LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070235.D
Acq On : 20 Dec 2021 12:55
Operator : JC/MD
Sample : M5044-19 10X
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 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: VN070235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.127	412	424	446	rVB3	62441	138980	1.67%	0.257%
2	5.071	1126	1149	1164	rBV2	73568	269607	3.25%	0.499%
3	5.613	1320	1351	1378	rVB4	45879	162762	1.96%	0.301%
4	7.045	1856	1885	1906	rBV3	157891	489780	5.90%	0.906%
5	7.321	1962	1988	2012	rBV2	48242	149295	1.80%	0.276%
6	8.021	2225	2249	2259	rBV2	846473	1992042	24.01%	3.684%
7	8.083	2260	2272	2290	rVV	1527986	3540064	42.66%	6.547%
8	8.171	2291	2305	2331	rVB2	377601	957218	11.54%	1.770%
9	8.295	2335	2351	2367	rVV4	66761	149908	1.81%	0.277%
10	8.437	2382	2404	2429	rBV	1001661	2310405	27.84%	4.273%
11	8.614	2436	2470	2494	rBV	772609	1988146	23.96%	3.677%
12	8.965	2580	2601	2630	rBV	2554889	5322559	64.14%	9.843%
13	9.456	2752	2784	2794	rBV5	161916	428761	5.17%	0.793%
14	9.510	2795	2804	2820	rVB2	130896	248016	2.99%	0.459%
15	9.730	2864	2886	2907	rVB7	56370	147193	1.77%	0.272%
16	9.882	2924	2943	2966	rBV	415404	852554	10.27%	1.577%
17	10.014	2967	2992	3007	rBV2	482800	1027589	12.38%	1.900%
18	10.210	3045	3065	3095	rBV7	79801	252290	3.04%	0.467%
19	10.371	3097	3125	3135	rBV3	158942	346408	4.17%	0.641%
20	10.440	3135	3151	3189	rVB	4236572	7981651	96.18%	14.761%
21	10.620	3206	3218	3233	rVB5	52243	126958	1.53%	0.235%
22	10.878	3296	3314	3337	rVV10	65283	191108	2.30%	0.353%
23	11.151	3407	3416	3434	rVB5	45870	113088	1.36%	0.209%
24	11.521	3538	3554	3582	rVB5	54335	183774	2.21%	0.340%
25	11.744	3618	3637	3657	rBV	4556915	8298235	100.00%	15.347%
26	11.950	3702	3714	3724	rBV2	69818	140464	1.69%	0.260%
27	12.731	3988	4005	4027	rVB	3608036	6409451	77.24%	11.853%
28	13.055	4118	4126	4138	rVB7	59185	97760	1.18%	0.181%
29	13.222	4172	4188	4203	rBV3	47962	129672	1.56%	0.240%
30	13.366	4231	4242	4253	rVB2	164582	262445	3.16%	0.485%
31	13.500	4274	4292	4298	rBV3	50349	121784	1.47%	0.225%
32	13.610	4323	4333	4339	rBV5	53066	91029	1.10%	0.168%
33	13.675	4341	4357	4399	rVB	3814274	6944788	83.69%	12.844%
34	13.836	4404	4417	4425	rBV2	137300	231862	2.79%	0.429%
35	13.997	4467	4477	4490	rVB9	60157	101213	1.22%	0.187%
36	14.150	4519	4534	4546	rVB7	75842	172896	2.08%	0.320%

LSC Area Percent Report

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ALS Vial : 7 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	14.214	4547	4558	4575	rBV	188947	322332	3.88%	0.596%
38	14.324	4588	4599	4612	rVB2	119653	217062	2.62%	0.401%
39	14.404	4615	4629	4642	rBV7	56768	116254	1.40%	0.215%
40	14.538	4671	4679	4689	rVB	131003	200257	2.41%	0.370%
41	14.619	4701	4709	4737	rVB5	82400	160922	1.94%	0.298%
42	14.809	4771	4780	4789	rBV3	60179	97861	1.18%	0.181%
43	14.917	4807	4820	4833	rBV4	103143	233439	2.81%	0.432%
44	15.193	4914	4923	4934	rVB4	75100	119205	1.44%	0.220%
45	15.507	5032	5040	5053	rVB	72734	127164	1.53%	0.235%
46	15.700	5107	5112	5133	rVB6	59824	106020	1.28%	0.196%

