

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122618\
 Data File : VX006819.D
 Acq On : 26 Dec 2018 15:36
 Operator : JC/MD
 Sample : J6549-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-8

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.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	1.276	16	20	25	rBV	31875	50224	1.45%	0.150%
2	1.489	51	55	65	rBV	618356	767735	22.13%	2.297%
3	1.642	67	80	84	rVB9	74773	258648	7.46%	0.774%
4	5.501	701	713	728	rBV	404262	1161421	33.48%	3.475%
5	5.659	728	739	755	rVB	746251	2098583	60.50%	6.279%
6	6.068	796	806	818	rBV	419550	1077482	31.06%	3.224%
7	6.860	926	936	949	rBV	1073118	2497530	72.00%	7.473%
8	8.714	1233	1240	1250	rBV	2304754	3468711	100.00%	10.379%
9	9.335	1336	1342	1347	rBV	35901	55315	1.59%	0.166%
10	9.585	1376	1383	1388	rVB2	24985	38129	1.10%	0.114%
11	10.110	1463	1469	1486	rVB	2223099	3023100	87.15%	9.045%
12	10.823	1581	1586	1592	rBV	82047	117235	3.38%	0.351%
13	11.134	1632	1637	1647	rBV	2010711	2531929	72.99%	7.576%
14	11.530	1698	1702	1708	rVB	41586	56923	1.64%	0.170%
15	11.804	1744	1747	1757	rVB	31703	53345	1.54%	0.160%
16	11.890	1757	1761	1767	rBV	45772	72995	2.10%	0.218%
17	11.987	1773	1777	1781	rBV4	29752	55425	1.60%	0.166%
18	12.079	1786	1792	1797	rVV	2491747	3159532	91.09%	9.454%
19	12.152	1801	1804	1810	rVB4	37263	51337	1.48%	0.154%
20	12.371	1835	1840	1847	rVB3	45216	87731	2.53%	0.262%
21	12.475	1847	1857	1861	rBV	190358	246196	7.10%	0.737%
22	12.518	1861	1864	1870	rVB4	33332	53095	1.53%	0.159%
23	12.737	1896	1900	1904	rBV4	27923	54335	1.57%	0.163%
24	12.823	1910	1914	1918	rBV	96193	127215	3.67%	0.381%
25	12.871	1920	1922	1925	rVV3	47320	48478	1.40%	0.145%
26	12.908	1925	1928	1931	rVV3	34375	40275	1.16%	0.121%
27	12.951	1931	1935	1940	rVV4	38225	81304	2.34%	0.243%
28	13.024	1944	1947	1953	rVB4	82692	126417	3.64%	0.378%
29	13.097	1954	1959	1962	rBV3	64254	82935	2.39%	0.248%
30	13.194	1972	1975	1977	rBV	71931	91194	2.63%	0.273%
31	13.268	1983	1987	1990	rBV2	56024	74086	2.14%	0.222%
32	13.316	1991	1995	1998	rVV	472060	578843	16.69%	1.732%
33	13.347	1998	2000	2005	rVB2	164661	212777	6.13%	0.637%
34	13.438	2011	2015	2018	rBV2	107625	144136	4.16%	0.431%

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Integration Parameters: RTEINT.P

Integrator: RTE
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 Sampling : 1
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35	13.475	2018	2021	2030	rVB6	162350	345164	9.95%	1.033%
36	13.560	2030	2035	2038	rBV4	55902	90859	2.62%	0.272%
37	13.597	2038	2041	2044	rBV4	29891	43100	1.24%	0.129%
38	13.652	2044	2050	2053	rBV6	81064	172072	4.96%	0.515%
39	13.731	2059	2063	2065	rBV3	97956	144189	4.16%	0.431%
40	13.792	2070	2073	2075	rVV2	119004	149760	4.32%	0.448%
41	13.822	2075	2078	2080	rVV3	94195	93443	2.69%	0.280%
42	13.853	2080	2083	2085	rVV4	61499	66779	1.93%	0.200%
43	13.896	2085	2090	2097	rVB6	224185	493555	14.23%	1.477%
44	13.987	2097	2105	2109	rBV5	114529	294727	8.50%	0.882%
45	14.091	2118	2122	2126	rVB	858743	897047	25.86%	2.684%
46	14.133	2126	2129	2131	rBV3	97104	112208	3.23%	0.336%
47	14.219	2141	2143	2145	rBV	46032	51019	1.47%	0.153%
48	14.286	2149	2154	2158	rVB2	254270	381123	10.99%	1.140%
49	14.377	2167	2169	2173	rVB4	49837	60417	1.74%	0.181%
50	14.432	2175	2178	2180	rVV	70840	75811	2.19%	0.227%
51	14.462	2180	2183	2190	rVB5	103739	246590	7.11%	0.738%
52	14.530	2190	2194	2196	rBV3	189584	289604	8.35%	0.867%
53	14.554	2196	2198	2204	rVB2	256038	340948	9.83%	1.020%
54	14.621	2204	2209	2213	rBV4	168364	284087	8.19%	0.850%
55	14.670	2213	2217	2224	rBV3	495938	729535	21.03%	2.183%
56	14.731	2224	2227	2231	rVB2	137961	203569	5.87%	0.609%
57	14.810	2231	2240	2243	rBV	1226919	1560916	45.00%	4.670%
58	14.847	2243	2246	2249	rVV4	111237	129148	3.72%	0.386%
59	14.901	2249	2255	2258	rVV6	142850	242863	7.00%	0.727%
60	14.932	2258	2260	2262	rVB	78306	63038	1.82%	0.189%
61	14.962	2263	2265	2269	rBV5	56519	94201	2.72%	0.282%
62	15.164	2293	2298	2301	rBV4	102243	195329	5.63%	0.584%
63	15.249	2307	2312	2314	rBV2	312482	525738	15.16%	1.573%
64	15.273	2314	2316	2320	rVV	397634	477962	13.78%	1.430%
65	15.340	2324	2327	2330	rVB2	168360	206371	5.95%	0.617%
66	15.444	2340	2344	2349	rVB7	83603	137605	3.97%	0.412%
67	15.554	2357	2362	2368	rBV2	632731	955332	27.54%	2.858%
68	15.688	2380	2384	2388	rVB6	81680	117226	3.38%	0.351%
69	15.761	2393	2396	2404	rVB2	149091	228853	6.60%	0.685%
70	16.169	2459	2463	2470	rBV8	51347	117015	3.37%	0.350%
71	16.456	2507	2510	2517	rVB	95962	159551	4.60%	0.477%

