LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

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: VN070246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.006	368	379	406	rVB	723696	1441562	4.94%	0.630%
2	3.422	516	534	553	rBV	148721	362986	1.24%	0.159%
3	4.197	792	823	853	rBV3	184368	641416	2.20%	0.280%
4	5.036	1102	1136	1150	rBV3	777171	2962804	10.15%	1.296%
5	5.586	1310	1341	1383	rBV	508470	1778601	6.10%	0.778%
6	6.093	1503	1530	1561	rBV2	214172	665910	2.28%	0.291%
7	6.871	1788	1820	1847	rBV2	125100	426478	1.46%	0.187%
8	7.029	1850	1879	1902	rVV	2209216	6780963	23.24%	2.965%
9	7.131	1903	1917	1940	rVB	278977	797419	2.73%	0.349%
10	7.831	2163	2178	2200	rVB2	190546	510899	1.75%	0.223%
11	8.019	2223	2248	2254	rBV2	917616	2065670	7.08%	0.903%
12	8.166	2285	2303	2329	rVB	4599120	11496761	39.40%	5.028%
13	8.287	2330	2348	2367	rBV2	1001615	2318178	7.95%	1.014%
14	8.432	2384	2402	2427	rBV	1097179	2562277	8.78%	1.121%
15	8.606	2430	2467	2491	rVV	11337694	29177192	100.00%	12.760%
16	8.700	2493	2502	2525	rVB4	266294	627889	2.15%	0.275%
17	8.820	2528	2547	2579	rVB3	413579	991466	3.40%	0.434%
18	8.965	2579	2601	2628	rBV	2869426	6367064	21.82%	2.784%
19	9.271	2704	2715	2745	rVB	138687	319607	1.10%	0.140%
20	9.453	2749	2783	2793	rBV	2764690	6743257	23.11%	2.949%
21	9.504	2793	2802	2819	rVB	2410260	4656857	15.96%	2.036%
22	9.588	2819	2833	2846	rBV	520690	1072582	3.68%	0.469%
23	9.727	2862	2885	2904	rVB2	720162	1835210	6.29%	0.803%
24	9.877	2923	2941	2966	rBV	5975194	12384517	42.45%	5.416%
25	10.011	2968	2991	3005	rBV	6415701	13584155	46.56%	5.940%
26	10.076	3006	3015	3022	rBV2	528635	822700	2.82%	0.360%
27	10.210	3045	3065	3095	rBV5	1459398	4344714	14.89%	1.900%
28	10.368	3108	3124	3137	rBV	3065894	5691603	19.51%	2.489%
29	10.440	3137	3151	3169	rBV	4772267	9259988	31.74%	4.049%
30	10.620	3203	3218	3233	rVB5	885240	1971580	6.76%	0.862%
31	10.778	3267	3277	3296	rVB4	354303	717277	2.46%	0.314%
32	10.883	3297	3316	3335	rBV8	927950	2460627	8.43%	1.076%
33	10.961	3336	3345	3359	rVB	632934	1103477	3.78%	0.483%
34	11.052	3359	3379	3392	rBV2	730096	1461927	5.01%	0.639%
35	11.151	3405	3416	3435	rVB	1170370	2502058	8.58%	1.094%
36	11.342	3480	3487	3499	rVB3	259785	405268	1.39%	0.177%

LSC Area Percent Report

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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

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

37	11.451	3519	3528	3536	rBV4	400155	638702	2.19%	0.279%
38	11.521	3537	3554	3581	rVB5	1471831	4247599	14.56%	1.858%
39	11.626	3581	3593	3605	rBV	1198438	2128566	7.30%	0.931%
40	11.744	3618	3637	3652	rBV2	4914028	9758648	33.45%	4.268%
41	11.811	3654	3662	3669	rBV	510251	733894	2.52%	0.321%
42	11.953	3707	3715	3723	rBV4	658822	996717	3.42%	0.436%
43	12.181	3791	3800	3811	rVB5	409844	651667	2.23%	0.285%
44	12.251	3816	3826	3835	rBV3	737639	1396131	4.79%	0.611%
45	12.366	3860	3869	3880	rVB	805289	1340297	4.59%	0.586%
46	12.446	3890	3899	3908	rBV5	359194	629960	2.16%	0.275%
47	12.583	3941	3950	3956	rBV	353405	638945	2.19%	0.279%
48	12.731	3991	4005	4026	rVB2	4231919	10354640	35.49%	4.528%
49	12.873	4049	4058	4065	rBV2	488741	885488	3.03%	0.387%
50	12.983	4089	4099	4105	rBV	498220	787170	2.70%	0.344%
51	13.053	4117	4125	4168	rVB7	1031962	3116685	10.68%	1.363%
52	13.222	4171	4188	4195	rBV	597920	1513023	5.19%	0.662%
53	13.283	4206	4211	4216	rBV2	273821	312478	1.07%	0.137%
54	13.366	4232	4242	4253	rVB	2074087	3234652	11.09%	1.415%
55	13.495	4273	4290	4297	rBV4	530514	1432853	4.91%	0.627%
56	13.605	4323	4331	4338	rBV2	508136	714079	2.45%	0.312%
57	13.675	4346	4357	4369	rBV	4947986	7796072	26.72%	3.409%
58	13.836	4406	4417	4425	rBV	1851175	3050614	10.46%	1.334%
59	13.997	4467	4477	4489	rBV4	790031	1383451	4.74%	0.605%
60	14.150	4521	4534	4546	rVB5	907194	2122104	7.27%	0.928%
61	14.214	4547	4558	4577	rBV	2842811	4863878	16.67%	2.127%
62	14.327	4589	4600	4612	rVB2	1599255	2853859	9.78%	1.248%
63	14.404	4615	4629	4642	rBV7	649261	1408742	4.83%	0.616%
64	14.538	4672	4679	4690	rVB	2051868	3068027	10.52%	1.342%
65	14.619	4701	4709	4719	rBV2	1234368	1764261	6.05%	0.772%
66	14.809	4771	4780	4788	rBV2	909608	1514829	5.19%	0.662%
67	14.917	4809	4820	4833	rBV6	1163059	2739057	9.39%	1.198%
68	15.193	4913	4923	4935	rBV5	1354833	2156771	7.39%	0.943%
69	15.305	4956	4965	4984	rVB5	1057836	2228969	7.64%	0.975%
70	15.466	5015	5025	5049	rVB8	608874	1520993	5.21%	0.665%
71	15.804	5140	5151	5168	rVB	692146	1373551	4.71%	0.601%

