

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112118\
 Data File : VX006117.D
 Acq On : 21 Nov 2018 12:07
 Operator : JC/MD
 Sample : J5967-05
 Misc : 5.01g/10ml/100ul/5.00mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FDSB-13(6-8)

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\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	1.751	64	98	99	rBV5	71078	506195	31.37%	4.510%
2	3.019	301	306	322	rVB2	7734	19223	1.19%	0.171%
3	4.934	606	620	628	rBV	9741	34804	2.16%	0.310%
4	5.507	701	714	727	rBV	174799	545296	33.79%	4.859%
5	5.653	727	738	757	rVB	319748	942035	58.38%	8.394%
6	6.068	796	806	819	rBV	202560	560405	34.73%	4.993%
7	6.860	924	936	952	rBV	475854	1177907	72.99%	10.495%
8	8.713	1233	1240	1253	rBV	999649	1613737	100.00%	14.379%
9	10.116	1462	1470	1485	rBV	956706	1383113	85.71%	12.324%
10	11.140	1632	1638	1654	rBV	804887	1080515	66.96%	9.628%
11	12.079	1787	1792	1802	rBV	1157150	1423962	88.24%	12.688%
12	12.384	1834	1842	1846	rBV	10072	27654	1.71%	0.246%
13	12.536	1862	1867	1870	rVB6	11338	20699	1.28%	0.184%