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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

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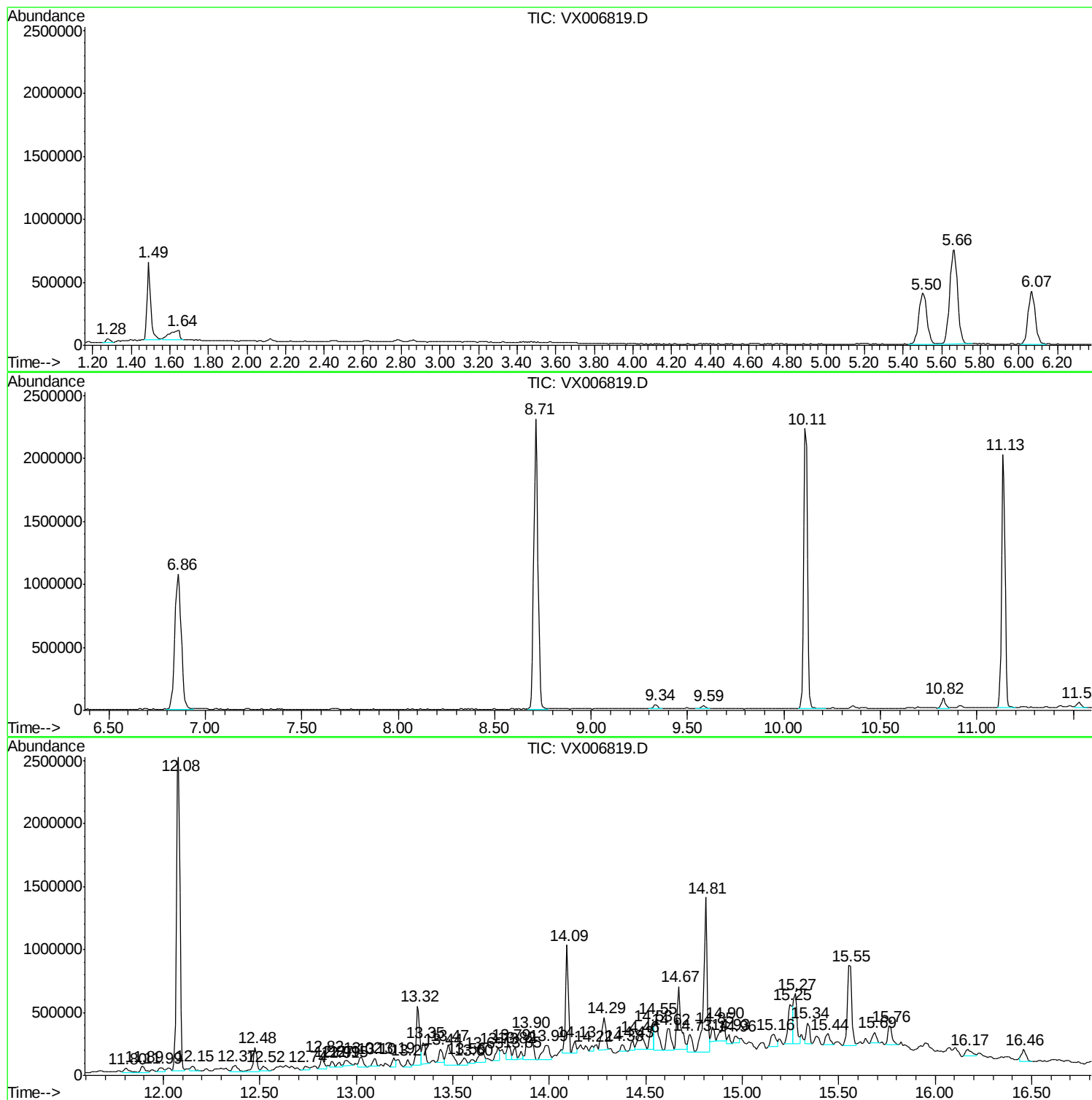
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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



