LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN070015.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	158	168	182	rVB	282549	435722	2.92%	0.238%
2	3.113	400	419	458	rBV	1613237	3832541	25.67%	2.091%
3	3.497	543	562	596	rBV	758618	1950406	13.06%	1.064%
4	3.703	622	639	659	rVB3	110613	259121	1.74%	0.141%
5	3.977	723	741	767	rVB3	218043	586798	3.93%	0.320%
6	4.245	817	841	871	rBV5	65845	233505	1.56%	0.127%
7	4.948	1076	1103	1121	rBV9	50429	200228	1.34%	0.109%
8	5.071	1123	1149	1154	rBV2	379525	1047134	7.01%	0.571%
9	5.613	1322	1351	1388	rBV3	641593	2224172	14.90%	1.213%
10	5.929	1445	1469	1497	rVB3	105865	332671	2.23%	0.181%
11	6.114	1510	1538	1569	rBV2	593917	1848481	12.38%	1.008%
12	6.283	1581	1601	1619	rBV4	86148	261597	1.75%	0.143%
13	6.399	1626	1644	1652	rBV2	57815	168308	1.13%	0.092%
14	6.466	1654	1669	1692	rVB2	215655	659094	4.41%	0.360%
15	6.600	1699	1719	1739	rBV5	124911	390997	2.62%	0.213%
16	6.898	1808	1830	1856	rBV4	248997	752417	5.04%	0.410%
17	7.042	1859	1884	1903	rBV3	493846	1498874	10.04%	0.818%
18	7.144	1903	1922	1942	rVV2	665809	1818860	12.18%	0.992%
19	7.844	2168	2183	2202	rVB3	268127	663272	4.44%	0.362%
20	8.024	2229	2250	2257	rBV	896139	2103093	14.09%	1.147%
21	8.083	2260	2272	2290	rVV4	2220164	5962769	39.94%	3.253%
22	8.174	2292	2306	2331	rVB2	1178327	3003220	20.12%	1.638%
23	8.295	2332	2351	2369	rBV	931292	2168326	14.52%	1.183%
24	8.442	2387	2406	2434	rBV2	1170204	3280354	21.97%	1.789%
25	8.617	2436	2471	2494	rVV	2596549	7726430	51.75%	4.215%
26	8.708	2498	2505	2528	rVB4	238616	545049	3.65%	0.297%
27	8.826	2529	2549	2581	rVB2	765276	1890758	12.66%	1.031%
28	8.968	2581	2602	2631	rBV	3098931	7000587	46.89%	3.819%
29	9.126	2649	2661	2675	rVB2	139306	272088	1.82%	0.148%
30	9.207	2675	2691	2694	rBV5	82277	151945	1.02%	0.083%
31	9.459	2753	2785	2797	rBV2	1331633	3347841	22.42%	1.826%
32	9.512	2797	2805	2823	rVB	540990	1031249	6.91%	0.563%
33	9.593	2823	2835	2844	rBV	150385	306809	2.06%	0.167%
34	9.641	2845	2853	2867	rVB2	188165	334409	2.24%	0.182%
35	9.732	2867	2887	2902	rBV5	149590	362236	2.43%	0.198%
36	9.883	2928	2943	2964	rVB2	1526870	3106931	20.81%	1.695%

LSC Area Percent Report

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Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

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

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Peak separation: 5

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Title : SW846 8260

37	9.976	2966	2978	2980	rBV	355271	486887	3.26%	0.266%
38	10.017	2982	2993	3007	rVB2	1941769	3801903	25.47%	2.074%
39	10.081	3007	3017	3026	rBV	523158	861834	5.77%	0.470%
40	10.218	3048	3068	3093	rBV	696930	1700290	11.39%	0.927%
41	10.322	3094	3107	3112	rBV2	151003	267307	1.79%	0.146%
42	10.371	3113	3125	3137	rVV	1282119	2273872	15.23%	1.240%
43	10.443	3137	3152	3166	rVV	4551162	8417812	56.38%	4.592%
44	10.505	3168	3175	3189	rVB	477541	849726	5.69%	0.464%
45	10.625	3205	3220	3234	rVB4	763384	1564438	10.48%	0.853%
46	10.786	3270	3280	3285	rBV6	115382	189515	1.27%	0.103%
47	10.867	3297	3310	3311	rBV2	331788	441769	2.96%	0.241%
48	10.963	3338	3346	3360	rVB3	159522	285209	1.91%	0.156%
49	11.055	3361	3380	3392	rBV3	163070	345685	2.32%	0.189%
50	11.157	3409	3418	3434	rVB	218553	451907	3.03%	0.247%
51	11.457	3521	3530	3538	rBV3	155631	226492	1.52%	0.124%
52	11.529	3547	3557	3582	rVB4	555950	1291048	8.65%	0.704%
53	11.629	3583	3594	3616	rBV	434607	786948	5.27%	0.429%
54	11.747	3621	3638	3654	rBV	4897481	8907645	59.66%	4.859%
55	11.846	3663	3675	3695	rVB	2548901	4411978	29.55%	2.407%
56	11.950	3697	3714	3742	rBV	7500622	14929703	100.00%	8.144%
57	12.280	3818	3837	3855	rVB	2476174	4594534	30.77%	2.506%
58	12.581	3940	3949	3959	rBV	290665	514865	3.45%	0.281%
59	12.734	3993	4006	4028	rVB2	4080915	7880705	52.79%	4.299%
60	12.921	4065	4076	4087	rVB	1172381	1832799	12.28%	1.000%
61	12.983	4087	4099	4107	rBV	4230420	7022896	47.04%	3.831%
62	13.058	4119	4127	4146	rVB2	2557302	4529962	30.34%	2.471%
63	13.222	4175	4188	4204	rBV	1472145	2652203	17.76%	1.447%
64	13.369	4230	4243	4258	rVB	6582889	10664934	71.43%	5.818%
65	13.611	4326	4333	4339	rBV3	152280	201902	1.35%	0.110%
66	13.675	4345	4357	4399	rVB2	4715893	11876217	79.55%	6.478%
67	13.841	4409	4419	4421	rBV	445670	558005	3.74%	0.304%
68	13.873	4423	4431	4438	rVV3	1213523	1812815	12.14%	0.989%
69	13.994	4467	4476	4488	rBV	822740	1201162	8.05%	0.655%
70	14.072	4497	4505	4515	rVB	321142	474030	3.18%	0.259%
71	14.134	4518	4528	4532	rBV	678825	997529	6.68%	0.544%
72	14.217	4549	4559	4572	rVB	1193429	1842114	12.34%	1.005%
73	14.327	4591	4600	4613	rVB3	729619	1205073	8.07%	0.657%
74	14.463	4642	4651	4660	rBV4	280515	457605	3.07%	0.250%
75	14.541	4674	4680	4687	rBV	366331	476537	3.19%	0.260%
76	14.579	4688	4694	4703	rVB	747308	995451	6.67%	0.543%

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Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A2-3-6.5

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Title : SW846 8260

77	14.622	4704	4710	4718	rVB2	343642	425169	2.85%	0.232%
78	14.764	4757	4763	4771	rVB2	197574	232466	1.56%	0.127%
79	14.812	4771	4781	4788	rBV2	573143	979265	6.56%	0.534%
80	14.850	4790	4795	4807	rVB4	665669	945943	6.34%	0.516%
81	14.930	4809	4825	4837	rBV4	931048	2292425	15.35%	1.250%
82	15.507	5031	5040	5053	rVB	575904	1020874	6.84%	0.557%
83	16.620	5442	5455	5490	rVB	568059	1384766	9.28%	0.755%

