LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

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\82X082218W.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	1.075	75	80	90	rBV	1430244	1894146	43.03%	5.200%
2	1.319	113	120	146	rBV	209321	1316528	29.91%	3.614%
3	2.446	299	305	319	rBV	64032	124035	2.82%	0.341%
4	2.617	328	333	342	rBV2	37983	83580	1.90%	0.229%
5	4.349	606	617	633	rBV	143403	390794	8.88%	1.073%
6	5.501	793	806	821	rBV	208415	593826	13.49%	1.630%
7	5.665	821	833	851	rVB	286219	812489	18.46%	2.231%
8	6.068	888	899	908	rBV	223485	573227	13.02%	1.574%
9	6.860	1019	1029	1045	rBV	451051	1053168	23.93%	2.891%
10	7.330	1099	1106	1118	rBV	22960	56367	1.28%	0.155%
11	8.714	1327	1333	1340	rBV	1088735	1698816	38.60%	4.664%
12	8.787	1340	1345	1353	rVB	88871	136210	3.09%	0.374%
13	10.116	1556	1563	1569	rBV	916443	1203908	27.35%	3.305%
14	10.256	1580	1586	1591	rBV	38324	51630	1.17%	0.142%
15	10.360	1597	1603	1610	rBV	104171	146714	3.33%	0.403%
16	10.445	1610	1617	1626	rBV	33404	49954	1.13%	0.137%
17	10.567	1632	1637	1648	rBV	305074	393535	8.94%	1.080%
18	10.701	1654	1659	1663	rBV	90125	120990	2.75%	0.332%
19	10.744	1663	1666	1672	rVB	35900	45179	1.03%	0.124%
20	10.811	1672	1677	1685	rBV2	114554	235488	5.35%	0.646%
21	11.140	1725	1731	1735	rBV	990821	1223690	27.80%	3.359%
22	11.189	1735	1739	1754	rVB	1288099	1533731	34.85%	4.211%
23	11.360	1759	1767	1773	rVB2	33298	50915	1.16%	0.140%
24	11.433	1773	1779	1784	rBV	110722	196974	4.48%	0.541%
25	11.475	1784	1786	1789	rVB	45627	47531	1.08%	0.130%
26	11.536	1794	1796	1805	rVB	48874	60187	1.37%	0.165%
27	11.628	1805	1811	1814	rBV	397654	489157	11.11%	1.343%
28	11.664	1814	1817	1826	rVB2	189809	263159	5.98%	0.722%
29	11.811	1835	1841	1846	rVB	209854	267995	6.09%	0.736%
30	11.884	1848	1853	1860	rBV	860094	1053190	23.93%	2.891%
31	12.030	1870	1877	1880	rVV3	130850	207044	4.70%	0.568%
32	12.079	1880	1885	1891	rVV	1238581	1544133	35.08%	4.239%
33	12.146	1891	1896	1902	rVB	138753	171999	3.91%	0.472%
34	12.213	1903	1907	1912	rBV2	60969	80041	1.82%	0.220%

LSC Area Percent Report

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Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

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\82X082218W.M
Title : SW846 8260

35	12.274	1912	1917	1929	rBV	3517201	4401513	100.00%	12.083%
36	12.372	1929	1933	1944	rVB3	129206	234864	5.34%	0.645%
37	12.518	1953	1957	1963	rVB	58372	78188	1.78%	0.215%
38	12.609	1963	1972	1978	rBV2	399450	808678	18.37%	2.220%
39	12.670	1978	1982	1985	rVB	96992	109591	2.49%	0.301%
40	12.756	1993	1996	2004	rVB3	92671	167772	3.81%	0.461%
41	12.902	2016	2020	2024	rVB2	46848	61749	1.40%	0.170%
42	12.981	2024	2033	2036	rBV	66477	110115	2.50%	0.302%
43	13.018	2036	2039	2046	rVB	522726	644590	14.64%	1.770%
44	13.170	2059	2064	2069	rBV3	122562	204617	4.65%	0.562%
45	13.225	2069	2073	2077	rVV2	222766	324047	7.36%	0.890%
46	13.262	2077	2079	2083	rVB4	38113	50738	1.15%	0.139%
47	13.353	2089	2094	2098	rVB2	351751	478689	10.88%	1.314%
48	13.481	2110	2115	2120	rVB	322574	389843	8.86%	1.070%
49	13.603	2131	2135	2138	rVV	58301	83827	1.90%	0.230%
50	13.640	2138	2141	2146	rVV3	85651	151629	3.44%	0.416%
51	13.707	2147	2152	2156	rVV2	447917	708556	16.10%	1.945%
52	13.743	2156	2158	2168	rVV3	377711	582539	13.23%	1.599%
53	13.914	2182	2186	2191	rVB	208333	266867	6.06%	0.733%
54	13.987	2192	2198	2201	rBV2	147898	231006	5.25%	0.634%
55	14.036	2201	2206	2219	rVV	1730202	2727654	61.97%	7.488%
56	14.133	2219	2222	2226	rVV	114439	148990	3.38%	0.409%
57	14.194	2226	2232	2235	rVV2	291721	406551	9.24%	1.116%
58	14.231	2235	2238	2242	rVV	1105130	1267748	28.80%	3.480%
59	14.292	2242	2248	2251	rVV	352401	657571	14.94%	1.805%
60	14.328	2251	2254	2259	rVV2	333738	442232	10.05%	1.214%
61	14.377	2259	2262	2268	rVV2	56468	103950	2.36%	0.285%
62	14.432	2268	2271	2275	rVV2	179490	216528	4.92%	0.594%
63	14.487	2275	2280	2284	rVV2	197977	259599	5.90%	0.713%
64	14.542	2284	2289	2294	rVB2	265800	338975	7.70%	0.931%
65	14.676	2306	2311	2313	rBV2	144237	242191	5.50%	0.665%
66	14.694	2313	2314	2318	rVV	122716	125075	2.84%	0.343%
67	14.731	2318	2320	2324	rVB2	67739	76113	1.73%	0.209%
68	14.786	2324	2329	2334	rBV2	181255	276495	6.28%	0.759%
69	14.841	2334	2338	2339	rBV	76061	83307	1.89%	0.229%
70	14.859	2339	2341	2347	rVB3	94071	152642	3.47%	0.419%
71	14.963	2355	2358	2364	rVB2	37998	64900	1.47%	0.178%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
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Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