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Instrument :
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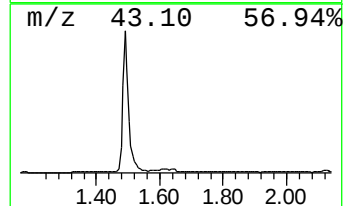
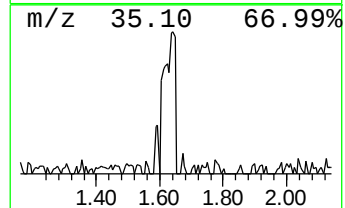
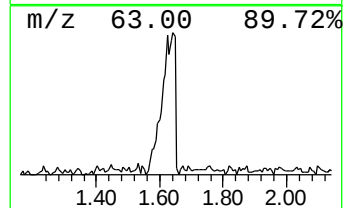
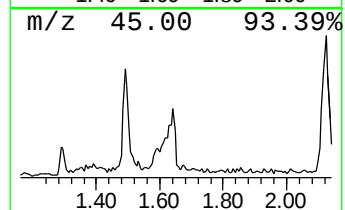
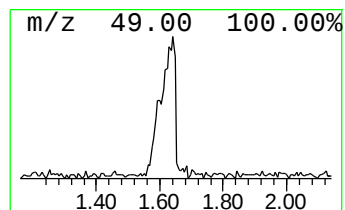
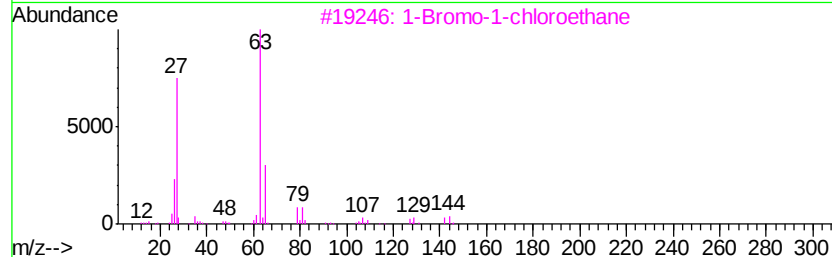
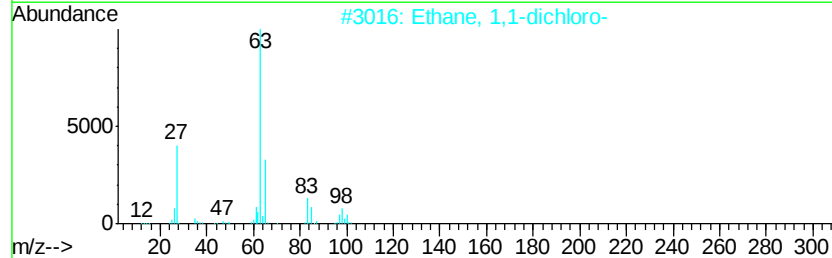
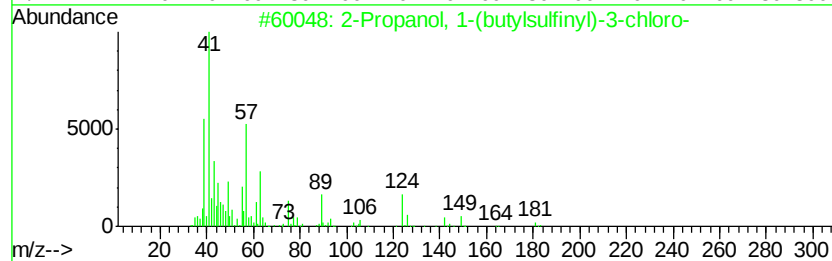
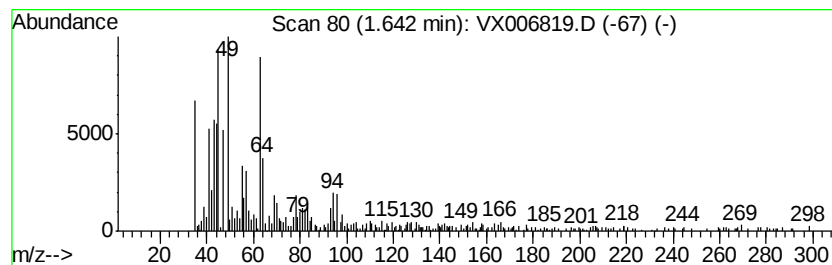
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown1.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	6.16 ug/l	258648	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(butylsulfinyl)-3-...	198	C7H15ClO2S	1000362-68-1	36
2			Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	18
3			1-Bromo-1-chloroethane	142	C2H4BrCl	000593-96-4	18
4			2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	17
5			S-Methyl methanethiosulphonate	126	C2H6O2S2	002949-92-0	12



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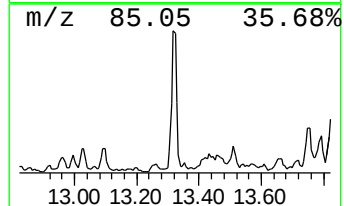
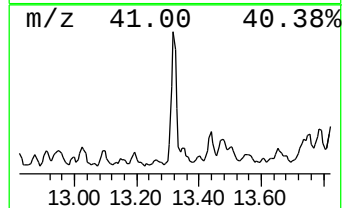
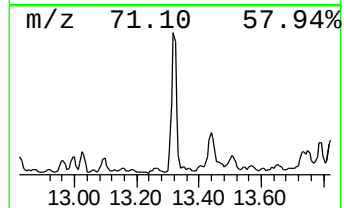
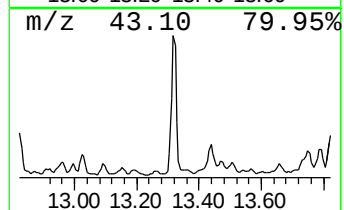
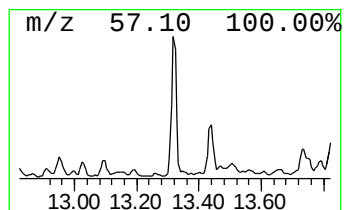
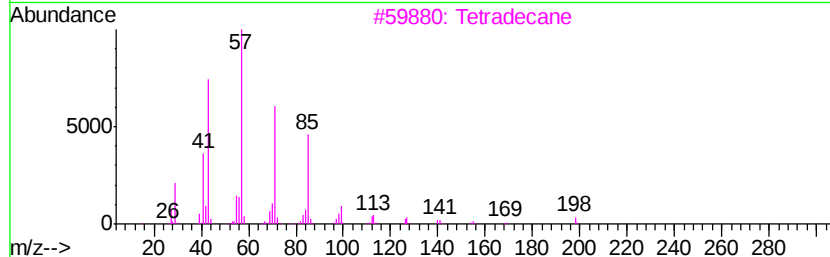
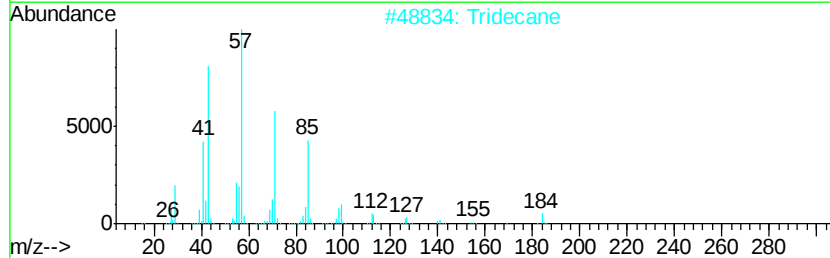
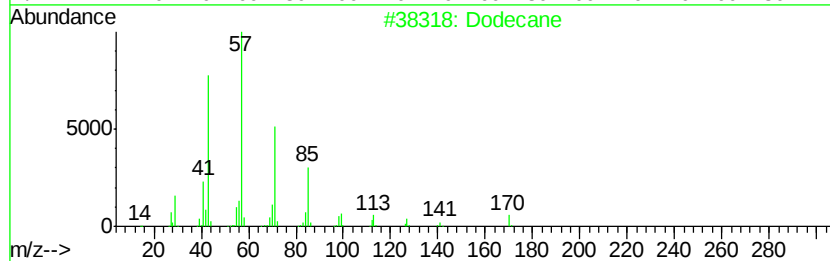
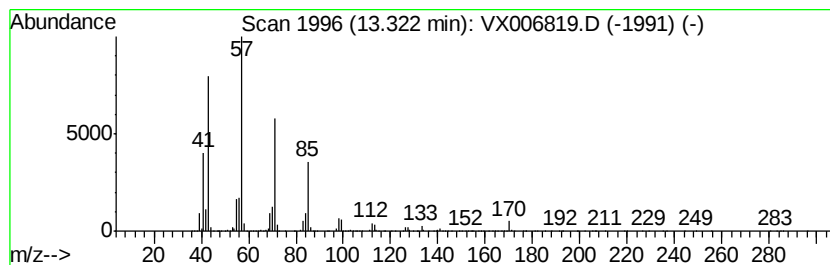
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	9.16 ug/l	578843	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane	170	C12H26	000112-40-3	90
2		Tridecane	184	C13H28	000629-50-5	86
3		Tetradecane	198	C14H30	000629-59-4	86
4		Hexadecane	226	C16H34	000544-76-3	83
5		Undecane	156	C11H24	001120-21-4	80