Sum of corrected areas: 228670311

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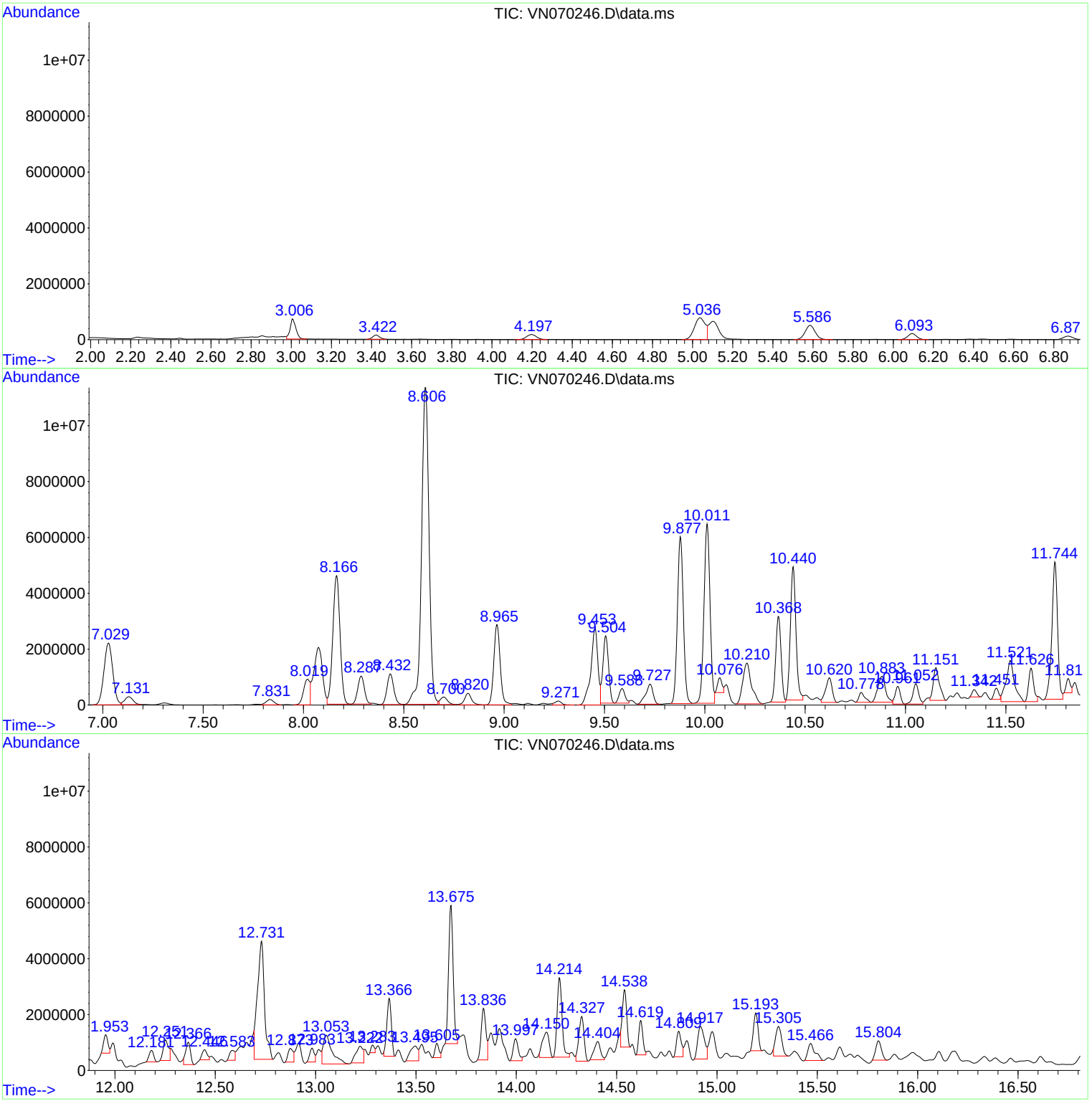
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

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\VN122021\
Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

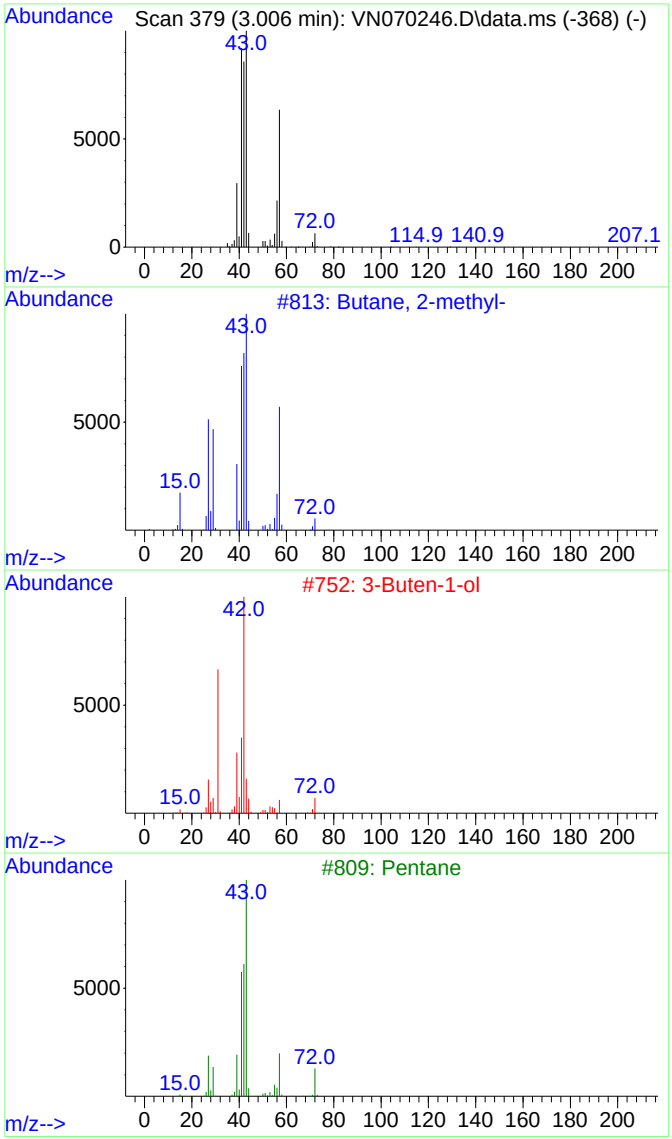
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

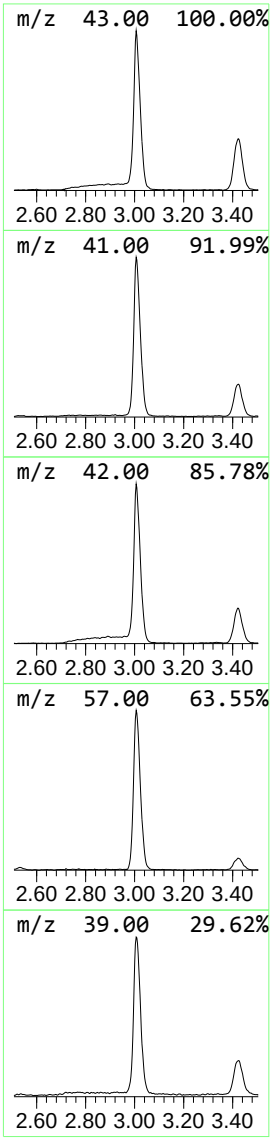
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.006	34.89 ug/l	1441560	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	42
4	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070246.D
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Sample : M5044-19
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

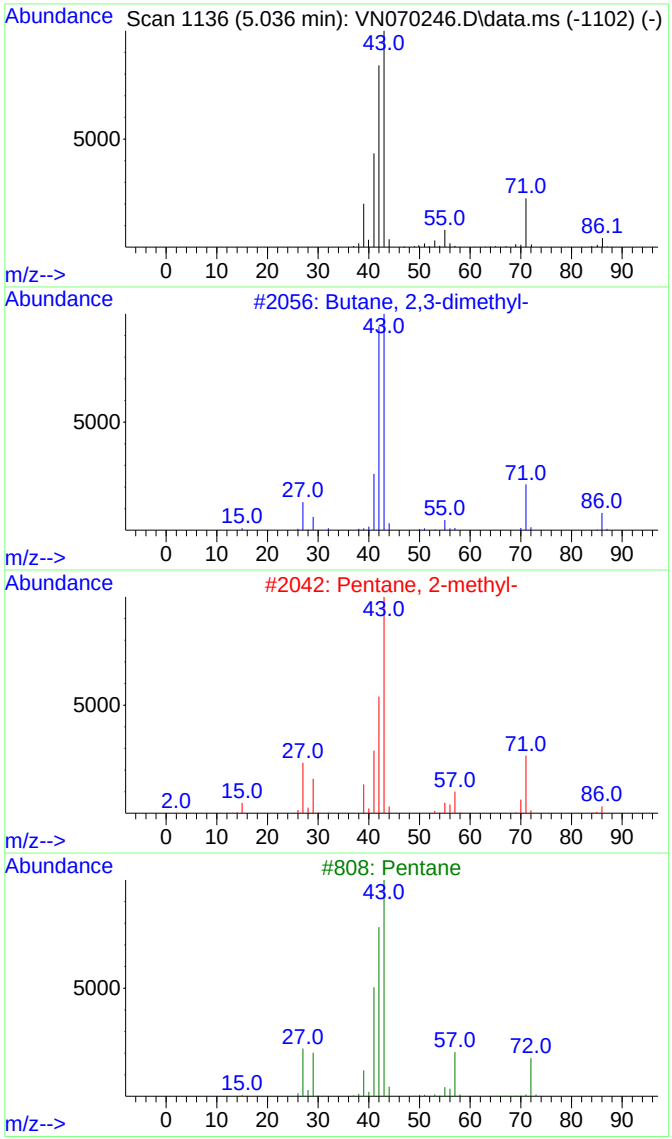
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

