

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
 Data File : VX020779.D
 Acq On : 27 Jan 2021 18:48
 Operator : JC/SP
 Sample : M1189-20
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41088

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\82X012521W.M
 Title : SW846 8260

Signal : TIC: VX020779.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.380	45	48	51	rVV	16155	17960	1.08%	0.142%
2	1.477	60	64	70	rBV	10246	17682	1.06%	0.140%
3	2.416	213	218	228	rVB	64292	109804	6.61%	0.866%
4	2.581	239	245	251	rVB	18106	31505	1.90%	0.249%
5	4.306	519	528	535	rBV4	5618	17265	1.04%	0.136%
6	4.642	575	583	593	rVB2	10843	33635	2.02%	0.265%
7	5.465	704	718	732	rBV	199184	567034	34.14%	4.474%
8	5.629	732	745	758	rVB	334345	918755	55.31%	7.249%
9	6.032	799	811	824	rBV	211434	562566	33.87%	4.439%
10	6.830	929	942	956	rBV	508432	1201654	72.34%	9.481%
11	7.269	1006	1014	1022	rBV2	26044	60843	3.66%	0.480%
12	8.696	1241	1248	1255	rBV	1090496	1661150	100.00%	13.106%
13	10.092	1471	1477	1489	rBV	1054935	1438768	86.61%	11.352%
14	10.232	1496	1500	1506	rBV2	11903	17667	1.06%	0.139%
15	10.336	1511	1517	1522	rBV	44149	62812	3.78%	0.496%
16	10.683	1569	1574	1578	rBV	42307	56508	3.40%	0.446%
17	10.842	1596	1600	1605	rVB	18338	22654	1.36%	0.179%
18	11.031	1620	1631	1641	rBV	723992	1157431	69.68%	9.132%
19	11.122	1641	1646	1656	rVB	900434	1206077	72.60%	9.516%
20	11.415	1690	1694	1699	rVV	43543	72705	4.38%	0.574%
21	11.488	1703	1706	1716	rVB	26862	39572	2.38%	0.312%
22	11.652	1728	1733	1737	rBV	26625	33500	2.02%	0.264%
23	11.787	1747	1755	1761	rBV	94960	129610	7.80%	1.023%
24	12.061	1794	1800	1806	rBV	1121583	1341277	80.74%	10.582%
25	12.122	1806	1810	1815	rVB	48620	62002	3.73%	0.489%
26	12.256	1827	1832	1834	rBV	125959	166448	10.02%	1.313%
27	12.280	1834	1836	1844	rVV2	71777	110648	6.66%	0.873%
28	12.354	1844	1848	1855	rVB3	29556	51179	3.08%	0.404%
29	12.585	1879	1886	1892	rVV3	30034	73305	4.41%	0.578%
30	12.652	1892	1897	1900	rVV	35679	45443	2.74%	0.359%
31	12.738	1906	1911	1919	rVB2	33450	54836	3.30%	0.433%
32	12.884	1931	1935	1940	rVB2	12214	17441	1.05%	0.138%
33	12.957	1940	1947	1951	rBV	26401	36751	2.21%	0.290%
34	13.000	1951	1954	1959	rVB	31989	38706	2.33%	0.305%
35	13.207	1984	1988	1993	rVB	35160	41173	2.48%	0.325%
36	13.329	2004	2008	2014	rVB2	91748	122204	7.36%	0.964%

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37	13.463	2025	2030	2037	rVB	71515	95564	5.75%	0.754%
38	13.579	2046	2049	2052	rVV	19039	26648	1.60%	0.210%
39	13.622	2052	2056	2062	rVV6	26060	58645	3.53%	0.463%
40	13.701	2066	2069	2075	rVB2	27141	41983	2.53%	0.331%
41	13.817	2081	2088	2096	rVB	42562	61986	3.73%	0.489%
42	13.890	2096	2100	2105	rBV	20837	28312	1.70%	0.223%
43	13.963	2107	2112	2117	rBV2	29453	42006	2.53%	0.331%
44	14.115	2133	2137	2140	rBV	20589	24850	1.50%	0.196%
45	14.268	2155	2162	2173	rBV2	61351	109743	6.61%	0.866%
46	14.408	2182	2185	2189	rBV	23151	29960	1.80%	0.236%
47	14.518	2199	2203	2210	rBV2	49263	66343	3.99%	0.523%
48	14.676	2221	2229	2233	rBV2	66900	110230	6.64%	0.870%
49	14.707	2233	2234	2240	rVB4	17418	18530	1.12%	0.146%
50	14.823	2248	2253	2257	rBV	55163	72937	4.39%	0.575%
51	14.932	2266	2271	2279	rBV	96703	143494	8.64%	1.132%
52	15.225	2315	2319	2327	rVB4	17799	42316	2.55%	0.334%
53	15.524	2364	2368	2373	rBV3	19895	32740	1.97%	0.258%
54	15.664	2386	2391	2394	rBV3	29141	43795	2.64%	0.346%
55	15.701	2394	2397	2404	rVB4	16448	25874	1.56%	0.204%

