

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
 Data File : VX006120.D
 Acq On : 21 Nov 2018 13:27
 Operator : JC/MD
 Sample : J5950-10
 Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SSI-FD-11132018

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\82X112018W.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	1.666	62	84	86	rBV3	63279	245266	14.32%	1.696%
2	5.507	702	714	728	rBV	180871	566891	33.10%	3.920%
3	5.659	728	739	753	rVB	340781	985661	57.55%	6.815%
4	6.068	796	806	824	rVB	215115	593647	34.66%	4.105%
5	6.860	926	936	957	rBV	495189	1234976	72.10%	8.539%
6	8.713	1231	1240	1249	rBV	1066586	1694374	98.93%	11.715%
7	10.116	1464	1470	1483	rBV	1039426	1466856	85.64%	10.142%
8	10.640	1550	1556	1560	rBV4	10876	20120	1.17%	0.139%
9	10.835	1585	1588	1592	rVB	15809	18475	1.08%	0.128%
10	11.085	1621	1629	1632	rBV3	19007	38682	2.26%	0.267%
11	11.140	1632	1638	1648	rVV	941919	1297299	75.74%	8.970%
12	11.243	1651	1655	1658	rVV2	28736	40407	2.36%	0.279%
13	11.487	1691	1695	1697	rBV	16931	20765	1.21%	0.144%
14	11.530	1697	1702	1707	rVB	216463	258038	15.07%	1.784%
15	11.689	1724	1728	1731	rBV2	26813	33270	1.94%	0.230%
16	11.737	1732	1736	1738	rVV	33154	38991	2.28%	0.270%
17	11.768	1738	1741	1744	rVV	85784	99142	5.79%	0.685%
18	11.835	1744	1752	1757	rVB6	30119	73129	4.27%	0.506%
19	11.890	1757	1761	1764	rBV2	40745	58857	3.44%	0.407%
20	11.945	1767	1770	1774	rVV2	36732	58561	3.42%	0.405%
21	11.993	1774	1778	1781	rVV2	36412	61463	3.59%	0.425%
22	12.030	1781	1784	1786	rVV4	26402	41049	2.40%	0.284%
23	12.079	1787	1792	1797	rVV	1268394	1712776	100.00%	11.842%
24	12.127	1797	1800	1802	rVV	89248	109543	6.40%	0.757%
25	12.152	1802	1804	1809	rVV	104701	133633	7.80%	0.924%
26	12.201	1809	1812	1813	rVV2	24300	30663	1.79%	0.212%
27	12.225	1813	1816	1823	rVB	94105	124546	7.27%	0.861%
28	12.371	1835	1840	1846	rVB5	42200	75576	4.41%	0.523%
29	12.432	1846	1850	1853	rBV5	12572	20879	1.22%	0.144%
30	12.475	1853	1857	1862	rVV	535029	592091	34.57%	4.094%
31	12.524	1862	1865	1871	rVB4	29739	52347	3.06%	0.362%
32	12.633	1874	1883	1890	rBV6	48125	134386	7.85%	0.929%
33	12.737	1897	1900	1903	rBV2	34473	39943	2.33%	0.276%
34	12.877	1920	1923	1928	rVB5	30078	37199	2.17%	0.257%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
 Data File : VX006120.D
 Acq On : 21 Nov 2018 13:27
 Operator : JC/MD
 Sample : J5950-10
 Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SSI-FD-11132018

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\82X112018W.M
 Title : SW846 8260