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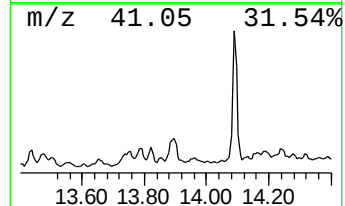
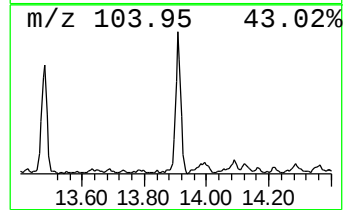
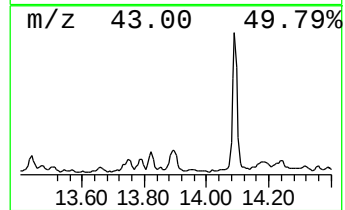
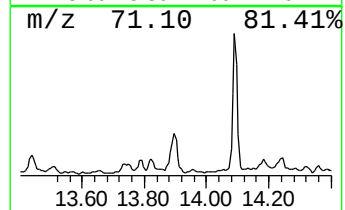
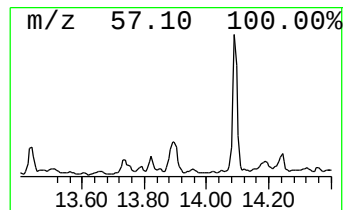
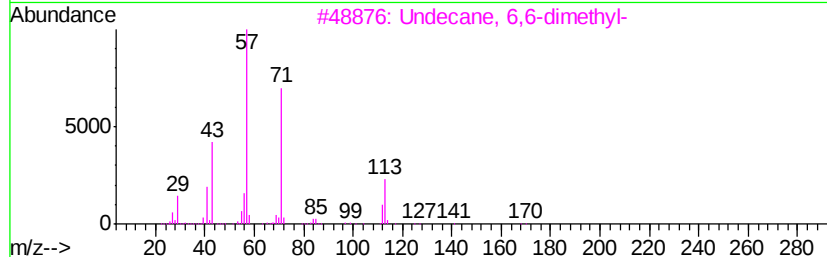
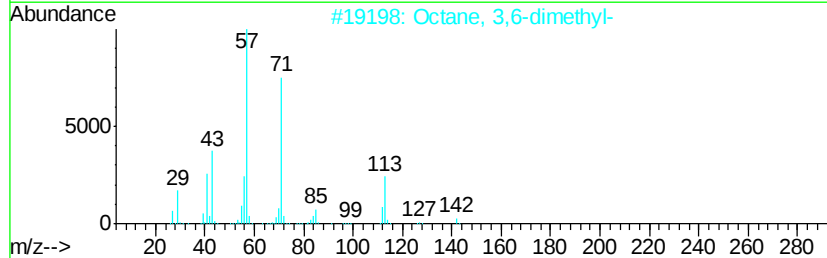
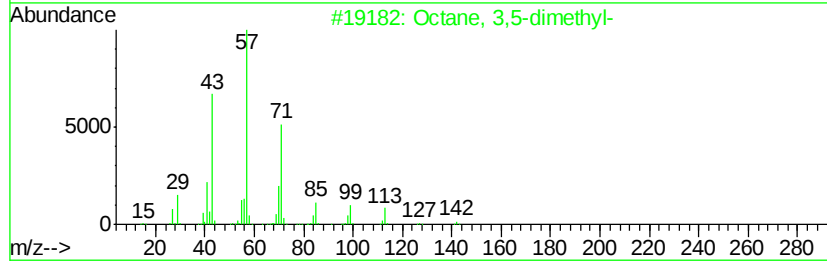
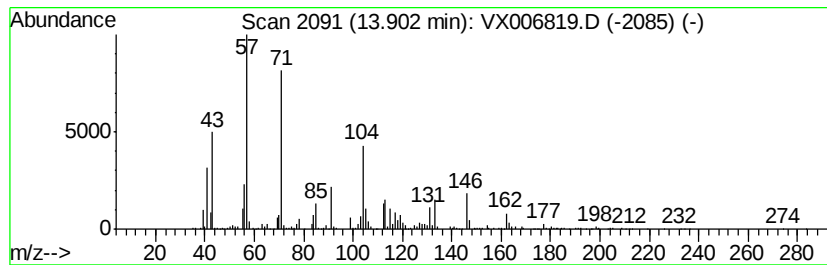
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Quant Title : SW846 8260

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

Peak Number 4 Octane, 3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	7.81 ug/l	493555	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	59
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
3		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59
4		Tridecane, 7-methyl-	198	C14H30	026730-14-3	58
5		Bacchotricuneatin c	342	C20H22O5	066563-30-2	55



