LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073139.D
Acq On : 26 Jun 2022 04:56
Operator : JC\MD
Sample : N3501-01 40X
Misc : 4.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
B2208-28

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\82N061722W.M
Title : SW846 8260

Signal : TIC: VN073139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.081	195	203	212	rBV2	47905	112361	5.94%	0.784%
2	3.457	259	267	282	rVB2	20688	54364	2.87%	0.379%
3	5.063	516	540	557	rBV3	50983	241387	12.76%	1.684%
4	5.528	608	619	633	rBV4	33098	117397	6.21%	0.819%
5	6.034	695	705	715	rVB4	18017	53393	2.82%	0.373%
6	6.963	852	863	872	rBV5	25790	81366	4.30%	0.568%
7	7.069	872	881	891	rVB3	19675	55623	2.94%	0.388%
8	7.239	902	910	924	rVB	16216	47869	2.53%	0.334%
9	7.951	1021	1031	1036	rBV	242401	606789	32.08%	4.234%
10	8.016	1036	1042	1050	rVV	505765	1194894	63.18%	8.337%
11	8.098	1051	1056	1069	rVB2	67492	170386	9.01%	1.189%
12	8.228	1069	1078	1086	rBV	46547	108864	5.76%	0.760%
13	8.369	1093	1102	1111	rBV	253971	578178	30.57%	4.034%
14	8.545	1116	1132	1144	rVV	222171	576922	30.50%	4.025%
15	8.645	1144	1149	1157	rVB5	10090	24955	1.32%	0.174%
16	8.757	1159	1168	1180	rVB3	21620	48876	2.58%	0.341%
17	8.904	1182	1193	1206	rBV	662551	1409378	74.52%	9.834%
18	9.392	1263	1276	1281	rBV3	43321	113826	6.02%	0.794%
19	9.445	1281	1285	1293	rVV3	29955	58978	3.12%	0.412%
20	9.816	1340	1348	1358	rBV	89281	180158	9.53%	1.257%
21	9.951	1358	1371	1378	rBV	91812	199137	10.53%	1.389%
22	10.016	1378	1382	1385	rBV2	16983	27266	1.44%	0.190%
23	10.151	1398	1405	1416	rVB3	25508	70237	3.71%	0.490%
24	10.304	1425	1431	1436	rBV3	24259	43432	2.30%	0.303%
25	10.374	1436	1443	1457	rBV	881659	1665464	88.05%	11.620%
26	10.557	1468	1474	1483	rVB7	18704	47809	2.53%	0.334%
27	11.463	1624	1628	1633	rBV6	12523	23192	1.23%	0.162%
28	11.568	1641	1646	1651	rBV2	12419	23807	1.26%	0.166%
29	11.680	1658	1665	1675	rBV	971817	1681693	88.91%	11.734%
30	11.780	1678	1682	1687	rVB	39189	68394	3.62%	0.477%
31	11.892	1694	1701	1709	rBV	87904	194664	10.29%	1.358%
32	12.215	1748	1756	1766	rBV	46437	92284	4.88%	0.644%
33	12.668	1826	1833	1844	rVB	809283	1395375	73.77%	9.736%
34	12.857	1860	1865	1869	rBV	30750	55813	2.95%	0.389%
35	12.921	1871	1876	1878	rBV2	21998	39775	2.10%	0.278%
36	12.951	1878	1881	1884	rVV	36039	51456	2.72%	0.359%

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Integration Parameters: RTEINT.P
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Title : SW846 8260

