LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

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\82N011822W.M
Title : SW846 8260

Signal : TIC: VN070855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.019	2225	2248	2259	rBV	579530	1374060	24.43%	2.402%
2	8.083	2260	2272	2294	rVV	1200603	2779963	49.43%	4.859%
3	8.166	2298	2303	2324	rVB6	30317	66494	1.18%	0.116%
4	8.292	2331	2350	2367	rBV4	71426	167329	2.98%	0.292%
5	8.434	2383	2403	2428	rBV	662044	1526162	27.14%	2.668%
6	8.614	2438	2470	2492	rBV2	132838	403222	7.17%	0.705%
7	8.826	2535	2549	2580	rVB4	117622	263732	4.69%	0.461%
8	8.965	2580	2601	2631	rBV	1615648	3399648	60.45%	5.943%
9	9.456	2755	2784	2795	rBV3	220824	529508	9.42%	0.926%
10	9.510	2796	2804	2820	rVB4	100610	190422	3.39%	0.333%
11	9.730	2866	2886	2903	rVB6	46936	115960	2.06%	0.203%
12	9.877	2924	2941	2965	rBV5	183728	395630	7.03%	0.692%
13	10.017	2981	2993	3004	rBV4	194655	351483	6.25%	0.614%
14	10.076	3004	3015	3025	rBV2	303432	558475	9.93%	0.976%
15	10.212	3046	3066	3093	rBV2	345236	823861	14.65%	1.440%
16	10.368	3112	3124	3134	rVV2	144623	257446	4.58%	0.450%
17	10.438	3134	3150	3181	rVV	2927493	5623964	100.00%	9.831%
18	10.620	3203	3218	3234	rVB2	401048	808681	14.38%	1.414%
19	10.781	3268	3278	3294	rVB3	124885	235672	4.19%	0.412%
20	10.872	3296	3312	3335	rBV3	130553	408155	7.26%	0.713%
21	10.961	3336	3345	3357	rVB2	108362	185098	3.29%	0.324%
22	11.049	3358	3378	3392	rBV2	215214	417463	7.42%	0.730%
23	11.151	3394	3416	3433	rBV	190475	501076	8.91%	0.876%
24	11.221	3433	3442	3449	rBV4	73121	121820	2.17%	0.213%
25	11.291	3461	3468	3477	rVB2	162234	221111	3.93%	0.387%
26	11.344	3478	3488	3500	rVB2	282322	466021	8.29%	0.815%
27	11.451	3517	3528	3537	rBV6	219719	369929	6.58%	0.647%
28	11.524	3538	3555	3580	rVB4	633368	1642887	29.21%	2.872%
29	11.626	3580	3593	3616	rBV	588162	1048509	18.64%	1.833%
30	11.741	3621	3636	3656	rBV	2260016	4113411	73.14%	7.190%
31	11.843	3663	3674	3693	rVB	692804	1211751	21.55%	2.118%
32	11.923	3695	3704	3705	rBV4	105660	115199	2.05%	0.201%
33	12.090	3755	3766	3772	rBV6	44278	86527	1.54%	0.151%
34	12.251	3813	3826	3840	rBV5	357211	762904	13.57%	1.334%
35	12.363	3860	3868	3880	rVB	451035	721793	12.83%	1.262%
36	12.452	3882	3901	3905	rBV7	319795	643148	11.44%	1.124%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

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\82N011822W.M
Title : SW846 8260

37	12.728	3993	4004	4014	rBV	1565339	2582302	45.92%	4.514%
38	12.916	4060	4074	4086	rVB	662354	1349556	24.00%	2.359%
39	13.055	4104	4126	4138	rBV2	1067663	2262778	40.23%	3.955%
40	13.216	4170	4186	4193	rBV2	273221	726179	12.91%	1.269%
41	13.281	4203	4210	4227	rVB2	577073	896130	15.93%	1.566%
42	13.366	4230	4242	4253	rBV	1445438	2337864	41.57%	4.087%
43	13.602	4324	4330	4337	rBV2	288888	342959	6.10%	0.600%
44	13.672	4346	4356	4376	rVB2	1925130	3841031	68.30%	6.714%
45	13.836	4408	4417	4423	rBV	380252	577539	10.27%	1.010%
46	13.871	4425	4430	4436	rVV2	471220	679869	12.09%	1.188%
47	13.908	4438	4444	4465	rVB5	874988	1811151	32.20%	3.166%
48	13.997	4467	4477	4486	rBV4	511002	858365	15.26%	1.500%
49	14.214	4548	4558	4569	rBV	1225488	1862581	33.12%	3.256%
50	14.324	4588	4599	4610	rVB3	616139	1039572	18.48%	1.817%
51	14.619	4702	4709	4717	rVB2	378569	456463	8.12%	0.798%
52	14.807	4771	4779	4789	rBV3	341798	575462	10.23%	1.006%
53	14.922	4808	4822	4834	rBV3	870768	2098732	37.32%	3.669%

