

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051822\
 Data File : VX028805.D
 Acq On : 18 May 2022 14:55
 Operator : JC/MD
 Sample : N2884-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31804

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	42	rBV	78187	219936	15.58%	2.339%
2	2.380	206	212	230	rVB	69807	121963	8.64%	1.297%
3	2.526	230	236	249	rBV2	20656	48456	3.43%	0.515%
4	4.233	506	516	528	rBV2	19061	51866	3.67%	0.551%
5	4.562	562	570	584	rBV2	5187	16034	1.14%	0.170%
6	5.391	694	706	720	rBV	164027	478439	33.90%	5.087%
7	5.556	722	733	748	rVB	279414	787210	55.77%	8.370%
8	5.958	786	799	816	rBV	183216	485335	34.39%	5.160%
9	6.111	816	824	833	rVV2	7391	19712	1.40%	0.210%
10	6.763	921	931	948	rBV	448131	1051663	74.51%	11.182%
11	7.214	997	1005	1012	rBV2	19884	46504	3.29%	0.494%
12	8.653	1234	1241	1248	rBV	887793	1411443	100.00%	15.007%
13	8.720	1248	1252	1256	rVV	11671	19779	1.40%	0.210%
14	8.769	1256	1260	1270	rVB2	14582	26288	1.86%	0.280%
15	9.238	1332	1337	1346	rBV	9407	16341	1.16%	0.174%
16	10.055	1465	1471	1482	rBV	939209	1231451	87.25%	13.094%
17	10.153	1483	1487	1493	rBV2	15619	23596	1.67%	0.251%
18	10.506	1541	1545	1555	rVB	18296	25848	1.83%	0.275%
19	10.683	1571	1574	1580	rVB	17219	23062	1.63%	0.245%
20	10.756	1581	1586	1594	rBV3	32939	58575	4.15%	0.623%
21	11.079	1634	1639	1645	rBV	718333	921278	65.27%	9.796%
22	11.134	1645	1648	1655	rVB	40349	51922	3.68%	0.552%
23	11.573	1716	1720	1723	rBV2	23992	32959	2.34%	0.350%