Sum of corrected areas: 183322506

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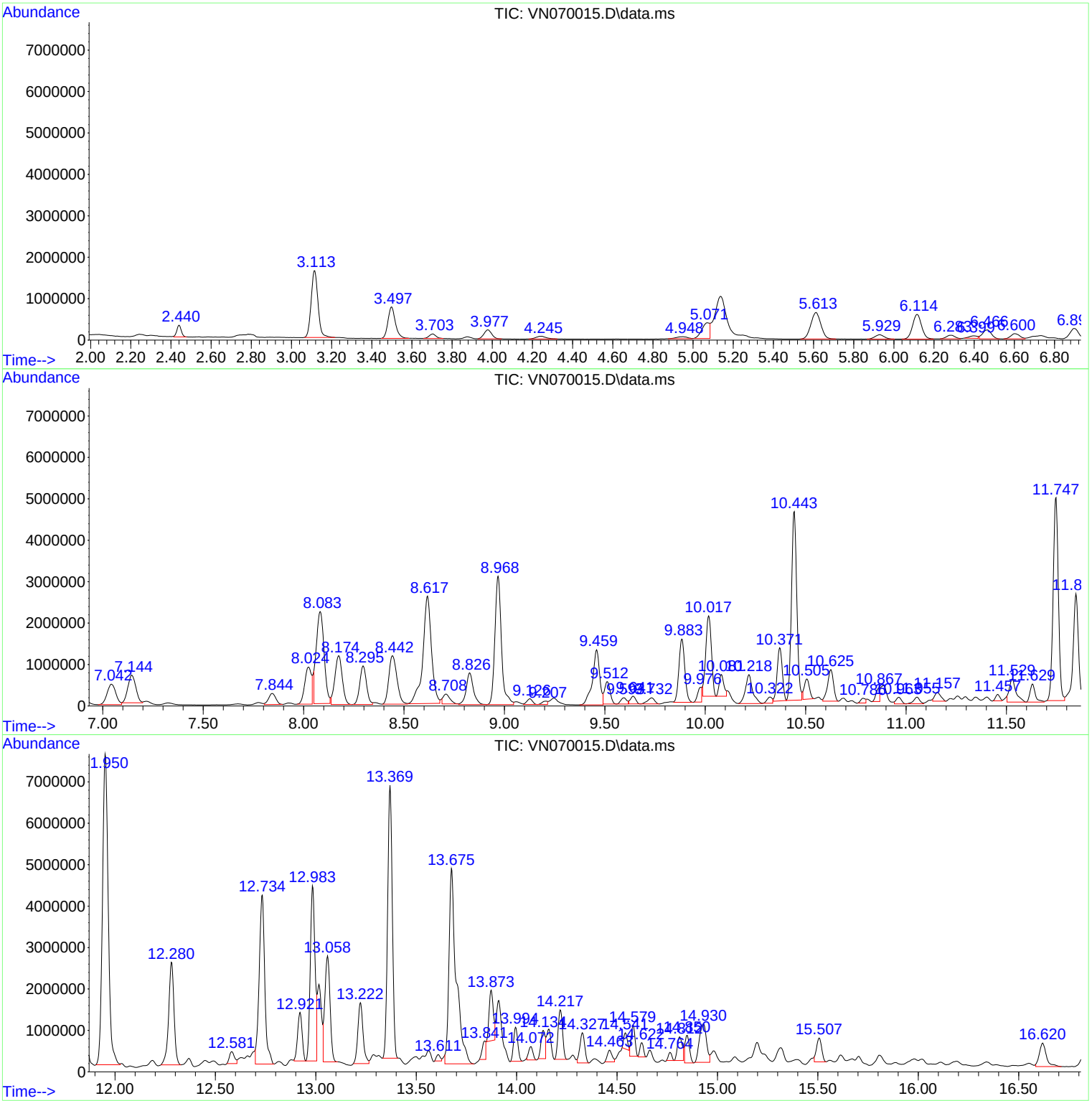
Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

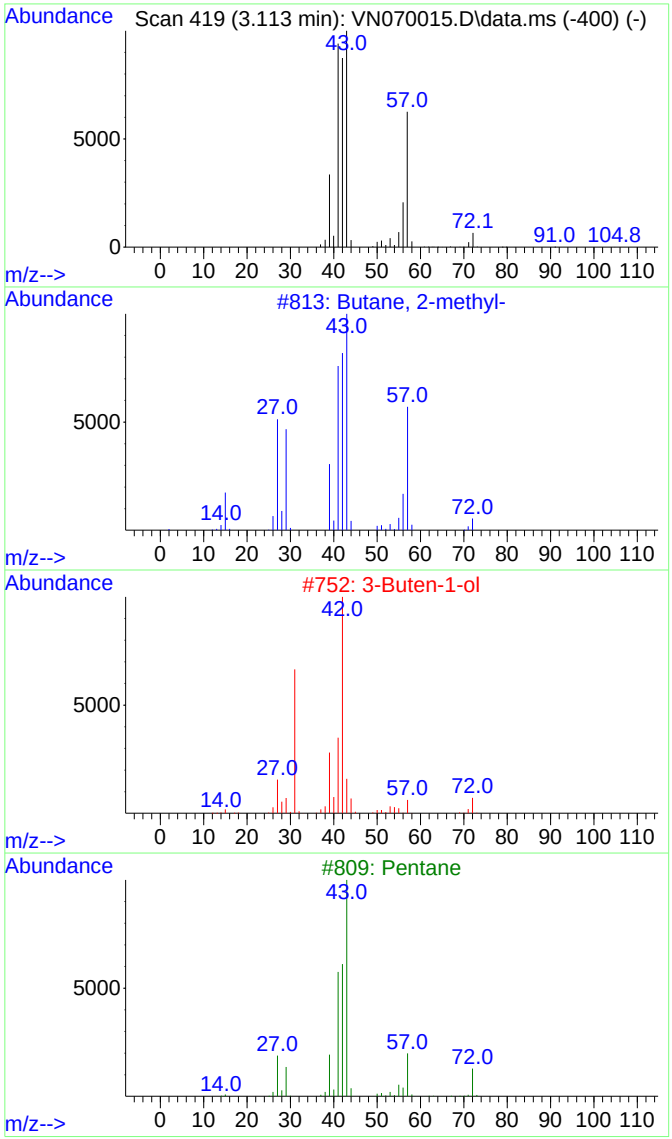
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

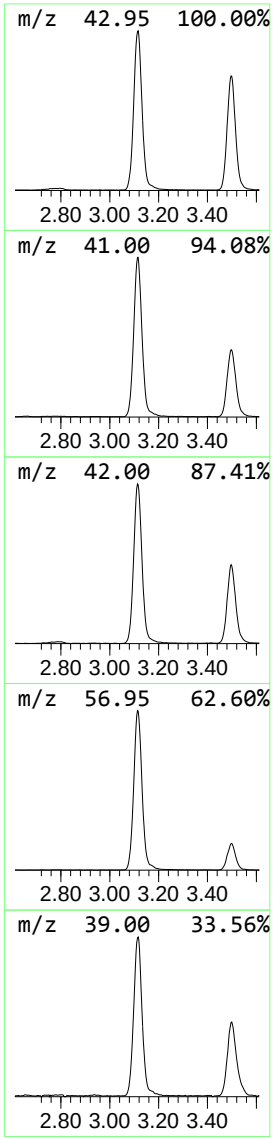
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.113	32.14 ug/l	3832540	Pentafluorobenzene	8.086

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	47
3	Pentane	72	C5H12	000109-66-0	36
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

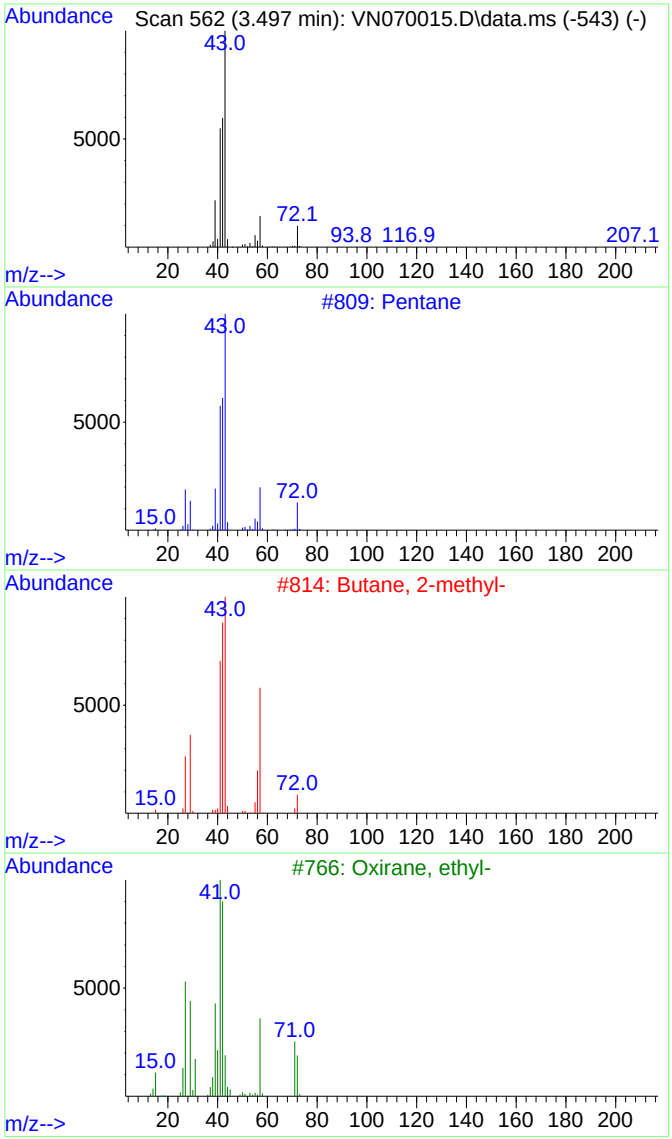
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