14	12.633	1881	1883	1889	rVB5	16181	27808	1.72%	0.248%
15	12.737	1896	1900	1904	rBV	22696	28448	1.76%	0.253%
16	12.877	1918	1923	1928	rVB4	20766	32766	2.03%	0.292%
17	12.944	1928	1934	1937	rBV6	14018	28889	1.79%	0.257%
18	13.060	1947	1953	1957	rBV4	23940	54095	3.35%	0.482%
19	13.268	1981	1987	1991	rBV2	23854	41684	2.58%	0.371%
20	13.353	1997	2001	2006	rVB4	26447	40022	2.48%	0.357%
21	13.438	2012	2015	2018	rBV	60341	77151	4.78%	0.687%
22	13.475	2018	2021	2024	rVB4	17889	26219	1.62%	0.234%
23	13.615	2040	2044	2047	rBV	18254	23349	1.45%	0.208%
24	13.658	2047	2051	2056	rBV7	8390	22528	1.40%	0.201%
25	13.761	2065	2068	2076	rBV6	29137	43810	2.71%	0.390%
26	13.859	2081	2084	2087	rVB4	28584	29893	1.85%	0.266%
27	13.902	2087	2091	2096	rBV2	152684	197696	12.25%	1.762%
28	14.048	2113	2115	2117	rBV2	19800	19565	1.21%	0.174%
29	14.127	2124	2128	2131	rBV3	46177	68733	4.26%	0.612%
30	14.328	2158	2161	2164	rBV4	29830	37200	2.31%	0.331%
31	14.371	2164	2168	2170	rBV3	26168	40365	2.50%	0.360%
32	14.670	2213	2217	2223	rBV	137737	184906	11.46%	1.648%
