LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072606.D
Acq On : 24 May 2022 23:20
Operator : JC\MD
Sample : N2968-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-31

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_N\methods\82N052422W.M
Title : SW846 8260

Signal : TIC: VN072606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	36	49	66	rBV	137668	652783	75.26%	8.797%
2	3.122	186	193	206	rVB5	14230	40596	4.68%	0.547%
3	3.510	249	259	266	rVB5	3691	10800	1.25%	0.146%
4	3.987	331	340	345	rBV4	3443	8938	1.03%	0.120%
5	4.569	428	439	444	rBV5	3985	13444	1.55%	0.181%
6	5.187	539	544	556	rVB5	6102	18871	2.18%	0.254%
7	5.351	560	572	585	rBV3	16853	60616	6.99%	0.817%
8	5.610	601	616	634	rBV3	176818	642705	74.10%	8.661%
9	6.475	754	763	764	rBV2	9246	13673	1.58%	0.184%
10	7.145	868	877	885	rBV3	13939	40144	4.63%	0.541%
11	8.016	1016	1025	1030	rBV	98985	233955	26.97%	3.153%
12	8.081	1030	1036	1046	rVB	172046	388976	44.84%	5.242%
13	8.445	1086	1098	1110	rBV3	153119	470497	54.24%	6.340%
14	8.963	1178	1186	1198	rBV	277875	559882	64.55%	7.545%
15	9.451	1265	1269	1275	rVB5	4631	9452	1.09%	0.127%
16	9.969	1352	1357	1362	rBV2	5923	9927	1.14%	0.134%
17	10.192	1390	1395	1405	rBV4	4368	9352	1.08%	0.126%
18	10.439	1428	1437	1444	rBV	429176	795021	91.66%	10.714%
19	10.498	1444	1447	1455	rVB2	8204	13468	1.55%	0.181%
20	10.639	1464	1471	1477	rVB	17552	31036	3.58%	0.418%
21	10.710	1477	1483	1490	rVB2	17613	31511	3.63%	0.425%
22	11.739	1650	1658	1670	rBV	457070	783681	90.35%	10.561%
23	11.839	1670	1675	1682	rVB	32200	55639	6.41%	0.750%
24	11.951	1686	1694	1703	rBV2	34830	66105	7.62%	0.891%
25	12.274	1744	1749	1756	rVB2	11468	19308	2.23%	0.260%
26	12.574	1794	1800	1807	rBV	42012	63806	7.36%	0.860%
27	12.727	1819	1826	1838	rBV	437679	732262	84.42%	9.868%
28	12.916	1852	1858	1866	rVB	33659	54688	6.30%	0.737%
29	13.216	1903	1909	1916	rVB	30728	45532	5.25%	0.614%
30	13.363	1929	1934	1941	rVB	13509	22413	2.58%	0.302%
31	13.492	1949	1956	1960	rBV4	4912	9525	1.10%	0.128%
32	13.669	1979	1986	2000	rBV	493824	867400	100.00%	11.689%
33	13.868	2009	2020	2027	rBV	168714	311695	35.93%	4.200%
34	14.057	2046	2052	2058	rVB3	6608	11334	1.31%	0.153%
35	14.210	2073	2078	2084	rBV	17786	26352	3.04%	0.355%
36	14.274	2084	2089	2092	rVV3	9669	14143	1.63%	0.191%

LSC Area Percent Report

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ALS Vial : 26 Sample Multiplier: 1

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Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Title : SW846 8260

37	14.321	2092	2097	2104	rVB2	52349	88628	10.22%	1.194%
38	14.533	2127	2133	2138	rBV	16458	27820	3.21%	0.375%
39	14.804	2173	2179	2187	rVB2	14063	23607	2.72%	0.318%
40	14.915	2192	2198	2206	rBV3	26897	60800	7.01%	0.819%
41	15.080	2220	2226	2230	rBV4	7565	13234	1.53%	0.178%
42	15.186	2238	2244	2249	rBV7	7764	14897	1.72%	0.201%
43	15.304	2256	2264	2271	rVB7	7900	18074	2.08%	0.244%
44	15.498	2287	2297	2304	rBV2	17313	34135	3.94%	0.460%

