylhex...	334 C18H38O3S	1000309-19-3 53



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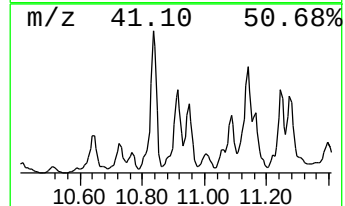
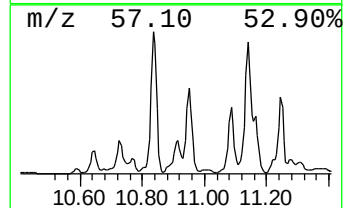
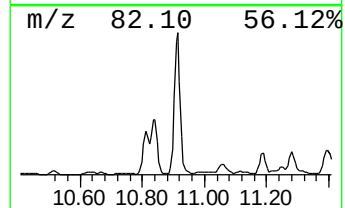
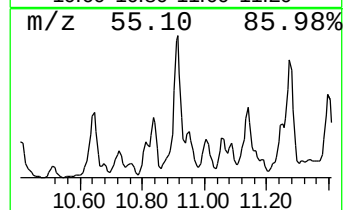
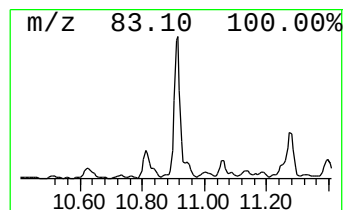
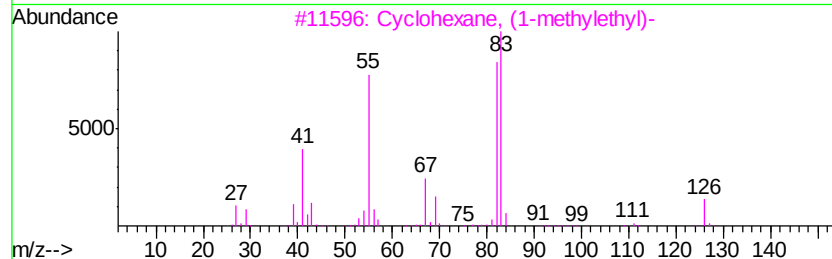
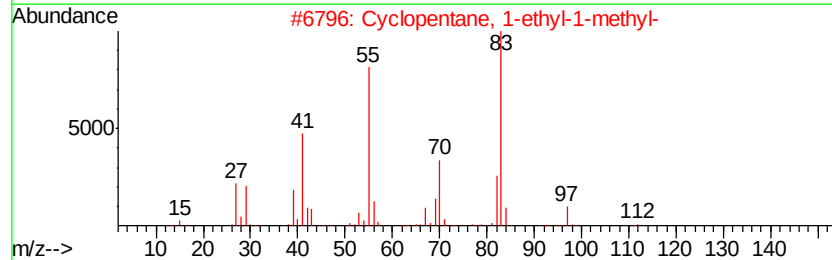
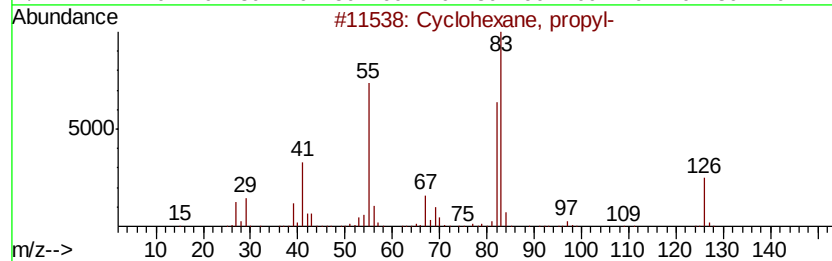
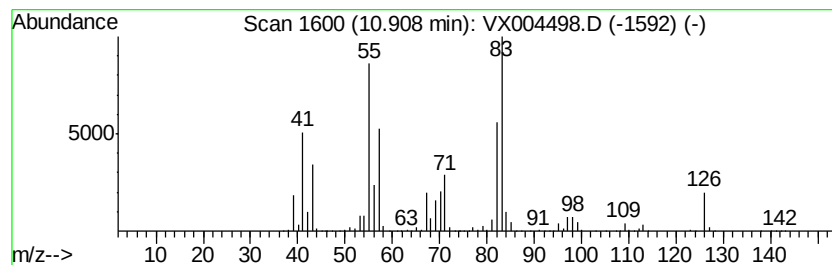
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Quant Title : SW846 8260