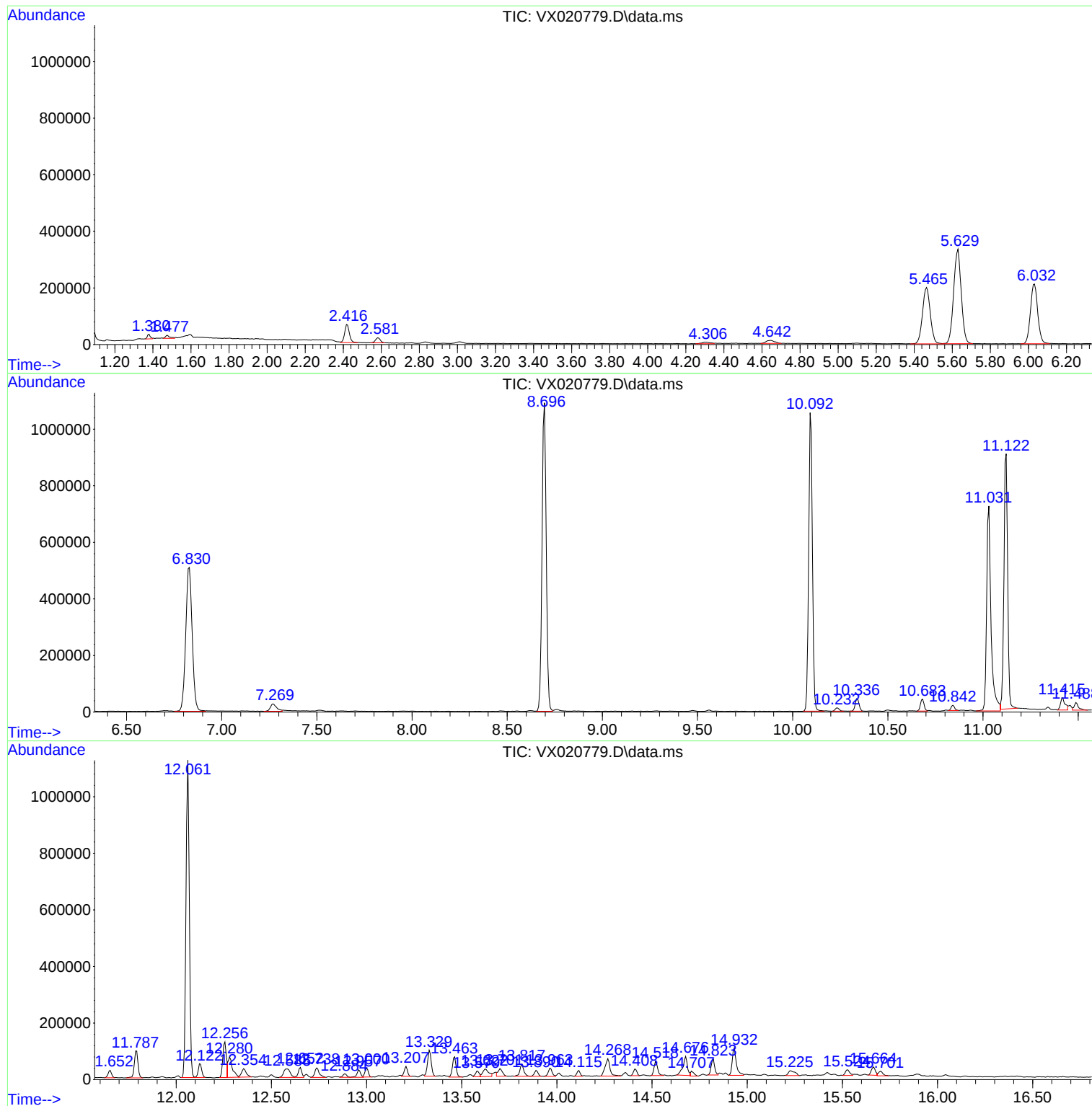
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



