

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061318\
 Data File : VX002534.D
 Acq On : 14 Jun 2018 03:35
 Operator : JC/MD
 Sample : J3383-11
 Misc : 6.10g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-40VR

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\82X060418W.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	1.069	75	79	93	rBV	852168	1072777	21.57%	1.680%
2	1.934	217	221	233	rVB	152409	226983	4.56%	0.356%
3	2.806	357	364	366	rBV2	89495	161918	3.26%	0.254%
4	2.855	366	372	384	rVB	447469	955738	19.21%	1.497%
5	3.135	409	418	437	rVB	323052	745690	14.99%	1.168%
6	3.489	466	476	491	rBV	533437	1197263	24.07%	1.875%
7	3.788	517	525	535	rVB	55021	138114	2.78%	0.216%
8	4.275	596	605	612	rVV	56395	170156	3.42%	0.267%
9	4.373	612	621	634	rVV	264115	770589	15.49%	1.207%
10	5.513	788	808	810	rBV	164887	451542	9.08%	0.707%
11	5.586	811	820	827	rVV3	481993	1833030	36.85%	2.871%
12	5.665	827	833	860	rVV2	282150	1331250	26.76%	2.085%
13	5.909	860	873	889	rVV	520828	1551863	31.20%	2.431%
14	6.068	889	899	915	rVV	172100	471401	9.48%	0.738%
15	6.251	915	929	937	rVV3	143496	531212	10.68%	0.832%
16	6.342	937	944	952	rVV2	161595	479206	9.63%	0.751%
17	6.446	952	961	973	rVB2	175387	501830	10.09%	0.786%
18	6.696	988	1002	1020	rBV	875002	2107501	42.37%	3.301%
19	6.866	1020	1030	1036	rBV	358827	957055	19.24%	1.499%
20	7.250	1083	1093	1099	rBV2	72299	161688	3.25%	0.253%
21	7.458	1114	1127	1138	rBV	1047536	2434667	48.95%	3.814%
22	7.567	1138	1145	1150	rBV	130402	270248	5.43%	0.423%
23	7.634	1150	1156	1166	rVB	176637	358787	7.21%	0.562%
24	7.732	1166	1172	1182	rVB	143097	281177	5.65%	0.440%
25	7.842	1182	1190	1198	rVB2	142558	301000	6.05%	0.471%
26	8.171	1236	1244	1247	rBV3	99993	200929	4.04%	0.315%
27	8.214	1247	1251	1254	rVV	87951	150119	3.02%	0.235%
28	8.256	1254	1258	1262	rVB2	136852	226869	4.56%	0.355%
29	8.342	1267	1272	1275	rVV	633218	1068524	21.48%	1.674%
30	8.378	1275	1278	1284	rVV	330893	527742	10.61%	0.827%
31	8.500	1293	1298	1303	rVV	675186	1126099	22.64%	1.764%
32	8.573	1307	1310	1319	rVB3	103415	193855	3.90%	0.304%
33	8.665	1319	1325	1329	rBV3	282750	566989	11.40%	0.888%
34	8.720	1329	1334	1343	rVB	880189	1529059	30.74%	2.395%

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35	8.835	1343	1353	1357	rBV	126644	252611	5.08%	0.396%
36	8.976	1370	1376	1382	rBV2	627047	989998	19.90%	1.551%
37	9.043	1382	1387	1398	rVB3	151027	331886	6.67%	0.520%
38	9.165	1398	1407	1413	rBV3	119967	262266	5.27%	0.411%
39	9.226	1413	1417	1420	rBV2	108563	158305	3.18%	0.248%
40	9.445	1448	1453	1458	rBV	127252	182407	3.67%	0.286%
41	9.561	1467	1472	1478	rBV3	218691	447505	9.00%	0.701%
42	9.622	1478	1482	1486	rVB2	155475	211484	4.25%	0.331%
43	9.677	1486	1491	1495	rBV3	68698	132607	2.67%	0.208%
44	9.823	1509	1515	1520	rBV5	82123	158906	3.19%	0.249%
45	9.878	1520	1524	1527	rVV2	107590	182672	3.67%	0.286%
46	9.927	1528	1532	1534	rVV2	126036	211830	4.26%	0.332%
47	9.963	1534	1538	1543	rVV	600262	852959	17.15%	1.336%
48	10.067	1547	1555	1559	rVV	496903	667496	13.42%	1.046%
49	10.116	1559	1563	1568	rVV	744643	1071116	21.53%	1.678%
50	10.256	1581	1586	1591	rVV	1105571	1452593	29.20%	2.275%
51	10.335	1591	1599	1600	rVV6	65648	162675	3.27%	0.255%
52	10.366	1600	1604	1609	rVV2	190897	304344	6.12%	0.477%
53	10.414	1609	1612	1623	rVB3	191763	351429	7.07%	0.550%
54	10.646	1645	1650	1654	rVV	135713	186198	3.74%	0.292%
55	10.725	1658	1663	1668	rBV	100945	169863	3.41%	0.266%
56	10.835	1674	1681	1685	rBV	145828	250474	5.04%	0.392%
57	10.914	1690	1694	1698	rVV3	96680	131758	2.65%	0.206%
58	11.024	1705	1712	1718	rBV	188398	280498	5.64%	0.439%
59	11.085	1718	1722	1726	rBV	113456	155772	3.13%	0.244%
60	11.146	1726	1732	1742	rVB2	966545	1670719	33.59%	2.617%
61	11.250	1745	1749	1752	rVB	195026	228705	4.60%	0.358%
62	11.365	1763	1768	1776	rVB	763375	944130	18.98%	1.479%
63	11.457	1778	1783	1787	rVV	705650	884125	17.77%	1.385%
64	11.512	1787	1792	1803	rVB	1206981	1702161	34.22%	2.666%
65	11.676	1814	1819	1826	rBV	158675	276125	5.55%	0.433%
66	11.811	1837	1841	1850	rVB	4079686	4974066	100.00%	7.792%
67	12.085	1880	1886	1891	rBV	1064746	1370764	27.56%	2.147%
68	12.146	1891	1896	1901	rBV	746245	1028171	20.67%	1.611%
69	12.304	1917	1922	1928	rBV	774544	1027318	20.65%	1.609%
70	12.378	1928	1934	1941	rVB3	1120014	1765463	35.49%	2.765%
71	12.481	1941	1951	1954	rBV2	135369	267305	5.37%	0.419%