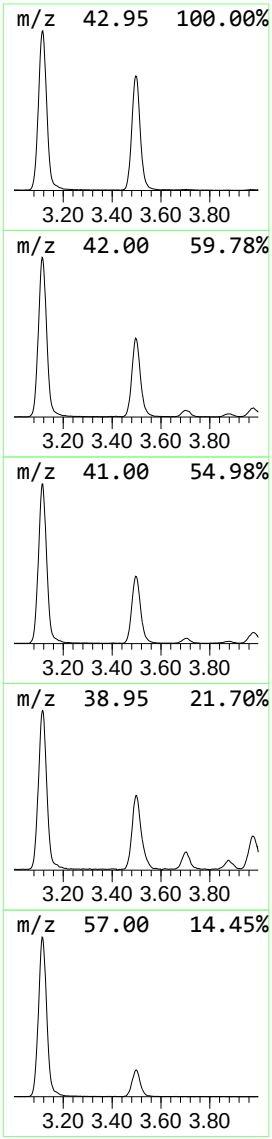
****

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.497	16.35 ug/l	1950410	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	64
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	47
4	Isobutylene epoxide	72	C4H8O	000558-30-5	9
5	Butanenitrile, 3-methyl-	83	C5H9N	000625-28-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
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Acq On : 11 Dec 2021 18:10
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Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

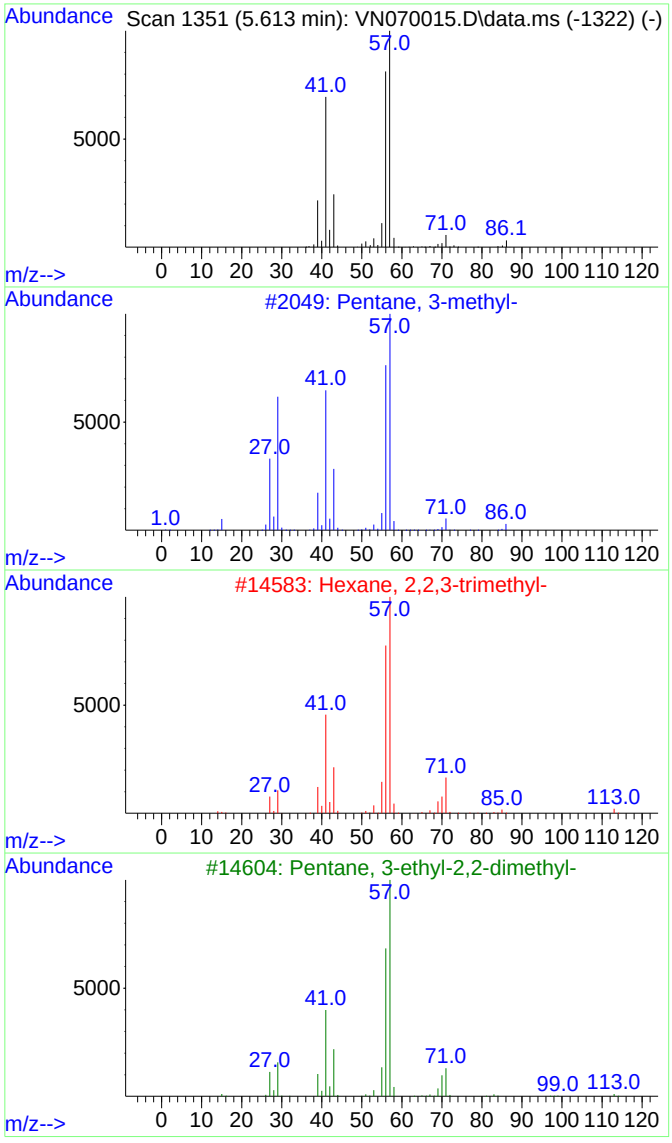
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

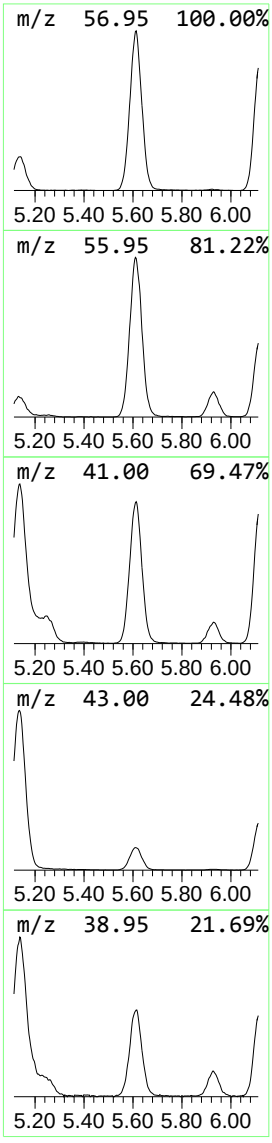
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.613	18.65 ug/l	2224170	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	43
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





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Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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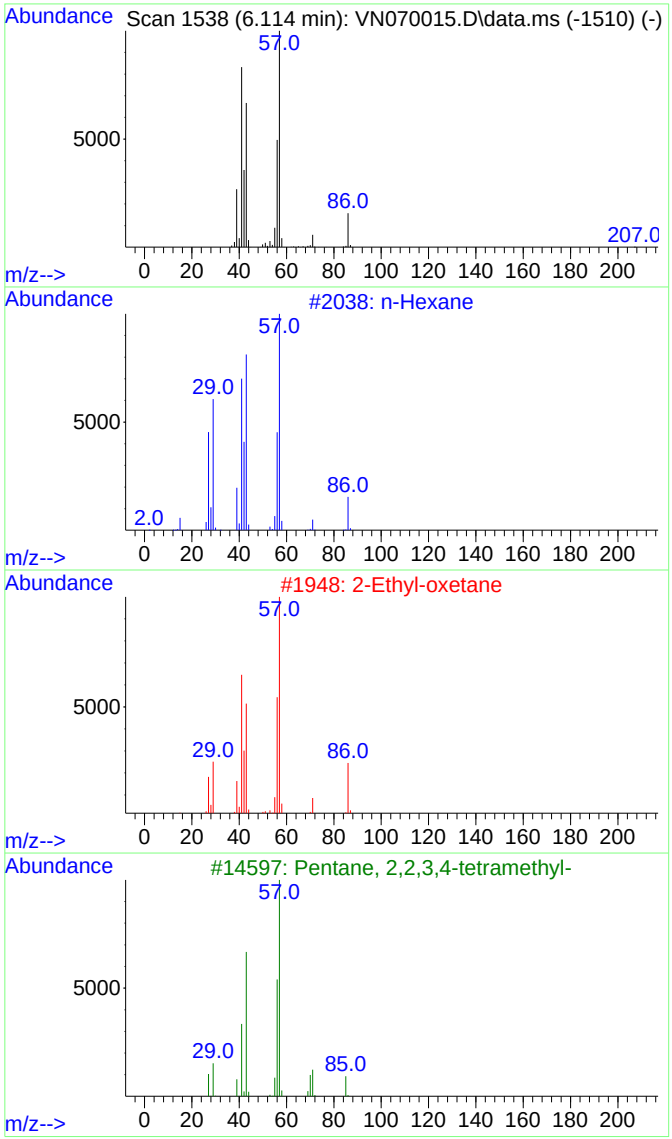
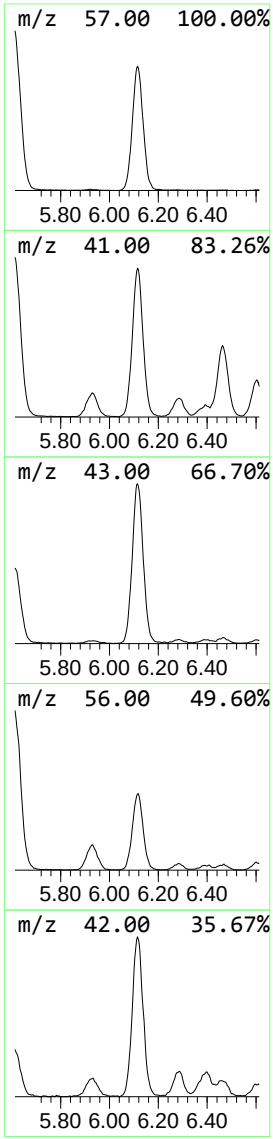
Peak Number 4 n-Hexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.114	15.50 ug/l	1848480	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	83
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35