Sum of corrected areas: 54072271

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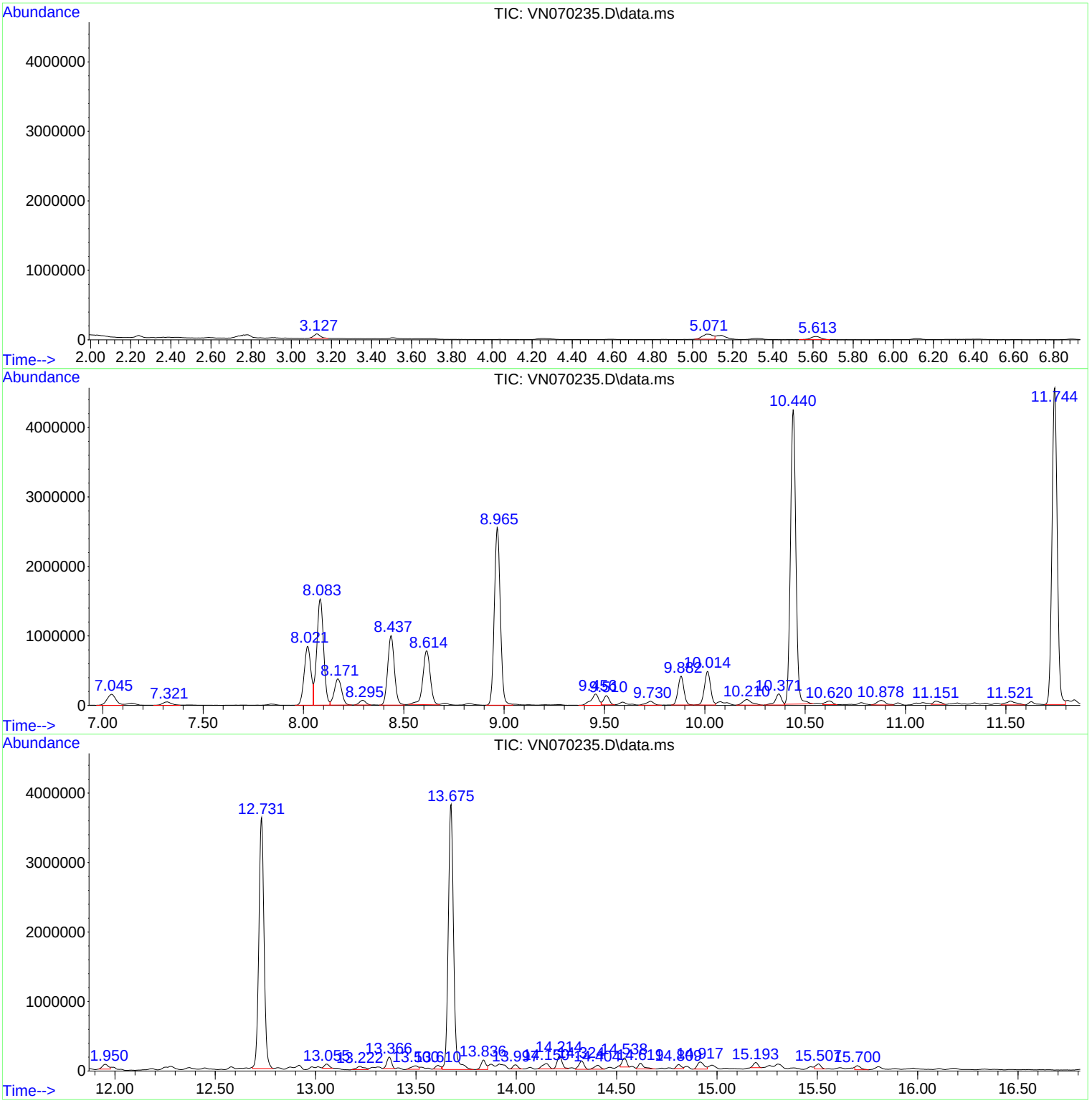
Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070235.D
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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