Sum of corrected areas: 57207047

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Operator : JC/MD
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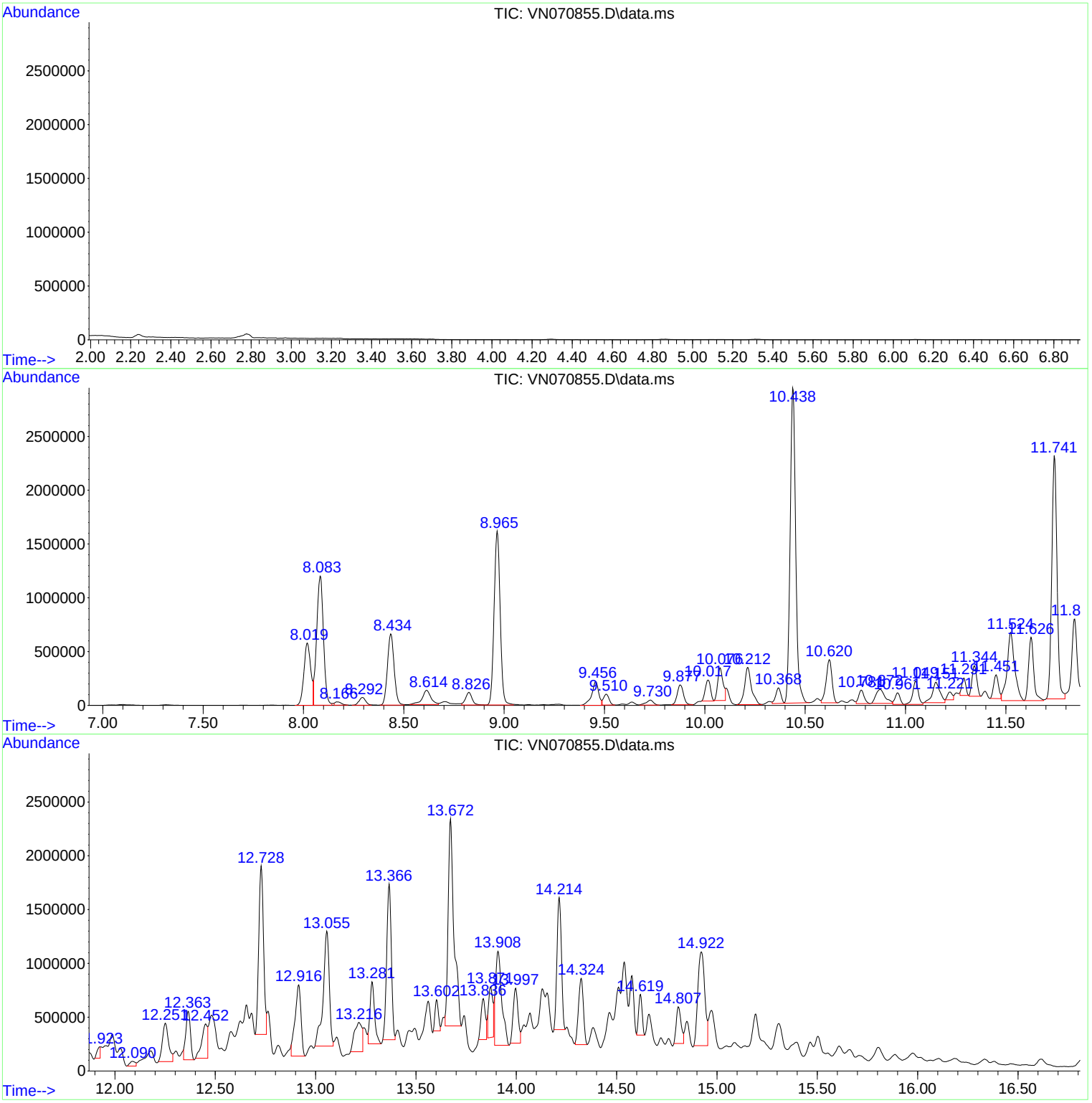
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
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MSVOA_N
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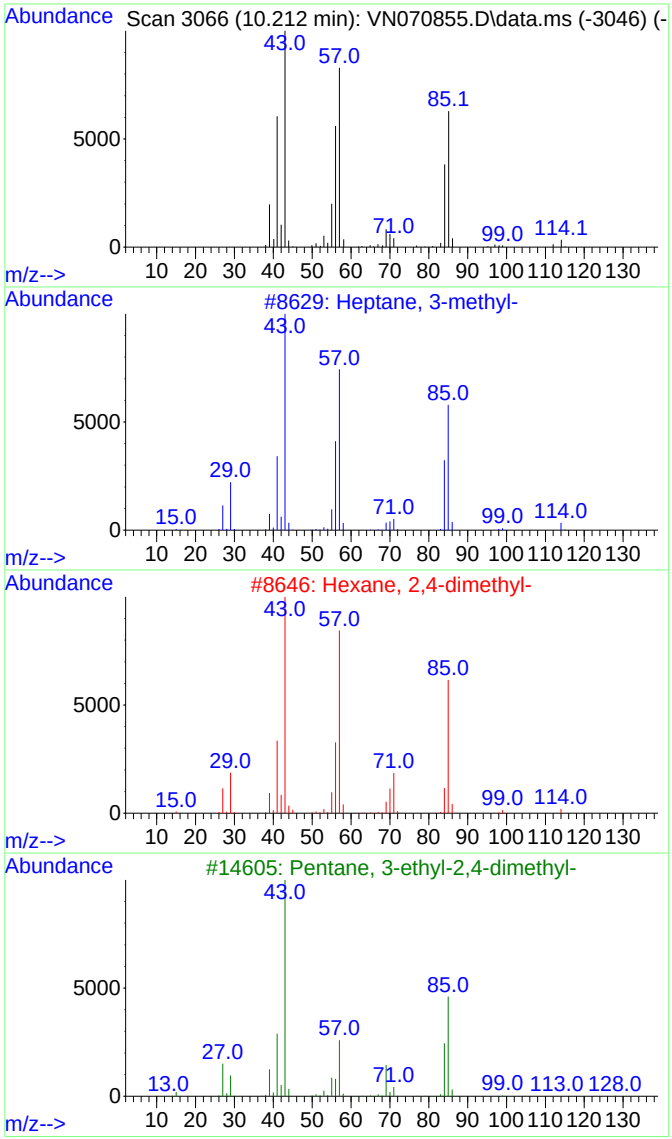
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

