

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041320\
 Data File : VX015650.D
 Acq On : 13 Apr 2020 18:19
 Operator : JC/SP
 Sample : L2239-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 Z5-S1GW-200407

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\82X032720W.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	1.064	20	29	43	rBV	3823696	4944662	91.67%	11.381%
2	2.332	232	237	242	rBV	42091	72137	1.34%	0.166%
3	2.417	245	251	261	rVB	77620	130007	2.41%	0.299%
4	4.643	608	616	629	rVB	133764	375191	6.96%	0.864%
5	5.100	684	691	698	rBV3	43079	119014	2.21%	0.274%
6	5.472	741	752	764	rBV	605146	1684756	31.23%	3.878%
7	5.636	768	779	793	rBV	1056440	2944661	54.59%	6.778%
8	6.033	836	844	858	rVB	668270	1755529	32.55%	4.041%
9	6.837	966	976	988	rBV	1609932	3868537	71.72%	8.904%
10	7.520	1082	1088	1096	rBV2	94645	194680	3.61%	0.448%
11	7.636	1101	1107	1114	rVV2	313969	610368	11.32%	1.405%
12	7.697	1114	1117	1126	rVB	28203	65437	1.21%	0.151%
13	8.697	1275	1281	1298	rBV	3388698	5364222	99.45%	12.347%
14	9.276	1369	1376	1389	rBV	244563	427610	7.93%	0.984%
15	9.563	1416	1423	1436	rBV	1988600	2720902	50.44%	6.263%
16	10.099	1505	1511	1522	rBV	3618346	4880180	90.47%	11.233%
17	10.617	1592	1596	1611	rBV	550993	839742	15.57%	1.933%
18	10.806	1621	1627	1631	rBV	248988	326800	6.06%	0.752%
19	10.843	1631	1633	1636	rVV	54918	61645	1.14%	0.142%
20	10.898	1638	1642	1650	rVB	70321	97975	1.82%	0.226%
21	11.068	1665	1670	1674	rBV	111648	149151	2.77%	0.343%
22	11.123	1674	1679	1686	rVV	3274794	4127781	76.52%	9.501%
23	11.629	1755	1762	1765	rBV	147963	190910	3.54%	0.439%
24	11.660	1765	1767	1770	rVV	87567	94128	1.75%	0.217%
25	11.696	1770	1773	1777	rVV	90424	123469	2.29%	0.284%
26	11.763	1777	1784	1787	rVV	208887	300981	5.58%	0.693%
27	11.800	1787	1790	1794	rVV	66232	86030	1.59%	0.198%
28	11.879	1797	1803	1809	rVB	202998	250522	4.64%	0.577%
