LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030149.D
Acq On : 20 Jul 2022 21:53
Operator : JC/MD
Sample : N3760-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1821

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\82X071222W.M
Title : SW846 8260

Signal : TIC: VX030149.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.544	67	75	83	rBV2	17472	30109	3.04%	0.433%
2	2.380	206	212	216	rBV	204782	330399	33.35%	4.752%
3	2.422	216	219	229	rVB	71896	117097	11.82%	1.684%
4	2.544	229	239	249	rBV	57145	112657	11.37%	1.620%
5	3.867	449	456	466	rBV5	3227	10500	1.06%	0.151%
6	4.568	560	571	586	rBV2	31108	91199	9.21%	1.312%
7	5.032	637	647	656	rBV6	2919	10700	1.08%	0.154%
8	5.391	695	706	722	rVB3	109343	316090	31.91%	4.547%
9	5.556	722	733	745	rBV	187691	531308	53.63%	7.642%
10	5.964	789	800	814	rBV	124337	334971	33.81%	4.818%
11	6.769	921	932	944	rBV	322854	753250	76.04%	10.834%
12	7.464	1042	1046	1056	rVB3	4857	10450	1.05%	0.150%
13	7.647	1071	1076	1087	rVB	20675	39669	4.00%	0.571%
14	8.415	1198	1202	1208	rVB4	8583	14271	1.44%	0.205%
15	8.580	1222	1229	1234	rBV2	8984	14566	1.47%	0.210%
16	8.653	1234	1241	1249	rBV	650750	990610	100.00%	14.249%
17	9.537	1381	1386	1392	rBV3	9849	16891	1.71%	0.243%
18	10.055	1463	1471	1484	rBV	629068	850743	85.88%	12.237%
19	11.085	1634	1640	1647	rBV	464303	581977	58.75%	8.371%
20	11.573	1714	1720	1732	rBV	138834	169012	17.06%	2.431%
21	11.829	1757	1762	1766	rBV	27418	36657	3.70%	0.527%
22	11.890	1766	1772	1777	rVV2	43802	72750	7.34%	1.046%
23	11.976	1781	1786	1789	rVV4	10724	17862	1.80%	0.257%
24	12.024	1789	1794	1802	rVV	619483	753473	76.06%	10.838%
25	12.104	1802	1807	1812	rVB2	42444	56465	5.70%	0.812%
26	12.225	1820	1827	1840	rBV	130065	273315	27.59%	3.931%
27	13.170	1978	1982	1986	rBV4	10421	17249	1.74%	0.248%
28	13.213	1986	1989	1997	rVB	29498	41536	4.19%	0.597%
29	13.579	2043	2049	2059	rVV8	11945	21176	2.14%	0.305%
30	13.731	2070	2074	2079	rBV	122813	158866	16.04%	2.285%
31	13.780	2079	2082	2089	rVB2	23517	32052	3.24%	0.461%
32	14.048	2119	2126	2131	rBV6	6564	13520	1.36%	0.194%
33	14.097	2131	2134	2142	rVB5	12472	20990	2.12%	0.302%
34	14.317	2165	2170	2176	rBV3	10609	18688	1.89%	0.269%
35	14.634	2219	2222	2232	rVB2	6887	11332	1.14%	0.163%
36	14.780	2241	2246	2252	rBV3	12504	16733	1.69%	0.241%

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Title : SW846 8260

37	16.097	2456	2462	2467	rBV5	7490	13666	1.38%	0.197%
38	16.328	2492	2500	2507	rBV2	27344	49550	5.00%	0.713%

