LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

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: VN070245.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.101	1106	1160	1187	rBV2	289876	1357955	5.86%	0.563%
2	5.581	1308	1339	1377	rBV2	206632	714214	3.08%	0.296%
3	6.093	1500	1530	1558	rBV4	256341	797668	3.44%	0.331%
4	6.444	1640	1661	1688	rVB2	166231	509622	2.20%	0.211%
5	6.586	1689	1714	1735	rBV3	83548	264229	1.14%	0.110%
6	6.881	1798	1824	1844	rBV4	168332	527396	2.28%	0.219%
7	7.026	1859	1878	1897	rBV3	194325	548785	2.37%	0.228%
8	7.128	1898	1916	1934	rBV2	234924	647520	2.80%	0.269%
9	7.766	2135	2154	2165	rBV4	154069	392189	1.69%	0.163%
10	7.831	2167	2178	2196	rVB2	195078	466138	2.01%	0.193%
11	8.021	2224	2249	2253	rBV2	990395	2148697	9.28%	0.891%
12	8.163	2290	2302	2327	rVB4	749269	1981512	8.56%	0.822%
13	8.287	2327	2348	2383	rBV	1242044	2923156	12.62%	1.213%
14	8.434	2383	2403	2433	rBV	1170966	2909959	12.57%	1.207%
15	8.609	2433	2468	2493	rBV	2427765	7727914	33.37%	3.206%
16	8.820	2524	2547	2576	rVB3	1037338	2527018	10.91%	1.048%
17	8.963	2576	2600	2627	rBV3	4038727	10277073	44.38%	4.264%
18	9.118	2646	2658	2672	rVB	482846	929481	4.01%	0.386%
19	9.193	2672	2686	2695	rVV	466670	949833	4.10%	0.394%
20	9.239	2697	2703	2728	rVB3	346478	741081	3.20%	0.307%
21	9.453	2749	2783	2794	rBV4	1622886	4479390	19.34%	1.858%
22	9.507	2795	2803	2819	rVV	815029	1572188	6.79%	0.652%
23	9.588	2821	2833	2840	rVV4	185790	362170	1.56%	0.150%
24	9.633	2841	2850	2865	rVB3	398233	780835	3.37%	0.324%
25	9.732	2866	2887	2901	rBV7	406450	1141208	4.93%	0.473%
26	9.877	2928	2941	2963	rBV2	2066180	4528271	19.55%	1.879%
27	9.971	2965	2976	2981	rBV	981194	1675368	7.23%	0.695%
28	10.014	2982	2992	3004	rVB3	2535786	4807930	20.76%	1.995%
29	10.076	3005	3015	3024	rBV	1598023	2789585	12.05%	1.157%
30	10.212	3047	3066	3092	rBV2	1768502	4123496	17.81%	1.711%
31	10.314	3093	3104	3112	rBV6	465251	884586	3.82%	0.367%
32	10.365	3113	3123	3136	rVB3	1456058	2622425	11.32%	1.088%
33	10.440	3136	3151	3172	rBV	5051630	10149353	43.83%	4.211%
34	10.542	3174	3189	3202	rVV7	389832	1219085	5.26%	0.506%
35	10.623	3204	3219	3232	rVV4	2148218	4517021	19.50%	1.874%
36	10.682	3233	3241	3250	rVB2	672991	996522	4.30%	0.413%

LSC Area Percent Report

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ClientSampleId :
DA-17-4.5

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	10.802	3268	3286	3295	rBV3	549053	1393249	6.02%	0.578%
38	10.859	3295	3307	3330	rVB6	1499661	4008480	17.31%	1.663%
39	10.961	3334	3345	3357	rVB5	486489	990613	4.28%	0.411%
40	11.049	3358	3378	3390	rBV6	441893	1176934	5.08%	0.488%
41	11.151	3391	3416	3432	rBV4	756583	2719160	11.74%	1.128%
42	11.253	3446	3454	3464	rVB4	584141	934157	4.03%	0.388%
43	11.454	3521	3529	3538	rBV4	392871	556554	2.40%	0.231%
44	11.524	3545	3555	3582	rVB4	1981204	4854711	20.96%	2.014%
45	11.626	3582	3593	3615	rBV	1537016	2912643	12.58%	1.208%
46	11.744	3624	3637	3653	rBV	5408990	9726397	42.00%	4.035%
47	11.843	3663	3674	3694	rVB	4082212	7060307	30.49%	2.929%
48	11.953	3699	3715	3738	rVB2	6520392	14336169	61.90%	5.948%
49	12.071	3753	3759	3773	rVB5	354575	529479	2.29%	0.220%
50	12.280	3817	3837	3854	rVB3	1263019	3074199	13.27%	1.275%
51	12.578	3937	3948	3959	rBV	3212500	5308321	22.92%	2.202%
52	12.731	3994	4005	4027	rVB2	4380581	9315808	40.23%	3.865%
53	12.817	4031	4037	4049	rVB6	382667	602415	2.60%	0.250%
54	12.919	4064	4075	4087	rBV	2727045	4371539	18.88%	1.814%
55	12.983	4087	4099	4106	rBV	4936156	8261838	35.68%	3.428%
56	13.055	4119	4126	4142	rVB	4184207	7317383	31.60%	3.036%
57	13.219	4176	4187	4204	rVB	2526978	4322116	18.66%	1.793%
58	13.366	4229	4242	4272	rVB	13441246	23158462	100.00%	9.608%
59	13.672	4345	4356	4364	rBV	5168371	8936394	38.59%	3.708%
60	13.838	4407	4418	4420	rBV	1096884	1363395	5.89%	0.566%
61	13.871	4421	4430	4438	rVV3	3282057	5240021	22.63%	2.174%
62	13.991	4467	4475	4489	rVB2	532143	848354	3.66%	0.352%
63	14.069	4494	4504	4514	rVB	666686	1019767	4.40%	0.423%
64	14.128	4515	4526	4532	rBV	1326175	2173950	9.39%	0.902%
65	14.214	4547	4558	4571	rVB	2300946	3600224	15.55%	1.494%
66	14.327	4589	4600	4612	rVB4	1179409	2008023	8.67%	0.833%
67	14.458	4640	4649	4661	rBV	394330	642615	2.77%	0.267%
68	14.538	4669	4679	4686	rBV	955734	1489737	6.43%	0.618%
69	14.576	4687	4693	4702	rVV	1123654	1571986	6.79%	0.652%
70	14.619	4703	4709	4718	rVB2	448677	548912	2.37%	0.228%
71	14.761	4754	4762	4769	rBV2	242114	316940	1.37%	0.131%
72	14.809	4770	4780	4789	rBV3	816894	1407016	6.08%	0.584%
73	14.925	4806	4823	4836	rBV5	1146812	2940509	12.70%	1.220%
74	15.196	4914	4924	4950	rVB3	447095	1132960	4.89%	0.470%
75	15.311	4956	4967	4986	rVB5	285225	640632	2.77%	0.266%
76	15.504	5028	5039	5054	rVB	718125	1359758	5.87%	0.564%

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Instrument :
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ClientSampleId :
DA-17-4.5

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	15.804	5138	5151	5171	rBV2	161124	340638	1.47%	0.141%
78	16.614	5441	5453	5471	rVB	245672	528734	2.28%	0.219%

