

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122618\
 Data File : VX006818.D
 Acq On : 26 Dec 2018 15:09
 Operator : JC/MD
 Sample : J6575-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS-122618-A

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	1.410	40	42	47	rBV	46134616	98194246	100.00%	26.885%
2	2.135	150	161	181	rBV	12500187	26176952	26.66%	7.167%
3	2.440	204	211	227	rVV	9353450	16320909	16.62%	4.469%
4	4.342	513	523	536	rBV	421350	1155918	1.18%	0.316%
5	4.689	569	580	592	rBV	573834	1685347	1.72%	0.461%
6	5.031	628	636	651	rVB2	276607	1021843	1.04%	0.280%
7	5.494	698	712	725	rBV2	398707	1162746	1.18%	0.318%
8	5.659	727	739	754	rVB	827965	2349526	2.39%	0.643%
9	5.945	772	786	797	rBV	2253433	5941324	6.05%	1.627%
10	6.061	797	805	814	rVV	416567	1043382	1.06%	0.286%
11	6.732	904	915	927	rBV	2355920	7808345	7.95%	2.138%
12	6.854	928	935	978	rVB2	1565629	5135145	5.23%	1.406%
13	7.543	1041	1048	1060	rBV	1039697	2000333	2.04%	0.548%
14	8.713	1234	1240	1247	rVB	2543945	3885632	3.96%	1.064%
15	9.500	1362	1369	1375	rBV	13634023	18891519	19.24%	5.172%
16	10.109	1464	1469	1476	rVB	2517063	3337978	3.40%	0.914%
17	10.353	1497	1509	1515	rVV	1368078	2362303	2.41%	0.647%
18	10.640	1550	1556	1561	rBV	798951	1185857	1.21%	0.325%
19	10.829	1580	1587	1592	rBV	37197004	46040752	46.89%	12.606%
20	10.914	1596	1601	1603	rBV	846324	1272609	1.30%	0.348%
21	11.139	1632	1638	1648	rVB2	2444035	3768550	3.84%	1.032%
22	11.432	1682	1686	1692	rBV	933774	1586912	1.62%	0.434%
23	11.530	1699	1702	1707	rVB	1929225	2302808	2.35%	0.630%
24	11.804	1744	1747	1757	rVB	1875678	2724892	2.78%	0.746%
25	11.889	1757	1761	1767	rBV	6525648	7978159	8.12%	2.184%
26	11.993	1774	1778	1781	rVV3	600873	1140145	1.16%	0.312%
27	12.023	1781	1783	1787	rVV2	1269759	1422771	1.45%	0.390%
28	12.078	1787	1792	1797	rVB2	2556758	3566596	3.63%	0.977%
29	12.158	1797	1805	1809	rBV3	2154446	3740548	3.81%	1.024%
30	12.273	1819	1824	1827	rBV	3010829	3949701	4.02%	1.081%
31	12.371	1836	1840	1846	rVB3	1704773	2979195	3.03%	0.816%
32	12.475	1846	1857	1861	rBV	3595407	4687510	4.77%	1.283%
33	12.517	1861	1864	1870	rVB3	840302	1293427	1.32%	0.354%
34	12.584	1870	1875	1877	rBV	707438	1029553	1.05%	0.282%

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35	12.639	1881	1884	1886	rVV	865806	1129924	1.15%	0.309%
36	12.755	1897	1903	1905	rBV2	605762	1247278	1.27%	0.341%
37	12.822	1910	1914	1918	rBV	8855425	9936805	10.12%	2.721%
38	12.944	1931	1934	1937	rBV3	652887	1032471	1.05%	0.283%
39	13.023	1943	1947	1953	rVB3	1467779	2473078	2.52%	0.677%
40	13.096	1953	1959	1962	rBV3	921572	1537932	1.57%	0.421%
41	13.151	1965	1968	1973	rVV	1285898	1570775	1.60%	0.430%
42	13.212	1973	1978	1984	rVB4	1626368	3032423	3.09%	0.830%
43	13.322	1990	1996	1998	rBV	3646867	4797688	4.89%	1.314%
44	13.346	1998	2000	2005	rVB2	2830571	3510972	3.58%	0.961%
45	13.474	2017	2021	2030	rVB2	4653163	6870005	7.00%	1.881%
46	13.560	2031	2035	2039	rBV3	787483	1323329	1.35%	0.362%
47	13.639	2044	2048	2053	rBV4	818977	1467392	1.49%	0.402%
48	13.730	2059	2063	2066	rBV3	688322	1263564	1.29%	0.346%
49	13.907	2086	2092	2097	rVB4	1699081	3498558	3.56%	0.958%
50	13.980	2097	2104	2110	rBV3	1175655	2571908	2.62%	0.704%
51	14.090	2119	2122	2126	rVB	3181477	3517143	3.58%	0.963%
52	14.133	2126	2129	2132	rBV2	886013	1093320	1.11%	0.299%
53	14.285	2149	2154	2158	rBV2	2229969	3230175	3.29%	0.884%
54	14.474	2181	2185	2191	rVB7	611636	1172306	1.19%	0.321%
55	14.535	2191	2195	2204	rVB5	1453583	3293702	3.35%	0.902%
56	14.614	2204	2208	2214	rBV5	577388	1105454	1.13%	0.303%
57	14.669	2214	2217	2224	rBV3	2090133	3517476	3.58%	0.963%
58	14.730	2224	2227	2231	rVB2	842446	1116326	1.14%	0.306%
59	14.785	2231	2236	2238	rBV3	1146257	1630593	1.66%	0.446%
60	14.810	2238	2240	2243	rVB	2376753	2253034	2.29%	0.617%
61	15.255	2307	2313	2320	rBV2	3214117	5253644	5.35%	1.438%
62	15.553	2357	2362	2368	rBV2	1051947	1644972	1.68%	0.450%