33	14.999	2268	2271	2272	rBV3	43734	49801	3.09%	0.444%
34	15.023	2272	2275	2284	rVB3	112341	202890	12.57%	1.808%

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ClientSampleId :
FDSB-13(6-8)

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

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35	15.279	2313	2317	2321	rVB	150592	191727	11.88%	1.708%
36	15.493	2348	2352	2357	rBV	150299	214726	13.31%	1.913%
37	15.761	2392	2396	2402	rBV5	84108	203281	12.60%	1.811%

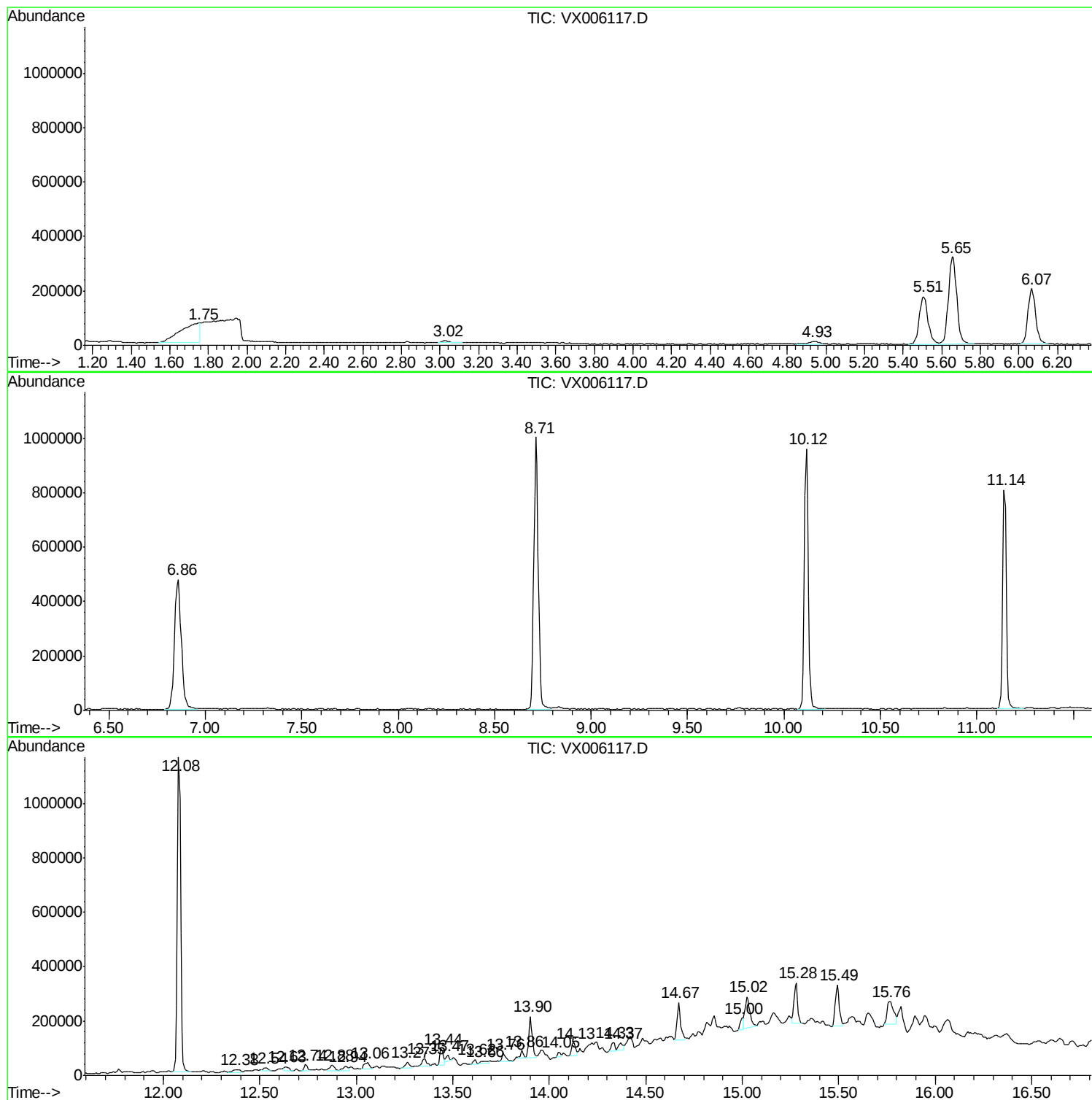
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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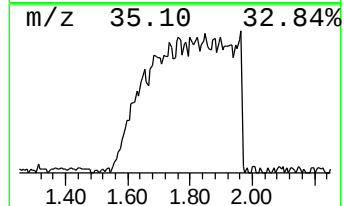
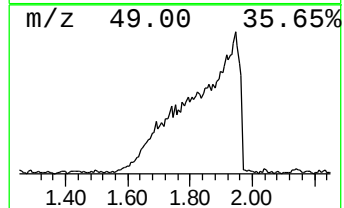
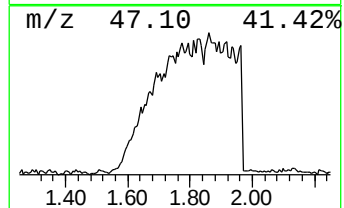
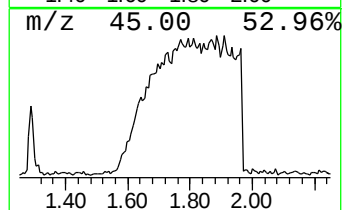
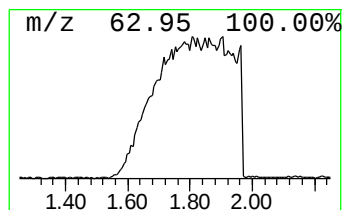
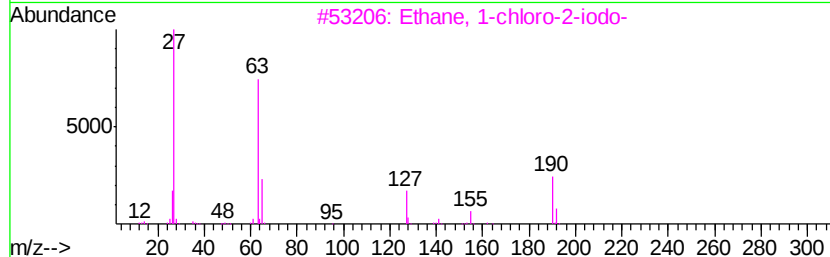
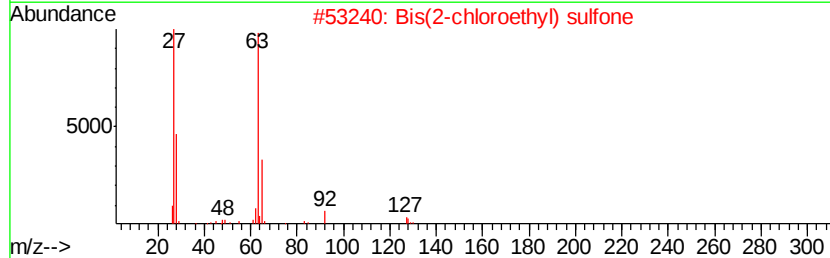
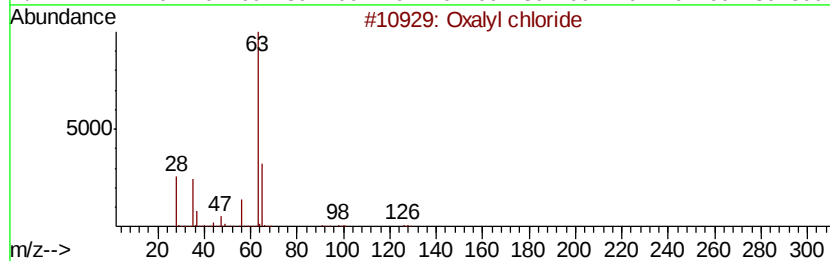
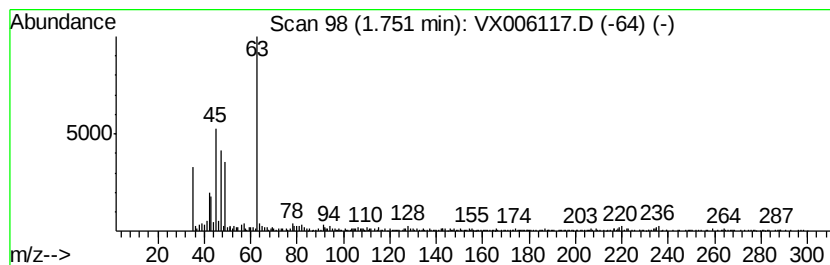