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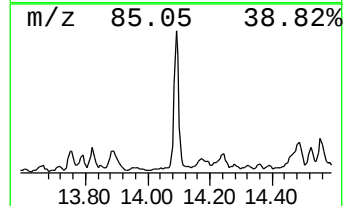
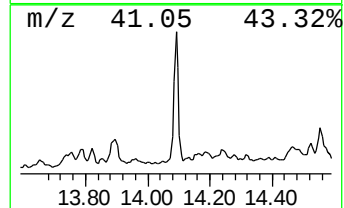
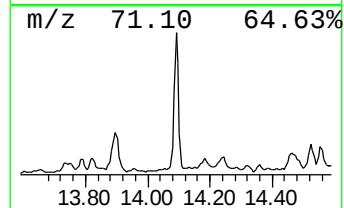
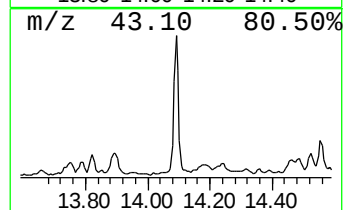
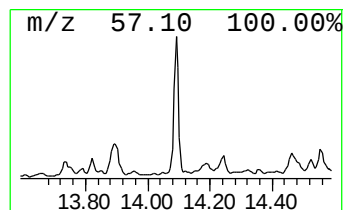
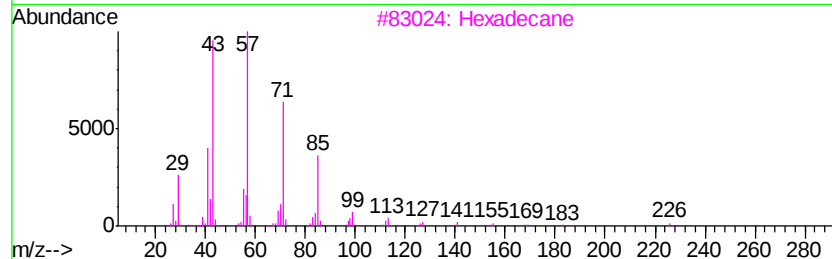
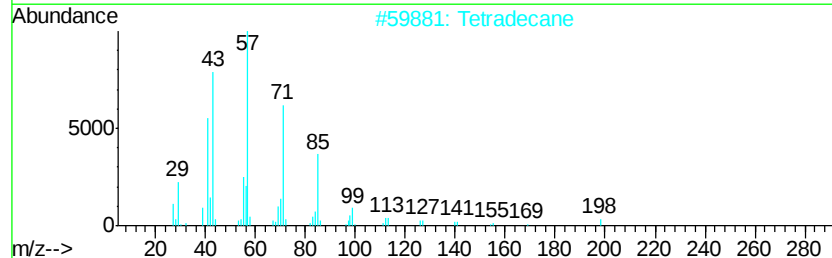
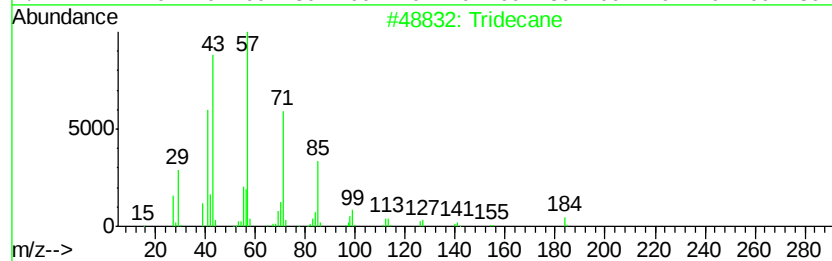
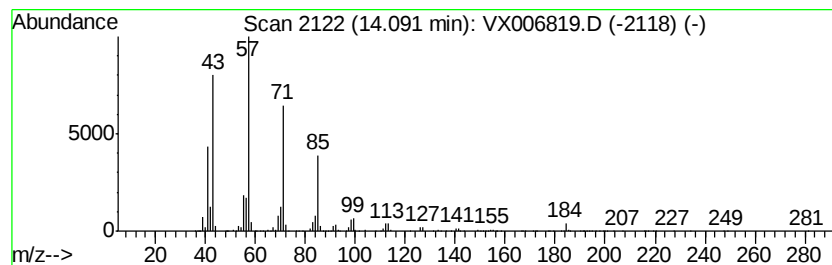
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 Quant Title : SW846 8260

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

 Peak Number 5 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	14.20 ug/l	897047	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	94
2	Tetradecane		198	C14H30	000629-59-4	91
3	Hexadecane		226	C16H34	000544-76-3	87
4	Dodecane		170	C12H26	000112-40-3	86
5	Decane, 2,3,6-trimethyl-		184	C13H28	062238-12-4	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006819.D
Acq On : 26 Dec 2018 15:36
Operator : JC/MD
Sample : J6549-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8