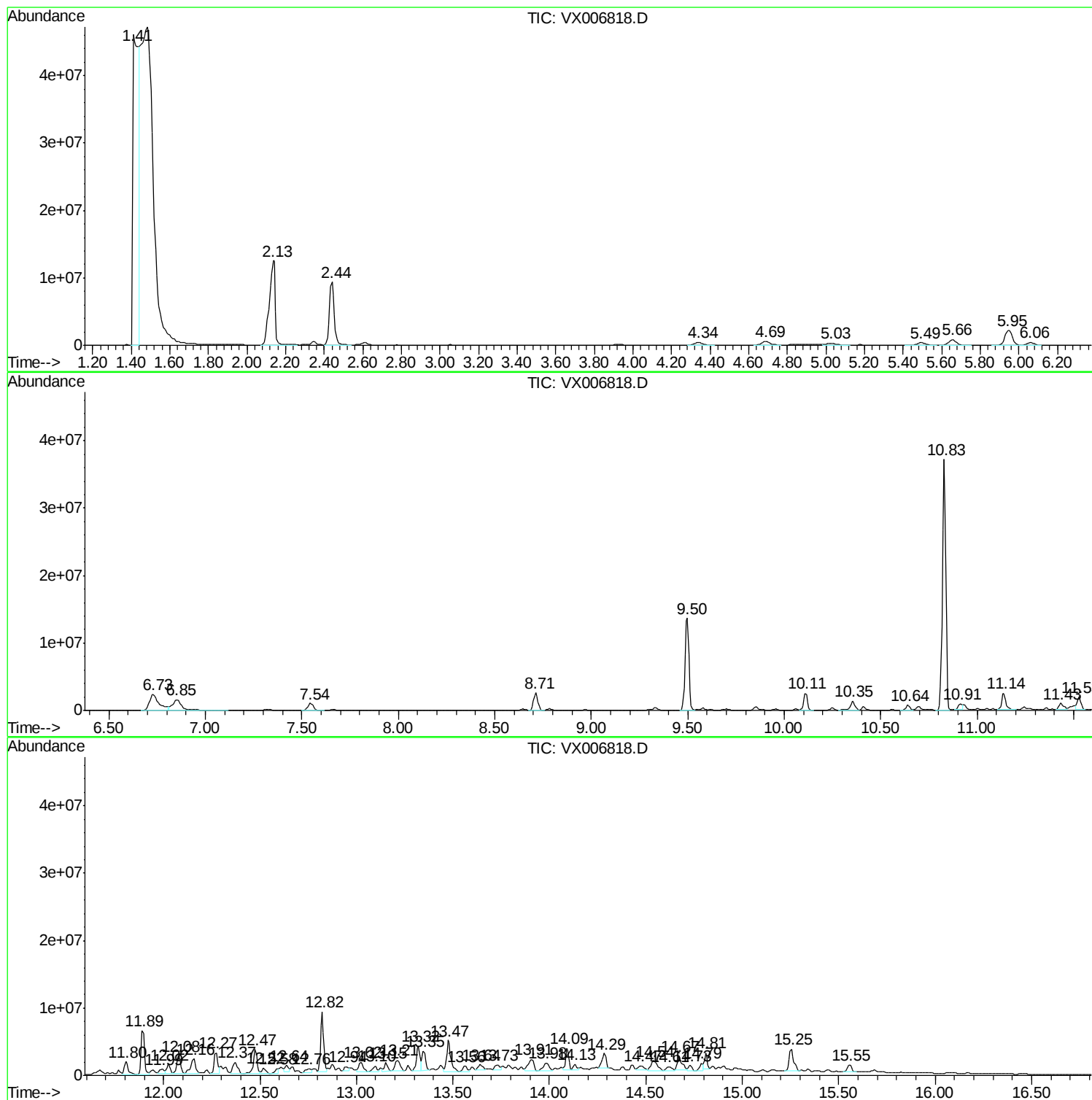
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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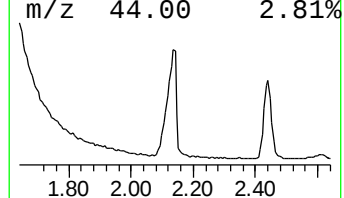
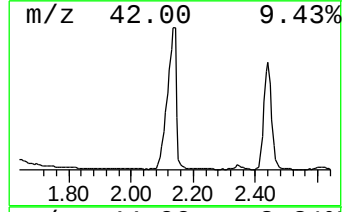
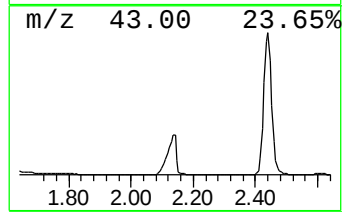
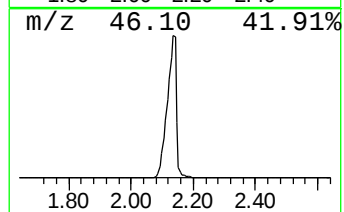
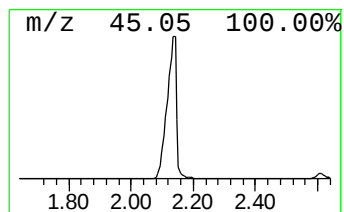
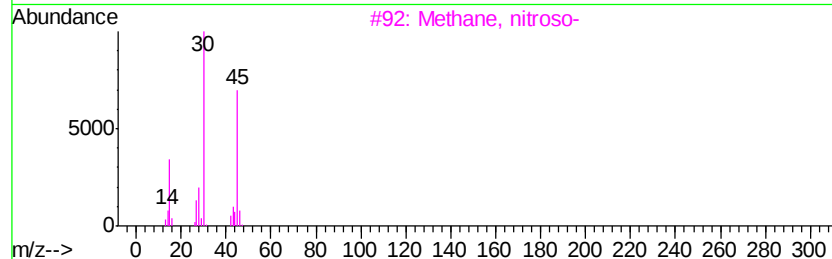
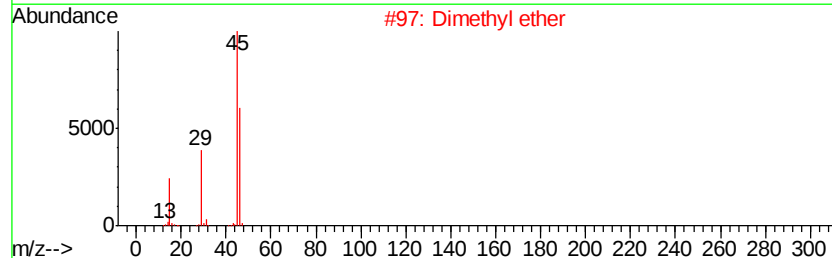
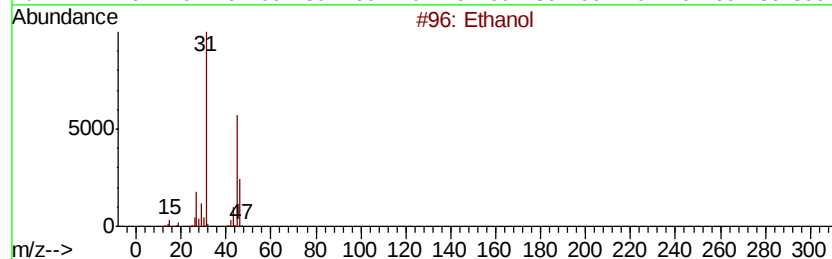
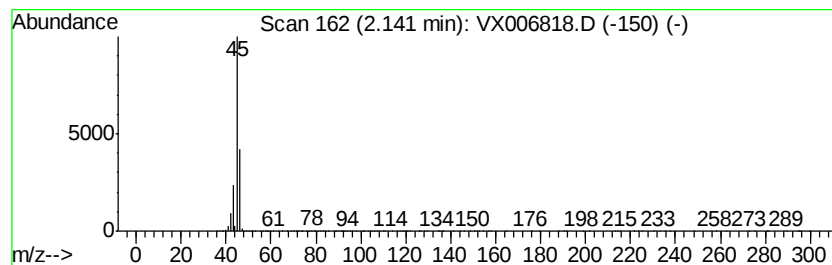
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	557.07 ug/l	26177000	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	83
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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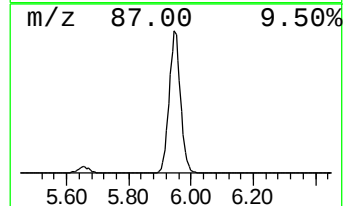
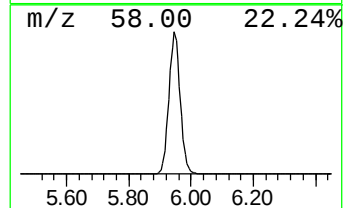
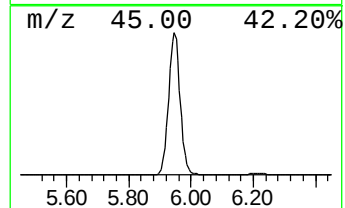
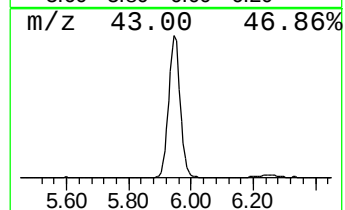
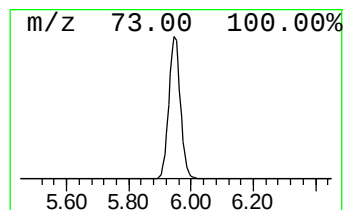
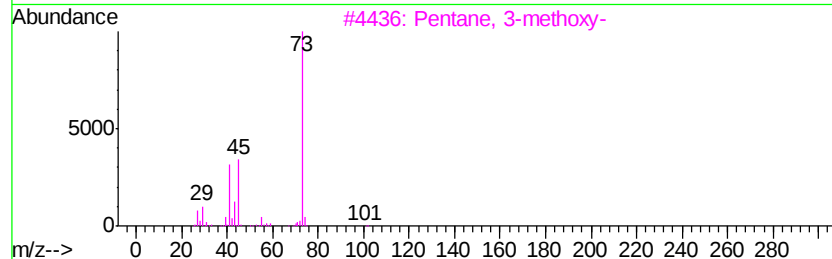
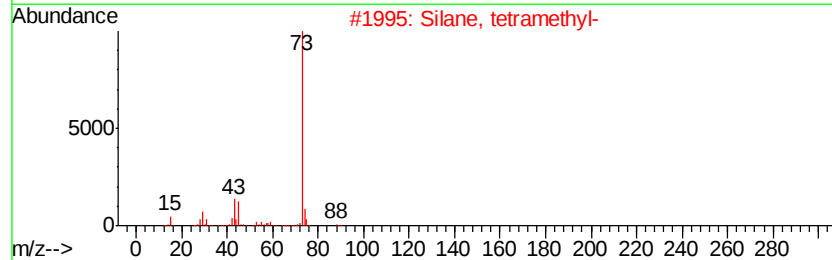
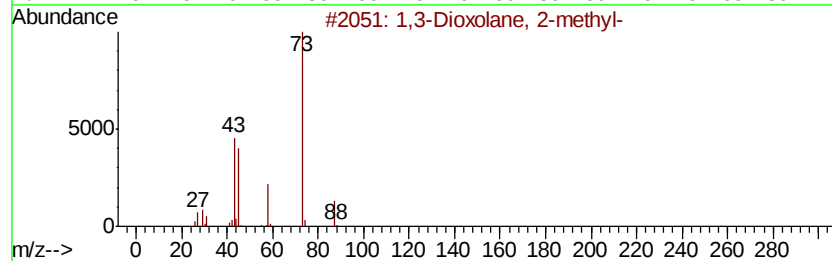
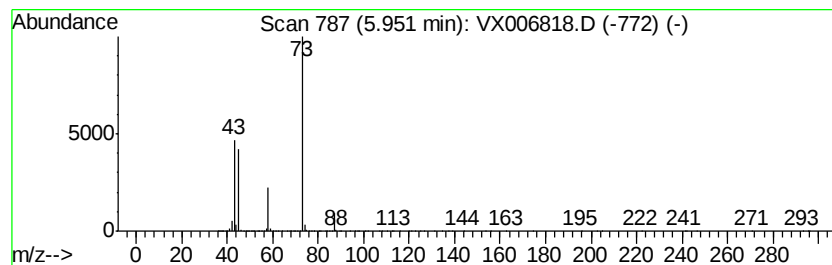
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxolane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	126.44 ug/l	5941320	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9