37	12.998	1884	1889	1894	rVB	65597	107796	5.70%	0.752%
38	13.157	1912	1916	1922	rVB	37503	63986	3.38%	0.446%
39	13.304	1936	1941	1947	rBV	178344	268045	14.17%	1.870%
40	13.610	1986	1993	2008	rBV	1059840	1891398	100.00%	13.197%
41	13.810	2023	2027	2029	rVV2	41163	63829	3.37%	0.445%
42	13.845	2029	2033	2037	rVB3	50075	82664	4.37%	0.577%
43	14.068	2067	2071	2073	rBV2	27554	42110	2.23%	0.294%
44	14.151	2082	2085	2089	rVB	50350	66693	3.53%	0.465%
45	14.515	2143	2147	2150	rBV2	29693	42447	2.24%	0.296%
46	15.427	2298	2302	2309	rVB	81085	156308	8.26%	1.091%
47	16.527	2486	2489	2494	rVB5	19880	31223	1.65%	0.218%

Sum of corrected areas: 14332261

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Instrument :
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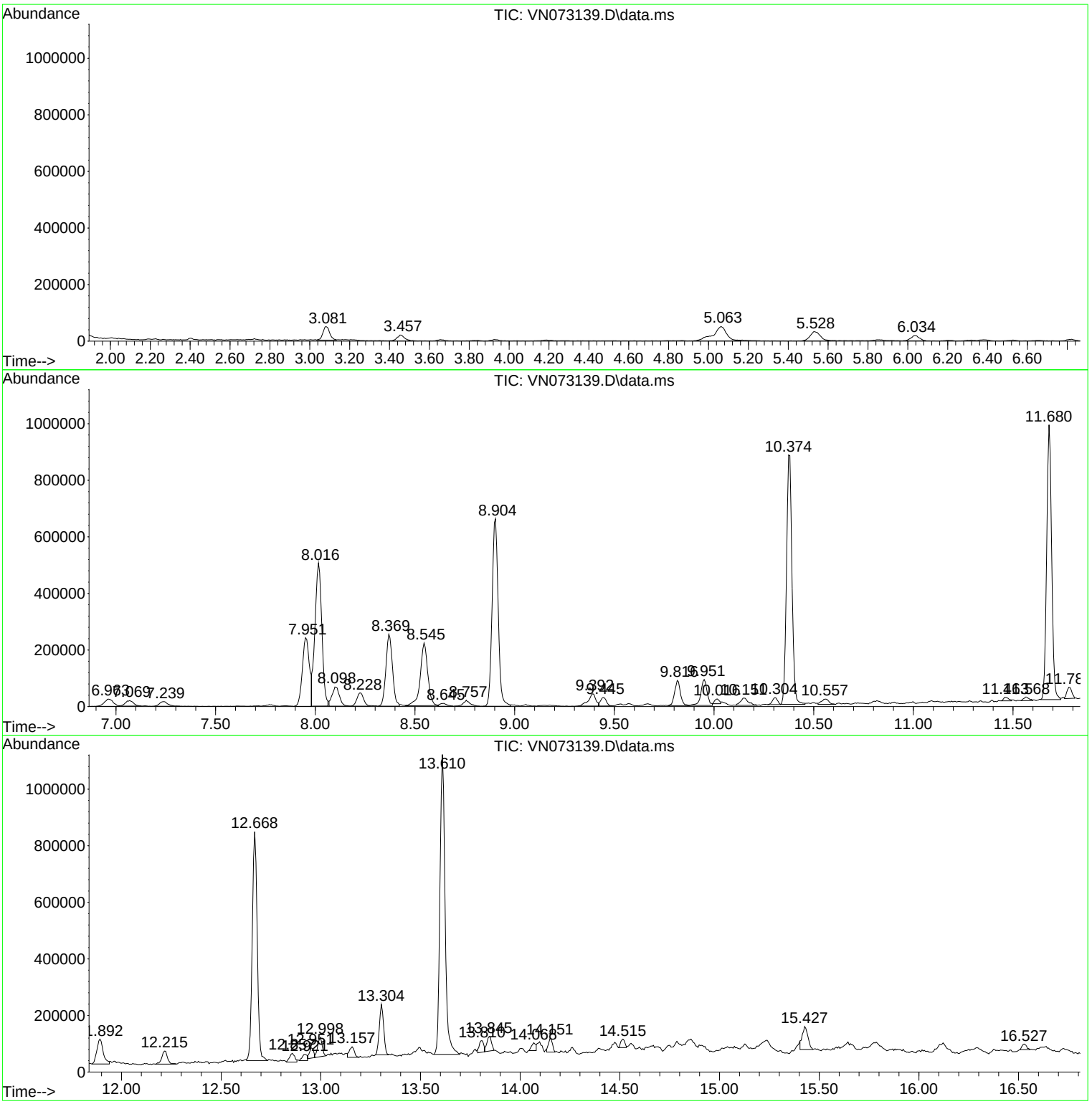
ClientSampleId :
B2208-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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_N\methods\82N061722W.M
Quant Title : SW846 8260

