

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091818\
 Data File : VX004656.D
 Acq On : 18 Sep 2018 14:29
 Operator : JC/MD
 Sample : J4906-05 50X
 Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SP-PIT-1

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	1.629	65	78	85	rVB4	8974	31914	2.69%	0.259%
2	3.513	379	387	397	rVB2	10386	23842	2.01%	0.193%
3	4.391	521	531	543	rVB2	8866	25169	2.12%	0.204%
4	5.501	702	713	723	rBV2	138181	395298	33.36%	3.206%
5	5.659	730	739	771	rVB2	196474	588629	49.68%	4.774%
6	5.921	771	782	795	rVB3	13262	42063	3.55%	0.341%
7	6.068	795	806	826	rBV	139334	375253	31.67%	3.043%
8	6.250	826	836	847	rVV7	6448	22527	1.90%	0.183%
9	6.452	860	869	878	rVB2	10217	28299	2.39%	0.229%
10	6.702	900	910	925	rVB3	21925	54854	4.63%	0.445%
11	6.860	925	936	949	rBV	319012	761756	64.29%	6.178%
12	7.458	1023	1034	1044	rBV2	59173	140009	11.82%	1.135%
13	7.848	1091	1098	1106	rVB3	10689	21422	1.81%	0.174%
14	8.025	1120	1127	1140	rVB4	11679	25906	2.19%	0.210%
15	8.342	1174	1179	1183	rBV	35093	58406	4.93%	0.474%
16	8.378	1183	1185	1193	rVB4	14949	22790	1.92%	0.185%
17	8.500	1200	1205	1210	rBV	21772	36614	3.09%	0.297%
18	8.665	1225	1232	1235	rBV2	40657	72295	6.10%	0.586%
19	8.713	1235	1240	1249	rVB	746501	1184946	100.00%	9.610%
20	8.841	1255	1261	1265	rBV	13948	23523	1.99%	0.191%
21	8.909	1269	1272	1278	rVB2	13537	21842	1.84%	0.177%
22	8.976	1278	1283	1289	rBV2	23999	38886	3.28%	0.315%
23	9.043	1289	1294	1305	rVB	32453	58074	4.90%	0.471%
24	9.165	1305	1314	1319	rBV	16099	29994	2.53%	0.243%
25	9.445	1353	1360	1365	rBV	27111	42537	3.59%	0.345%
26	9.567	1374	1380	1385	rBV3	20671	46950	3.96%	0.381%
27	9.622	1385	1389	1394	rVB	44685	59108	4.99%	0.479%
28	9.677	1394	1398	1403	rBV	48887	77286	6.52%	0.627%
29	9.817	1416	1421	1426	rBV3	15827	25181	2.13%	0.204%
30	9.878	1426	1431	1437	rBV4	24537	60370	5.09%	0.490%
31	9.963	1441	1445	1449	rVB	43810	61678	5.21%	0.500%
32	10.067	1455	1462	1465	rBV	48581	67363	5.68%	0.546%
33	10.116	1465	1470	1476	rVV	652406	874975	73.84%	7.096%
34	10.189	1476	1482	1485	rVV3	9570	19763	1.67%	0.160%

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 Title : SW846 8260

35	10.244	1486	1491	1497	rVB3	12706	27113	2.29%	0.220%
36	10.335	1497	1506	1508	rBV3	26829	51527	4.35%	0.418%
37	10.378	1508	1513	1516	rVV2	34931	64133	5.41%	0.520%
38	10.414	1516	1519	1530	rVB2	23353	46334	3.91%	0.376%
39	10.512	1530	1535	1543	rBV5	15855	31538	2.66%	0.256%
40	10.646	1550	1557	1565	rVB4	40225	75191	6.35%	0.610%
41	10.725	1565	1570	1575	rBV3	17104	28126	2.37%	0.228%
42	10.835	1580	1588	1592	rBV2	91604	141187	11.92%	1.145%
43	10.914	1592	1601	1604	rBV3	62821	102023	8.61%	0.827%
44	10.951	1604	1607	1612	rVB	35535	45962	3.88%	0.373%
45	11.018	1612	1618	1621	rBV3	18714	30154	2.54%	0.245%
46	11.085	1626	1629	1632	rVB	21819	24338	2.05%	0.197%
47	11.140	1632	1638	1649	rVB	748144	993646	83.86%	8.058%
48	11.243	1649	1655	1658	rBV	44038	68556	5.79%	0.556%
49	11.274	1658	1660	1671	rVB3	43586	62079	5.24%	0.503%
50	11.359	1671	1674	1677	rBV	20382	25765	2.17%	0.209%
51	11.451	1684	1689	1692	rBV3	17221	28445	2.40%	0.231%
52	11.487	1692	1695	1700	rBV3	34650	47590	4.02%	0.386%
53	11.536	1700	1703	1708	rVB2	26278	39794	3.36%	0.323%
54	11.682	1721	1727	1732	rVB5	23596	51719	4.36%	0.419%
55	11.737	1732	1736	1738	rBV2	22256	27950	2.36%	0.227%
56	11.768	1738	1741	1745	rBV	87712	95386	8.05%	0.774%
57	11.945	1767	1770	1775	rVB3	47677	66580	5.62%	0.540%
58	11.999	1775	1779	1782	rBV	44365	54652	4.61%	0.443%
59	12.079	1787	1792	1798	rVV	895935	1106600	93.39%	8.974%
60	12.128	1798	1800	1802	rVV	37366	37522	3.17%	0.304%
61	12.158	1802	1805	1809	rVV2	47584	55147	4.65%	0.447%
62	12.225	1809	1816	1824	rVB3	52544	96748	8.16%	0.785%
63	12.304	1824	1829	1836	rVB	55488	85749	7.24%	0.695%
64	12.371	1836	1840	1846	rBV3	62964	110713	9.34%	0.898%
65	12.475	1851	1857	1862	rBV3	30669	59080	4.99%	0.479%
66	12.524	1862	1865	1870	rVB3	35551	57371	4.84%	0.465%
67	12.640	1871	1884	1886	rBV5	57353	168015	14.18%	1.363%
68	12.670	1886	1889	1897	rVB	70057	120490	10.17%	0.977%
69	12.743	1897	1901	1902	rBV2	41049	52378	4.42%	0.425%
70	12.877	1920	1923	1928	rVB5	23176	31731	2.68%	0.257%
71	12.944	1928	1934	1945	rBV7	73620	225627	19.04%	1.830%