35	12.957	1928	1936	1941	rVV5	47193	127438	7.44%	0.881%
36	13.030	1945	1948	1955	rVB5	42896	65976	3.85%	0.456%
37	13.097	1955	1959	1962	rBV2	28684	35316	2.06%	0.244%
38	13.322	1992	1996	1998	rBV	80198	91725	5.36%	0.634%
39	13.353	1998	2001	2006	rVB4	39033	54357	3.17%	0.376%
40	13.438	2012	2015	2018	rBV2	27939	31870	1.86%	0.220%
41	13.475	2018	2021	2024	rVV5	13718	17319	1.01%	0.120%
42	13.645	2045	2049	2054	rBV7	11660	22004	1.28%	0.152%
43	13.737	2060	2064	2065	rBV2	15679	18535	1.08%	0.128%
44	13.792	2070	2073	2076	rVV	27418	30103	1.76%	0.208%
45	13.822	2076	2078	2081	rVB2	23226	22720	1.33%	0.157%
46	13.895	2086	2090	2098	rVB2	60756	94065	5.49%	0.650%
47	14.097	2118	2123	2126	rBV	127010	140967	8.23%	0.975%
48	14.158	2131	2133	2136	rBV2	16911	21923	1.28%	0.152%
49	14.273	2150	2152	2159	rVB6	19375	32270	1.88%	0.223%
50	14.462	2179	2183	2186	rBV2	35073	58332	3.41%	0.403%
51	14.487	2186	2187	2191	rVV3	27275	24379	1.42%	0.169%
52	14.529	2191	2194	2196	rVV2	27466	30070	1.76%	0.208%
53	14.560	2196	2199	2205	rVB2	54514	108897	6.36%	0.753%
54	14.621	2205	2209	2214	rVB	40852	55992	3.27%	0.387%
55	14.670	2214	2217	2220	rBV	103119	123818	7.23%	0.856%
56	14.810	2236	2240	2244	rBV	208963	248618	14.52%	1.719%
57	14.846	2244	2246	2250	rVB4	45336	57756	3.37%	0.399%
58	14.901	2250	2255	2259	rBV4	37241	62379	3.64%	0.431%
59	15.164	2293	2298	2301	rBV3	39760	73518	4.29%	0.508%
60	15.243	2308	2311	2313	rBV	22666	25943	1.51%	0.179%
61	15.279	2313	2317	2320	rVV	145289	187095	10.92%	1.294%
62	15.340	2323	2327	2332	rVB	74437	106078	6.19%	0.733%
63	15.444	2341	2344	2348	rBV5	14320	20034	1.17%	0.139%
64	15.560	2358	2363	2369	rVB2	176402	244660	14.28%	1.692%
65	15.694	2381	2385	2389	rBV5	22095	42317	2.47%	0.293%
66	15.968	2426	2430	2435	rVB4	17879	35073	2.05%	0.243%
67	16.176	2459	2464	2466	rBV5	18352	32514	1.90%	0.225%
68	16.230	2471	2473	2478	rVB2	19463	28597	1.67%	0.198%
69	16.462	2506	2511	2520	rVB	46102	80850	4.72%	0.559%

