LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 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: VX033245.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	41	44	51	rVB	10501	11547	1.60%	0.207%
2	2.392	205	214	226	rBV	114686	230484	32.02%	4.134%
3	2.593	236	247	258	rBV4	2567	12739	1.77%	0.228%
4	2.703	260	265	273	rVV	4929	10062	1.40%	0.180%
5	2.989	296	312	324	rBV3	10425	52225	7.25%	0.937%
6	3.331	360	368	378	rVB4	4252	10293	1.43%	0.185%
7	3.696	419	428	441	rVB2	5899	15962	2.22%	0.286%
8	4.227	503	515	530	rBV	117870	323540	44.94%	5.803%
9	4.568	560	571	588	rBV	24218	74416	10.34%	1.335%
10	5.385	692	705	721	rBV2	62518	183029	25.43%	3.283%
11	5.556	721	733	748	rVV	129837	371659	51.63%	6.666%
12	5.958	789	799	810	rBV	63577	168707	23.44%	3.026%
13	6.763	922	931	948	rVB	195913	463952	64.45%	8.321%
14	7.464	1040	1046	1052	rBV2	6283	12751	1.77%	0.229%
15	7.580	1060	1065	1072	rVB2	9475	18550	2.58%	0.333%
16	8.135	1145	1156	1173	rBV	13910	33475	4.65%	0.600%
17	8.439	1199	1206	1212	rBV2	4144	8798	1.22%	0.158%
18	8.574	1222	1228	1234	rBV	20943	34761	4.83%	0.623%
19	8.647	1234	1240	1248	rVV	288638	448874	62.36%	8.050%
20	8.720	1248	1252	1257	rVV	9126	14543	2.02%	0.261%
21	8.781	1257	1262	1269	rVV4	6346	15157	2.11%	0.272%
22	8.854	1269	1274	1280	rVB5	3897	7904	1.10%	0.142%
23	8.970	1288	1293	1299	rBV2	9910	19956	2.77%	0.358%
24	9.537	1382	1386	1394	rVB3	4643	8129	1.13%	0.146%
25	10.055	1462	1471	1483	rBV	394897	531109	73.78%	9.525%
26	10.159	1483	1488	1491	rBV2	6545	10240	1.42%	0.184%
27	10.195	1491	1494	1500	rVB	5924	8188	1.14%	0.147%
28	10.299	1507	1511	1518	rVB	11111	17615	2.45%	0.316%
29	10.445	1530	1535	1541	rVB	72813	95309	13.24%	1.709%
30	10.506	1541	1545	1552	rVB	7538	10082	1.40%	0.181%
31	10.659	1560	1570	1572	rBV2	34718	54754	7.61%	0.982%
32	10.683	1572	1574	1581	rVB	32303	35726	4.96%	0.641%
33	10.756	1581	1586	1594	rBV2	18101	37898	5.26%	0.680%
34	11.079	1634	1639	1645	rBV	257611	329556	45.78%	5.910%
35	11.305	1673	1676	1682	rVB2	5007	7412	1.03%	0.133%
36	11.427	1690	1696	1701	rVV2	10558	17670	2.45%	0.317%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 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