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	117.92 ug/l	2341470	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	68
2		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	49
3		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	49
4		Cyclohexane, methyl-	98	C7H14	000108-87-2	46
5		trans--4-Nonene	126	C9H18	010405-85-3	30



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

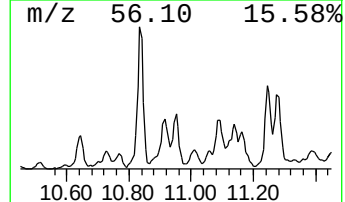
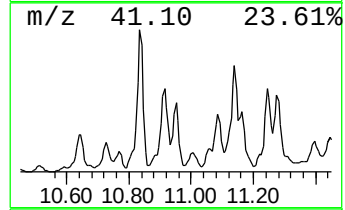
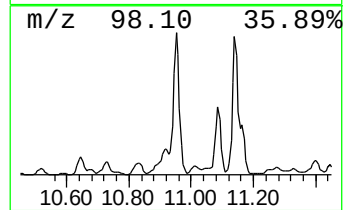
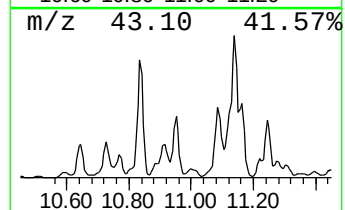
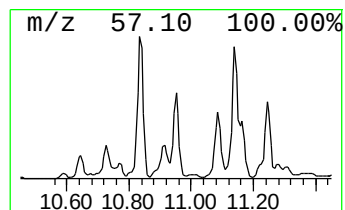
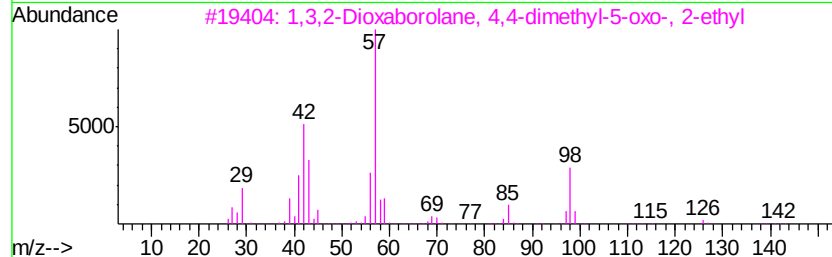
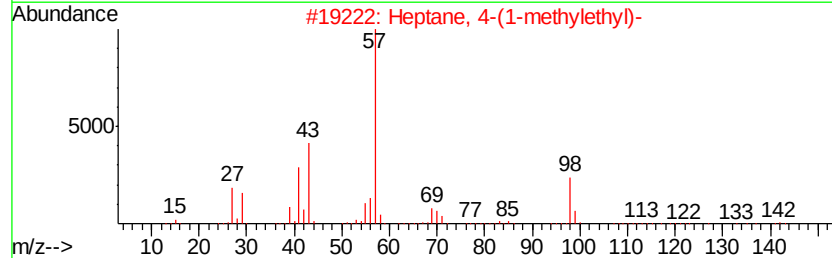
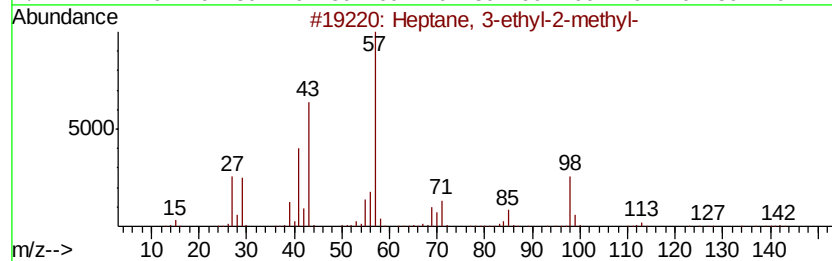
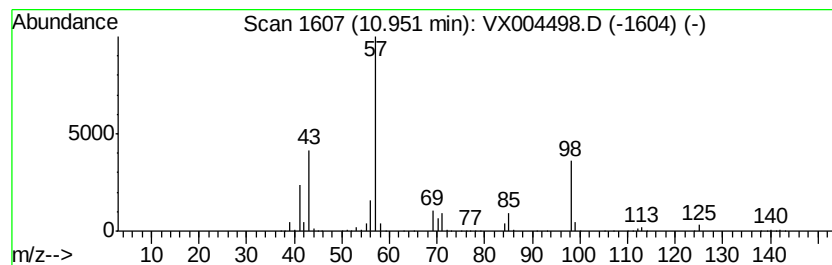
Instrument :
MSVOA_X
ClientSampleId :
EP1-SUT-4USTS-S