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72	12.524	1954	1958	1965	rVB	304061	373067	7.50%	0.584%
73	12.591	1965	1969	1971	rBV	575579	702371	14.12%	1.100%
74	12.615	1971	1973	1978	rVV	547659	627393	12.61%	0.983%
75	12.676	1978	1983	1986	rVV	878805	1143831	23.00%	1.792%
76	12.707	1986	1988	1992	rVV	157079	174757	3.51%	0.274%
77	12.762	1992	1997	2005	rVB3	387797	657081	13.21%	1.029%
78	12.908	2017	2021	2025	rVB2	182733	214340	4.31%	0.336%
79	12.981	2025	2033	2037	rBV	574039	819528	16.48%	1.284%
80	13.024	2037	2040	2045	rVB	798207	955098	19.20%	1.496%
81	13.103	2045	2053	2056	rBV3	224919	491036	9.87%	0.769%
82	13.231	2069	2074	2077	rVB2	456311	578110	11.62%	0.906%
83	13.274	2077	2081	2084	rVB2	158694	189928	3.82%	0.298%
84	13.322	2084	2089	2091	rBV2	259456	405312	8.15%	0.635%
85	13.353	2091	2094	2100	rVV2	816373	1098184	22.08%	1.720%
86	13.432	2104	2107	2112	rVB2	182678	237884	4.78%	0.373%
87	13.487	2112	2116	2124	rVB4	139430	267354	5.37%	0.419%
88	13.566	2124	2129	2132	rBV2	163453	233051	4.69%	0.365%
89	13.609	2132	2136	2138	rBV	233551	289465	5.82%	0.453%
90	13.646	2138	2142	2148	rVB3	257870	448850	9.02%	0.703%
91	13.731	2152	2156	2161	rVB2	213300	342146	6.88%	0.536%
92	13.841	2169	2174	2179	rVB	322081	429946	8.64%	0.673%
93	13.987	2192	2198	2203	rBV4	175491	317729	6.39%	0.498%
94	14.036	2203	2206	2209	rVV2	104815	136956	2.75%	0.215%
95	14.097	2213	2216	2219	rVB3	125917	143403	2.88%	0.225%
96	14.139	2219	2223	2227	rBV2	245425	296538	5.96%	0.465%
97	14.280	2241	2246	2255	rVV	225349	372320	7.49%	0.583%
98	14.438	2268	2272	2276	rVB	151473	177626	3.57%	0.278%
99	14.700	2311	2315	2325	rVB	506229	687424	13.82%	1.077%
100	14.847	2332	2339	2348	rVB2	181478	276589	5.56%	0.433%