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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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Title : SW846 8260

72	15.249	2401	2405	2413	rVB	97016	168105	3.82%	0.461%
73	15.444	2434	2437	2446	rVB3	33914	70516	1.60%	0.194%
74	15.554	2450	2455	2459	rBV3	52912	82906	1.88%	0.228%
75	15.688	2472	2477	2481	rBV	48836	82850	1.88%	0.227%
76	15.725	2481	2483	2491	rVB	33780	55302	1.26%	0.152%
77	16.627	2625	2631	2640	rBV	56245	115890	2.63%	0.318%

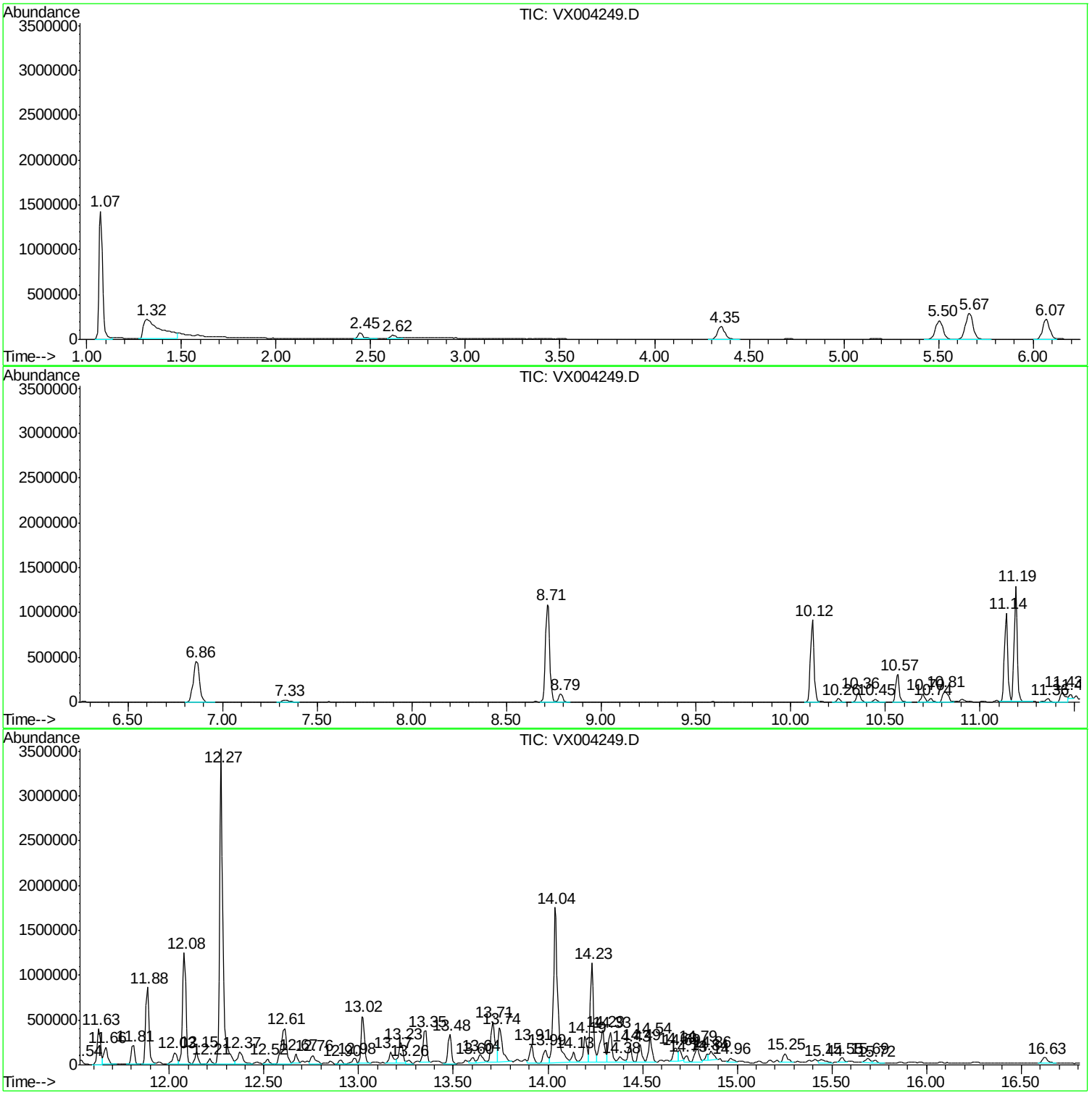
Sum of corrected areas: 36425838

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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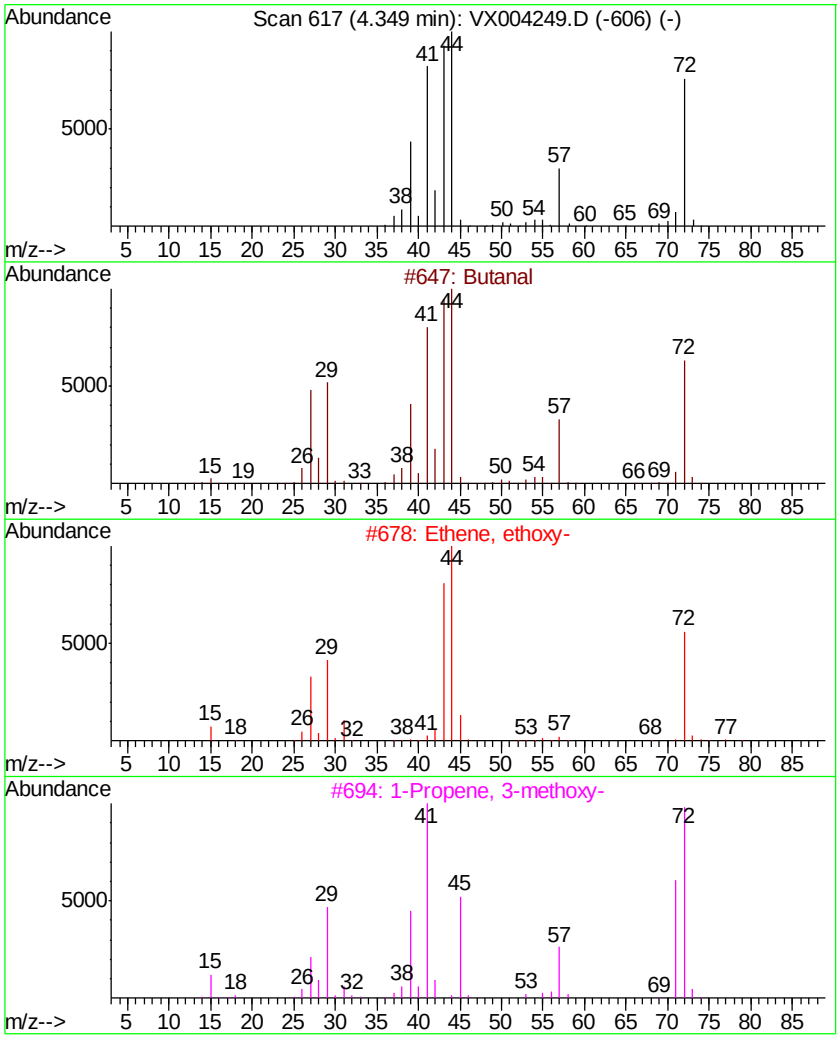
