LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

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: VN070247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	83	92	128	rVB4	57082	177935	1.65%	0.220%
2	7.024	1849	1877	1900	rBV4	45423	139679	1.30%	0.173%
3	7.351	1979	1999	2030	rBV2	37568	123841	1.15%	0.153%
4	8.019	2223	2248	2258	rBV2	907098	2275341	21.15%	2.819%
5	8.080	2259	2271	2291	rVV	1719686	4027845	37.44%	4.990%
6	8.161	2291	2301	2325	rVB2	106481	260509	2.42%	0.323%
7	8.284	2331	2347	2364	rVB3	65725	145208	1.35%	0.180%
8	8.432	2379	2402	2431	rBV	1141113	2697827	25.08%	3.342%
9	8.603	2450	2466	2514	rVB2	394541	1132706	10.53%	1.403%
10	8.818	2529	2546	2563	rBV3	66317	145749	1.35%	0.181%
11	8.963	2577	2600	2629	rBV	2827322	6104356	56.74%	7.562%
12	9.451	2757	2782	2792	rBV2	146396	323507	3.01%	0.401%
13	9.504	2793	2802	2818	rVB3	110806	216570	2.01%	0.268%
14	9.877	2921	2941	2964	rVB2	310575	663543	6.17%	0.822%
15	10.011	2975	2991	3005	rBV4	367370	772085	7.18%	0.956%
16	10.076	3005	3015	3045	rVB4	147754	391511	3.64%	0.485%
17	10.212	3050	3066	3093	rVB3	150085	361764	3.36%	0.448%
18	10.368	3109	3124	3135	rBV	335132	634871	5.90%	0.786%
19	10.440	3135	3151	3171	rVV	4443461	8428445	78.34%	10.441%
20	10.620	3205	3218	3233	rVB3	154565	295117	2.74%	0.366%
21	11.151	3407	3416	3435	rVB2	84552	167868	1.56%	0.208%
22	11.524	3546	3555	3580	rVB3	203091	456673	4.24%	0.566%
23	11.626	3582	3593	3615	rBV2	156113	288298	2.68%	0.357%
24	11.744	3619	3637	3654	rBV	4840382	8708104	80.94%	10.788%
25	11.956	3709	3716	3724	rBV2	121331	166804	1.55%	0.207%
26	12.731	3991	4005	4027	rVB	4160746	7720687	71.76%	9.564%
27	12.983	4090	4099	4106	rBV	228287	362975	3.37%	0.450%
28	13.050	4116	4124	4144	rVB3	508089	989600	9.20%	1.226%
29	13.366	4231	4242	4254	rVB	1150723	1820415	16.92%	2.255%
30	13.675	4343	4357	4397	rVB2	5242302	10758602	100.00%	13.328%
31	13.838	4409	4418	4421	rBV3	216267	288375	2.68%	0.357%
32	13.871	4423	4430	4435	rVV3	558727	866831	8.06%	1.074%
33	13.908	4438	4444	4466	rVB2	904768	1690984	15.72%	2.095%
34	13.991	4467	4475	4489	rVB2	298495	415190	3.86%	0.514%
35	14.069	4497	4504	4514	rVB	166469	225902	2.10%	0.280%
36	14.131	4517	4527	4532	rBV	477170	753340	7.00%	0.933%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

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

37	14.217	4548	4559	4576	rBV	1006818	1636416	15.21%	2.027%
38	14.324	4590	4599	4611	rVB3	430754	722242	6.71%	0.895%
39	14.461	4642	4650	4661	rBV3	223966	369319	3.43%	0.458%
40	14.538	4672	4679	4686	rBV	554903	778907	7.24%	0.965%
41	14.579	4687	4694	4702	rVB	868495	1179059	10.96%	1.461%
42	14.622	4703	4710	4718	rVB3	424434	508404	4.73%	0.630%
43	14.761	4755	4762	4770	rBV2	239674	311509	2.90%	0.386%
44	14.809	4771	4780	4787	rBV4	530491	900864	8.37%	1.116%
45	14.847	4789	4794	4806	rVB3	692376	998921	9.28%	1.237%
46	14.925	4808	4823	4835	rBV4	956575	2455230	22.82%	3.042%
47	15.193	4915	4923	4951	rVB4	625098	1596539	14.84%	1.978%
48	15.311	4957	4967	4984	rVB6	499105	1112404	10.34%	1.378%
49	15.466	5017	5025	5029	rBV6	190978	278277	2.59%	0.345%
50	15.504	5032	5039	5052	rVB	525472	888308	8.26%	1.100%
51	15.611	5070	5079	5089	rBV4	220639	374329	3.48%	0.464%
52	15.804	5141	5151	5167	rVB2	319067	669691	6.22%	0.830%
53	16.614	5441	5453	5483	rVB	389917	943933	8.77%	1.169%

