LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

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: VN070136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.559	1300	1331	1363	rVB3	102328	359208	1.12%	0.116%
2	6.074	1494	1523	1552	rBV3	128681	403825	1.26%	0.130%
3	7.016	1846	1874	1894	rBV4	180091	560430	1.74%	0.181%
4	7.118	1895	1912	1936	rVB2	145536	417992	1.30%	0.135%
5	8.019	2223	2248	2255	rBV2	945088	2239046	6.96%	0.722%
6	8.161	2287	2301	2324	rVB2	631766	1619957	5.04%	0.522%
7	8.284	2327	2347	2365	rBV	782591	1816154	5.65%	0.586%
8	8.432	2383	2402	2429	rBV	1129888	2605798	8.10%	0.840%
9	8.606	2432	2467	2492	rBV	2808694	7880400	24.50%	2.542%
10	8.818	2524	2546	2576	rVB2	852638	1853621	5.76%	0.598%
11	8.963	2579	2600	2628	rBV	2986890	6562029	20.40%	2.117%
12	9.451	2747	2782	2793	rBV2	1511260	3675057	11.42%	1.185%
13	9.505	2794	2802	2819	rVV	857634	1677182	5.21%	0.541%
14	9.588	2819	2833	2842	rVV	256592	534345	1.66%	0.172%
15	9.633	2843	2850	2864	rVV2	234007	422017	1.31%	0.136%
16	9.727	2864	2885	2900	rVB5	246506	613789	1.91%	0.198%
17	9.877	2903	2941	2963	rVV	2634368	5695308	17.71%	1.837%
18	10.011	2963	2991	3005	rVV2	3567099	8401202	26.12%	2.710%
19	10.076	3005	3015	3045	rVB2	1593931	4091843	12.72%	1.320%
20	10.213	3046	3066	3092	rBV2	1639602	3939164	12.25%	1.271%
21	10.368	3109	3124	3137	rBV	3184252	5680541	17.66%	1.832%
22	10.441	3137	3151	3175	rVB	4786366	9296363	28.90%	2.998%
23	10.623	3203	3219	3234	rVB2	2111720	4185772	13.01%	1.350%
24	10.784	3268	3279	3284	rBV2	205561	350796	1.09%	0.113%
25	10.886	3296	3317	3334	rVB7	988409	2866641	8.91%	0.925%
26	10.961	3336	3345	3359	rVB	395179	701193	2.18%	0.226%
27	11.052	3359	3379	3391	rBV4	414994	855972	2.66%	0.276%
28	11.154	3407	3417	3433	rVB	610673	1248774	3.88%	0.403%
29	11.454	3520	3529	3538	rBV2	398588	601113	1.87%	0.194%
30	11.527	3545	3556	3582	rVB4	1546732	3570542	11.10%	1.152%
31	11.626	3582	3593	3617	rBV	1221313	2196963	6.83%	0.709%
32	11.747	3620	3638	3653	rBV	4773113	8913169	27.71%	2.875%
33	11.846	3665	3675	3693	rVB	3402842	5791252	18.00%	1.868%
34	11.953	3697	3715	3739	rVB2	8623807	17852697	55.50%	5.758%
35	12.184	3792	3801	3813	rVB5	372415	635114	1.97%	0.205%
36	12.254	3817	3827	3832	rBV5	556703	900622	2.80%	0.290%

LSC Area Percent Report

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Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

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
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