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 Heptane, 3-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.95	71.04 ug/l	1410510	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	80	
2	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	53	
3	1,3,2-Dioxaborolane, 4,4-dimethv...	142	C6H11B03	1000063-89-2	50	
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	47	
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	47	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

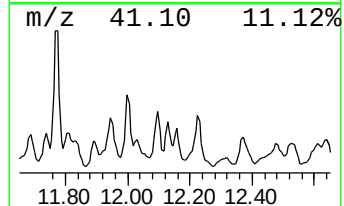
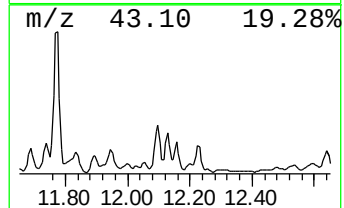
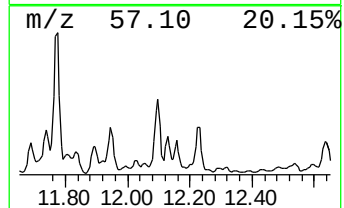
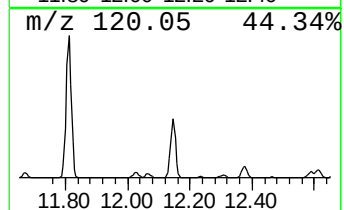
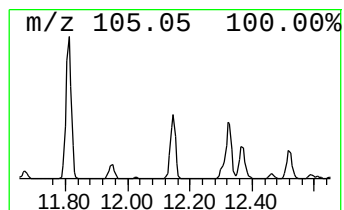
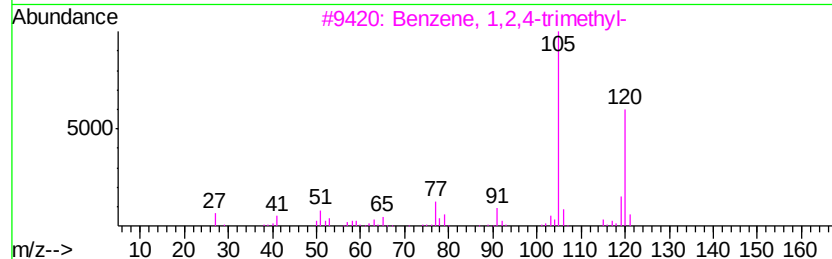
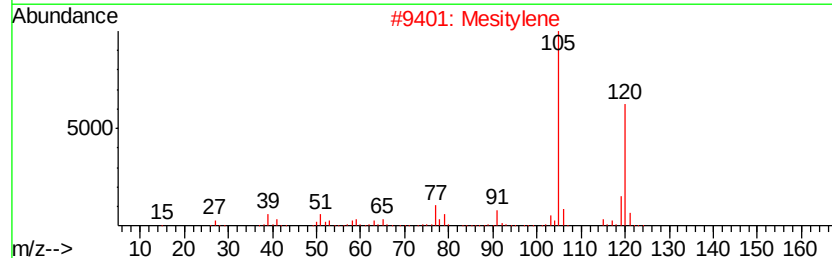
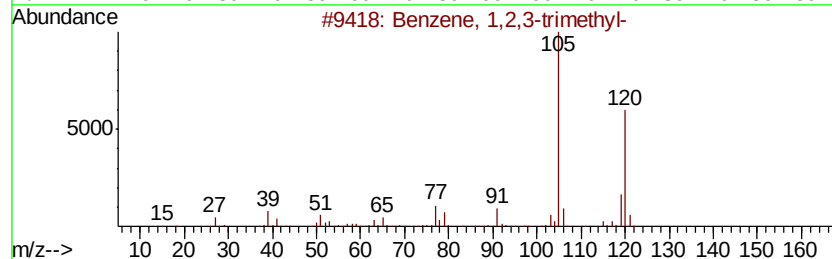
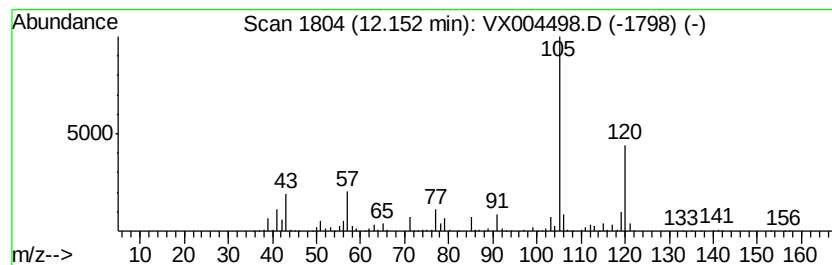
Instrument :
MSVOA_X
ClientSampleId :
EP1-SUT-4USTS-S

