LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120622\
Data File : VX033270.D
Acq On : 06 Dec 2022 19:41
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	40	44	49	rBV	8759	9395	1.38%	0.172%
2	2.386	206	213	226	rBV	113687	220259	32.35%	4.043%
3	2.593	237	247	251	rBV3	2312	7473	1.10%	0.137%
4	2.989	297	312	327	rBV3	9745	45059	6.62%	0.827%
5	3.331	359	368	377	rVB	4281	9981	1.47%	0.183%
6	3.696	418	428	441	rBV2	5202	14050	2.06%	0.258%
7	4.233	504	516	529	rBV	107383	293144	43.05%	5.381%
8	4.562	563	570	591	rVB	23161	71084	10.44%	1.305%
9	5.391	693	706	721	rBV2	68042	201557	29.60%	3.700%
10	5.550	721	732	747	rVV	134781	384766	56.51%	7.063%
11	5.958	787	799	810	rBV	66711	176922	25.98%	3.248%
12	6.763	921	931	947	rBV	199702	474439	69.68%	8.709%
13	7.251	1005	1011	1015	rBV5	2722	7062	1.04%	0.130%
14	7.464	1038	1046	1052	rBV2	5647	11606	1.70%	0.213%
15	7.580	1061	1065	1072	rVB	9112	16127	2.37%	0.296%
16	8.141	1146	1157	1168	rBV2	13508	30824	4.53%	0.566%
17	8.439	1200	1206	1214	rBV3	3829	8413	1.24%	0.154%
18	8.574	1223	1228	1234	rBV	20004	32778	4.81%	0.602%
19	8.653	1234	1241	1248	rVV	275243	437871	64.31%	8.038%
20	8.720	1248	1252	1257	rVV	6991	12477	1.83%	0.229%
21	8.775	1257	1261	1269	rVV3	6205	15489	2.27%	0.284%
22	8.848	1270	1273	1285	rVB4	3426	7961	1.17%	0.146%
23	8.970	1286	1293	1300	rBV2	9836	19436	2.85%	0.357%
24	9.433	1363	1369	1375	rBV	4030	7046	1.03%	0.129%
25	9.537	1381	1386	1398	rVB4	4417	9195	1.35%	0.169%
26	10.055	1461	1471	1484	rBV	401032	549463	80.70%	10.087%
27	10.159	1484	1488	1493	rBV3	5395	9041	1.33%	0.166%
28	10.305	1507	1512	1518	rVB	6395	10548	1.55%	0.194%
29	10.445	1528	1535	1541	rVV	67291	89548	13.15%	1.644%
30	10.506	1541	1545	1550	rVB2	6694	8760	1.29%	0.161%
31	10.659	1562	1570	1572	rBV2	31312	48567	7.13%	0.892%
32	10.683	1572	1574	1582	rVB	30109	34938	5.13%	0.641%
33	10.756	1582	1586	1594	rBV2	17044	35660	5.24%	0.655%
34	11.079	1634	1639	1645	rBV	293163	373505	54.86%	6.856%
35	11.427	1691	1696	1701	rBV2	8779	13143	1.93%	0.241%
36	11.476	1701	1704	1713	rVB2	6619	10278	1.51%	0.189%