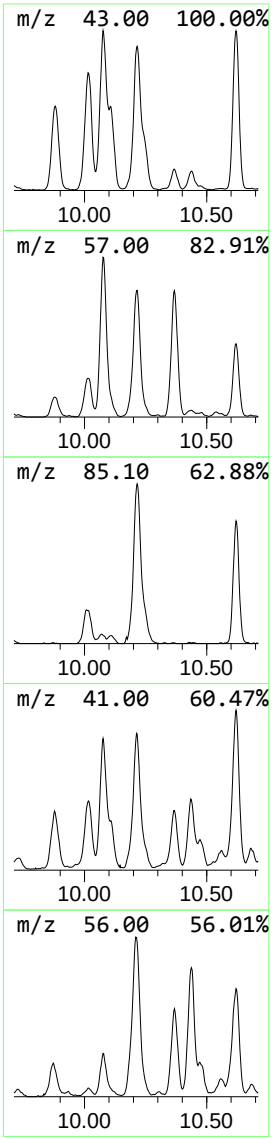
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Heptane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.212	12.12 ug/l	823861	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	58
3	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	53
5	Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

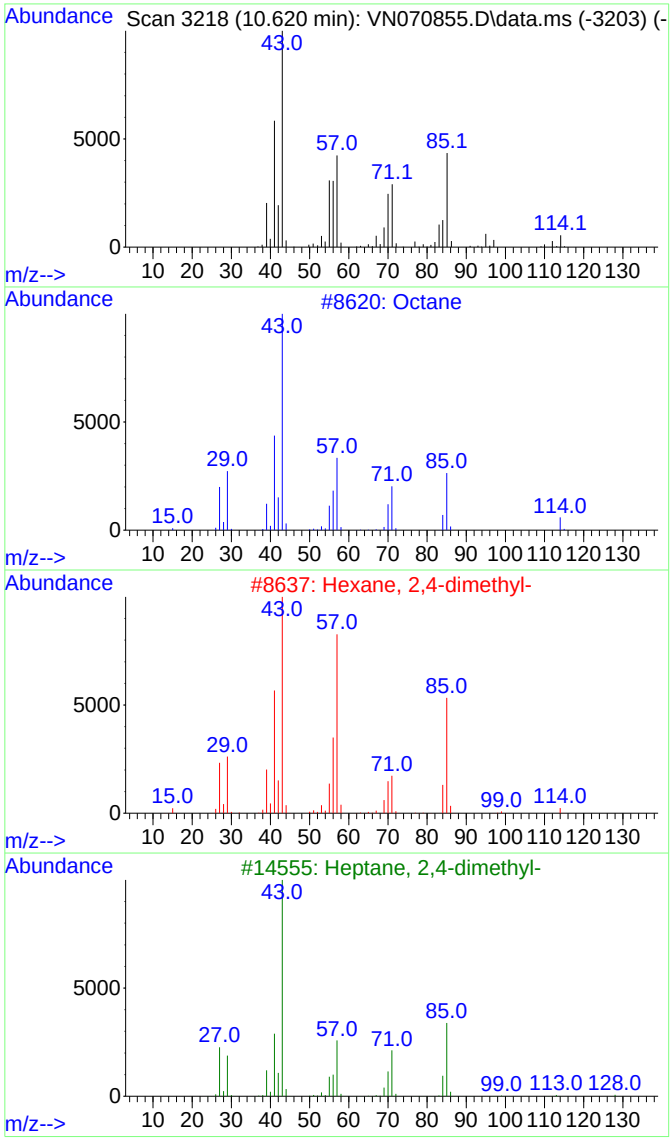
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

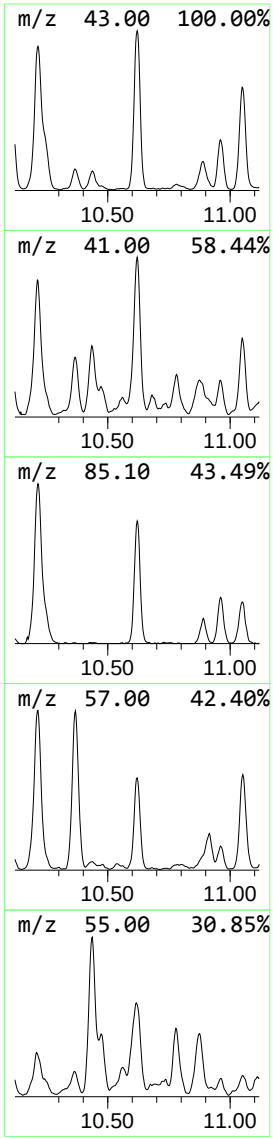
****

Peak Number 2 Octane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.620	9.83 ug/l	808681	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	87
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	68
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	50
5	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

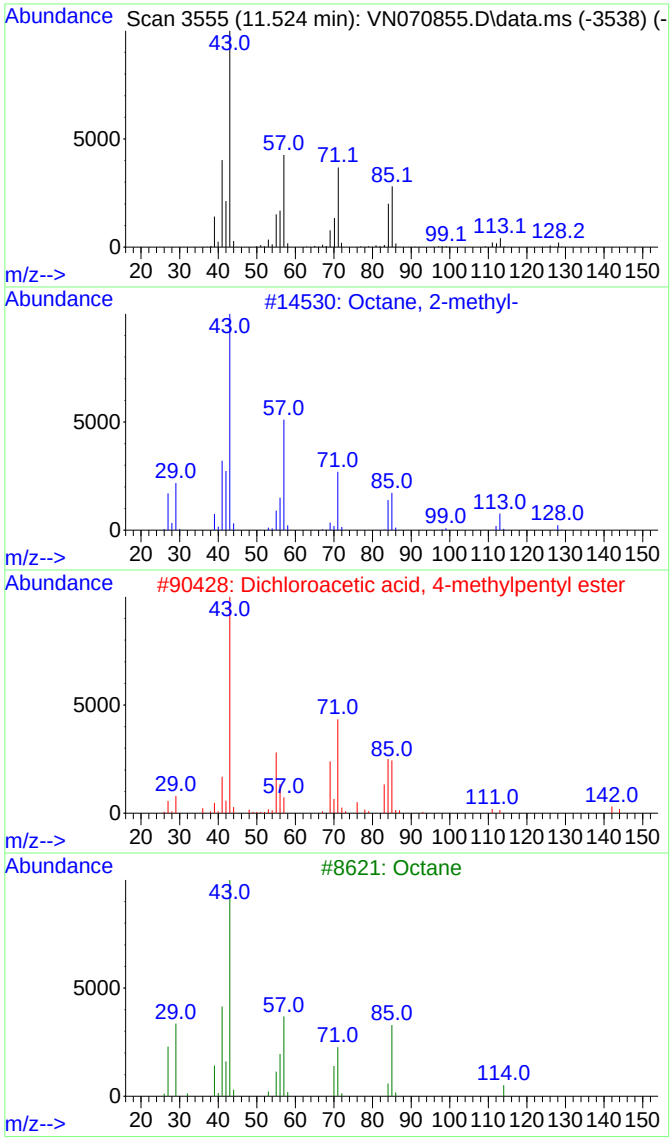
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