29	12.062	1828	1833	1841	rVB	4379939	5394062	100.00%	12.416%
30	12.257	1860	1865	1878	rBV	553927	841430	15.60%	1.937%
31	12.629	1921	1926	1937	rBV2	239541	403189	7.47%	0.928%

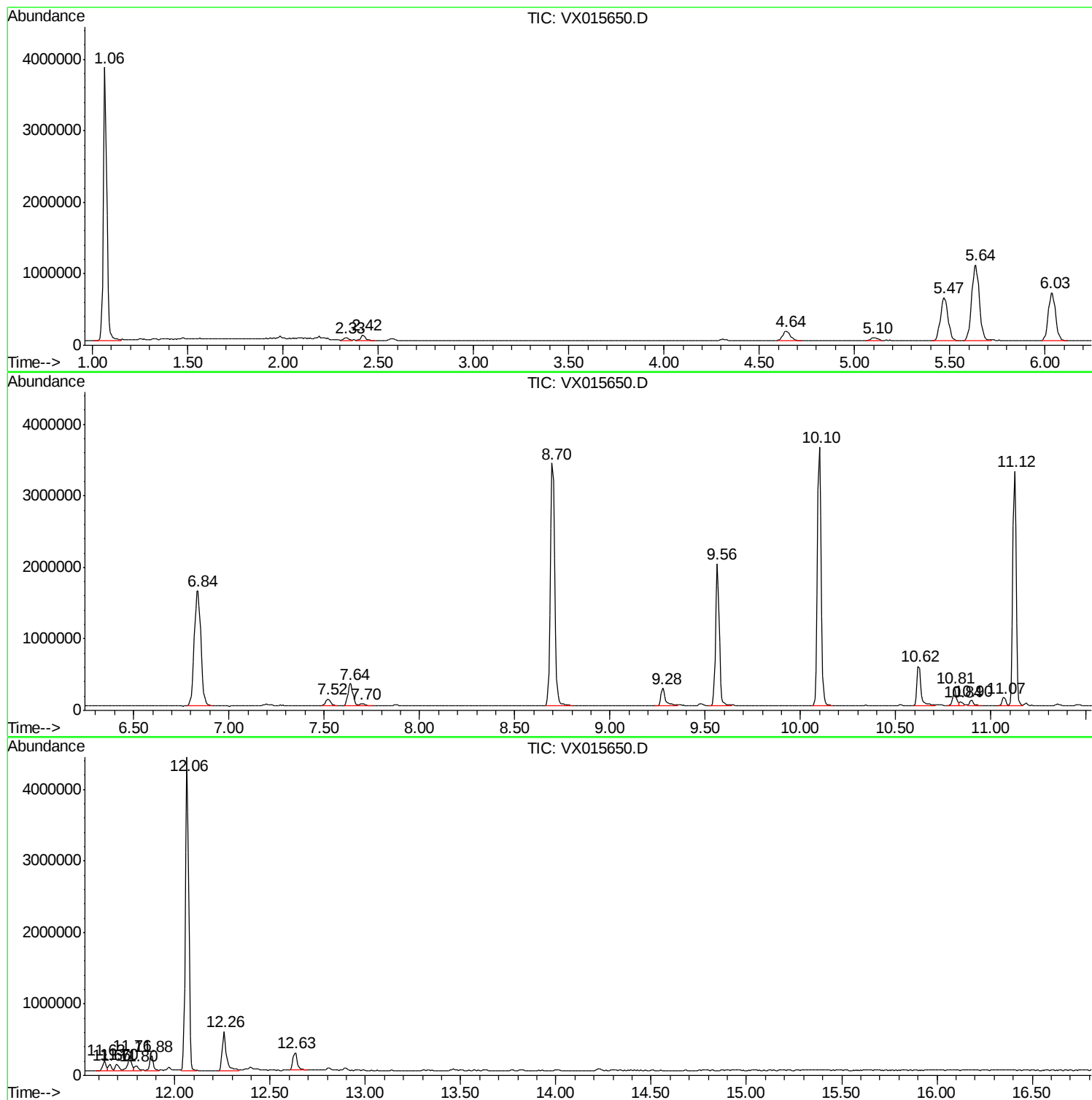
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ClientSampleId :
Z5-S1GW-200407

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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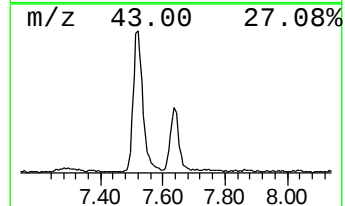
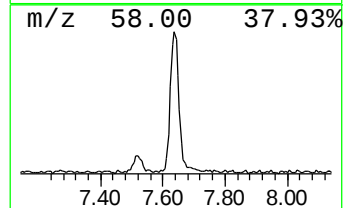
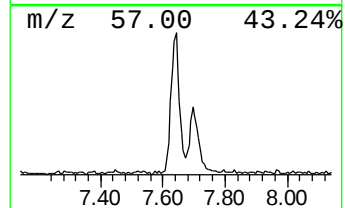
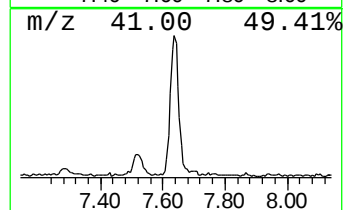
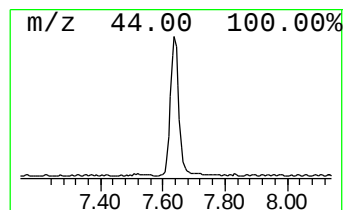
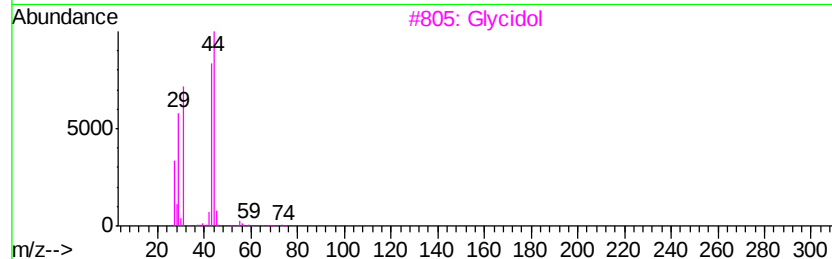
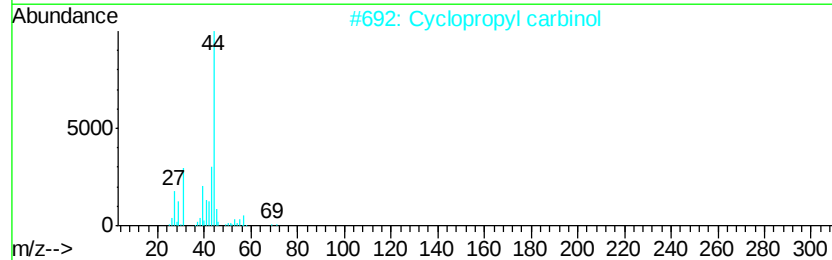
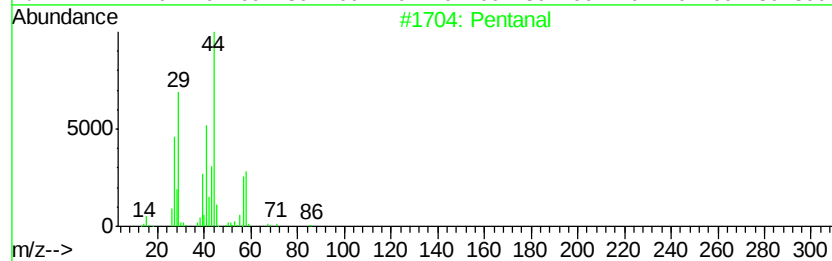
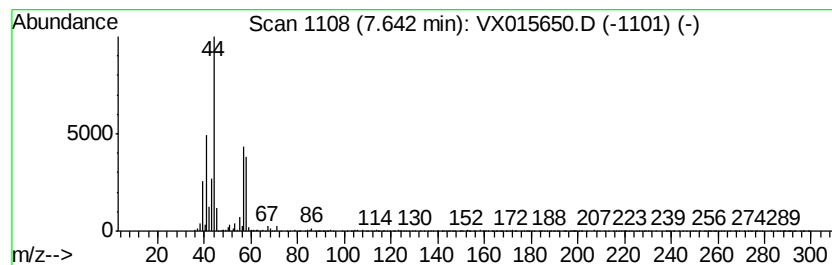
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
 Quant Title : SW846 8260

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