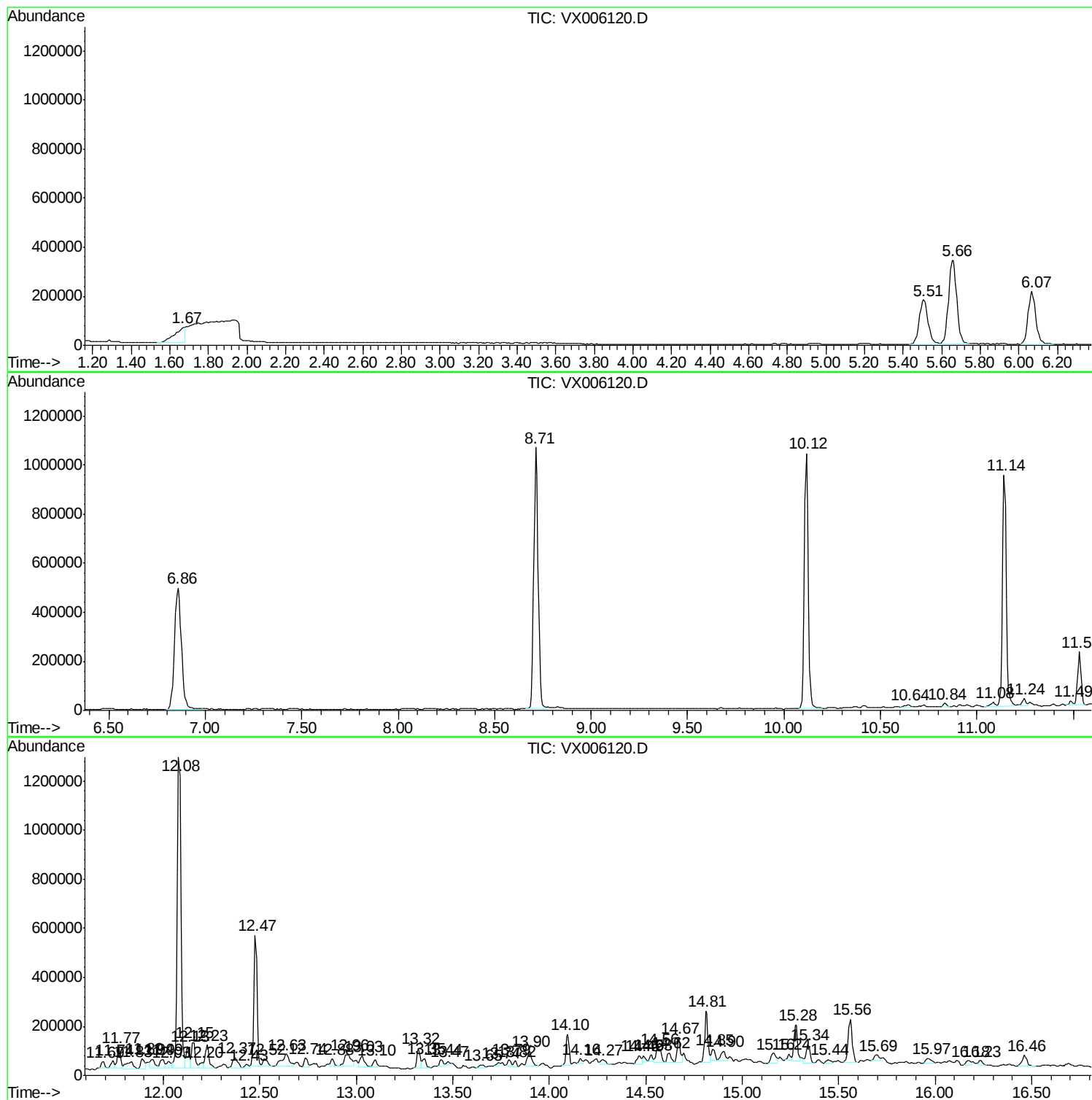
Sum of corrected areas: 14463009

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

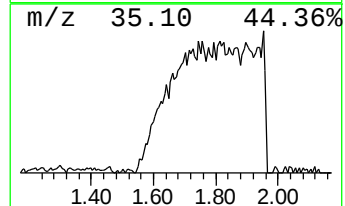
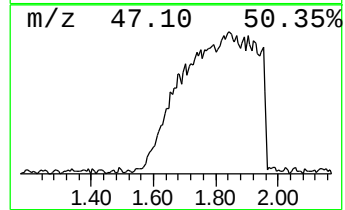
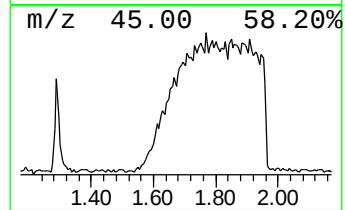
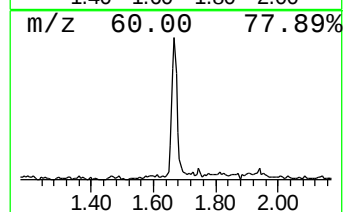
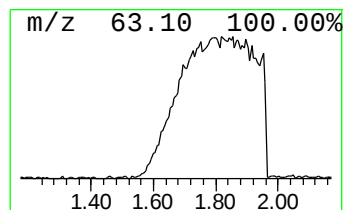
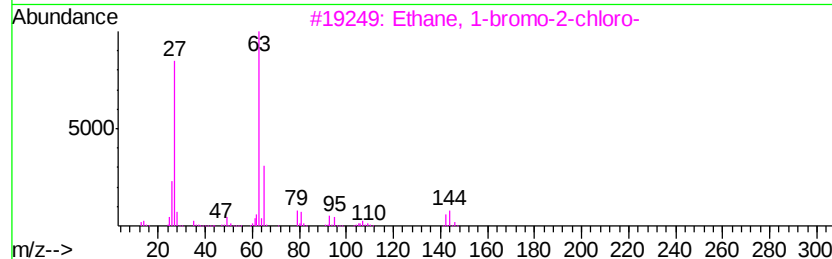
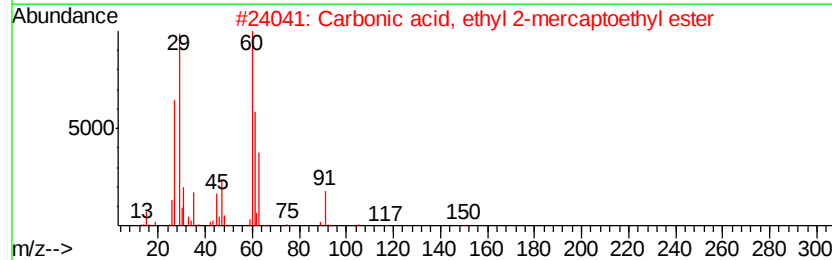
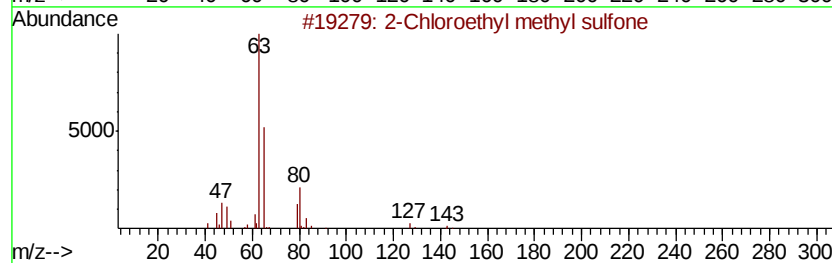
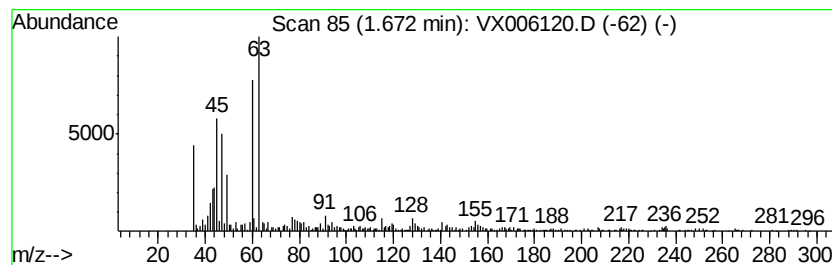
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Chloroethyl methyl sulfone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	12.44 ug/l	245266	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Chloroethyl methyl sulfone	142	C3H7ClO2S	050890-51-2	45
2		Carbonic acid, ethyl 2-mercaptoe...	150	C5H10O3S	005628-96-6	34
3		Ethane, 1-bromo-2-chloro-	142	C2H4BrCl	000107-04-0	30
4		Oxalyl chloride	126	C2Cl2O2	000079-37-8	28
5		Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	23