24	11.604	1723	1725	1734	rVV2	19643	32582	2.31%	0.346%
25	11.689	1734	1739	1747	rVB	24527	32537	2.31%	0.346%
26	11.829	1755	1762	1765	rBV3	13619	22662	1.61%	0.241%
27	11.872	1765	1769	1778	rVV	71698	115535	8.19%	1.228%
28	11.951	1779	1782	1786	rVV3	9689	17930	1.27%	0.191%
29	12.024	1789	1794	1801	rVB	883850	1114230	78.94%	11.847%
30	12.219	1821	1826	1837	rBV	590274	801029	56.75%	8.517%
31	12.305	1837	1840	1854	rVV7	26389	60836	4.31%	0.647%
32	13.847	2090	2093	2100	rVB2	11576	16365	1.16%	0.174%
33	13.914	2100	2104	2110	rBV3	14724	21596	1.53%	0.230%

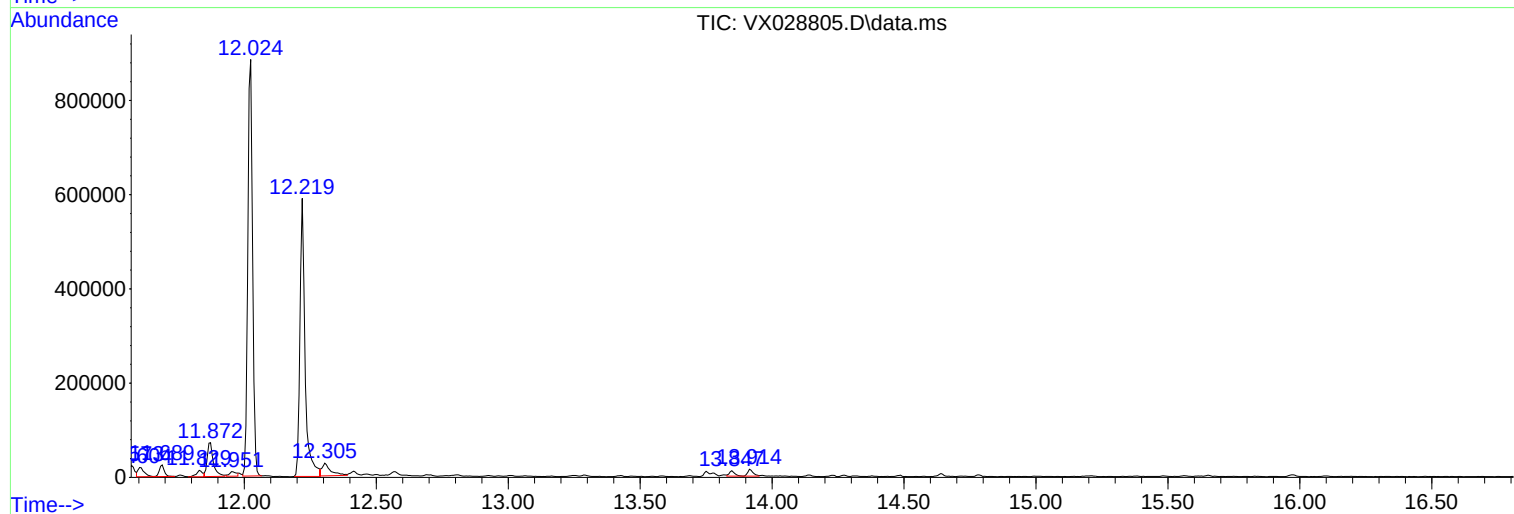
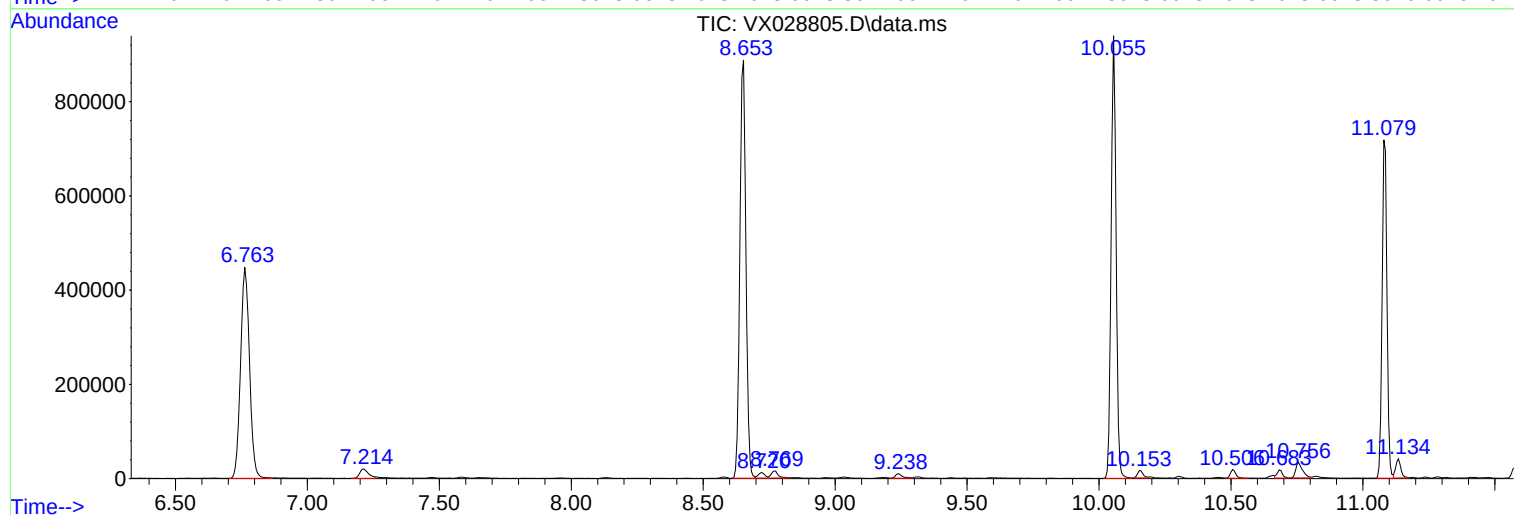
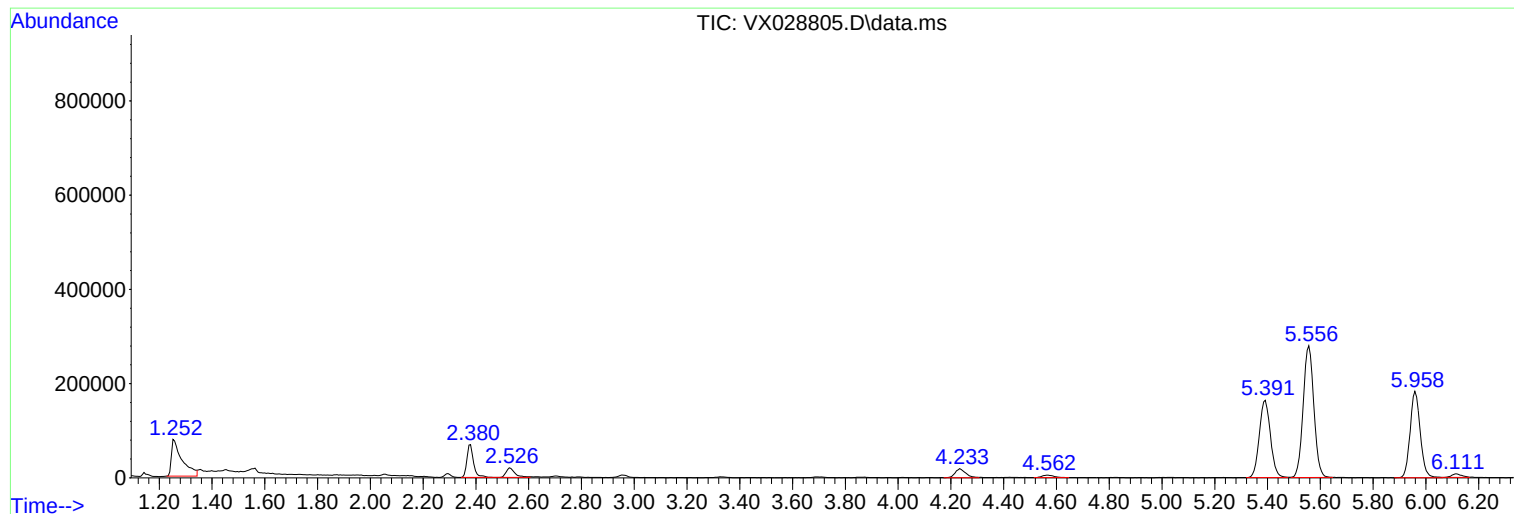
