

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD012221\
 Data File : VD068152.D
 Acq On : 22 Jan 2021 13:43
 Operator : VA/SY
 Sample : M1189-05
 Misc : 3.81G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 41048

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_D\Method\82D011921S.M
 Title : SW846 8260

Signal : TIC: VD068152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.320	63	68	78	rBV	40516	74624	2.54%	0.404%
2	4.967	509	518	519	rBV3	15440	31210	1.06%	0.169%
3	7.920	1009	1020	1025	rBV	382719	930287	31.66%	5.042%
4	7.985	1025	1031	1040	rVB	710763	1584696	53.93%	8.588%
5	8.332	1080	1090	1101	rBV	373974	862040	29.34%	4.672%
6	8.867	1170	1181	1200	rBV	1075611	2170213	73.86%	11.761%
7	9.355	1259	1264	1271	rVB4	17263	34999	1.19%	0.190%
8	10.232	1407	1413	1423	rBV	28311	53306	1.81%	0.289%
9	10.344	1423	1432	1439	rVV	1630953	2938386	100.00%	15.924%
10	10.408	1441	1443	1455	rVV3	45073	85649	2.91%	0.464%
11	10.526	1455	1463	1469	rVB7	14296	30002	1.02%	0.163%
12	11.432	1609	1617	1627	rVV8	10187	33827	1.15%	0.183%
13	11.649	1645	1654	1665	rBV	1346254	2334605	79.45%	12.652%
14	11.744	1665	1670	1675	rBV	27646	46942	1.60%	0.254%
15	11.855	1682	1689	1699	rVB3	55290	118286	4.03%	0.641%
16	12.179	1731	1744	1752	rBV4	66606	159596	5.43%	0.865%
17	12.479	1788	1795	1801	rBV7	15730	33808	1.15%	0.183%
18	12.632	1814	1821	1831	rVB	952668	1604412	54.60%	8.695%
19	12.832	1847	1855	1860	rVB2	34119	67065	2.28%	0.363%
20	12.914	1860	1869	1873	rBV	213188	377584	12.85%	2.046%
21	13.055	1888	1893	1898	rBV	57385	90014	3.06%	0.488%
22	13.143	1900	1908	1913	rVV6	31969	60150	2.05%	0.326%
23	13.267	1924	1929	1934	rBV	35521	59793	2.03%	0.324%
24	13.326	1934	1939	1946	rVB	379614	590148	20.08%	3.198%
25	13.573	1975	1981	1991	rVV	929443	1610610	54.81%	8.728%
26	13.667	1991	1997	2007	rVB	1086721	1655763	56.35%	8.973%
27	13.767	2011	2014	2018	rBV3	31502	42831	1.46%	0.232%
28	13.814	2018	2022	2026	rVB3	31719	46752	1.59%	0.253%
29	13.896	2032	2036	2041	rVB2	46862	66128	2.25%	0.358%
30	14.032	2055	2059	2061	rBV	35165	43852	1.49%	0.238%
31	14.120	2068	2074	2078	rBV	80574	119556	4.07%	0.648%
32	14.220	2088	2091	2096	rVB6	23107	35847	1.22%	0.194%
33	14.285	2096	2102	2108	rBV10	16612	38378	1.31%	0.208%
34	14.361	2111	2115	2121	rBV6	20943	43717	1.49%	0.237%
35	14.443	2121	2129	2133	rVV6	38374	93160	3.17%	0.505%
36	14.479	2133	2135	2139	rVB	33065	39566	1.35%	0.214%

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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

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Title : SW846 8260

37	14.749	2178	2181	2187	rVV3	42444	61331	2.09%	0.332%
38	14.820	2188	2193	2197	rVV4	29000	62758	2.14%	0.340%
39	14.867	2198	2201	2209	rVB5	36832	70831	2.41%	0.384%
40	15.367	2279	2286	2290	rBV4	26659	49666	1.69%	0.269%