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Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

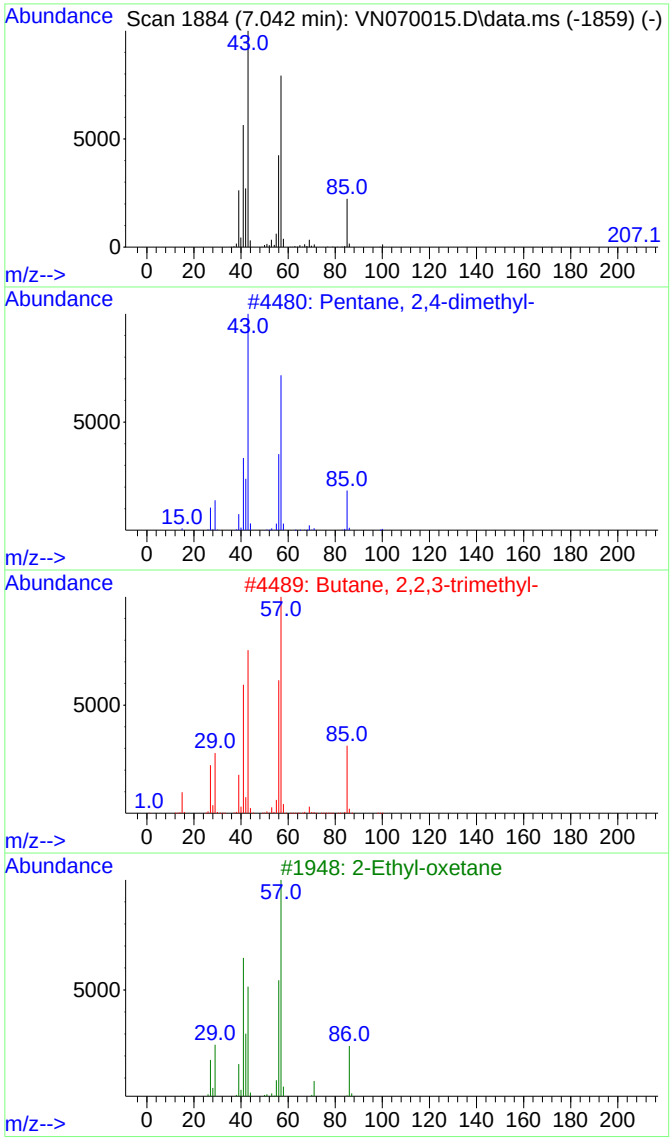
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

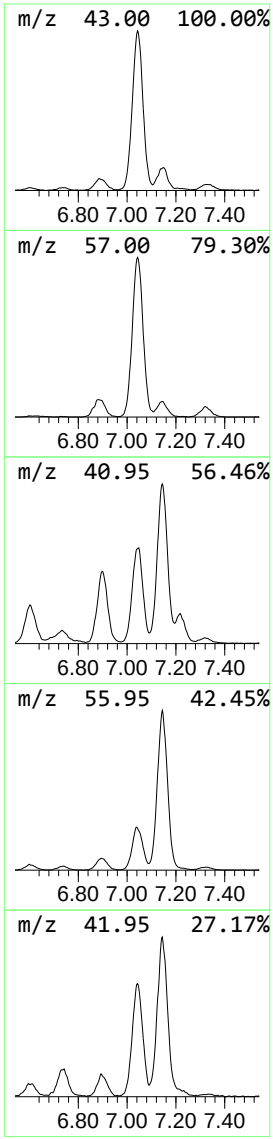
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.042	12.57 ug/l	1498870	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	53
4	n-Hexane	86	C6H14	000110-54-3	53
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

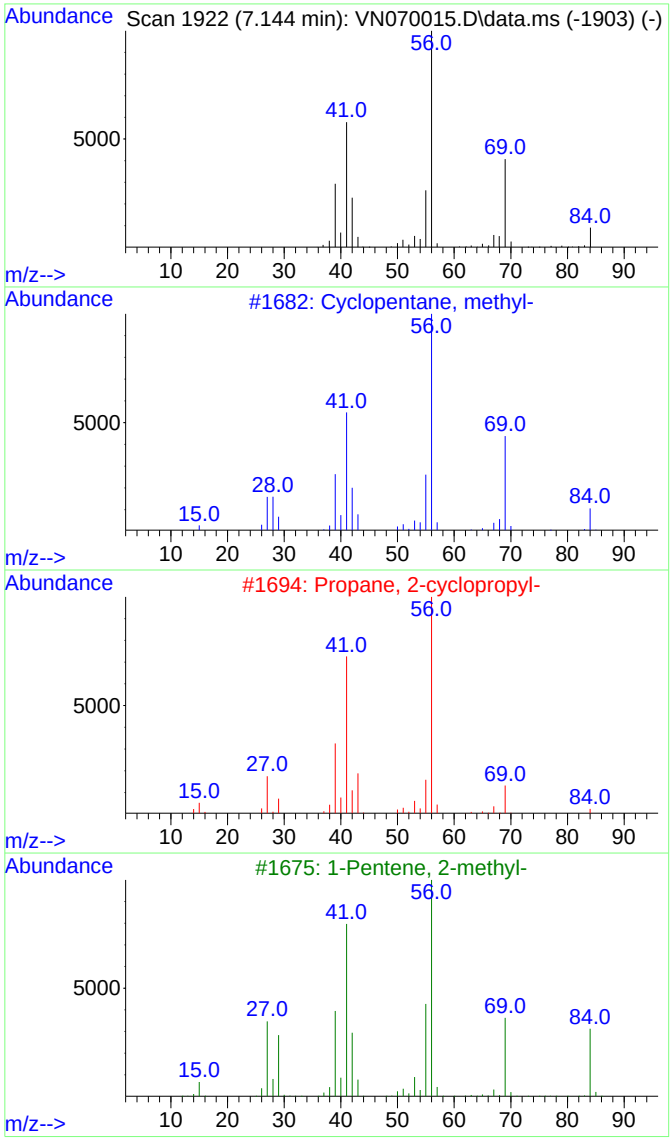
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

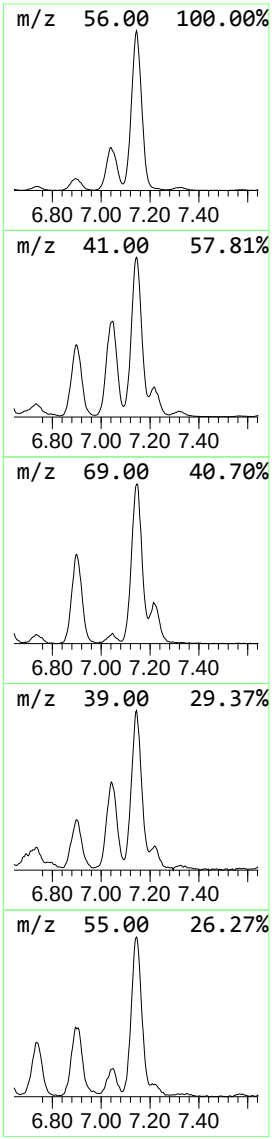
****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.144	15.25 ug/l	1818860	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	50
5	Cyclobutane	56	C4H8	000287-23-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