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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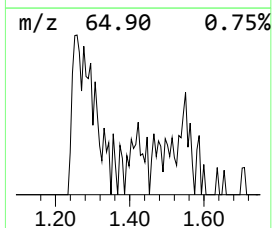
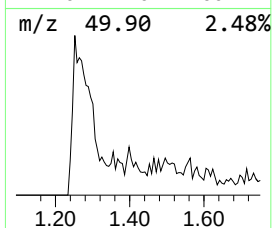
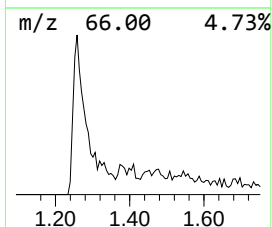
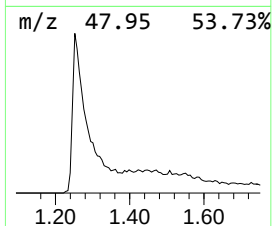
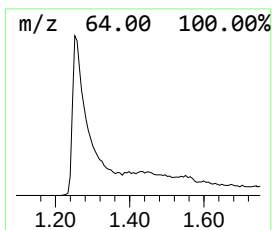
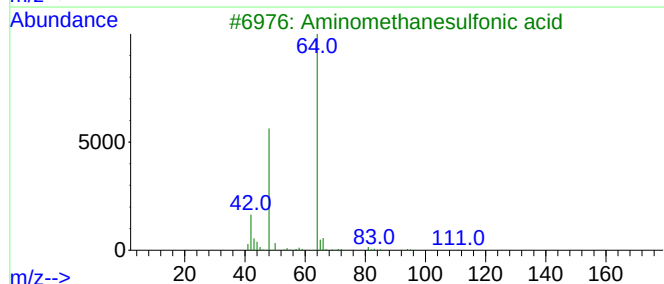
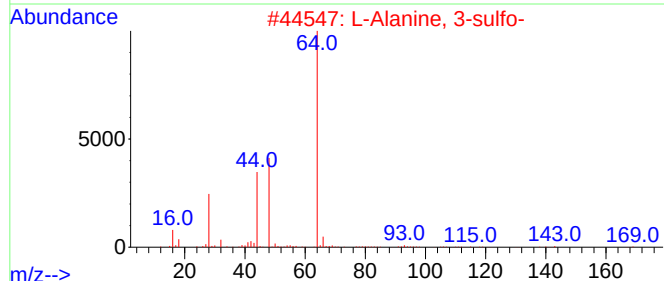
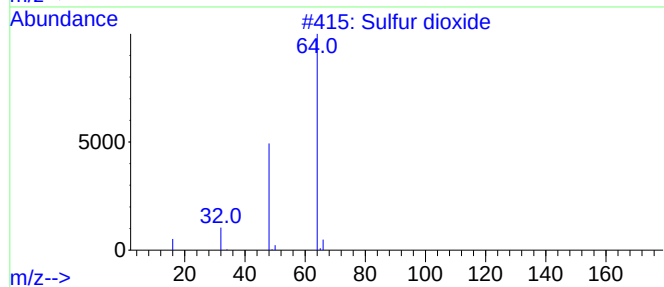
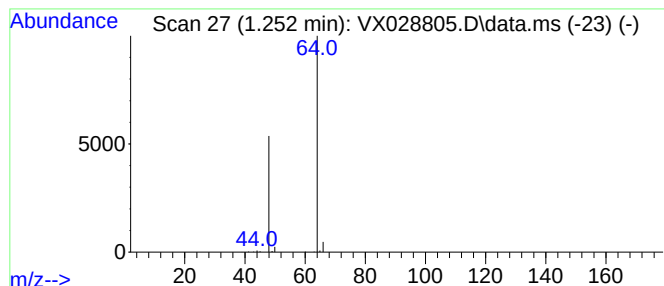
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	13.97 ug/l	219936	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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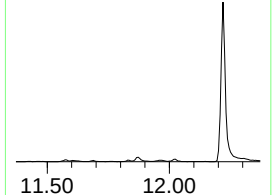
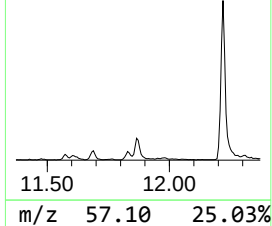