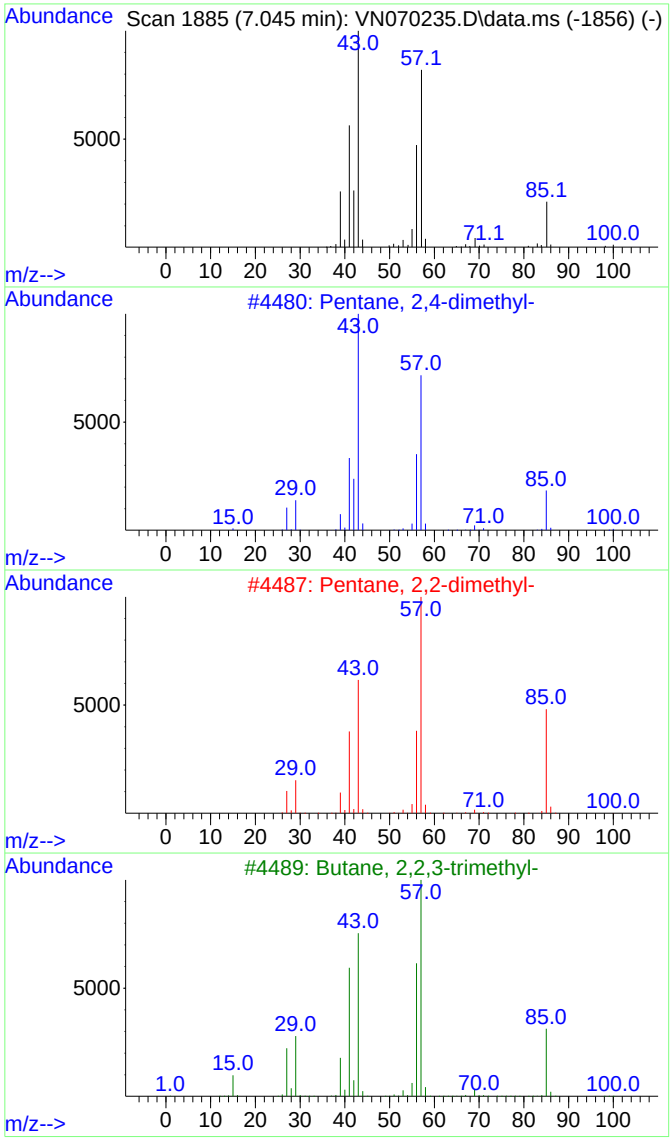
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

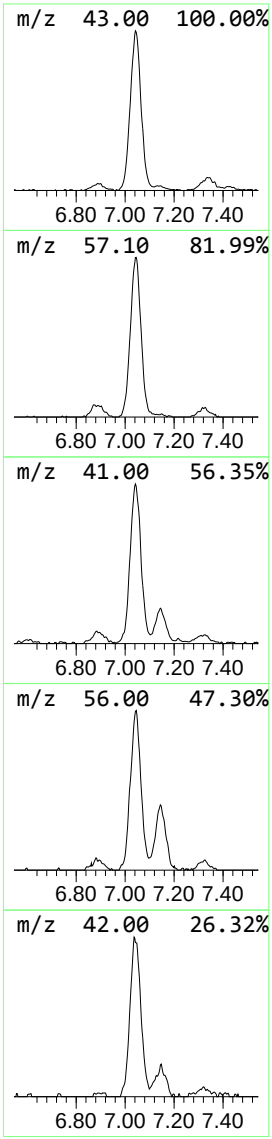
****

Peak Number 1 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	6.92 ug/l	489780	Pentafluorobenzene	8.083