Sum of corrected areas: 7420725

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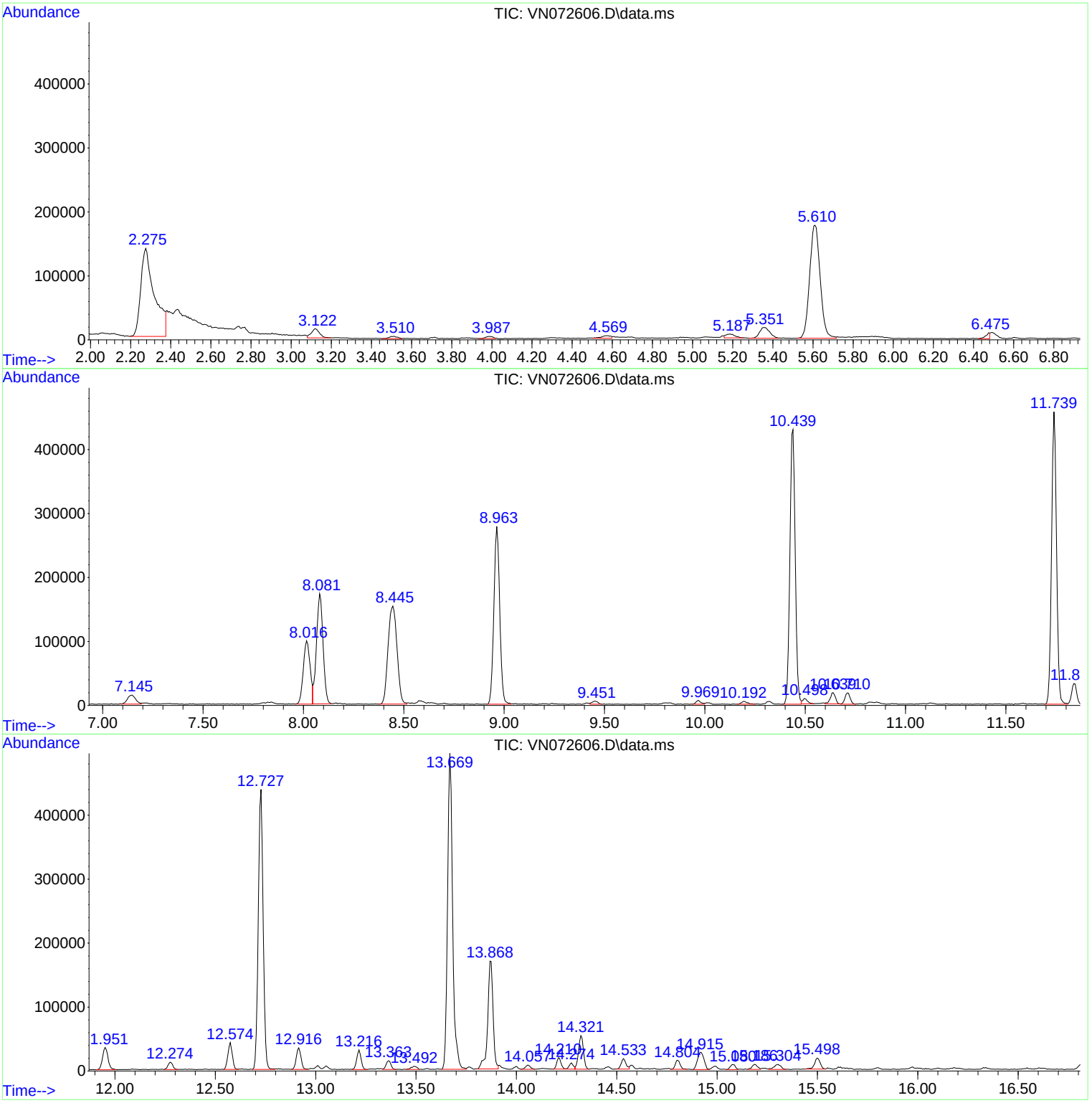
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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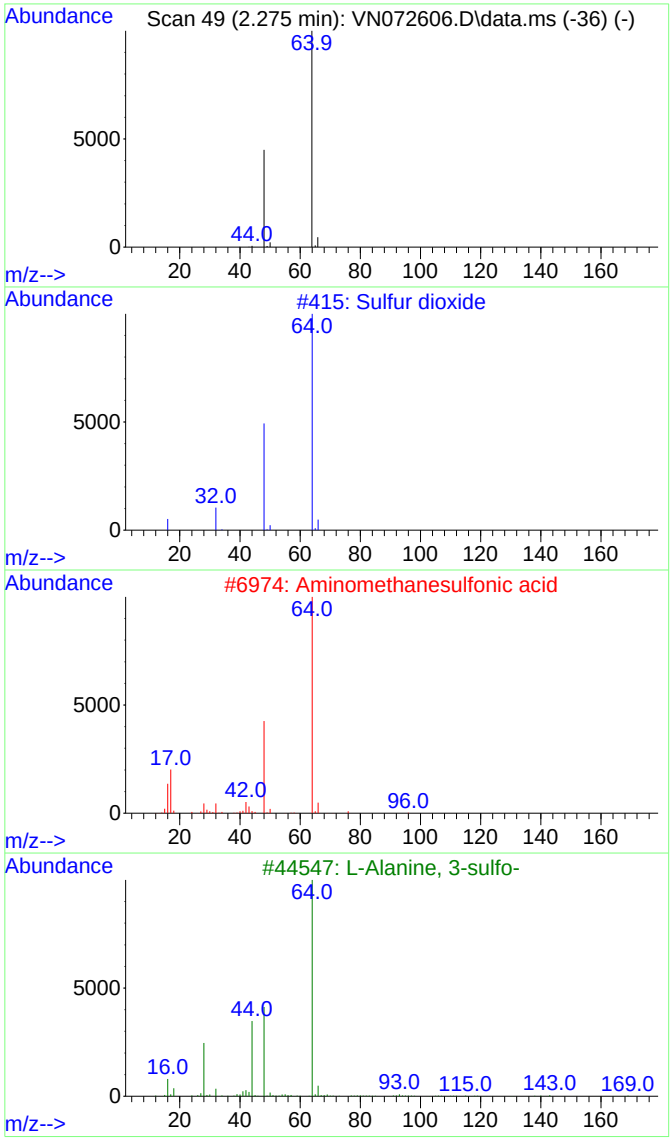
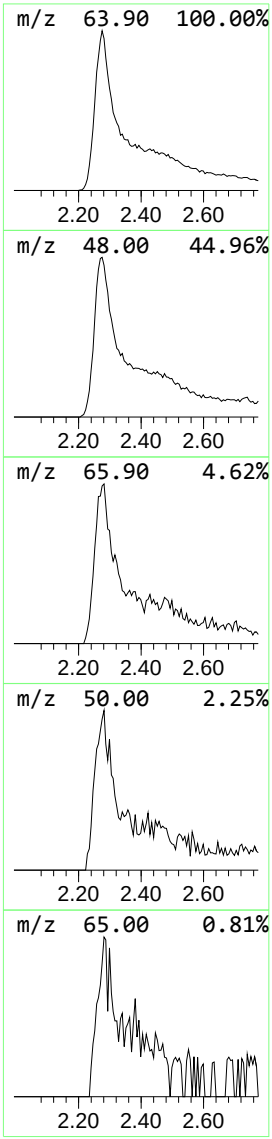