Sum of corrected areas: 241032372

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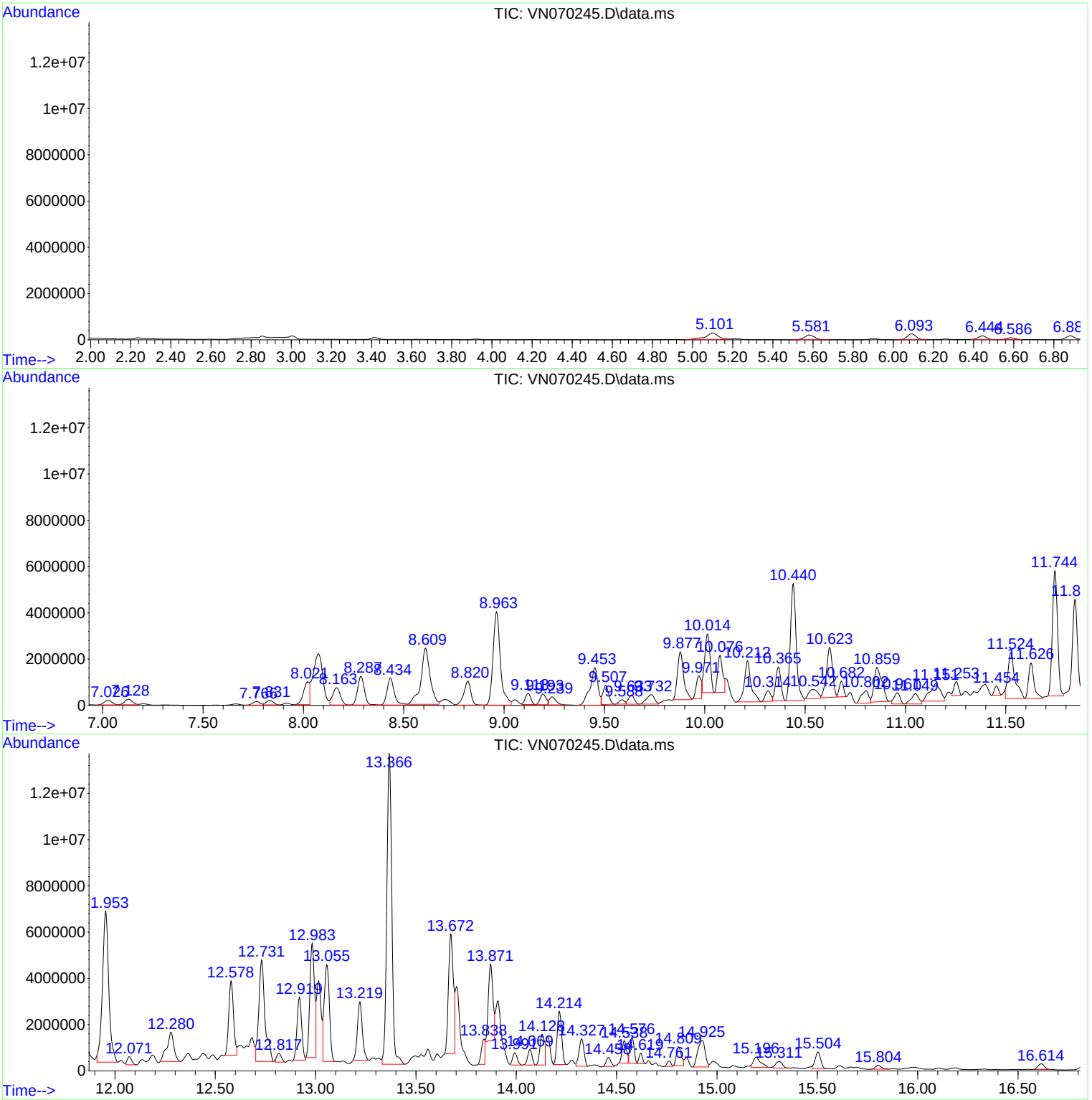
Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

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\VN122021\
Data File : VN070245.D
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

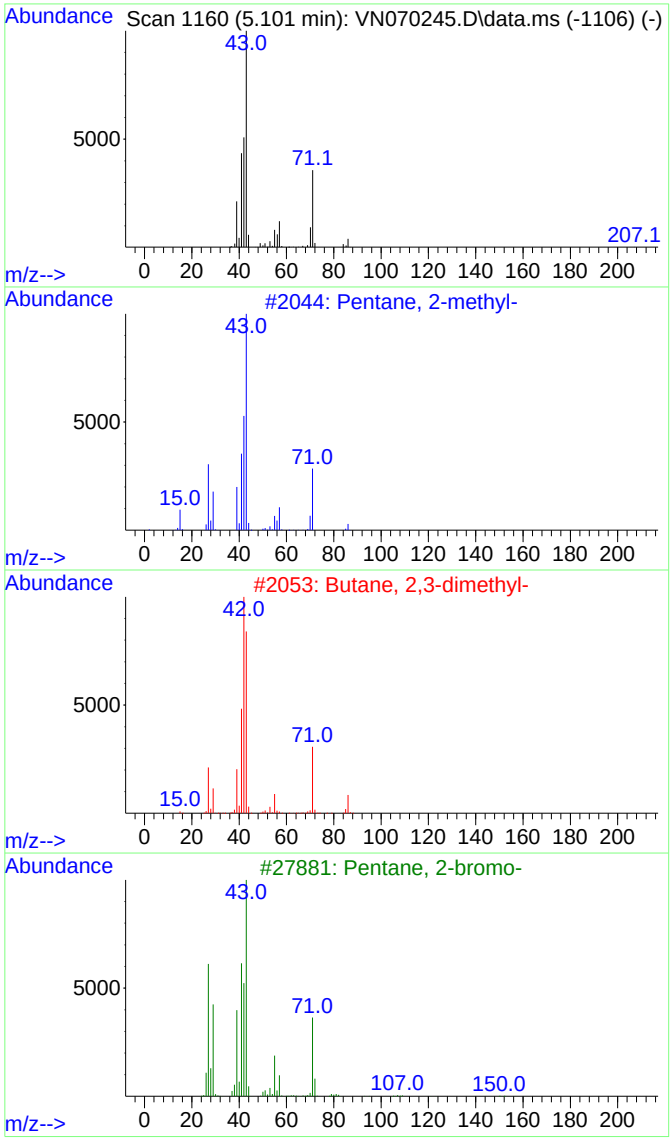
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

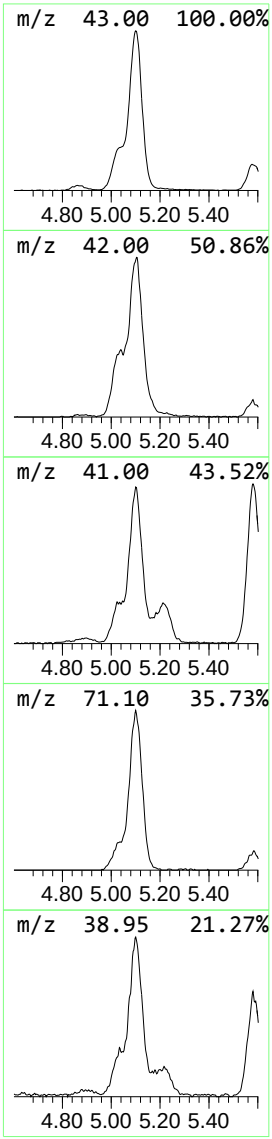
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.101	31.60 ug/l	1357960	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	45
4	Butanoic acid, 3-methyl-2-oxo-, ...	130	C6H10O3	003952-67-8	38
5	Pentane	72	C5H12	000109-66-0	28





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Data File : VN070245.D
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Operator : JC/MD
Sample : M5044-17
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

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

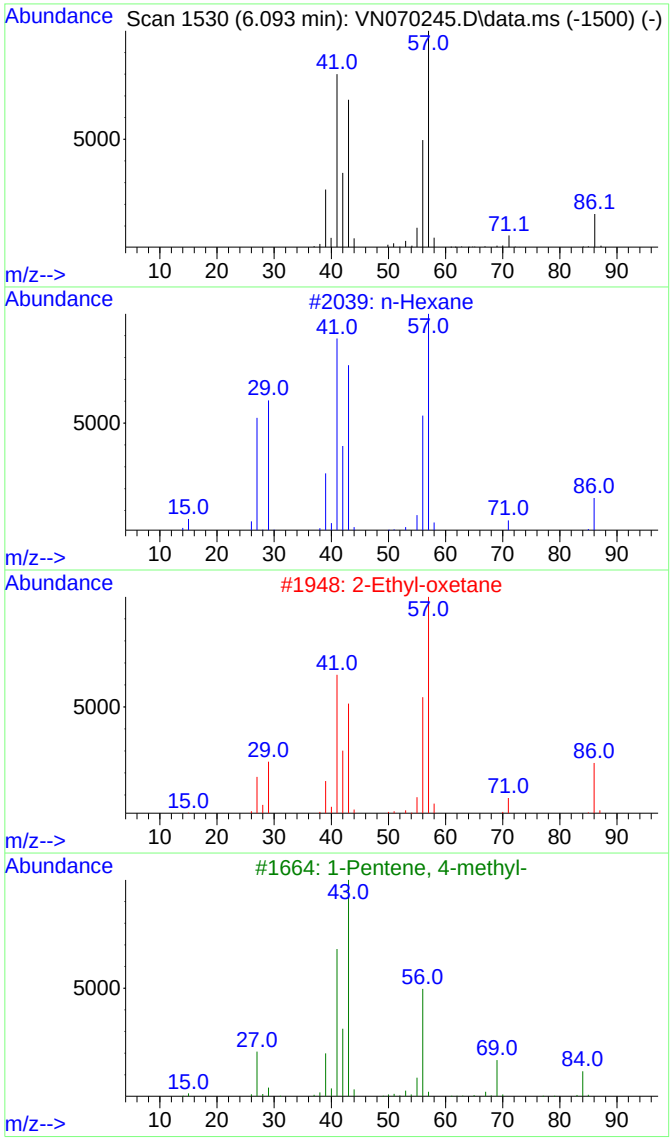
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