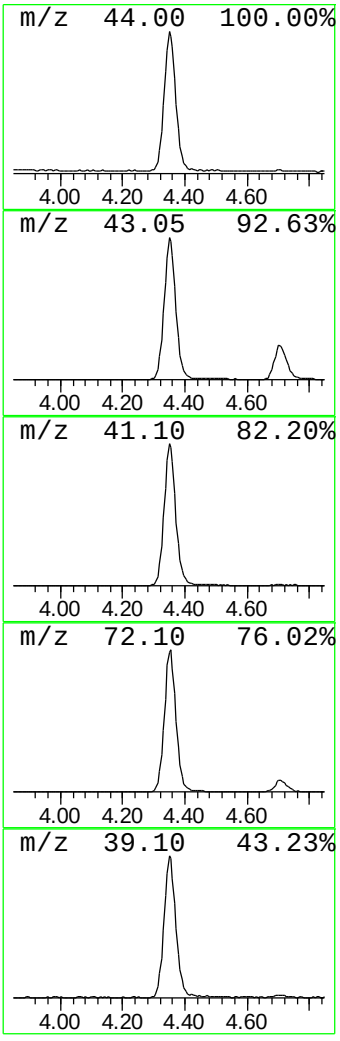
Peak Number 2 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	24.05 ug/l	390794	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

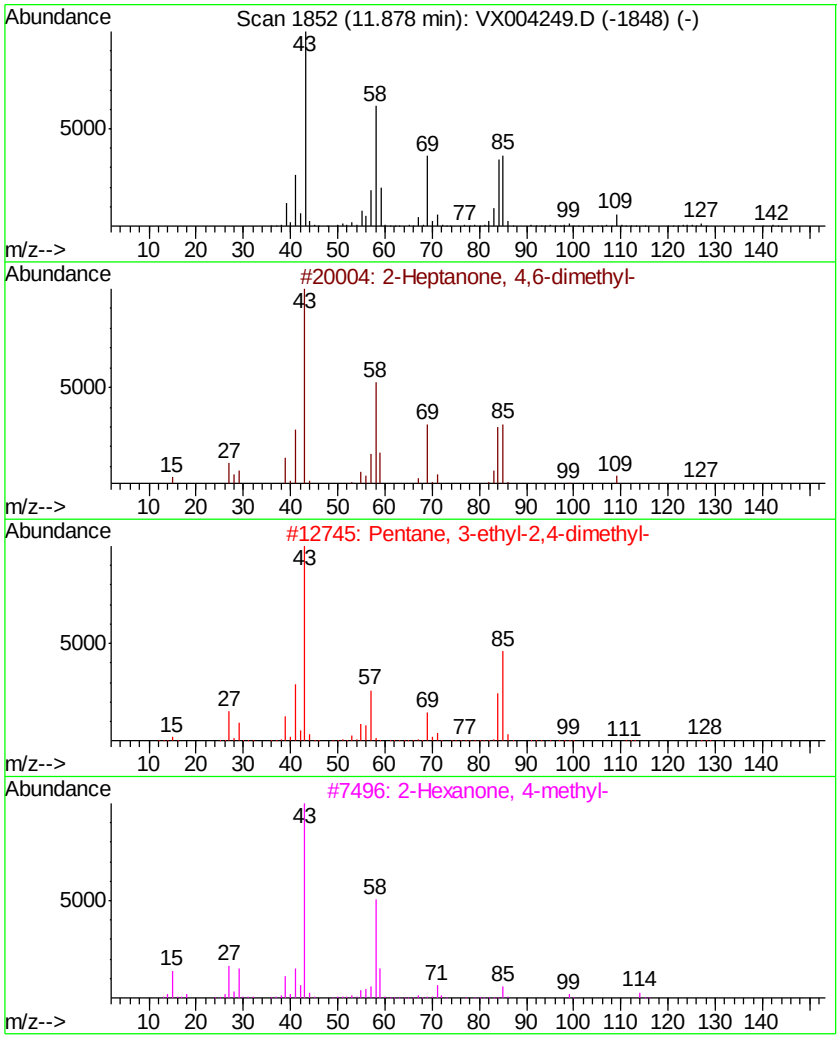
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

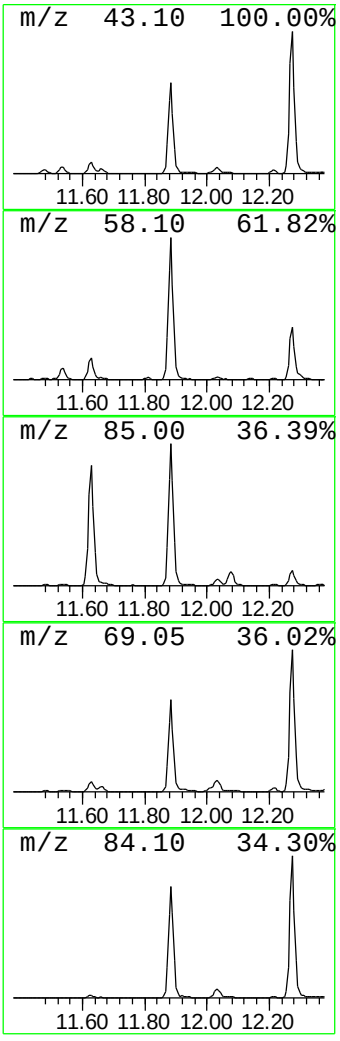
****

Peak Number 3 2-Heptanone, 4,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	34.10 ug/l	1053190	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	38
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	38
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	38
5	Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