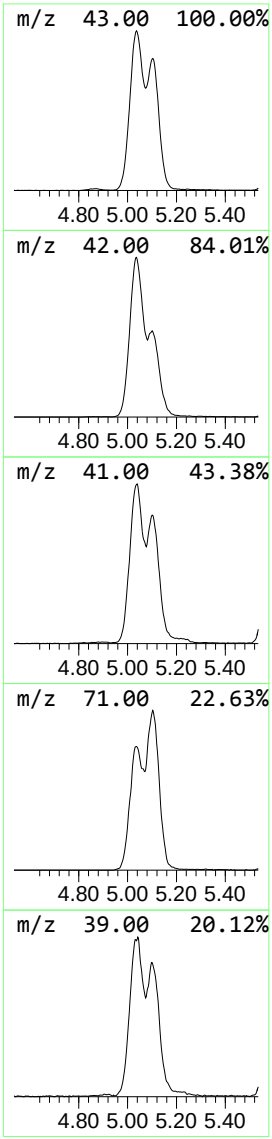
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.036	71.72 ug/l	2962800	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3	Pentane	72	C5H12	000109-66-0	38
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	38
5	Tetrahydrofuran	72	C4H8O	000109-99-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

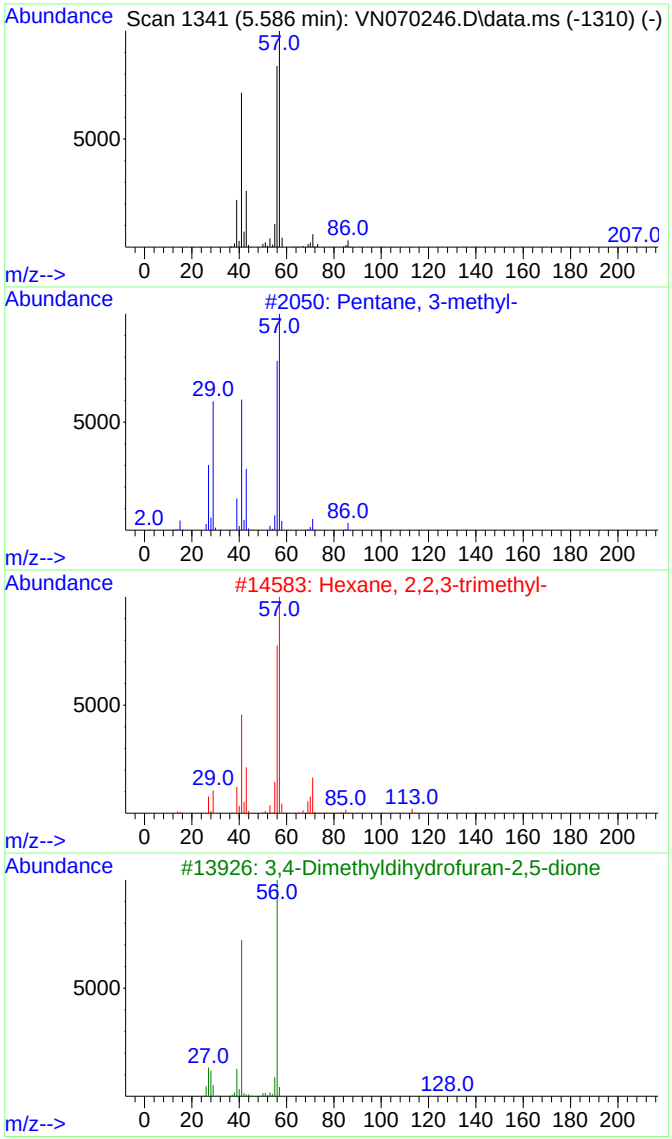
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

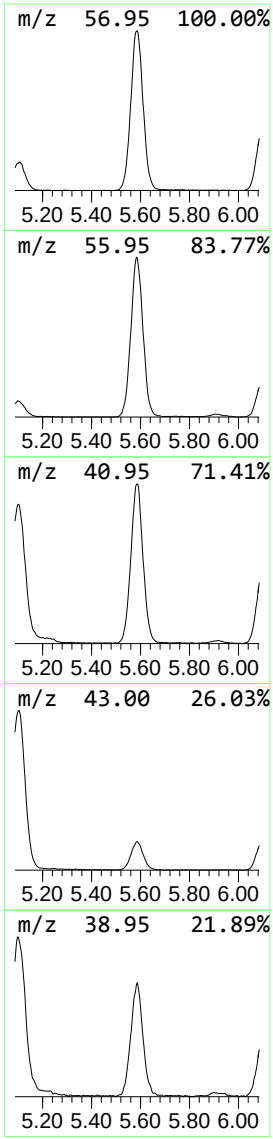
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.586	43.05 ug/l	1778600	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	50
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

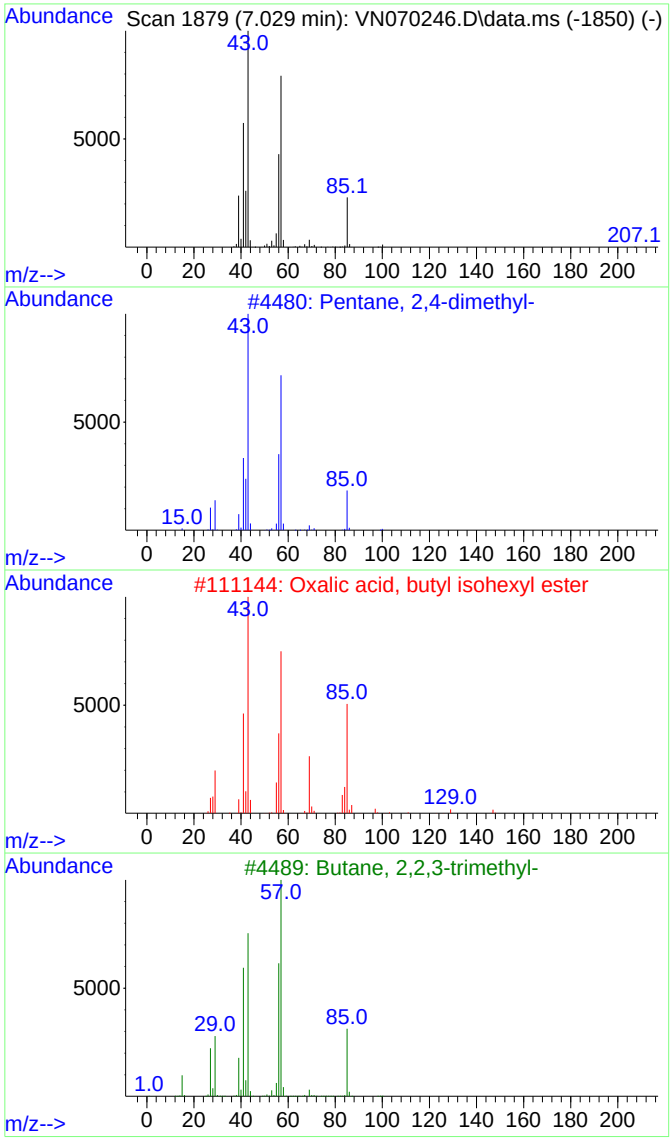
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

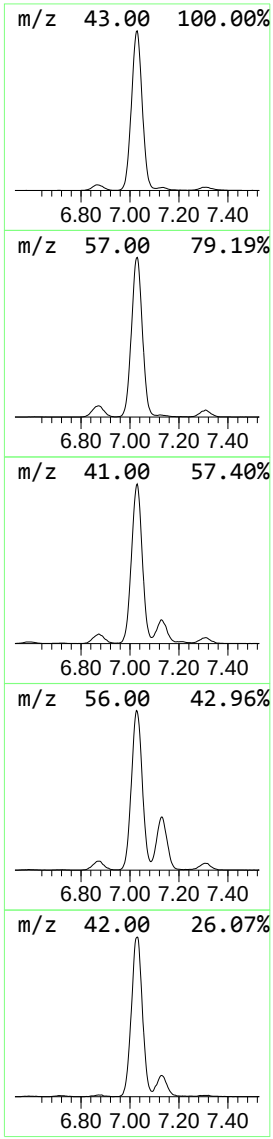
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.029	164.13 ug/l	6780960	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	72
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	56
5	n-Hexane	86	C6H14	000110-54-3	53