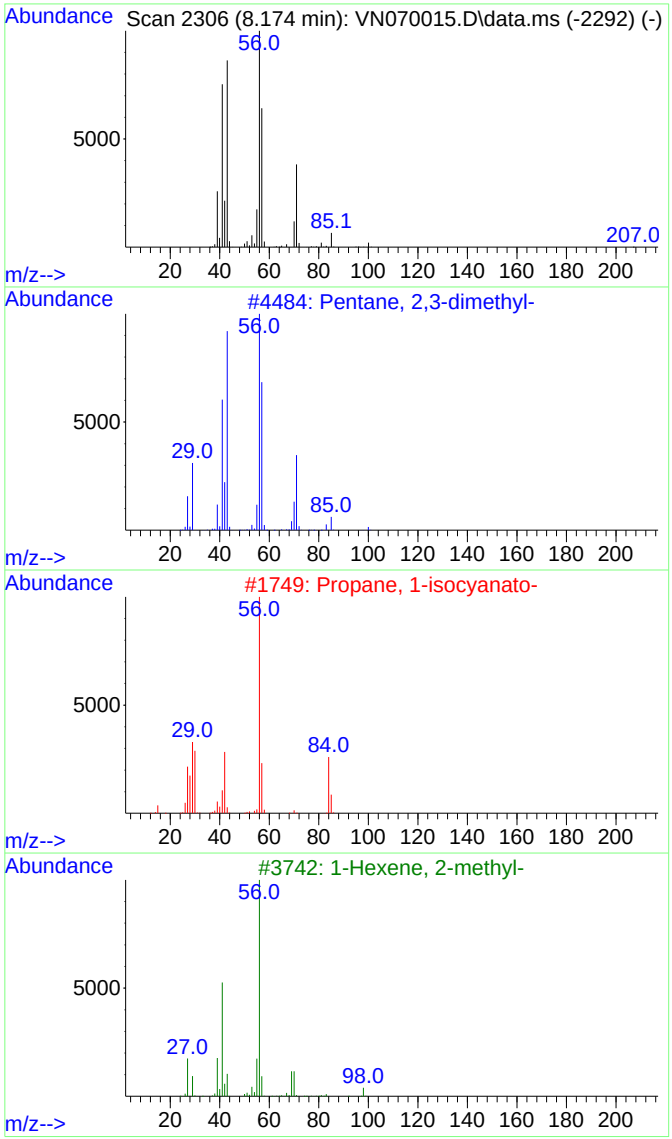
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

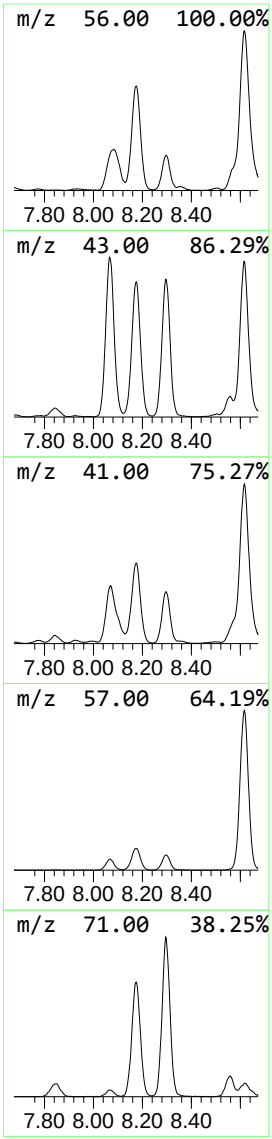
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	25.18 ug/l	3003220	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	43
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	28
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	25





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

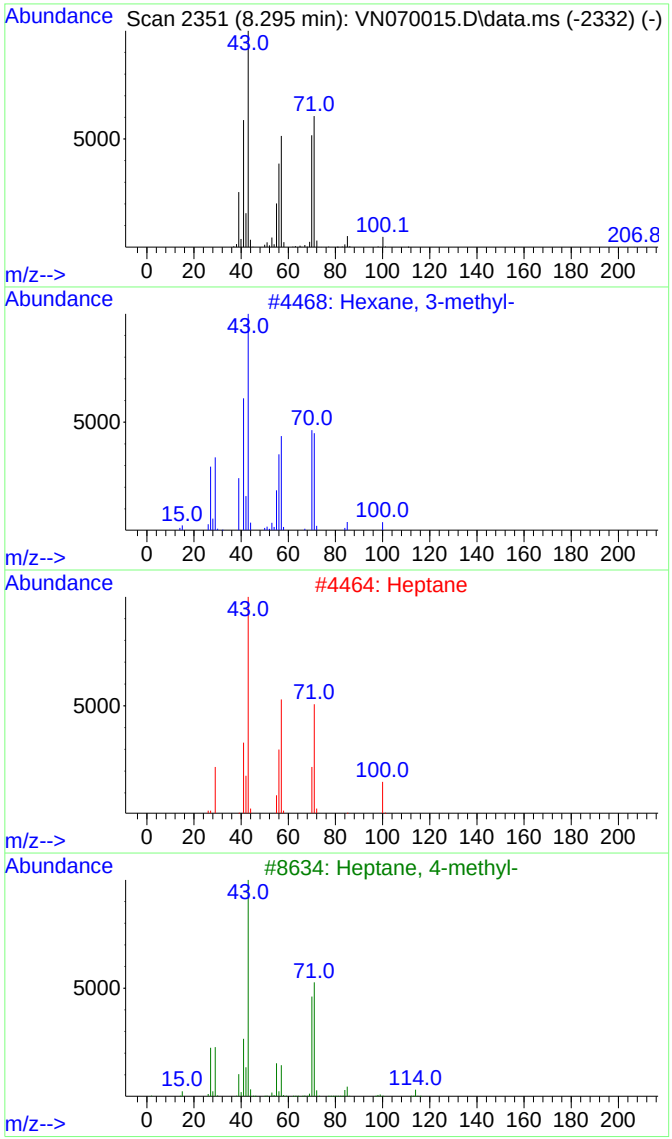
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

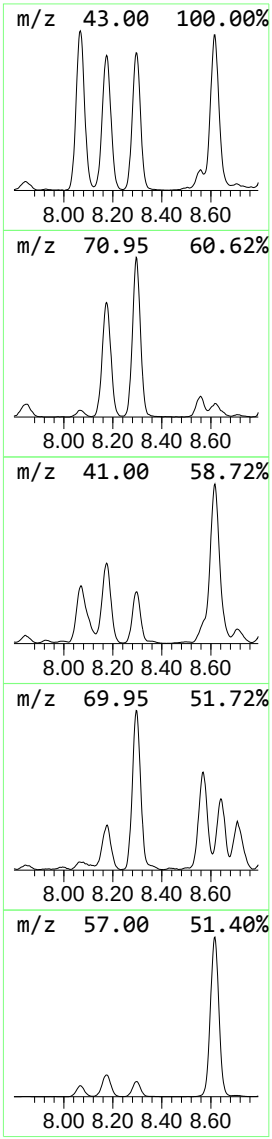
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.295	18.18 ug/l	2168330	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

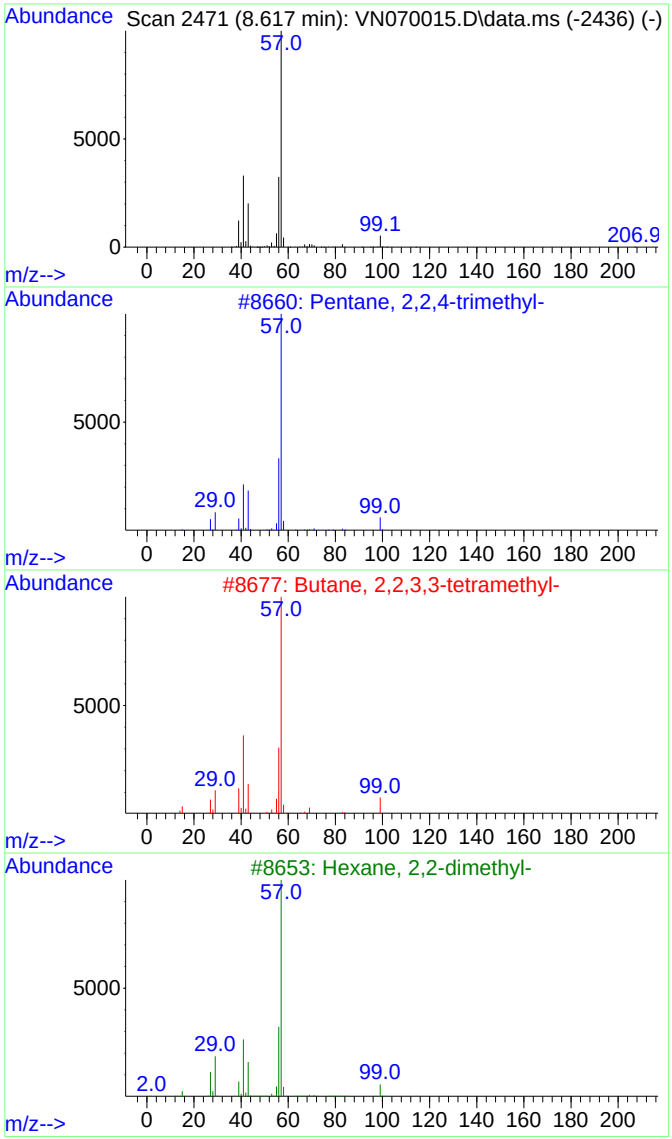
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