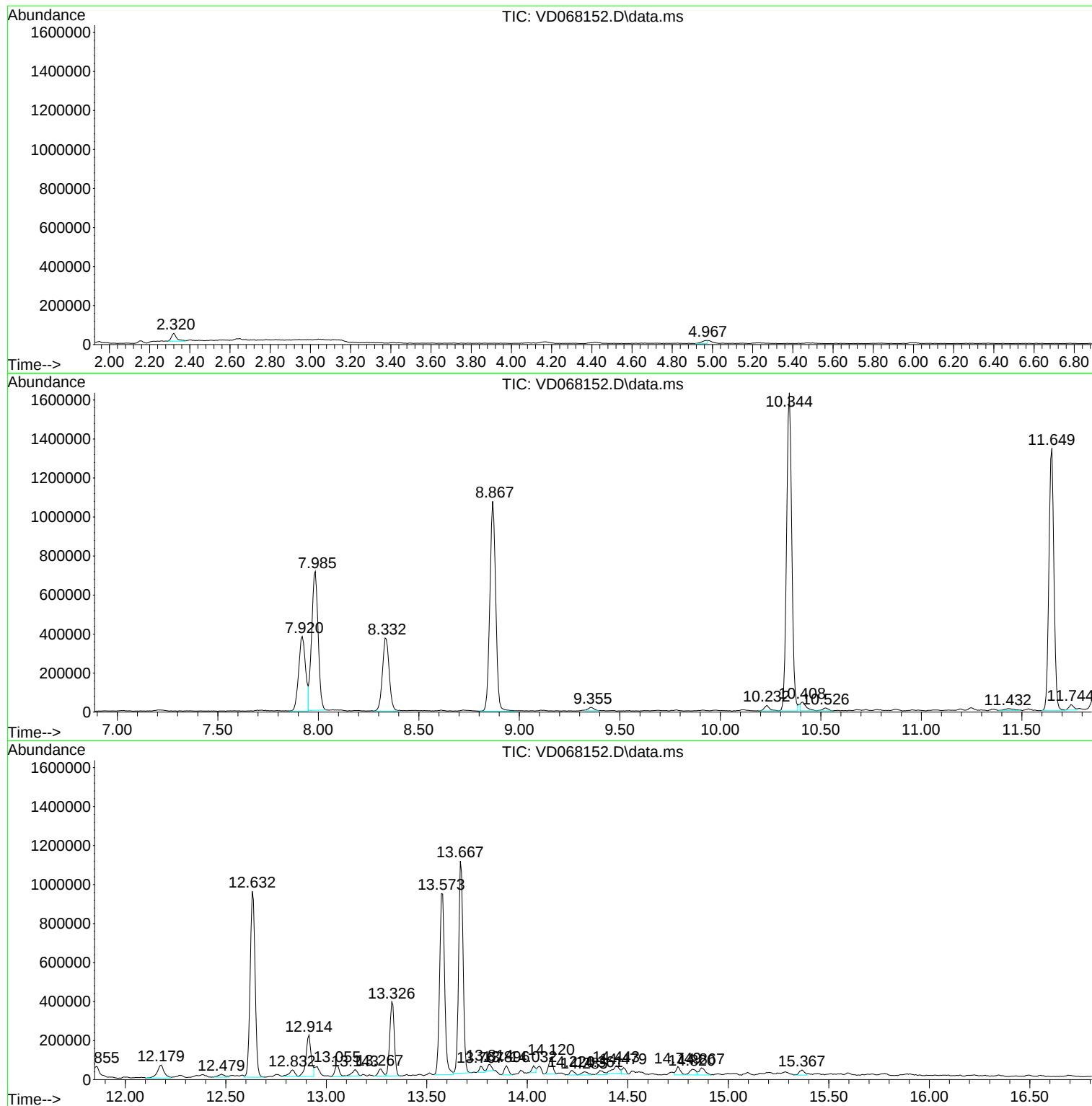
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D011921S.M
Quant Title : SW846 8260