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 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.15	50.47 ug/l	4478960	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

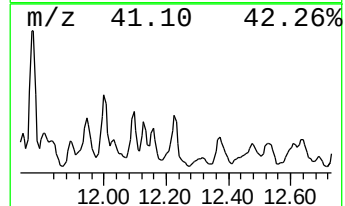
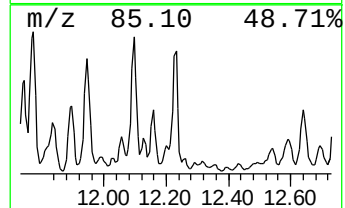
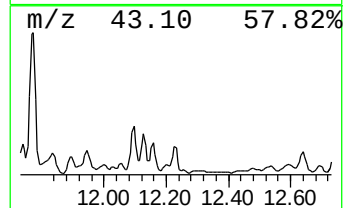
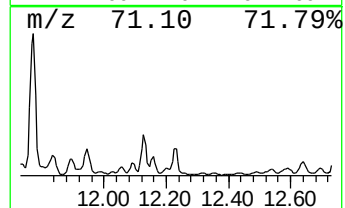
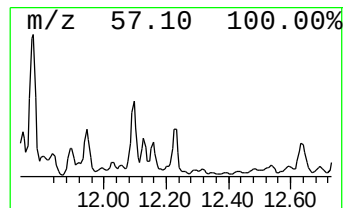
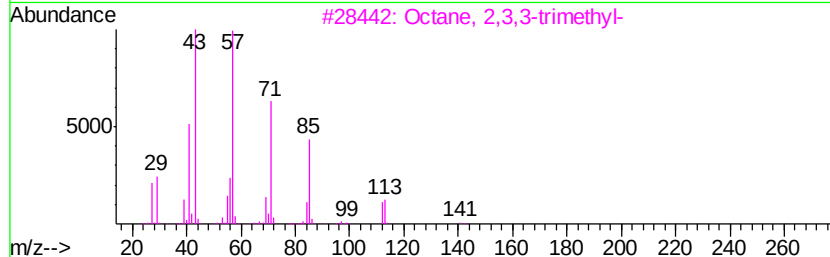
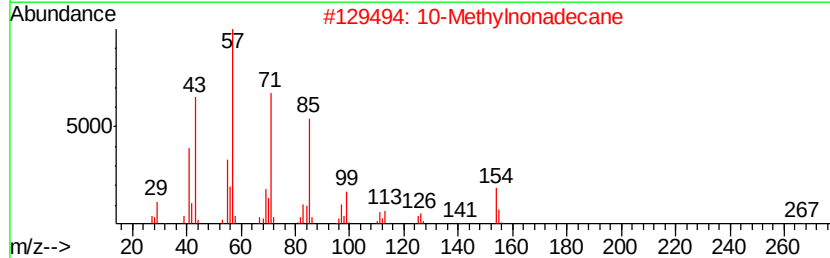
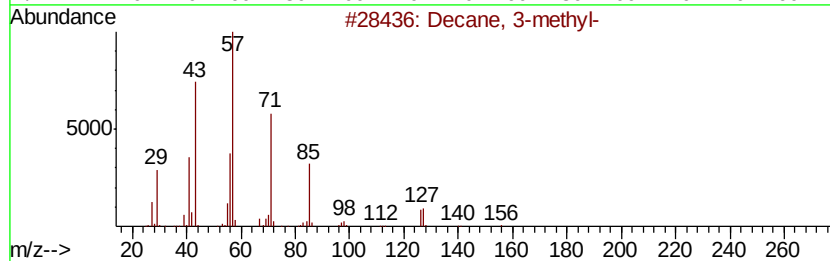
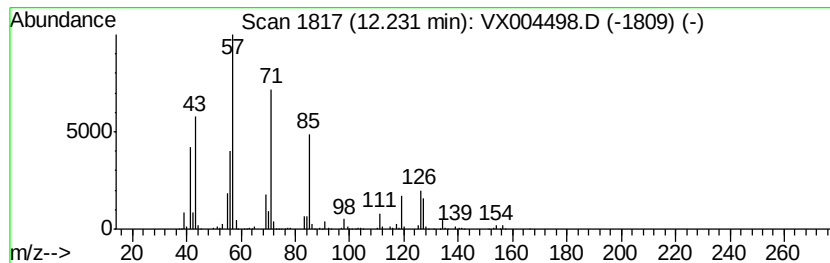
Instrument :
MSVOA_X
ClientSampleId :
EP1-SUT-4USTS-S