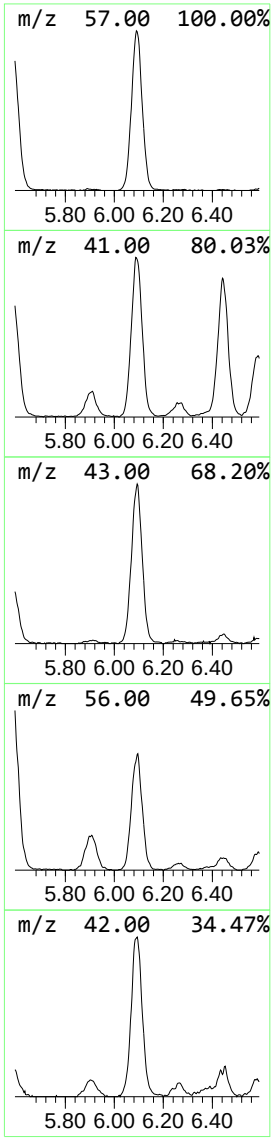
****

Peak Number 2 n-Hexane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.093	18.56 ug/l	797668	Pentafluorobenzene	8.080

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	50
3	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35





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DA-17-4.5

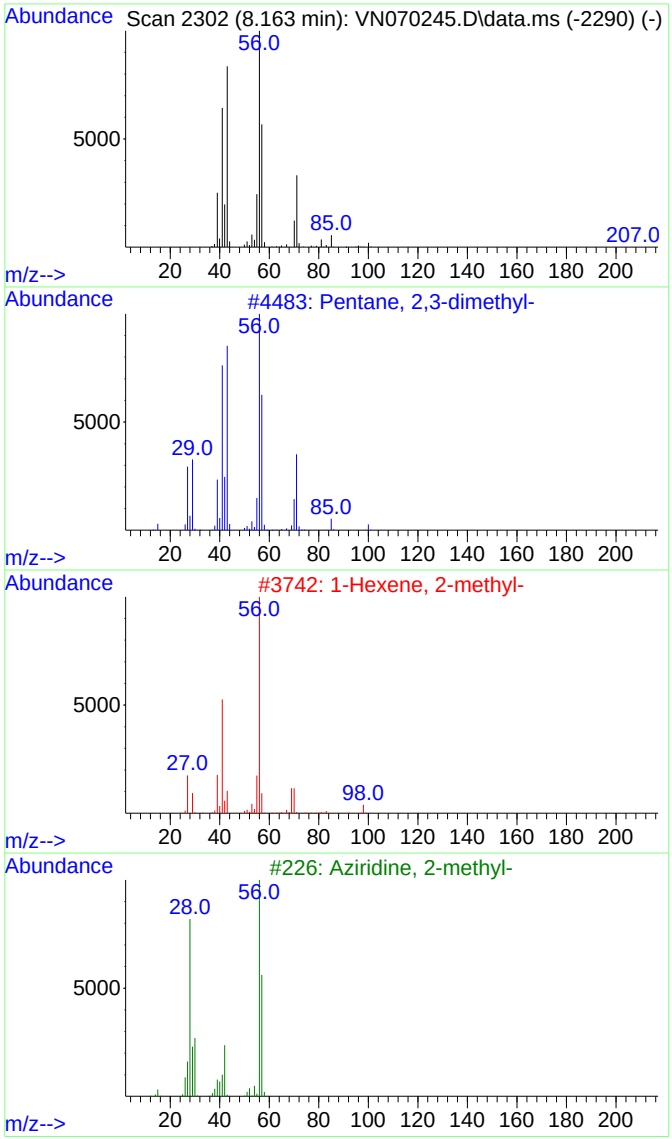
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

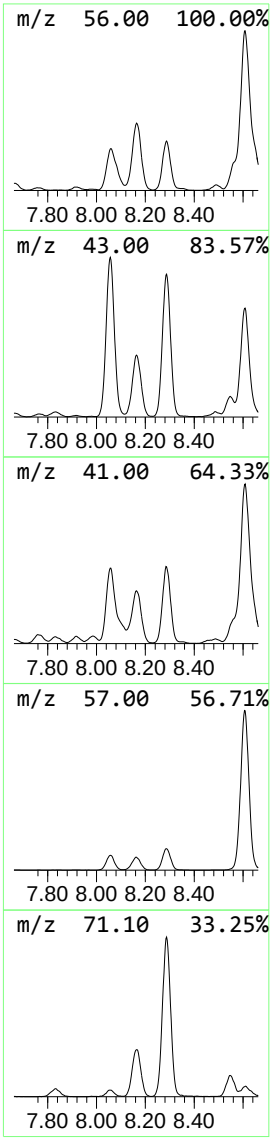
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.163	46.11 ug/l	1981510	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	38
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	38





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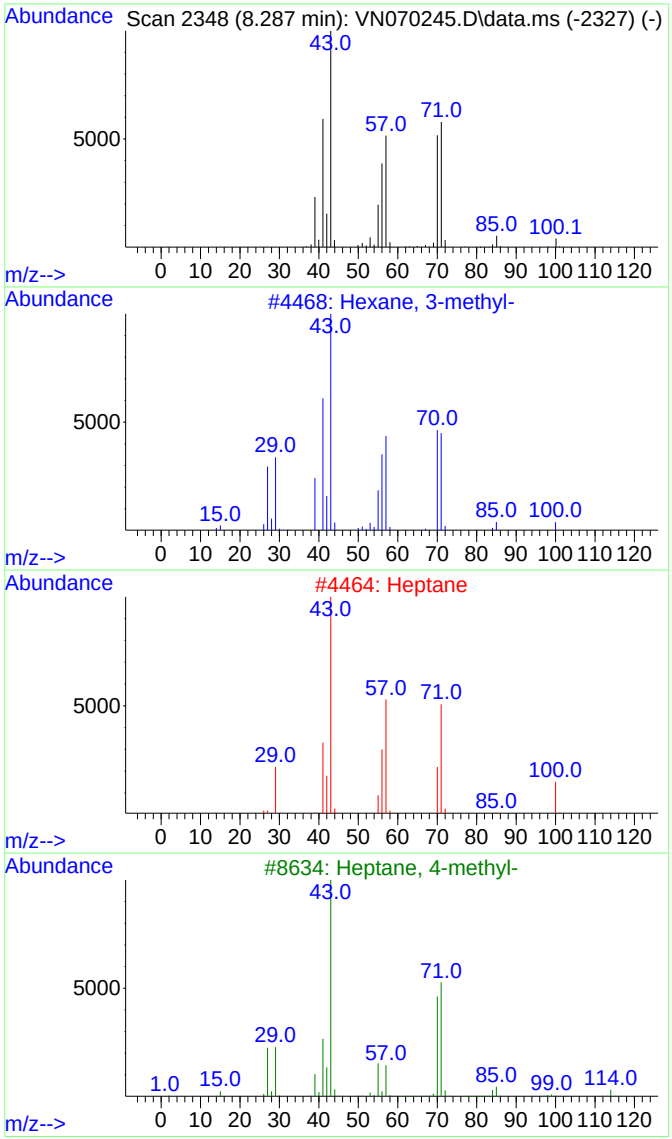
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