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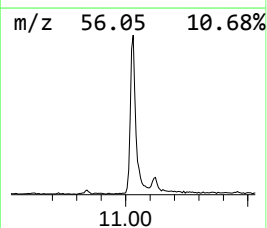
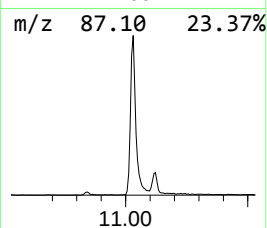
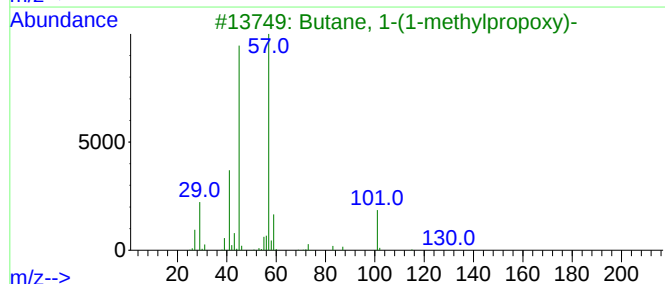
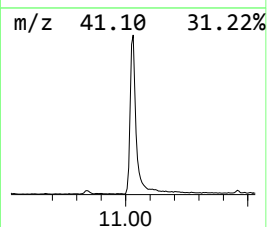
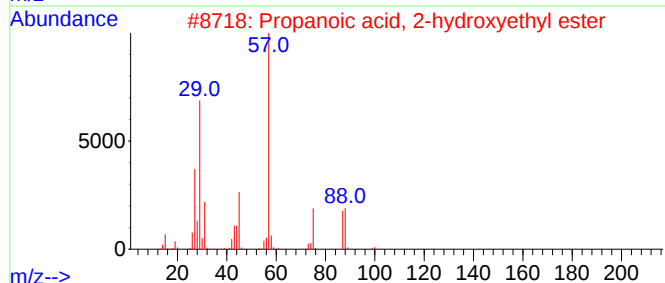
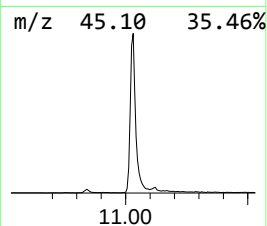
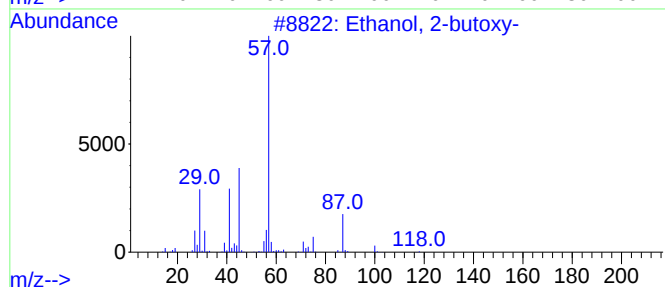
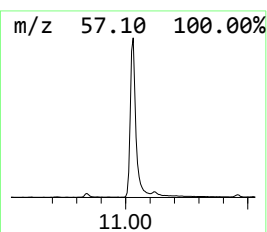
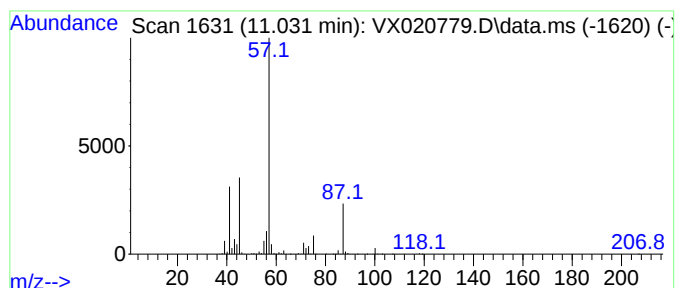
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Quant Title : SW846 8260

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

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.031	40.22 ug/l	1157430	Chlorobenzene-d5	10.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	91
2			Propanoic acid, 2-hydroxyethyl e...	118	C5H10O3	024567-27-9	39
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	38
4			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	37
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	36