Sum of corrected areas: 80723409

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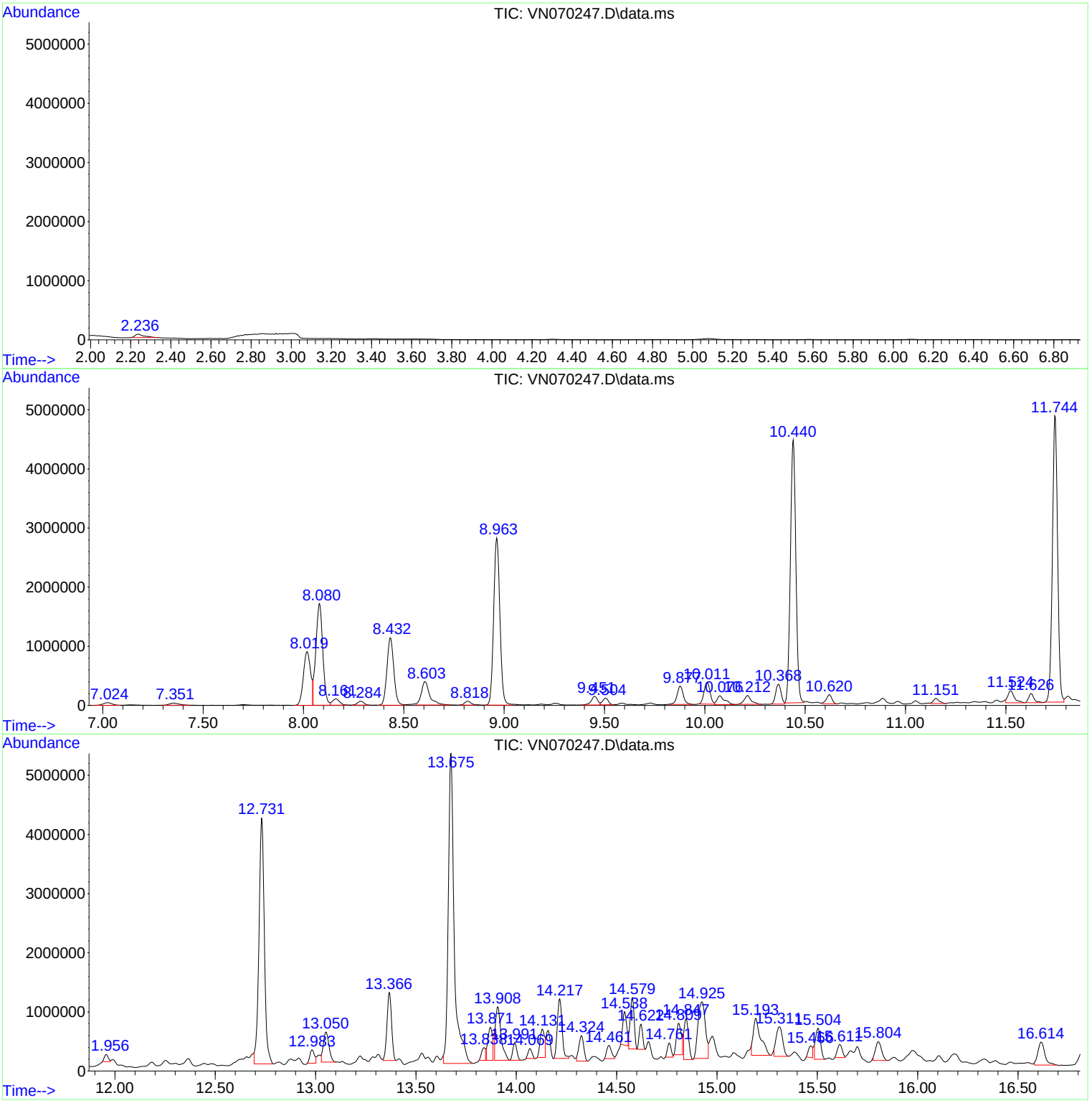
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

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 : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