37	11.482	1701	1705	1714	rVB	6660	10753	1.49%	0.193%
38	11.573	1714	1720	1723	rBV3	7720	11408	1.58%	0.205%
39	11.610	1723	1726	1728	rVV3	8087	13323	1.85%	0.239%
40	11.634	1728	1730	1734	rVB	10009	10252	1.42%	0.184%
41	11.756	1743	1750	1754	rBV2	9431	12646	1.76%	0.227%
42	11.805	1754	1758	1761	rVV	11655	16681	2.32%	0.299%
43	11.841	1761	1764	1767	rVV3	12364	20254	2.81%	0.363%
44	11.890	1770	1772	1780	rVB3	8691	13966	1.94%	0.250%
45	12.024	1788	1794	1802	rVB	385088	508329	70.61%	9.117%
46	12.152	1808	1815	1820	rVB5	4060	8709	1.21%	0.156%
47	12.219	1820	1826	1838	rBV	498572	719867	100.00%	12.911%
48	12.311	1838	1841	1846	rVB6	12029	21641	3.01%	0.388%
49	12.414	1853	1858	1863	rBV	173015	216566	30.08%	3.884%
50	12.567	1878	1883	1889	rBV5	8239	15761	2.19%	0.283%
51	12.695	1901	1904	1911	rVB5	5942	9237	1.28%	0.166%
52	12.768	1911	1916	1918	rBV4	6227	9334	1.30%	0.167%
53	12.798	1918	1921	1927	rVB5	8402	13844	1.92%	0.248%
54	13.170	1978	1982	1988	rBV7	4826	10406	1.45%	0.187%
55	13.286	1995	2001	2007	rVV9	6785	13761	1.91%	0.247%
56	13.341	2007	2010	2015	rVV3	7333	9330	1.30%	0.167%
57	13.420	2018	2023	2030	rVB	16226	28222	3.92%	0.506%
58	13.658	2059	2062	2068	rBV8	4305	8946	1.24%	0.160%
59	13.774	2077	2081	2084	rBV	20742	27244	3.78%	0.489%
60	13.804	2084	2086	2090	rVV	13500	15545	2.16%	0.279%
61	13.847	2090	2093	2099	rVV6	8378	12536	1.74%	0.225%
62	13.914	2100	2104	2110	rVB4	7942	12587	1.75%	0.226%
63	14.134	2136	2140	2144	rVB2	5238	8149	1.13%	0.146%
64	14.640	2216	2223	2226	rBV	16004	25734	3.57%	0.462%
65	14.780	2240	2246	2250	rBV	12983	17483	2.43%	0.314%
66	15.475	2356	2360	2365	rBV3	5532	8256	1.15%	0.148%
67	15.615	2378	2383	2386	rBV3	7011	12035	1.67%	0.216%
68	15.841	2412	2420	2426	rBV5	3379	7540	1.05%	0.135%
69	15.969	2436	2441	2449	rBV8	8967	18381	2.55%	0.330%