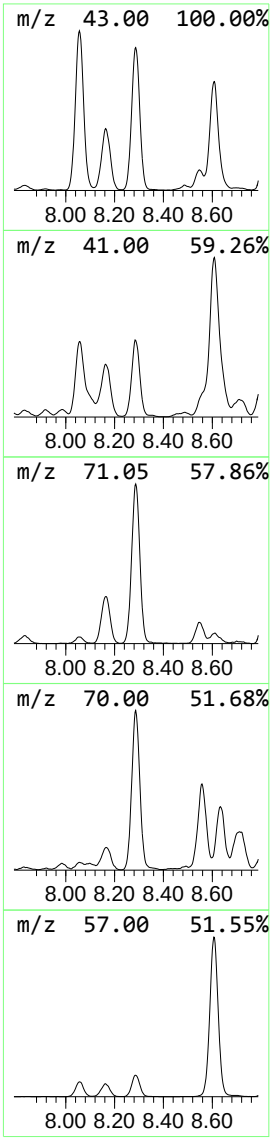
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	68.02 ug/l	2923160	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	72
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	50





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

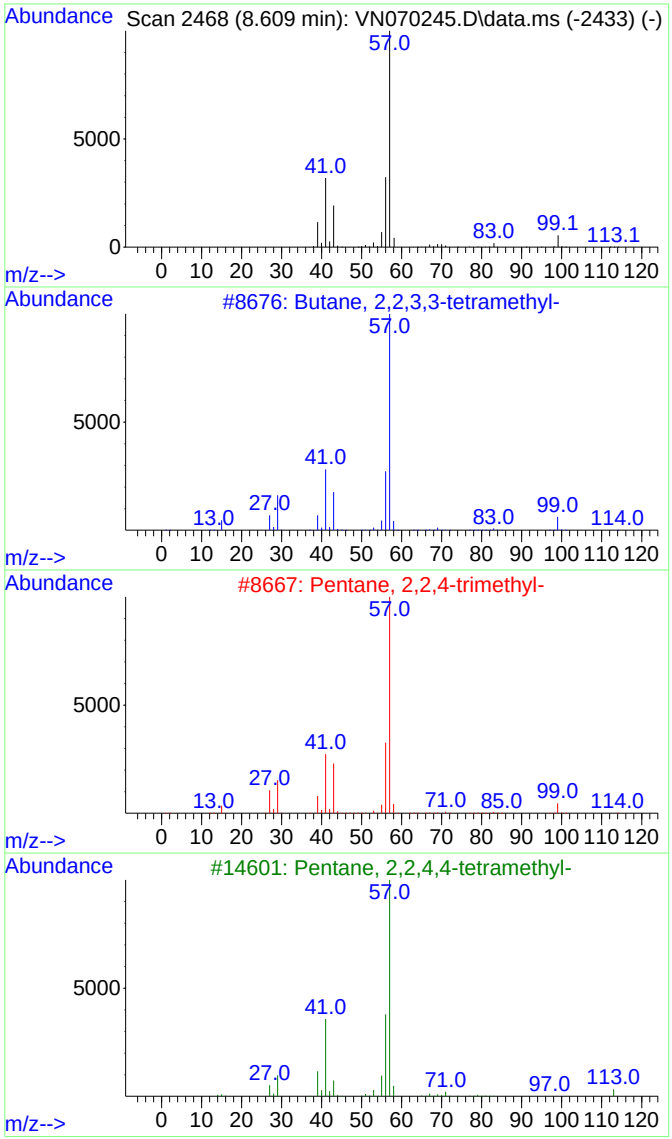
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

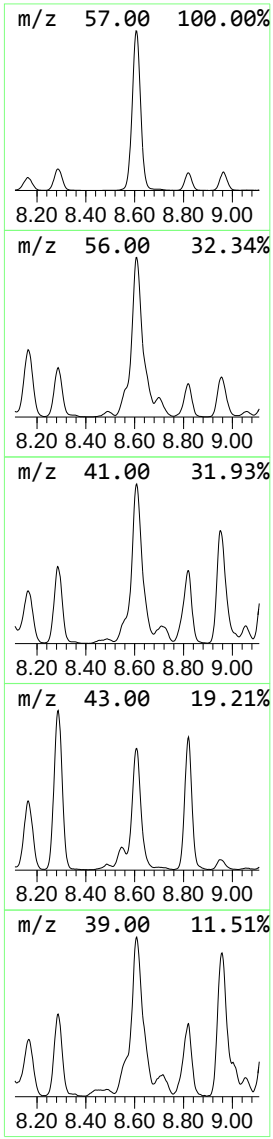
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.609	37.60 ug/l	7727910	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	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59





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Data File : VN070245.D
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Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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ClientSampleId :
DA-17-4.5

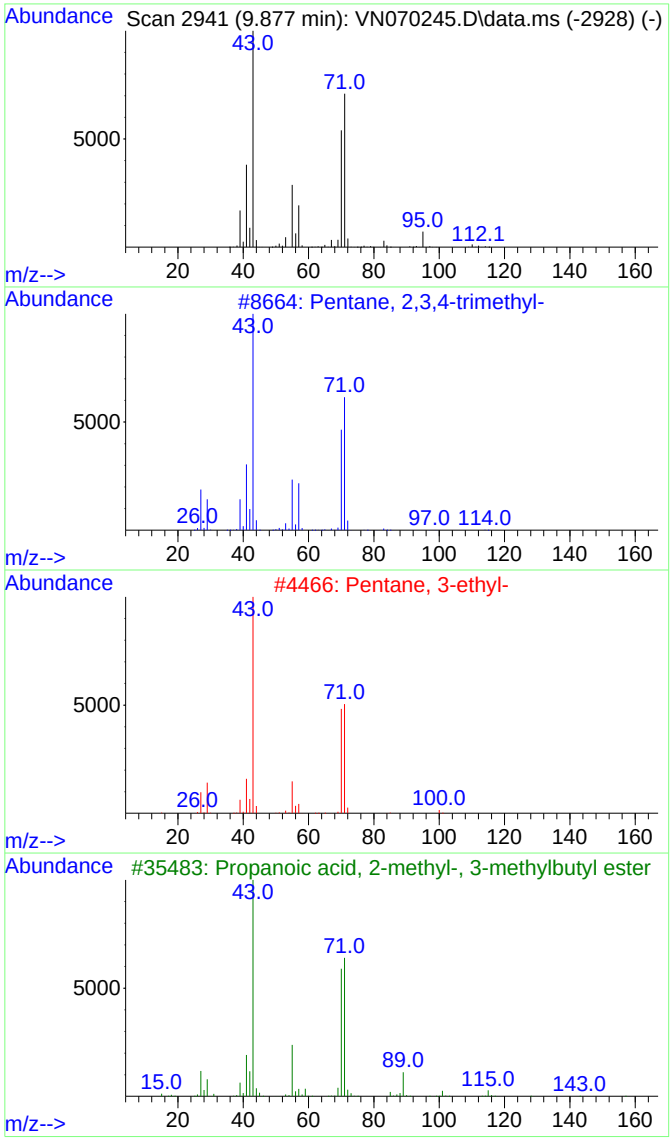
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

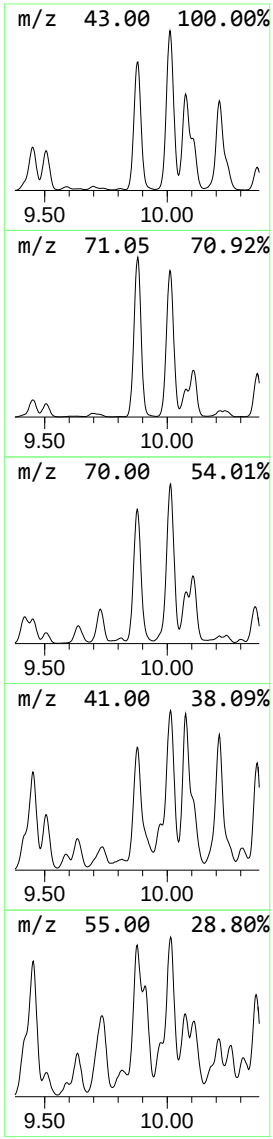
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	22.03 ug/l	4528270	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	56
3	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	56
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	56
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