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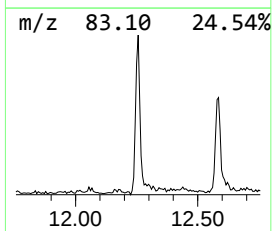
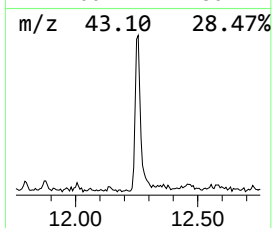
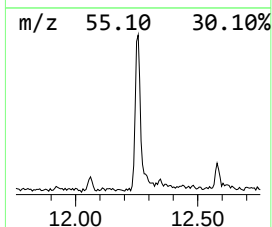
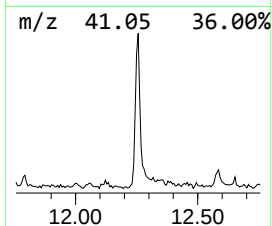
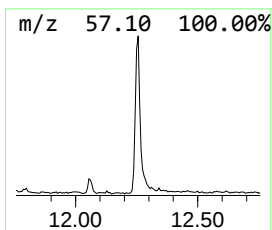
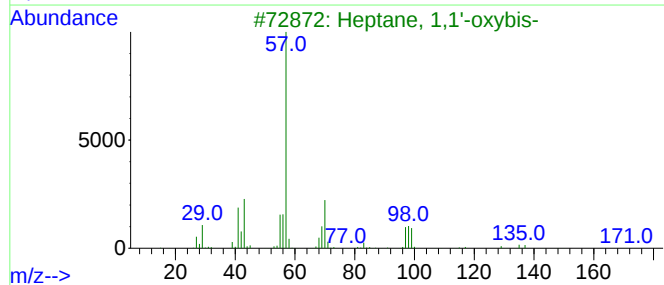
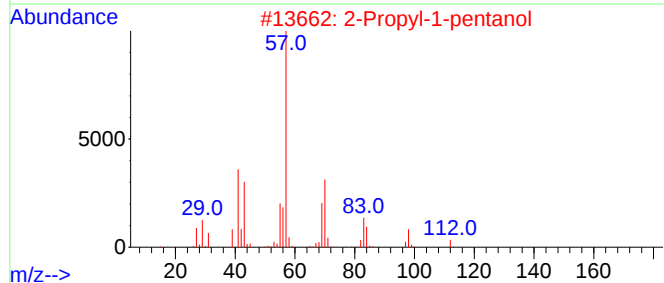
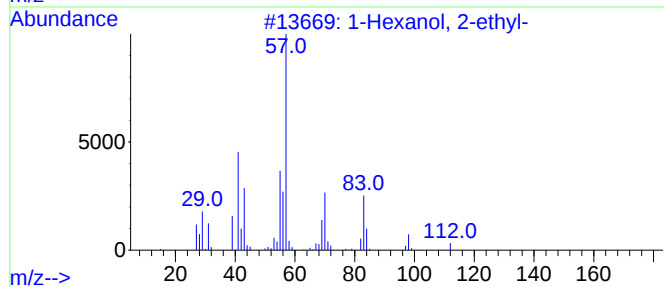
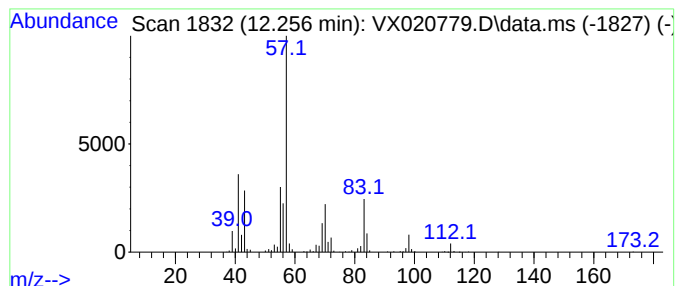
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	6.20 ug/l	166448	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	58
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
4			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	47
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