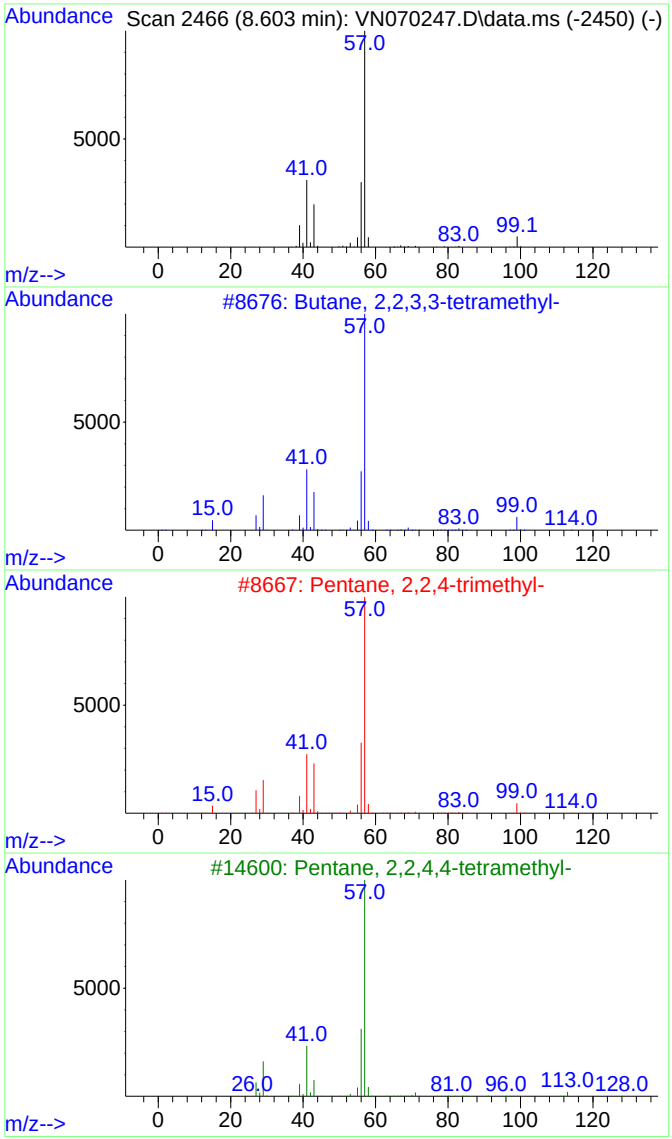
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

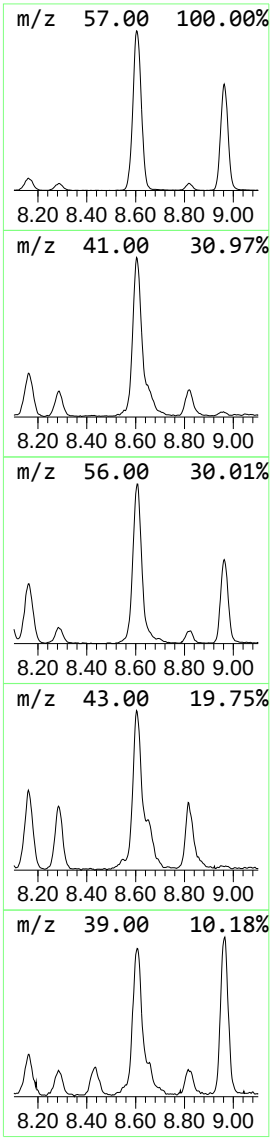
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.603	9.28 ug/l	1132710	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
4	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

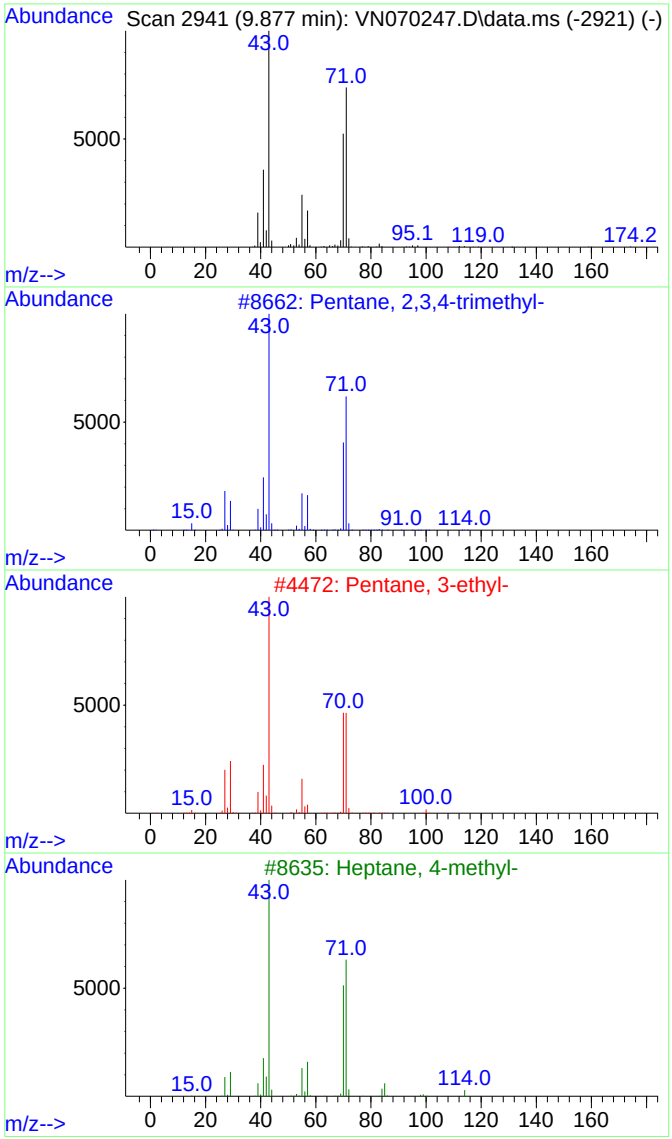
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