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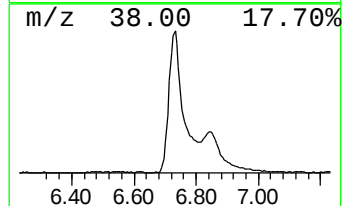
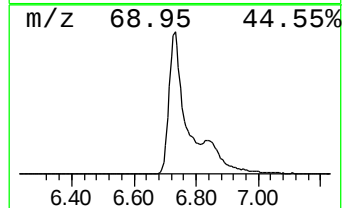
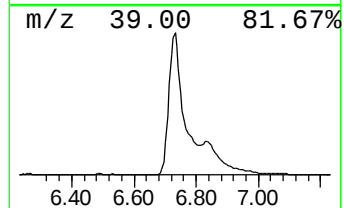
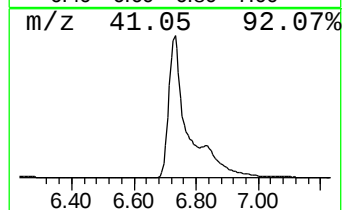
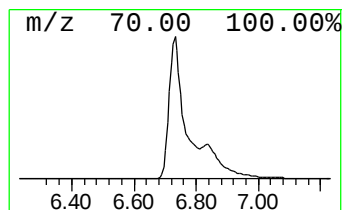
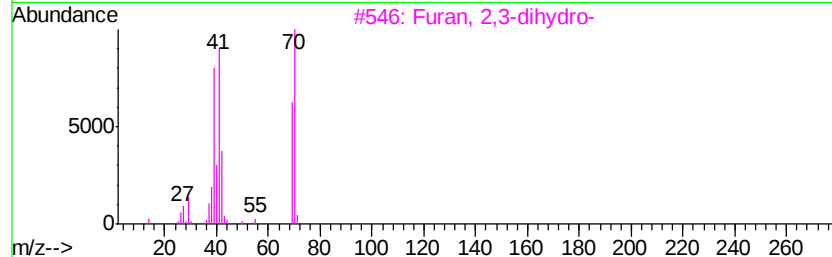
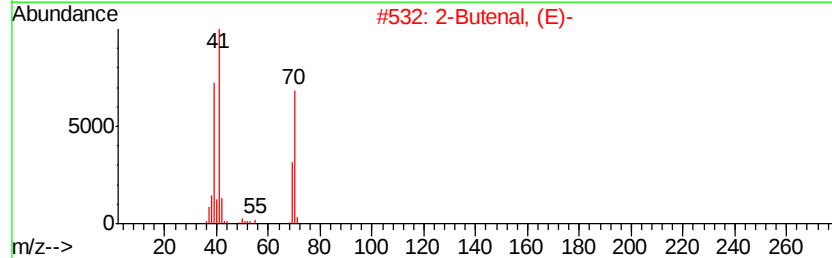
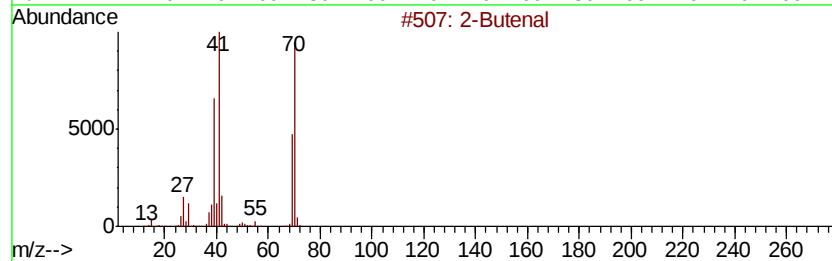
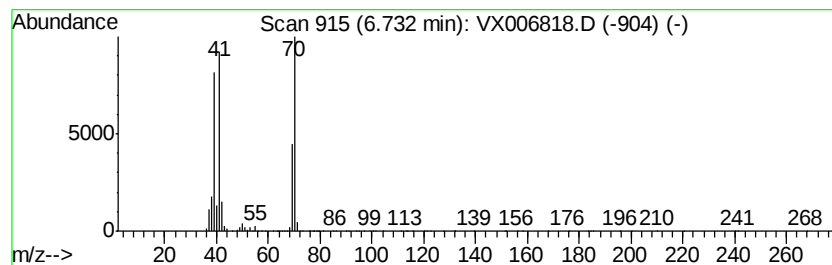
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-Butenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	76.03 ug/l	7808350	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenal	70	C4H6O	004170-30-3	91
2		2-Butenal, (E)-	70	C4H6O	000123-73-9	91
3		Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90
4		Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	90
5		Methacrolein	70	C4H6O	000078-85-3	90