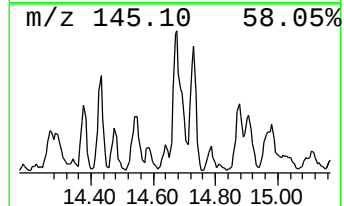
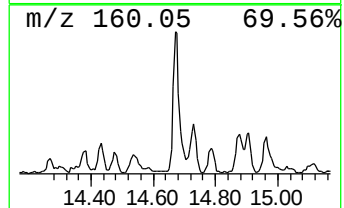
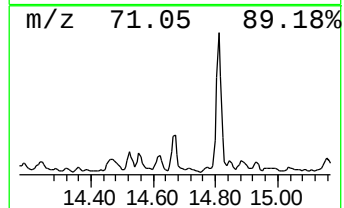
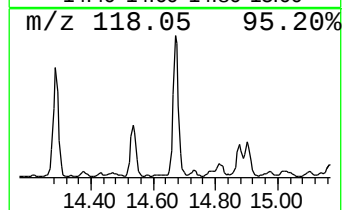
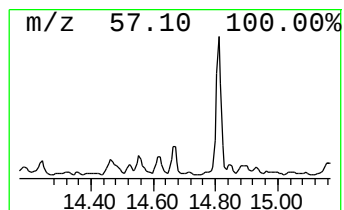
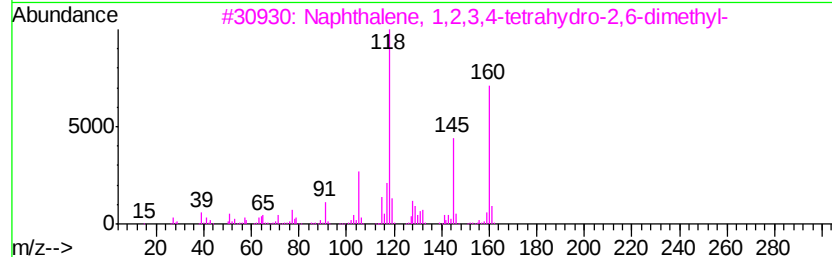
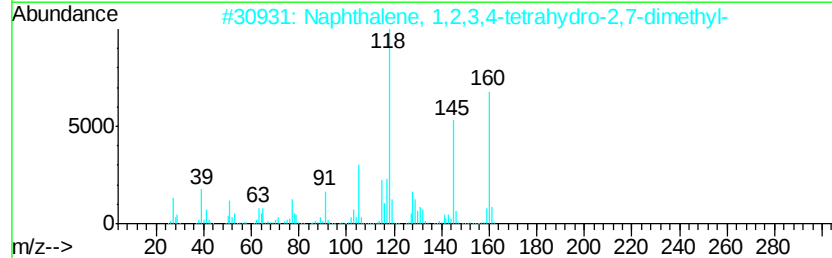
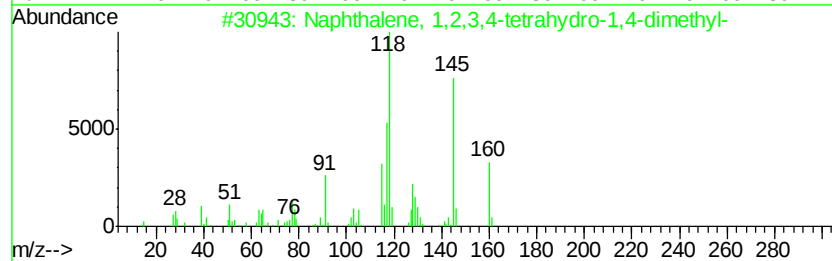
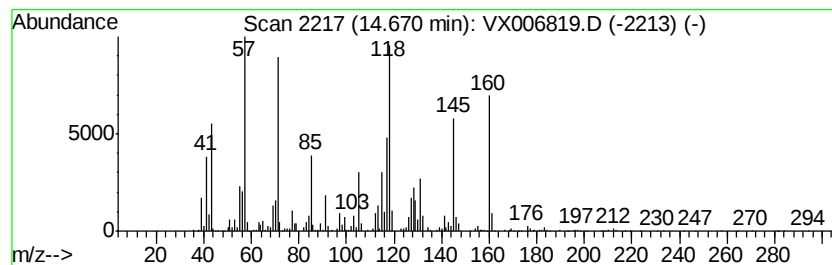
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	11.55 ug/l	729535	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	89
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	50
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	42
4		1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	38
5		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006819.D
Acq On : 26 Dec 2018 15:36
Operator : JC/MD
Sample : J6549-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8

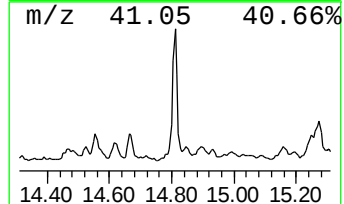
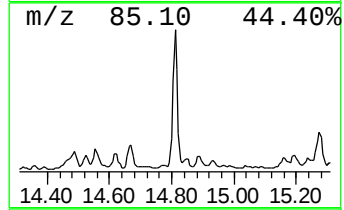
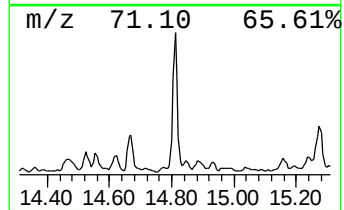
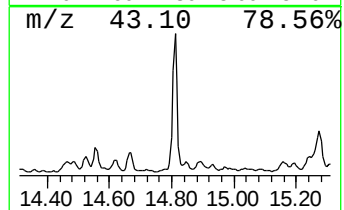
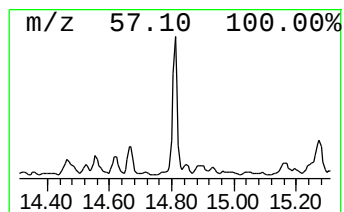
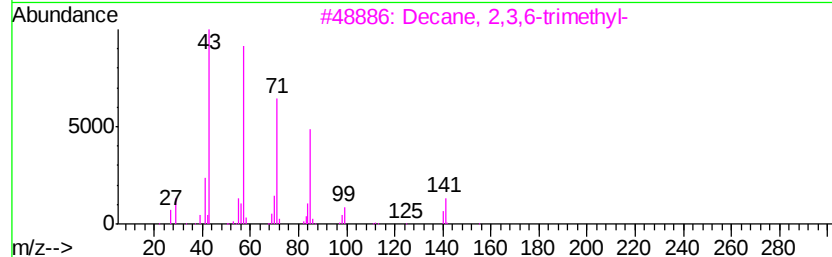
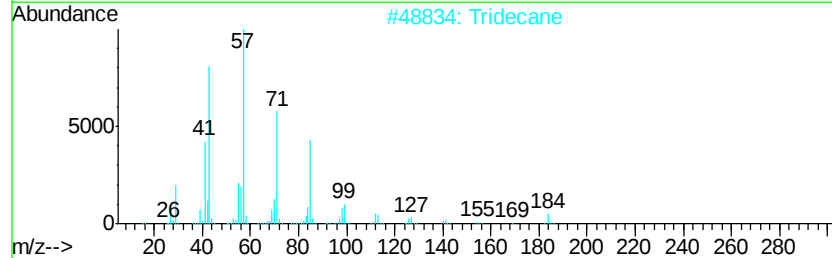
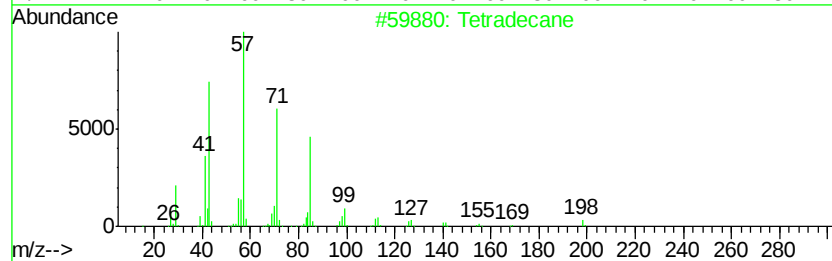
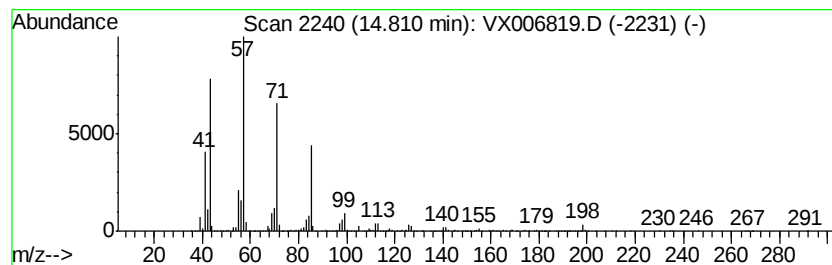
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Quant Title : SW846 8260