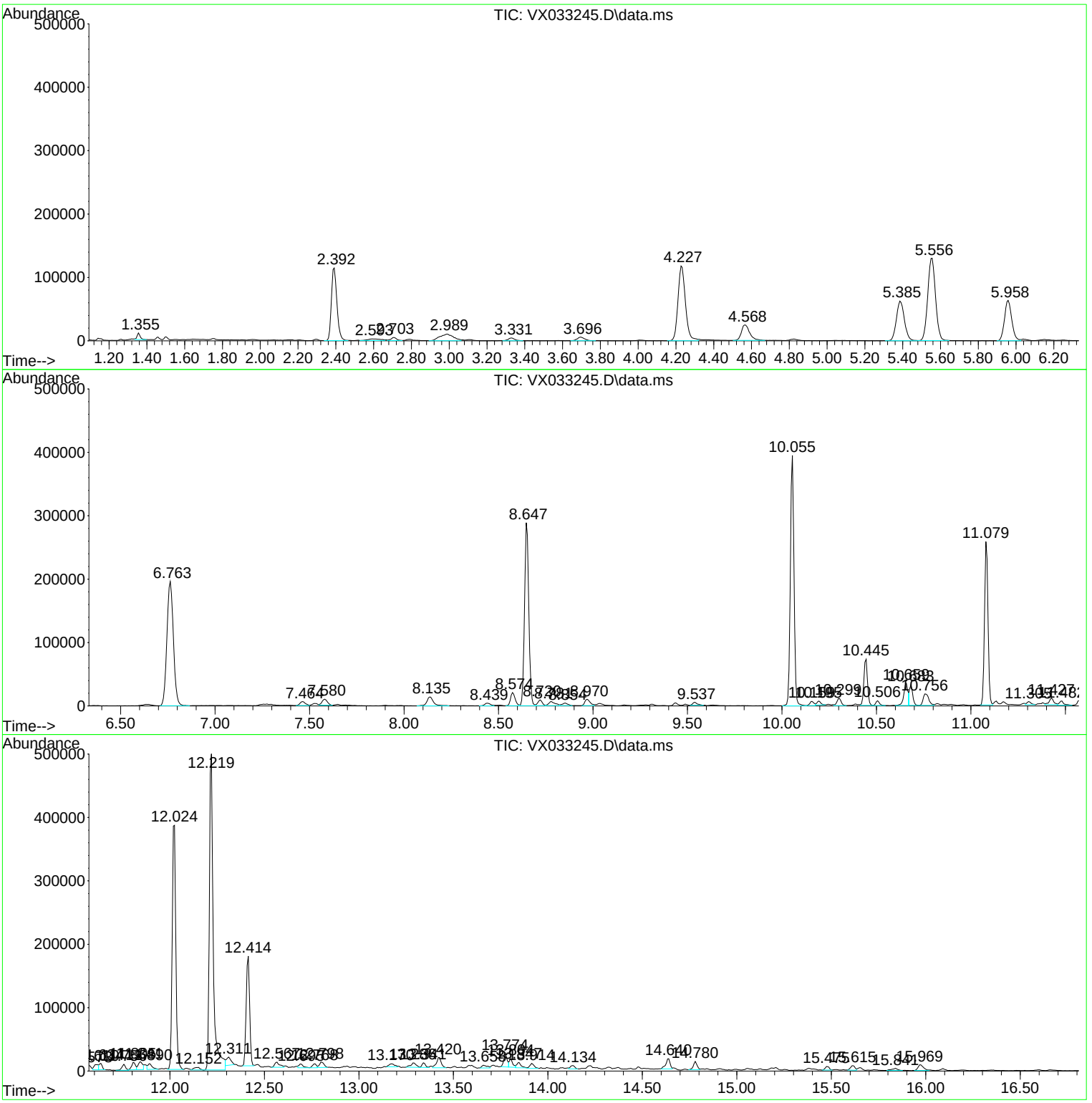
Sum of corrected areas: 5575798

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

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

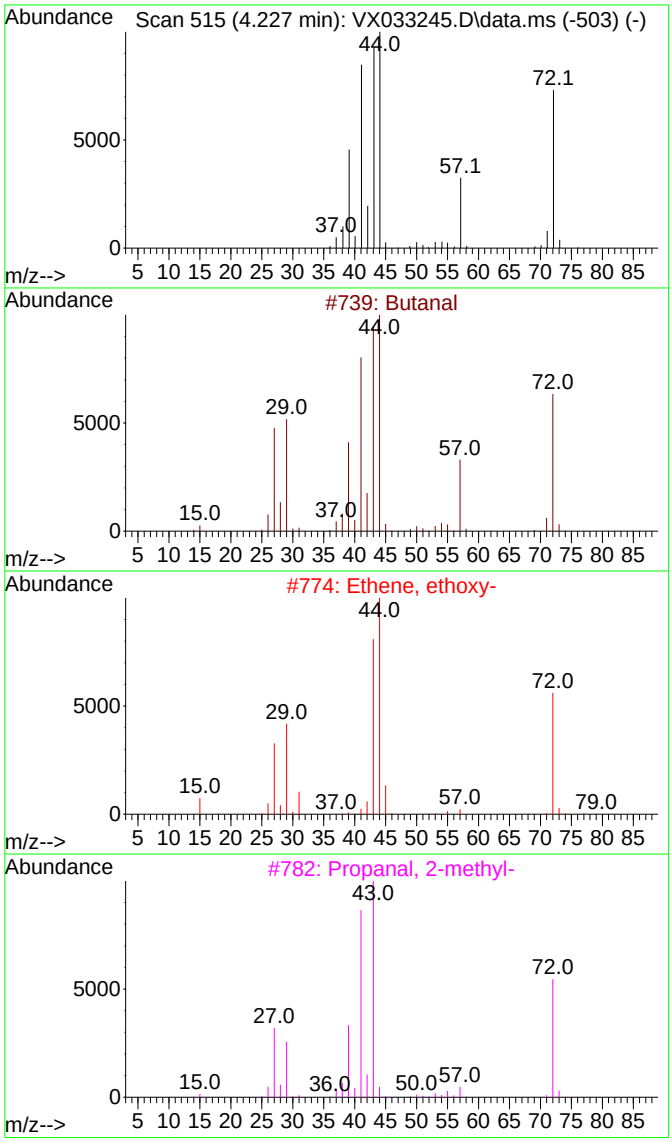
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