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Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

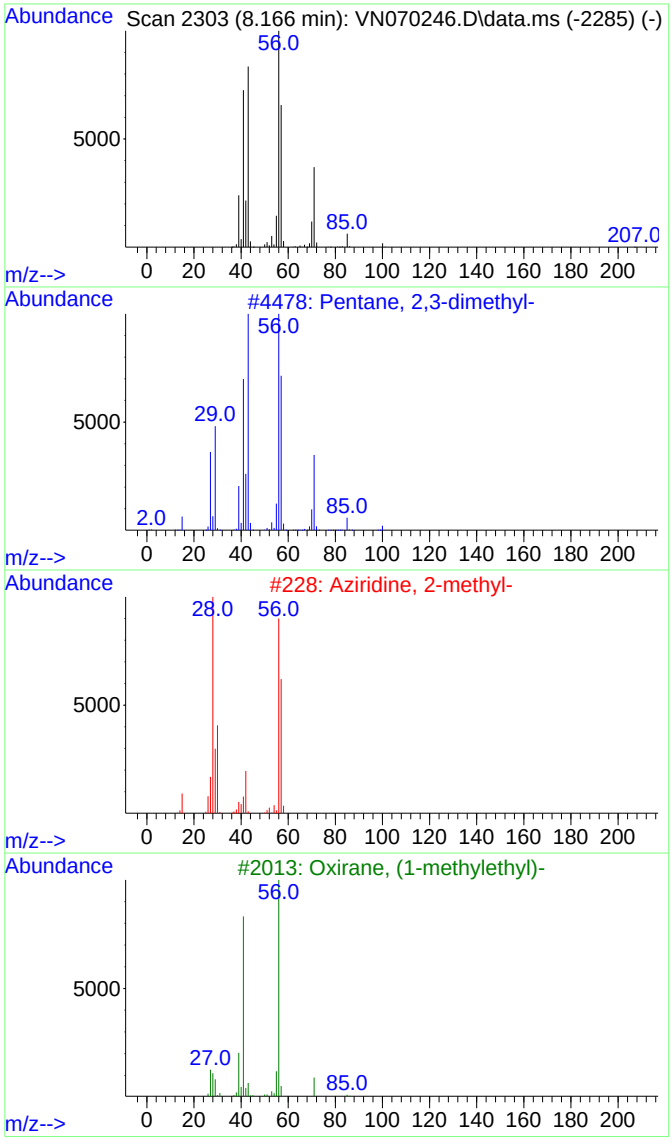
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

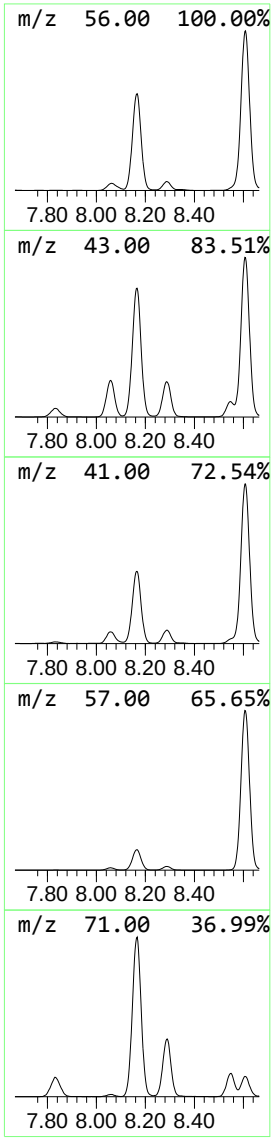
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.166	278.28 ug/l	11496800	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
4	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	36





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

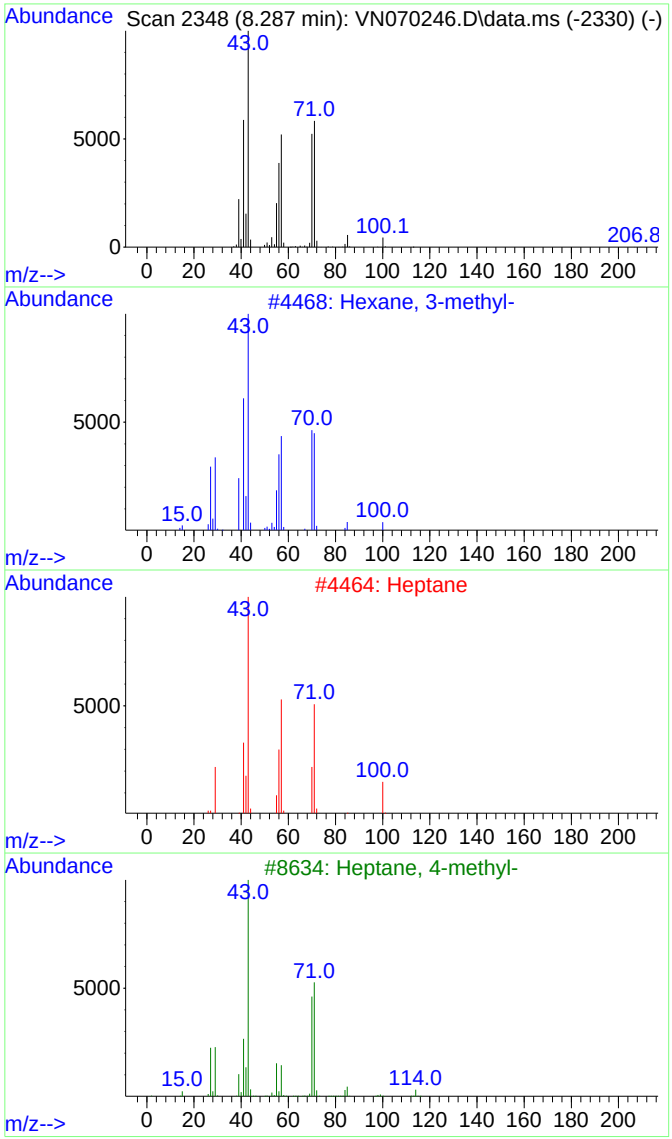
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

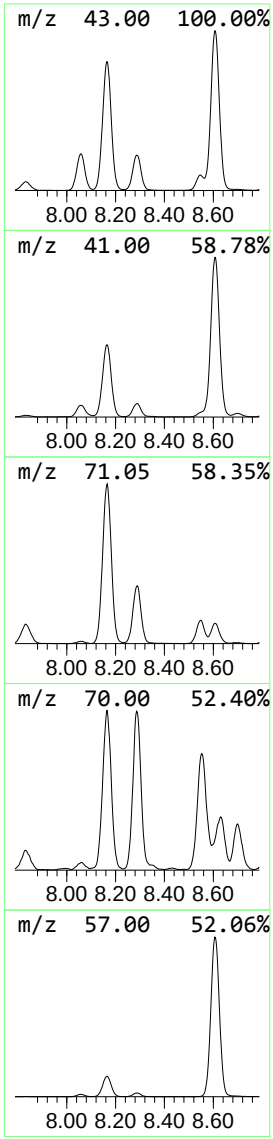
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	56.11 ug/l	2318180	Pentafluorobenzene	8.080

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	64
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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