****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	83.91 ug/l	652783	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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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ClientSampleId :
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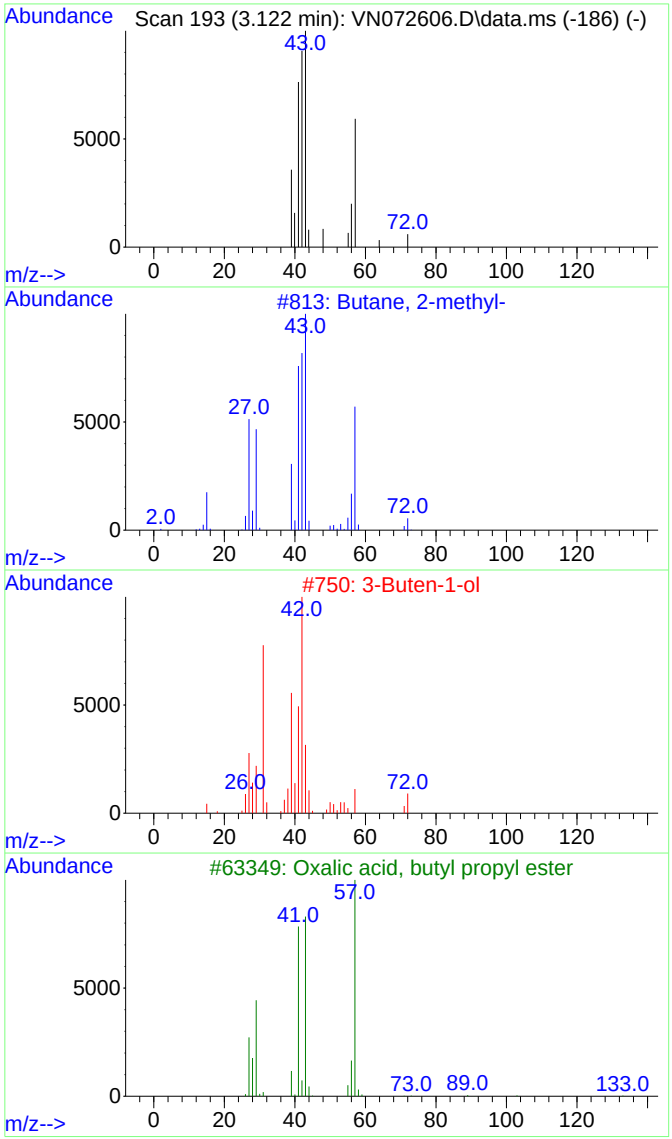
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