Sum of corrected areas: 6952349

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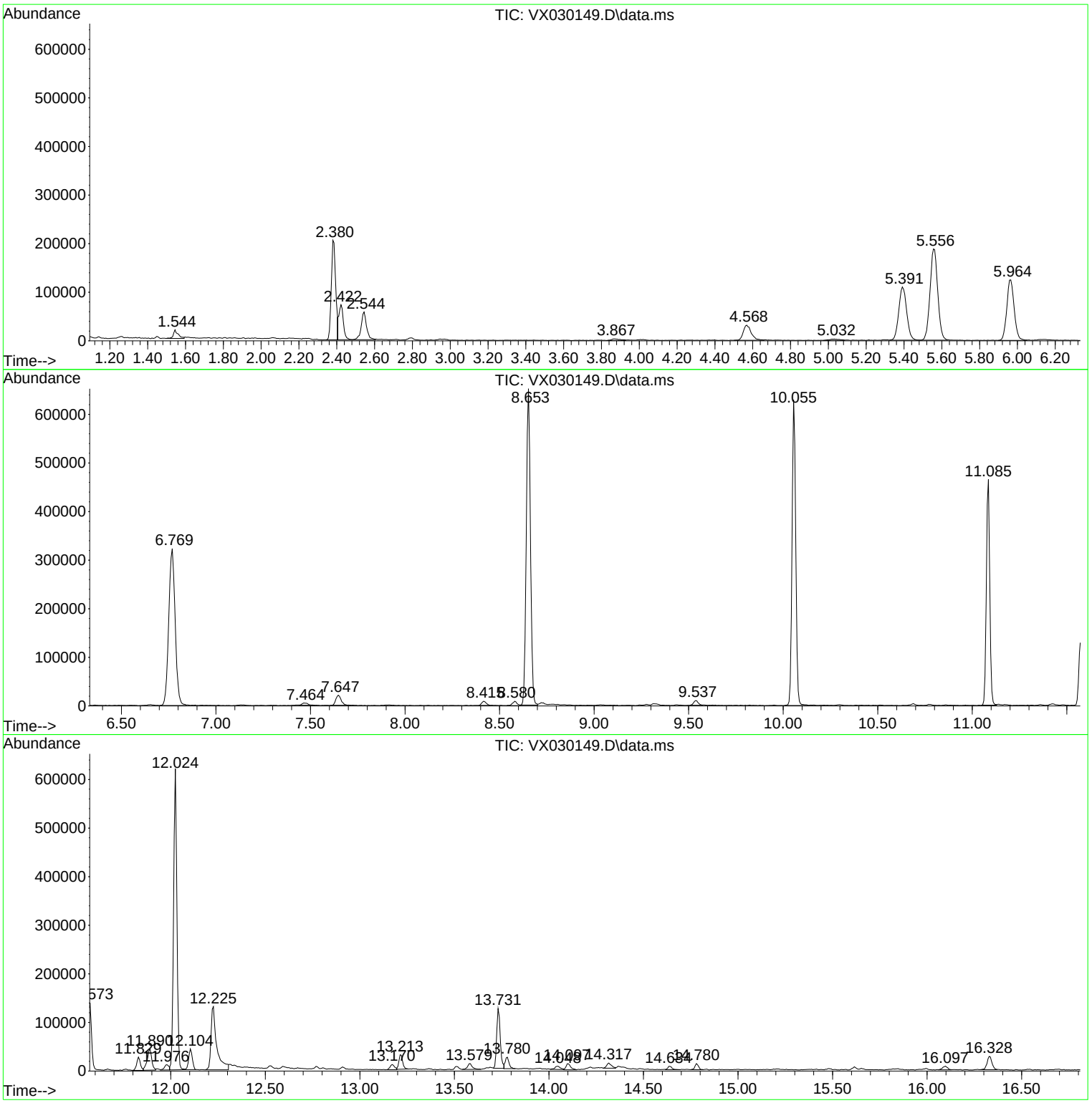
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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



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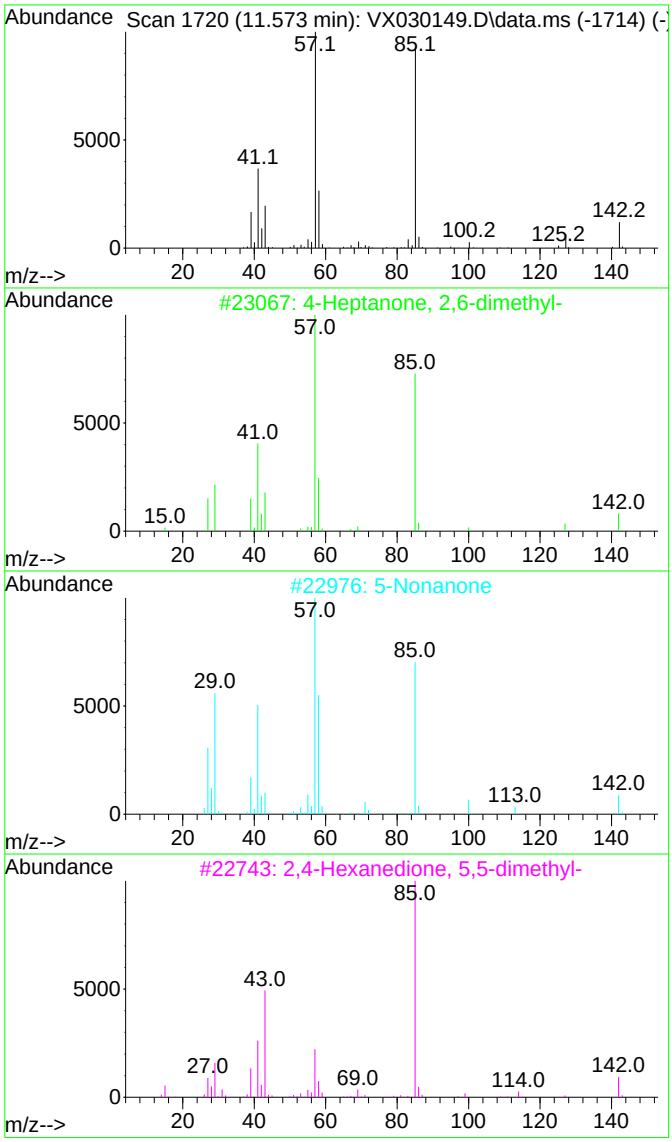
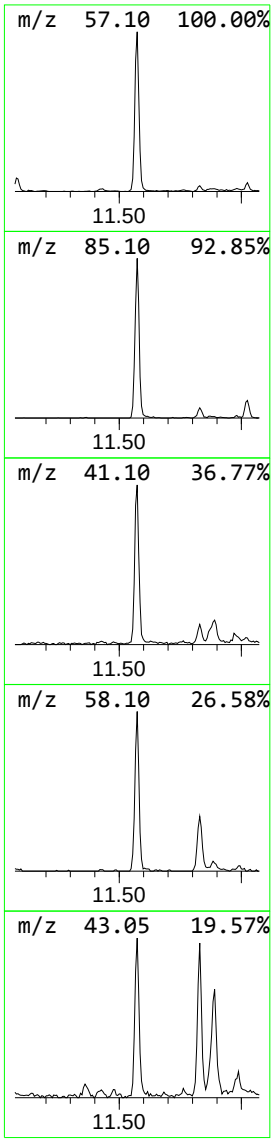
****
Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	11.22 ug/l	169012	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	59
4	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	50