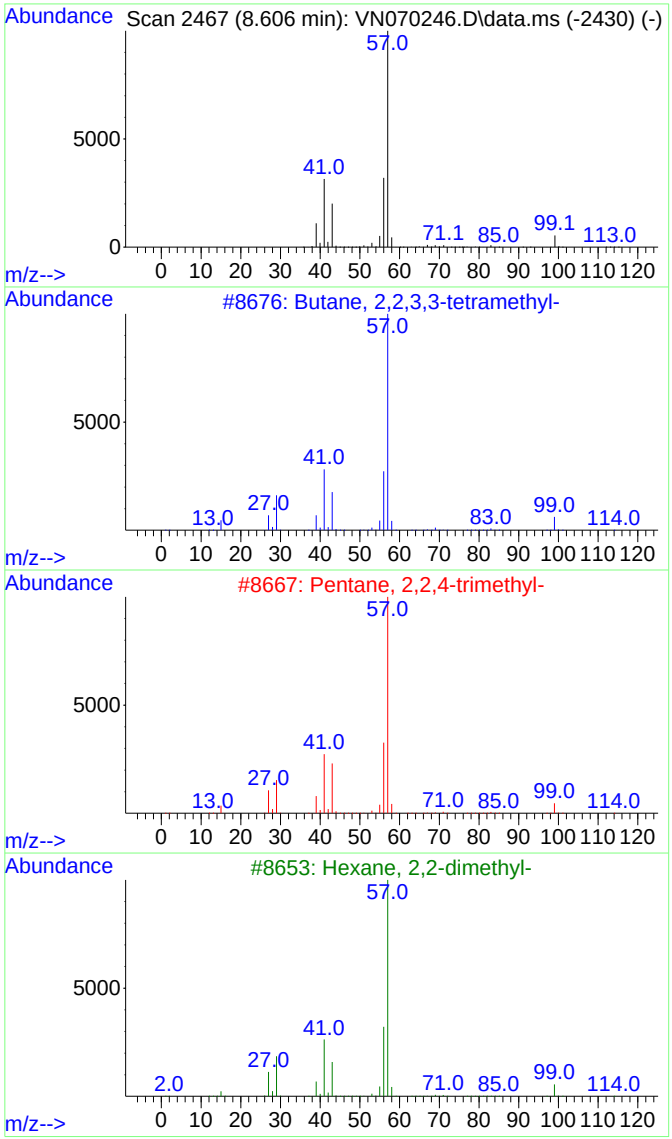
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

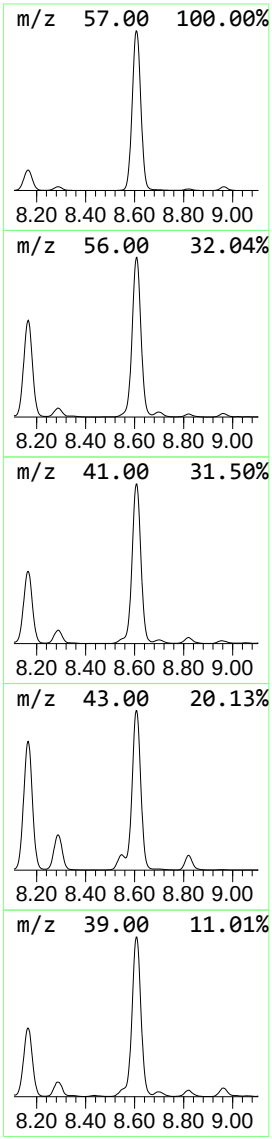
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.606	229.13 ug/l	29177200	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5	Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	39





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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

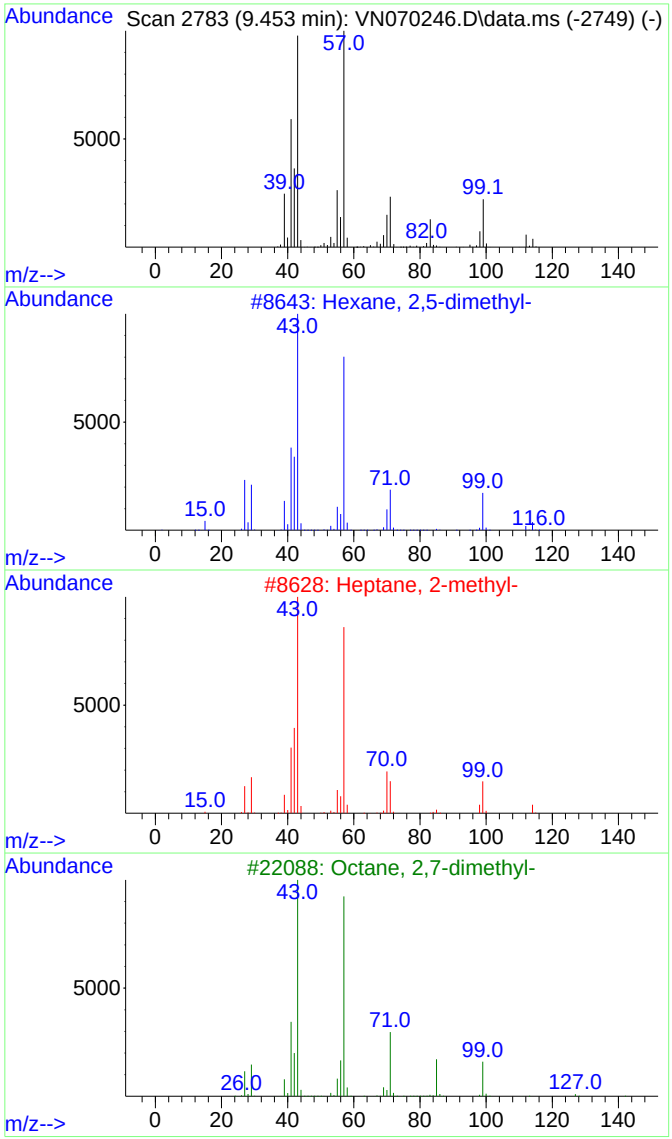
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

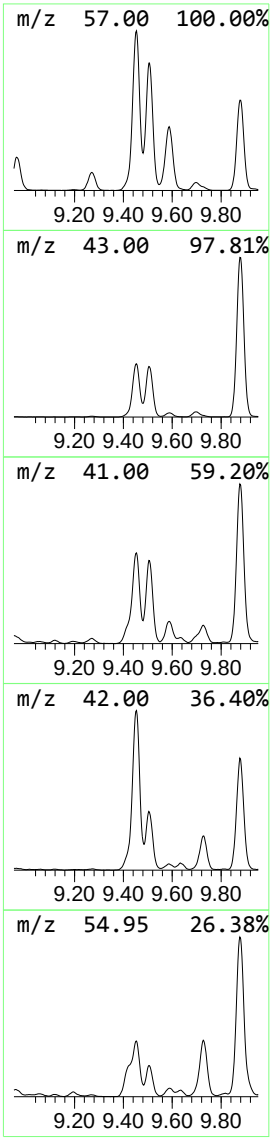
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexane, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.453	52.95 ug/l	6743260	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	87
2	Heptane, 2-methyl-	114	C8H18	000592-27-8	49
3	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	43
4	2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	43
5	2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	43





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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

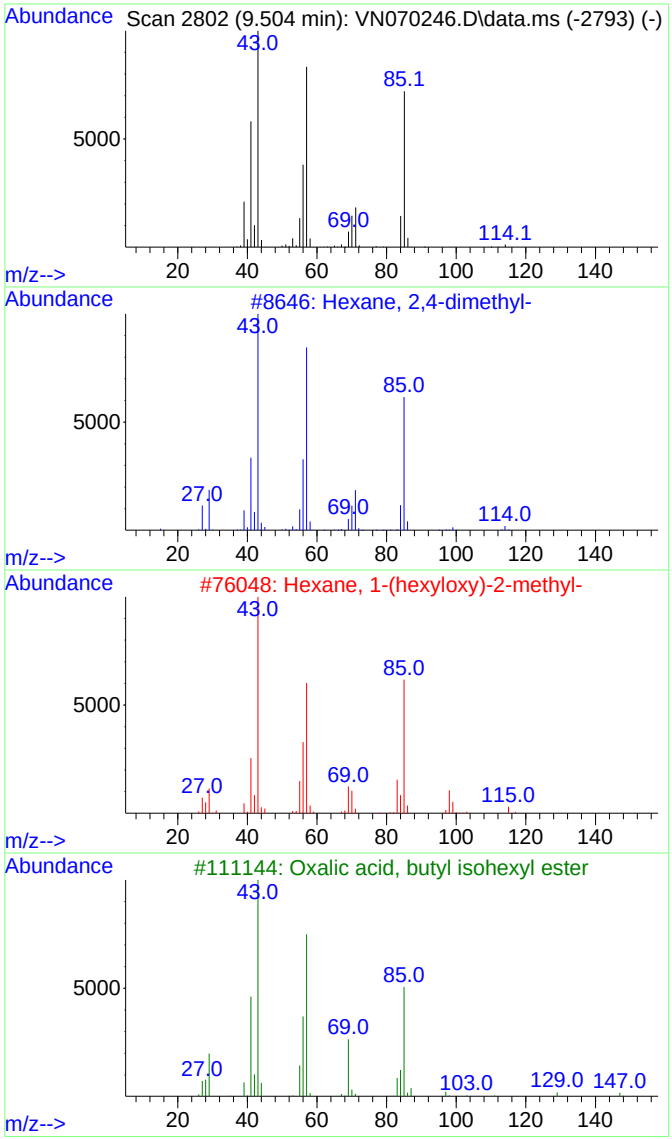
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