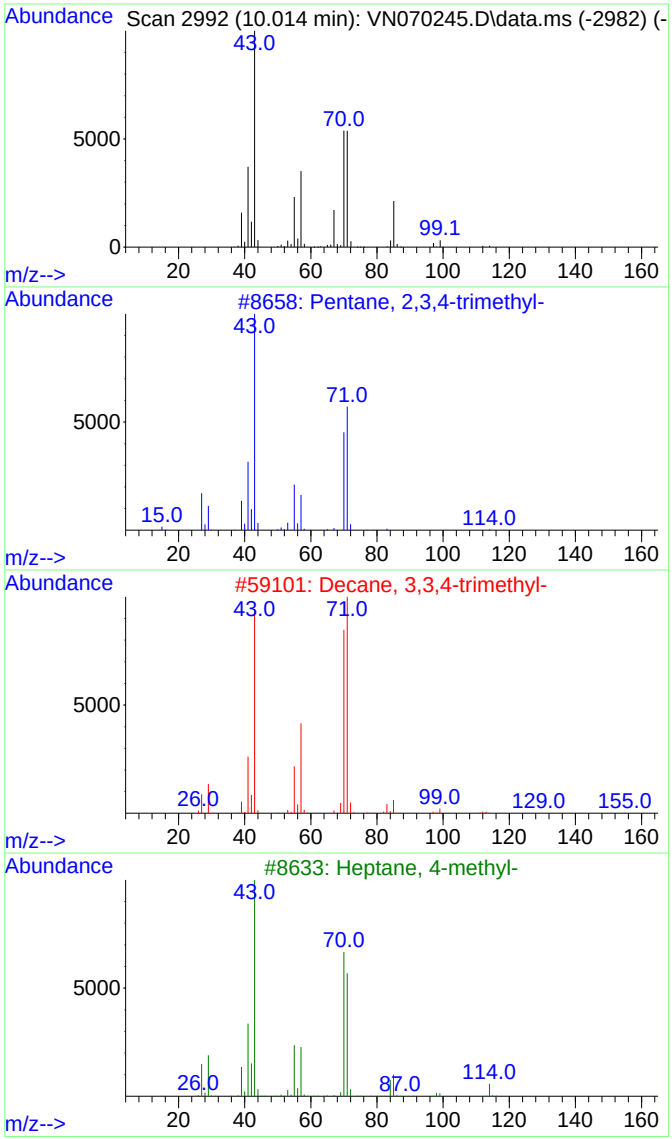
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

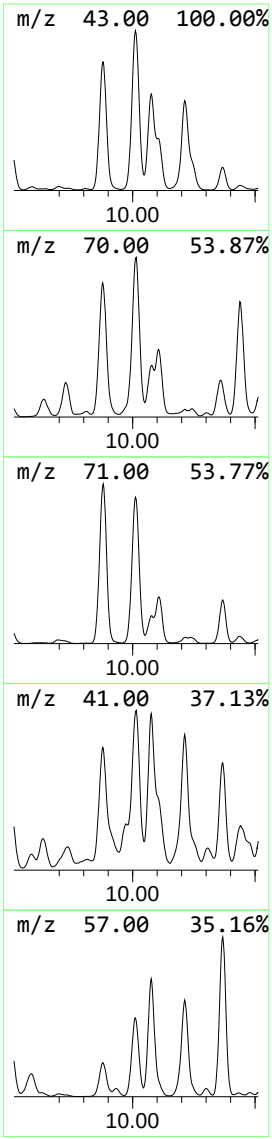
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Decane, 3,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	23.39 ug/l	4807930	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	76
2	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

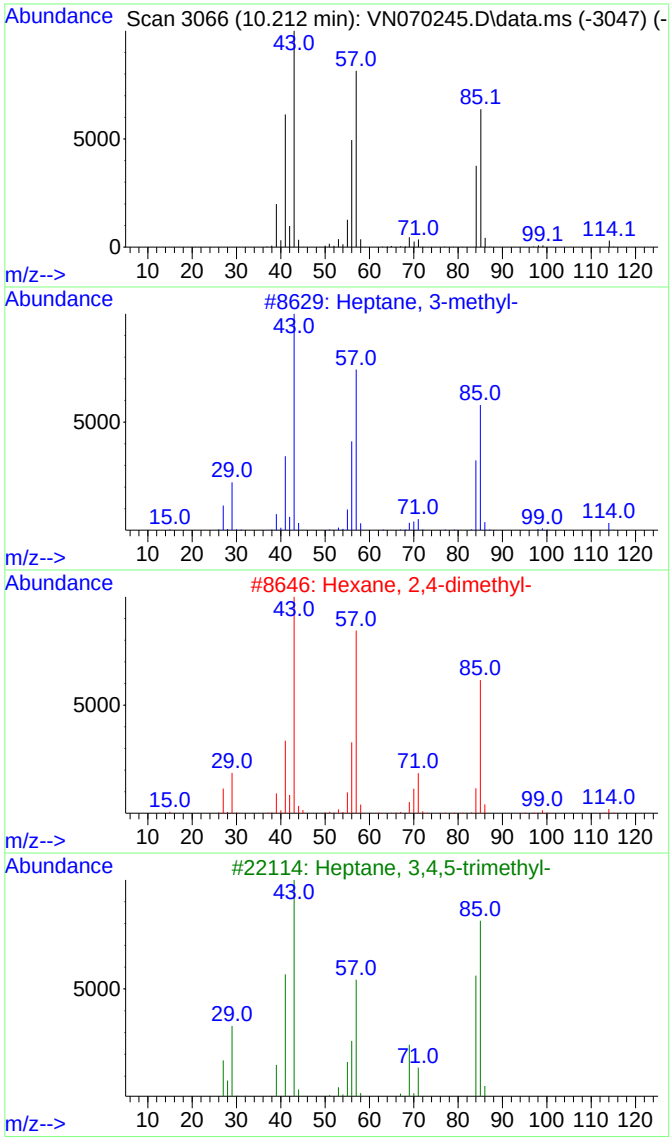
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

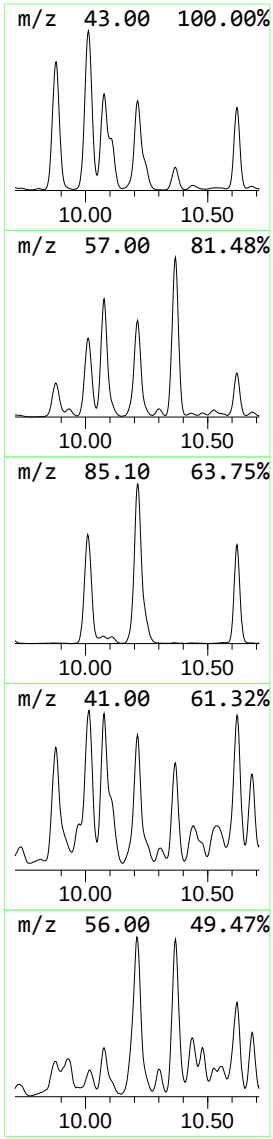
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.212	20.06 ug/l	4123500	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
3	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
4	Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	53
5	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	53





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Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

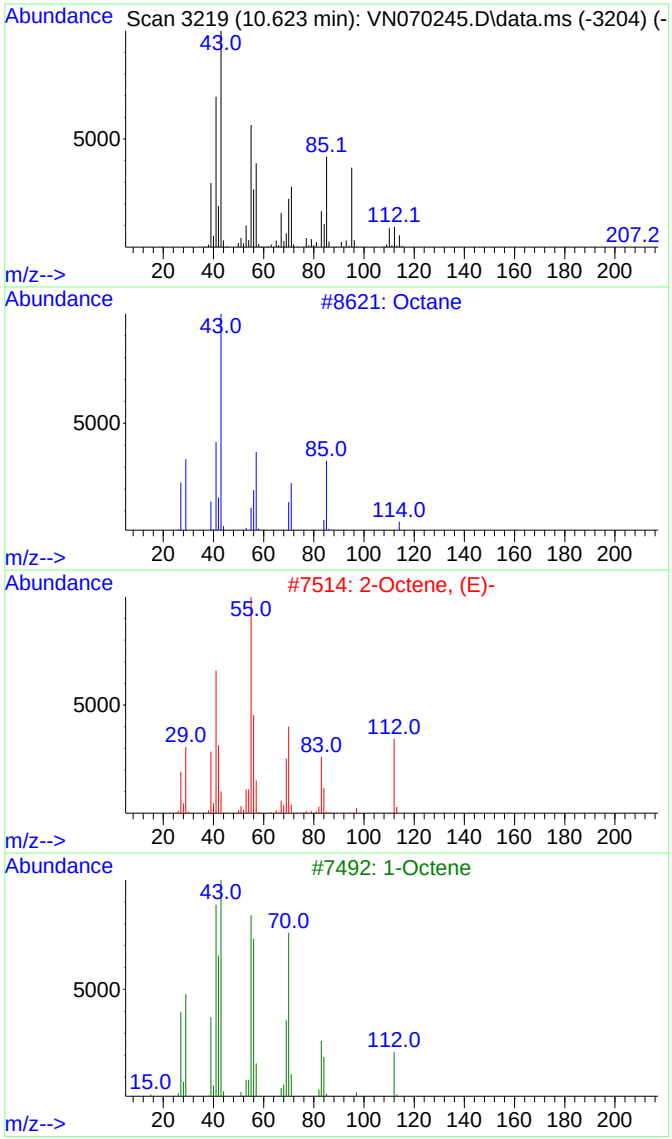
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