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

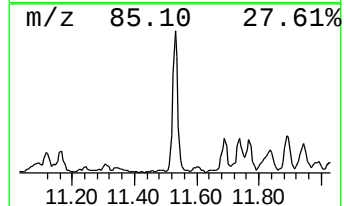
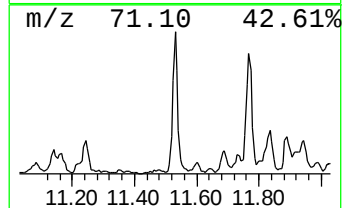
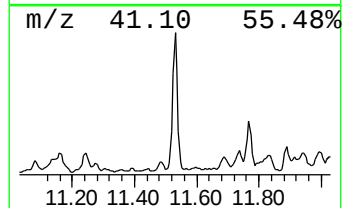
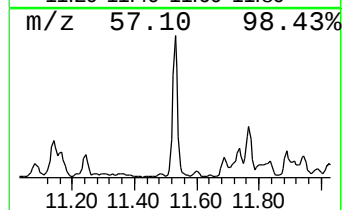
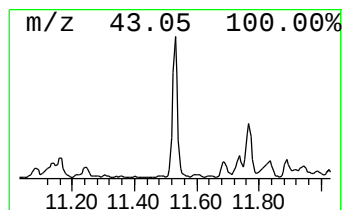
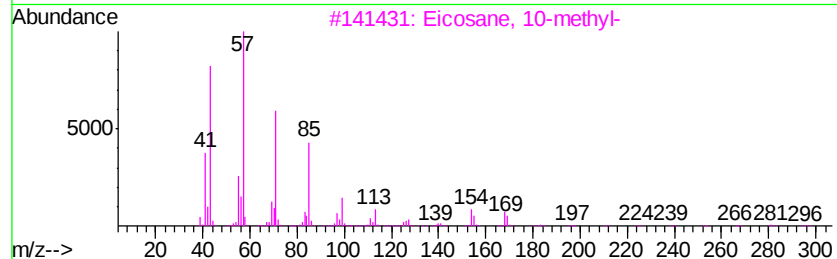
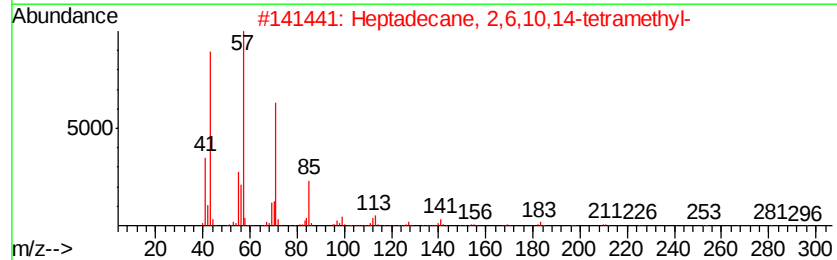
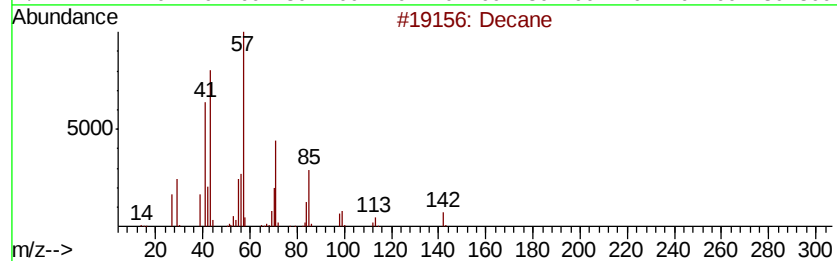
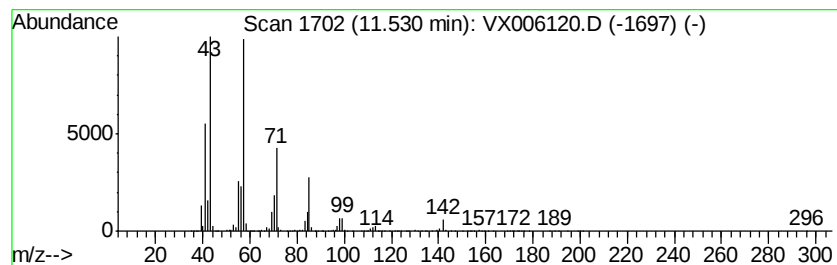
Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 2 Decane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	7.53 ug/l	258038	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane		142 C10H22	000124-18-5 93
2	Heptadecane, 2,6,10,14-tetramethyl-		296 C21H44	018344-37-1 74
3	Eicosane, 10-methyl-		296 C21H44	054833-23-7 72
4	Hexadecane		226 C16H34	000544-76-3 64
5	Dodecane		170 C12H26	000112-40-3 64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