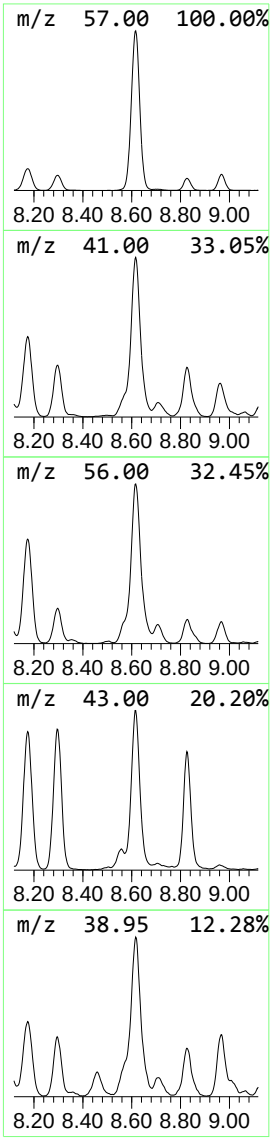
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	55.18 ug/l	7726430	1,4-Difluorobenzene	8.968

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





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Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

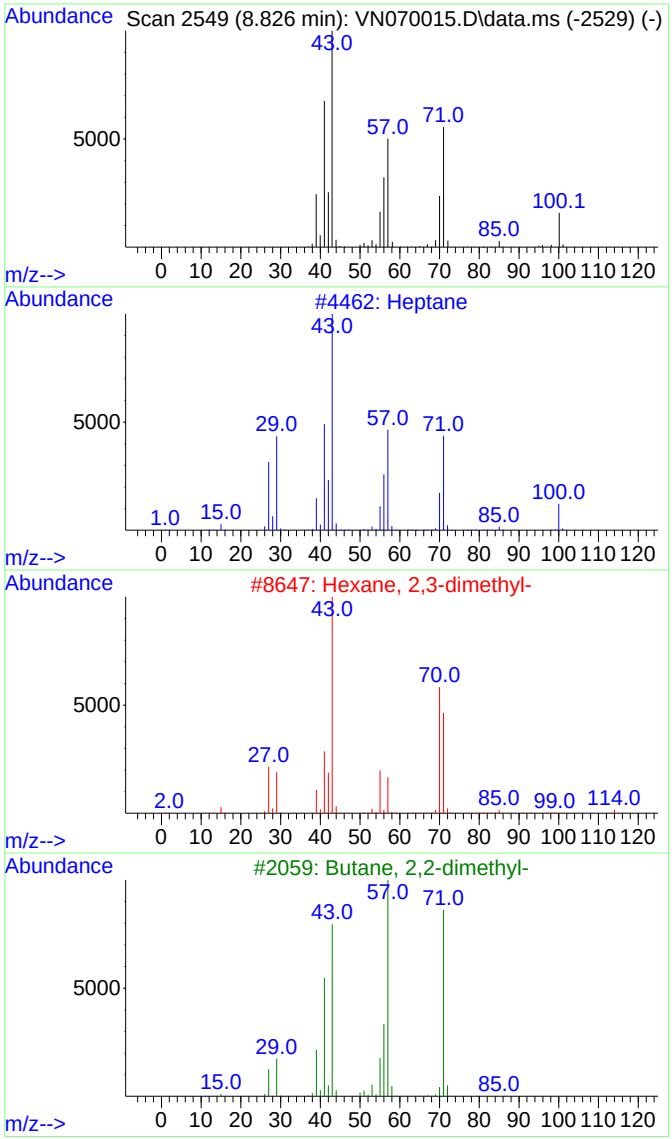
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

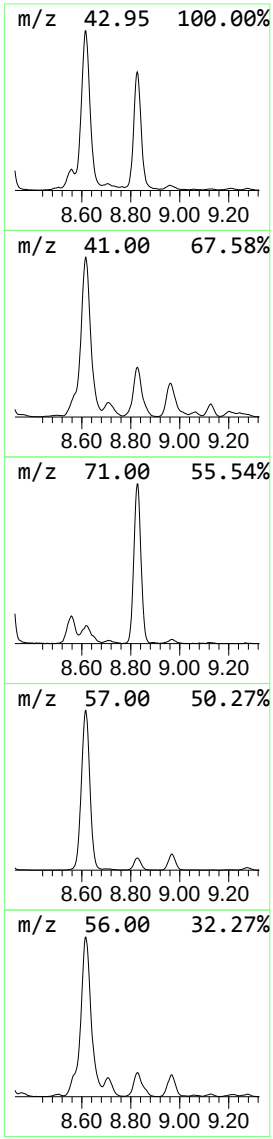
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Heptane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	13.50 ug/l	1890760	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	94
2	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	37





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

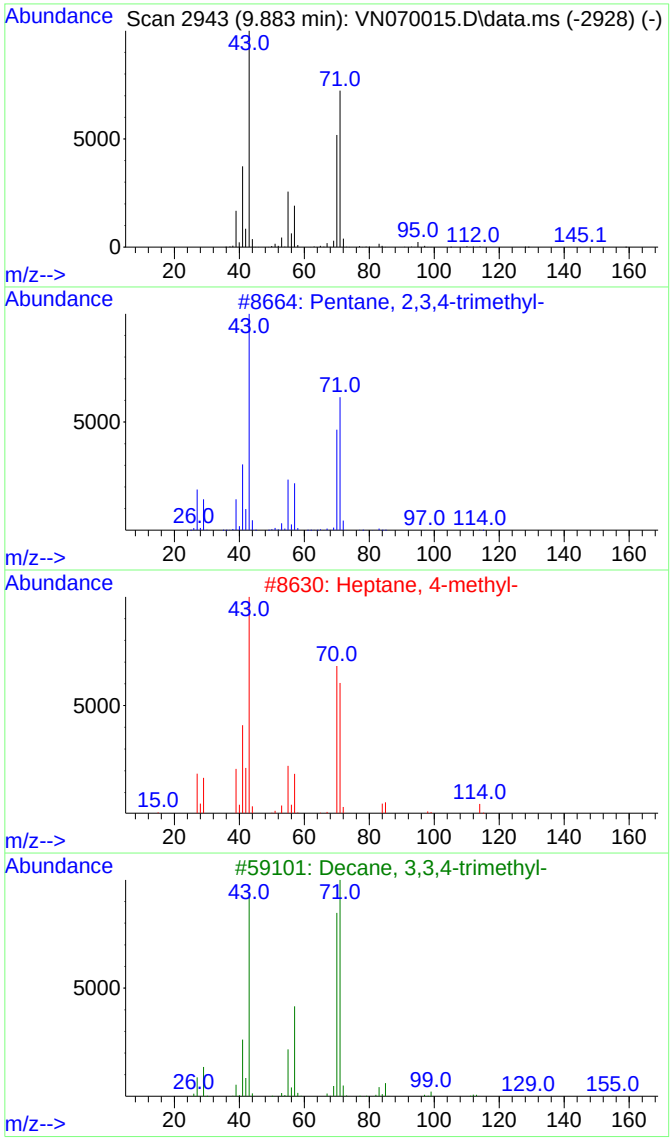
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