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.75	26.87 ug/l	506195	Pentafluorobenzene	5.66		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalyl chloride	126	C2Cl2O2	000079-37-8	40
2		Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	25
3		Ethane, 1-chloro-2-iodo-	190	C2H4ClI	000624-70-4	9
4		Isopropylthiophosphondiamide	138	C3H11N2PS	1000306-03-6	9
5		1,3-Dioxonane, 5,5,6,6,7,7,8,8-o...	274	C7H6F8O2	036301-47-0	9



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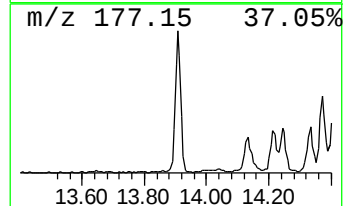
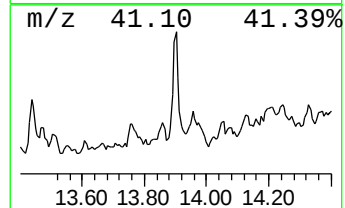
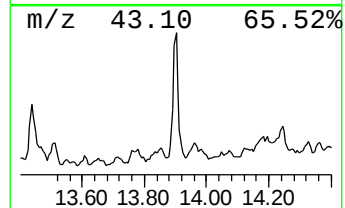
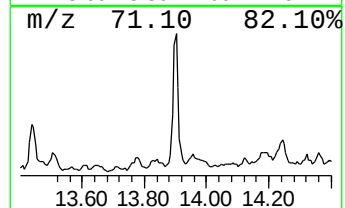
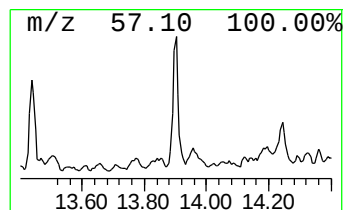
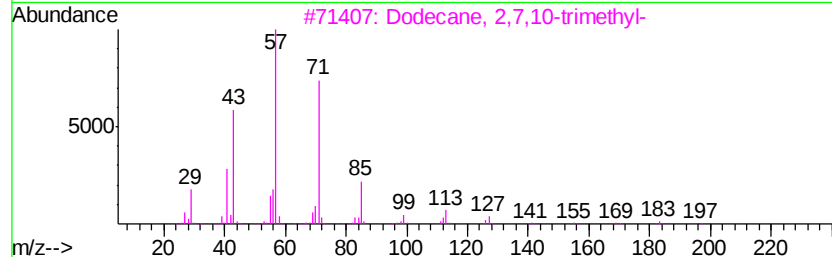
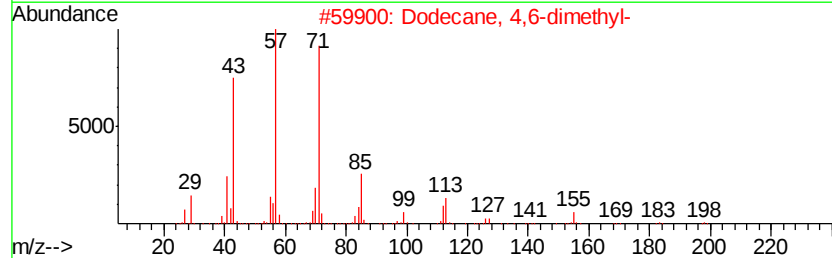
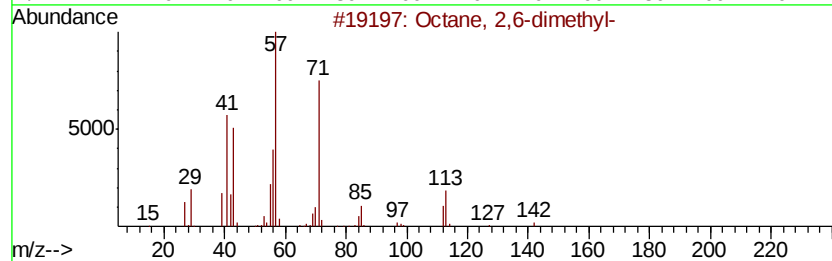
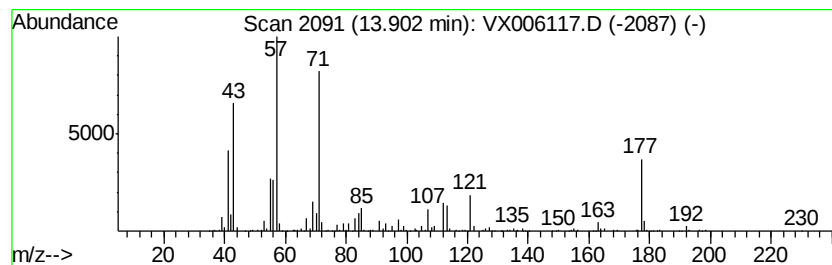
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	6.94 ug/l	197696	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
2	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	58
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	53