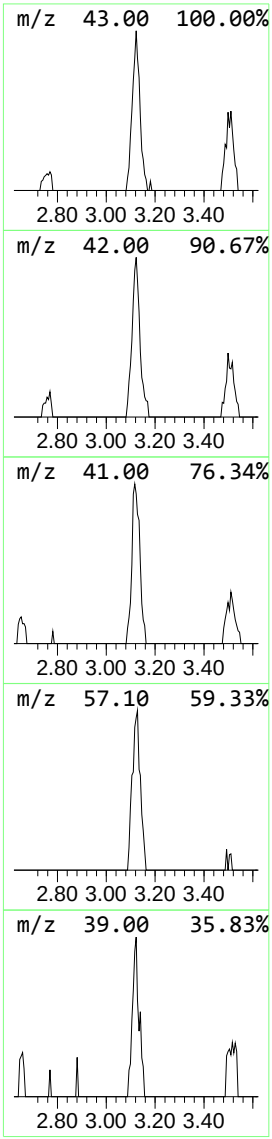
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	5.22 ug/l	40596	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	37
3	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	9
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	9
5	Pentane	72	C5H12	000109-66-0	9





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MSVOA_N
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TIC Library : C:\Database\NIST20.L
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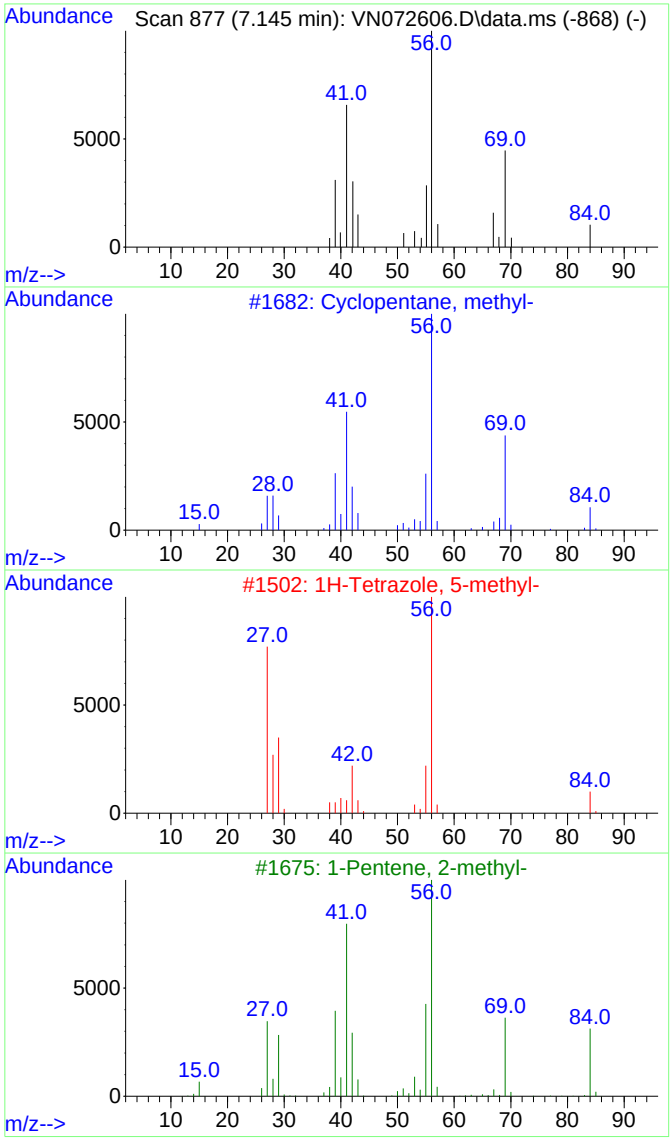
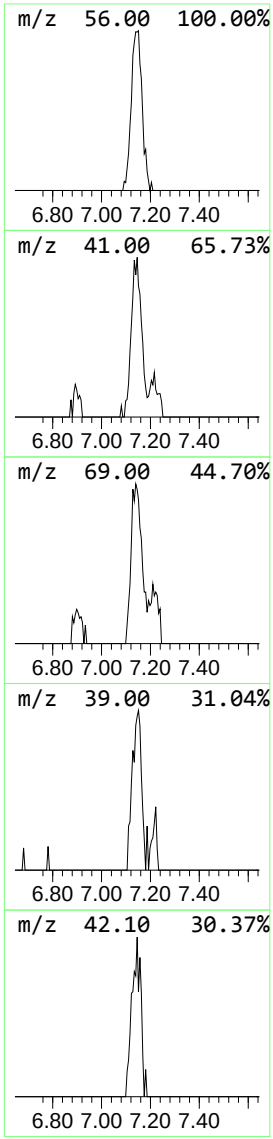
****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	5.16 ug/l	40144	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	40
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	40