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Title : SW846 8260

37	11.573	1716	1720	1723	rBV	7698	11351	1.67%	0.208%
38	11.604	1723	1725	1727	rVV3	7058	9347	1.37%	0.172%
39	11.634	1727	1730	1734	rVB2	9461	12787	1.88%	0.235%
40	11.756	1744	1750	1754	rBV5	6956	10541	1.55%	0.194%
41	11.811	1754	1759	1761	rVV	11028	15646	2.30%	0.287%
42	11.841	1761	1764	1767	rVV2	11337	18498	2.72%	0.340%
43	11.890	1770	1772	1780	rVB4	7141	12838	1.89%	0.236%
44	12.024	1788	1794	1801	rVB	429621	541916	79.59%	9.948%
45	12.219	1821	1826	1839	rBV	486593	680865	100.00%	12.499%
46	12.414	1853	1858	1863	rBV	170573	206470	30.32%	3.790%
47	12.567	1879	1883	1891	rVB5	8650	16972	2.49%	0.312%
48	12.768	1911	1916	1918	rVV4	7384	11938	1.75%	0.219%
49	12.805	1918	1922	1928	rVB6	8603	15501	2.28%	0.285%
50	13.286	1999	2001	2007	rVB5	4783	7405	1.09%	0.136%
51	13.341	2007	2010	2015	rBV3	6788	9104	1.34%	0.167%
52	13.426	2018	2024	2030	rVB	15373	25105	3.69%	0.461%
53	13.597	2047	2052	2057	rBV7	3388	7973	1.17%	0.146%
54	13.658	2057	2062	2067	rBV5	3973	7962	1.17%	0.146%
55	13.774	2077	2081	2084	rBV	13203	18699	2.75%	0.343%
56	13.804	2084	2086	2089	rVV	12257	13156	1.93%	0.242%
57	13.847	2089	2093	2100	rVV5	11166	18080	2.66%	0.332%
58	13.914	2100	2104	2110	rVB2	11249	15708	2.31%	0.288%
59	14.134	2132	2140	2145	rBV	8498	12833	1.88%	0.236%
60	14.640	2216	2223	2227	rBV2	7728	12520	1.84%	0.230%
61	14.780	2240	2246	2250	rBV	6129	8257	1.21%	0.152%
62	15.969	2431	2441	2449	rBV5	8832	18155	2.67%	0.333%