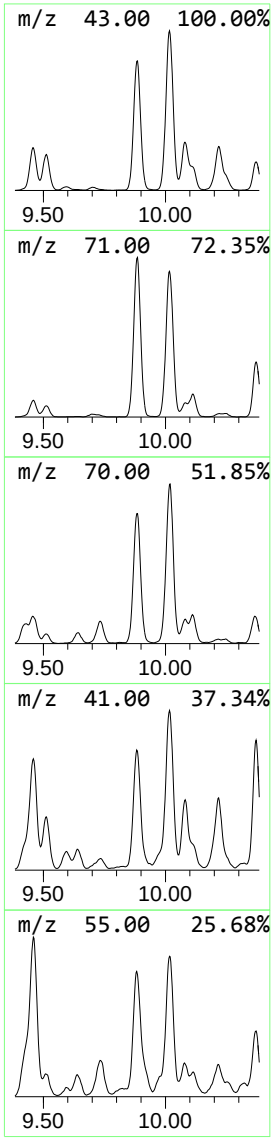
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	22.19 ug/l	3106930	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
4	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

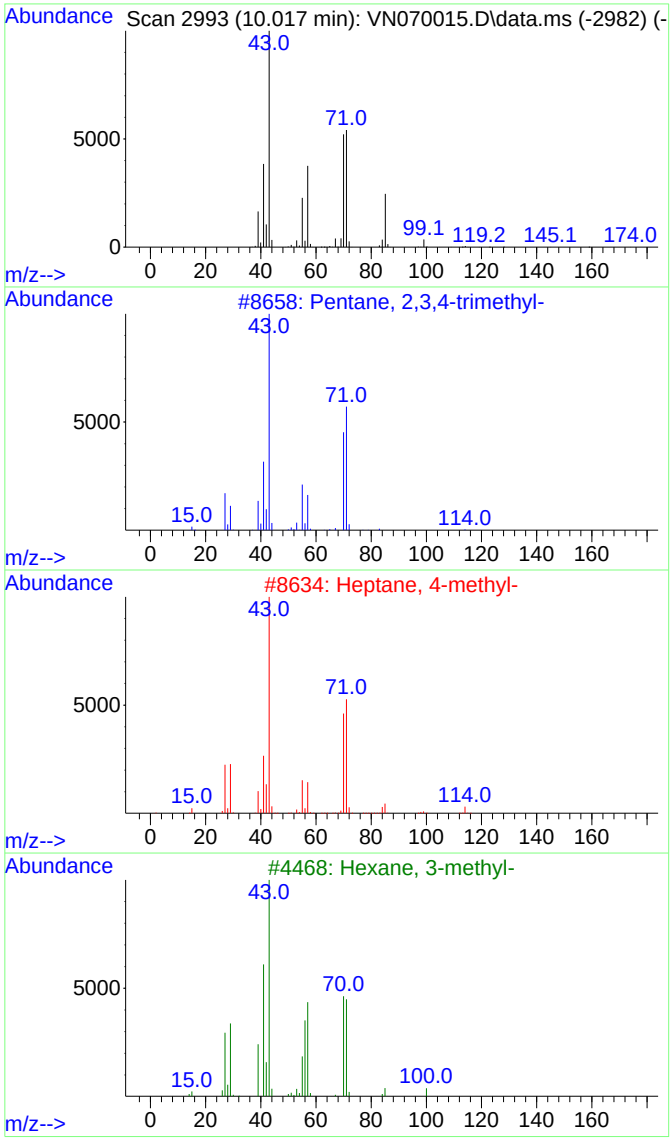
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

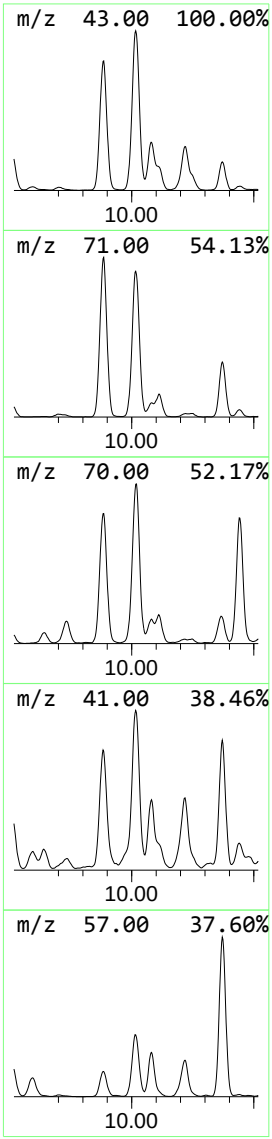
****

Peak Number 12 Heptane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.017	27.15 ug/l	3801900	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	68
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
4	Pentane, 3-ethyl-	100	C7H16	000617-78-7	59
5	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	59





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

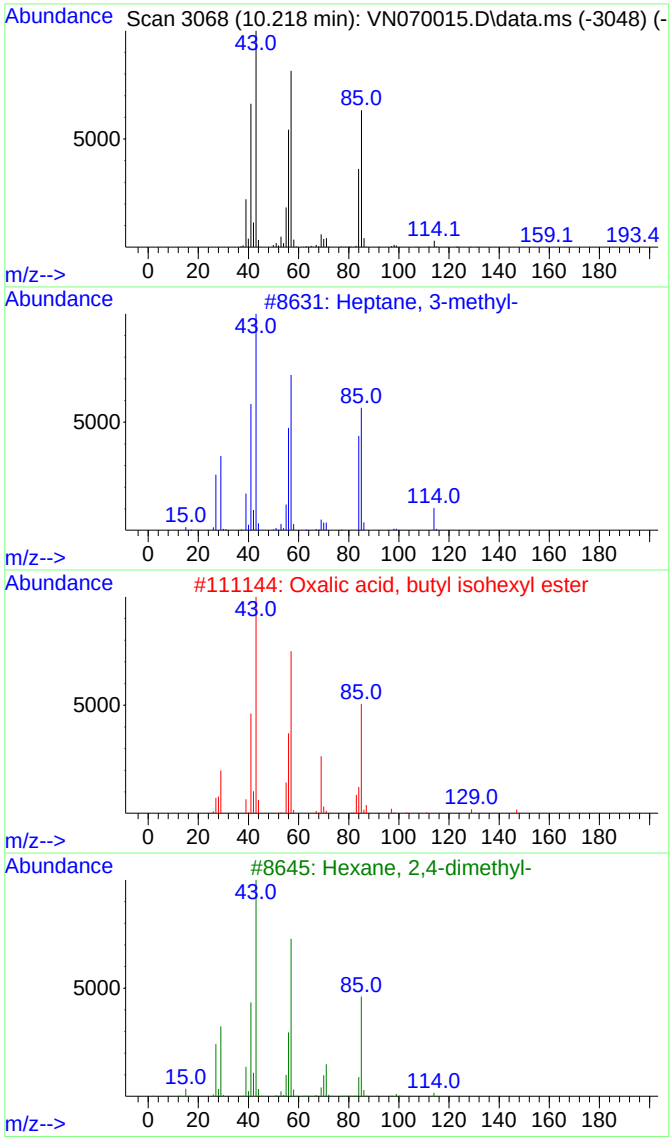
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

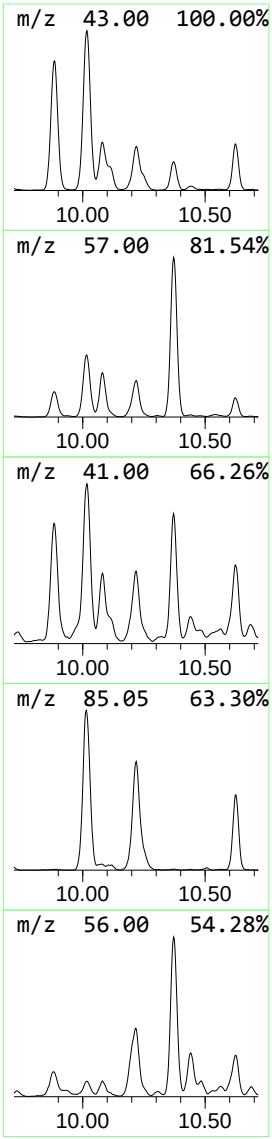
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Heptane, 3-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.218	12.14 ug/l	1700290	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	83
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	78
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4	Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	53
5	Butanoic acid, 3-methyl-, butyl ...	158	C9H18O2	000109-19-3	53





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Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