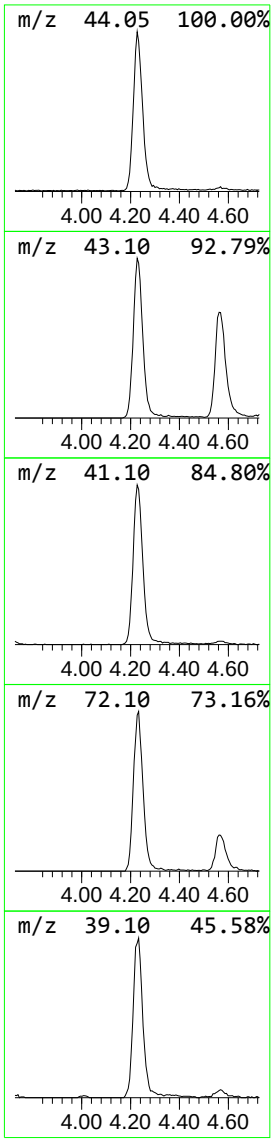
****

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	43.53 ug/l	323540	Pentafluorobenzene	5.556

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	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

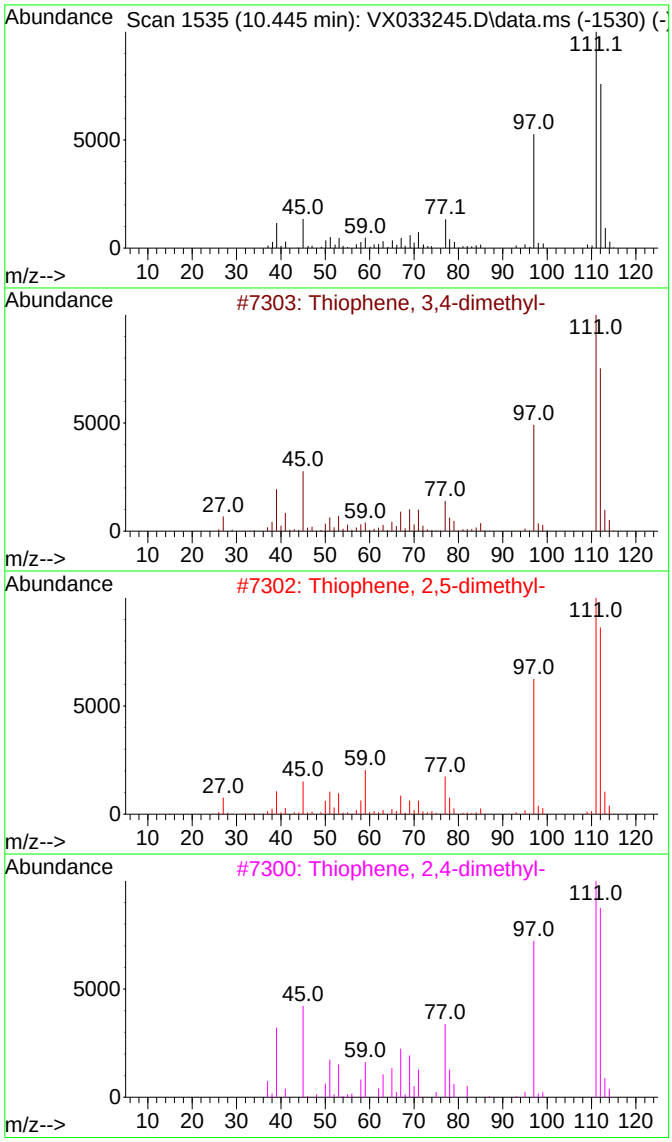
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