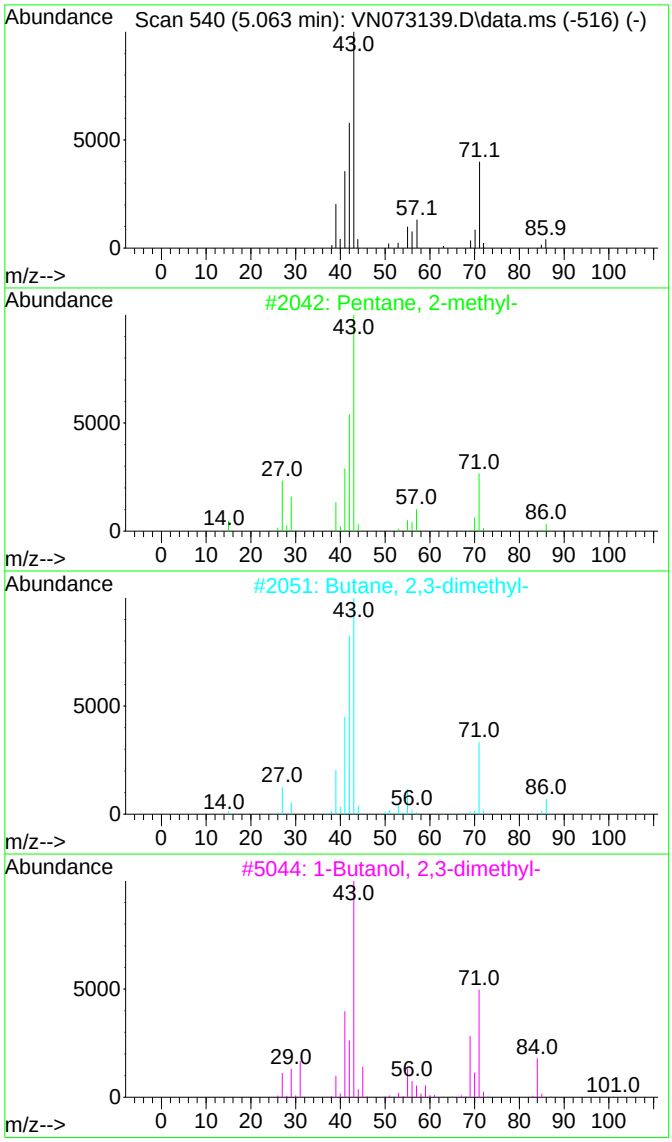
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

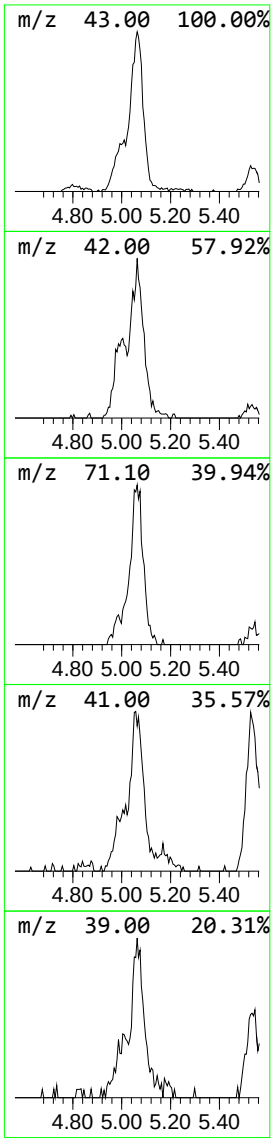
****

Peak Number 1 Pentane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	10.10 ug/l	241387	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5	Pentane	72	C5H12	000109-66-0	32