Sum of corrected areas: 5447492

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ClientSampleId :
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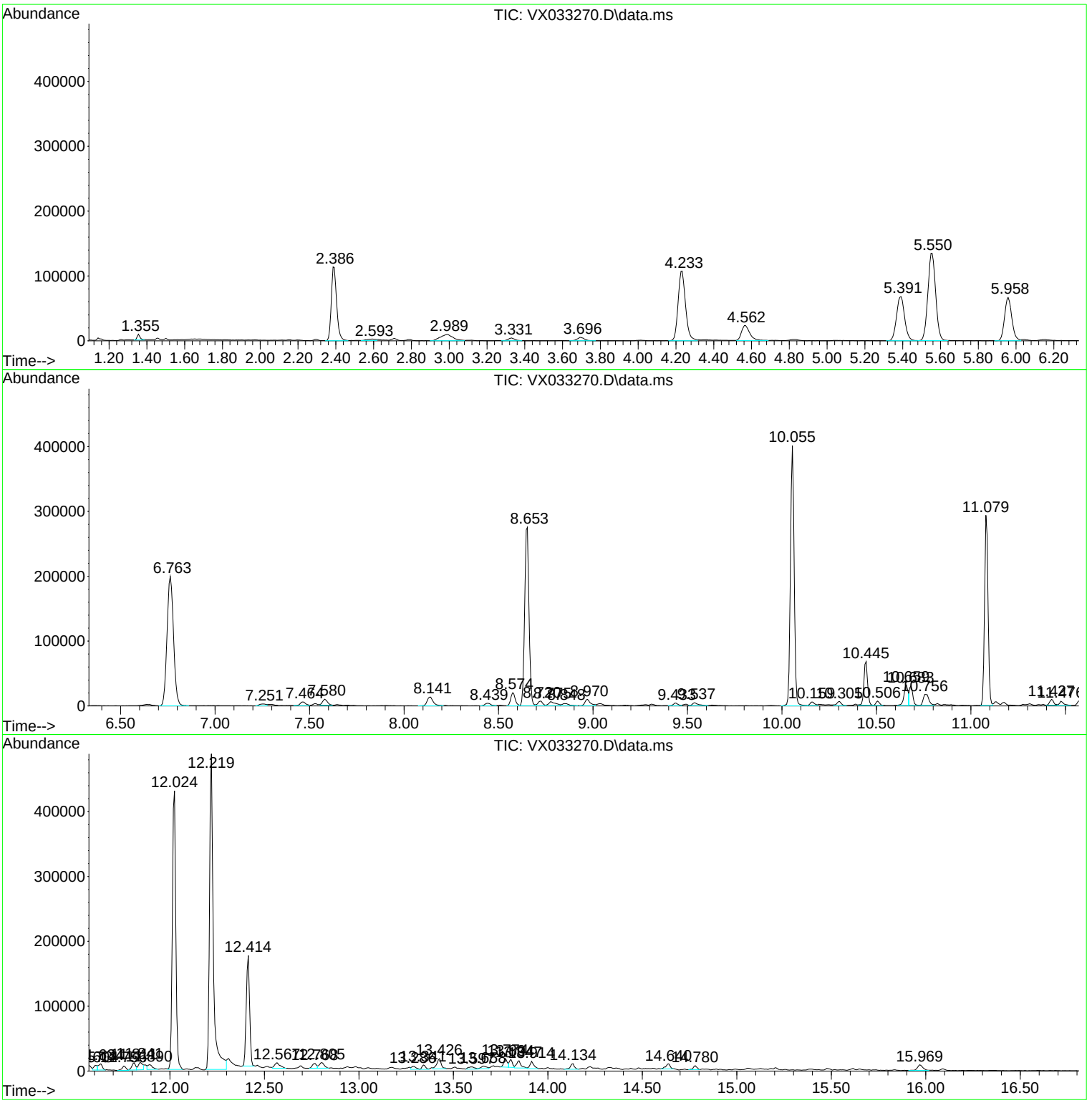
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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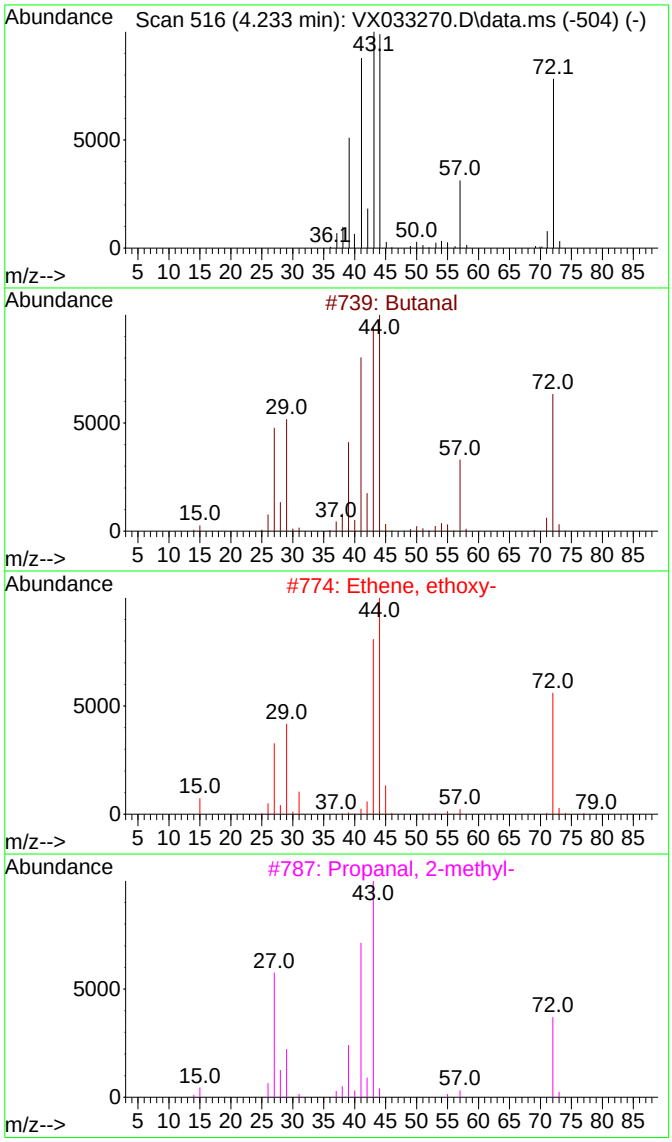
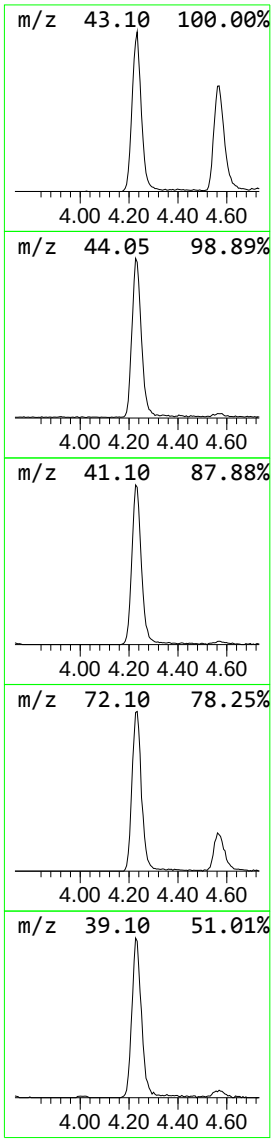
****