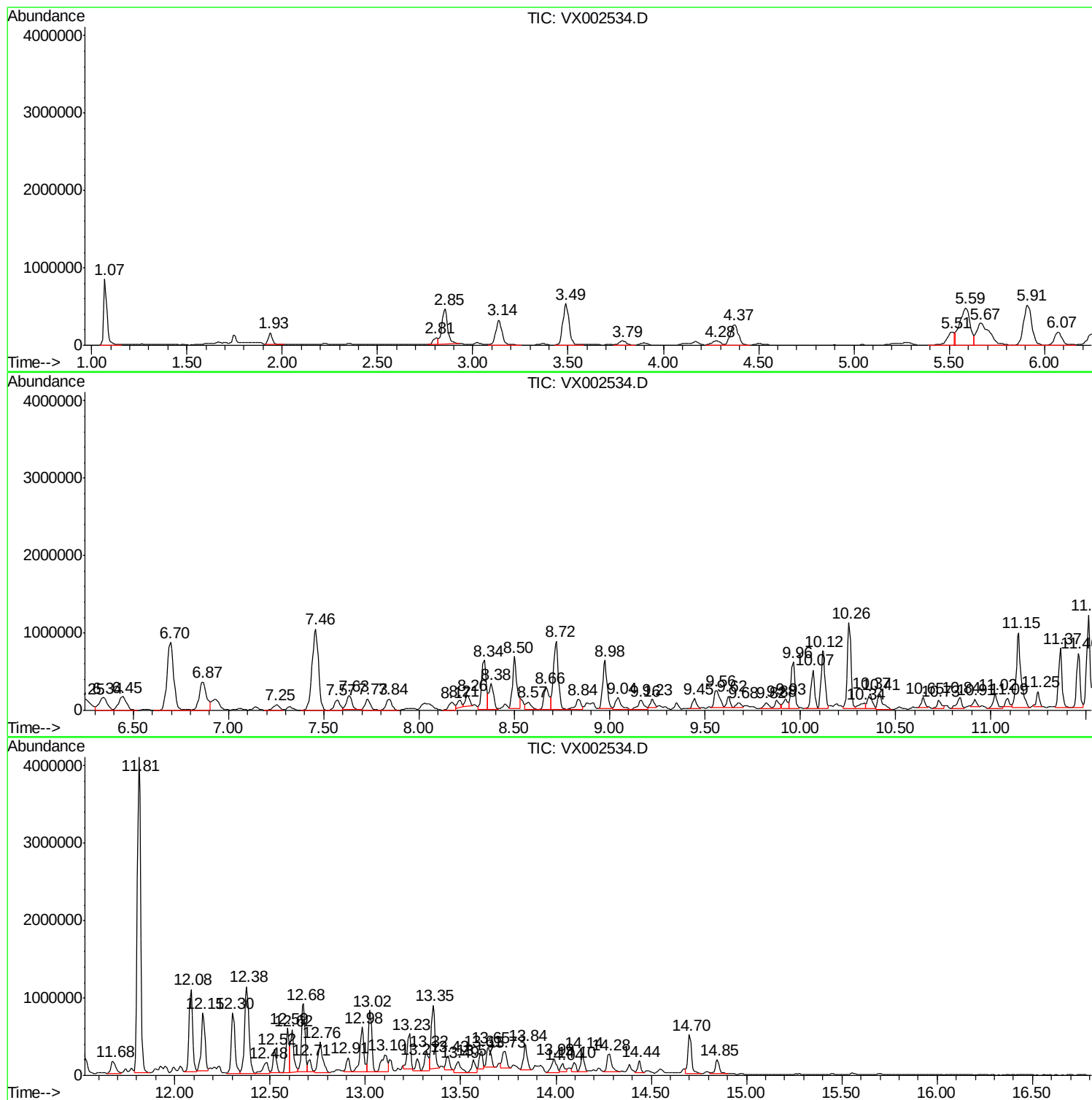
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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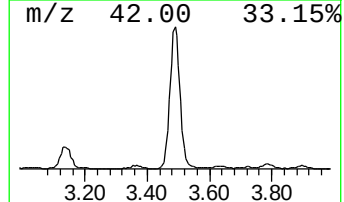
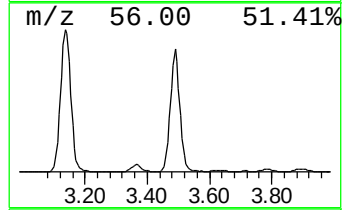
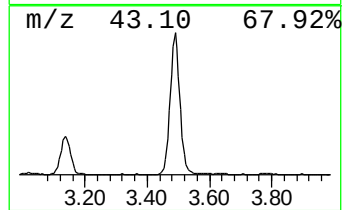
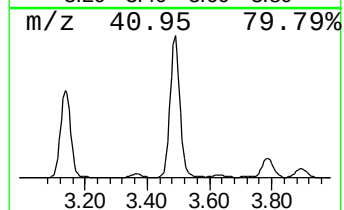
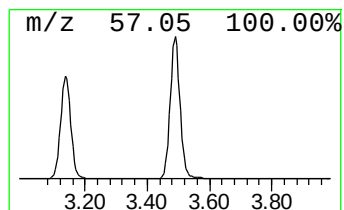
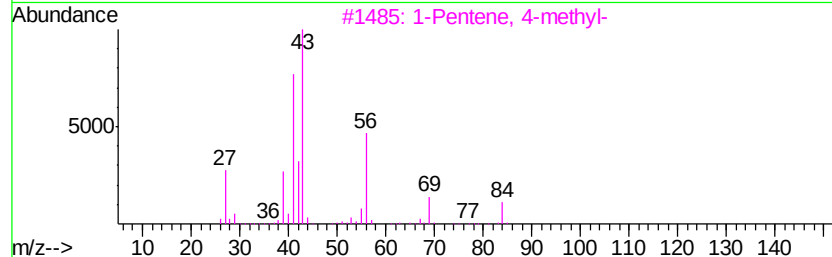
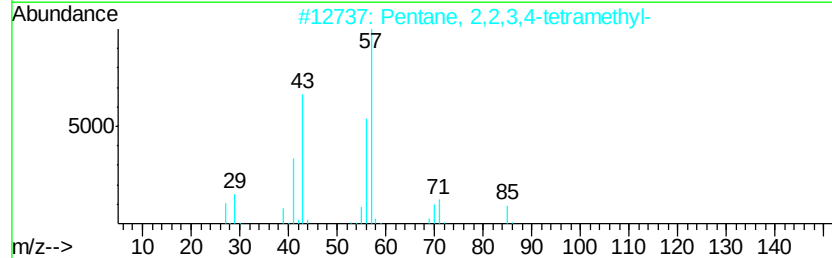
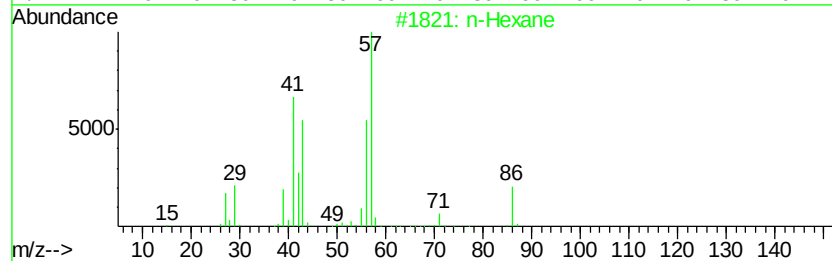
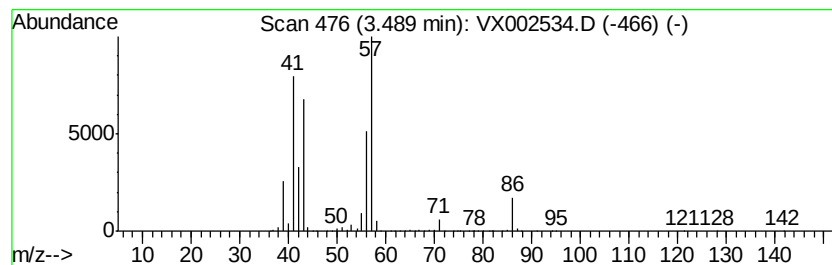
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Hexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	44.97 ug/l	1197260	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	94
2		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
3		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
4		Butanal, 2-methyl-	86	C5H10O	000096-17-3	35
5		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35