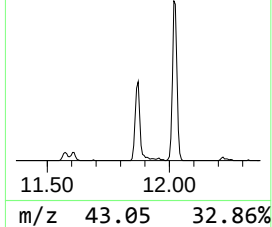
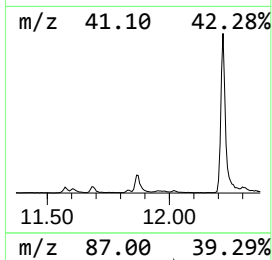
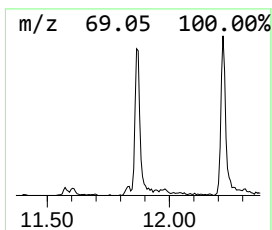
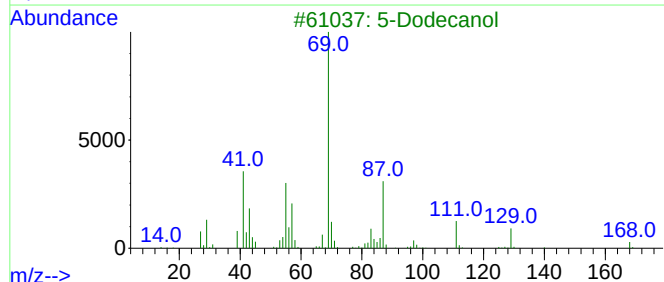
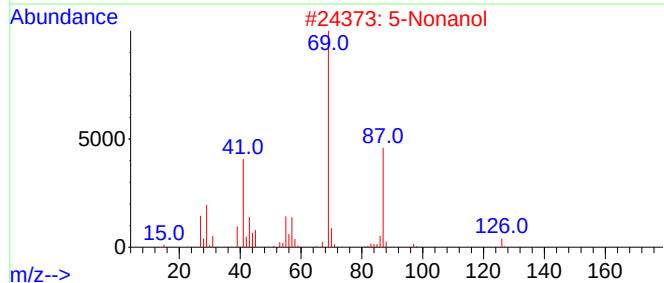
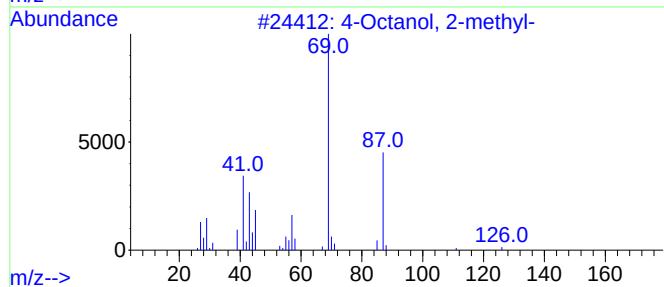
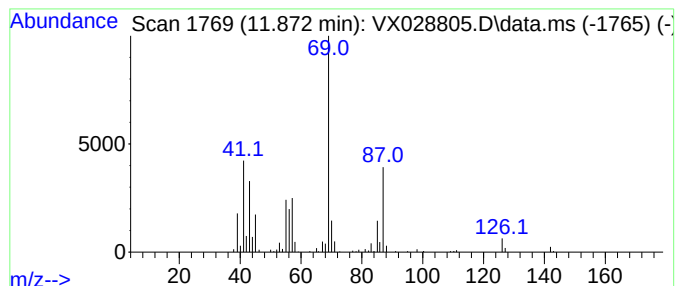
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Octanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.872	5.18 ug/l	115535	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64
2			5-Nonanol	144	C9H20O	000623-93-8	64
3			5-Dodecanol	186	C12H26O	010203-33-5	64
4			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	64
5			2-Butenoic acid, butyl ester	142	C8H14O2	007299-91-4	59



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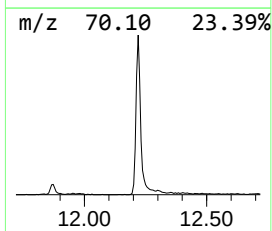