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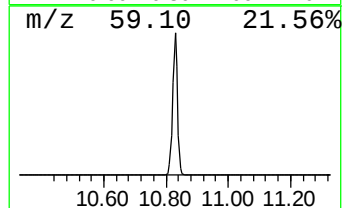
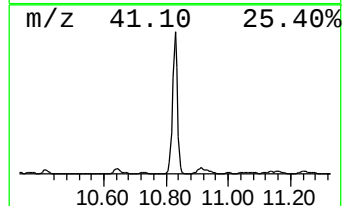
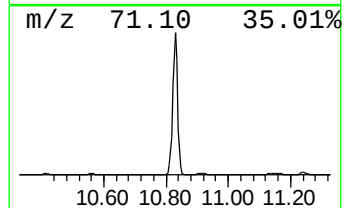
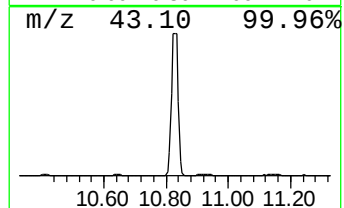
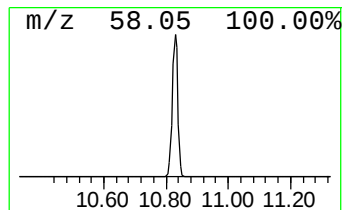
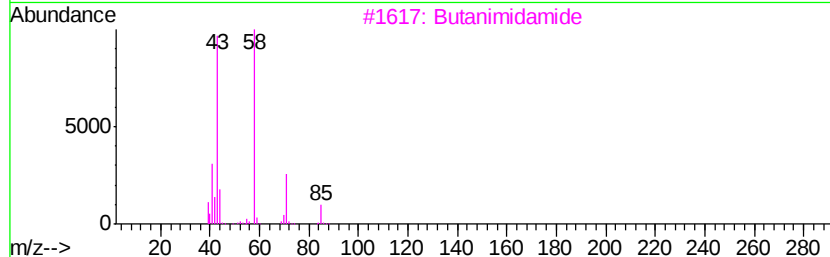
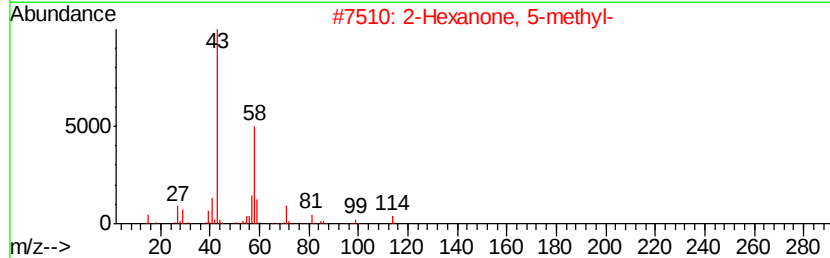
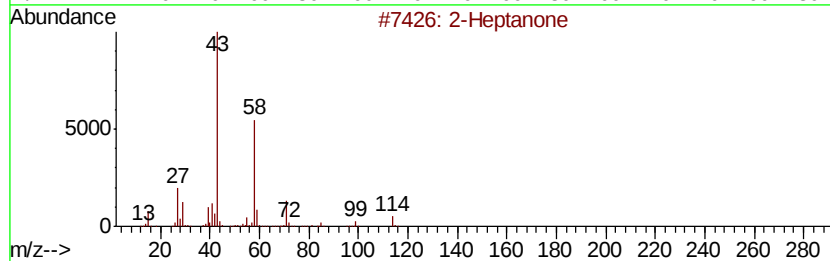
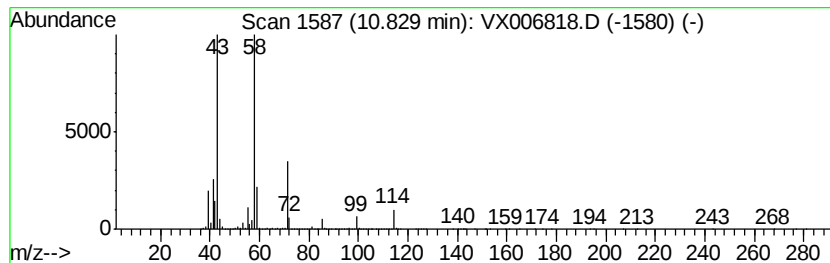
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Peak Number 5 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	689.65 ug/l	46040800	Chlorobenzene-d5	10.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone	114	C7H14O	000110-43-0	87
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72
3		Butanimidamide	86	C4H10N2	000107-90-4	59
4		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	59
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	47