4	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	50
5	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	49



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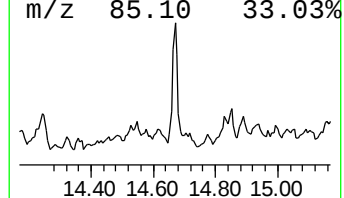
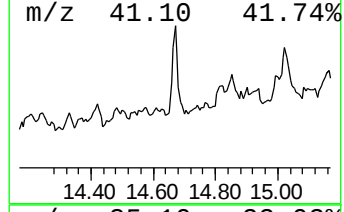
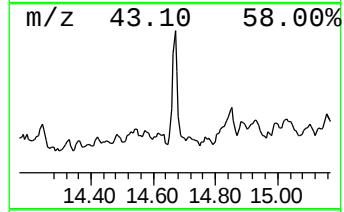
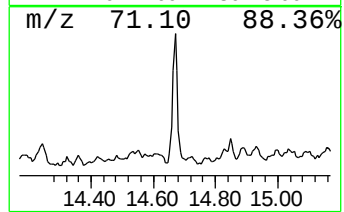
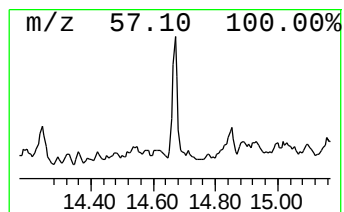
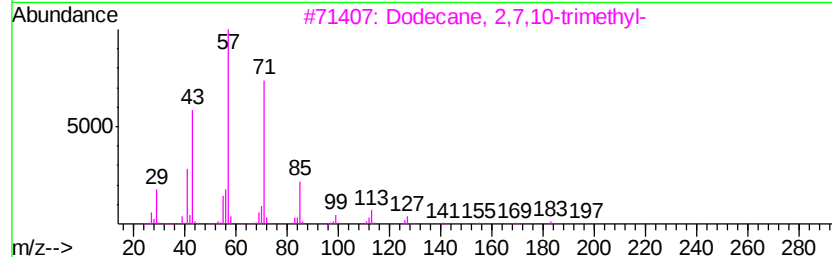
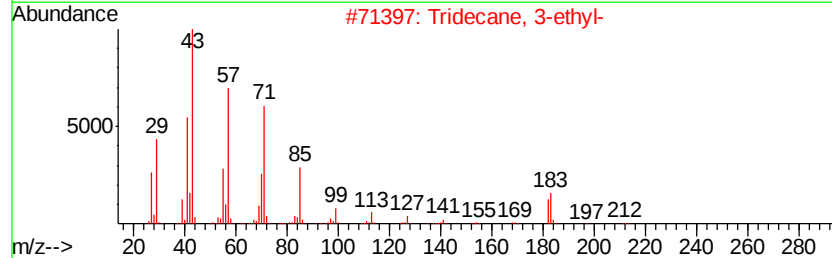
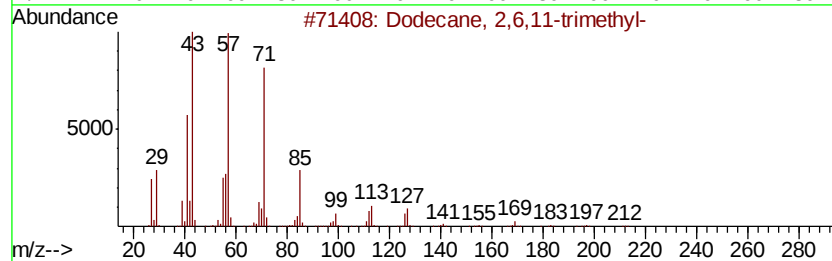
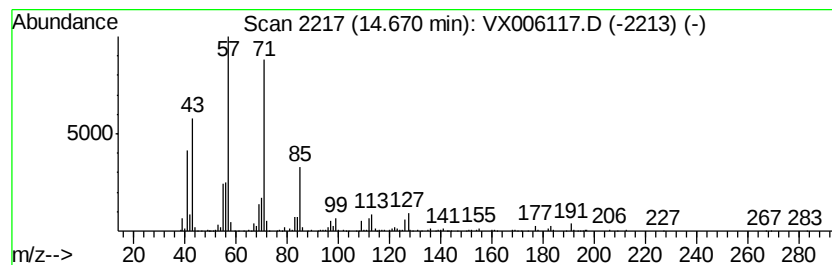
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane, 2,6,11-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	6.49 ug/l	184906	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	90
2		Tridecane, 3-ethyl-	212	C15H32	013286-73-2	80
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
5		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64



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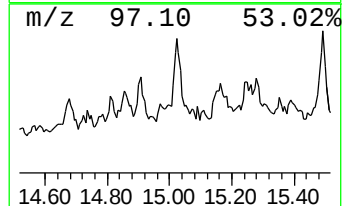
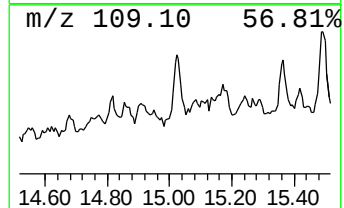