 Peak Number 2 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	7.89 ug/l	610368	1,4-Difluorobenzene	6.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal		86	C5H10O	000110-62-3	90
2	Cyclopropyl carbinol		72	C4H8O	002516-33-8	45
3	Glycidol		74	C3H6O2	000556-52-5	38
4	Butanal, 3-methyl-		86	C5H10O	000590-86-3	33
5	2-Heptanamine, 5-methyl-		129	C8H19N	053907-81-6	9



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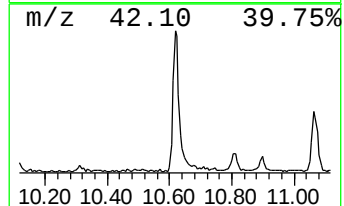
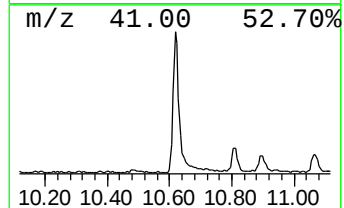
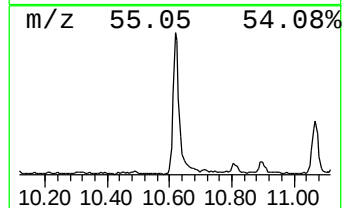
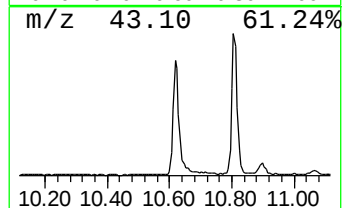
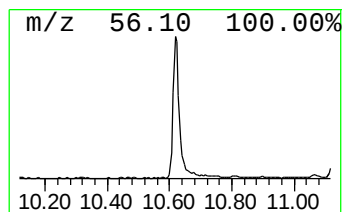
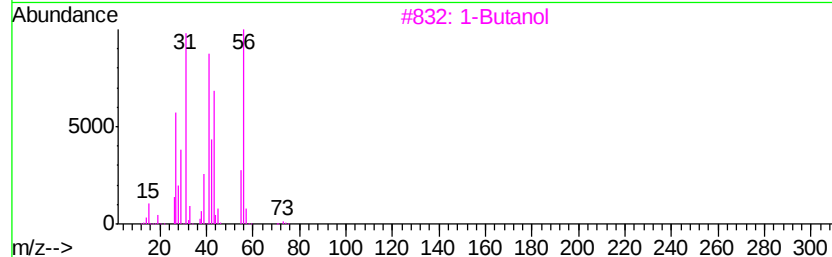
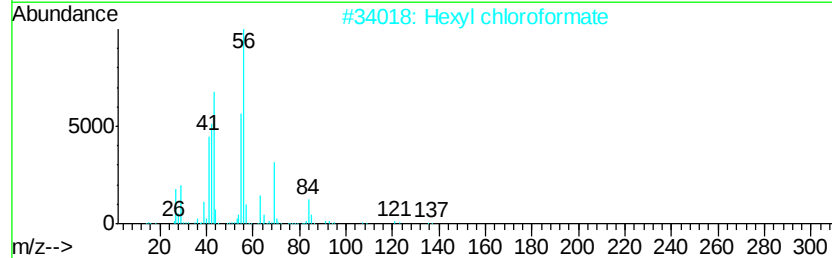
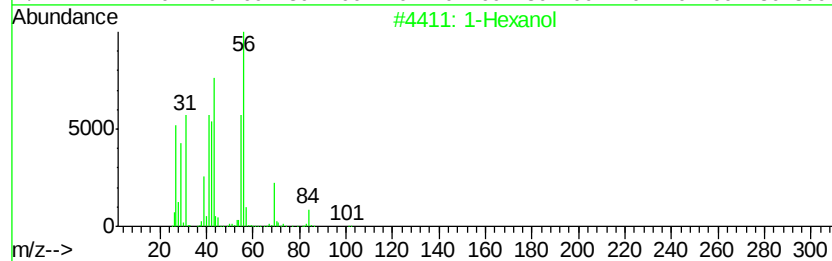
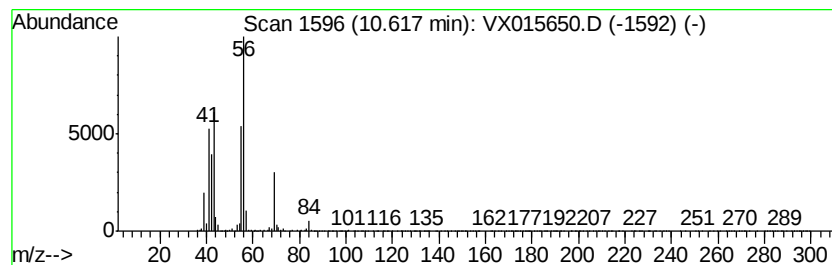
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Peak Number 3 1-Hexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.62	8.60 ug/l	839742	Chlorobenzene-d5	10.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	83