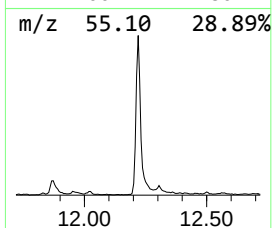
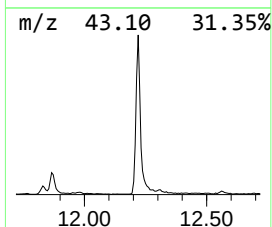
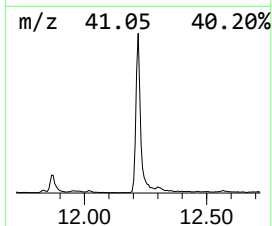
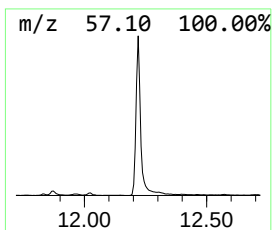
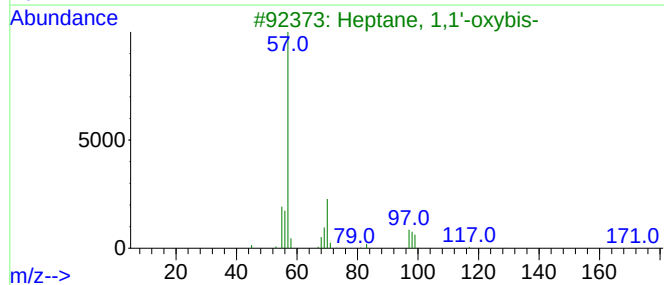
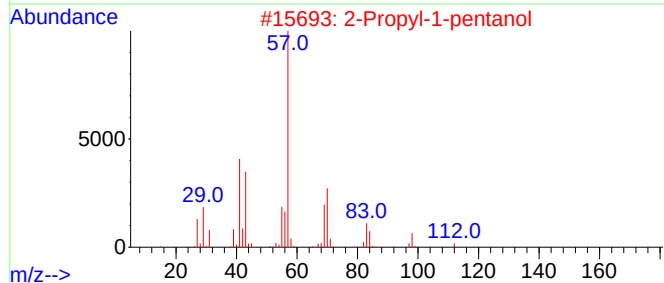
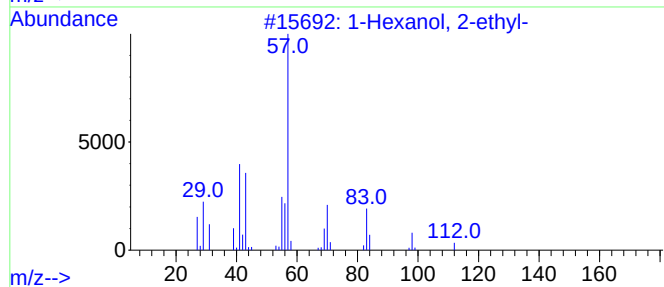
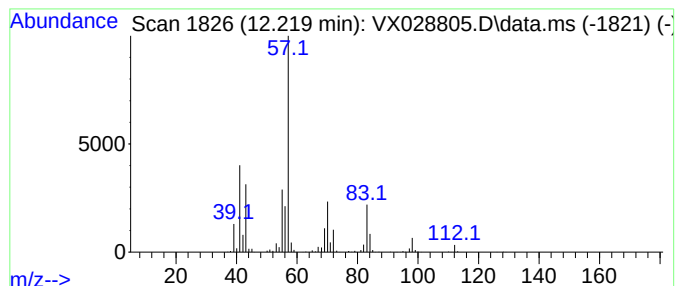
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
12.219	35.95 ug/l	801029	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	43



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	14.0	ug/l	219936	1	5.556	787210	50.0
4-Octanol, 2-me...	11.872	5.2	ug/l	115535	4	12.024	1114230	50.0
1-Hexanol, 2-et...	12.219	36.0	ug/l	801029	4	12.024	1114230	50.0