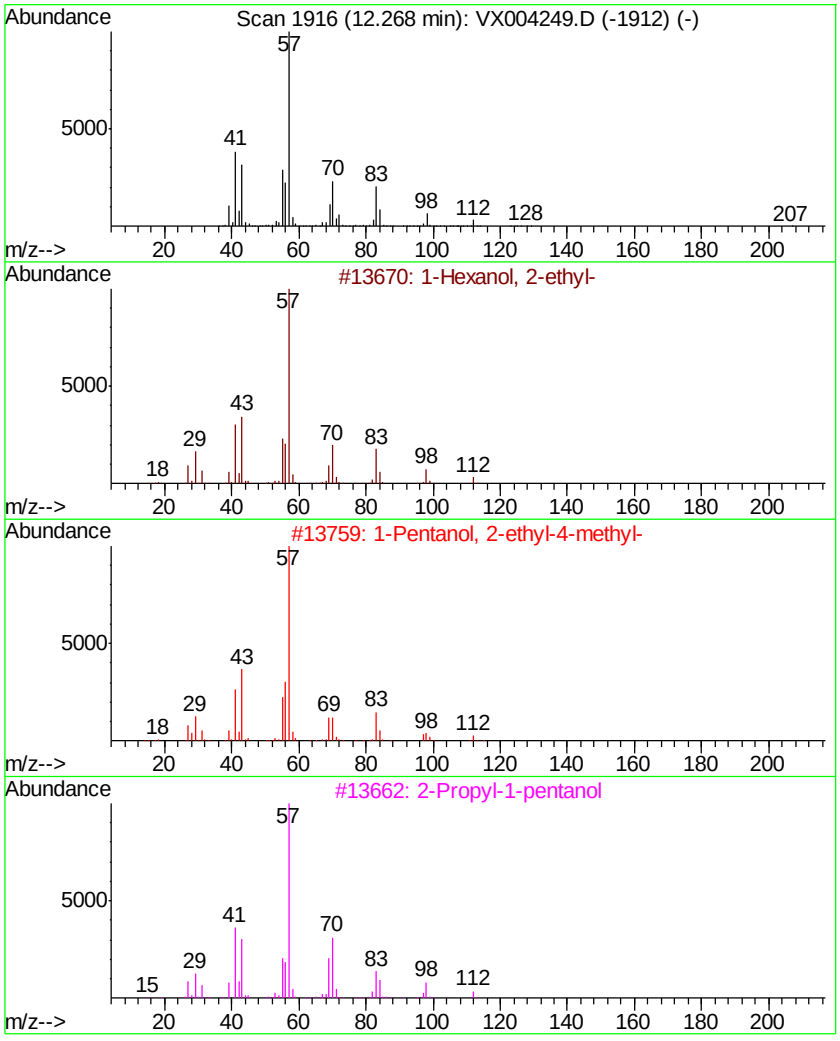
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

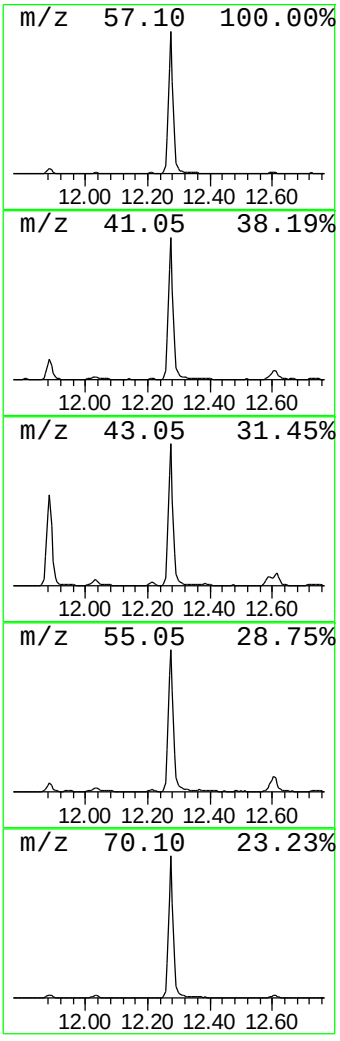
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	142.52 ug/l	4401510	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

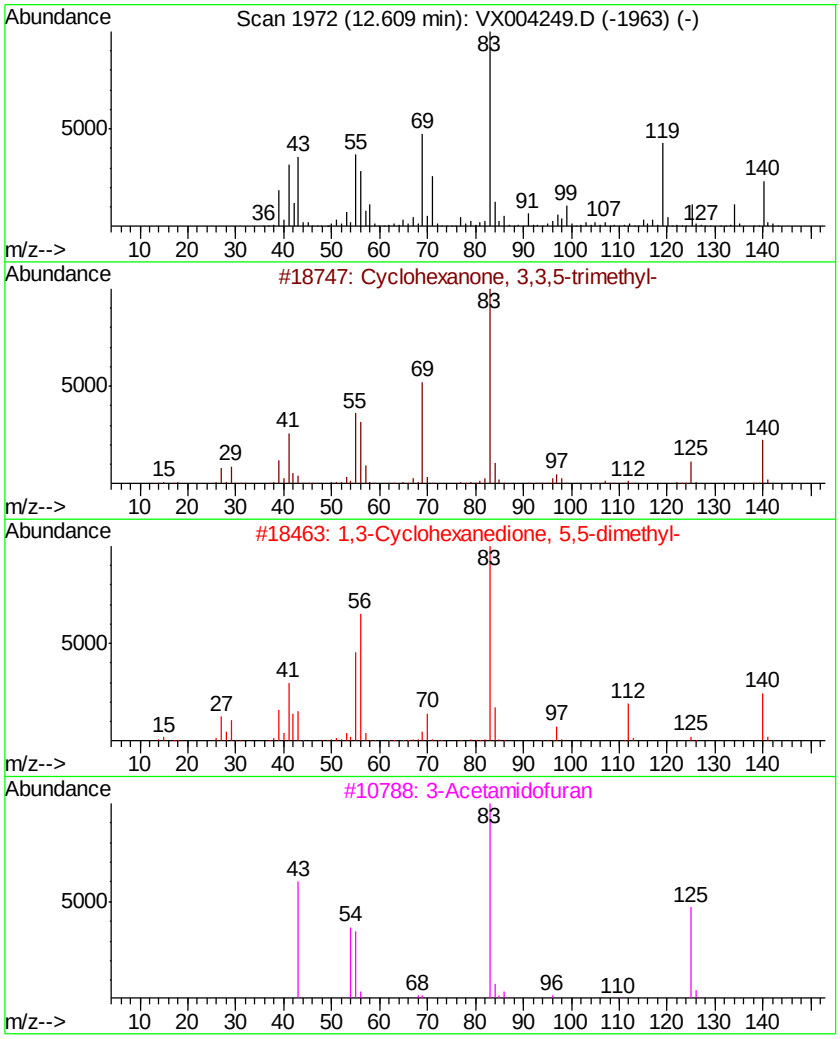
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