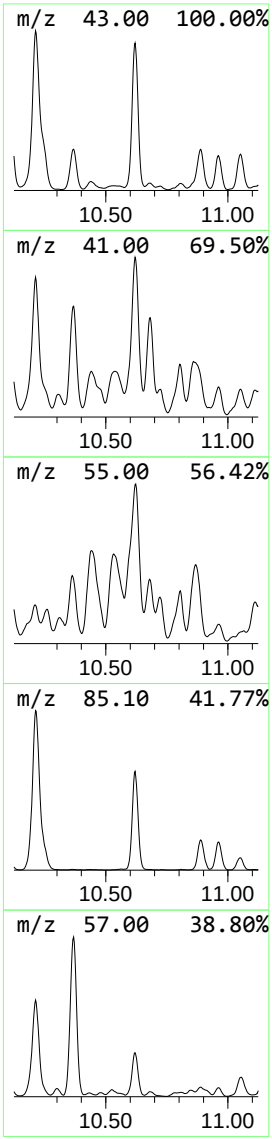
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Octane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.623	23.22 ug/l	4517020	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	64
2	2-Octene, (E)-	112	C8H16	013389-42-9	38
3	1-Octene	112	C8H16	000111-66-0	38
4	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	38
5	4-Octene, (E)-	112	C8H16	014850-23-8	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

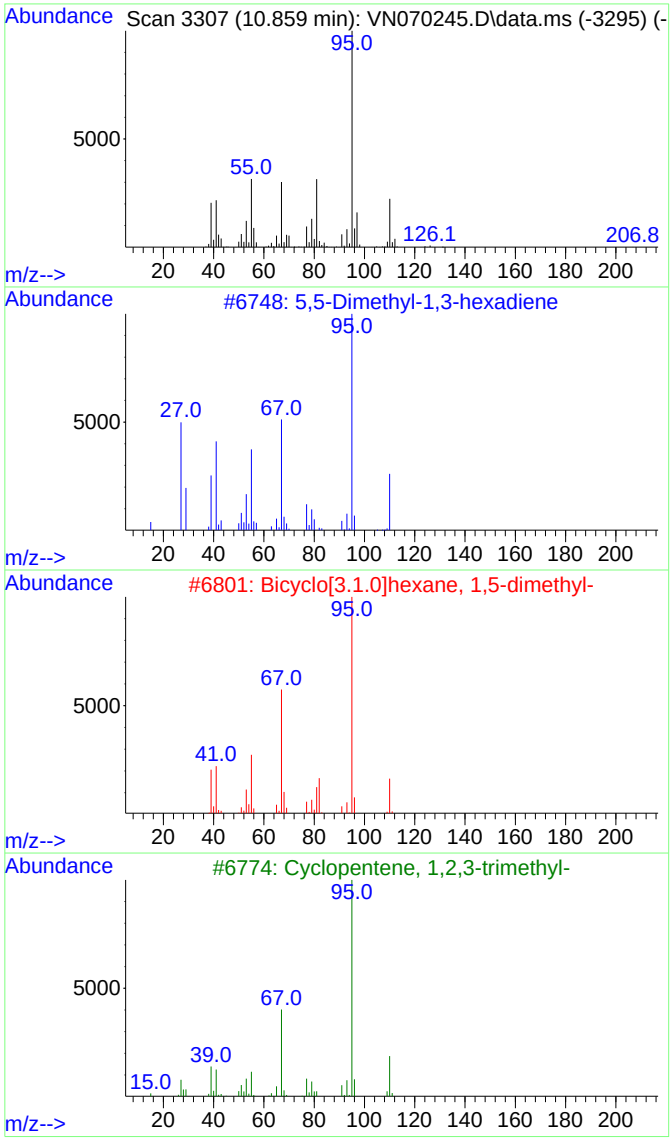
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

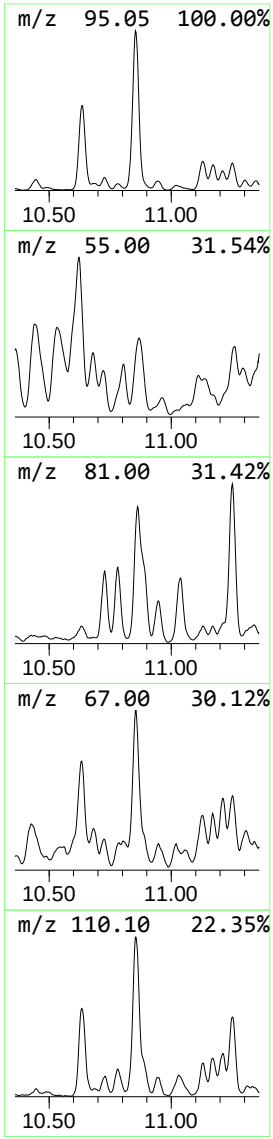
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 5,5-Dimethyl-1,3-hexadiene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.859	20.61 ug/l	4008480	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	87
2	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	81
3	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	81
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	74
5	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

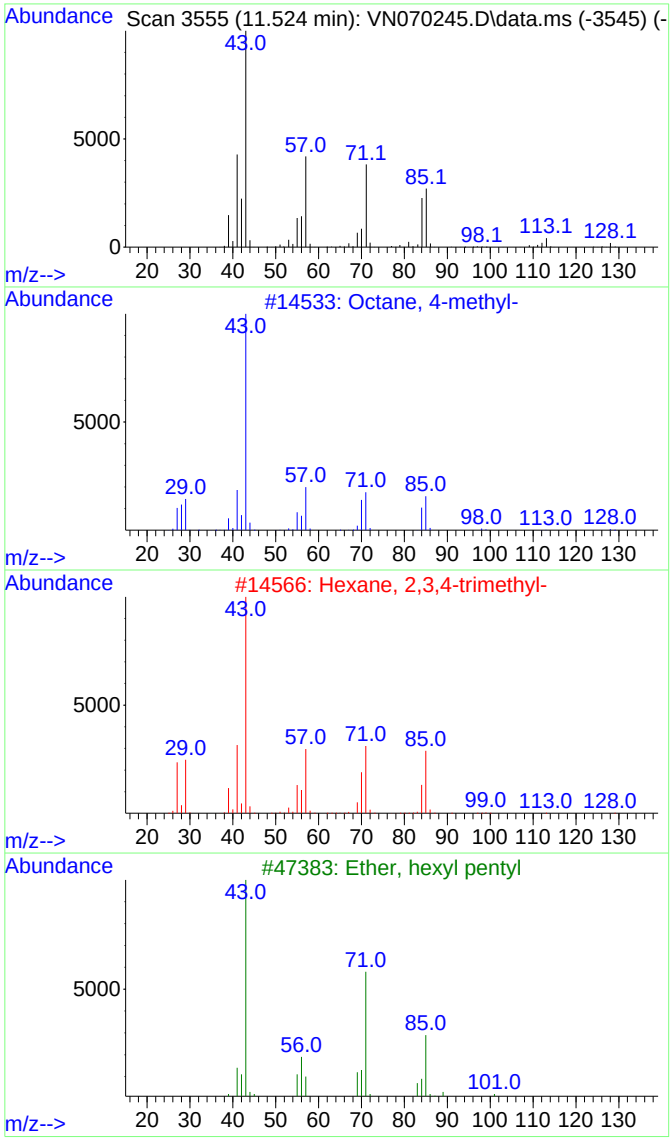
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