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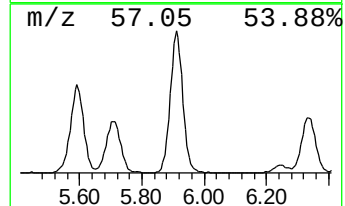
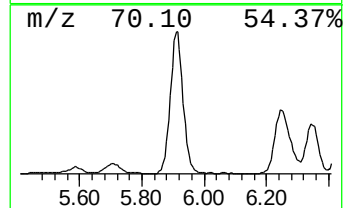
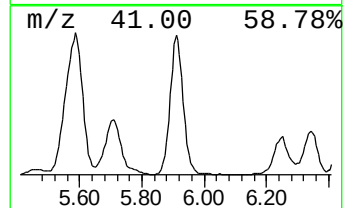
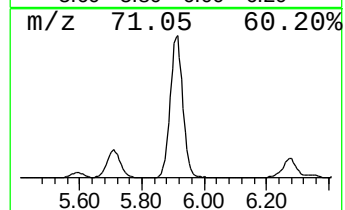
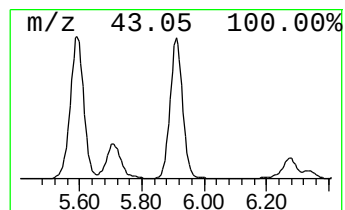
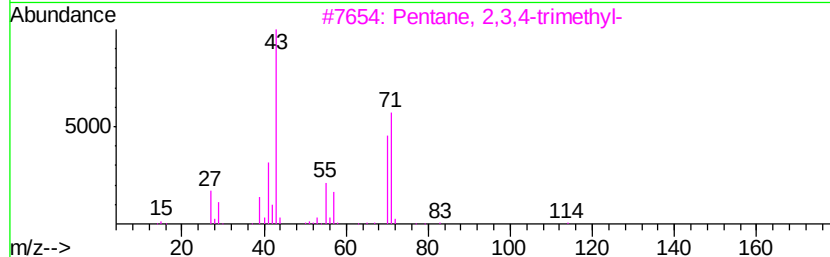
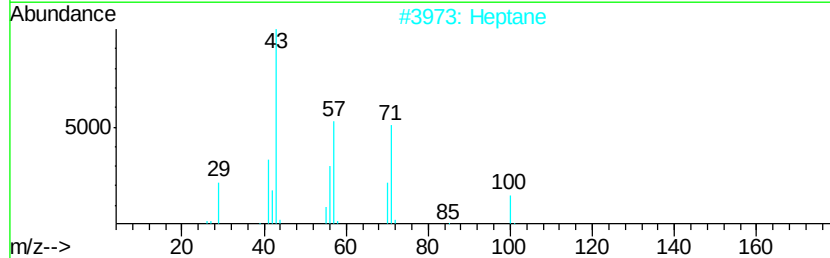
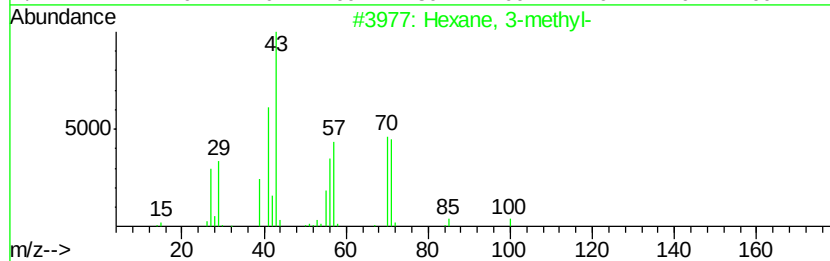
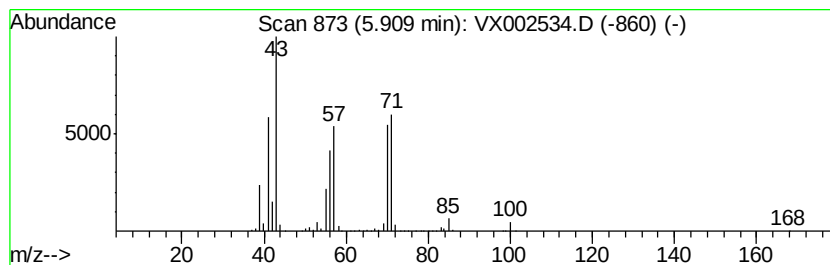
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.91	58.29 ug/l	1551860	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2		Heptane	100	C7H16	000142-82-5	80
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4		Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	47



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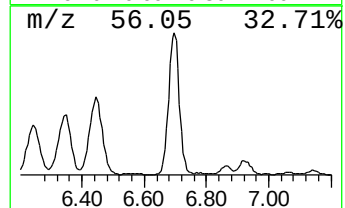
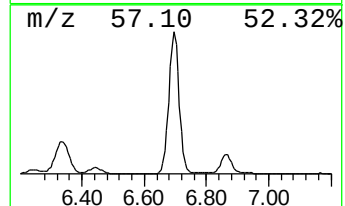
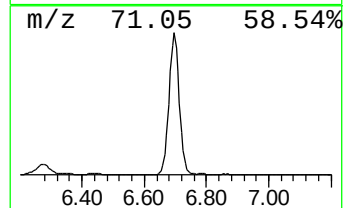
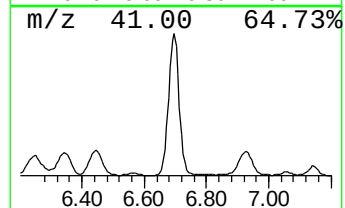
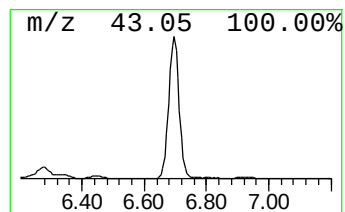
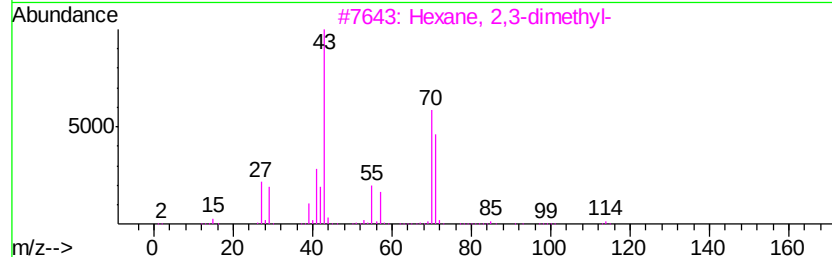
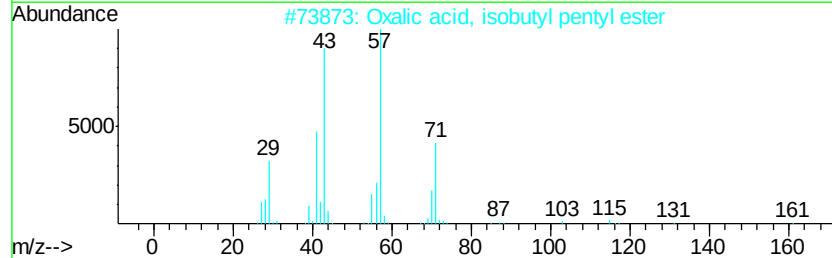
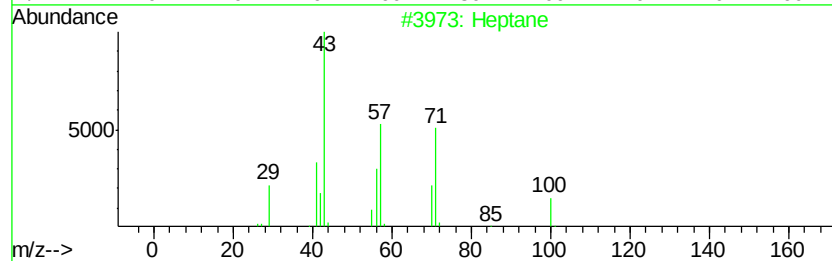
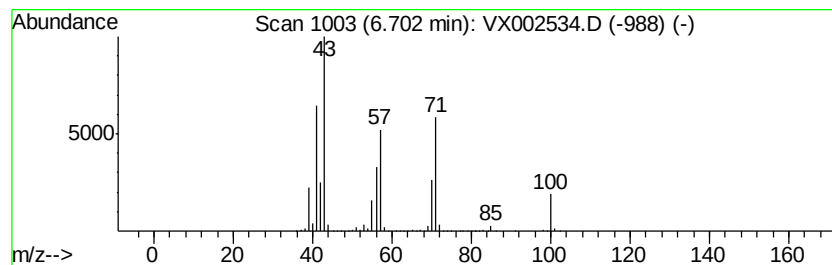
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	110.10 ug/l	2107500	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	53
3		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
4		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
B-40VR