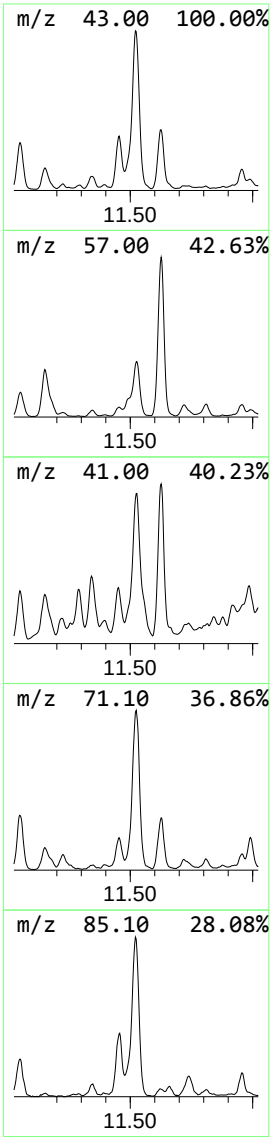
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.524	19.97 ug/l	1642890	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	64
2	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	59
3	Octane	114	C8H18	000111-65-9	59
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	58
5	Dodecane, 5-methyl-	184	C13H28	017453-93-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

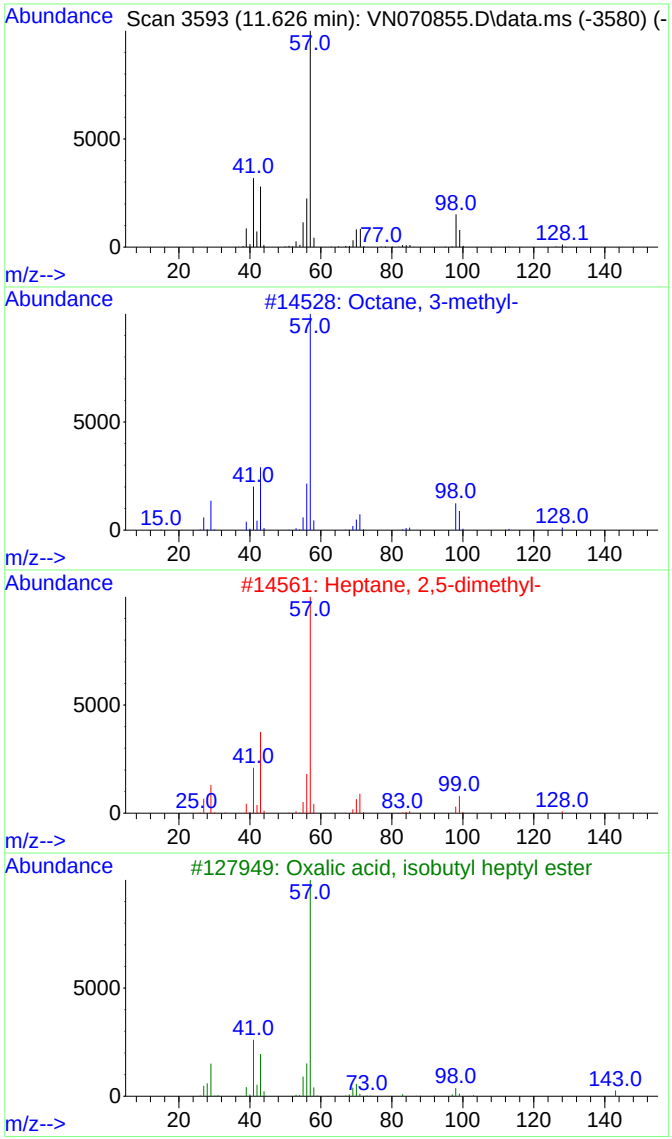
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

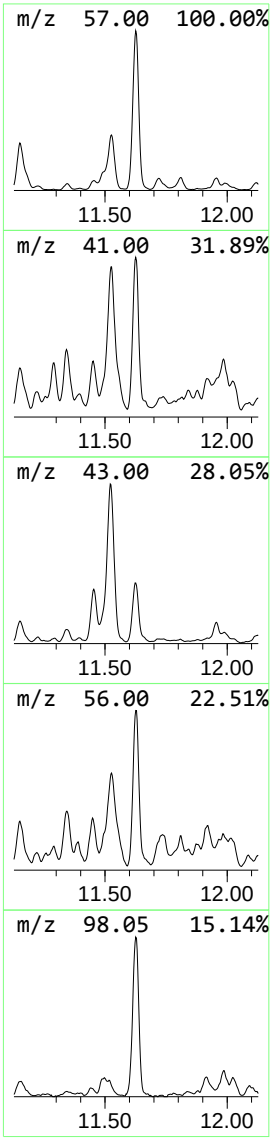
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.626	12.74 ug/l	1048510	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	87
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	80
3	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	64
4	Undecane, 6-methyl-	170	C12H26	017302-33-9	59
5	Heptane, 3-ethyl-	128	C9H20	015869-80-4	52