37	12.366	3862	3869	3880	rVB2	573121	901825	2.80%	0.291%
38	12.581	3940	3949	3958	rBV	644728	1175055	3.65%	0.379%
39	12.731	3993	4005	4016	rVB2	3138600	5673553	17.64%	1.830%
40	12.876	4049	4059	4063	rBV2	390996	594063	1.85%	0.192%
41	12.921	4065	4076	4087	rVB	3099077	4862611	15.12%	1.568%
42	12.983	4087	4099	4107	rBV	10534123	17824556	55.41%	5.749%
43	13.058	4119	4127	4168	rVB2	7561361	14128034	43.92%	4.557%
44	13.222	4172	4188	4205	rBV	4315318	7878202	24.49%	2.541%
45	13.369	4229	4243	4257	rBV	19631244	32167300	100.00%	10.375%
46	13.498	4275	4291	4296	rBV4	511964	1228824	3.82%	0.396%
47	13.608	4325	4332	4338	rBV3	467152	642585	2.00%	0.207%
48	13.675	4346	4357	4363	rBV	5038973	8178543	25.43%	2.638%
49	13.841	4407	4419	4421	rBV2	2003663	2598706	8.08%	0.838%
50	13.871	4422	4430	4437	rVV2	6129055	10702191	33.27%	3.452%
51	13.908	4439	4444	4467	rVV4	6082296	11913703	37.04%	3.843%
52	13.994	4467	4476	4489	rVB2	1479859	2236216	6.95%	0.721%
53	14.069	4495	4504	4515	rVB	1293707	1999499	6.22%	0.645%
54	14.131	4516	4527	4533	rBV	2905344	4791983	14.90%	1.546%
55	14.217	4548	4559	4572	rVB	5364453	8329030	25.89%	2.686%
56	14.327	4590	4600	4612	rVB4	2574592	4279020	13.30%	1.380%
57	14.461	4639	4650	4662	rBV2	1183811	2125188	6.61%	0.685%
58	14.541	4671	4680	4687	rBV	2247261	3462915	10.77%	1.117%
59	14.579	4687	4694	4703	rVV	3239607	4723354	14.68%	1.523%
60	14.622	4703	4710	4718	rVV2	1788138	2527620	7.86%	0.815%
61	14.662	4720	4725	4740	rVB	1094311	1510304	4.70%	0.487%
62	14.764	4755	4763	4770	rBV	976552	1269559	3.95%	0.409%
63	14.809	4771	4780	4788	rBV2	2421871	4038749	12.56%	1.303%
64	14.930	4808	4825	4837	rBV4	3748088	9065930	28.18%	2.924%
65	15.086	4877	4883	4899	rVB3	311132	548438	1.70%	0.177%
66	15.196	4902	4924	4935	rBV5	1877432	4735141	14.72%	1.527%
67	15.314	4956	4968	4986	rVB5	1476437	3354612	10.43%	1.082%
68	15.507	5016	5040	5053	rBV	2015711	4303944	13.38%	1.388%
69	15.614	5069	5080	5091	rBV4	662643	1189862	3.70%	0.384%
70	15.804	5137	5151	5168	rBV2	803114	1730268	5.38%	0.558%
71	16.617	5440	5454	5491	rVB	950414	2333227	7.25%	0.753%