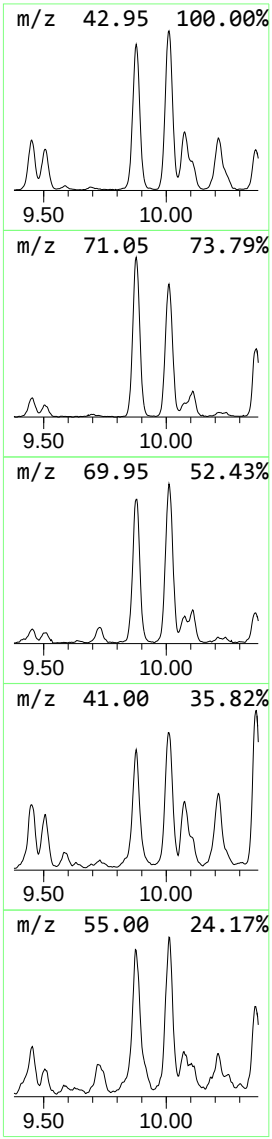
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	5.43 ug/l	663543	1,4-Difluorobenzene	8.963

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	Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

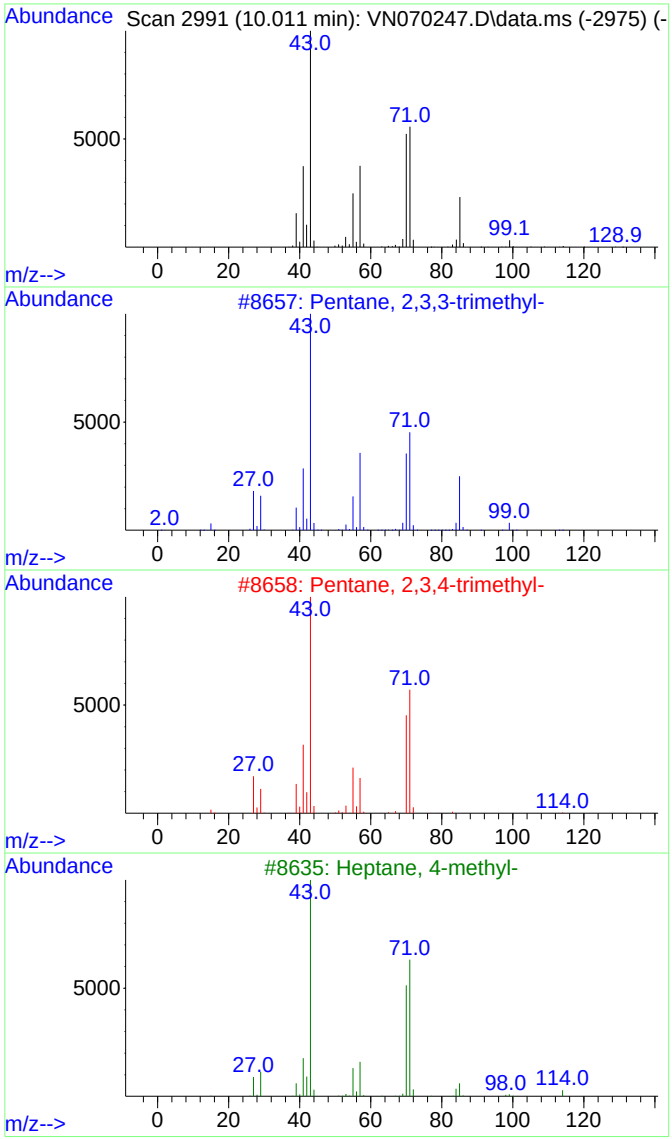
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

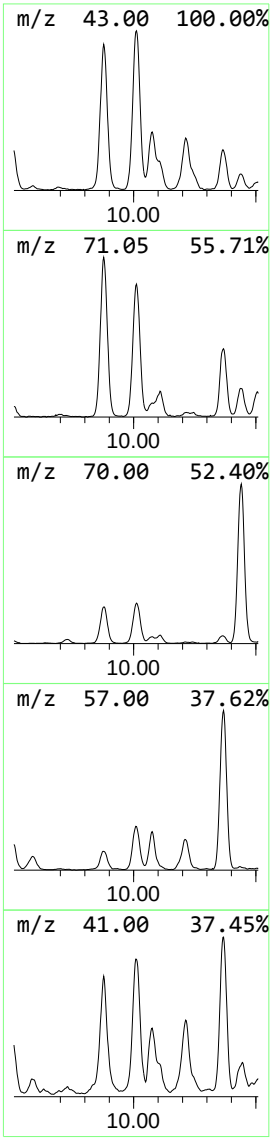
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.011	6.32 ug/l	772085	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	74
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Diisoamyl ether	158	C10H22O	000544-01-4	59
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
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Operator : JC/MD
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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