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Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

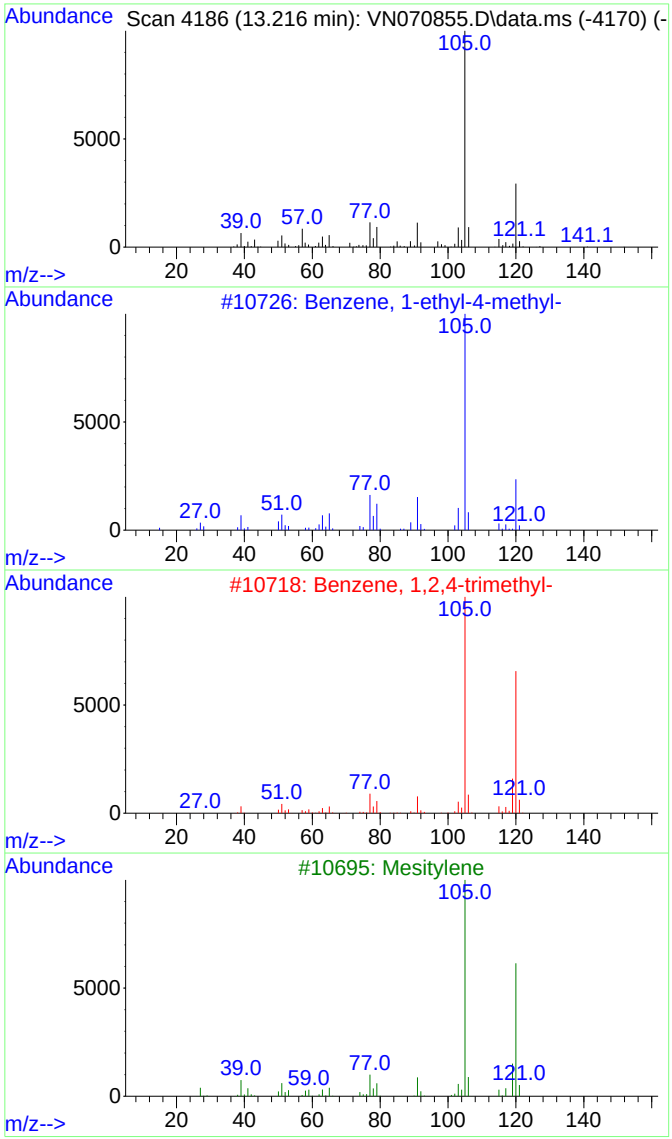
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

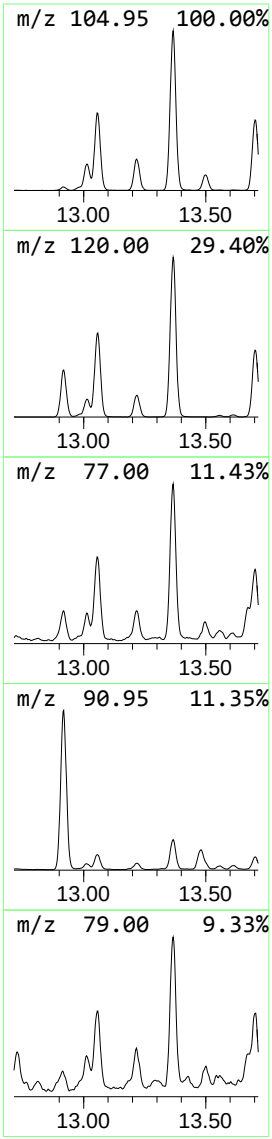
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	9.45 ug/l	726179	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3	Mesitylene	120	C9H12	000108-67-8	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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Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

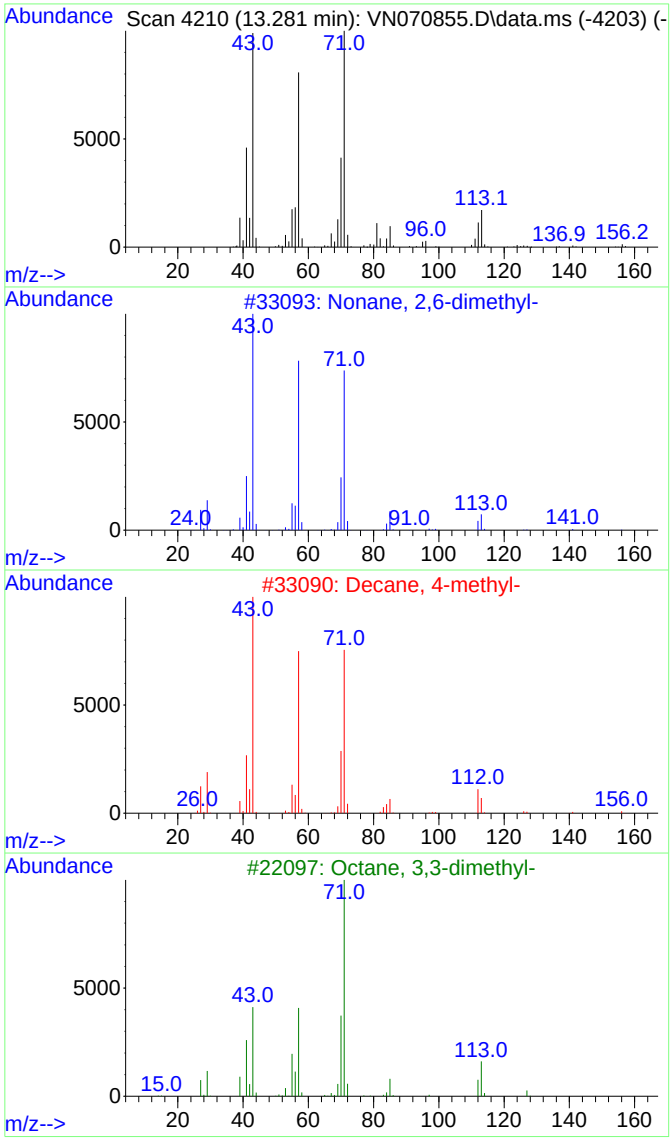
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