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	50
5	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	50





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Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

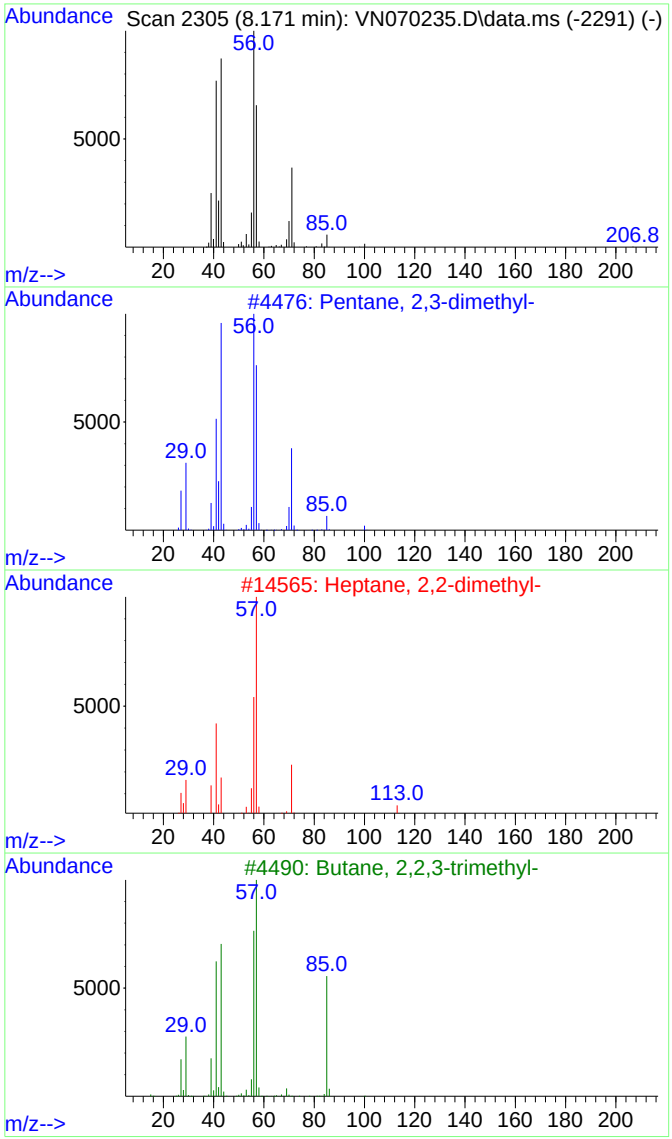
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

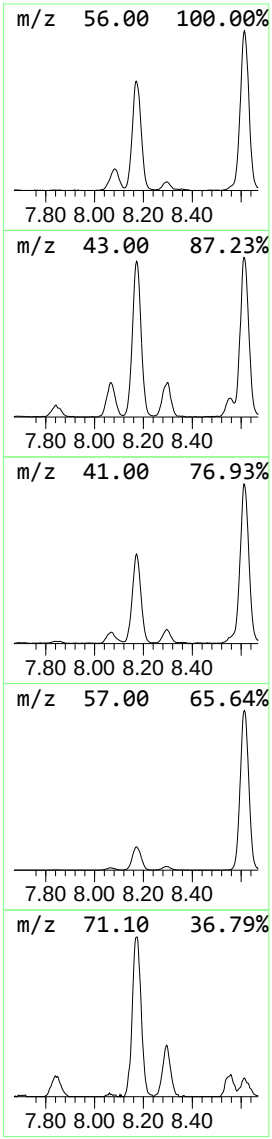
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.171	13.52 ug/l	957218	Pentafluorobenzene	8.083