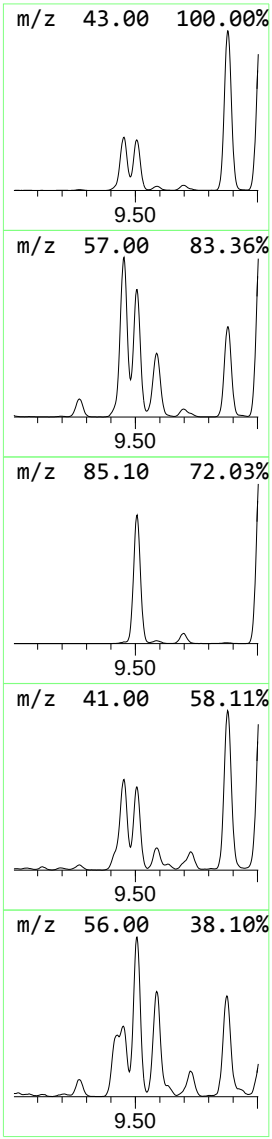
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexane, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.504	36.57 ug/l	4656860	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	90
2	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	83
3	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	78
4	Nonane, 5-methyl-	142	C10H22	015869-85-9	72
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59





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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

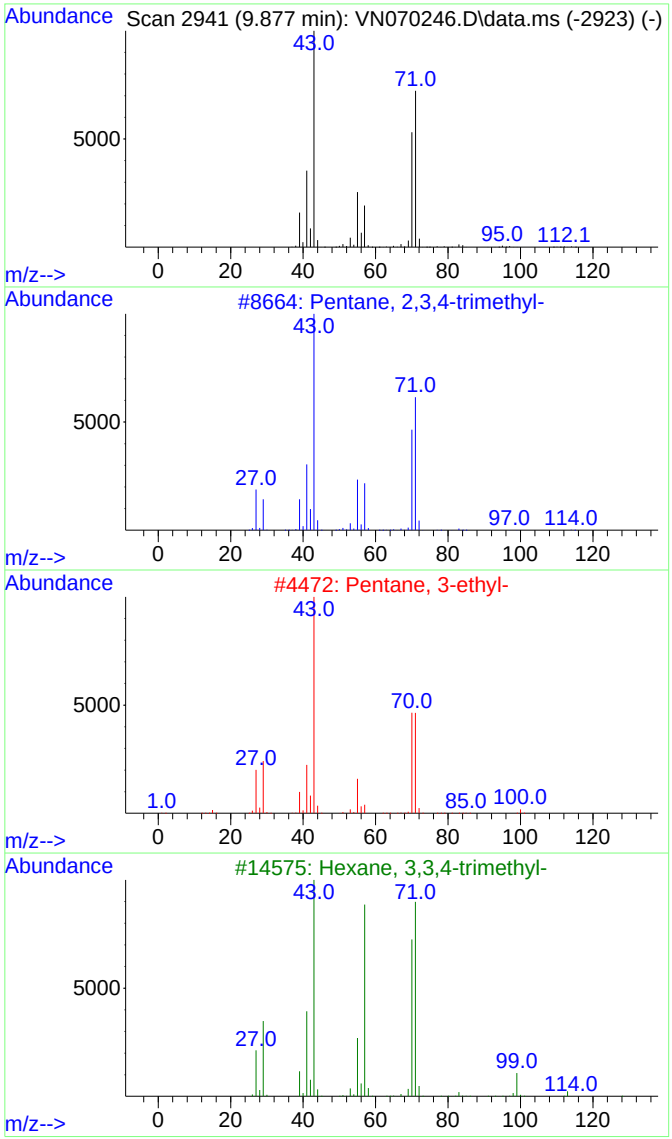
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

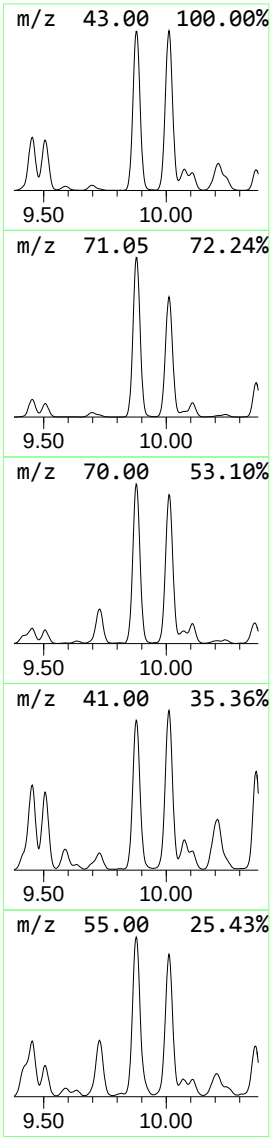
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	97.25 ug/l	12384500	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	74
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64





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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

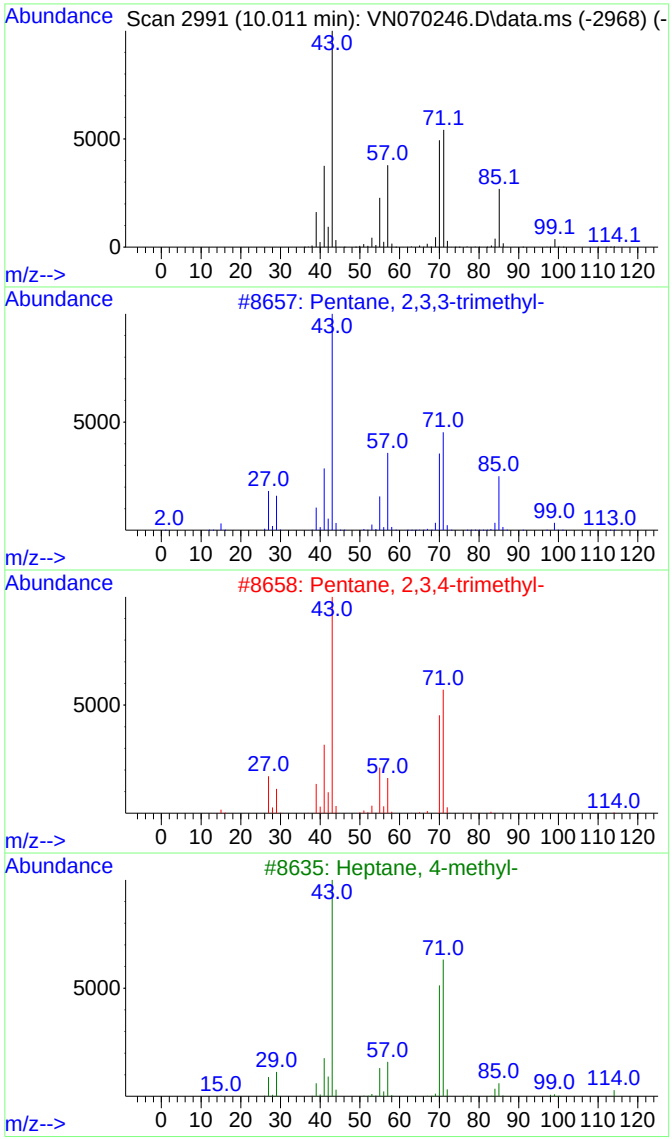
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

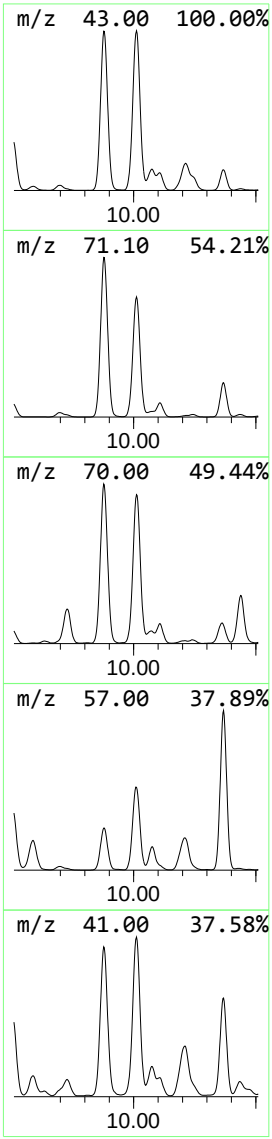
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.011	106.68 ug/l	13584200	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	68
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