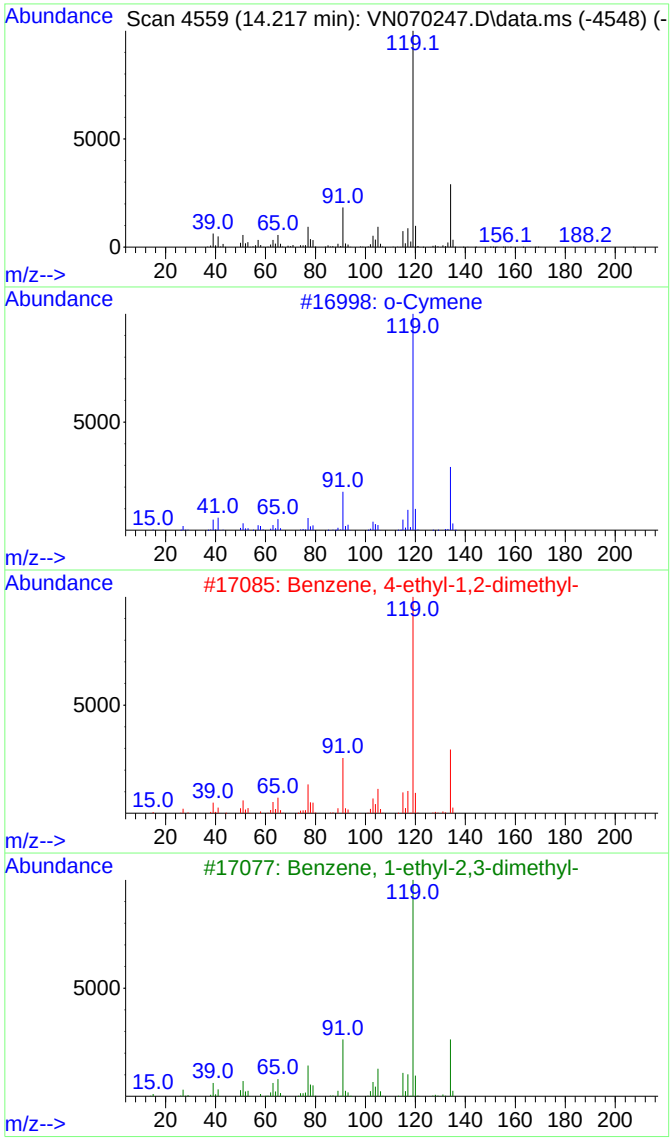
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

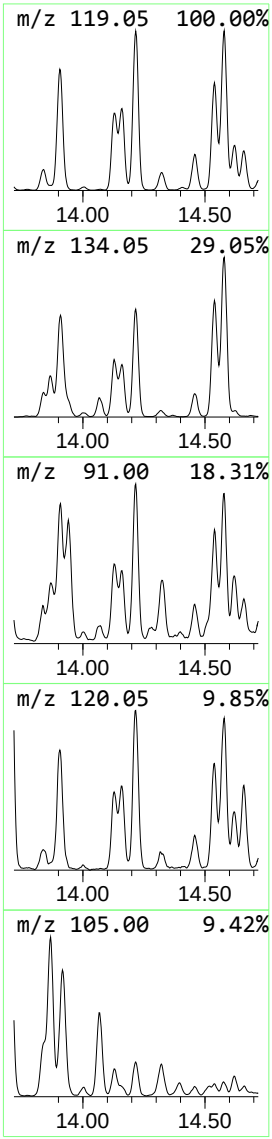
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	7.61 ug/l	1636420	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





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Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