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 Decane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	36.39 ug/l	3228750	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane, 3-methyl-	156 C11H24	013151-34-3	87
2	10-Methylnonadecane	282 C20H42	056862-62-5	53
3	Octane, 2,3,3-trimethyl-	156 C11H24	062016-30-2	50
4	Tridecane	184 C13H28	000629-50-5	50
5	Pentane, 2,2,3,4-tetramethyl-	128 C9H20	001186-53-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

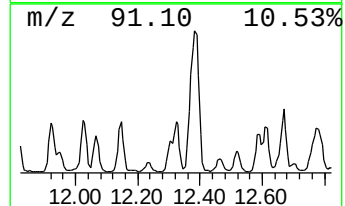
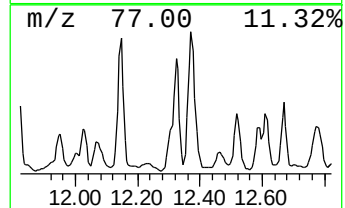
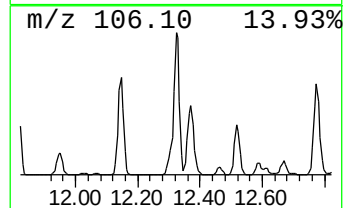
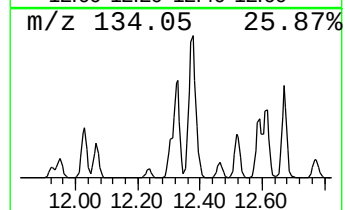
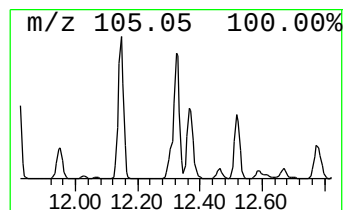
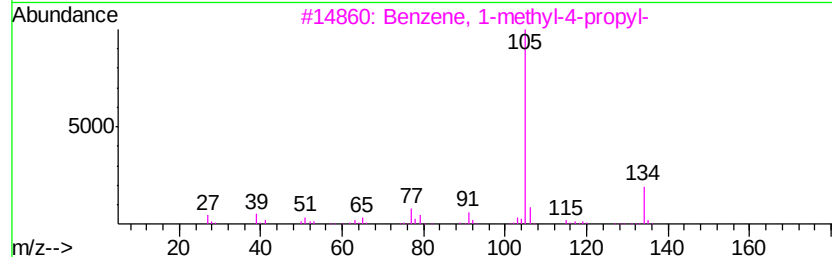
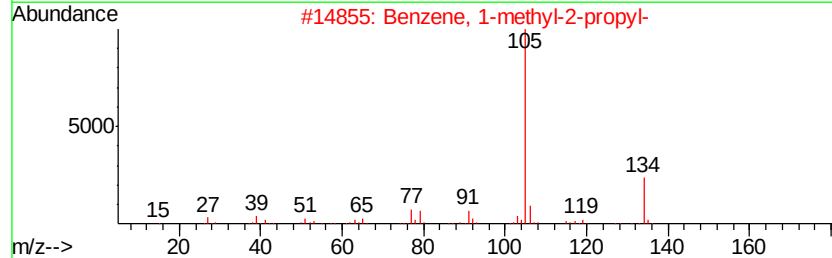
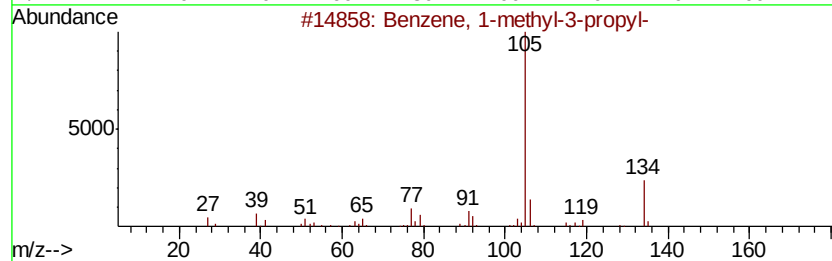
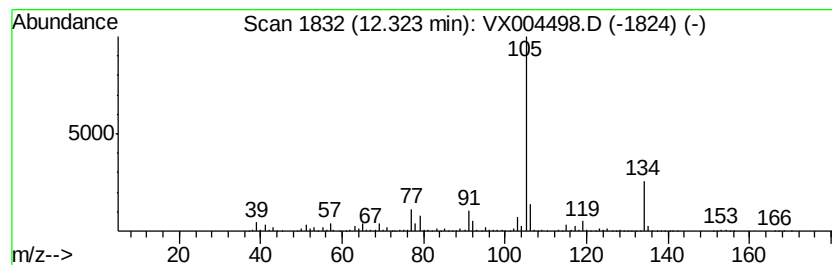
Instrument :
MSVOA_X
ClientSampleId :
EP1-SUT-4USTS-S