Sum of corrected areas: 310040501

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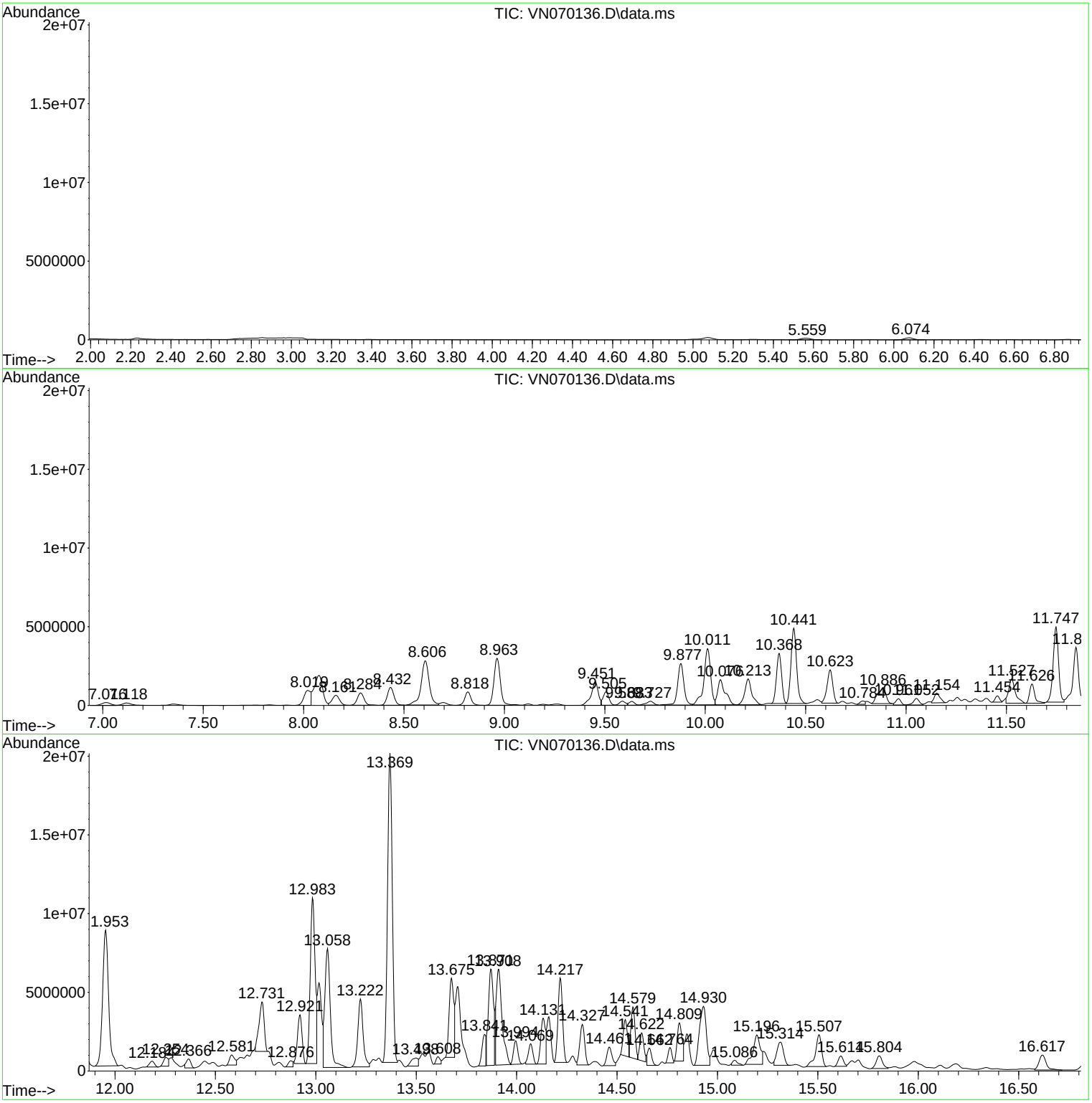
Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

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\VN121621\
Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
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Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

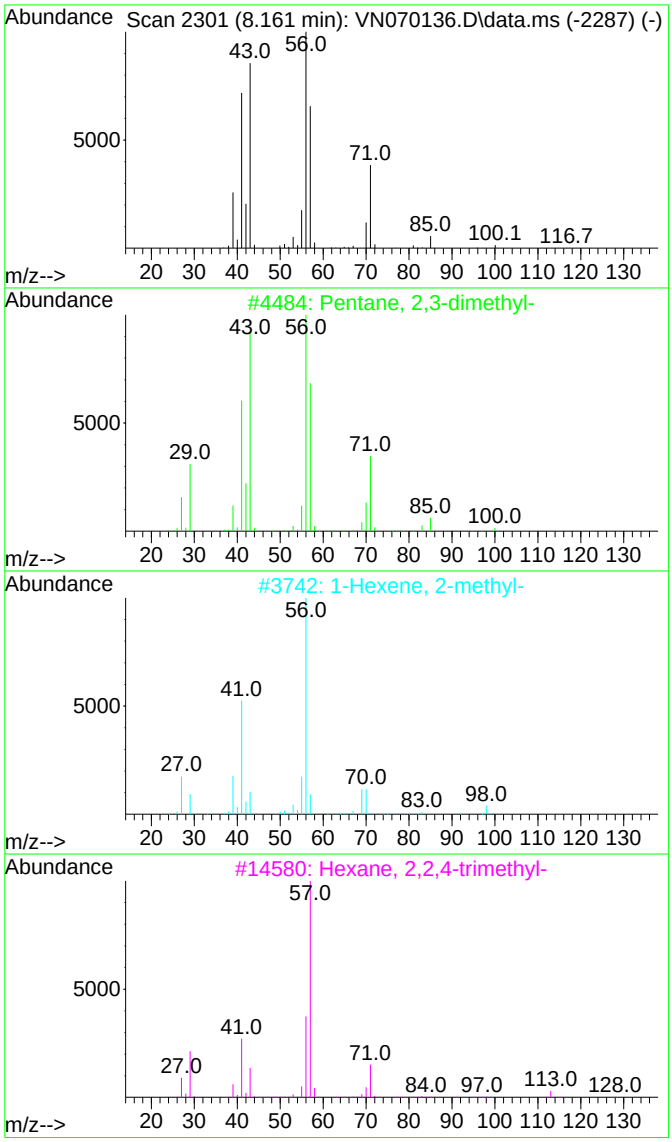
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