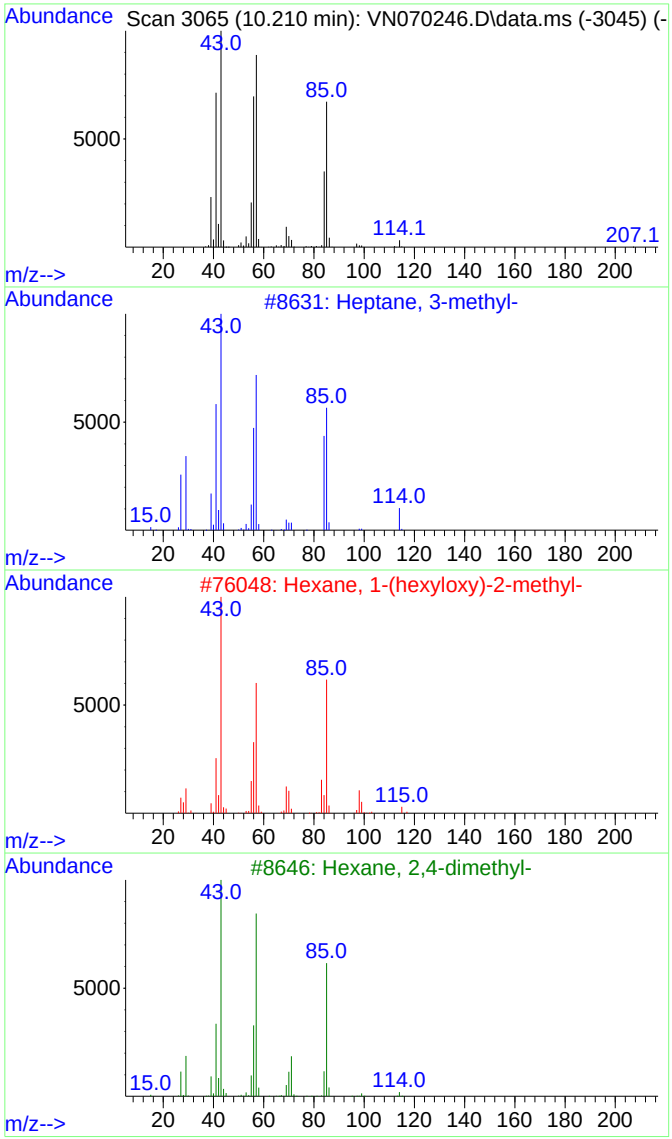
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

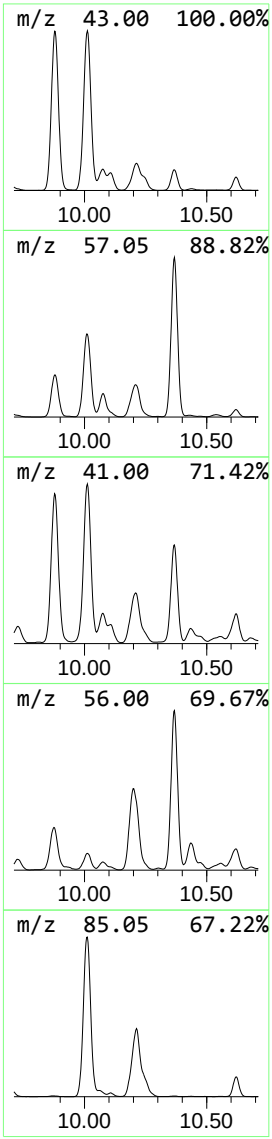
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Heptane, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	34.12 ug/l	4344710	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	83
2	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	72
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
5	Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	53





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Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

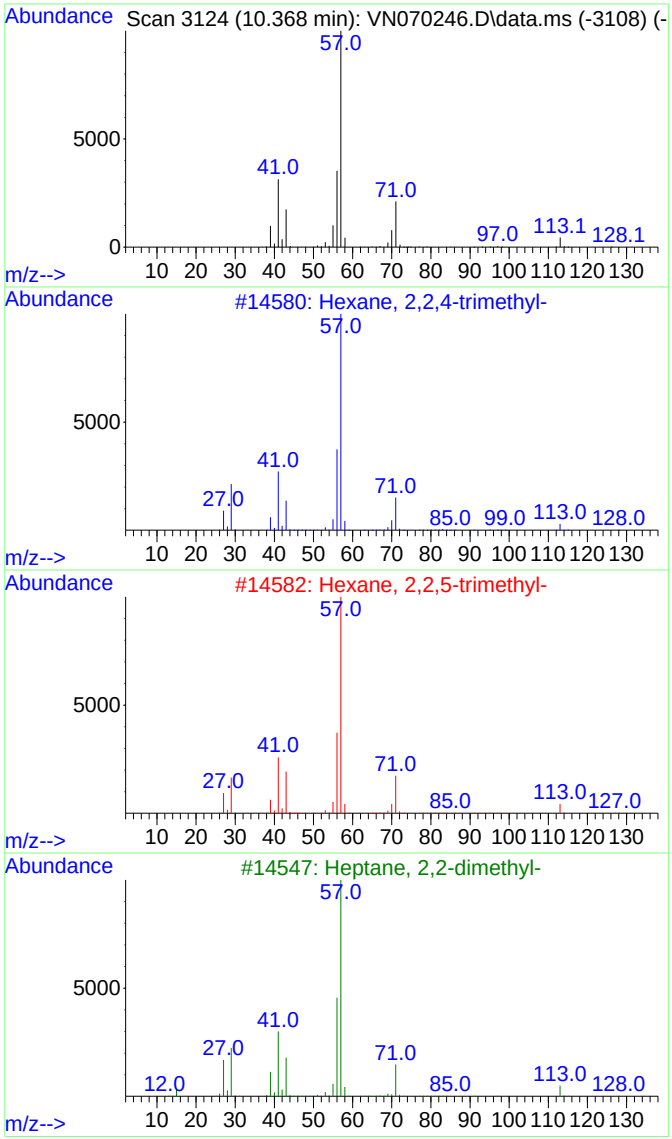
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

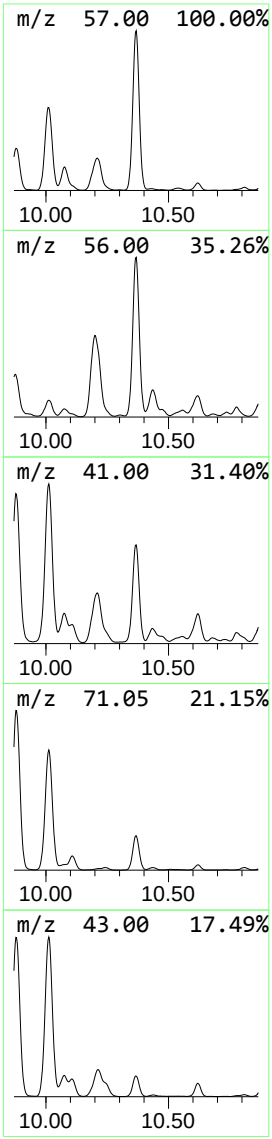
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	29.16 ug/l	5691600	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	90
2	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	83
3	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50





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Data File : VN070246.D
Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