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72	13.030	1945	1948	1953	rVB4	29430	41748	3.52%	0.339%
73	13.103	1953	1960	1962	rBV4	98105	198213	16.73%	1.607%
74	13.152	1962	1968	1978	rVB4	119332	392657	33.14%	3.184%
75	13.316	1991	1995	1996	rVV4	18398	24259	2.05%	0.197%
76	13.347	1996	2000	2006	rVV2	111649	181480	15.32%	1.472%
77	13.402	2006	2009	2011	rVV3	17312	23042	1.94%	0.187%
78	13.438	2011	2015	2019	rVV2	61227	91867	7.75%	0.745%
79	13.481	2019	2022	2031	rVV7	34947	93217	7.87%	0.756%
80	13.560	2033	2035	2038	rVV4	19207	26342	2.22%	0.214%
81	13.603	2038	2042	2045	rVV	29809	46902	3.96%	0.380%
82	13.639	2045	2048	2053	rVB3	28970	45981	3.88%	0.373%
83	13.725	2059	2062	2066	rBV2	22174	31376	2.65%	0.254%
84	13.835	2076	2080	2083	rVV	60822	91196	7.70%	0.740%
85	13.895	2086	2090	2098	rVB2	85088	189538	16.00%	1.537%
86	13.987	2099	2105	2109	rVB7	19086	43374	3.66%	0.352%
87	14.133	2125	2129	2132	rBV3	18760	26580	2.24%	0.216%
88	14.322	2148	2160	2174	rVV5	69605	338777	28.59%	2.747%
89	14.548	2191	2197	2205	rVB6	21474	57777	4.88%	0.469%
90	14.700	2218	2222	2226	rVB	73904	88965	7.51%	0.721%
91	14.786	2232	2236	2239	rBV4	13561	24873	2.10%	0.202%
92	14.840	2242	2245	2252	rVV	40924	58943	4.97%	0.478%
93	15.273	2308	2316	2320	rBV2	18836	34932	2.95%	0.283%
94	15.450	2341	2345	2348	rBV3	11795	21084	1.78%	0.171%
95	15.493	2348	2352	2355	rVV4	20579	41802	3.53%	0.339%
96	15.548	2356	2361	2370	rVB4	36616	85747	7.24%	0.695%
97	15.694	2379	2385	2387	rBV	22911	38464	3.25%	0.312%
98	15.724	2387	2390	2401	rVB2	23976	53783	4.54%	0.436%
99	15.913	2411	2421	2426	rBV6	9583	33549	2.83%	0.272%
100	16.176	2459	2464	2472	rVB2	23889	48015	4.05%	0.389%

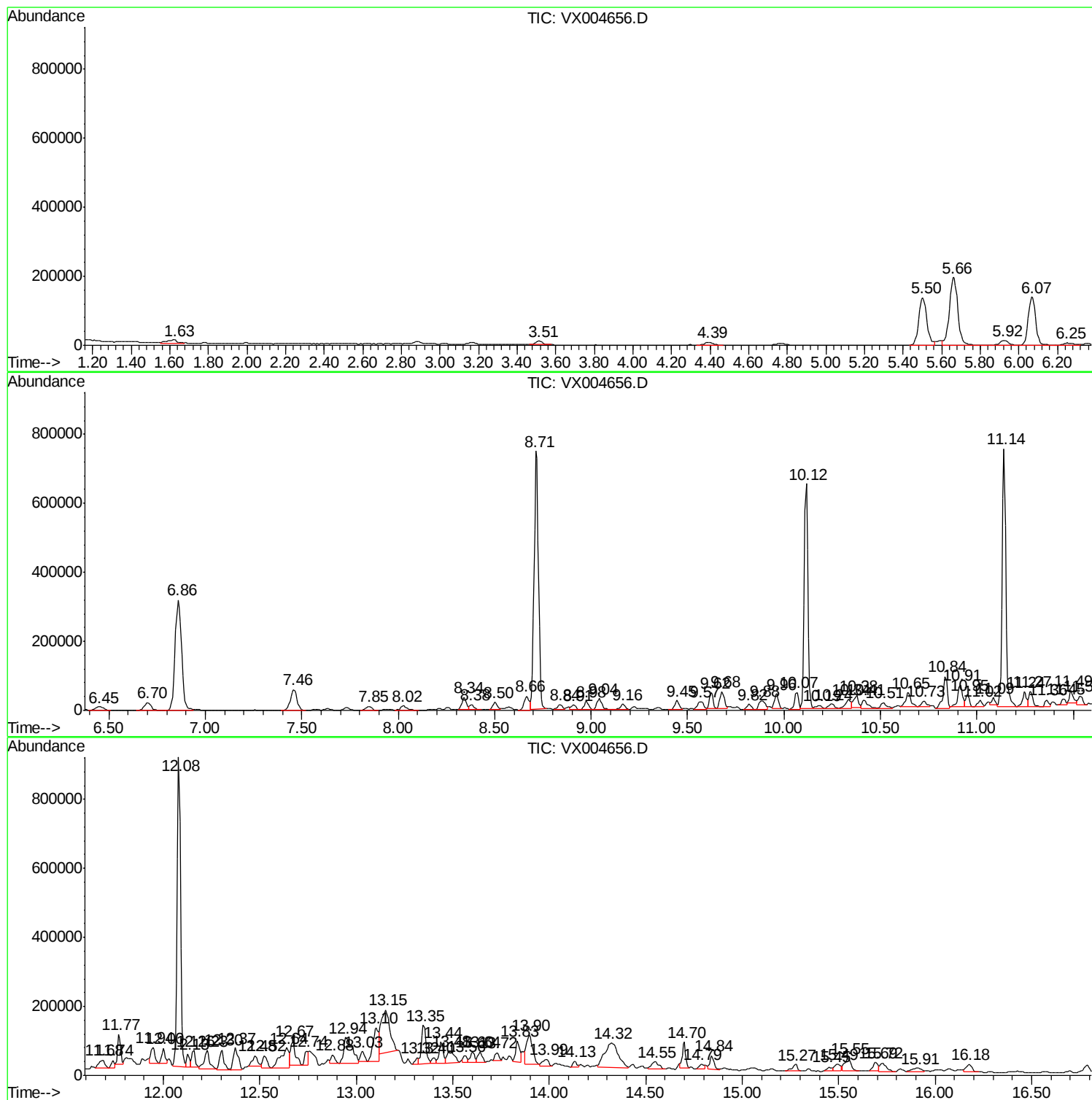
Sum of corrected areas: 12330964

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Instrument :
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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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
SP-PIT-1