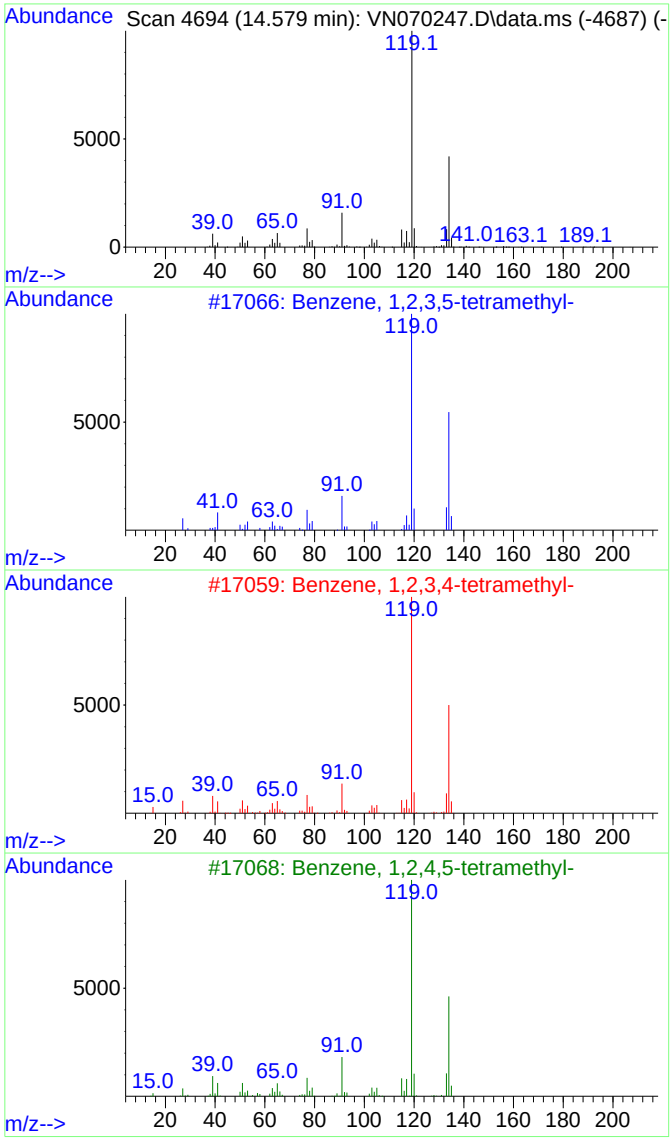
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

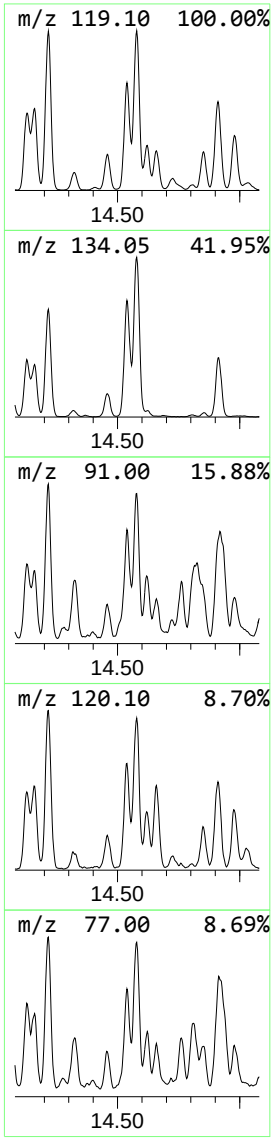
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.579	5.48 ug/l	1179060	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





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ALS Vial : 19 Sample Multiplier: 1

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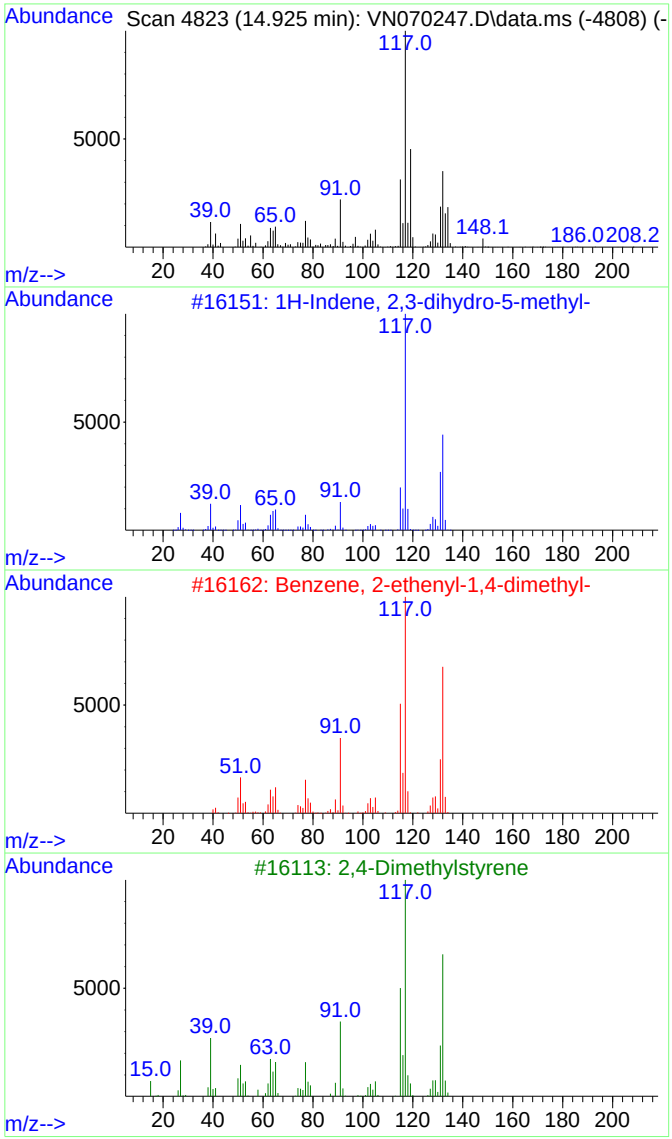
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