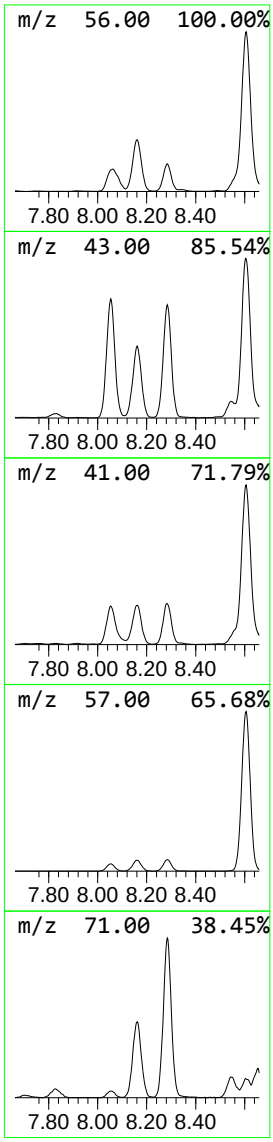
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	36.18 ug/l	1619960	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	38
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	36
4	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	32
5	Heptane	100	C7H16	000142-82-5	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

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

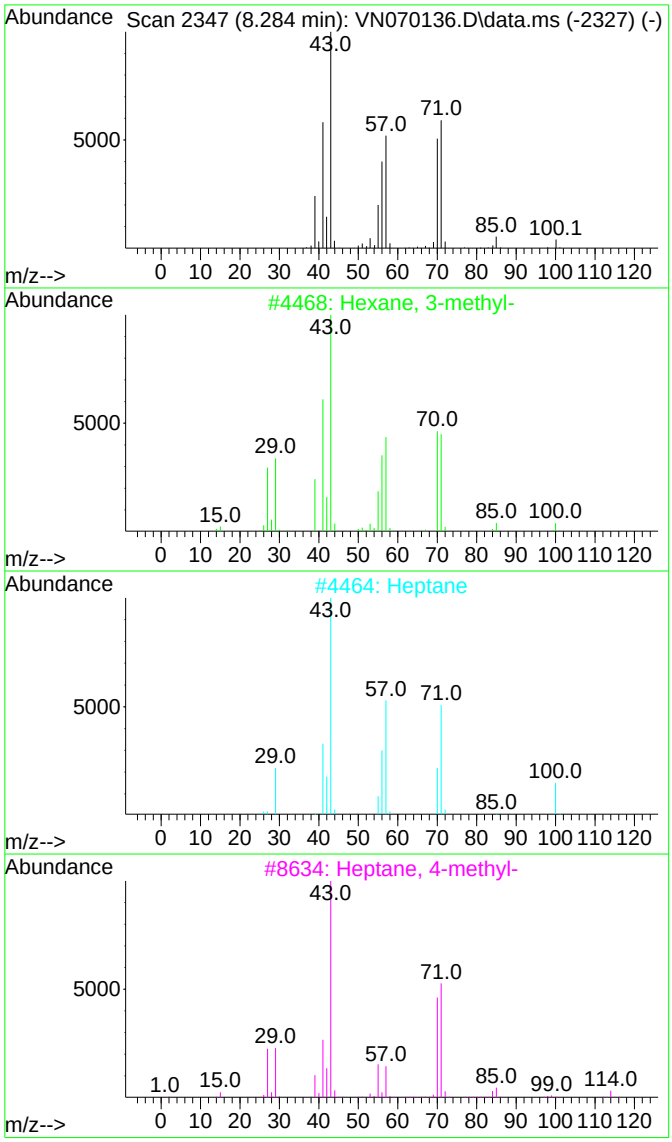
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