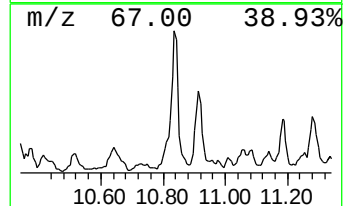
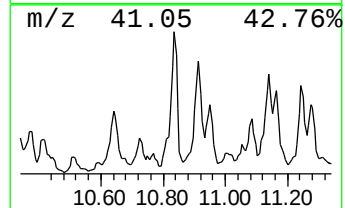
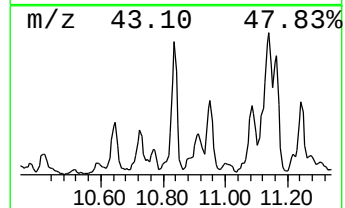
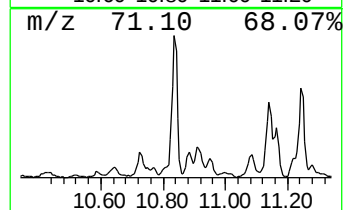
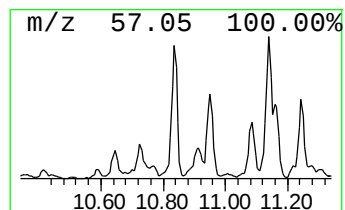
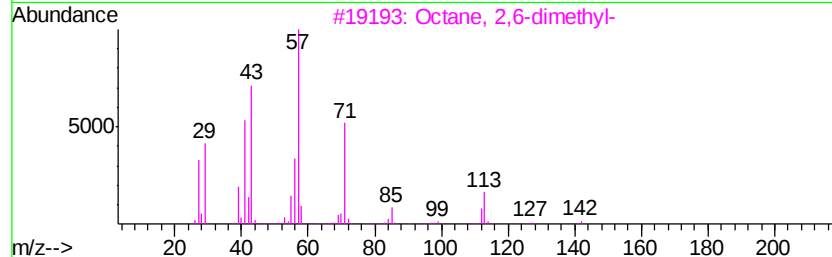
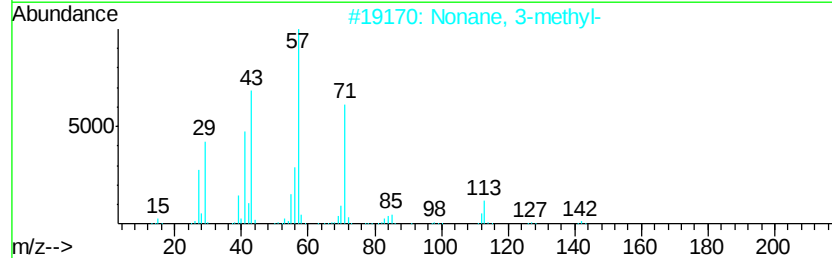
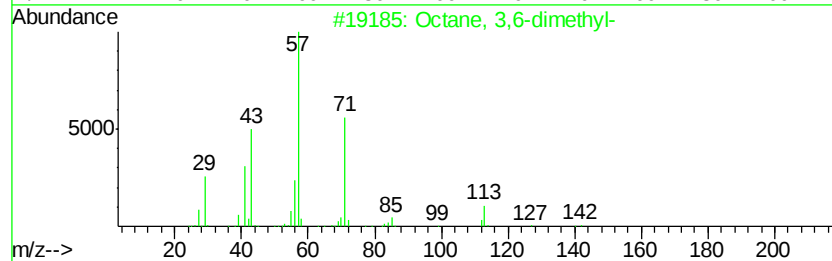
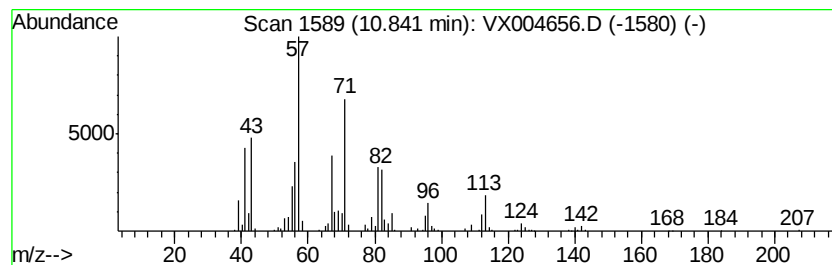
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	8.07 ug/l	141187	Chlorobenzene-d5	10.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	60
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	60
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	60
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	38