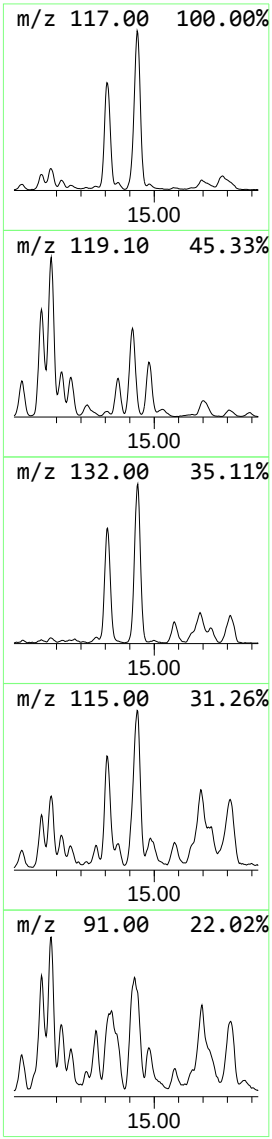
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.925	11.41 ug/l	2455230	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3	2,4-Dimethylstyrene	132	C10H12	002234-20-0	90
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70





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Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

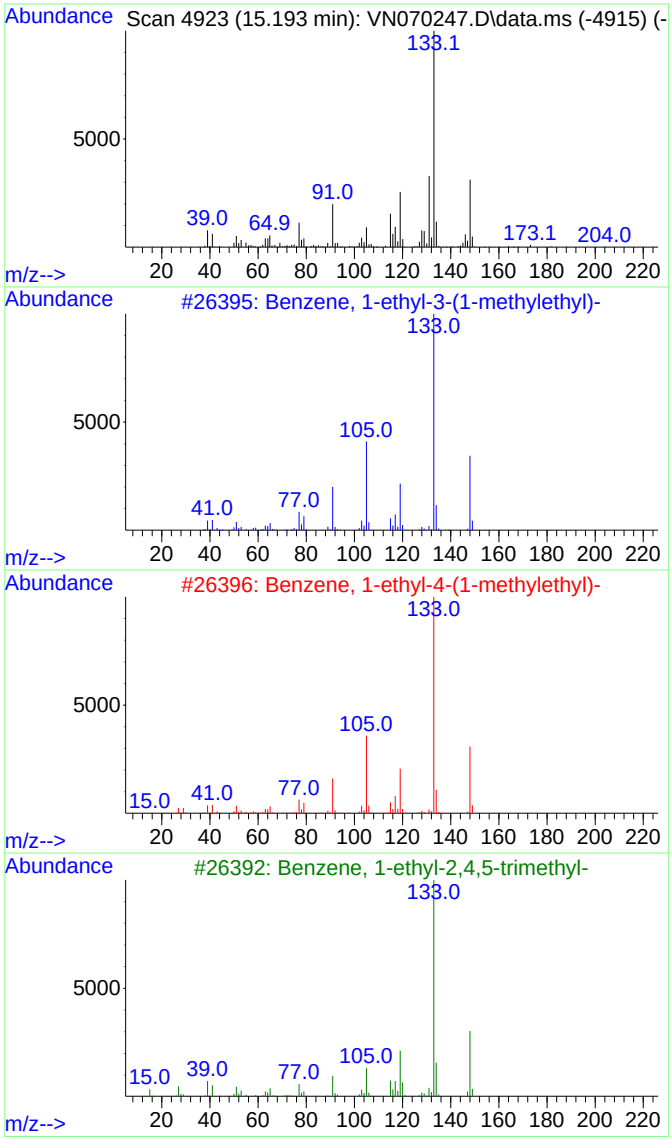
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

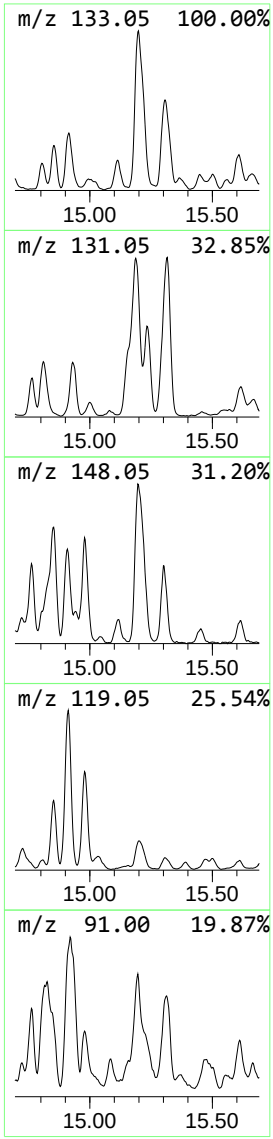
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-(1-methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.193	7.42 ug/l	1596540	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	81
2	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	81
3	Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	72
4	4-tert-Butyltoluene	148	C11H16	000098-51-1	70
5	Benzene, pentamethyl-	148	C11H16	000700-12-9	70