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 Benzene, 1-methyl-3-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	32.35 ug/l	2870970	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-methyl-3-propyl-	134 C10H14	001074-43-7 95
2		Benzene, 1-methyl-2-propyl-	134 C10H14	001074-17-5 91
3		Benzene, 1-methyl-4-propyl-	134 C10H14	001074-55-1 90
4		Benzene, (1-methylpropyl)-	134 C10H14	000135-98-8 72
5		2-Tolylloxirane	134 C9H10O	002783-26-8 64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

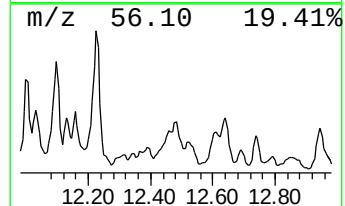
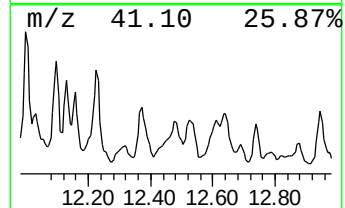
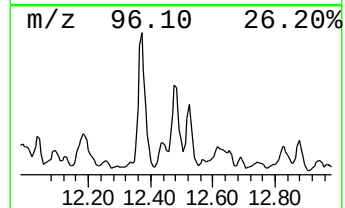
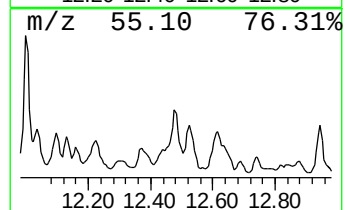
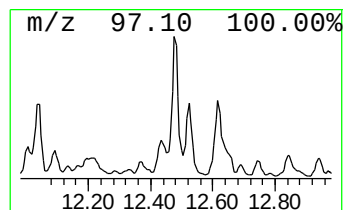
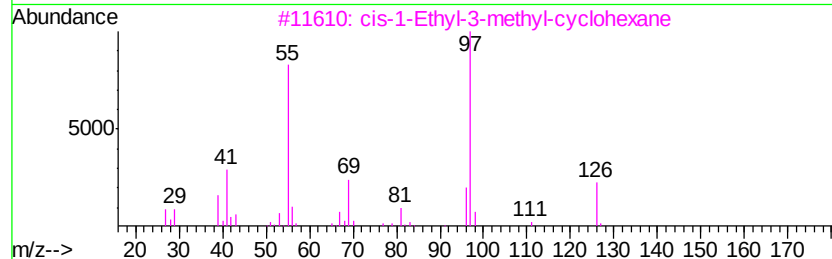
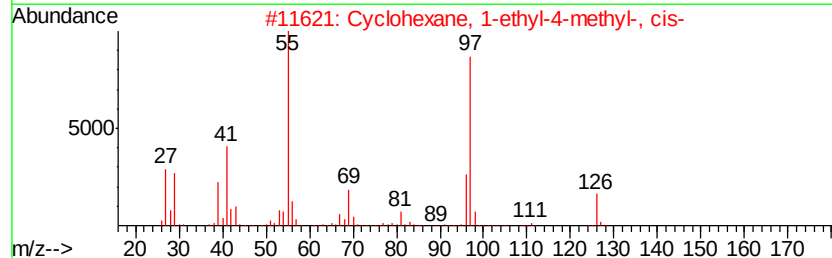
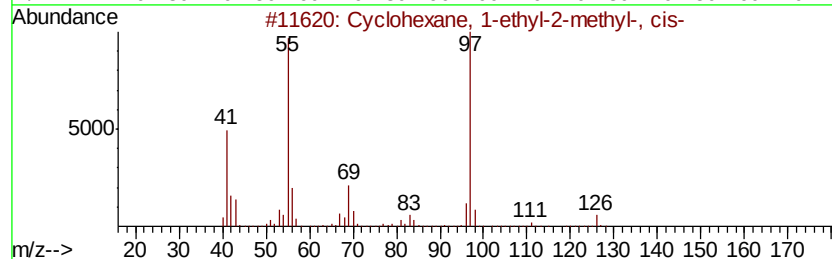
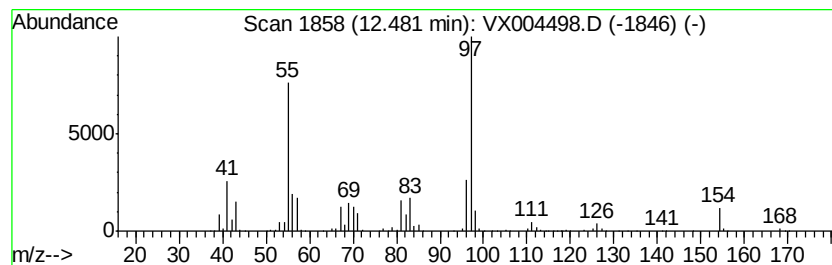
Instrument :
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ClientSampleId :
EP1-SUT-4USTS-S

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 10 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	35.58 ug/l	3156930	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126 C9H18	004923-77-7 64