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Instrument :
MSVOA_N
ClientSampleId :
B2208-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

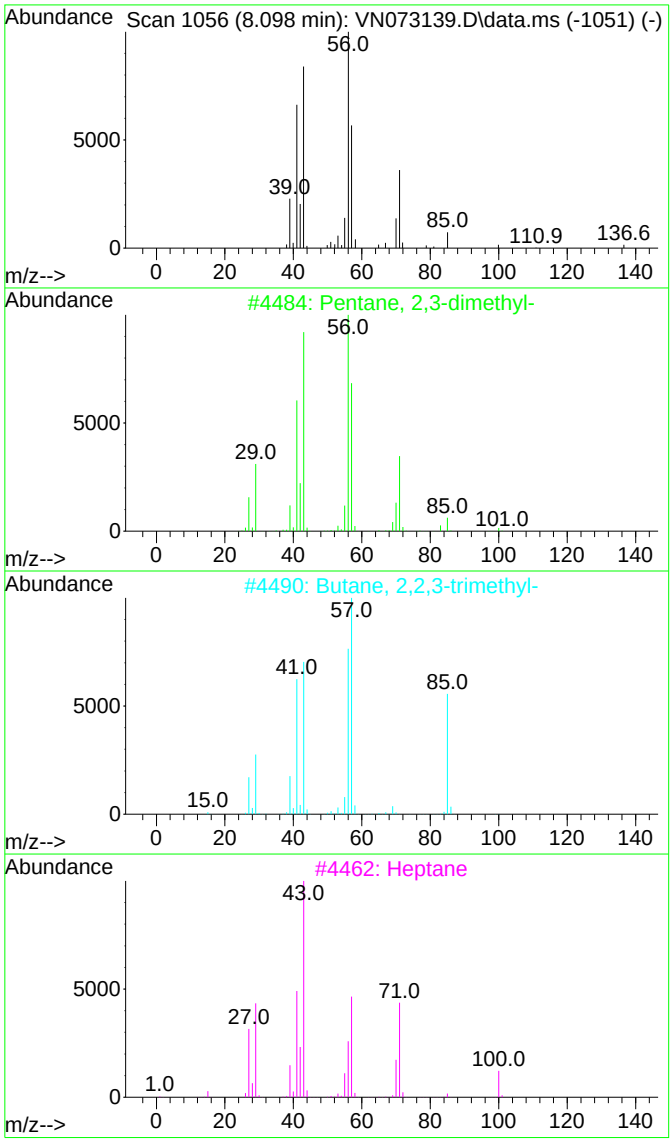
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

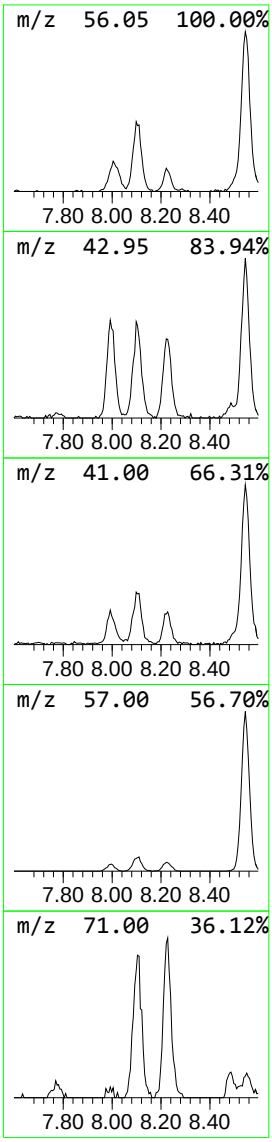
****

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	7.13 ug/l	170386	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	47
3	Heptane	100	C7H16	000142-82-5	47
4	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	43
5	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	40