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	38.09 ug/l	293144	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25
5	Isobutylene epoxide	72	C4H8O	000558-30-5	16





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Instrument :
MSVOA_X
ClientSampleId :
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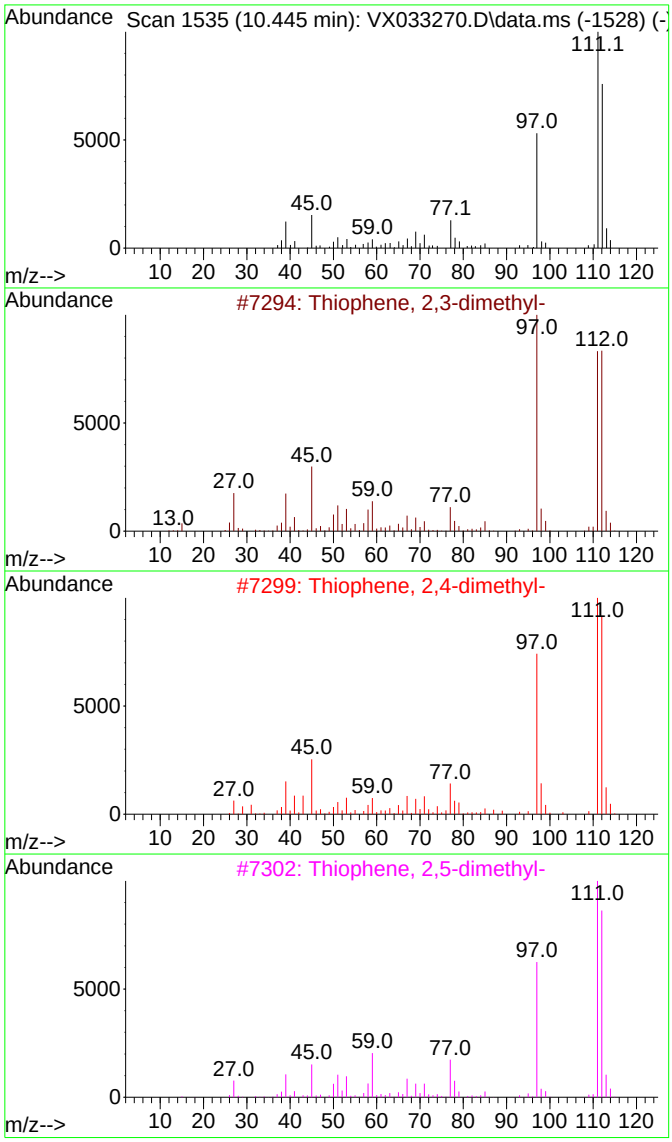
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

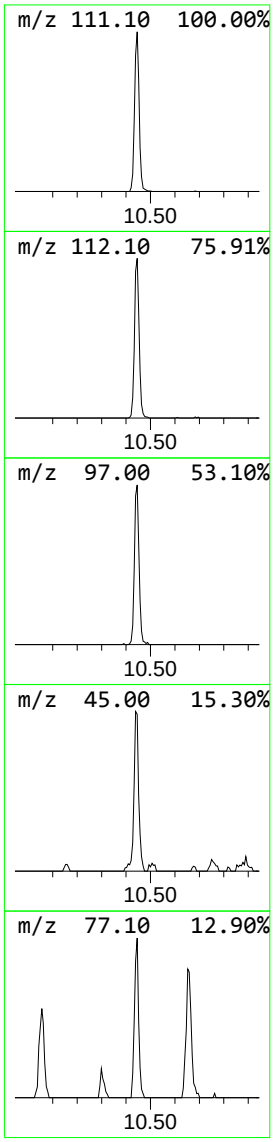
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Thiophene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	8.15 ug/l	89548	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	94
2	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	91
3	Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
4	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	90
5	2-Thiophenecarboxaldehyde	112	C5H4OS	000098-03-3	59