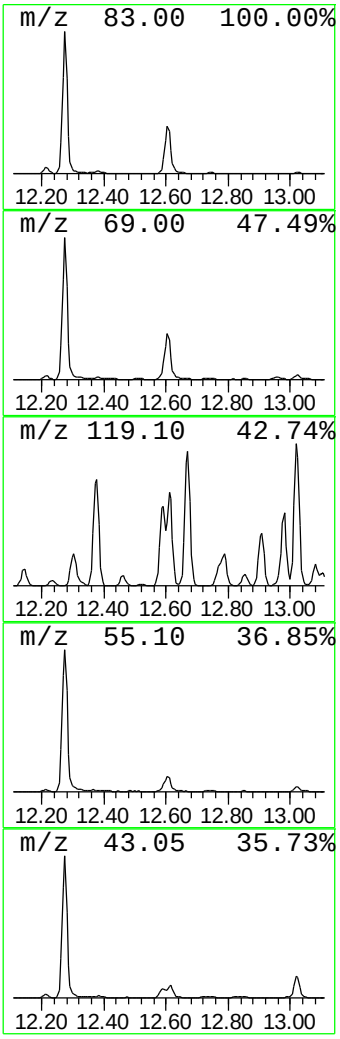
****

Peak Number 5 Cyclohexanone, 3,3,5-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	26.19 ug/l	808678	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
2	1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	43
3	3-Acetamidofuran	125	C6H7NO2	059445-85-1	38
4	2,4,6-Trimethyl-3-heptene	140	C10H20	1000113-56-9	38
5	1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
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Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

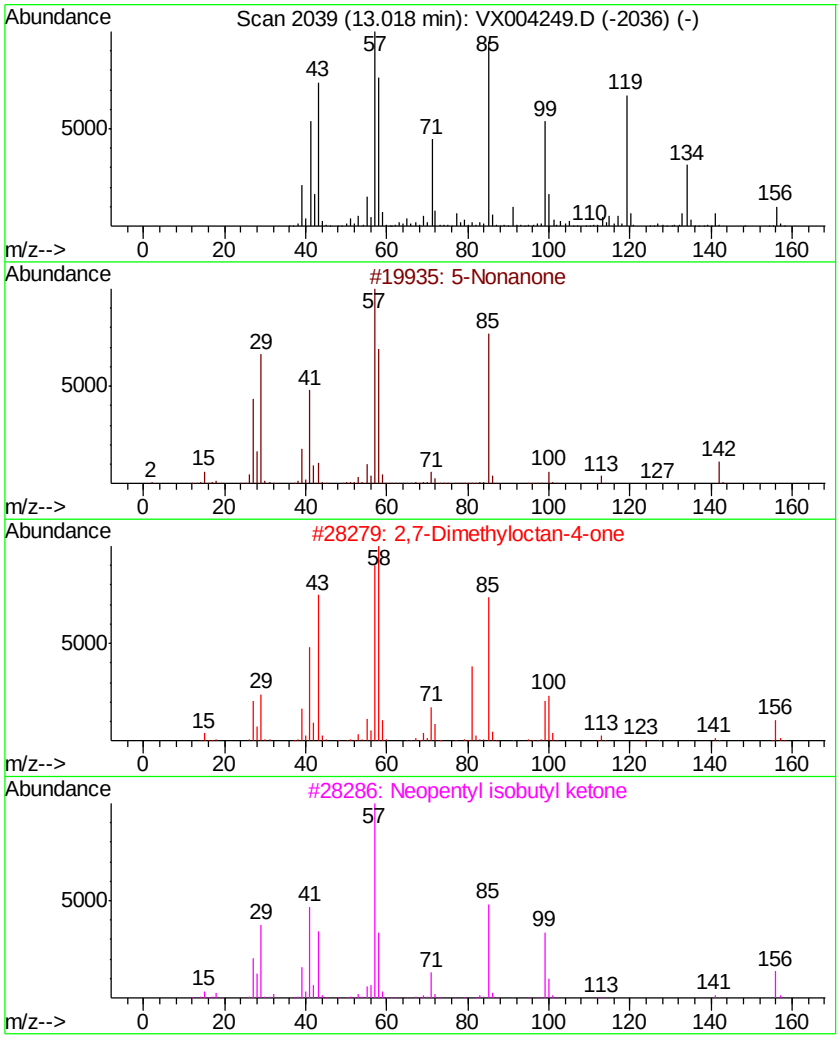
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

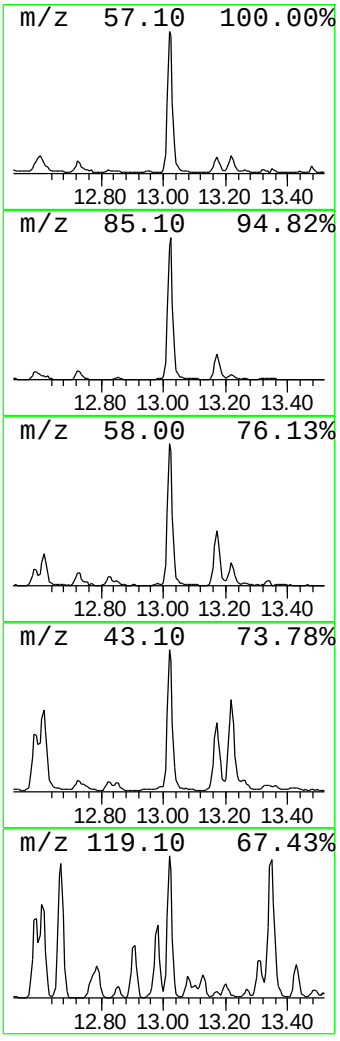
****

Peak Number 6 unknown13.02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	20.87 ug/l	644590	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nonanone	142	C9H18O	000502-56-7	43
2	2,7-Dimethyloctan-4-one	156	C10H20O	059387-92-7	43
3	Neopentyl isobutyl ketone	156	C10H20O	040239-19-8	43
4	Thiazole	85	C3H3NS	000288-47-1	38
5	1-t-Butyl-2-hexanone	156	C10H20O	022319-52-4	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