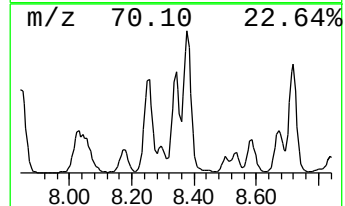
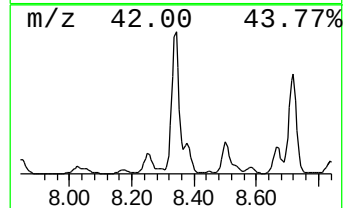
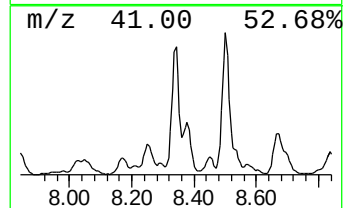
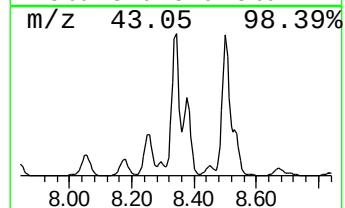
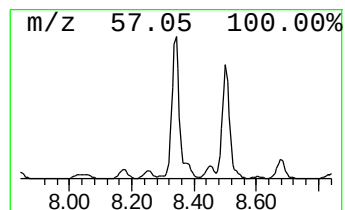
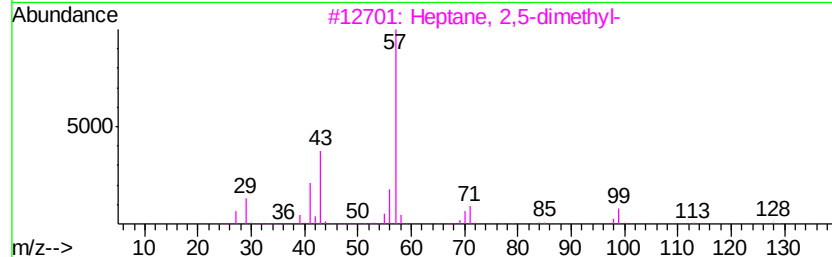
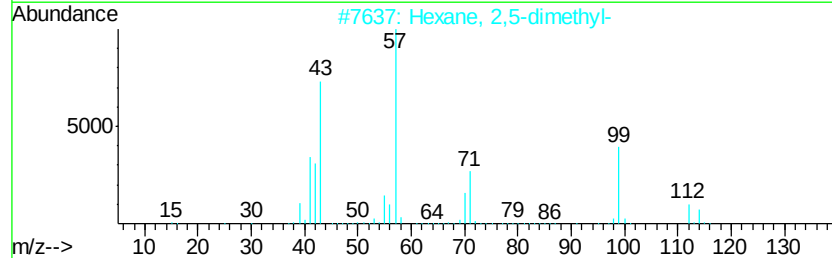
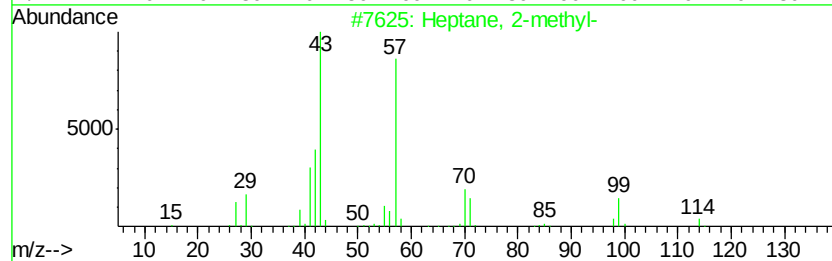
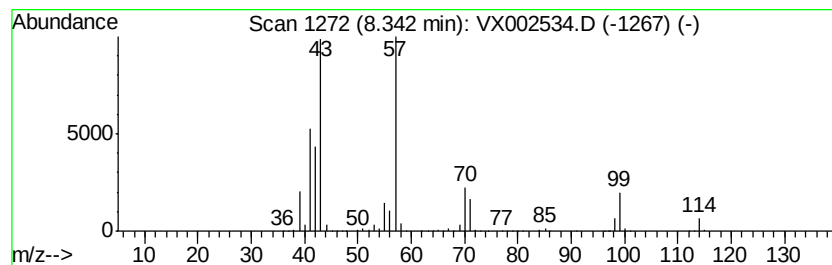
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Quant Title : SW846 8260

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

Peak Number 5 Heptane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	55.82 ug/l	1068520	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2-methyl-	114	C8H18	000592-27-8	94
2		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	87
3		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	38
4		Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	38
5		1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10µ/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