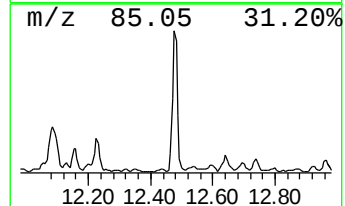
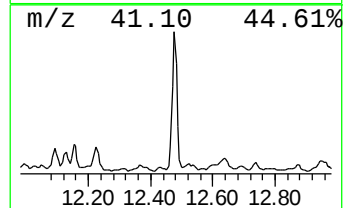
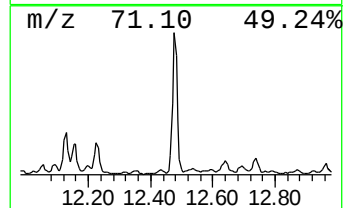
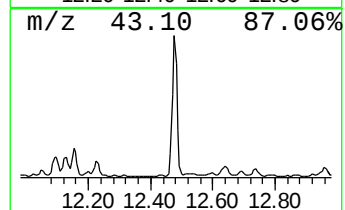
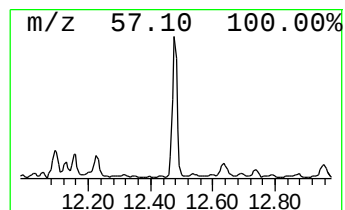
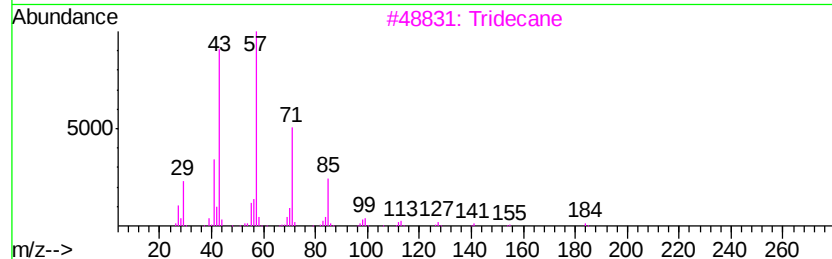
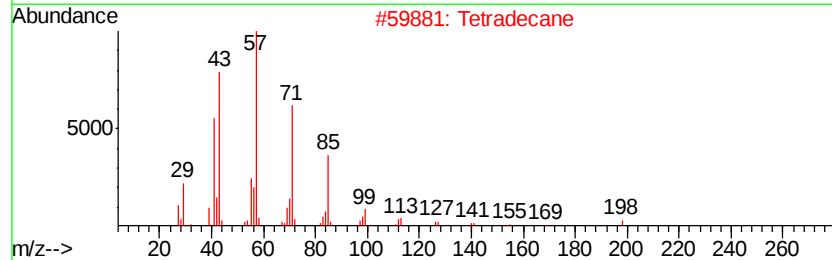
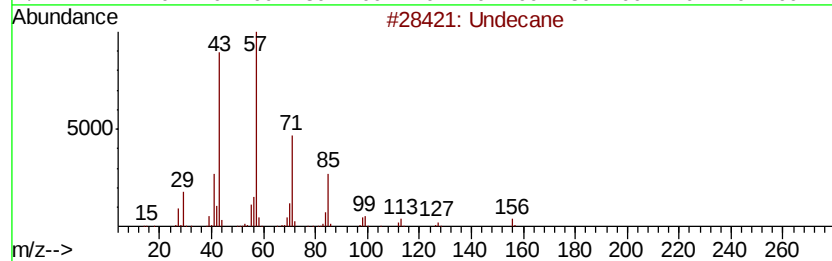
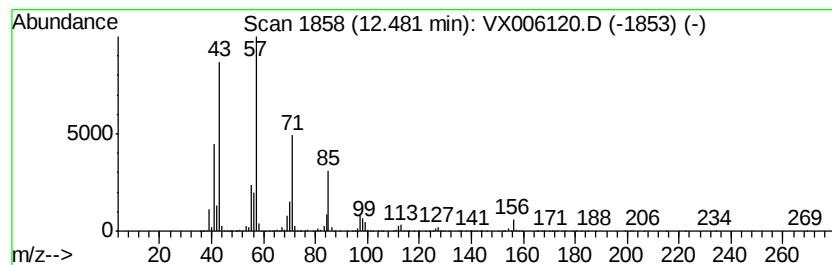
Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 3 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	17.28 ug/l	592091	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	90
2	Tetradecane	198 C14H30	000629-59-4	86
3	Tridecane	184 C13H28	000629-50-5	80
4	Decane, 2,3,7-trimethyl-	184 C13H28	062238-13-5	64
5	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
 Data File : VX006120.D
 Acq On : 21 Nov 2018 13:27
 Operator : JC/MD
 Sample : J5950-10
 Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleID :
 SSI-FD-11132018