3	1-Butanol	74	C4H10O	000071-36-3	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	64



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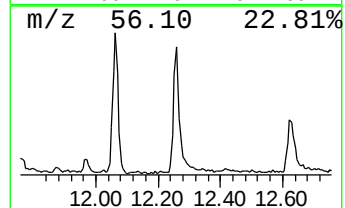
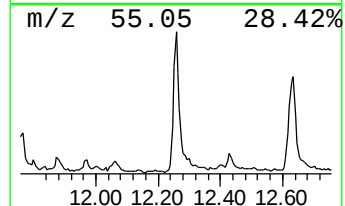
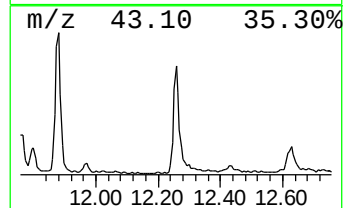
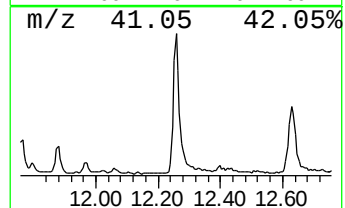
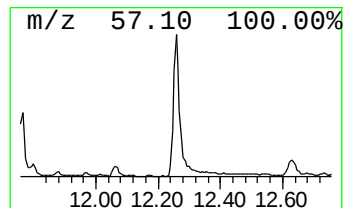
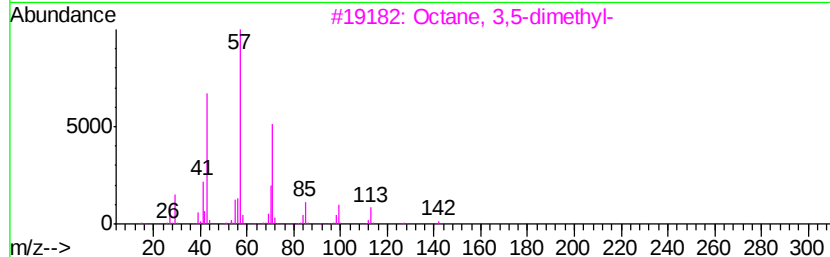
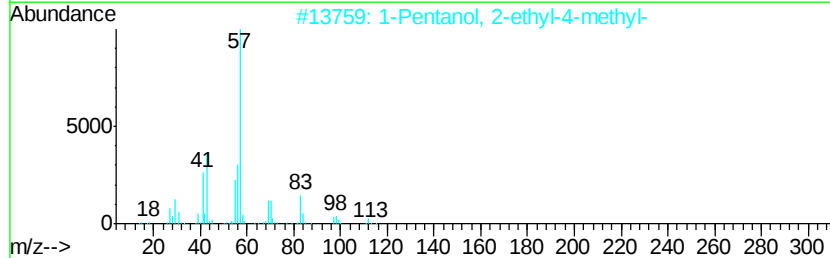
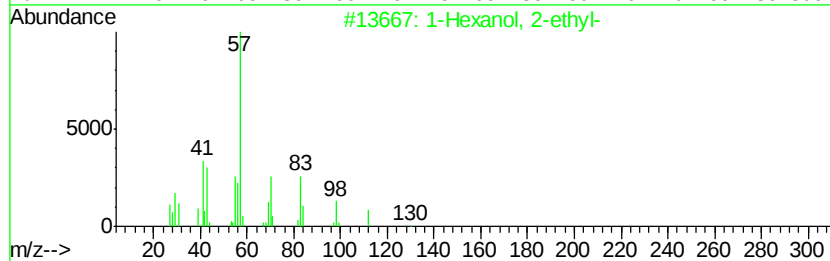
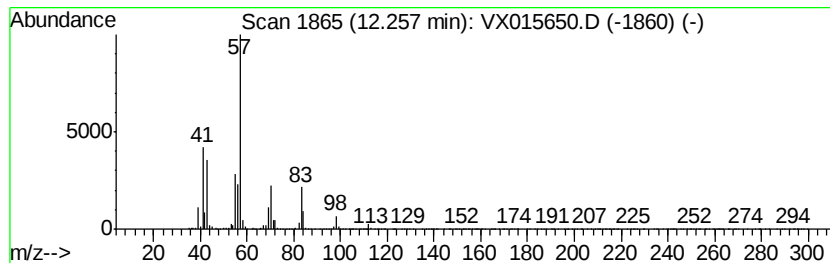
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	7.80 ug/l	841430	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5		Decanal	156	C10H20O	000112-31-2	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	7.64	7.9	ug/l	610368	2	6.84	3868540	50.0
1-Hexanol	10.62	8.6	ug/l	839742	3	10.10	4880180	50.0
1-Hexanol, 2-ethyl-	12.26	7.8	ug/l	841430	4	12.06	5394060	50.0