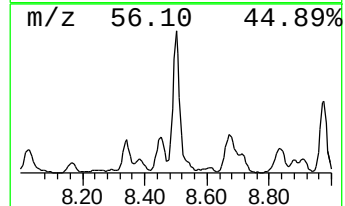
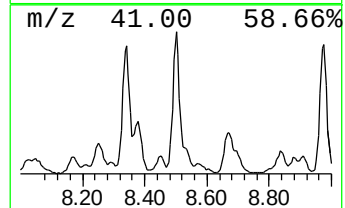
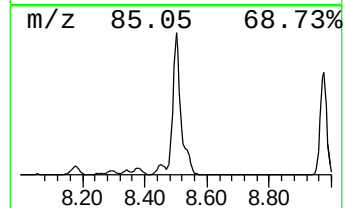
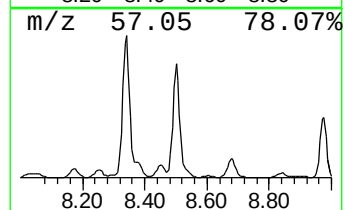
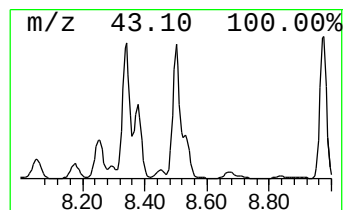
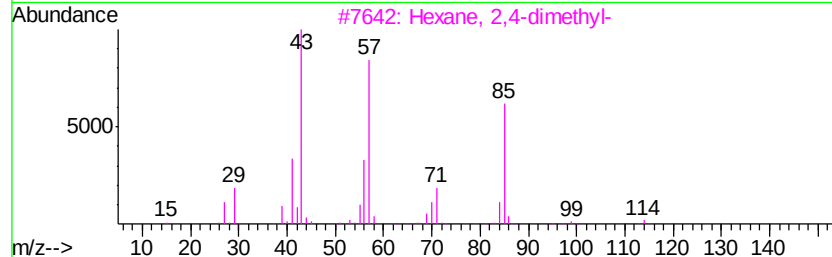
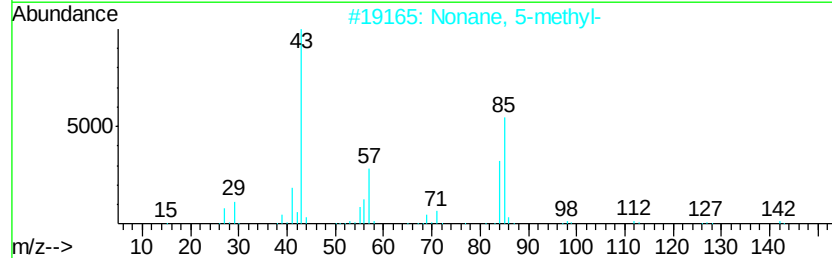
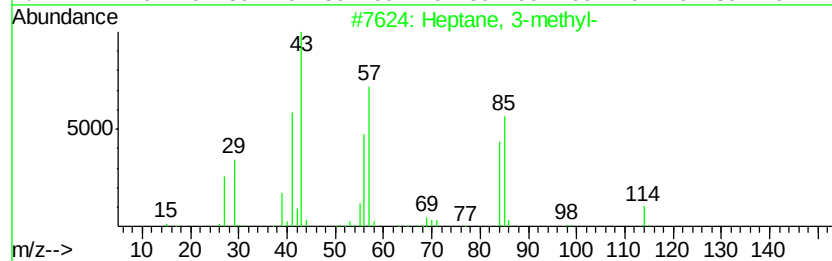
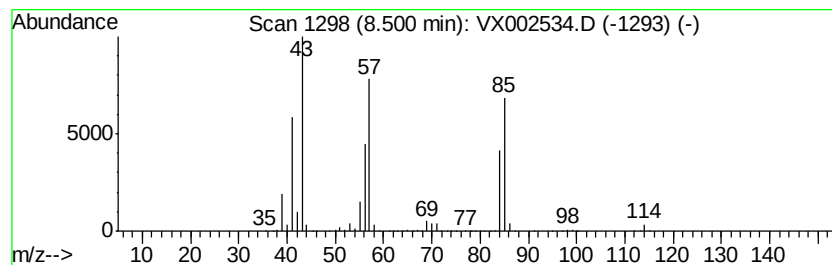
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Quant Title : SW846 8260

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

Peak Number 6 Heptane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.50	52.57 ug/l	1126100	Chlorobenzene-d5	10.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	94
2	Nonane, 5-methyl-	142	C10H22	015869-85-9	64
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	59
5	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
B-40VR

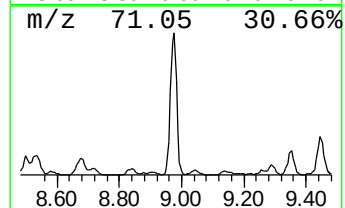
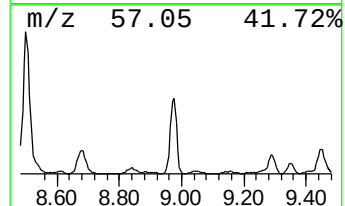
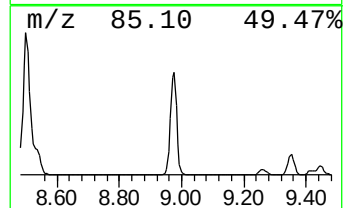
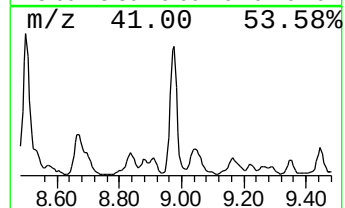
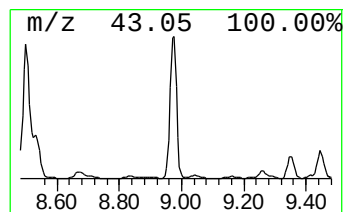
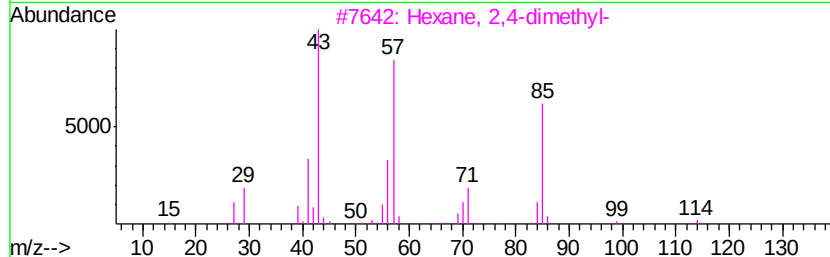
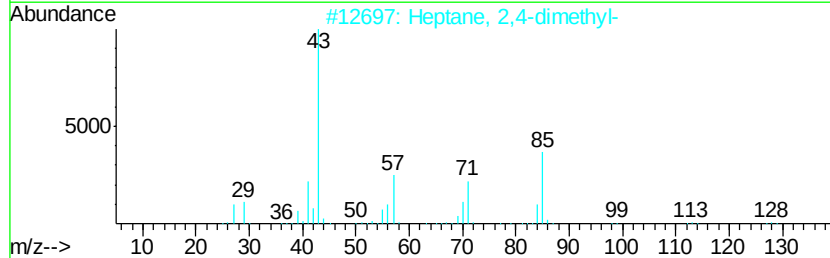
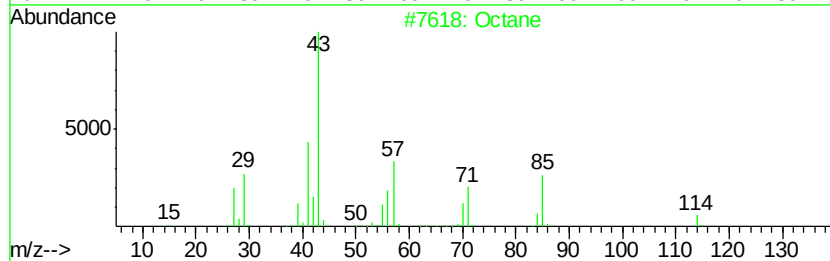
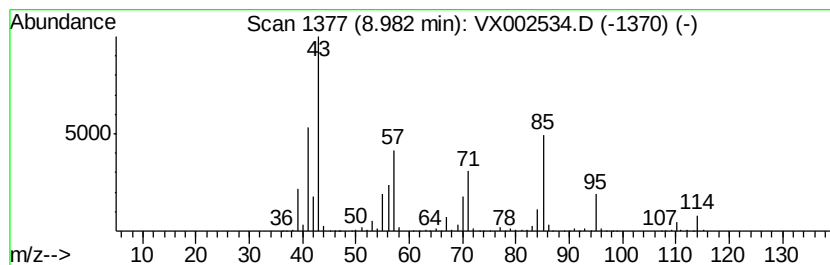
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Quant Title : SW846 8260