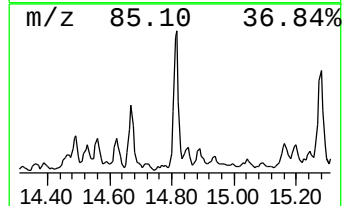
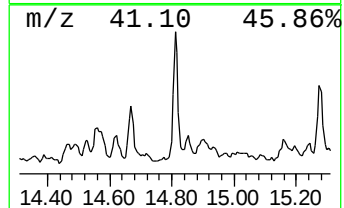
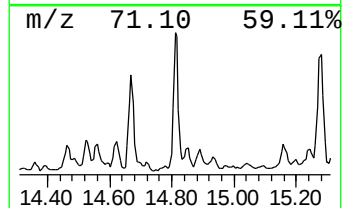
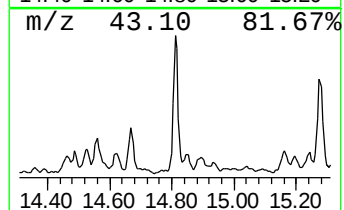
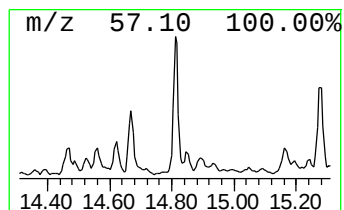
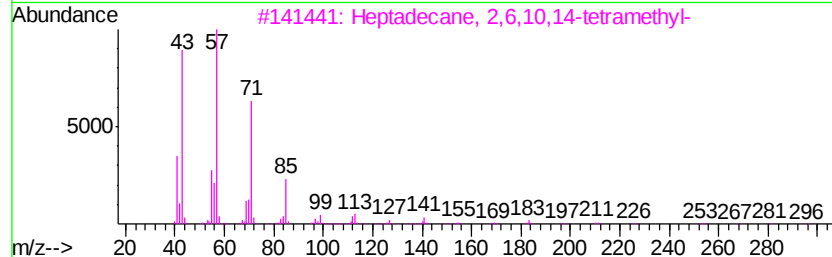
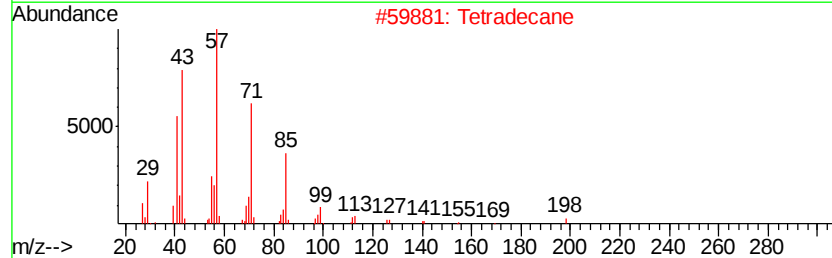
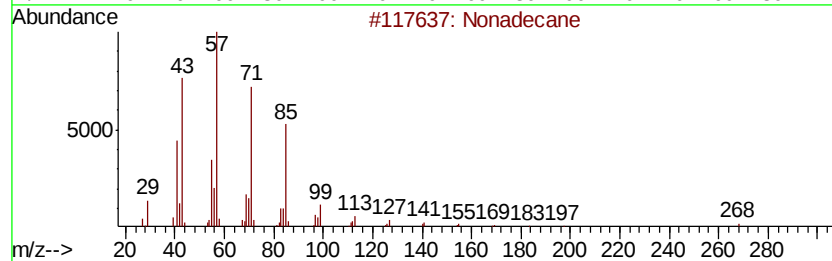
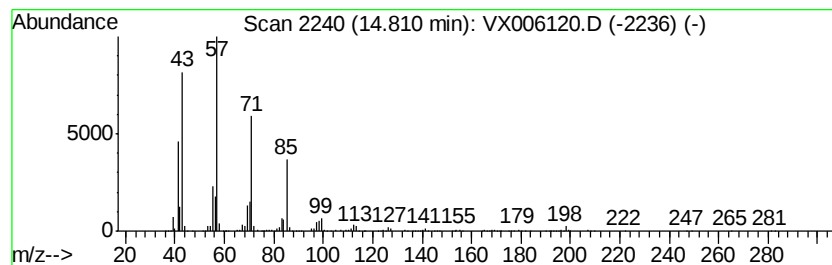
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
 Quant Title : SW846 8260

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

 Peak Number 4 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	7.26 ug/l	248618	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		Tetradecane	198	C14H30	000629-59-4	87
3		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	78
4		Hexadecane	226	C16H34	000544-76-3	78
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