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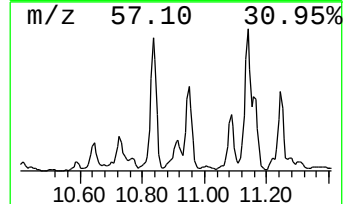
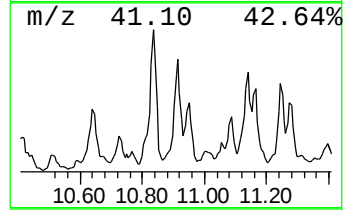
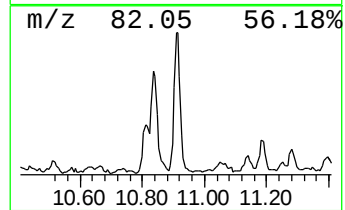
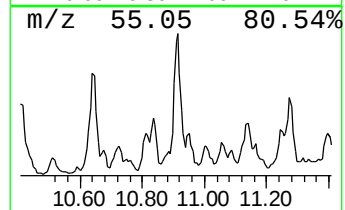
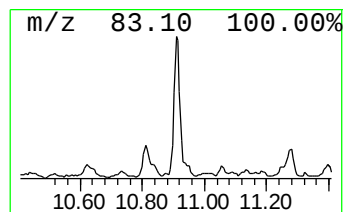
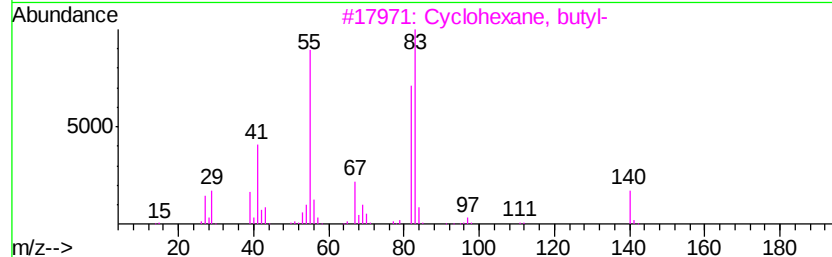
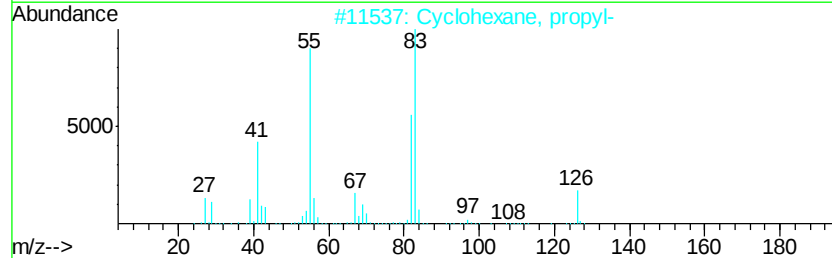
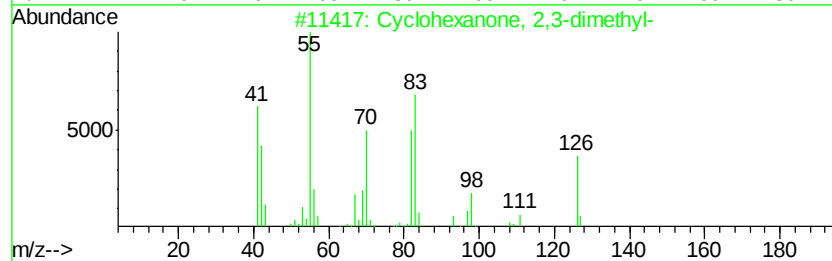
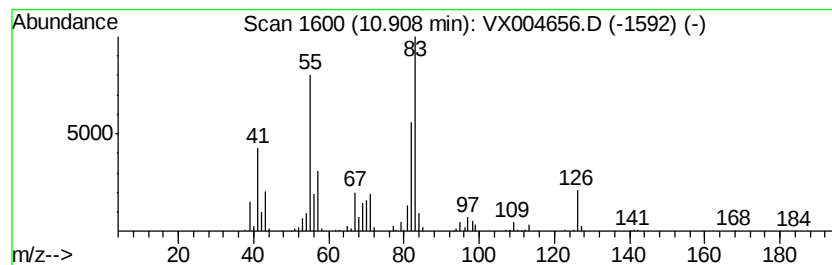
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexanone, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.91	5.83 ug/l	102023	Chlorobenzene-d5		10.12	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	74
2		Cvclohexane, propyl-	126	C9H18	001678-92-8	72
3		Cvclohexane, butyl-	140	C10H20	001678-93-9	59
4		Cvclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	58
5		Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	53



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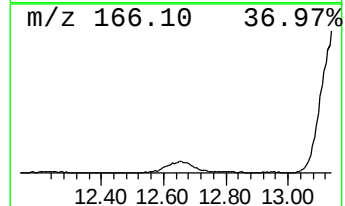
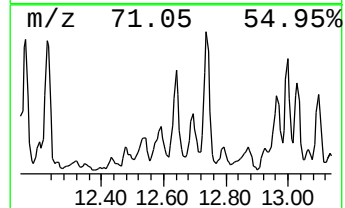
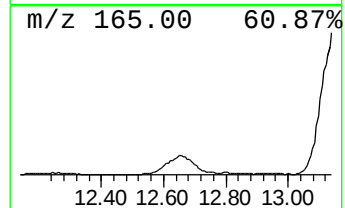
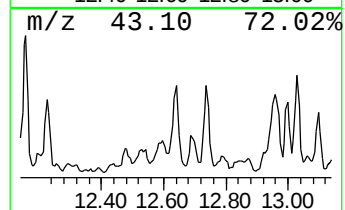
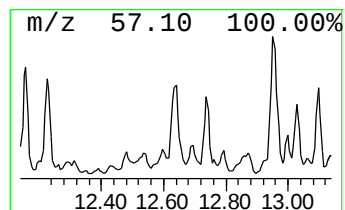
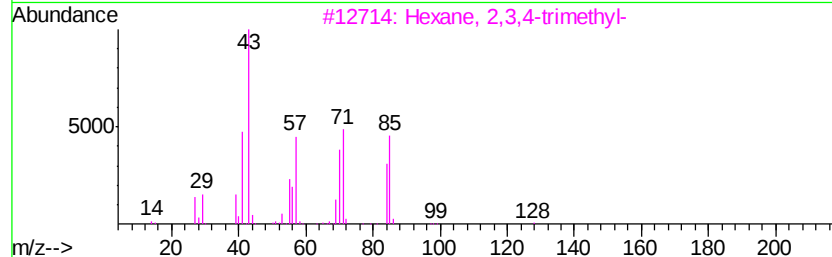
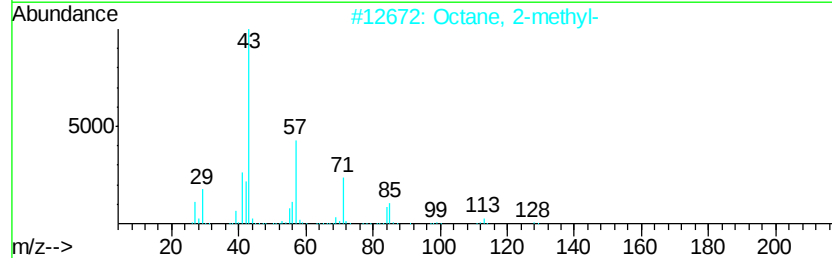
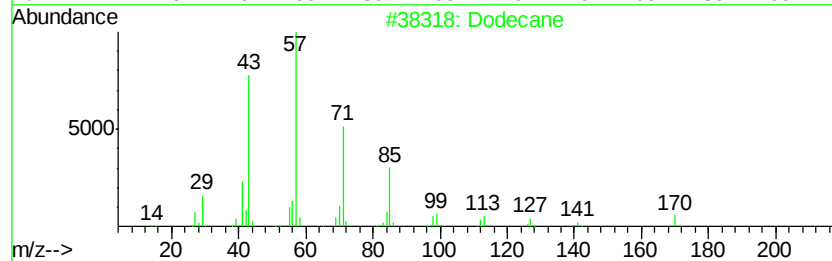
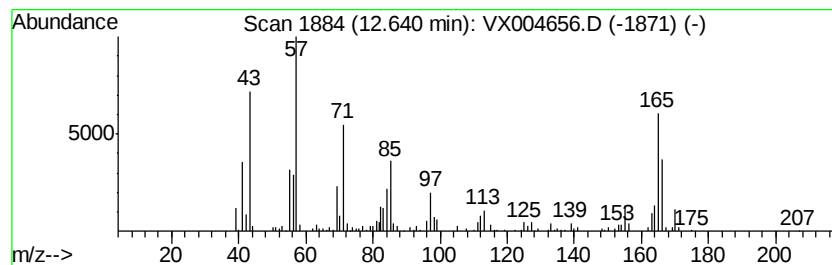
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MSVOA_X
ClientSampled :
SP-PIT-1