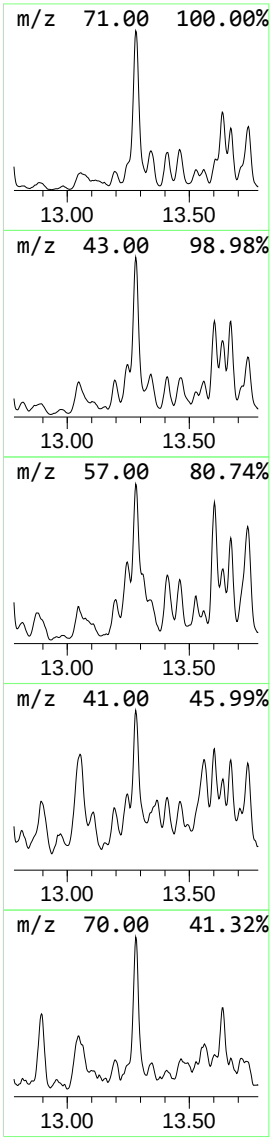
****

Peak Number 6 Nonane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.281	11.67 ug/l	896130	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	80
2	Decane, 4-methyl-	156	C11H24	002847-72-5	74
3	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
4	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	64
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64





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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

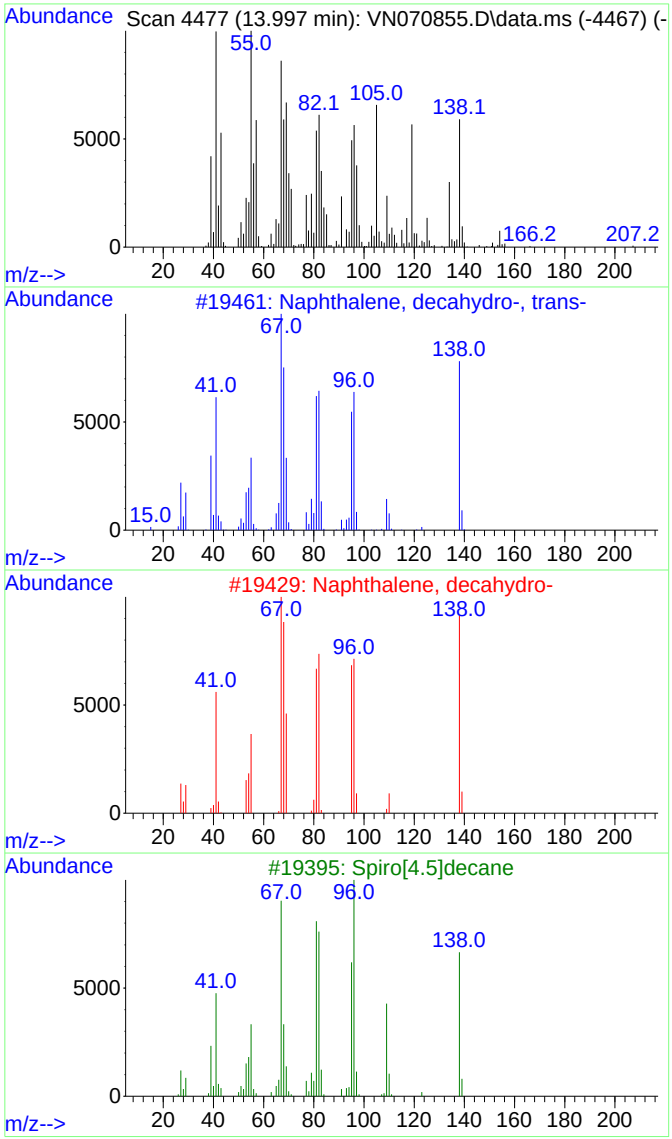
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

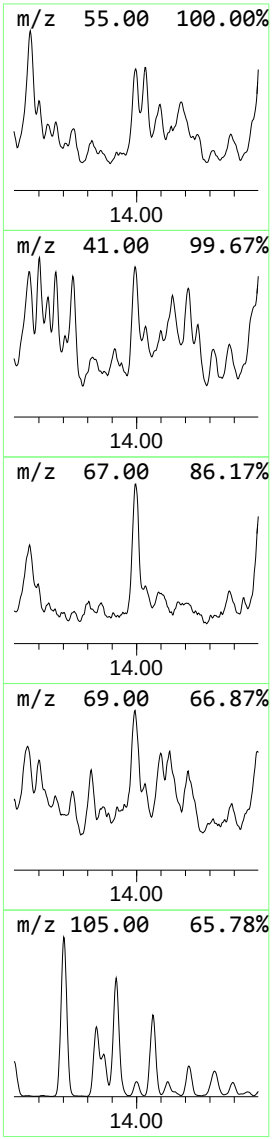
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, decahydro-, tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	11.17 ug/l	858365	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	94
3	Spiro[4.5]decane	138	C10H18	000176-63-6	76
4	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
5	4-Isopropenylcyclohexanone	138	C9H14O	022460-53-3	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