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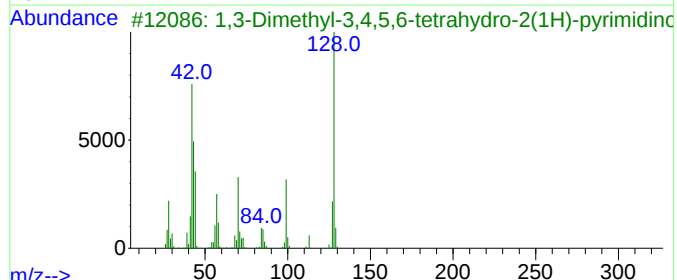
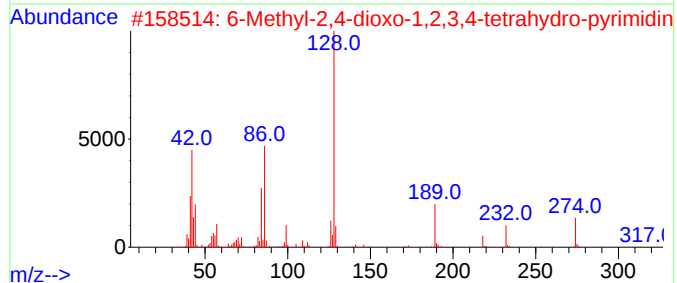
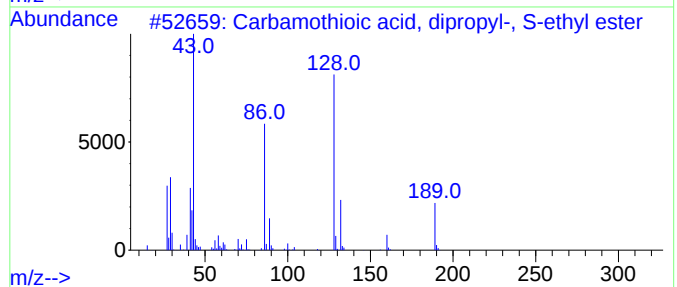
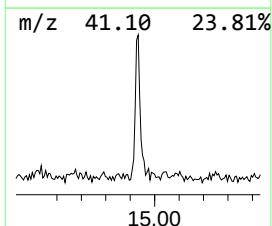
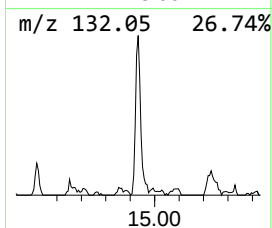
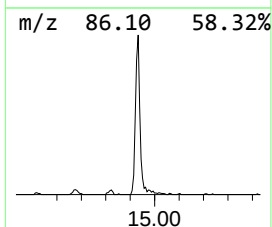
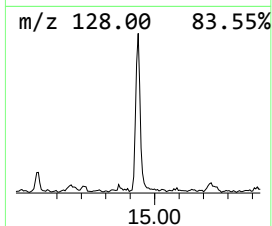
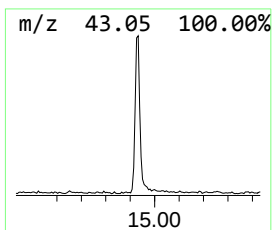
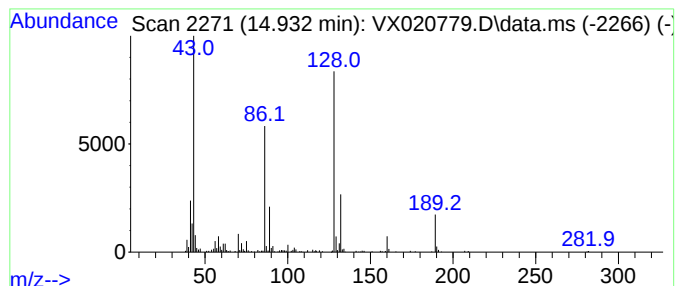
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Peak Number 3 Carbamothioic acid, dipropyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.932	5.35 ug/l	143494	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbamothioic acid, dipropyl-, S...	189	C9H19NOS	000759-94-4	93
2			6-Methyl-2,4-dioxo-1,2,3,4-tetra...	317	C13H23N3O4S	1000275-98-8	42
3			1,3-Dimethyl-3,4,5,6-tetrahydro...	128	C6H12N2O	007226-23-5	35
4			2-Amino-4,5-dimethylthiazole	128	C5H8N2S	002289-75-0	35
5			2-(E)-Pentenoic acid, (4S)-amino...	219	C13H17NO2	244033-75-8	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-butoxy-	11.031	40.2	ug/l	1157430	3	10.092	1438770	50.0
1-Hexanol, 2-et...	12.256	6.2	ug/l	166448	4	12.061	1341280	50.0
Carbamothioic a...	14.932	5.3	ug/l	143494	4	12.061	1341280	50.0