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 unknown12.64 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	7.59 ug/l	168015	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane	170 C12H26	000112-40-3	38
2	Octane, 2-methyl-	128 C9H20	003221-61-2	30
3	Hexane, 2,3,4-trimethyl-	128 C9H20	000921-47-1	27
4	Tetradecane, 2,6,10-trimethyl-	240 C17H36	014905-56-7	27
5	Tridecane	184 C13H28	000629-50-5	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

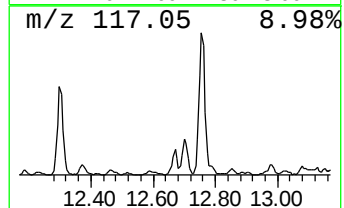
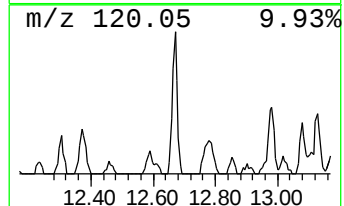
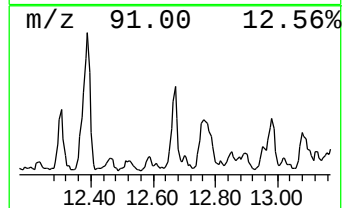
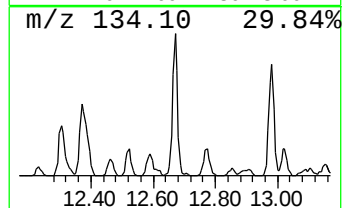
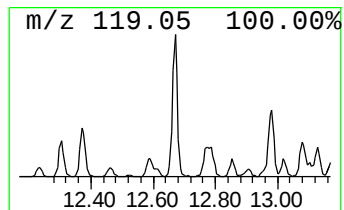
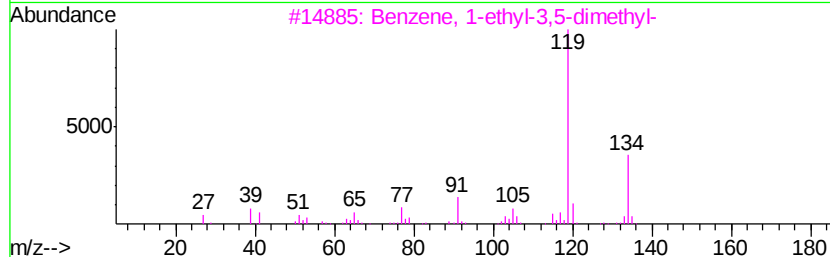
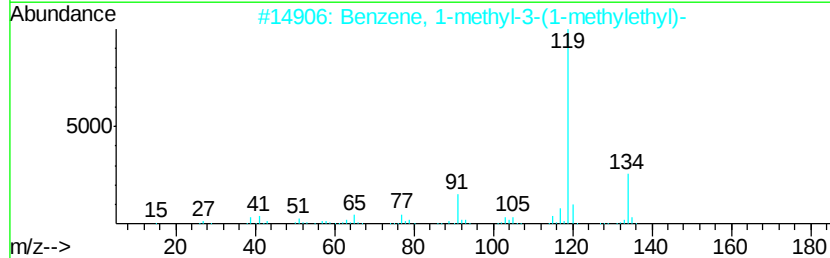
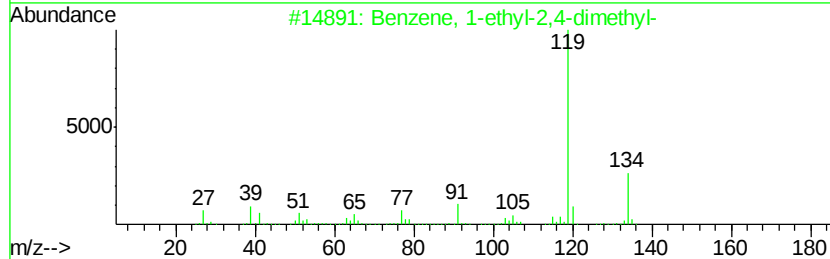
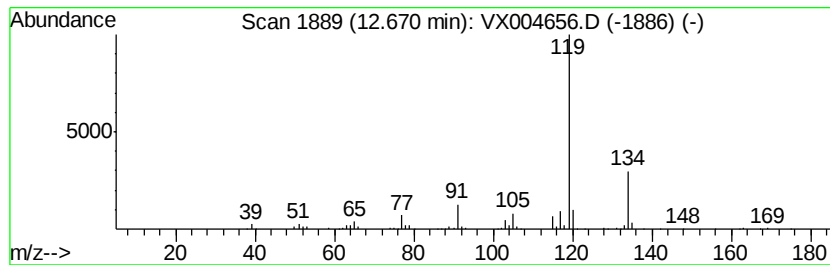
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	5.44 ug/l	120490	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
2		Benzene, 1-methyl-3-(1-methylethyl-)	134	C10H14	000535-77-3	94
3		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5		p-Cymene	134	C10H14	000099-87-6	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