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	004926-78-7 59
3		cis-1-Ethyl-3-methyl-cyclohexane	126 C9H18	019489-10-2 59
4		Cyclohexane, 1-methyl-3-pentyl-	168 C12H24	054411-02-8 59
5		Oxalic acid, cyclohexylmethyl is...	270 C15H26O4	1000309-68-3 59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091218\
Data File : VX004498.D
Acq On : 12 Sep 2018 16:49
Operator : JC/MD
Sample : J4724-16 50X
Misc : 4.95g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-SUT-4USTS-S

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
Cyclohexane, 1-et...	10.65	54.1	ug/l	1073660	3	10.12	992811	50.0
Octane, 2,5-dimet...	10.73	39.2	ug/l	778955	3	10.12	992811	50.0
Octane, 2,6-dimet...	10.84	143.3	ug/l	2846300	3	10.12	992811	50.0
Cyclohexane, propyl-	10.91	117.9	ug/l	2341470	3	10.12	992811	50.0
Heptane, 3-ethyl-...	10.95	71.0	ug/l	1410510	3	10.12	992811	50.0
Benzene, 1,2,3-tr...	12.15	50.5	ug/l	4478960	4	12.08	4436900	50.0
Decane, 3-methyl-	12.23	36.4	ug/l	3228750	4	12.08	4436900	50.0
Benzene, 1-methyl...	12.32	32.4	ug/l	2870970	4	12.08	4436900	50.0
Cyclohexane, 1-et...	12.48	35.6	ug/l	3156930	4	12.08	4436900	50.0