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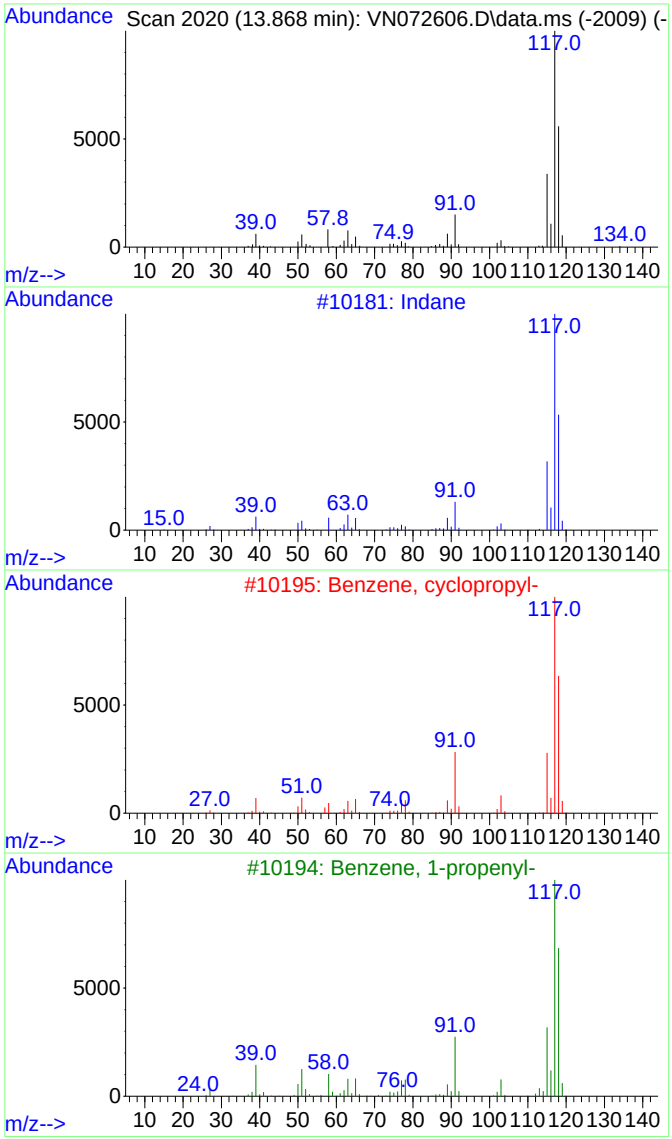
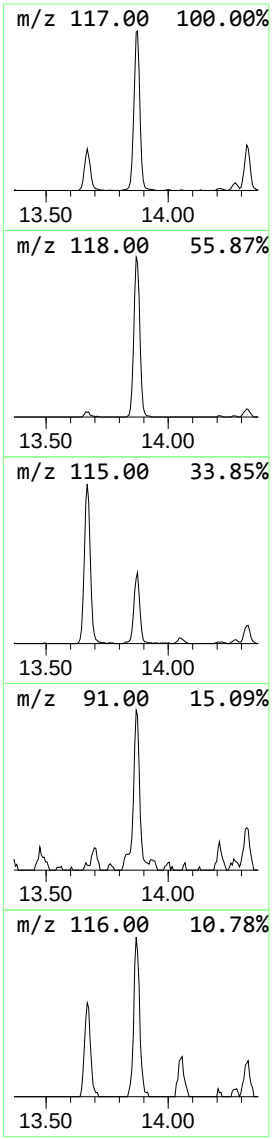
****
Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	17.97 ug/l	311695	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	80
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	80
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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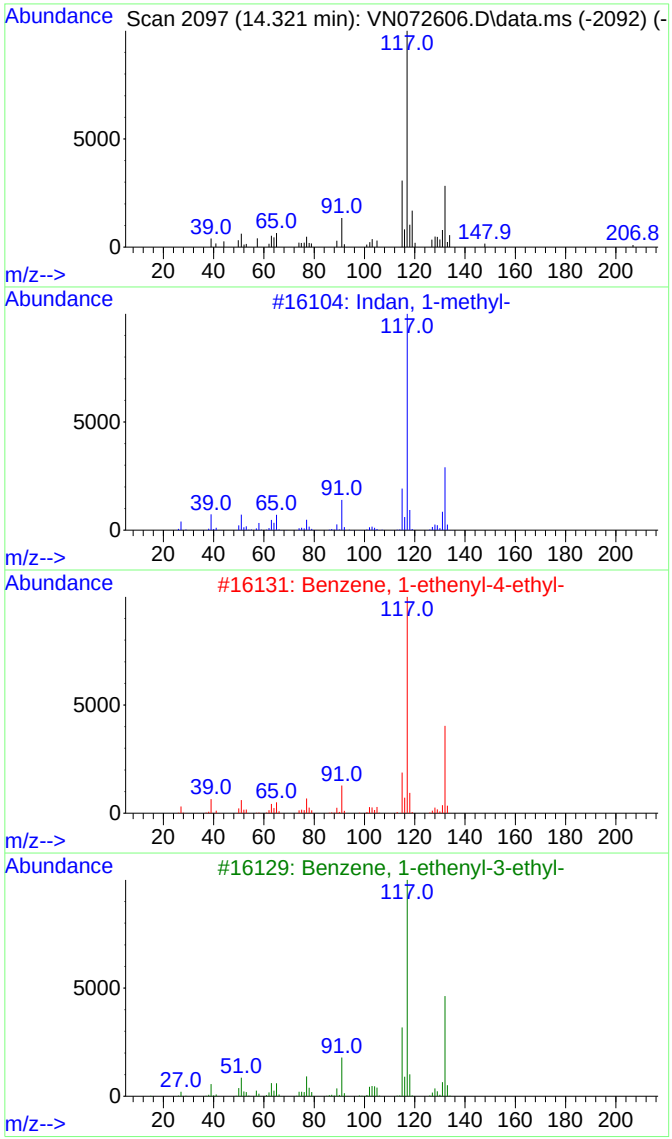
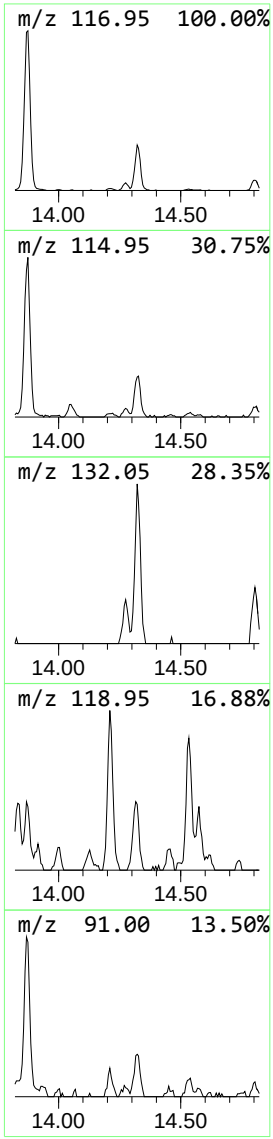
****
Peak Number 5 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	5.11 ug/l	88628	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	76
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74
4	Benzene, 1-pentenyl-	146	C11H14	000826-18-6	53
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	46





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	2.275	83.9	ug/l	652783	1	8.081	388976	50.0
Butane, 2-methyl-	3.122	5.2	ug/l	40596	1	8.081	388976	50.0
Cyclopentane, m...	7.145	5.2	ug/l	40144	1	8.081	388976	50.0
Indane	13.868	18.0	ug/l	311695	4	13.669	867400	50.0
Indan, 1-methyl-	14.321	5.1	ug/l	88628	4	13.669	867400	50.0