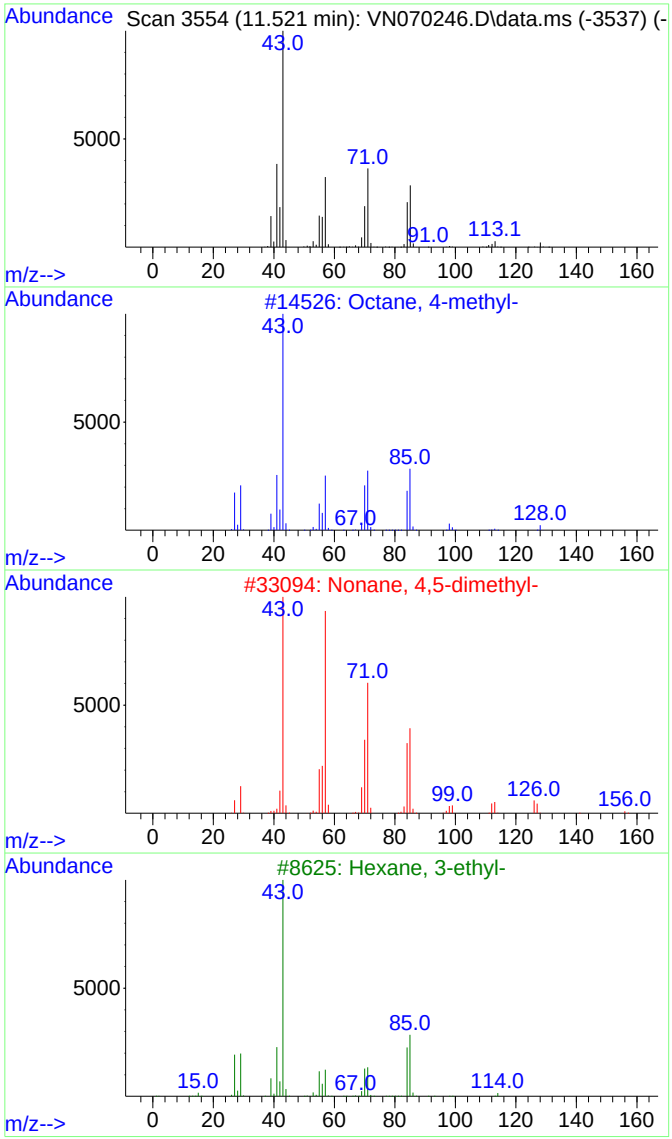
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

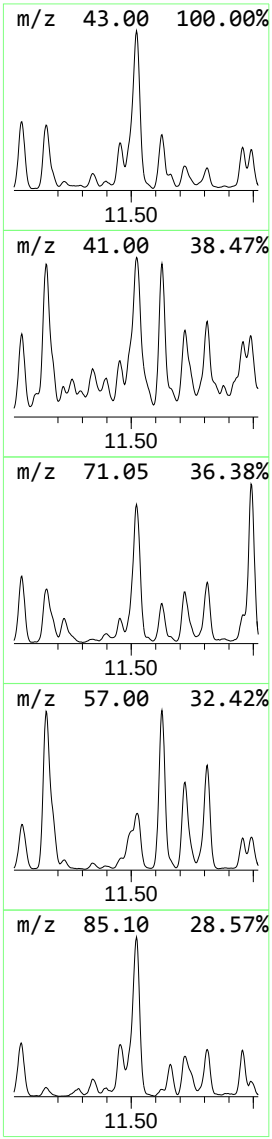
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Octane, 4-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.521	21.76 ug/l	4247600	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	91
2	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	78
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	64
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
5	Octane	114	C8H18	000111-65-9	64





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Acq On : 20 Dec 2021 17:35
Operator : JC/MD
Sample : M5044-19
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

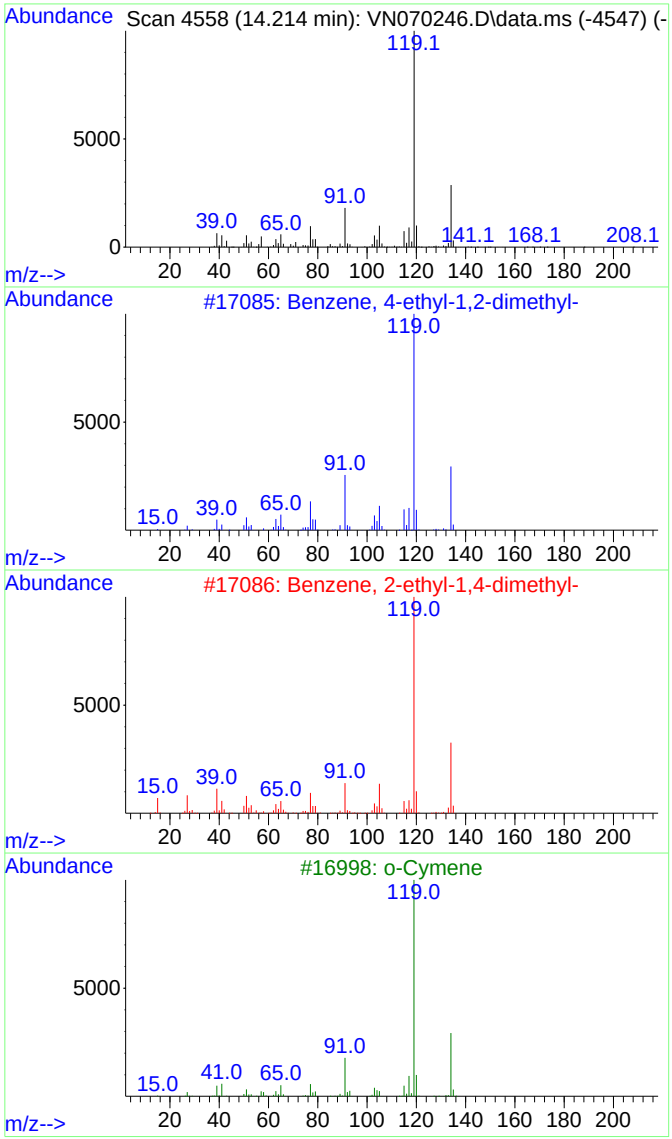
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

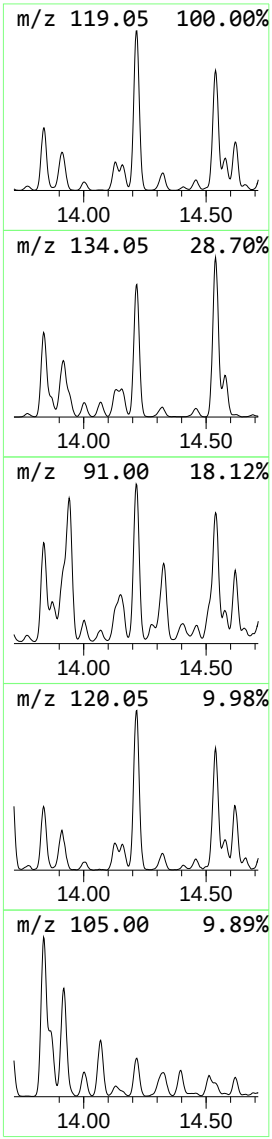
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	31.19 ug/l	4863880	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	p-Cymene	134	C10H14	000099-87-6	95





Tentatively Identified Compound (LSC) summary

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Operator : JC/MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

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-	3.006	34.9	ug/l	1441560	1	8.080	2065670	50.0
Butane, 2,3-dim...	5.036	71.7	ug/l	2962800	1	8.080	2065670	50.0
Pentane, 3-methyl-	5.586	43.0	ug/l	1778600	1	8.080	2065670	50.0
Pentane, 2,4-di...	7.029	164.1	ug/l	6780960	1	8.080	2065670	50.0
Pentane, 2,3-di...	8.166	278.3	ug/l	11496800	1	8.080	2065670	50.0
Hexane, 3-methyl-	8.287	56.1	ug/l	2318180	1	8.080	2065670	50.0
Butane, 2,2,3,3...	8.606	229.1	ug/l	29177200	2	8.965	6367060	50.0
Hexane, 2,5-dim...	9.453	53.0	ug/l	6743260	2	8.965	6367060	50.0
Hexane, 2,4-dim...	9.504	36.6	ug/l	4656860	2	8.965	6367060	50.0
Pentane, 2,3,4-...	9.877	97.3	ug/l	12384500	2	8.965	6367060	50.0
Pentane, 2,3,3-...	10.011	106.7	ug/l	13584200	2	8.965	6367060	50.0
Heptane, 3-methyl-	10.210	34.1	ug/l	4344710	2	8.965	6367060	50.0
Hexane, 2,2,4-t...	10.368	29.2	ug/l	5691600	3	11.744	9758650	50.0
Octane, 4-methyl-	11.521	21.8	ug/l	4247600	3	11.744	9758650	50.0
Benzene, 4-ethy...	14.214	31.2	ug/l	4863880	4	13.675	7796070	50.0