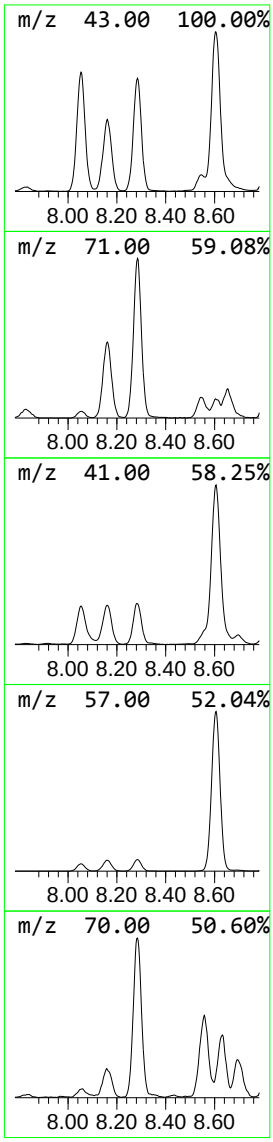
****

Peak Number 2 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	40.56 ug/l	1816150	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	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

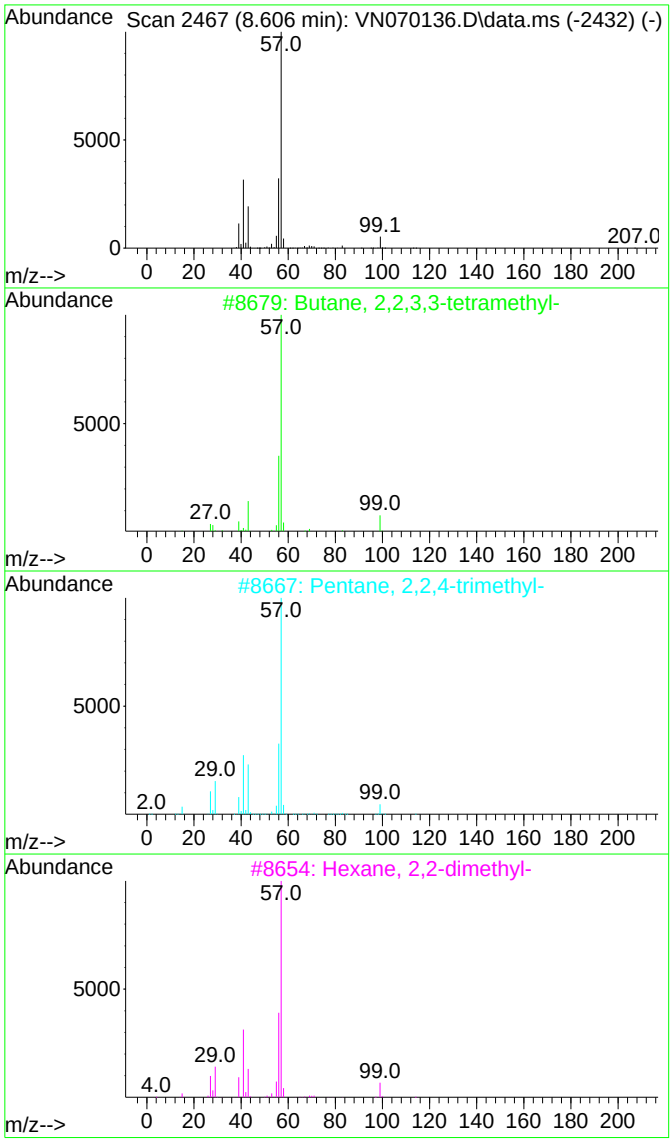
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