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SS-122618-A

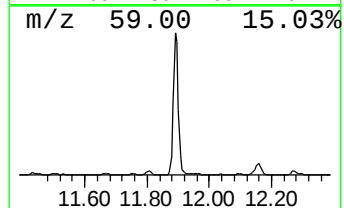
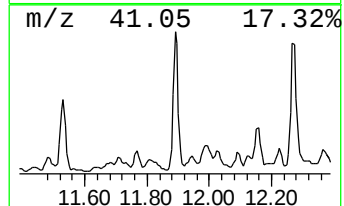
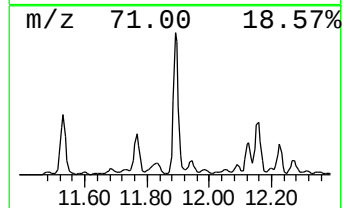
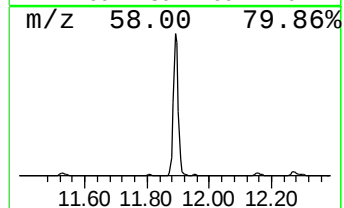
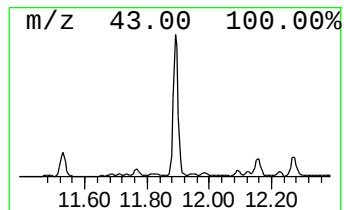
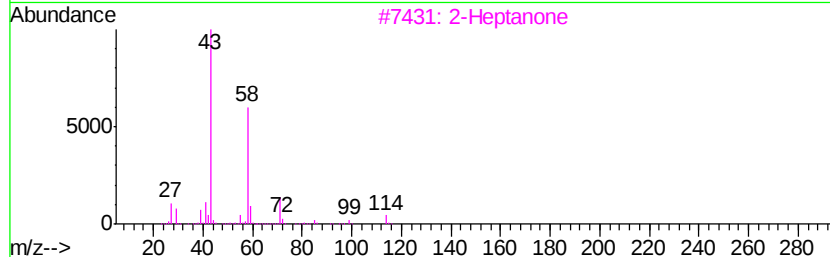
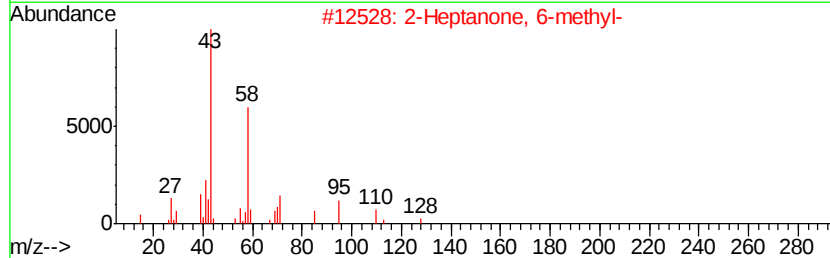
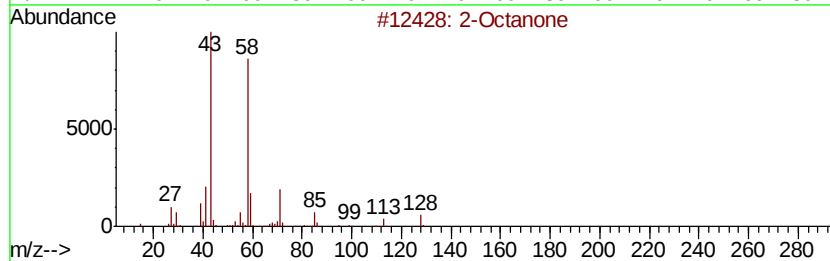
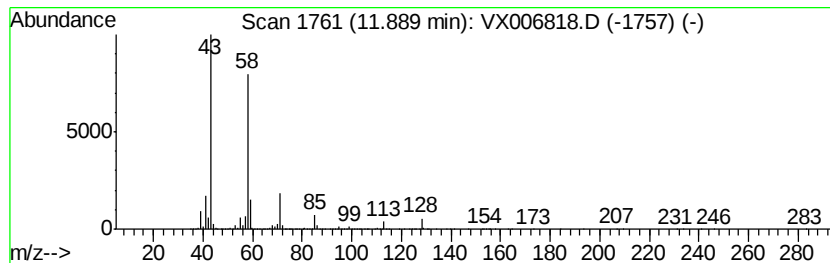
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Quant Title : SW846 8260

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

Peak Number 6 2-Octanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	111.85 ug/l	7978160	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone		128	C8H16O	000111-13-7	94
2	2-Heptanone, 6-methyl-		128	C8H16O	000928-68-7	90
3	2-Heptanone		114	C7H14O	000110-43-0	72
4	2-Hexanone		100	C6H12O	000591-78-6	64
5	2-Hexanone, 5-methyl-		114	C7H14O	000110-12-3	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006818.D
Acq On : 26 Dec 2018 15:09
Operator : JC/MD
Sample : J6575-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS-122618-A