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MSVOA_N
ClientSampleId :
B2208-28

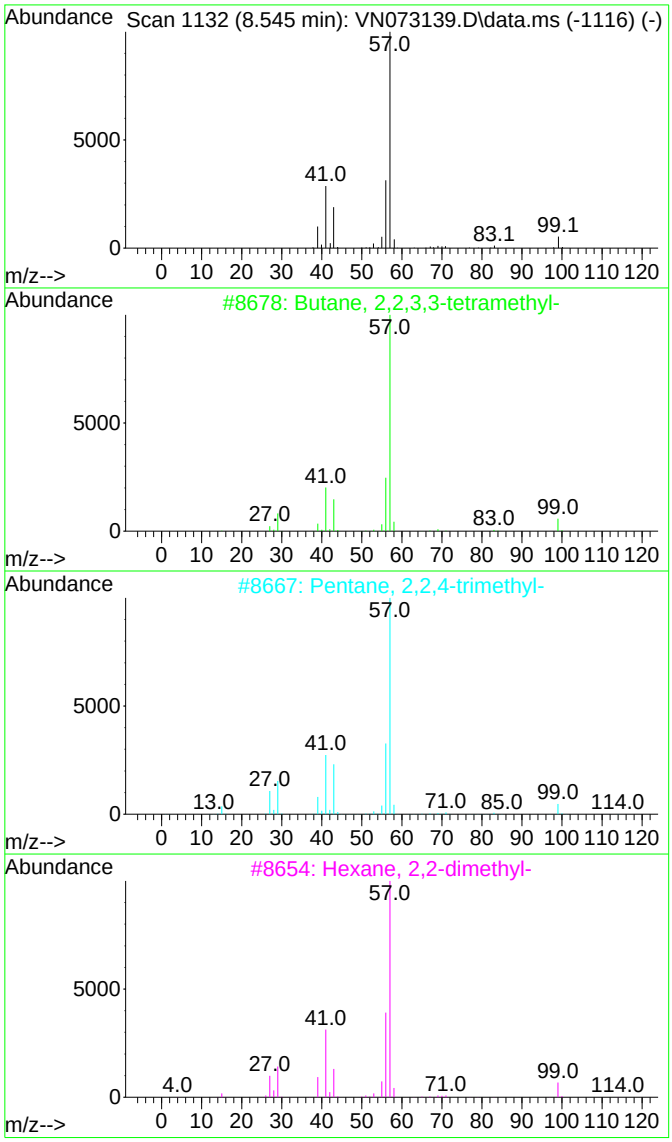
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

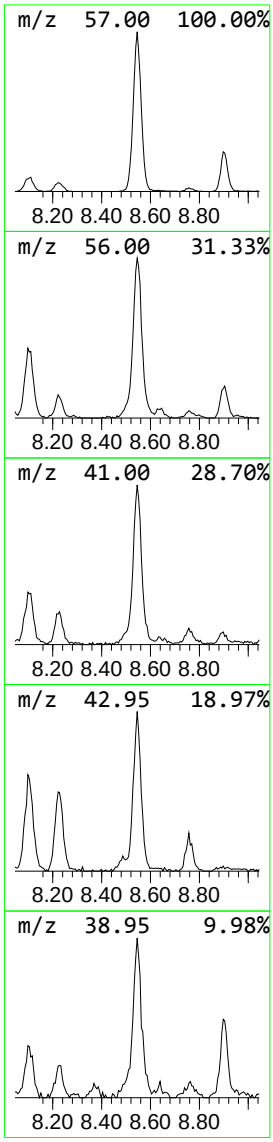
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	20.47 ug/l	576922	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