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ClientSampleId :
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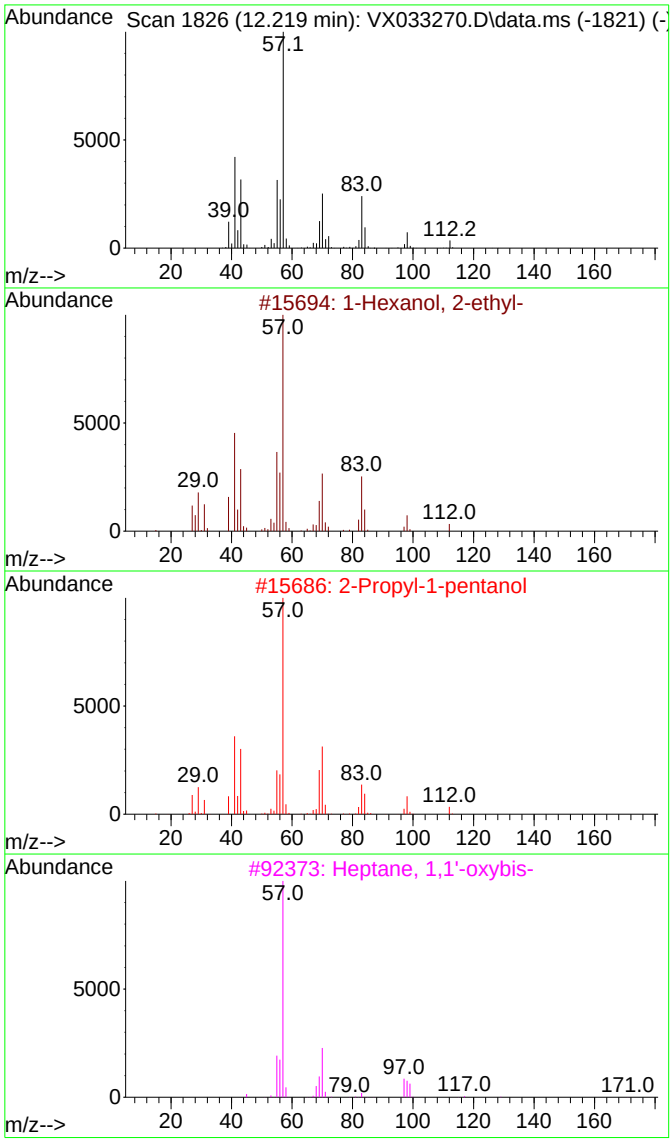
Quant Title : SW846 8260

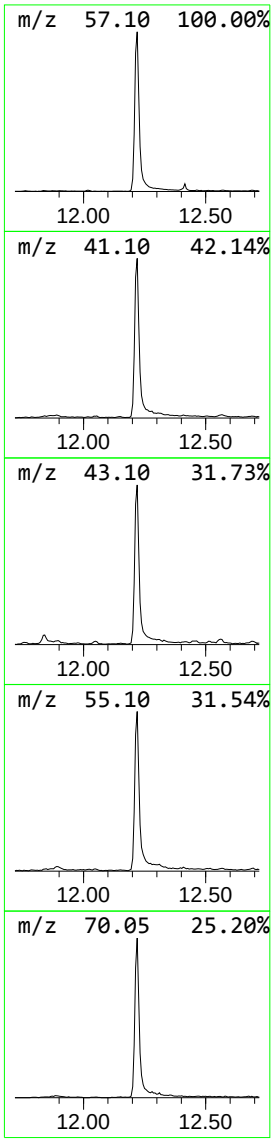
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	62.82 ug/l	680865	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	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47
5	Carbonic acid, butyl 2-ethylhexy...	230	C13H26O3	1000357-84-4	42