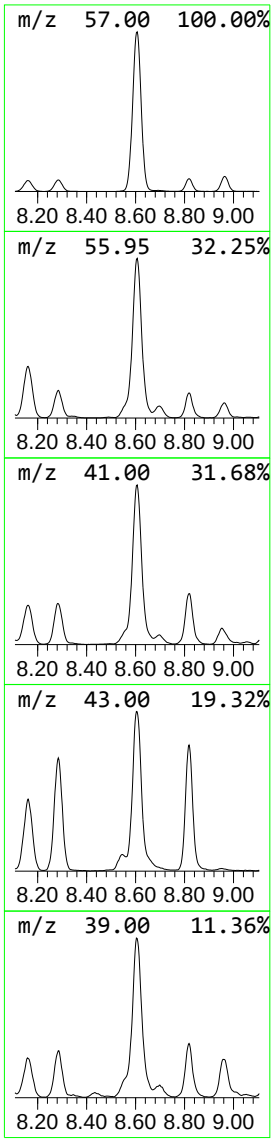
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.606	60.05 ug/l	7880400	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	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59





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Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

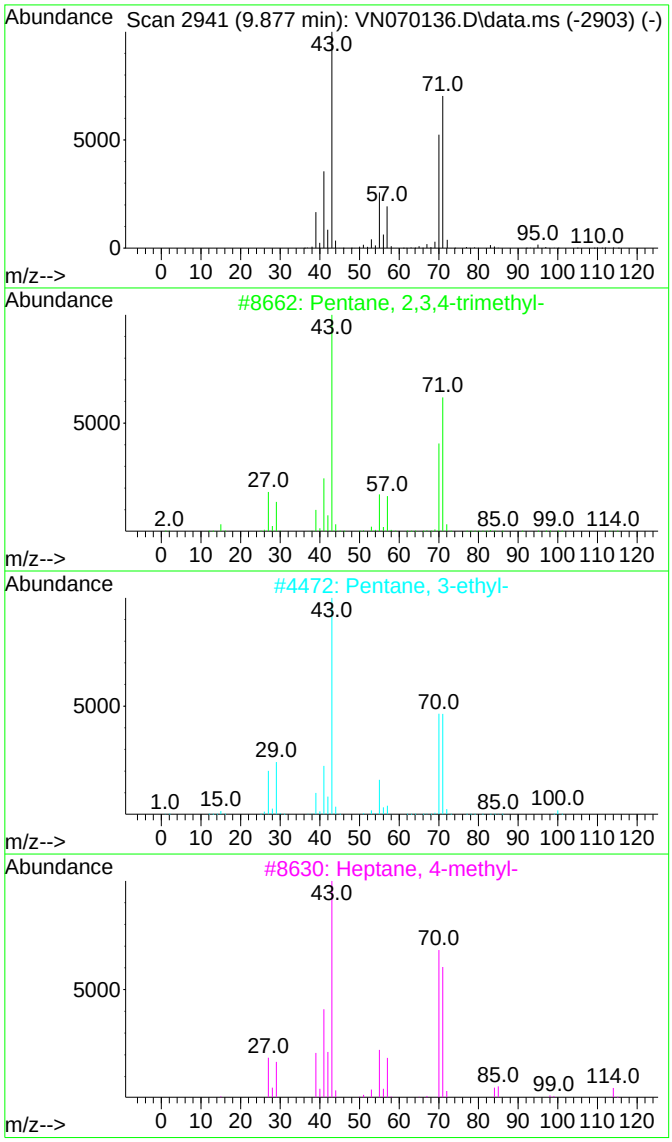
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