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MSVOA_N
ClientSampleId :
B2208-28

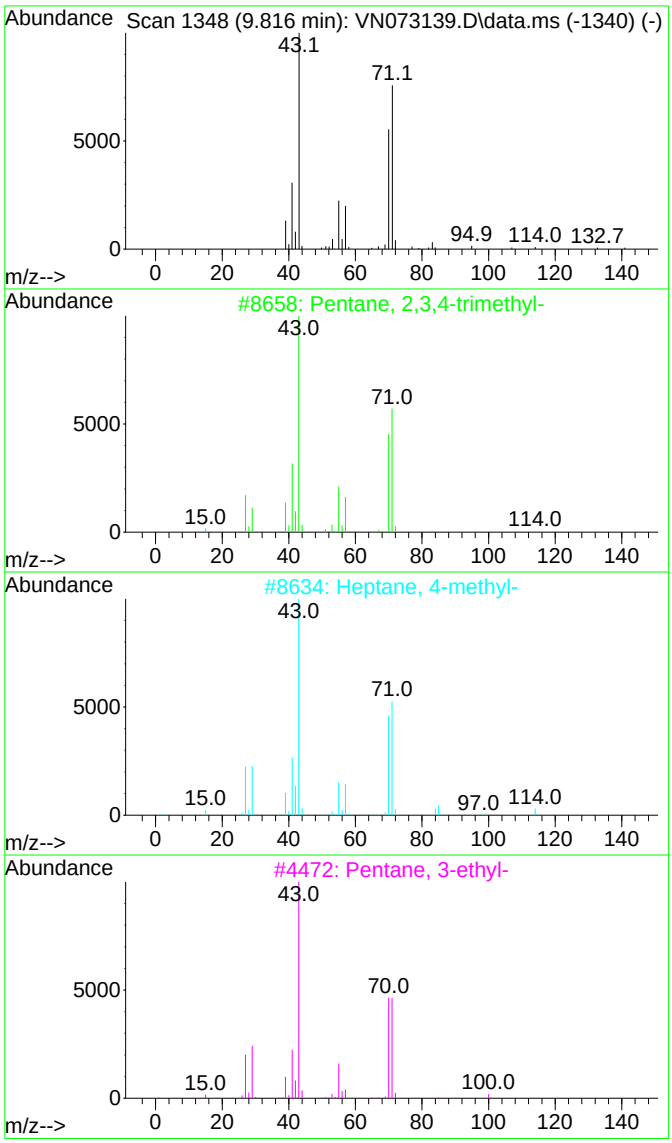
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

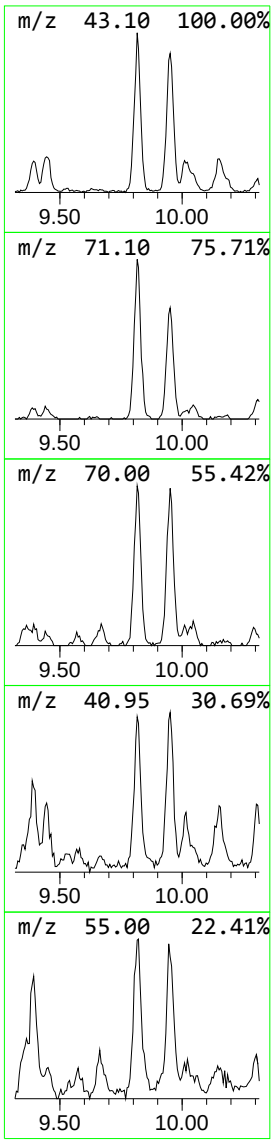
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	6.39 ug/l	180158	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
5	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78