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

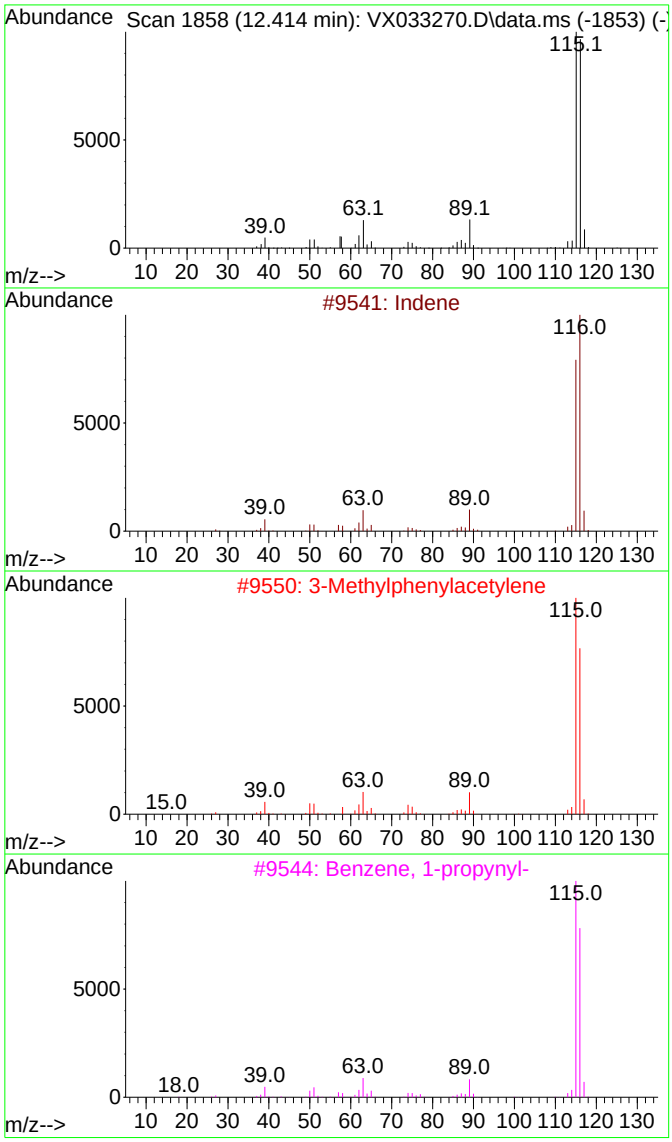
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

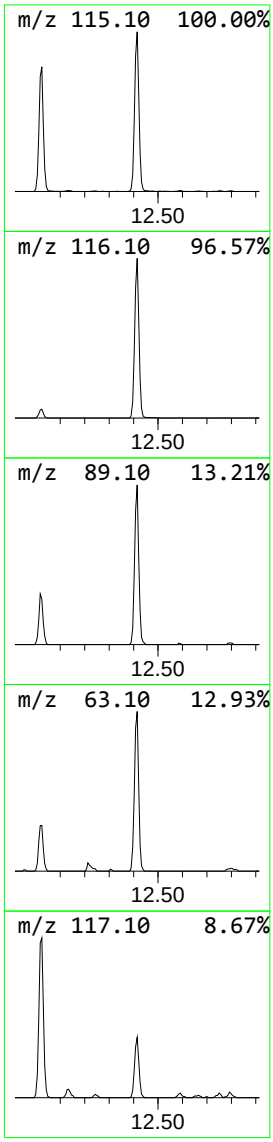
****

Peak Number 4 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	19.05 ug/l	206470	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90





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
Butanal	4.233	38.1	ug/l	293144	1	5.550	384766	50.0
Thiophene, 2,3-...	10.445	8.2	ug/l	89548	3	10.055	549463	50.0
1-Hexanol, 2-et...	12.219	62.8	ug/l	680865	4	12.024	541916	50.0
Indene	12.414	19.1	ug/l	206470	4	12.024	541916	50.0