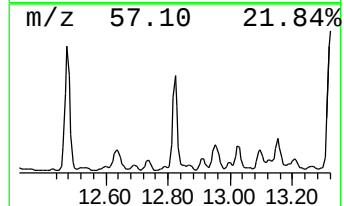
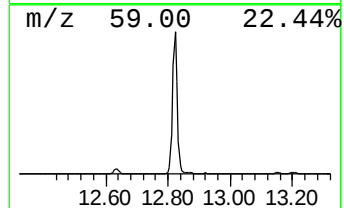
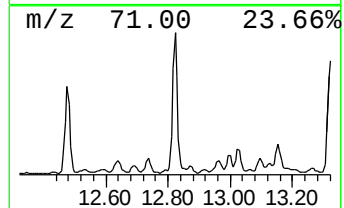
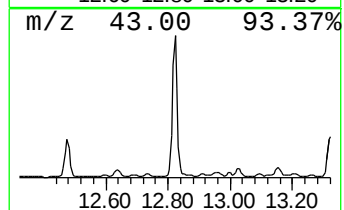
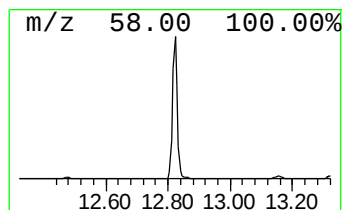
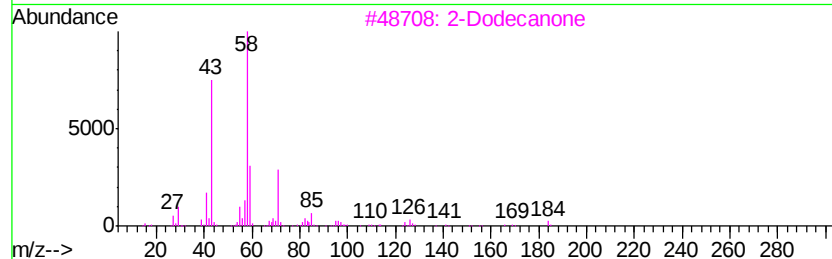
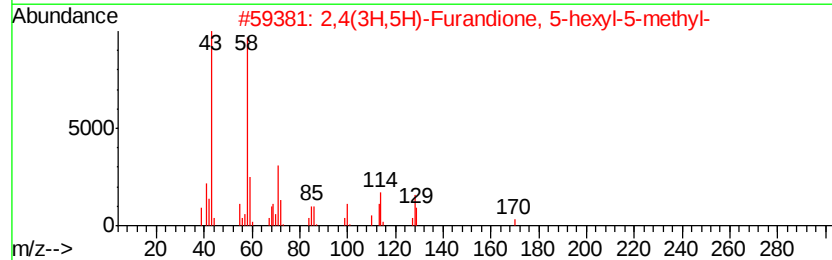
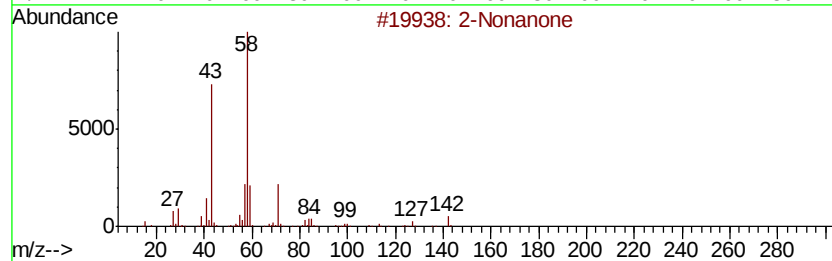
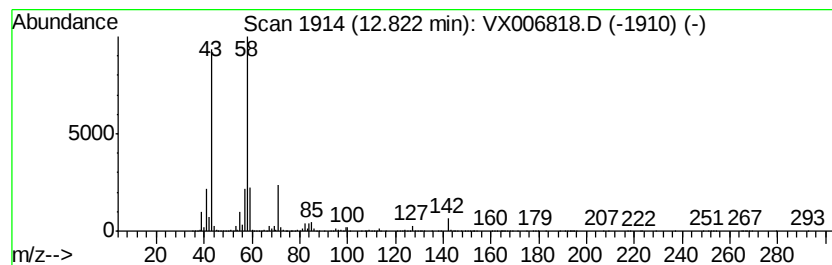
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Quant Title : SW846 8260

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

Peak Number 7 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	139.30 ug/l	9936810	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanone	142	C9H18O	000821-55-6	97
2		2,4(3H,5H)-Furandione, 5-hexyl-5-methyl-	198	C11H18O3	054852-79-8	64
3		2-Dodecanone	184	C12H24O	006175-49-1	64
4		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	58
5		2-Octanone	128	C8H16O	000111-13-7	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006818.D
Acq On : 26 Dec 2018 15:09
Operator : JC/MD
Sample : J6575-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS-122618-A