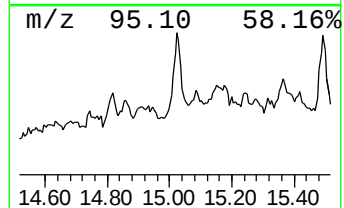
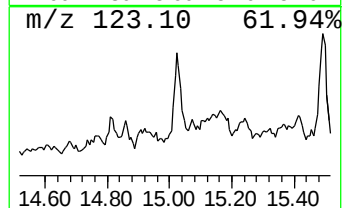
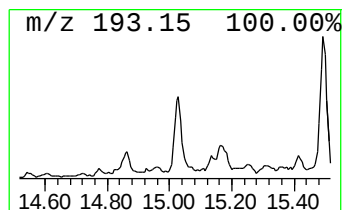
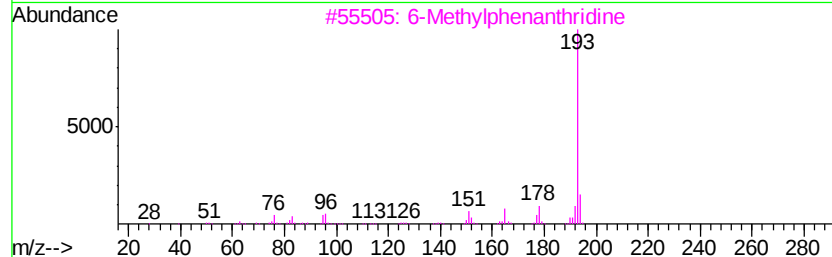
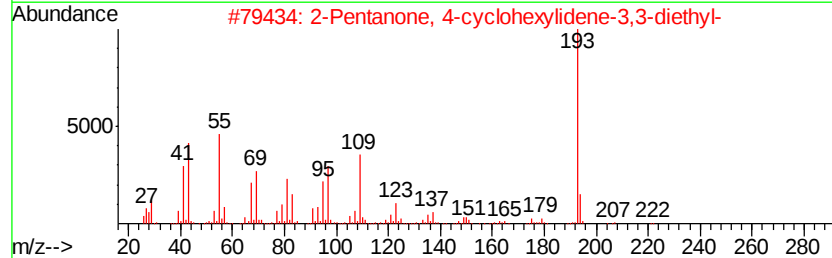
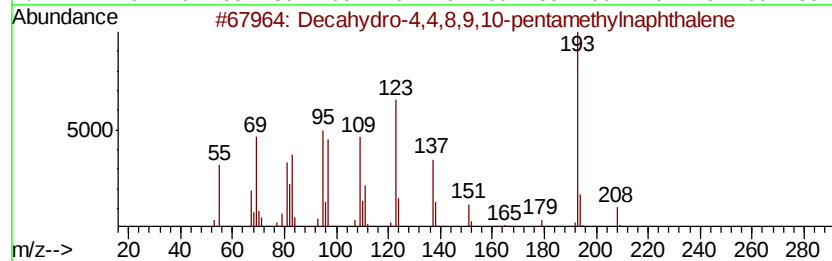
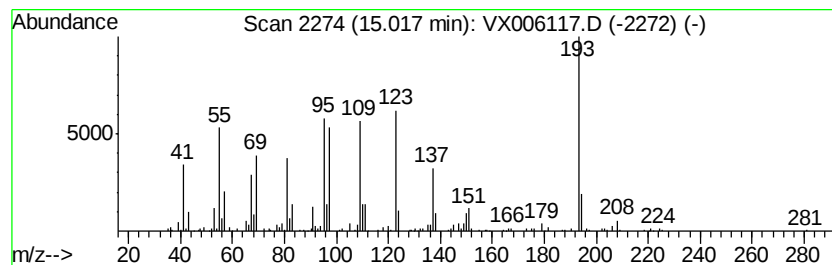
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Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	7.12 ug/l	202890	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3	91
2	2-Pentanone, 4-cyclohexylidene-3...	222 C15H26O	313253-65-5	53
3	6-Methylphenanthridine	193 C14H11N	003955-65-5	27
4	Ethanone, 1-(1-ethyl-1H-pyrazol-...	138 C7H10N2O	1000316-95-0	18
5	2-Cyclopenten-1-one, 2,3,4,5-tet...	138 C9H14O	054458-61-6	18



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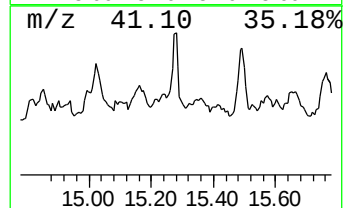
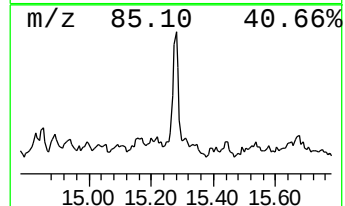
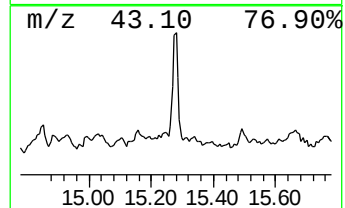
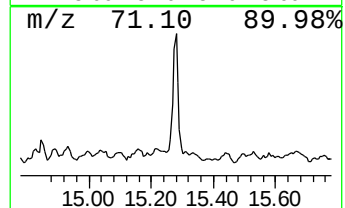
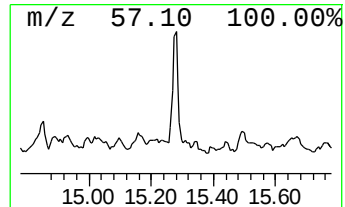
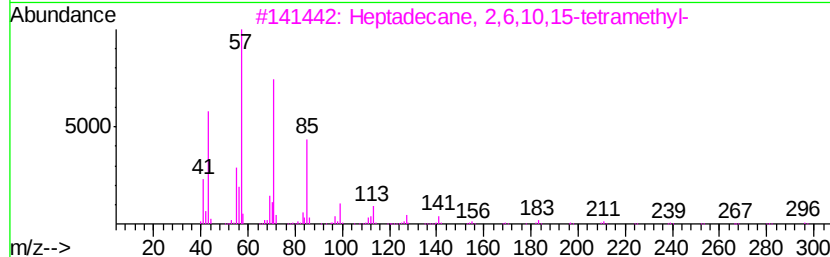