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



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Instrument :
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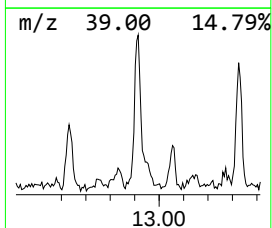
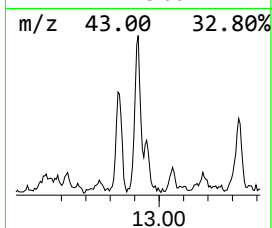
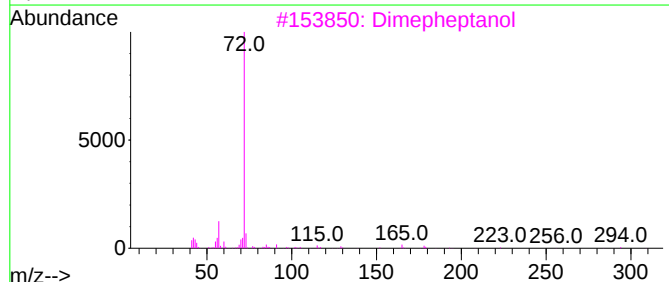
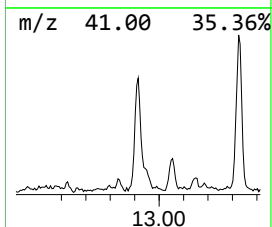
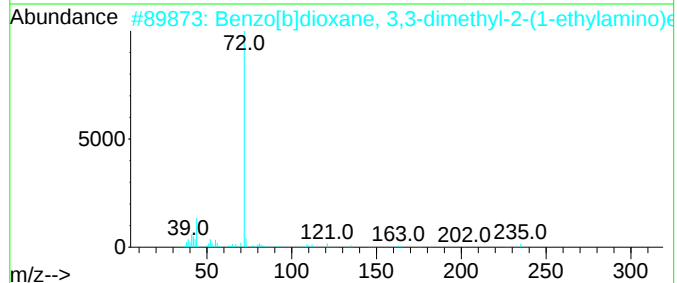
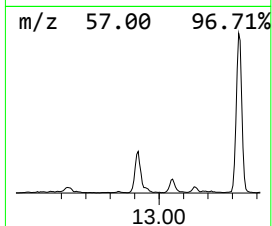
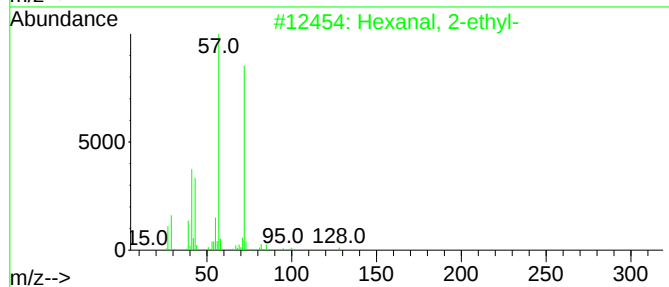
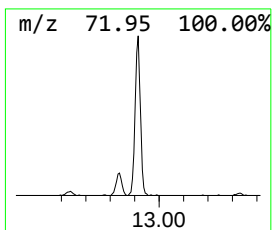
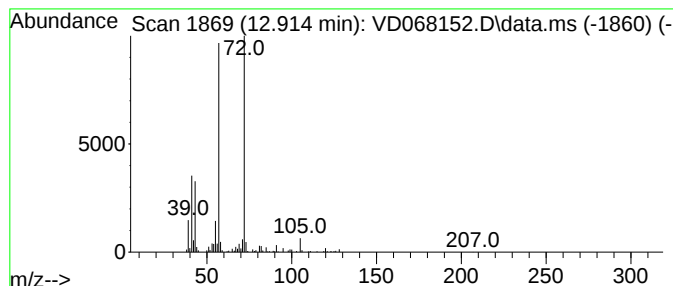
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D011921S.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanal, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.914	11.72 ug/l	377584	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	90
2			Benzo[b]dioxane, 3,3-dimethyl-2-...	235	C14H21NO2	003523-36-2	50
3			Dimepheptanol	311	C21H29NO	000545-90-4	45
4			2-Ethylamino-1-phenylpropanol	179	C11H17NO	1000298-69-2	42
5			(1R,2R)-(-)-N-Methylpseudoephedrine	179	C11H17NO	014222-20-9	42