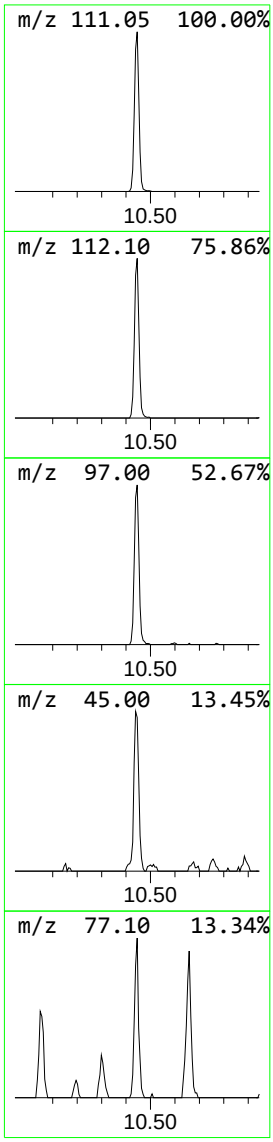
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	8.97 ug/l	95309	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	91
2	Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
3	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	87
4	Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	86
5	2-Thiophenecarboxaldehyde	112	C5H4OS	000098-03-3	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

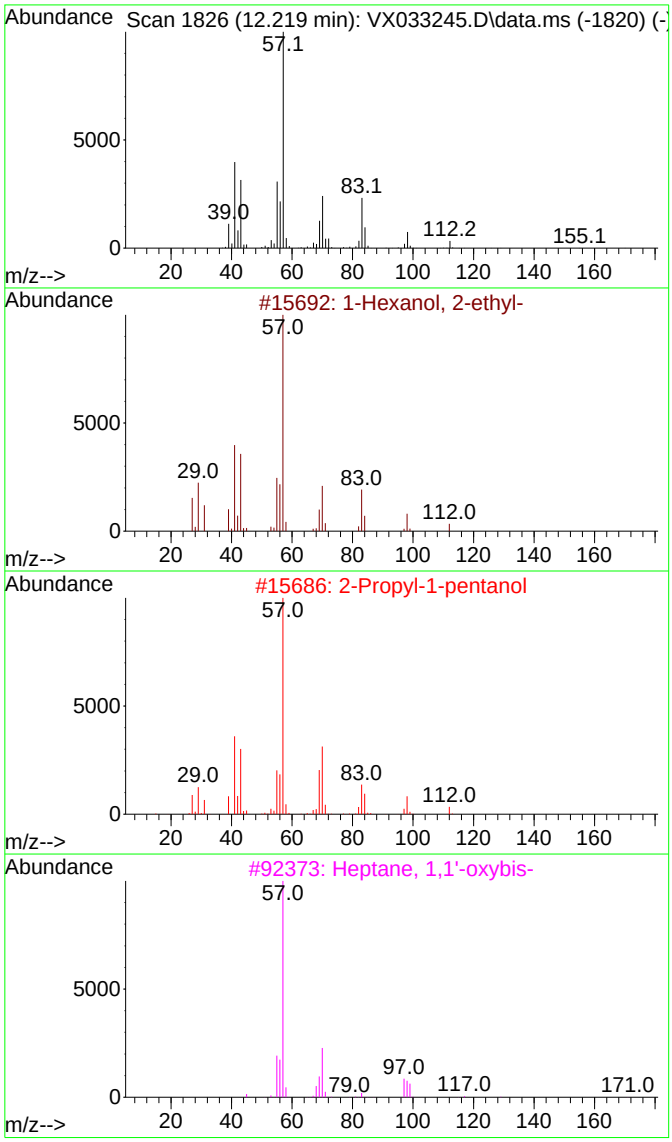
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

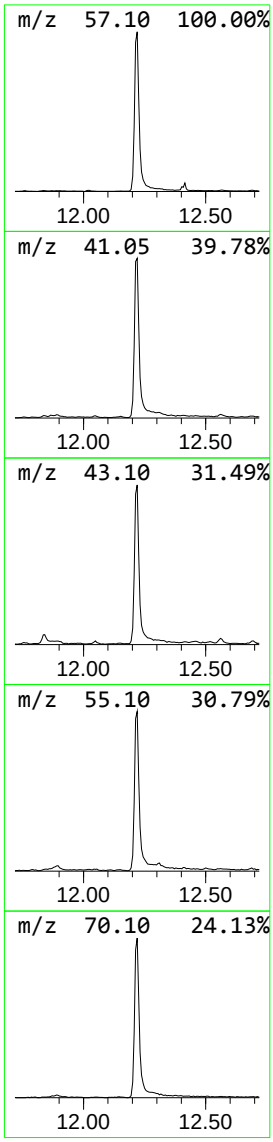
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	70.81 ug/l	719867	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	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	43
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31910