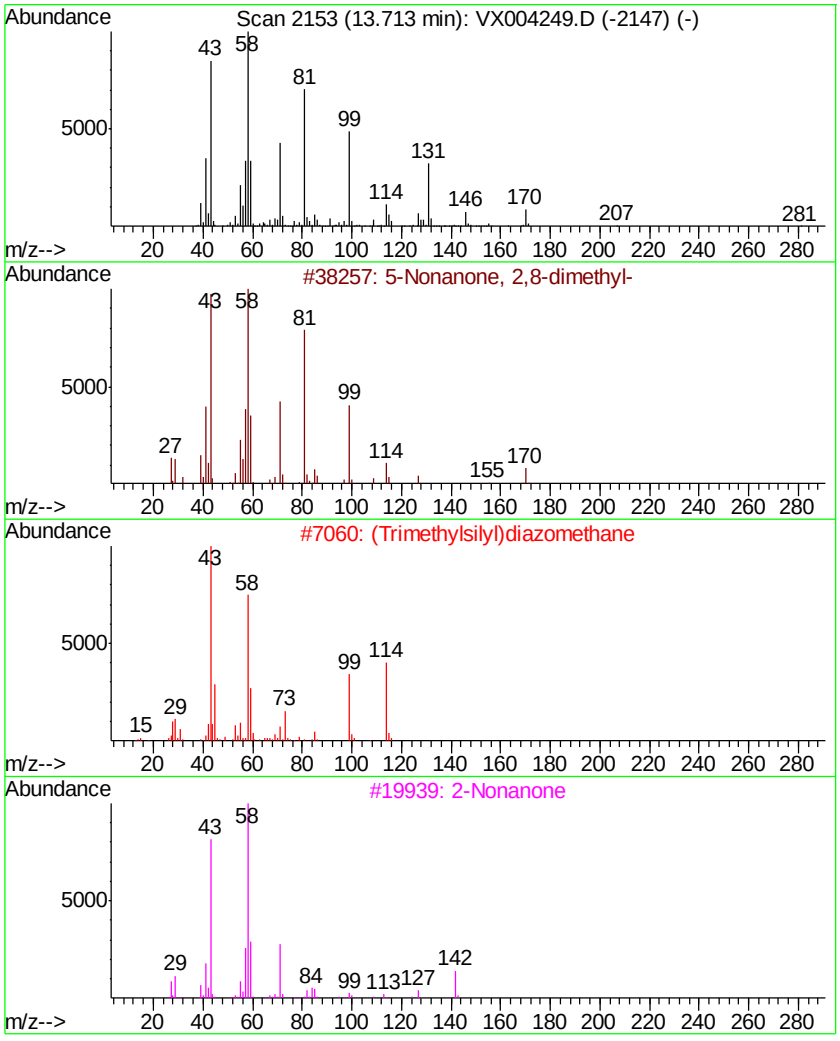
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