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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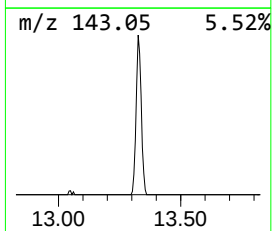
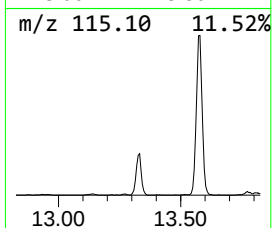
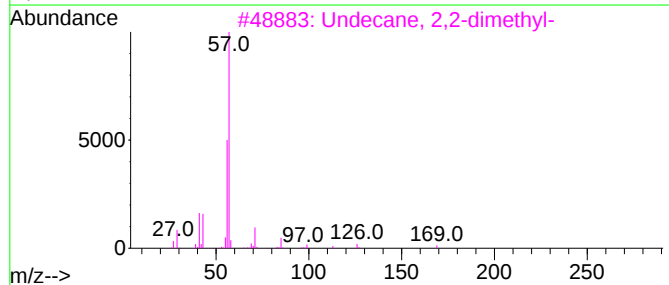
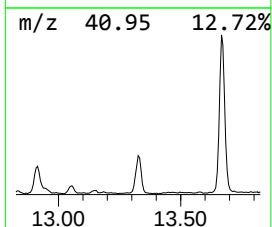
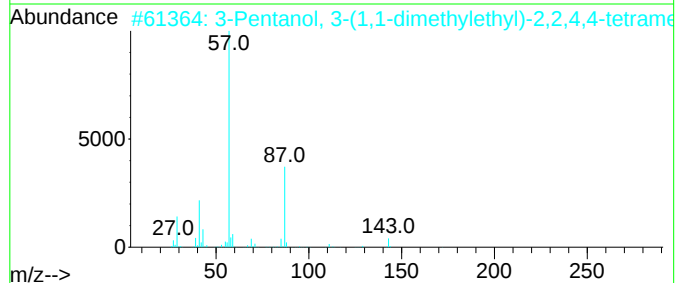
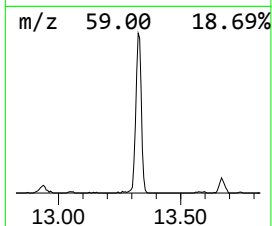
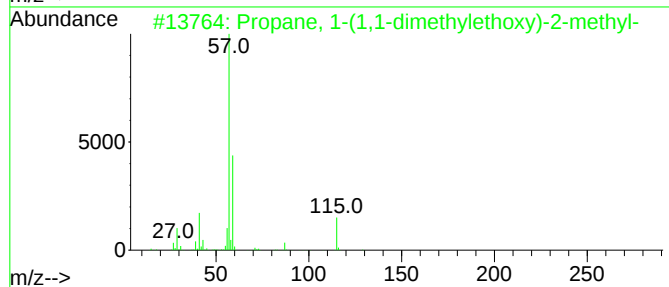
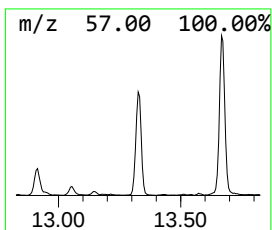
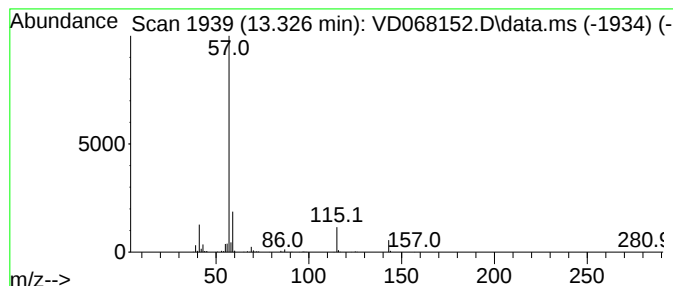
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D011921S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.326 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.326	18.32 ug/l	590148	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-(1,1-dimethylethoxy)-...	130	C8H18O	033021-02-2	23
2			3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	9
3			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	9
4			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9
5			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	5