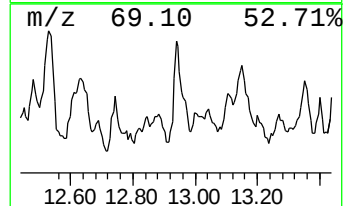
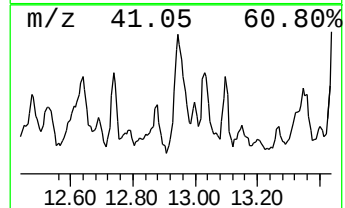
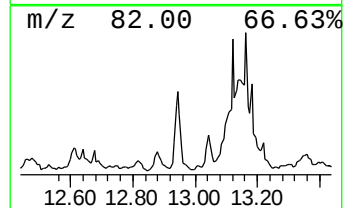
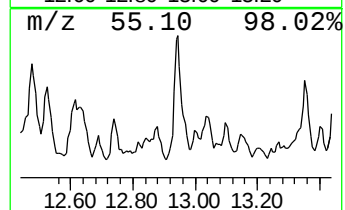
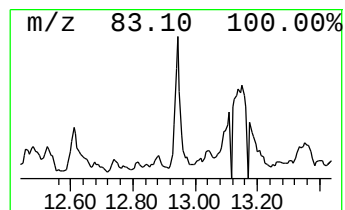
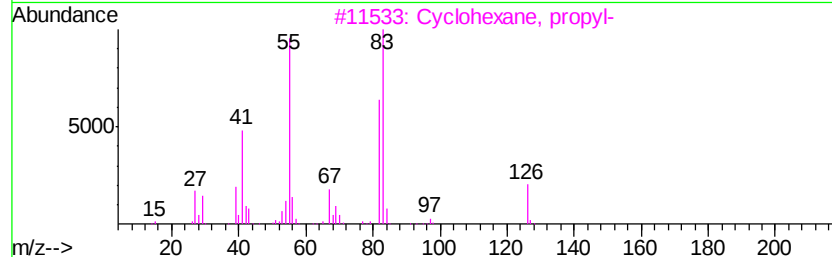
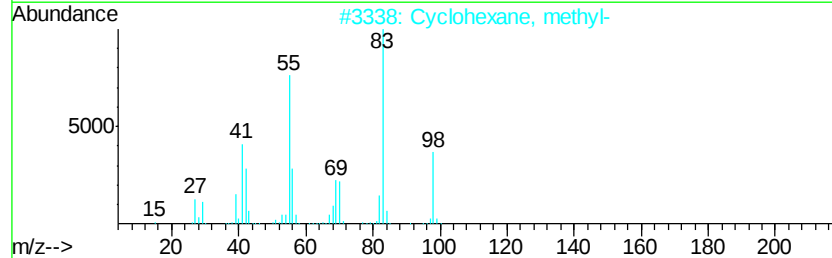
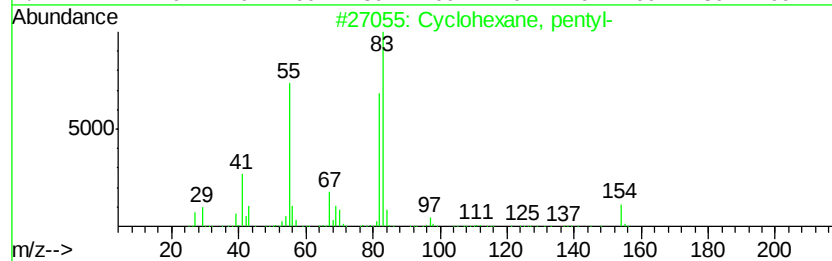
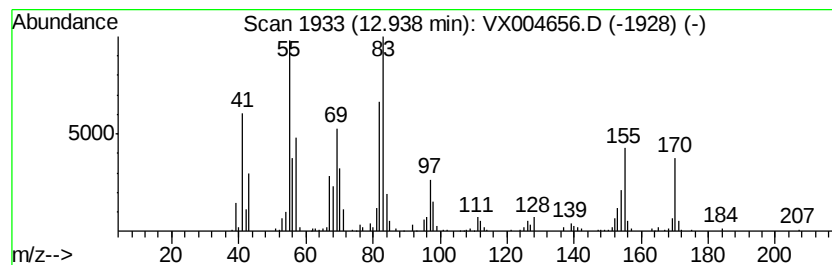
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, pentyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	10.19 ug/l	225627	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, pentyl-	154	C11H22	004292-92-6	52
2		Cyclohexane, methyl-	98	C7H14	000108-87-2	46
3		Cyclohexane, propyl-	126	C9H18	001678-92-8	46
4		Cyclohexane, ethyl-	112	C8H16	001678-91-7	46
5		Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