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

Peak Number 7 Tetradecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	24.70 ug/l	1560920	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	97
2		Tridecane	184	C13H28	000629-50-5	93
3		Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	80
4		Bacchotricuneatin c	342	C20H22O5	066563-30-2	68
5		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006819.D
Acq On : 26 Dec 2018 15:36
Operator : JC/MD
Sample : J6549-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8

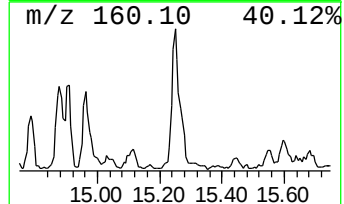
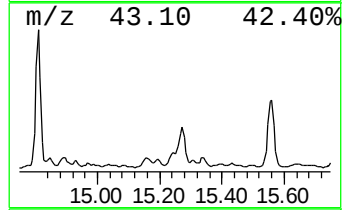
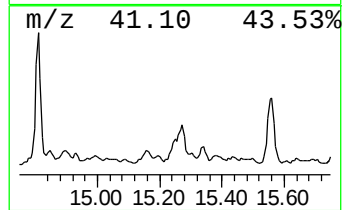
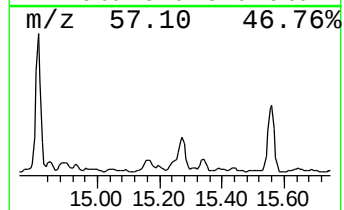
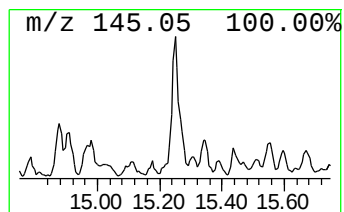
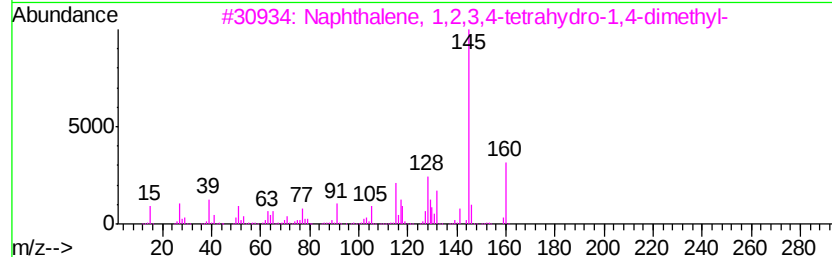
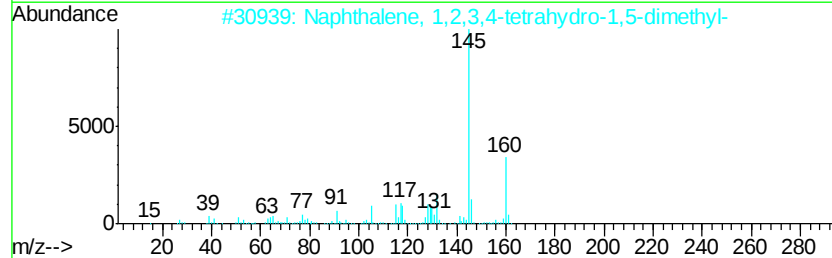
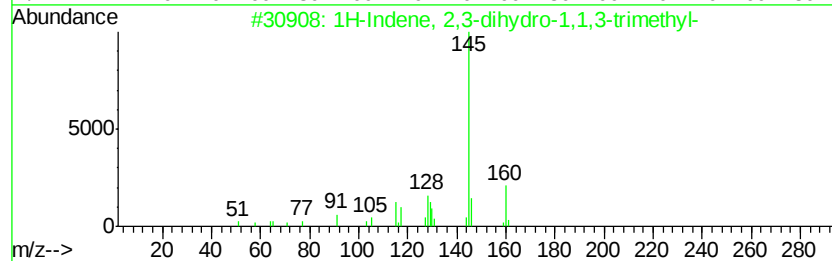
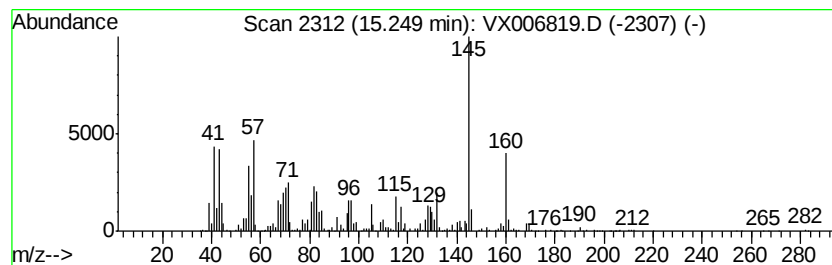
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	8.32 ug/l	525738	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	93
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	93
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91
4		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	91
5		Ethanone, 1-(2,3-dihydro-1H-inde...	160	C11H12O	004228-10-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006819.D
Acq On : 26 Dec 2018 15:36
Operator : JC/MD
Sample : J6549-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8