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Quant Title : SW846 8260

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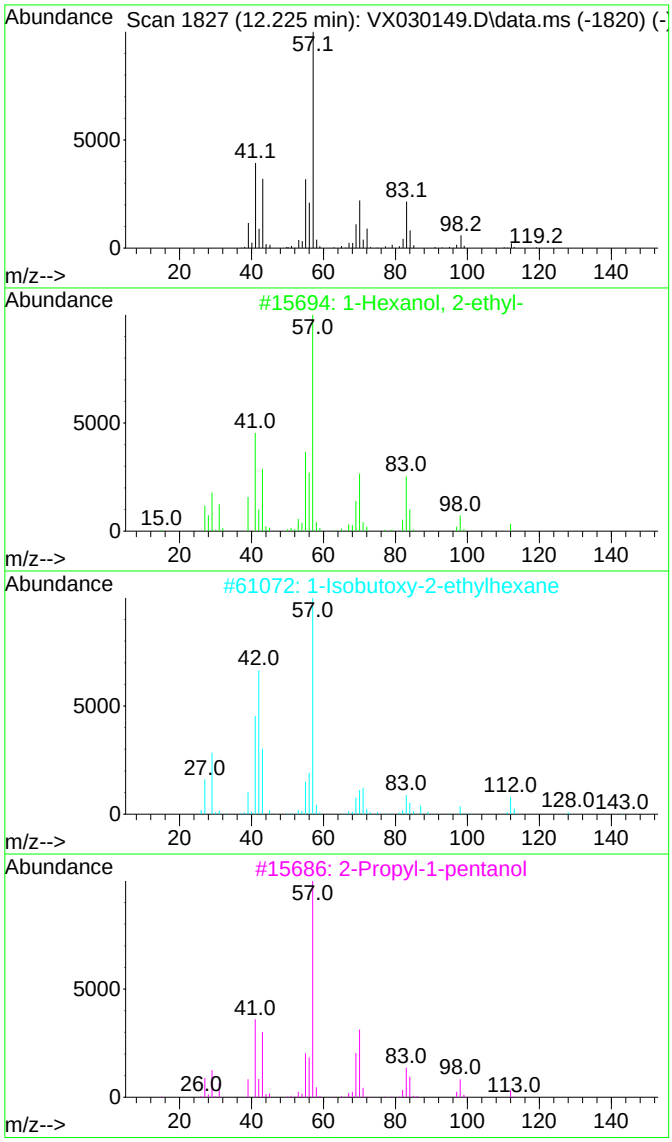
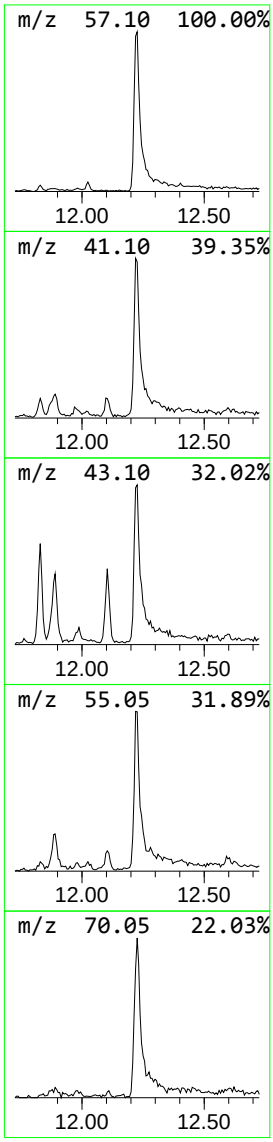
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.226	18.14 ug/l	273315	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	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Heptanone, 2,...	11.573	11.2	ug/l	169012	4	12.024	753473	50.0
1-Hexanol, 2-et...	12.226	18.1	ug/l	273315	4	12.024	753473	50.0