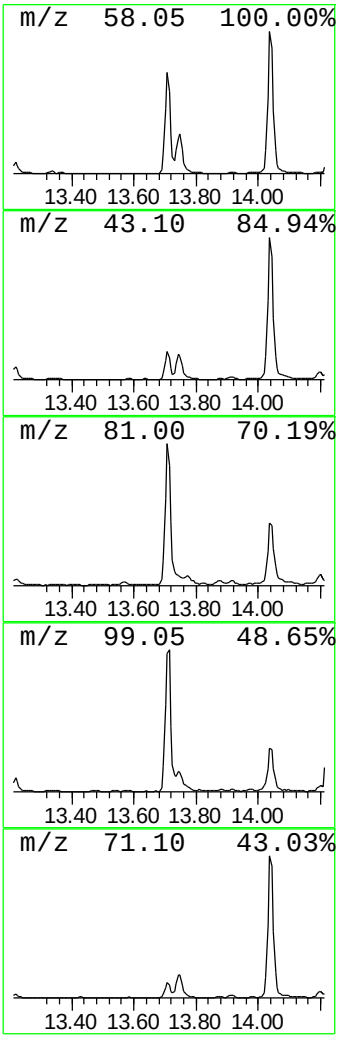
****

Peak Number 7 5-Nonanone, 2,8-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	22.94 ug/l	708556	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nonanone, 2,8-dimethyl-	170	C11H22O	002050-99-9	92
2	(Trimethylsilyl)diazomethane	114	C4H10N2Si	018107-18-1	53
3	2-Nonanone	142	C9H18O	000821-55-6	50
4	2-Undecanone	170	C11H22O	000112-12-9	50
5	2-Methoxyethyl 2-ethylhexanoate	202	C11H22O3	205983-99-9	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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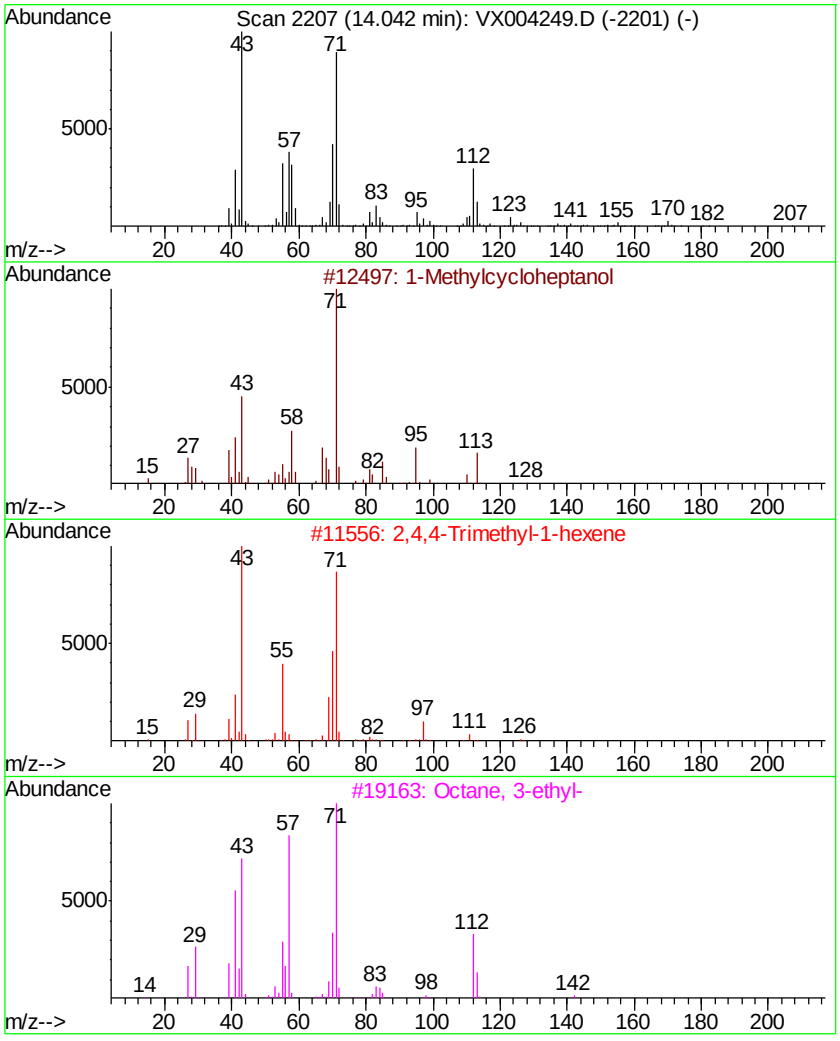
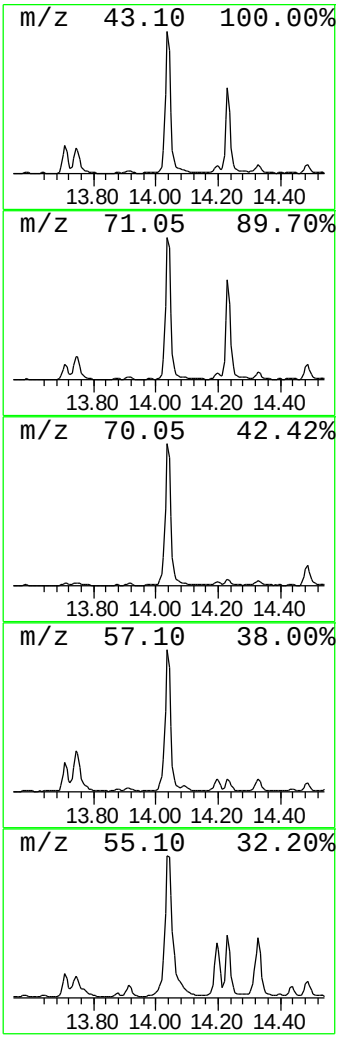
Peak Number 8 1-Methylcycloheptanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	88.32 ug/l	2727650	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylcycloheptanol	128	C8H16O	003761-94-2	50
2	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	47
3	Octane, 3-ethyl-	142	C10H22	005881-17-4	47
4	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	40
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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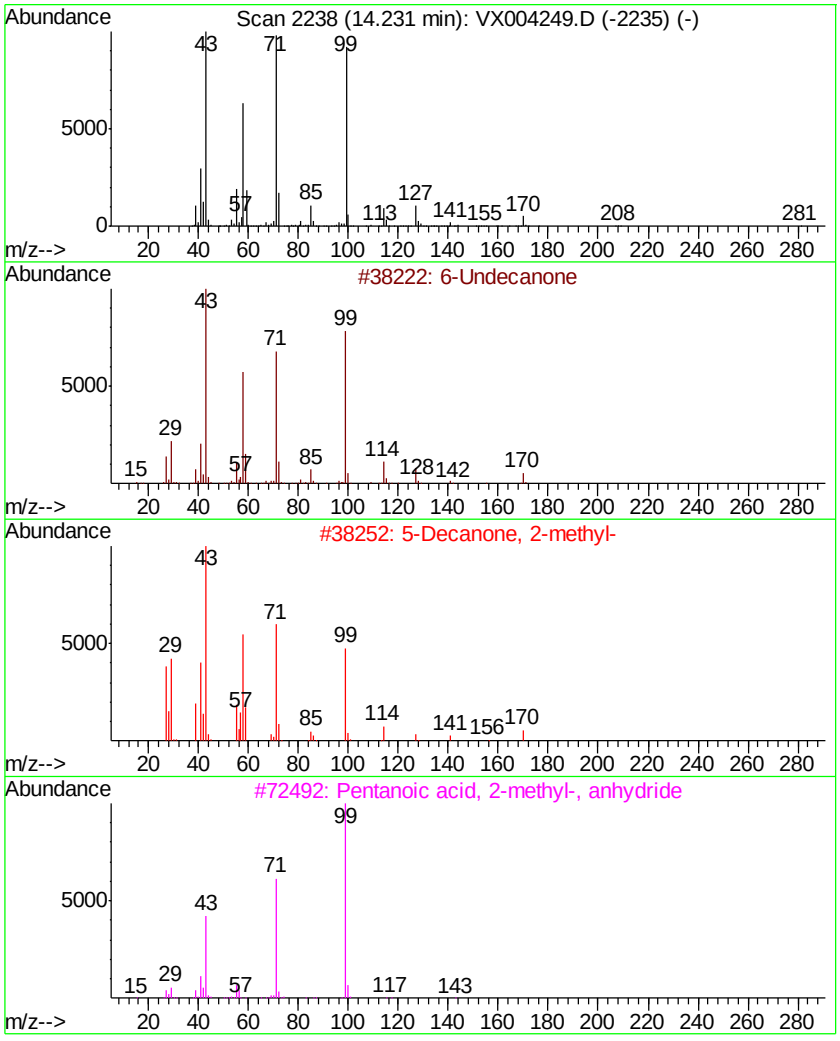
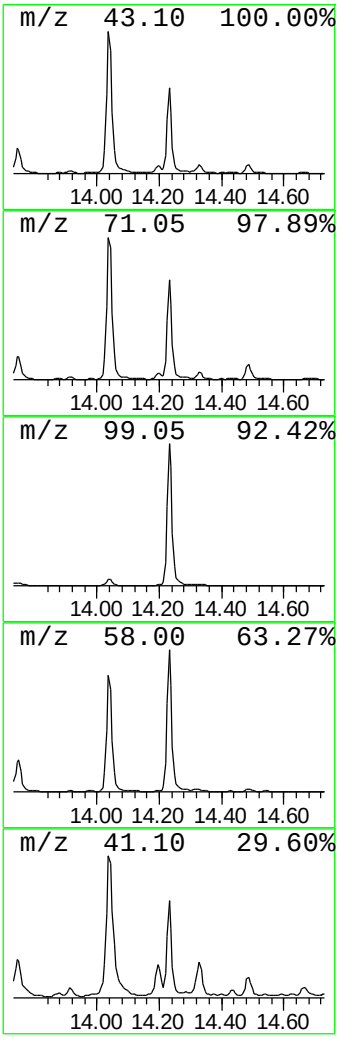
Peak Number 9 6-Undecanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	41.05 ug/l	1267750	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Undecanone	170	C11H22O	000927-49-1	93