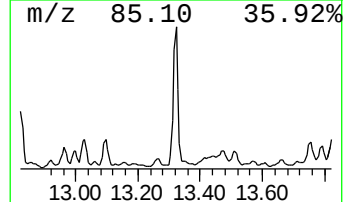
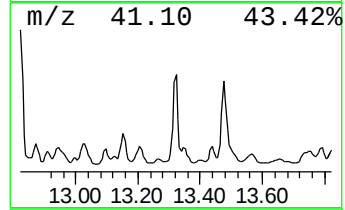
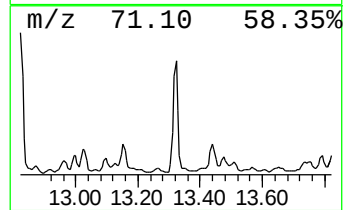
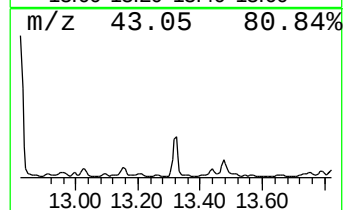
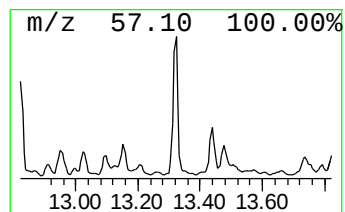
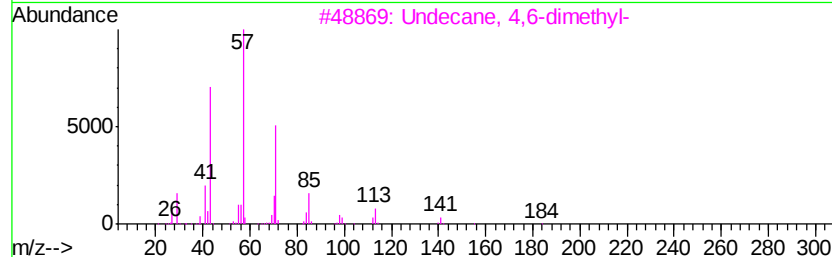
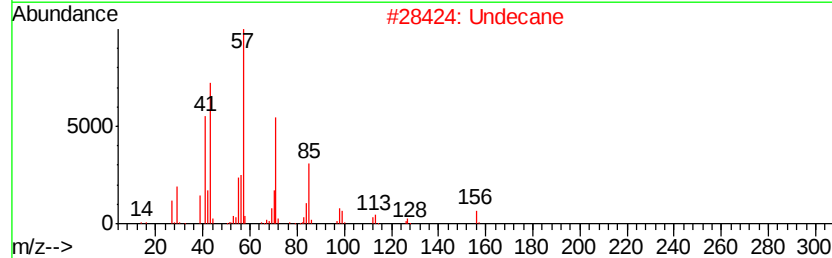
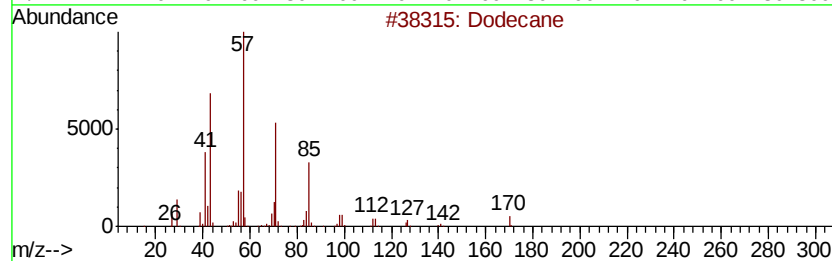
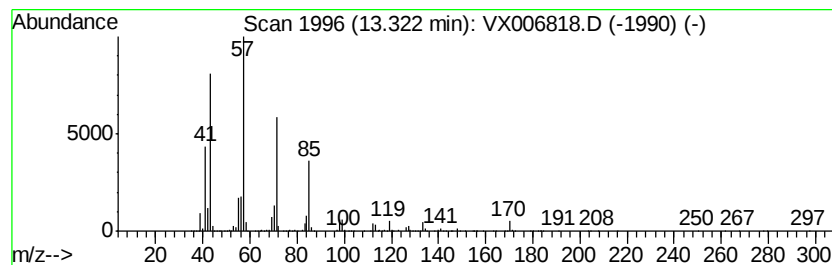
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	67.26 ug/l	4797690	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane	170	C12H26	000112-40-3	96
2		Undecane	156	C11H24	001120-21-4	87
3		Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	83
4		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	83
5		Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006818.D
Acq On : 26 Dec 2018 15:09
Operator : JC/MD
Sample : J6575-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
SS-122618-A

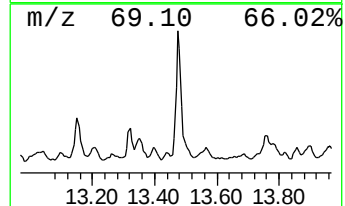
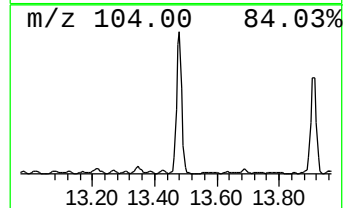
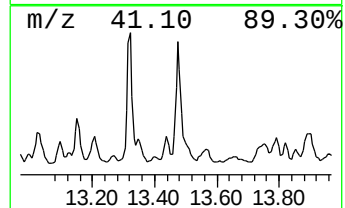
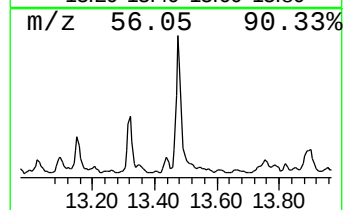
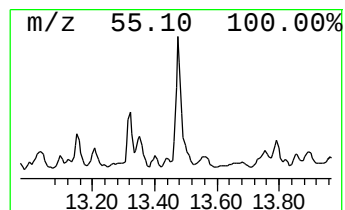
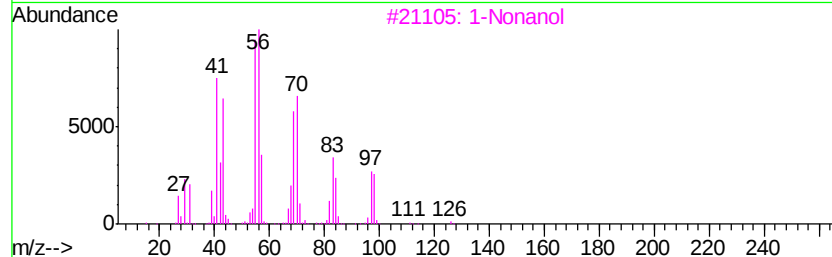
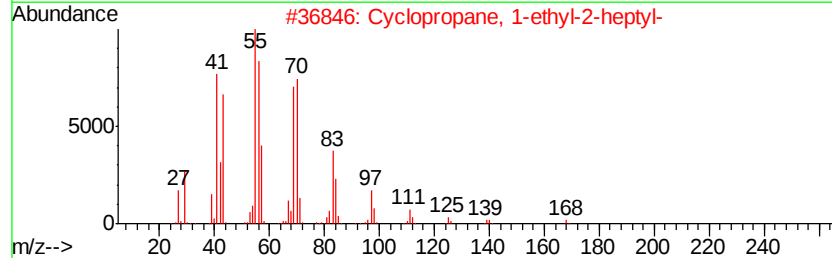
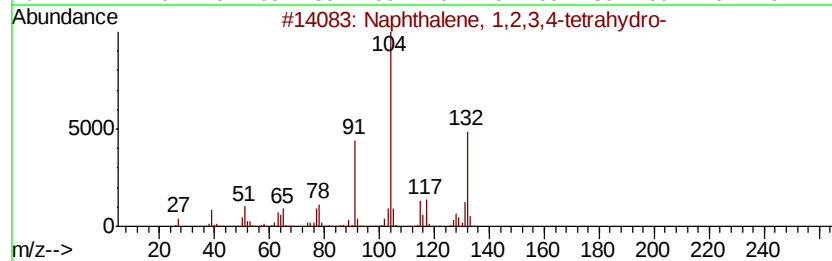
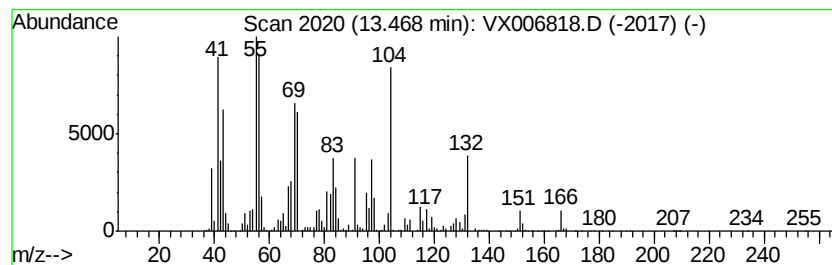
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	96.31 ug/l	6870010	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	55
2		Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	55
3		1-Nonanol	144	C9H20O	000143-08-8	53
4		Cycloheptane	98	C7H14	000291-64-5	50
5		Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122618\
Data File : VX006818.D
Acq On : 26 Dec 2018 15:09
Operator : JC/MD
Sample : J6575-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