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Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

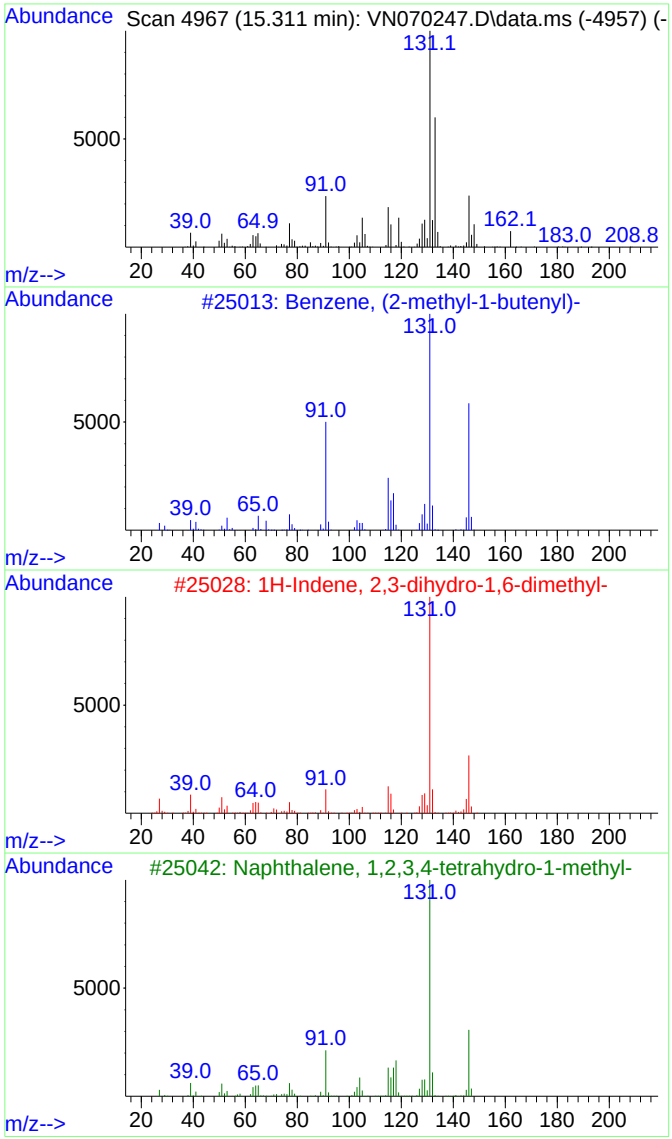
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

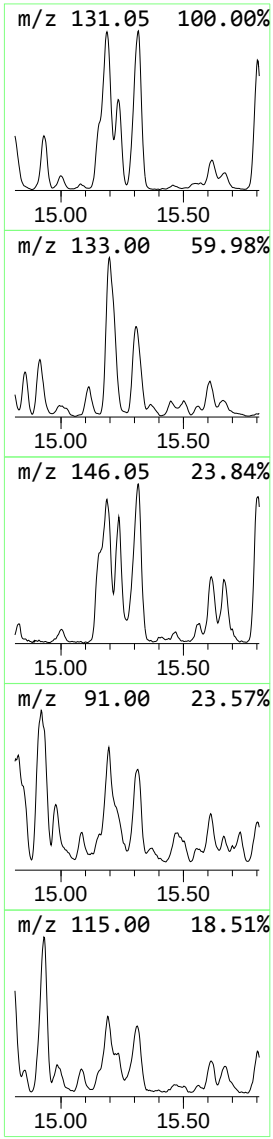
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.311	5.17 ug/l	1112400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	91
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	64
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070247.D
Acq On : 20 Dec 2021 18:01
Operator : JC/MD
Sample : M5011-12
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-5-(12.5-13)

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, 2,2,3,3...	8.603	9.3	ug/l	1132710	2	8.963	6104360	50.0
Pentane, 2,3,4-...	9.877	5.4	ug/l	663543	2	8.963	6104360	50.0
Pentane, 2,3,3-...	10.011	6.3	ug/l	772085	2	8.963	6104360	50.0
o-Cymene	14.217	7.6	ug/l	1636420	4	13.675	10758600	50.0
Benzene, 1,2,3,...	14.579	5.5	ug/l	1179060	4	13.675	10758600	50.0
1H-Indene, 2,3-...	14.925	11.4	ug/l	2455230	4	13.675	10758600	50.0
Benzene, 1-ethy...	15.193	7.4	ug/l	1596540	4	13.675	10758600	50.0
Benzene, (2-met...	15.311	5.2	ug/l	1112400	4	13.675	10758600	50.0