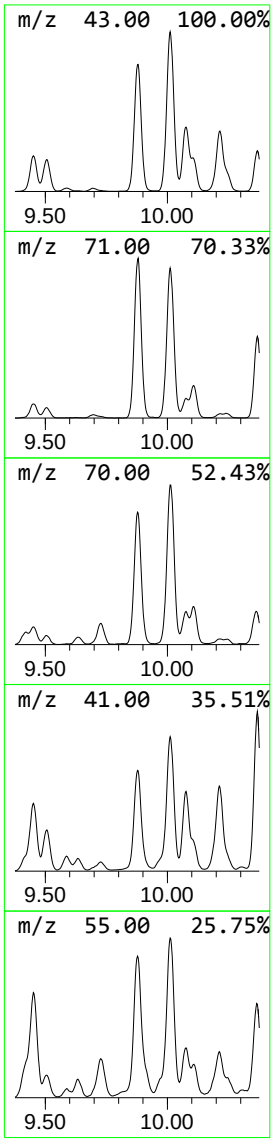
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	43.40 ug/l	5695310	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	83
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	74
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

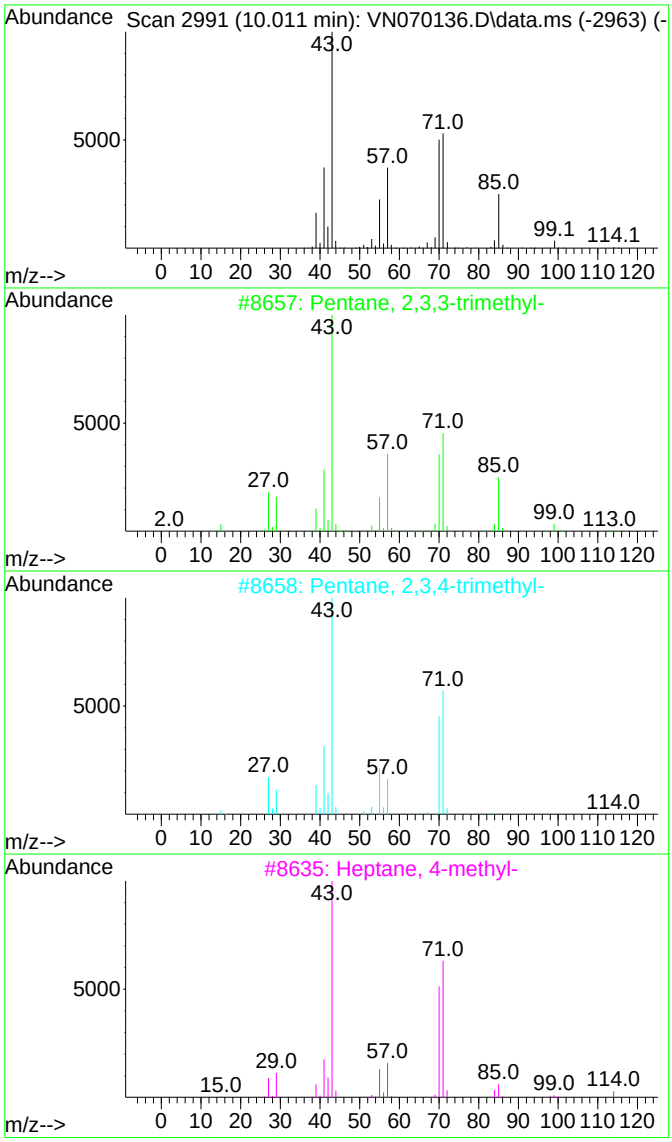
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

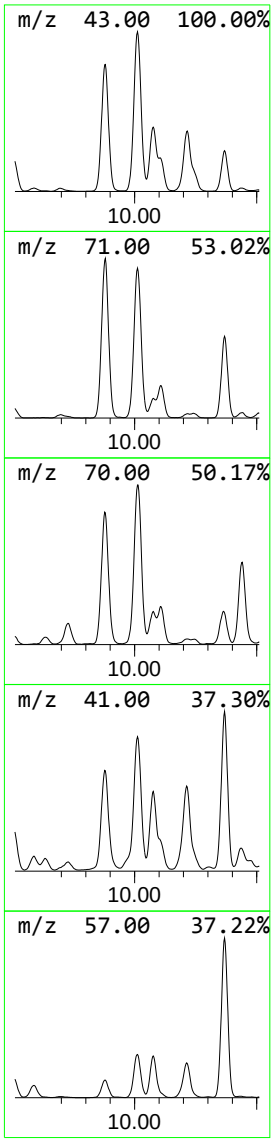
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.011	64.01 ug/l	8401200	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	90
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	76
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	53