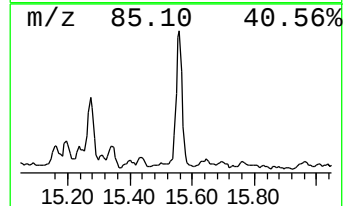
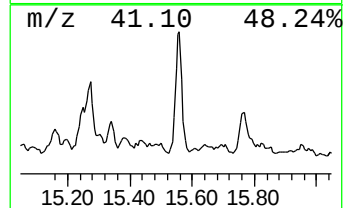
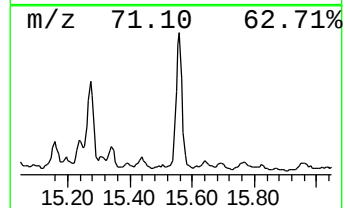
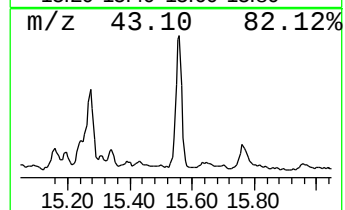
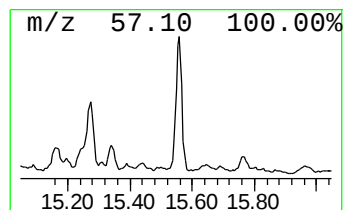
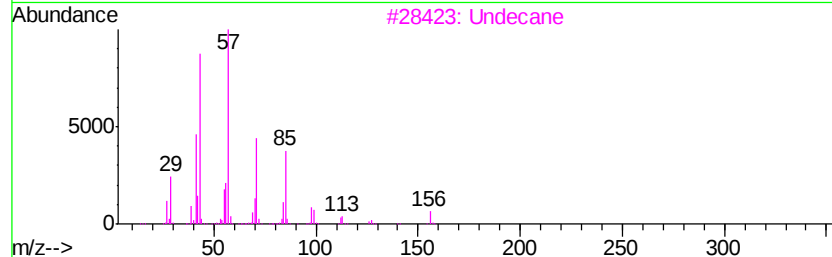
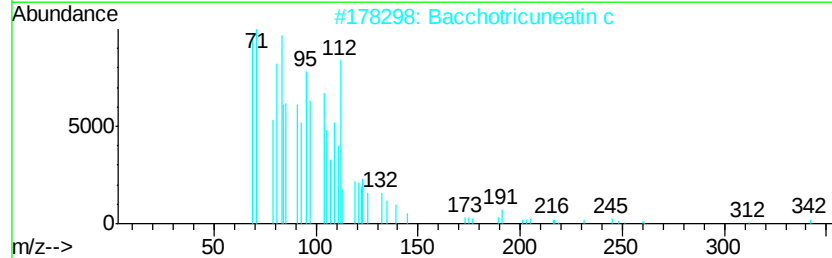
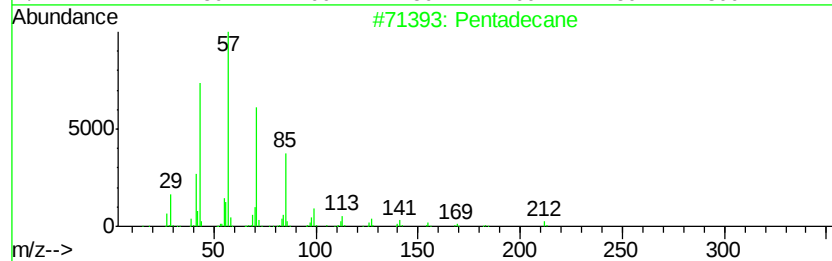
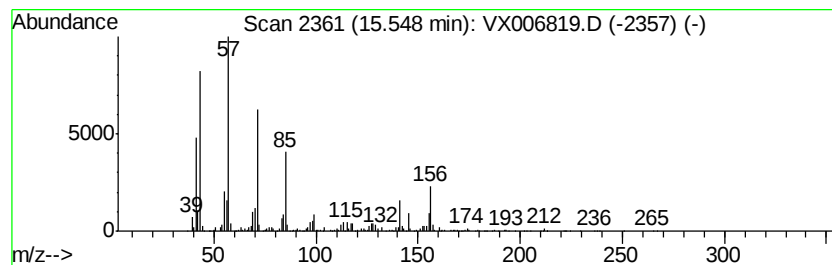
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Quant Title : SW846 8260

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

Peak Number 10 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	15.12 ug/l	955332	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	95
2		Bacchotricuneatin c	342	C20H22O5	066563-30-2	95
3		Undecane	156	C11H24	001120-21-4	80
4		Tetradecane	198	C14H30	000629-59-4	74
5		Tridecane, 7-propyl-	226	C16H34	055045-09-5	74



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122618\
Data File : VX006819.D
Acq On : 26 Dec 2018 15:36
Operator : JC/MD
Sample : J6549-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.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
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Dodecane	13.32	9.2	ug/l	578843	4	12.08	3159530	50.0
Octane, 3,5-dimet...	13.90	7.8	ug/l	493555	4	12.08	3159530	50.0
Tridecane	14.09	14.2	ug/l	897047	4	12.08	3159530	50.0
Naphthalene, 1,2,...	14.67	11.6	ug/l	729535	4	12.08	3159530	50.0
Tetradecane	14.81	24.7	ug/l	1560920	4	12.08	3159530	50.0
1H-Indene, 2,3-di...	15.25	8.3	ug/l	525738	4	12.08	3159530	50.0
Pentadecane	15.55	15.1	ug/l	955332	4	12.08	3159530	50.0