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40
5	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	38





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Acq On : 20 Dec 2021 12:55
Operator : JC/MD
Sample : M5044-19 10X
Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

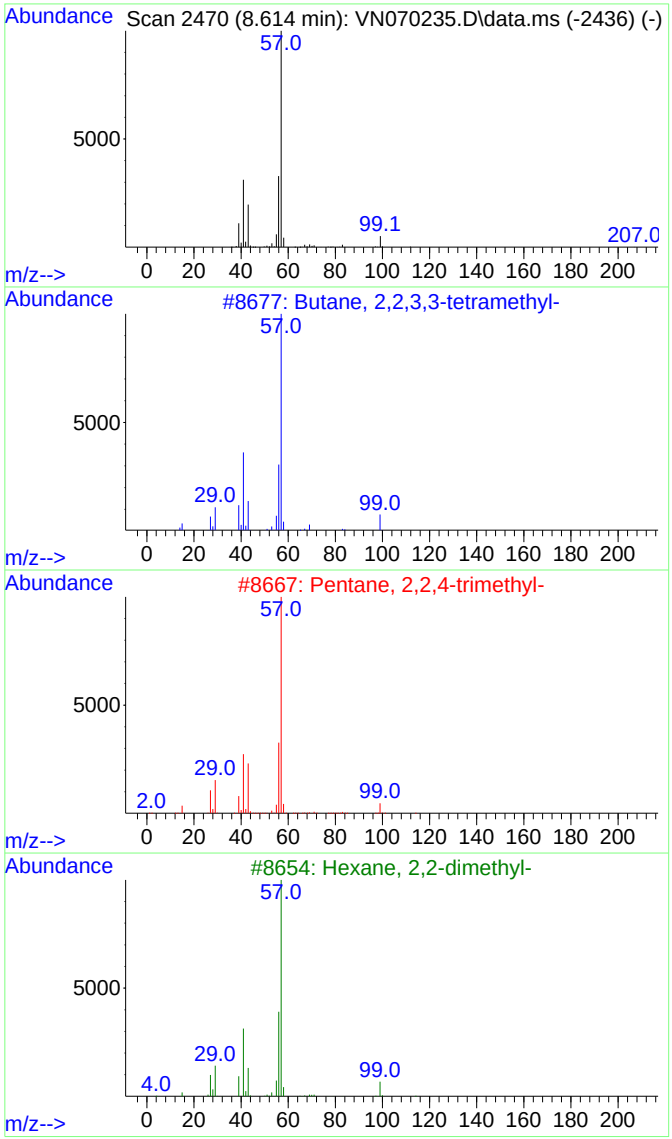
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

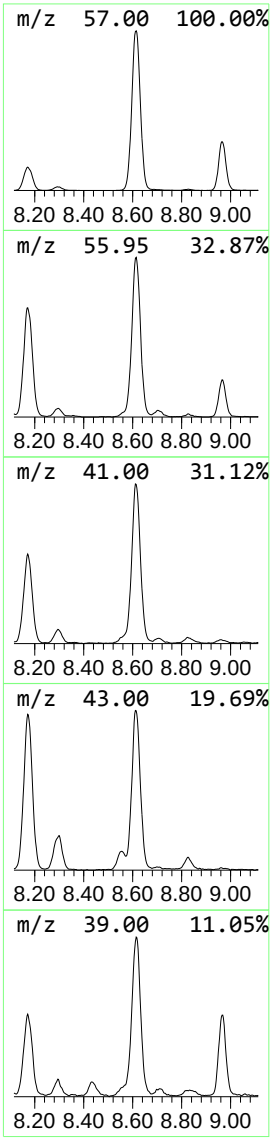
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	18.68 ug/l	1988150	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	72
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	59
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





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Operator : JC/MD
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Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-19-5.0