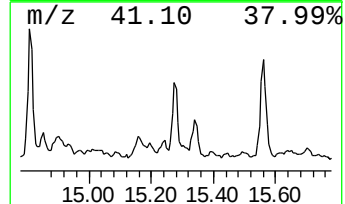
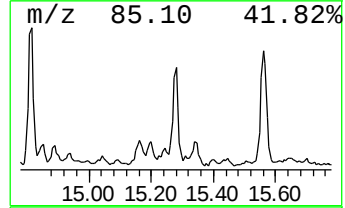
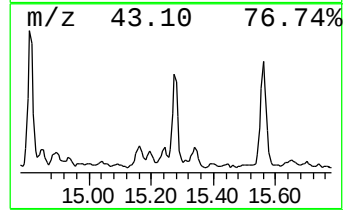
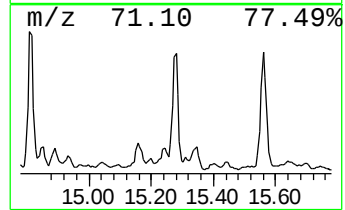
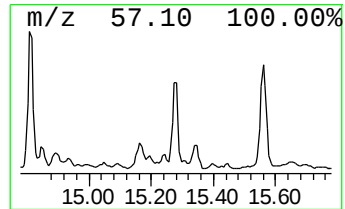
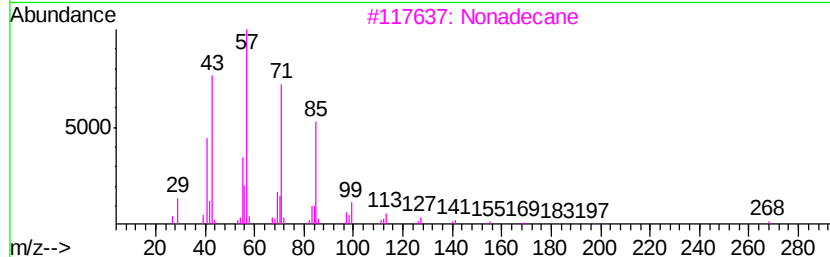
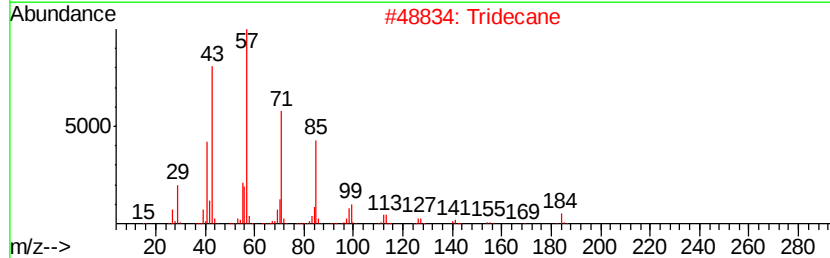
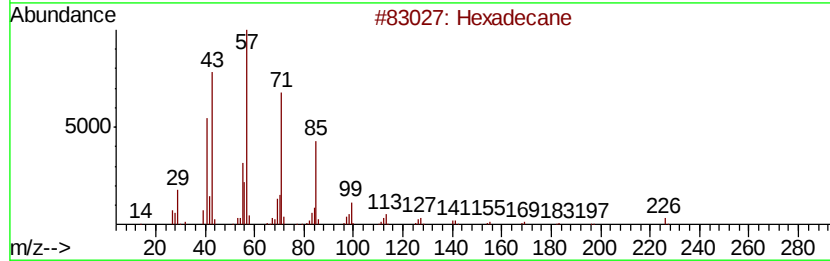
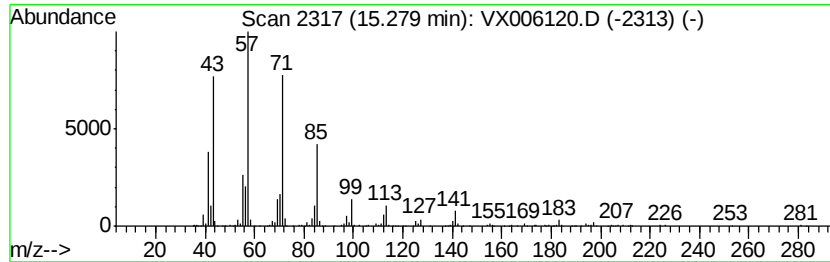
Instrument :
MSVOA_X
ClientSampled :
SSI-FD-11132018

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.46 ug/l	187095	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	93
2	Tridecane	184 C13H28	000629-50-5	91
3	Nonadecane	268 C19H40	000629-92-5	91
4	Tetradecane	198 C14H30	000629-59-4	90
5	Dodecane, 2-methyl-6-propyl-	226 C16H34	055045-08-4	86