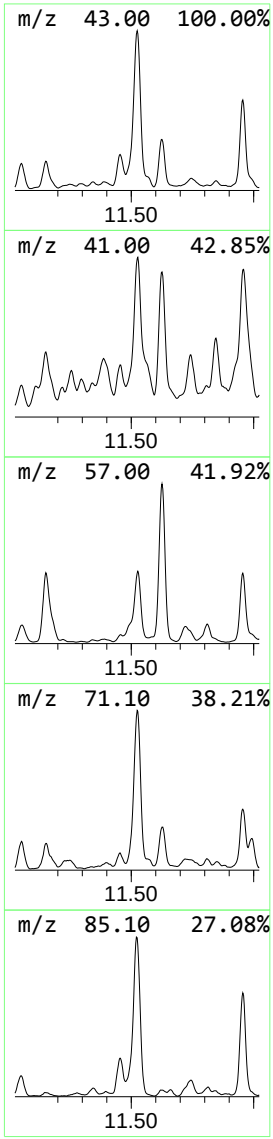
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Octane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.524	24.96 ug/l	4854710	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	64
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
3	Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
5	Octane, 2-methyl-	128	C9H20	003221-61-2	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

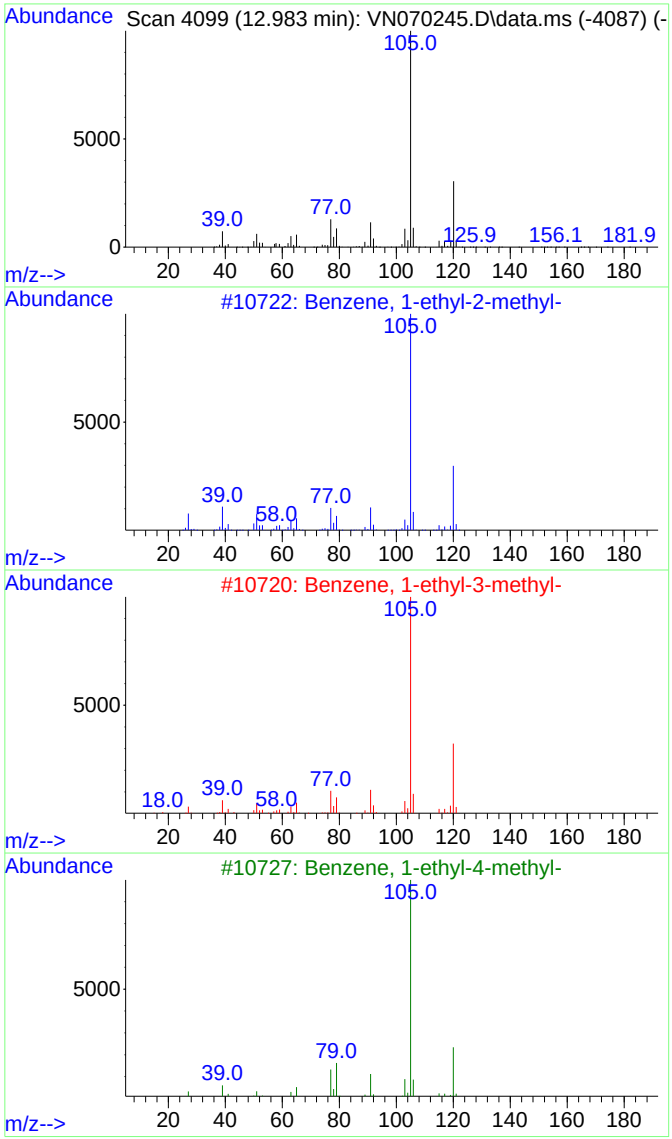
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

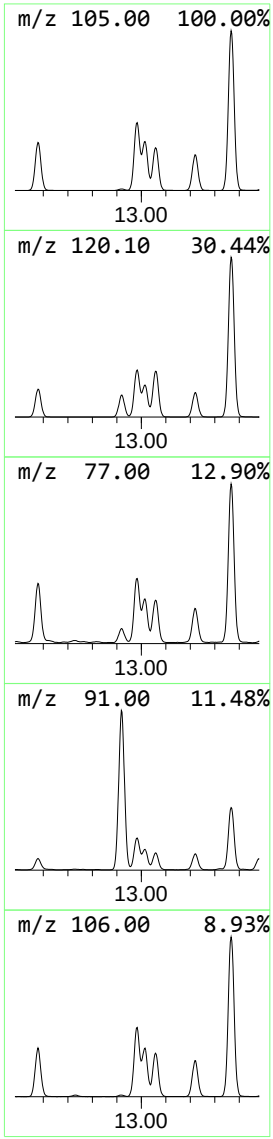
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	46.23 ug/l	8261840	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	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

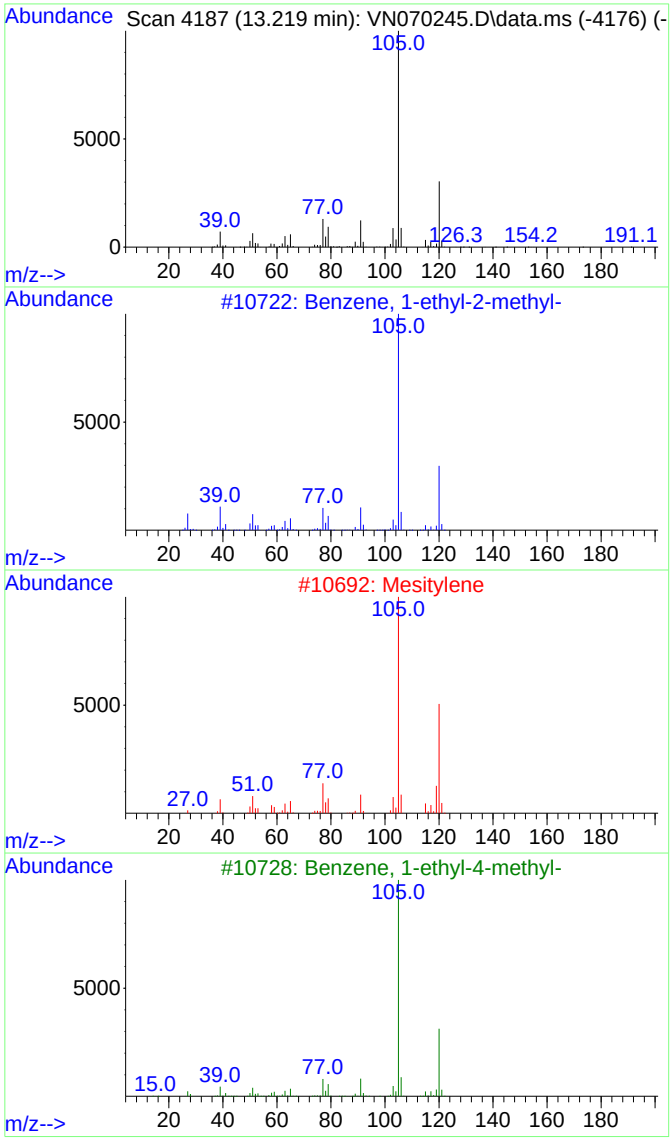
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

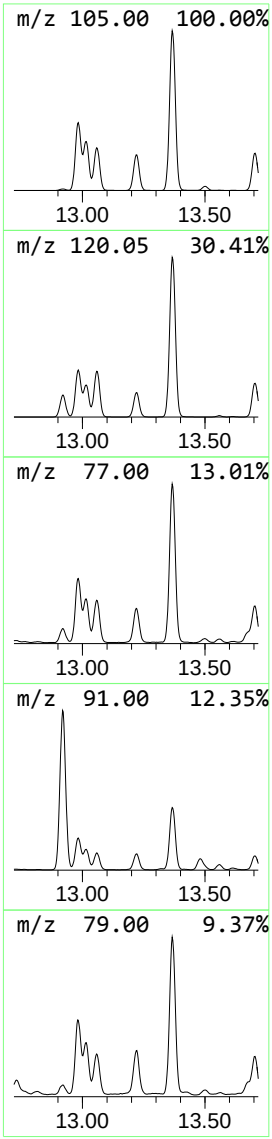
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	24.18 ug/l	4322120	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	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