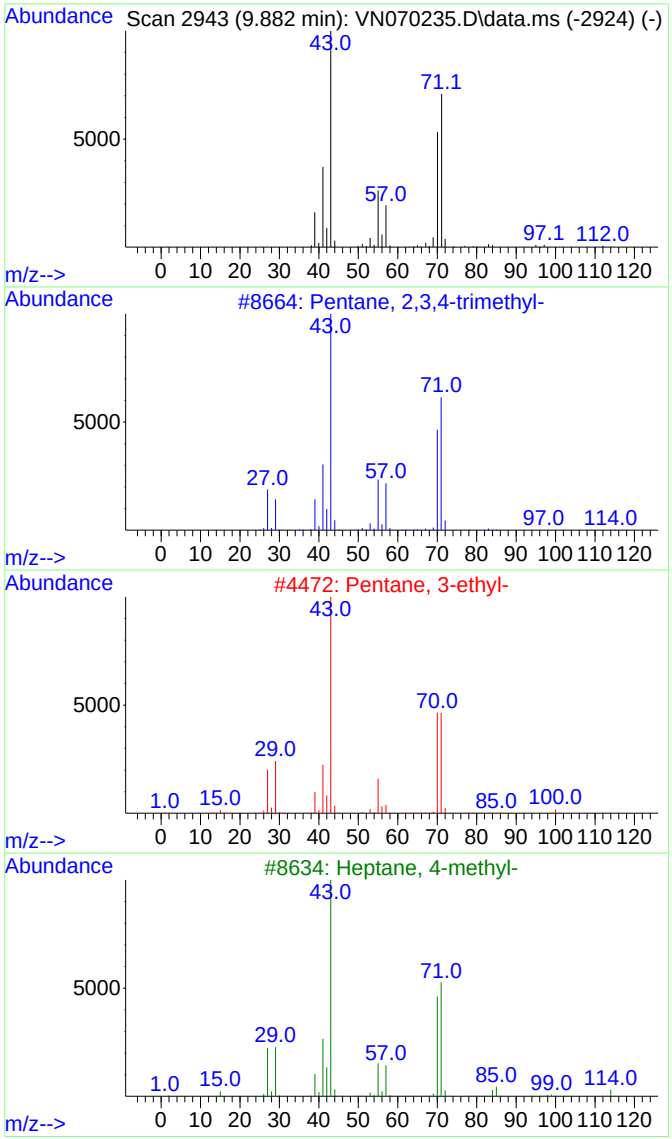
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

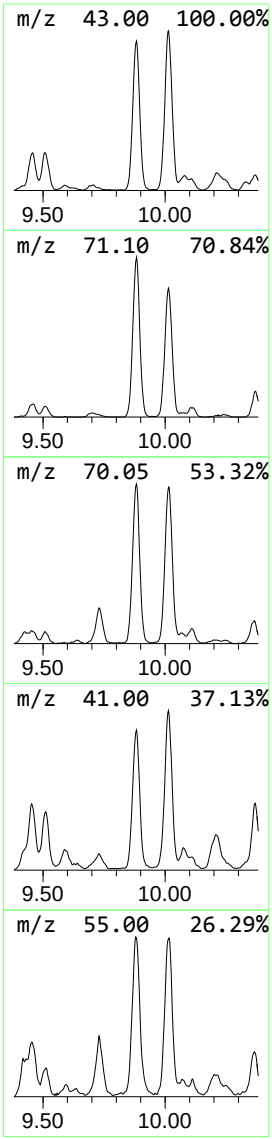
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.882	8.01 ug/l	852554	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	90
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	56





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Misc : 6.60g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 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