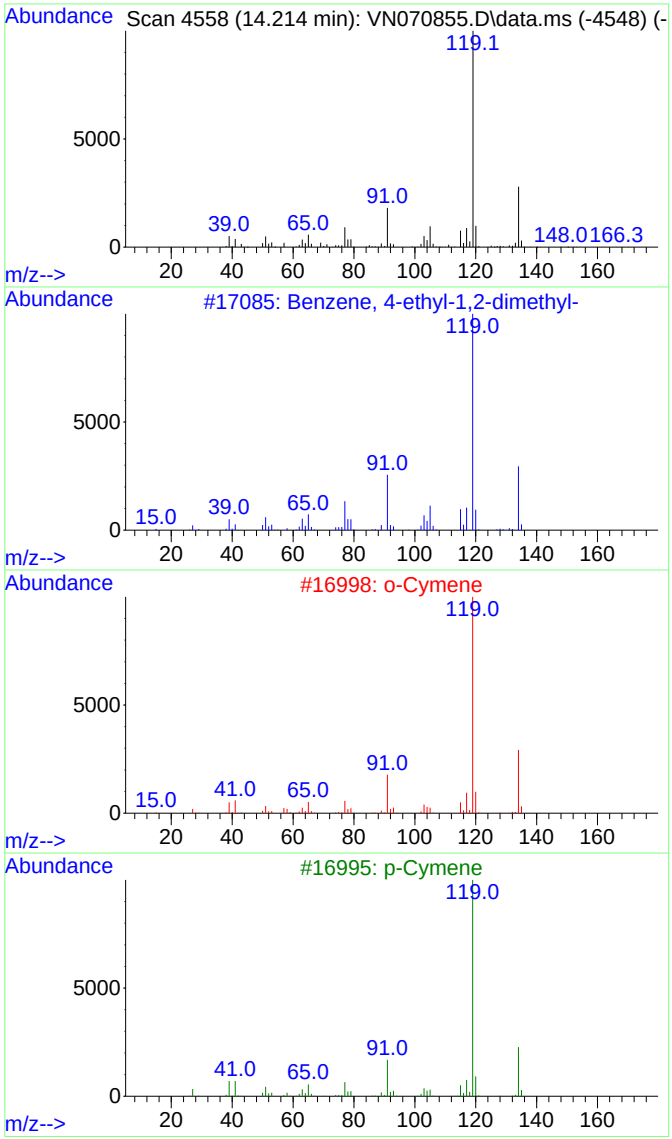
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

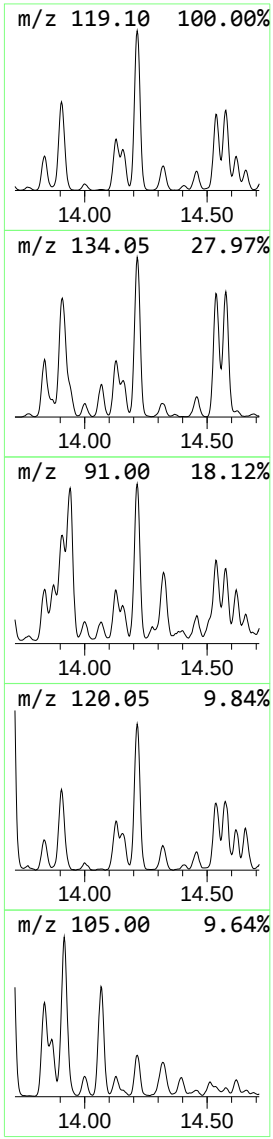
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	24.25 ug/l	1862580	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	o-Cymene	134	C10H14	000527-84-4	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

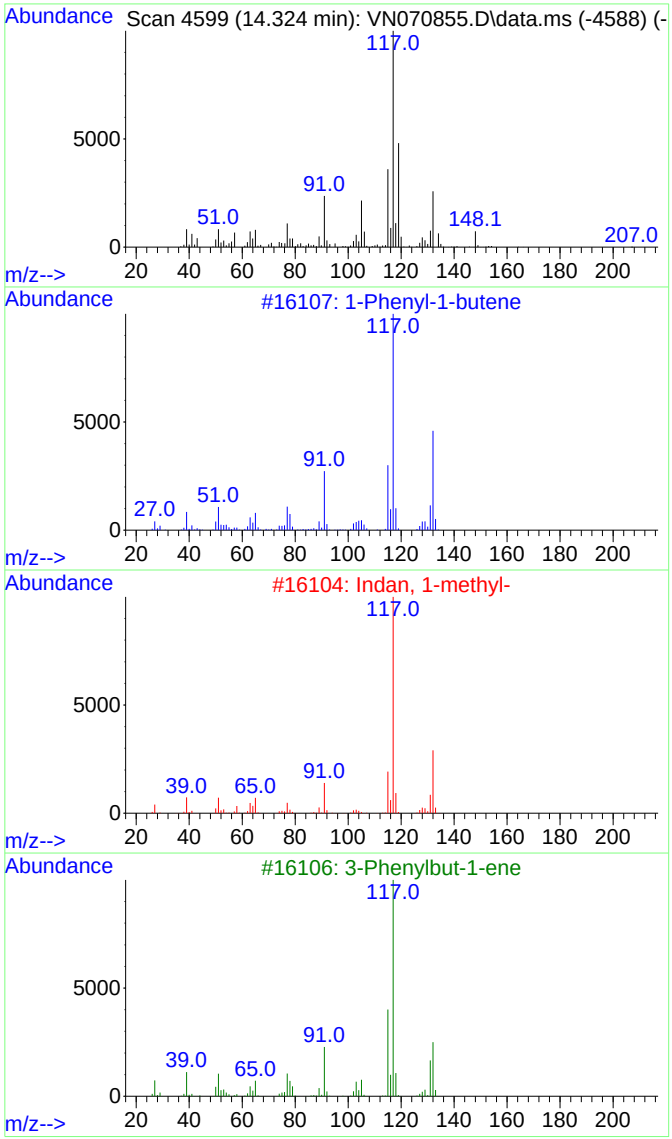
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