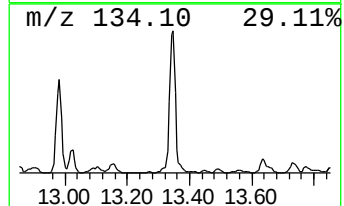
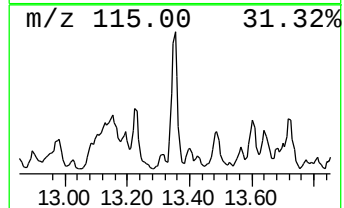
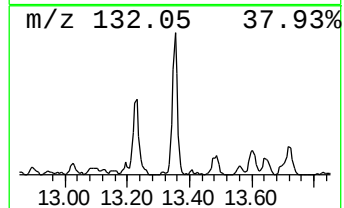
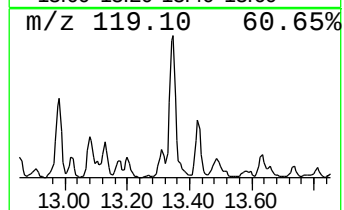
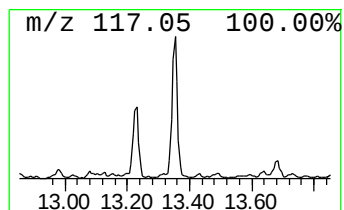
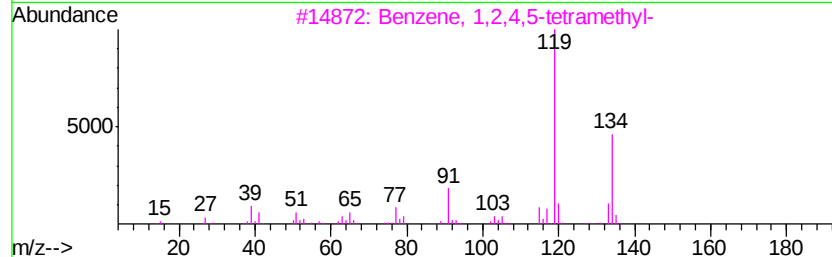
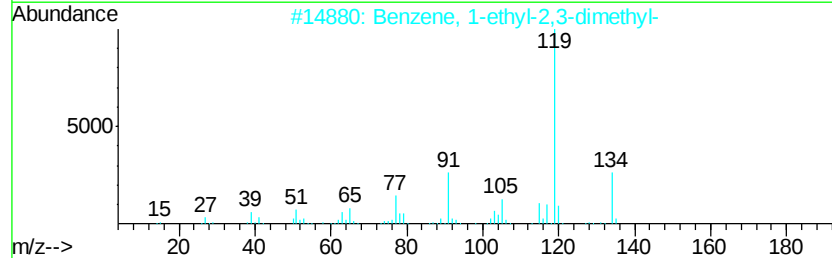
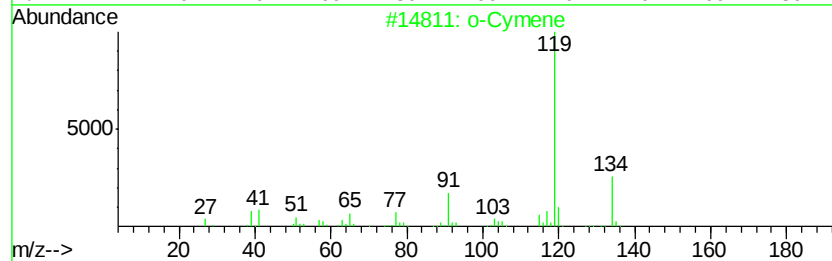
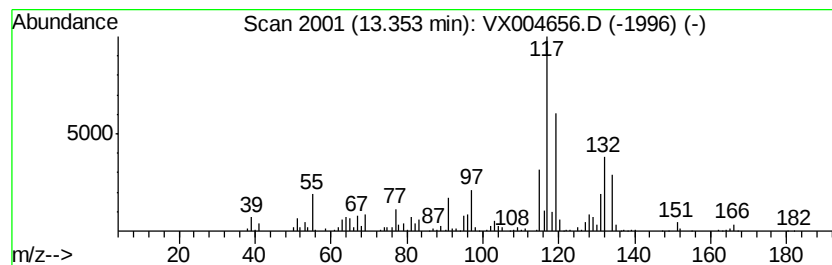
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	8.20 ug/l	181480	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	60
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	60
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	53
4		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	53
5		p-Cymene	134	C10H14	000099-87-6	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

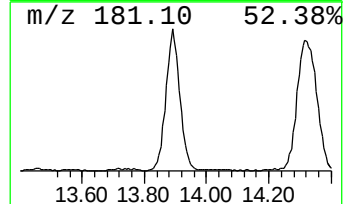
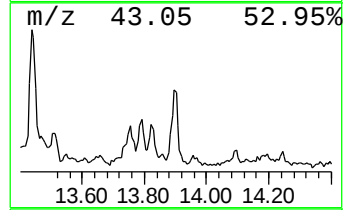
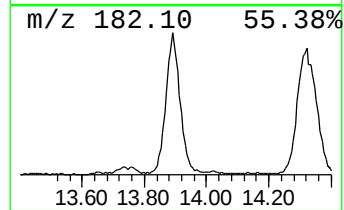
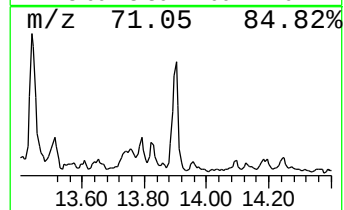
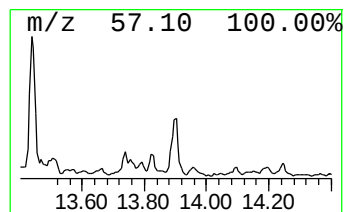
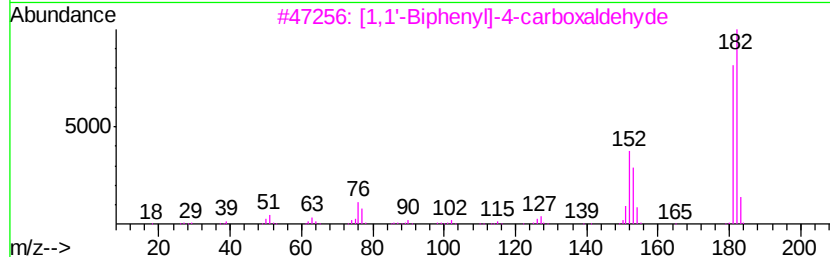
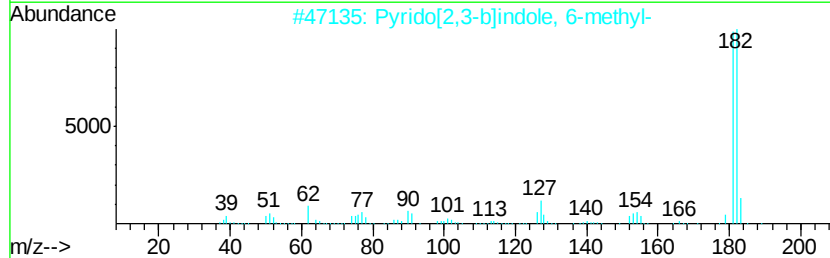
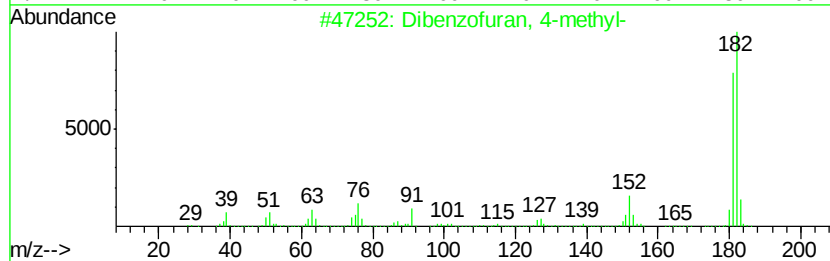
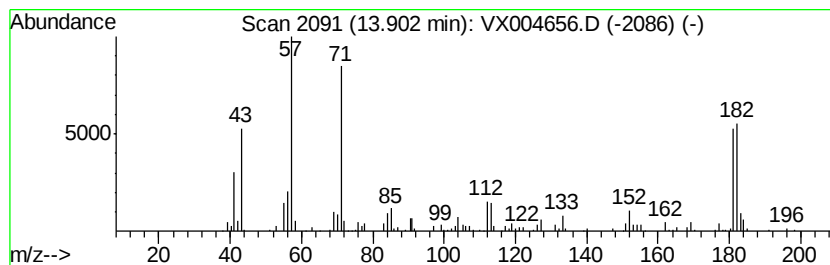
Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