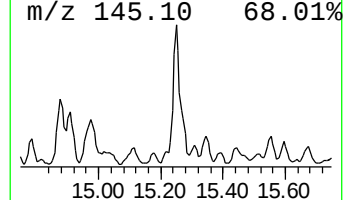
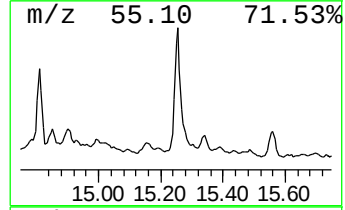
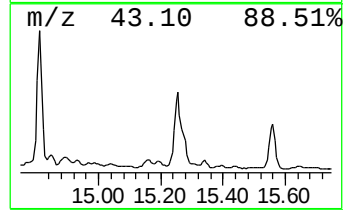
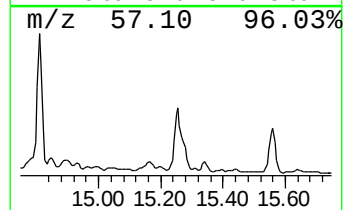
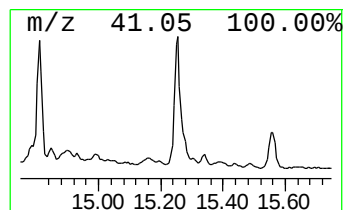
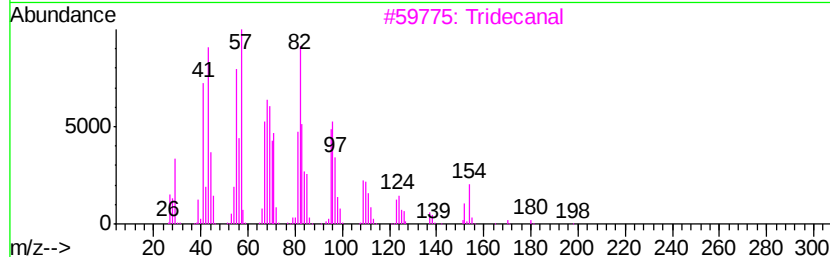
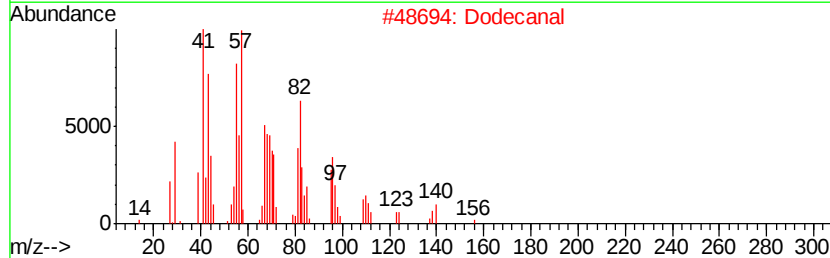
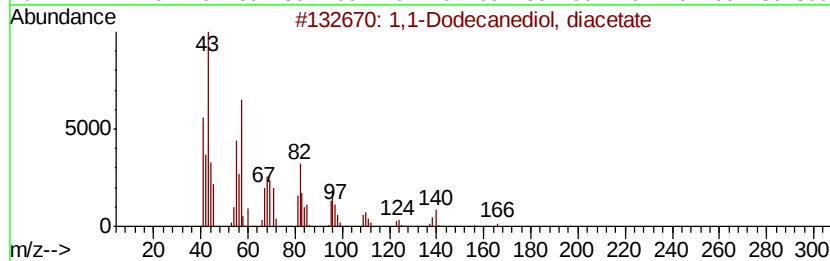
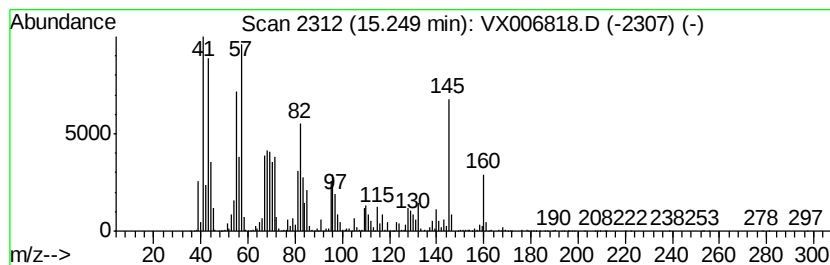
Instrument :
MSVOA_X
ClientSampleId :
SS-122618-A

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 10 1,1-Dodecanediol, diacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	73.65 ug/l	5253640	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,1-Dodecanediol, diacetate	286 C16H30O4	056438-07-4	81
2	Dodecanal	184 C12H24O	000112-54-9	76
3	Tridecanal	198 C13H26O	010486-19-8	76
4	Tetradecanal	212 C14H28O	000124-25-4	76
5	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	60



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX122618\
Data File : VX006818.D
Acq On : 26 Dec 2018 15:09
Operator : JC/MD
Sample : J6575-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS-122618-A

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.14	557.1	ug/l	26177000	1	5.66	2349530	50.0
1,3-Dioxolane, 2-...	5.95	126.4	ug/l	5941320	1	5.66	2349530	50.0
2-Butenal	6.73	76.0	ug/l	7808350	2	6.86	5135150	50.0
2-Heptanone	10.83	689.6	ug/l	46040800	3	10.11	3337980	50.0
2-Octanone	11.89	111.8	ug/l	7978160	4	12.08	3566600	50.0
2-Nonanone	12.82	139.3	ug/l	9936810	4	12.08	3566600	50.0
Dodecane	13.32	67.3	ug/l	4797690	4	12.08	3566600	50.0
Naphthalene, 1,2,...	13.47	96.3	ug/l	6870010	4	12.08	3566600	50.0
1,1-Dodecanediol,...	15.25	73.7	ug/l	5253640	4	12.08	3566600	50.0