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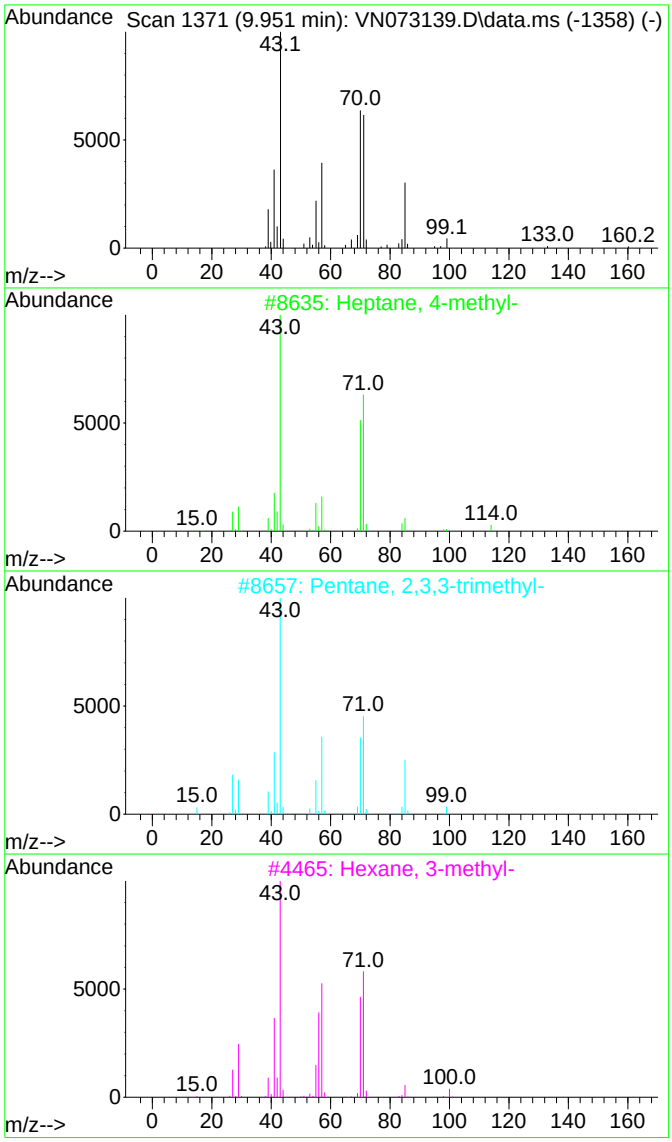
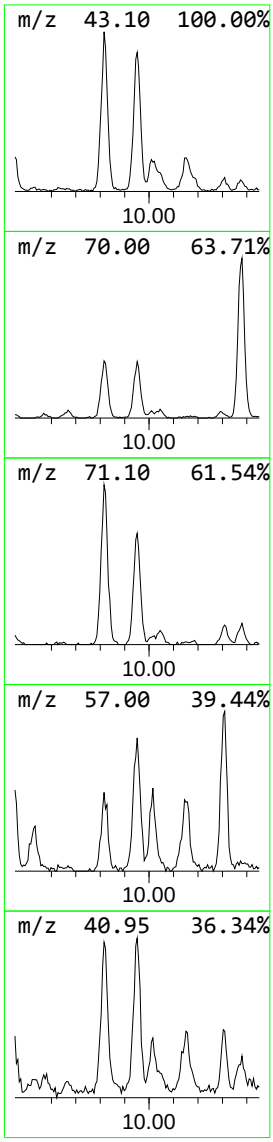
****

Peak Number 5 Heptane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	7.06 ug/l	199137	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 4-methyl-	114	C8H18	000589-53-7	72
2	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	72
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2-methyl-	5.063	10.1	ug/l	241387	1	8.016	1194890	50.0
Pentane, 2,3-di...	8.098	7.1	ug/l	170386	1	8.016	1194890	50.0
Butane, 2,2,3,3...	8.545	20.5	ug/l	576922	2	8.904	1409380	50.0
Pentane, 2,3,4-...	9.816	6.4	ug/l	180158	2	8.904	1409380	50.0
Heptane, 4-methyl-	9.951	7.1	ug/l	199137	2	8.904	1409380	50.0