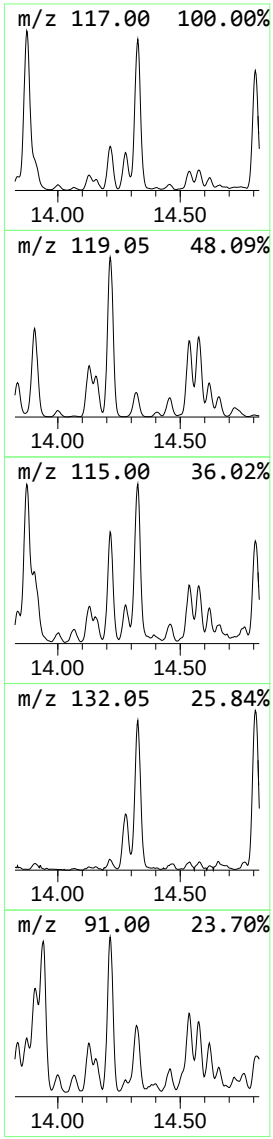
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	13.53 ug/l	1039570	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
2	Indan, 1-methyl-	132	C10H12	000767-58-8	64
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

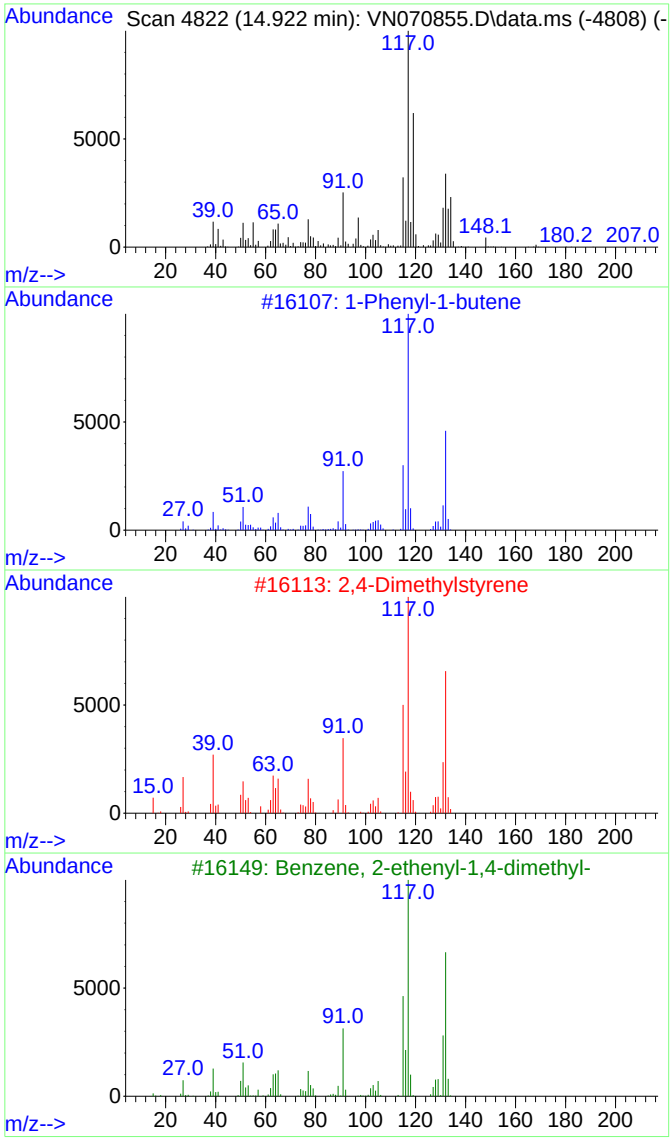
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

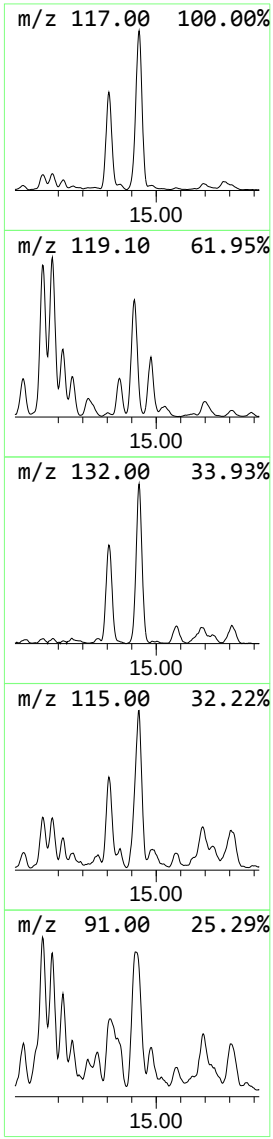
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,4-Dimethylstyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	27.32 ug/l	2098730	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	86
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070855.D
Acq On : 31 Jan 2022 16:34
Operator : JC/MD
Sample : N1337-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.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
Heptane, 3-methyl-	10.212	12.1	ug/l	823861	2	8.965	3399650	50.0
Octane	10.620	9.8	ug/l	808681	3	11.741	4113410	50.0
Octane, 2-methyl-	11.524	20.0	ug/l	1642890	3	11.741	4113410	50.0
Octane, 3-methyl-	11.626	12.7	ug/l	1048510	3	11.741	4113410	50.0
Benzene, 1-ethy...	13.216	9.4	ug/l	726179	4	13.672	3841030	50.0
Nonane, 2,6-dim...	13.281	11.7	ug/l	896130	4	13.672	3841030	50.0
Naphthalene, de...	13.997	11.2	ug/l	858365	4	13.672	3841030	50.0
Benzene, 4-ethy...	14.214	24.3	ug/l	1862580	4	13.672	3841030	50.0
1-Phenyl-1-butene	14.324	13.5	ug/l	1039570	4	13.672	3841030	50.0
2,4-Dimethylsty...	14.922	27.3	ug/l	2098730	4	13.672	3841030	50.0