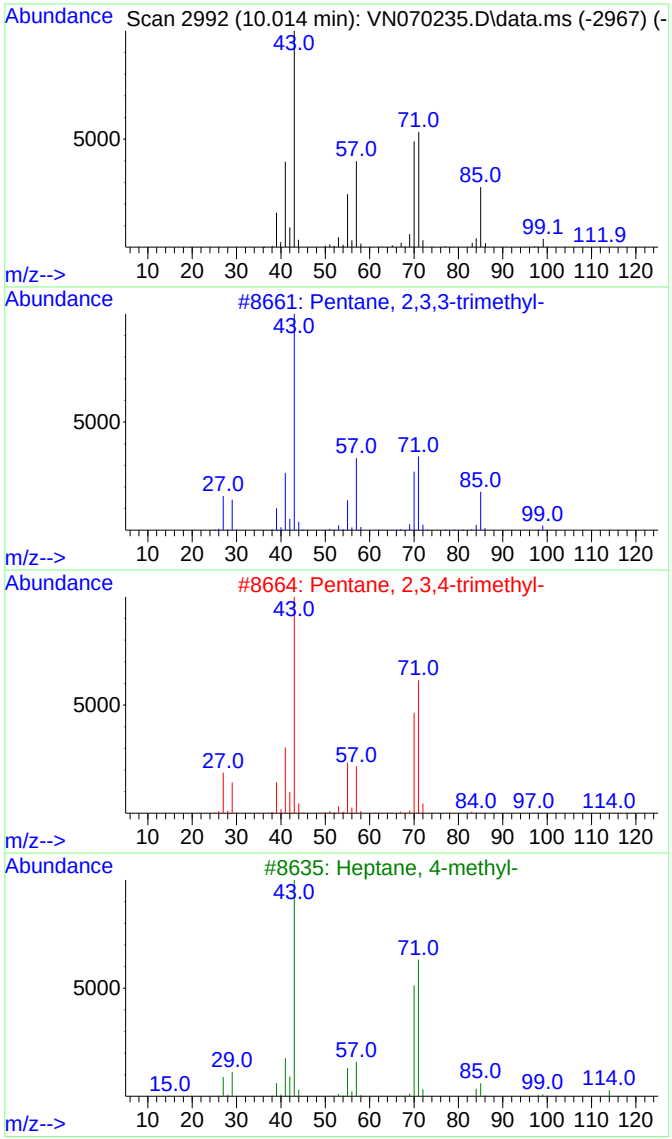
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

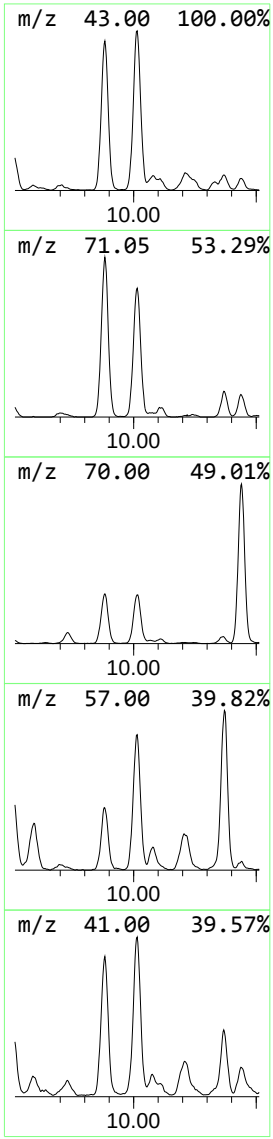
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	9.65 ug/l	1027590	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	83
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	74
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	72
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





Tentatively Identified Compound (LSC) summary

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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
Pentane, 2,4-di...	7.045	6.9	ug/l	489780	1	8.083	3540060	50.0
Pentane, 2,3-di...	8.171	13.5	ug/l	957218	1	8.083	3540060	50.0
Butane, 2,2,3,3...	8.614	18.7	ug/l	1988150	2	8.965	5322560	50.0
Pentane, 2,3,4-...	9.882	8.0	ug/l	852554	2	8.965	5322560	50.0
Pentane, 2,3,3-...	10.014	9.7	ug/l	1027590	2	8.965	5322560	50.0