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

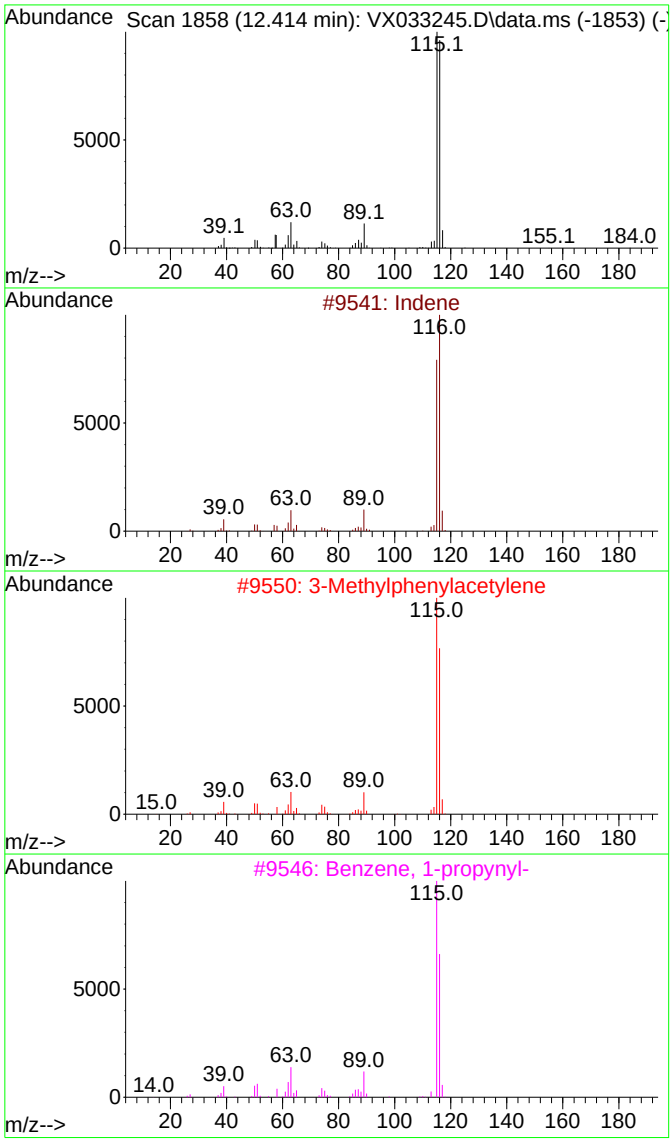
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

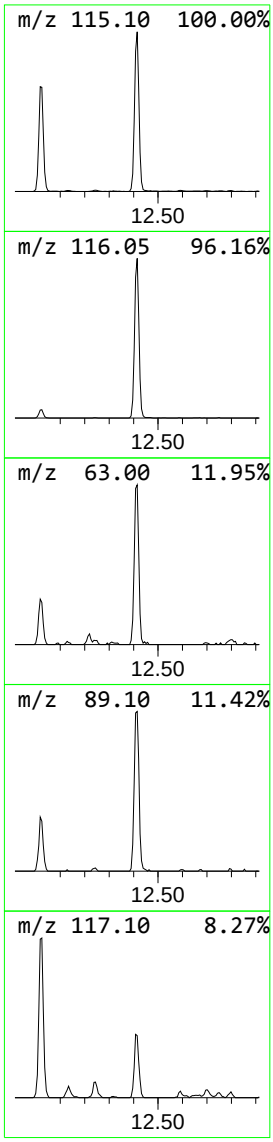
****

Peak Number 4 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	21.30 ug/l	216566	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	87
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
Data File : VX033245.D
Acq On : 05 Dec 2022 22:45
Operator : JC/MD
Sample : N5859-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	4.227	43.5	ug/l	323540	1	5.556	371659	50.0
Thiophene, 3,4-...	10.445	9.0	ug/l	95309	3	10.055	531109	50.0
1-Hexanol, 2-et...	12.219	70.8	ug/l	719867	4	12.024	508329	50.0
Indene	12.414	21.3	ug/l	216566	4	12.024	508329	50.0