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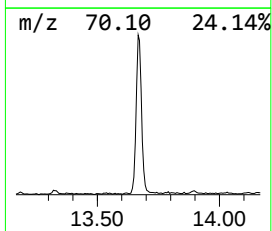
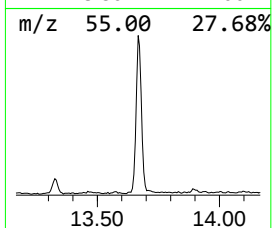
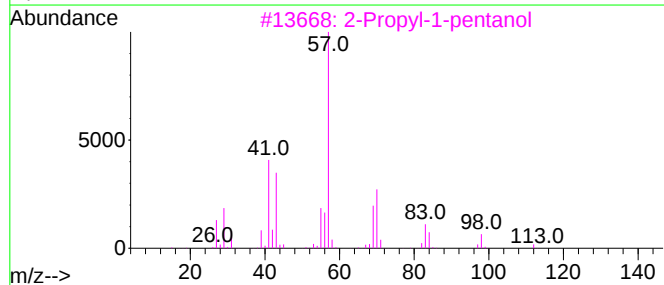
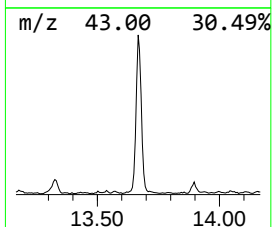
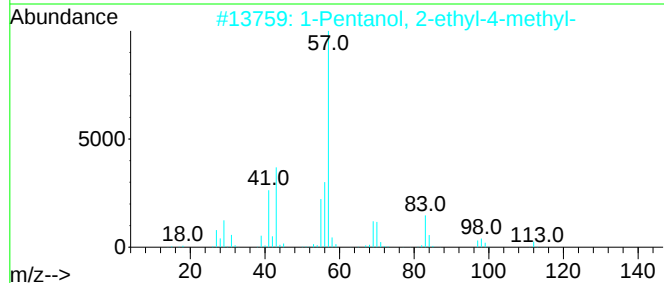
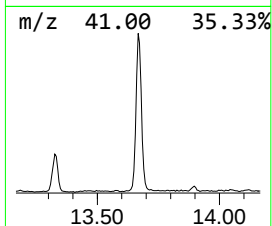
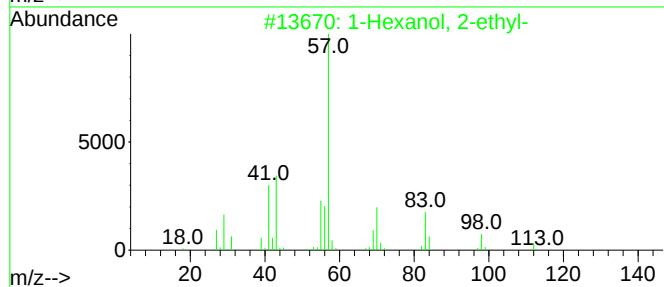
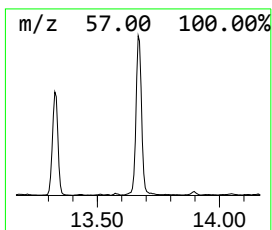
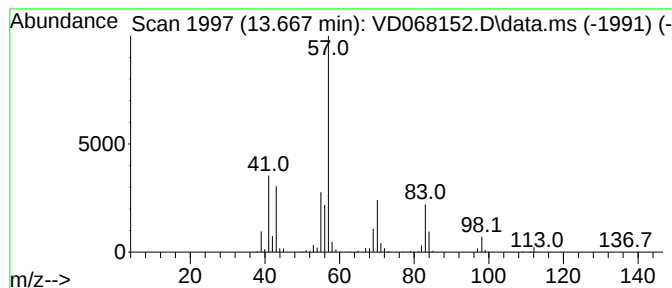
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D011921S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.667	51.40 ug/l	1655760	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal, 2-ethyl-	12.914	11.7	ug/l	377584	4	13.573	1610610	50.0
unknown13.326	13.326	18.3	ug/l	590148	4	13.573	1610610	50.0
1-Hexanol, 2-et...	13.667	51.4	ug/l	1655760	4	13.573	1610610	50.0