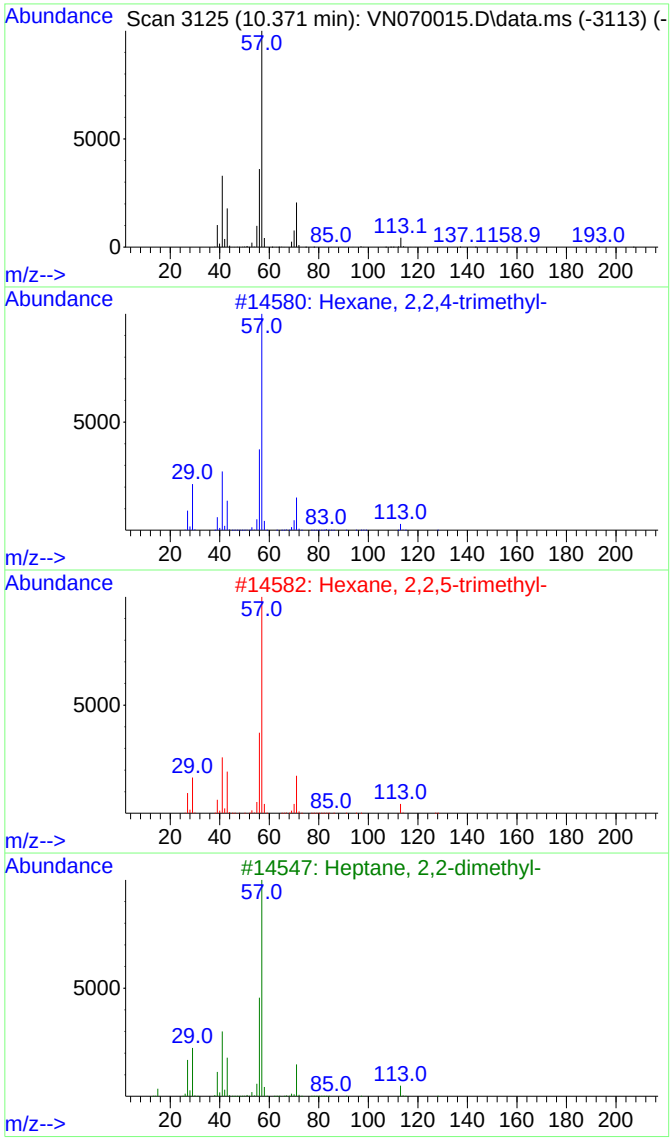
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

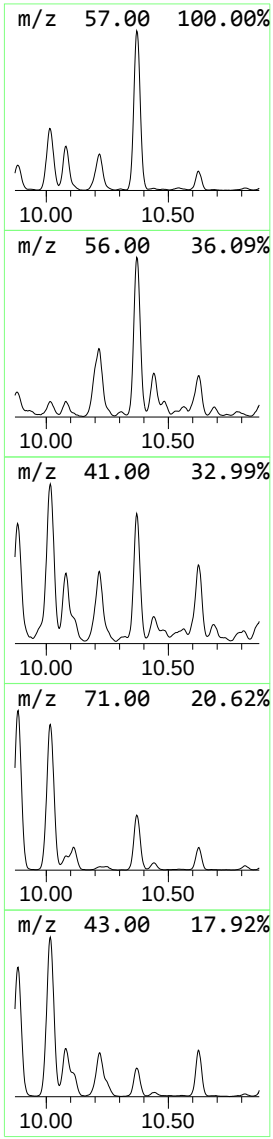
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Hexane, 2,2,4-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.371	12.76 ug/l	2273870	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	86
2	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	83
3	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	59
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
5	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	45





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Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

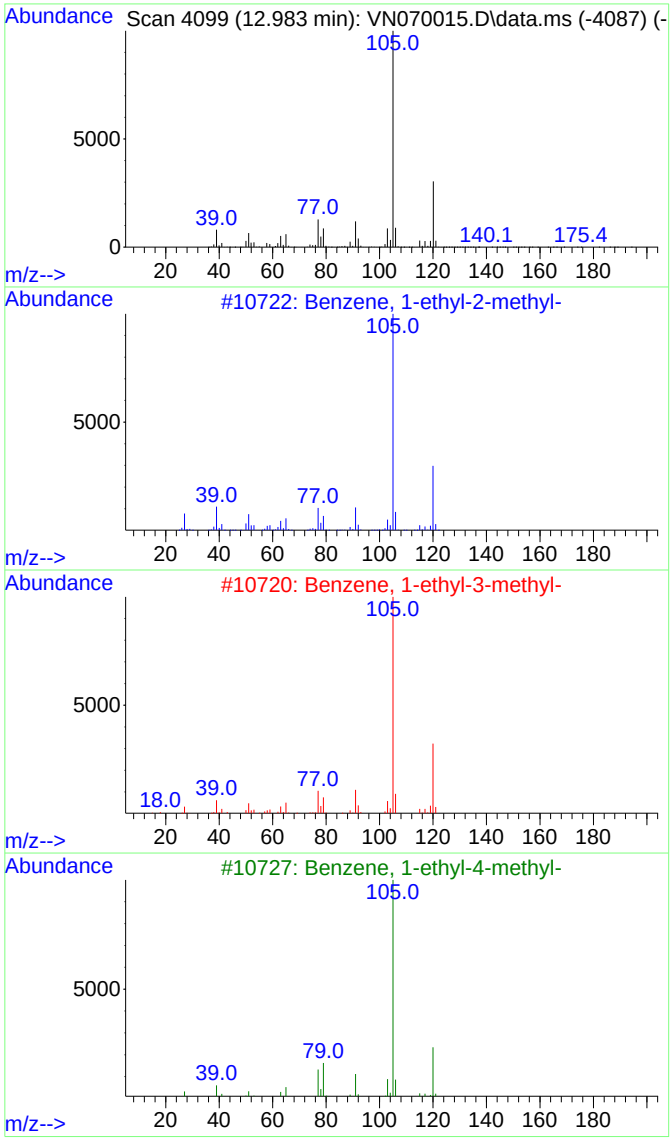
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

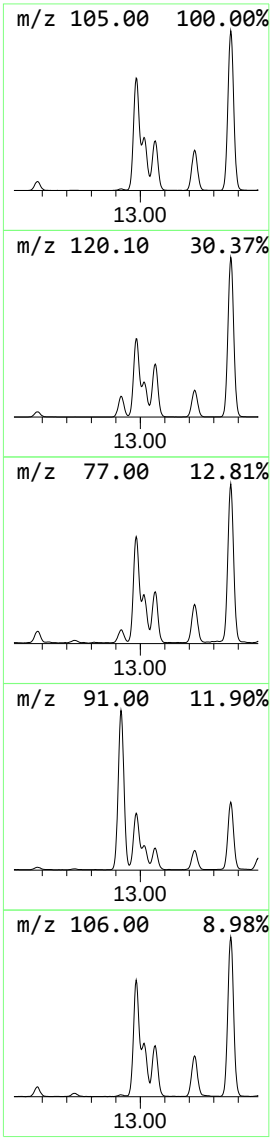
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	29.57 ug/l	7022900	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070015.D
Acq On : 11 Dec 2021 18:10
Operator : JC/MD
Sample : M4873-02 10X
Misc : 6.27g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-3-6.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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
Butane, 2-methyl-	3.113	32.1	ug/l	3832540	1	8.086	5962770	50.0
Pentane	3.497	16.4	ug/l	1950410	1	8.086	5962770	50.0
Pentane, 3-methyl-	5.613	18.6	ug/l	2224170	1	8.086	5962770	50.0
n-Hexane	6.114	15.5	ug/l	1848480	1	8.086	5962770	50.0
Pentane, 2,4-di...	7.042	12.6	ug/l	1498870	1	8.086	5962770	50.0
Cyclopentane, m...	7.144	15.3	ug/l	1818860	1	8.086	5962770	50.0
Pentane, 2,3-di...	8.174	25.2	ug/l	3003220	1	8.086	5962770	50.0
Hexane, 3-methyl-	8.295	18.2	ug/l	2168330	1	8.086	5962770	50.0
Pentane, 2,2,4-...	8.617	55.2	ug/l	7726430	2	8.968	7000590	50.0
Heptane	8.826	13.5	ug/l	1890760	2	8.968	7000590	50.0
Pentane, 2,3,4-...	9.883	22.2	ug/l	3106930	2	8.968	7000590	50.0
Heptane, 4-methyl-	10.017	27.1	ug/l	3801900	2	8.968	7000590	50.0
Heptane, 3-methyl-	10.218	12.1	ug/l	1700290	2	8.968	7000590	50.0
Hexane, 2,2,4-t...	10.371	12.8	ug/l	2273870	3	11.746	8907650	50.0
Benzene, 1-ethy...	12.983	29.6	ug/l	7022900	4	13.675	11876200	50.0