2	5-Decanone, 2-methyl-	170	C11H22O	054410-89-8	91
3	Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	50
4	Hexanethioic acid, S-propyl ester	174	C9H18OS	002432-78-2	50
5	Cyclohexanol, 1-methyl-	114	C7H14O	000590-67-0	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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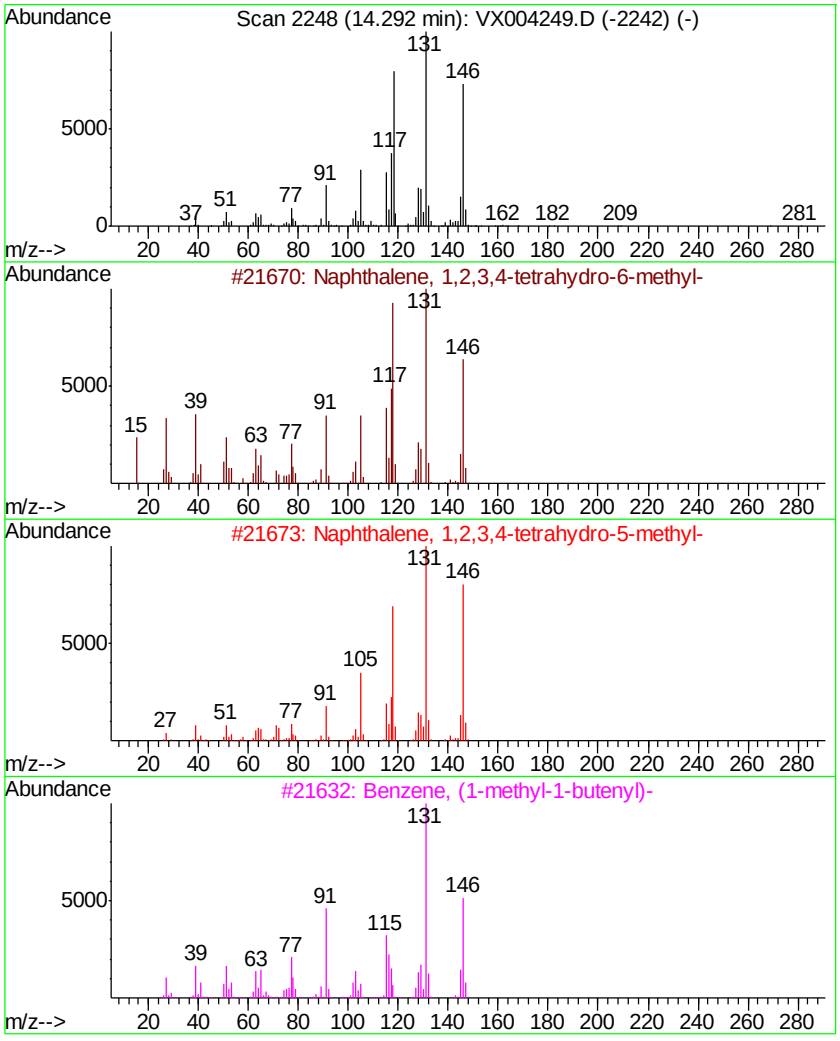
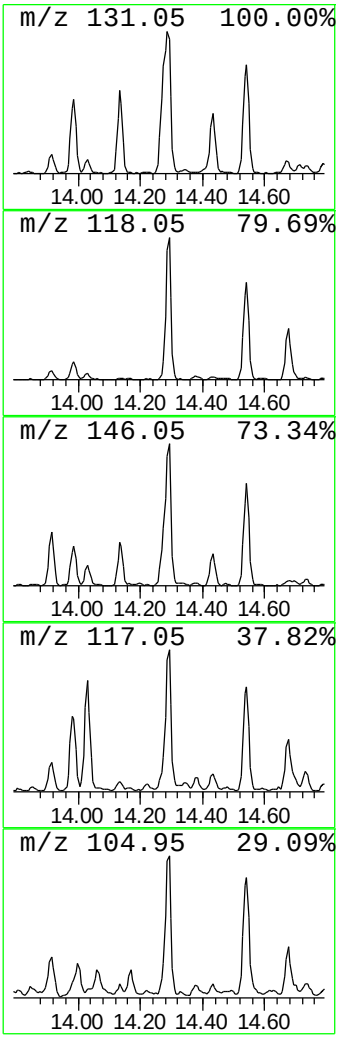
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	21.29 ug/l	657571	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	64
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
Data File : VX004249.D
Acq On : 24 Aug 2018 16:15
Operator : JC/MD
Sample : J4652-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SONO-W

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	4.35	24.1	ug/l	390794	1	5.67	812489	50.0
2-Heptanone, 4,6-...	11.88	34.1	ug/l	1053190	4	12.08	1544130	50.0
1-Hexanol, 2-ethyl-	12.27	142.5	ug/l	4401510	4	12.08	1544130	50.0
Cyclohexanone, 3,...	12.61	26.2	ug/l	808678	4	12.08	1544130	50.0
unknown13.02	13.02	20.9	ug/l	644590	4	12.08	1544130	50.0
5-Nonanone, 2,8-d...	13.71	22.9	ug/l	708556	4	12.08	1544130	50.0
1-Methylcyclohept...	14.04	88.3	ug/l	2727650	4	12.08	1544130	50.0
6-Undecanone	14.23	41.0	ug/l	1267750	4	12.08	1544130	50.0
Naphthalene, 1,2,...	14.29	21.3	ug/l	657571	4	12.08	1544130	50.0