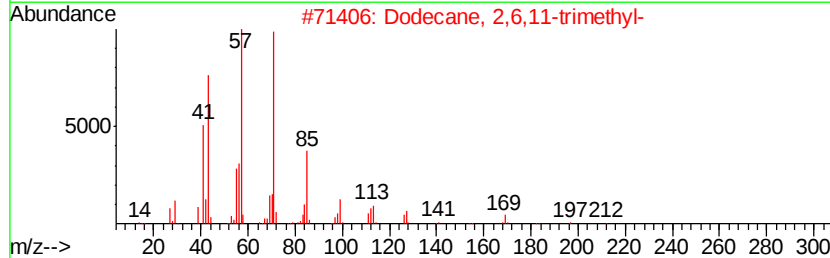
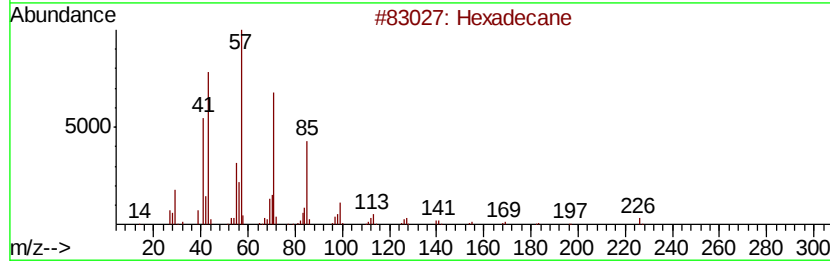
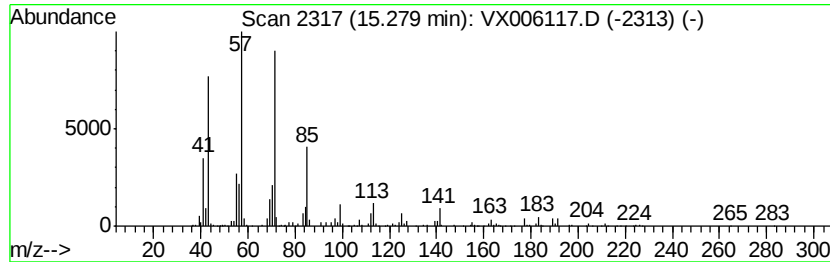
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.28	6.73 ug/l	191727	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	81
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Decane, 2-methyl-	156	C11H24	006975-98-0	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112118\
Data File : VX006117.D
Acq On : 21 Nov 2018 12:07
Operator : JC/MD
Sample : J5967-05
Misc : 5.01µl/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

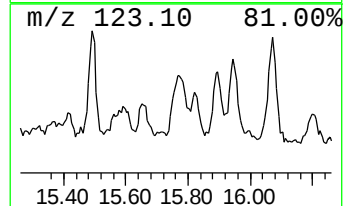
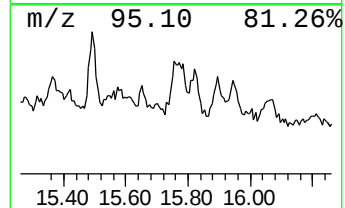
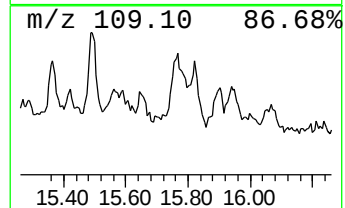
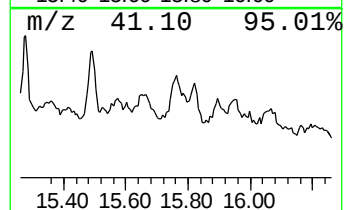
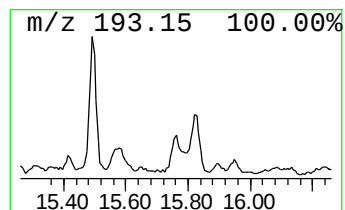
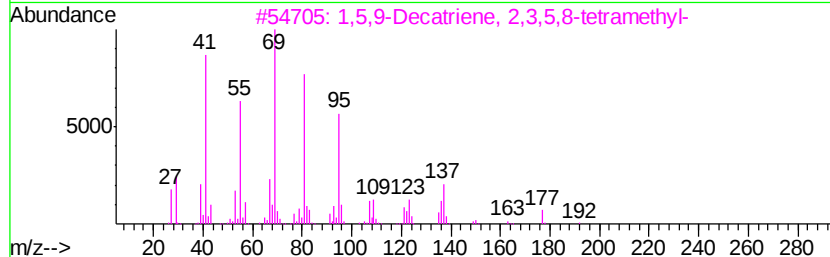
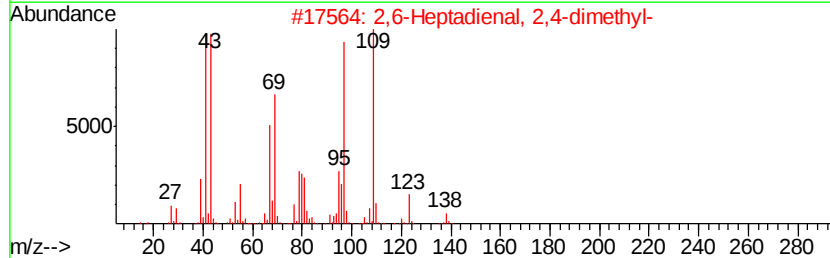
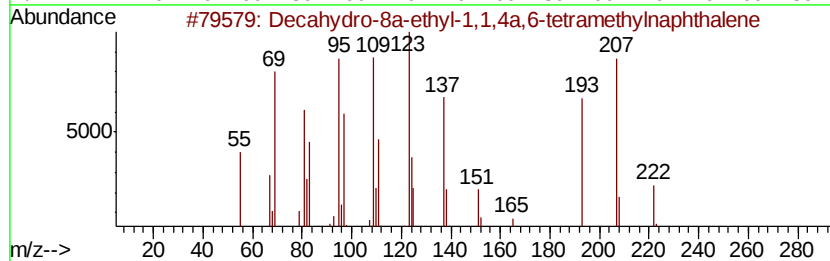
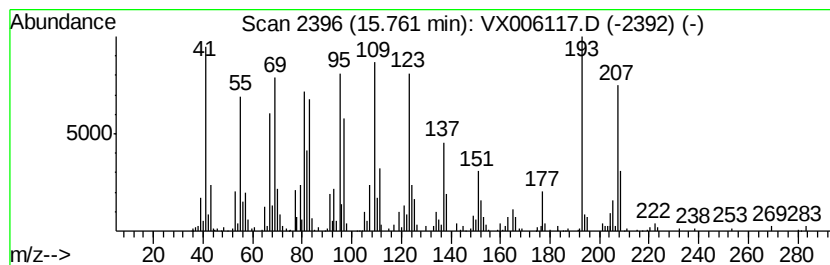
Instrument :
MSVOA_X
ClientSampleId :
FDSB-13(6-8)

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 7 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	7.14 ug/l	203281	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222 C16H30	1000100-23-6	52
2	2,6-Heptadienal, 2,4-dimethyl-	138 C9H14O	085136-08-9	38
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192 C14H24	230646-72-7	38
4	Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3	35
5	2-Cyclopenten-1-one, 2,3,4,5-tet...	138 C9H14O	054458-61-6	15



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112118\
Data File : VX006117.D
Acq On : 21 Nov 2018 12:07
Operator : JC/MD
Sample : J5967-05
Misc : 5.01g/10ml/100ul/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FDSB-13(6-8)

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
unknown1.75	1.75	26.9	ug/l	506195	1	5.66	942035	50.0
Octane, 2,6-dimet...	13.90	6.9	ug/l	197696	4	12.08	1423960	50.0
Dodecane, 2,6,11-...	14.67	6.5	ug/l	184906	4	12.08	1423960	50.0
Decahydro-4,4,8,9...	15.02	7.1	ug/l	202890	4	12.08	1423960	50.0
Hexadecane	15.28	6.7	ug/l	191727	4	12.08	1423960	50.0
Decahydro-8a-ethy...	15.76	7.1	ug/l	203281	4	12.08	1423960	50.0