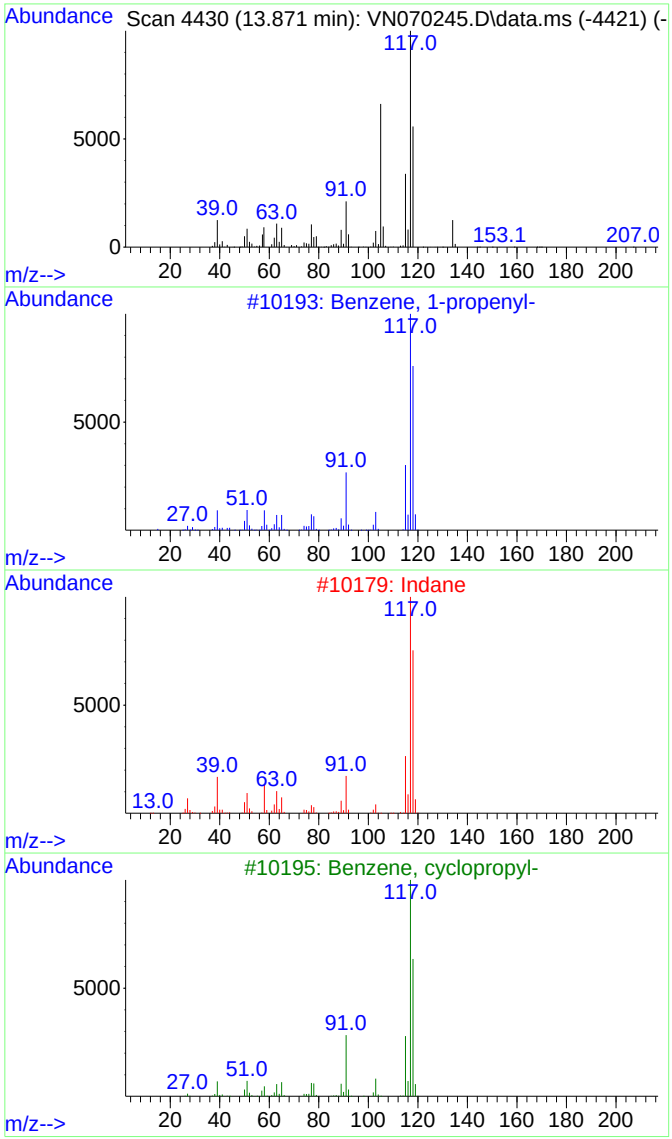
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

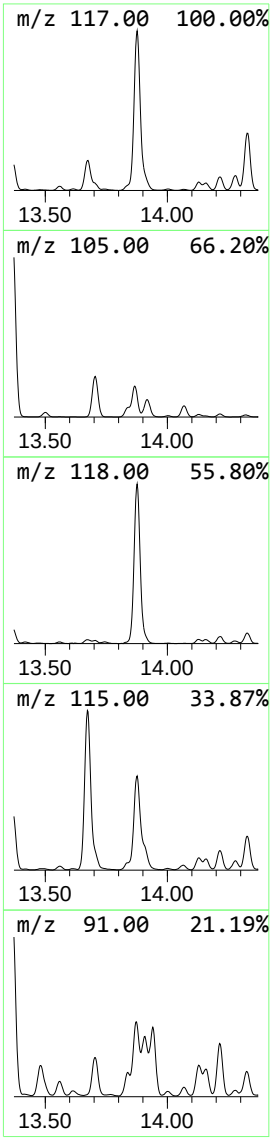
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	29.32 ug/l	5240020	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	92
2	Indane	118	C9H10	000496-11-7	70
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70





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Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

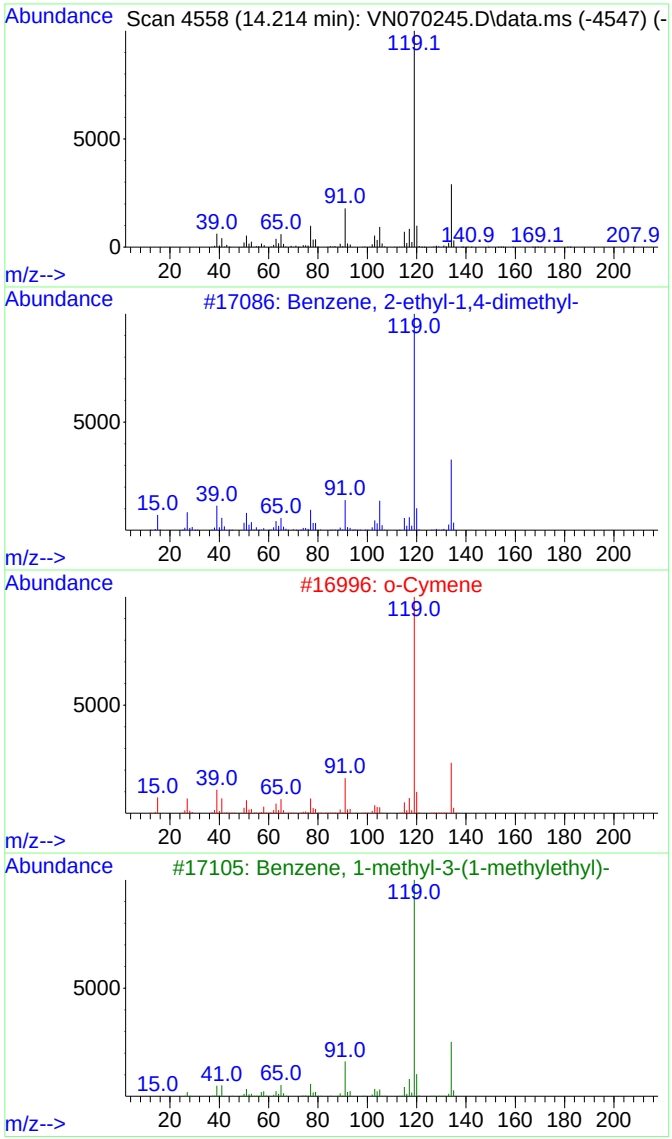
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

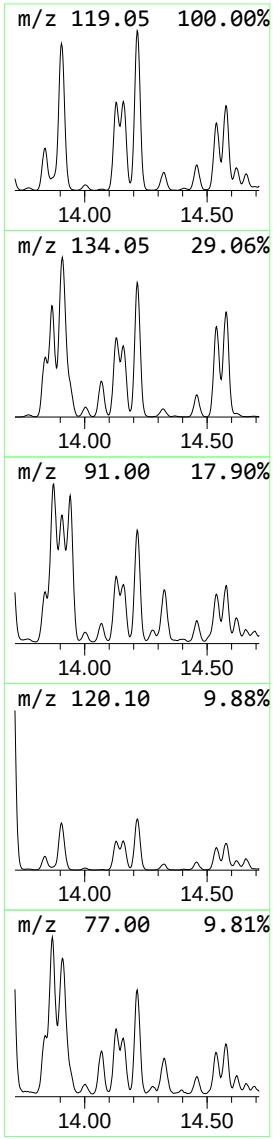
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	20.14 ug/l	3600220	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070245.D
Acq On : 20 Dec 2021 17:10
Operator : JC/MD
Sample : M5044-17
Misc : 6.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-17-4.5

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
Pentane, 2-methyl-	5.101	31.6	ug/l	1357960	1	8.080	2148700	50.0
n-Hexane	6.093	18.6	ug/l	797668	1	8.080	2148700	50.0
Pentane, 2,3-di...	8.163	46.1	ug/l	1981510	1	8.080	2148700	50.0
Hexane, 3-methyl-	8.287	68.0	ug/l	2923160	1	8.080	2148700	50.0
Butane, 2,2,3,3...	8.609	37.6	ug/l	7727910	2	8.965	10277100	50.0
Pentane, 2,3,4-...	9.877	22.0	ug/l	4528270	2	8.965	10277100	50.0
Decane, 3,3,4-t...	10.014	23.4	ug/l	4807930	2	8.965	10277100	50.0
Heptane, 3-methyl-	10.212	20.1	ug/l	4123500	2	8.965	10277100	50.0
Octane	10.623	23.2	ug/l	4517020	3	11.746	9726400	50.0
5,5-Dimethyl-1,...	10.859	20.6	ug/l	4008480	3	11.746	9726400	50.0
Octane, 4-methyl-	11.524	25.0	ug/l	4854710	3	11.746	9726400	50.0
Benzene, 1-ethy...	12.983	46.2	ug/l	8261840	4	13.675	8936390	50.0
Benzene, 1-ethy...	13.219	24.2	ug/l	4322120	4	13.675	8936390	50.0
Benzene, 1-prop...	13.871	29.3	ug/l	5240020	4	13.675	8936390	50.0
Benzene, 2-ethy...	14.214	20.1	ug/l	3600220	4	13.675	8936390	50.0