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

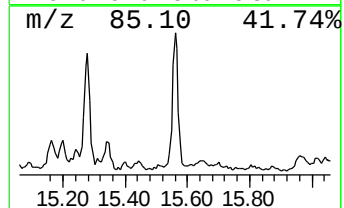
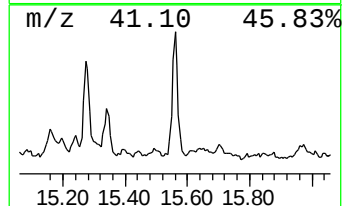
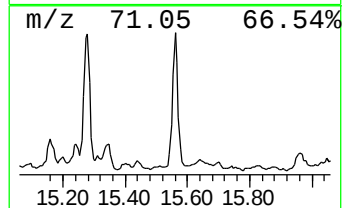
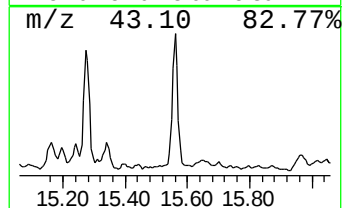
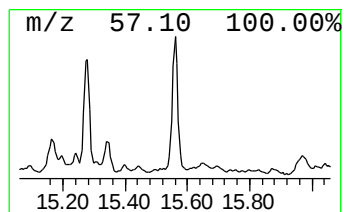
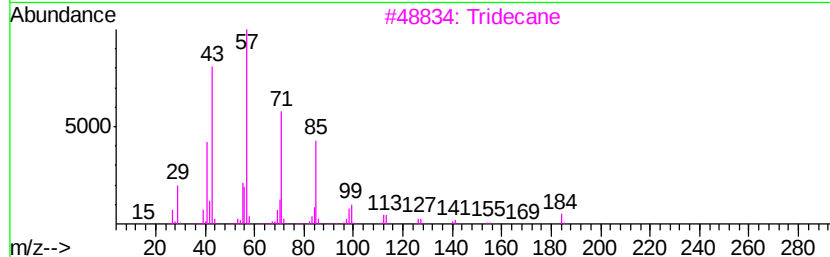
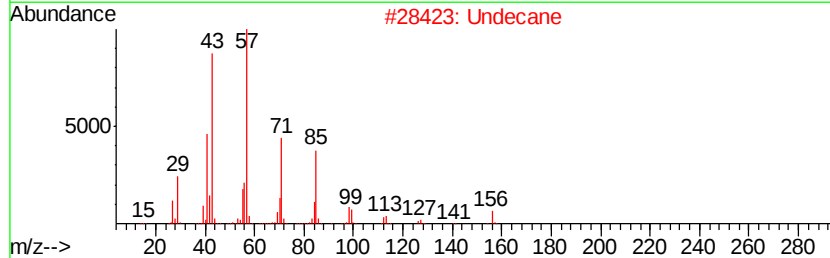
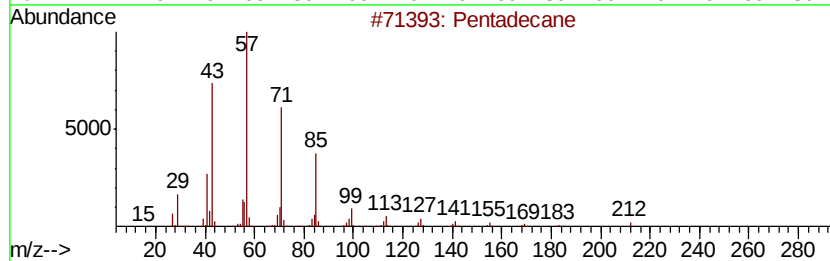
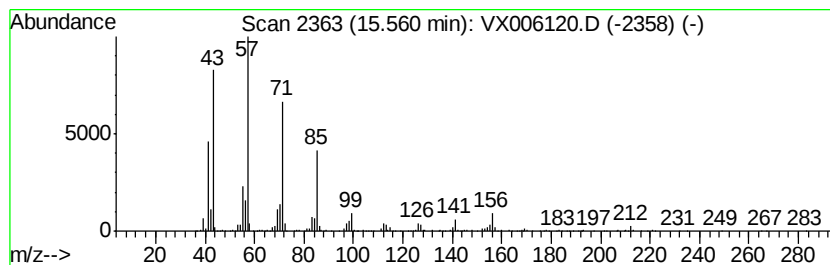
Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.56	7.14 ug/l	244660	1,4-Dichlorobenzene-d4		12.08
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Undecane	156	C11H24	001120-21-4	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Hexadecane	226	C16H34	000544-76-3	83
5	Dodecane	170	C12H26	000112-40-3	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112118\
Data File : VX006120.D
Acq On : 21 Nov 2018 13:27
Operator : JC/MD
Sample : J5950-10
Misc : 6.68g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SSI-FD-11132018

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.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
2-Chloroethyl met...	1.67	12.4	ug/l	245266	1	5.66	985661	50.0
Decane	11.53	7.5	ug/l	258038	4	12.08	1712780	50.0
Undecane	12.48	17.3	ug/l	592091	4	12.08	1712780	50.0
Nonadecane	14.81	7.3	ug/l	248618	4	12.08	1712780	50.0
Hexadecane	15.28	5.5	ug/l	187095	4	12.08	1712780	50.0
Pentadecane	15.56	7.1	ug/l	244660	4	12.08	1712780	50.0