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

Peak Number 7 Octane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	46.21 ug/l	989998	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane	114	C8H18	000111-65-9	94
2		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
3		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4		Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	59
5		Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

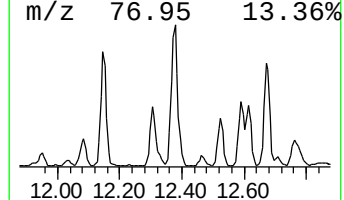
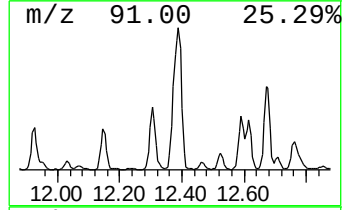
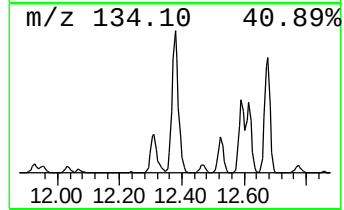
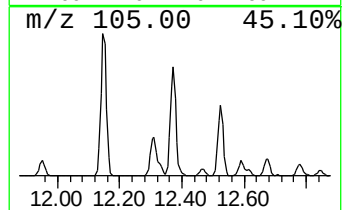
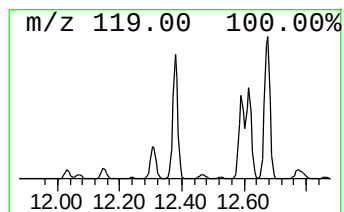
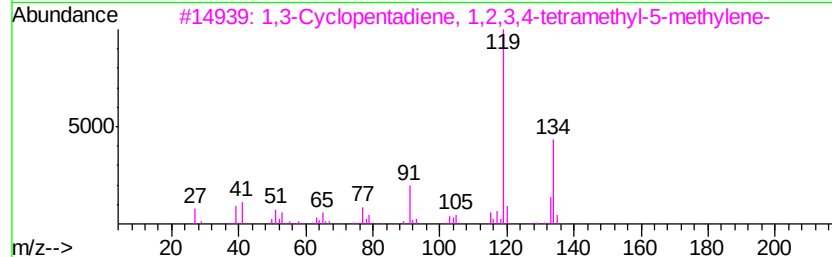
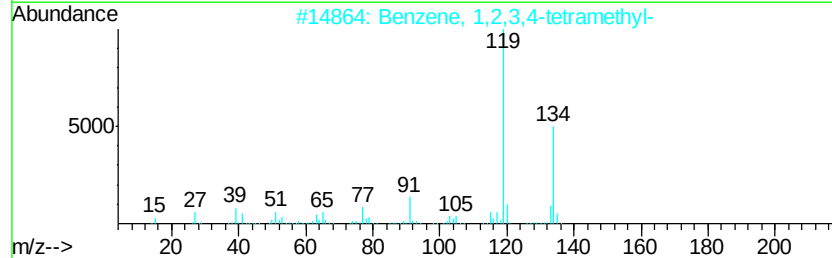
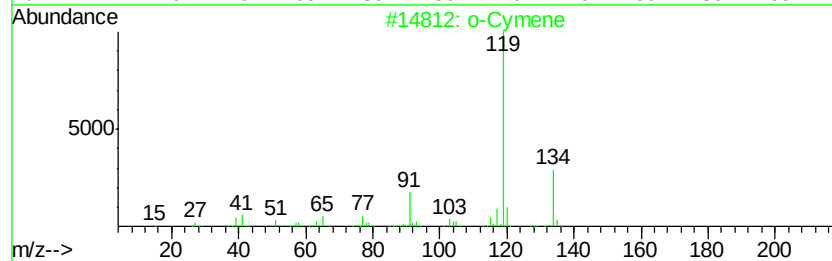
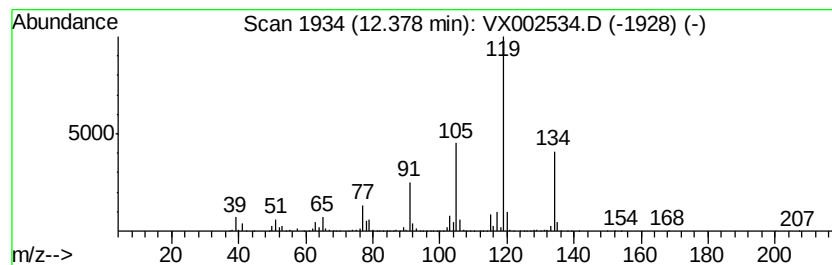
Instrument :
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ClientSampleId :
B-40VR