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 Dibenzofuran, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	8.56 ug/l	189538	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzofuran, 4-methyl-	182	C13H10O	007320-53-8	55
2	Pyrido[2,3-b]indole, 6-methyl-	182	C12H10N2	108349-67-3	46
3	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	45
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	30
5	8H-Thiazolo[5,4-c]azepin-8-one, ...	182	C8H10N2OS	031967-03-0	30



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08q/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

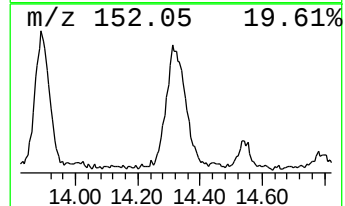
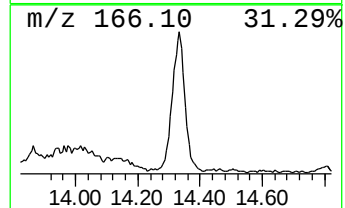
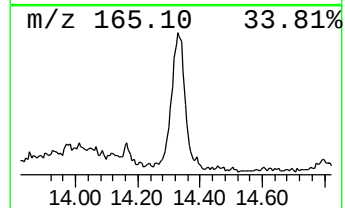
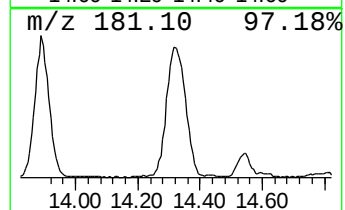
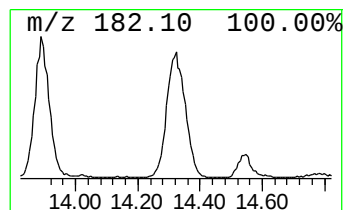
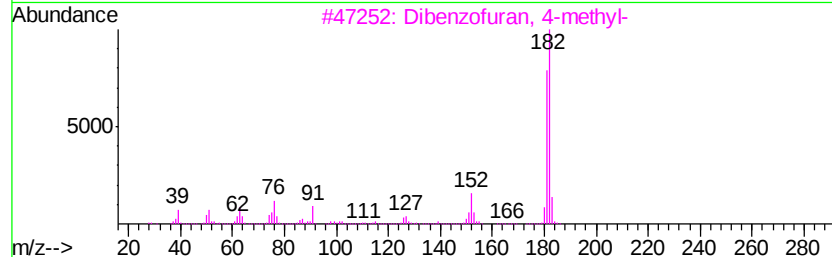
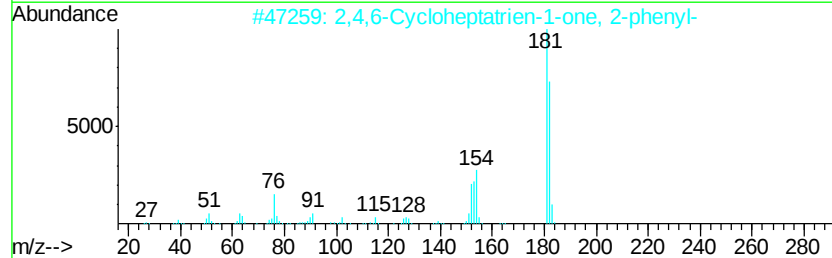
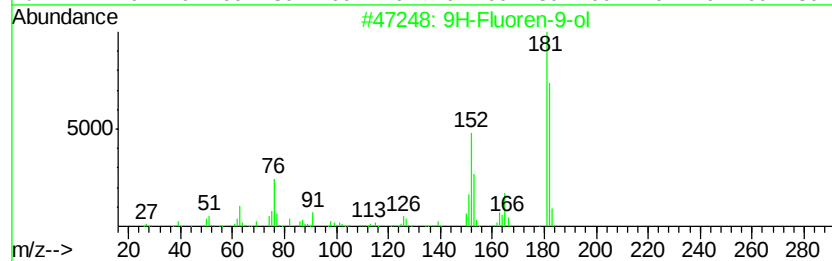
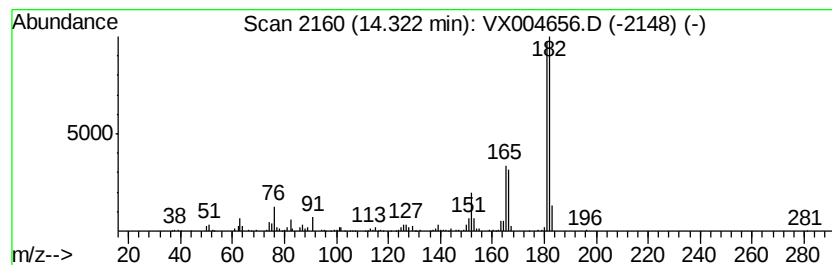
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

Peak Number 10 9H-Fluoren-9-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	15.31 ug/l	338777	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9H-Fluoren-9-ol	182	C13H10O	001689-64-1	87
2		2,4,6-Cycloheptatrien-1-one, 2-p...	182	C13H10O	014562-09-5	64
3		Dibenzofuran, 4-methyl-	182	C13H10O	007320-53-8	60
4		[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	59
5		2-Hydroxyfluorene	182	C13H10O	002443-58-5	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004656.D
Acq On : 18 Sep 2018 14:29
Operator : JC/MD
Sample : J4906-05 50X
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-PIT-1

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
Octane, 3,6-dimet...	10.84	8.1	ug/l	141187	3	10.12	874975	50.0
Cyclohexanone, 2,...	10.91	5.8	ug/l	102023	3	10.12	874975	50.0
unknown12.64	12.64	7.6	ug/l	168015	4	12.08	1106600	50.0
Benzene, 1-ethyl-...	12.67	5.4	ug/l	120490	4	12.08	1106600	50.0
Cyclohexane, pentyl-	12.94	10.2	ug/l	225627	4	12.08	1106600	50.0
o-Cymene	13.35	8.2	ug/l	181480	4	12.08	1106600	50.0
Dibenzofuran, 4-m...	13.90	8.6	ug/l	189538	4	12.08	1106600	50.0
9H-Fluoren-9-ol	14.32	15.3	ug/l	338777	4	12.08	1106600	50.0