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	64.40 ug/l	1765460	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		o-Cymene	134 C10H14	000527-84-4 94
2		Benzene, 1,2,3,4-tetramethyl-	134 C10H14	000488-23-3 91
3		1,3-Cyclopentadiene, 1,2,3,4-tet...	134 C10H14	076089-59-3 91
4		Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14	000934-74-7 91
5		Benzene, 1,2,3,5-tetramethyl-	134 C10H14	000527-53-7 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-40VR

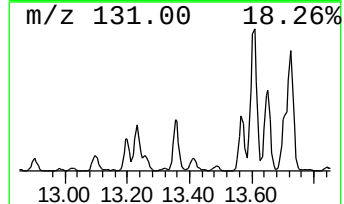
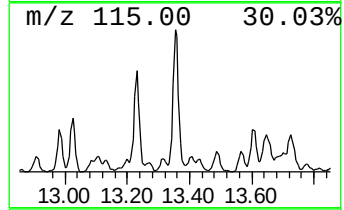
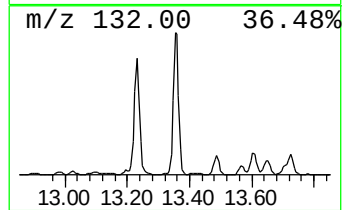
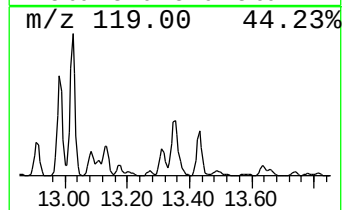
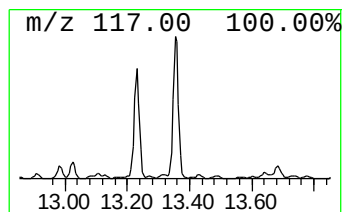
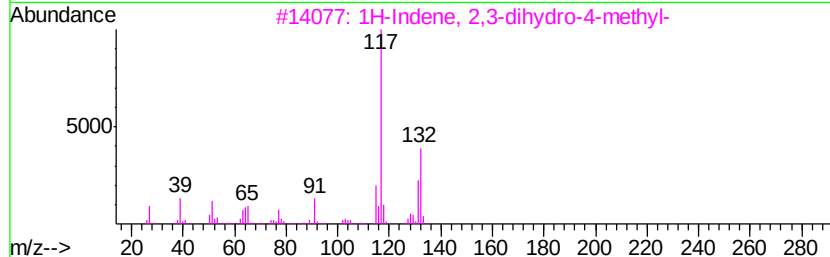
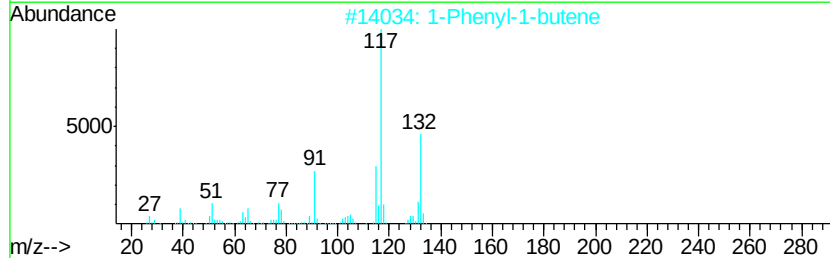
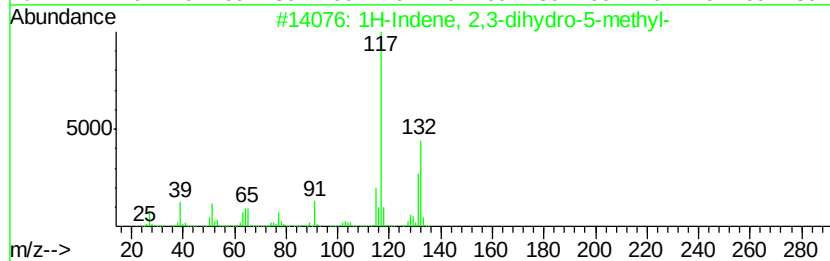
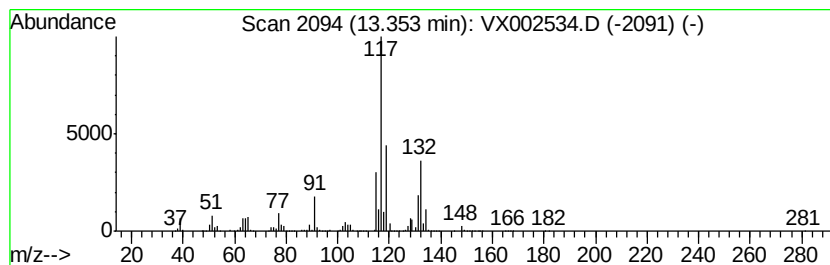
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	40.06 ug/l	1098180	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	93
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	92
4		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	76



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_X\DATA\VX061318\
Data File : VX002534.D
Acq On : 14 Jun 2018 03:35
Operator : JC/MD
Sample : J3383-11
Misc : 6.10g/5mL/100uL/5.0mL/MSV0A_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSV0A_X
ClientSampleId :
B-40VR

Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_X\METHOD\82X060418W.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
n-Hexane	3.49	45.0	ug/l	1197260	1	5.67	1331250	50.0
Hexane, 3-methyl-	5.91	58.3	ug/l	1551860	1	5.67	1331250	50.0
Heptane	6.70	110.1	ug/l	2107500	2	6.87	957055	50.0
Heptane, 2-methyl-	8.34	55.8	ug/l	1068520	2	6.87	957055	50.0
Heptane, 3-methyl-	8.50	52.6	ug/l	1126100	3	10.12	1071120	50.0
Octane	8.98	46.2	ug/l	989998	3	10.12	1071120	50.0
o-Cymene	12.38	64.4	ug/l	1765460	4	12.08	1370760	50.0
1H-Indene, 2,3-di...	13.35	40.1	ug/l	1098180	4	12.08	1370760	50.0