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Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

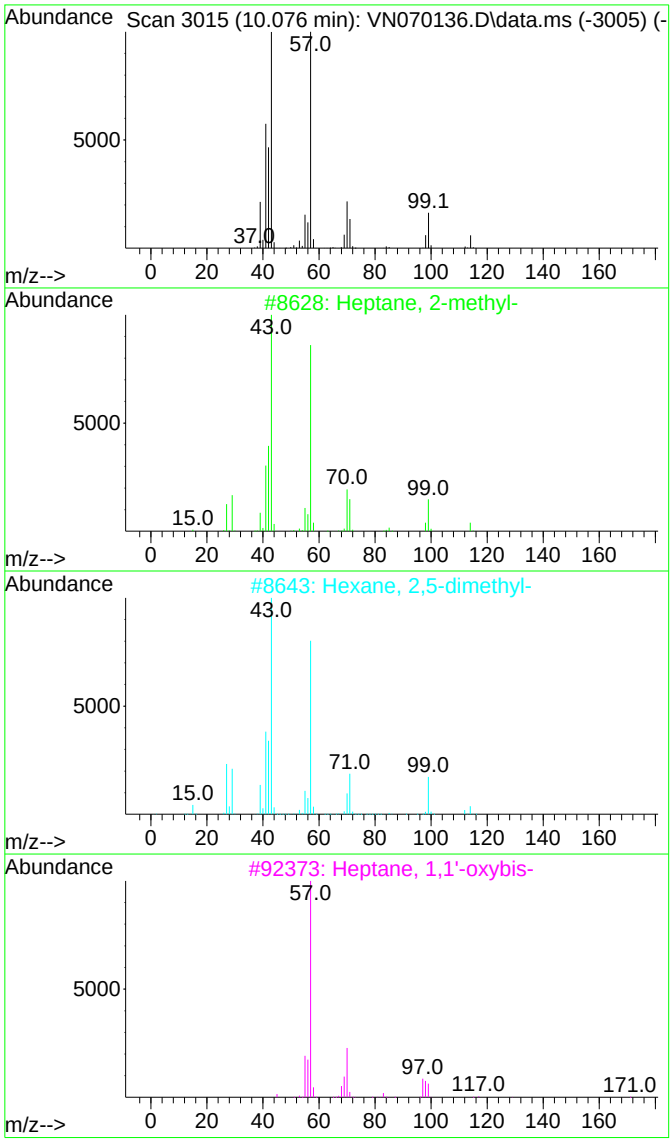
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

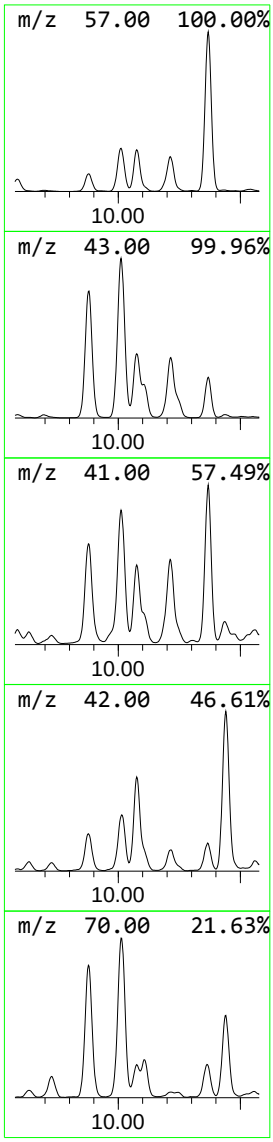
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.076	31.18 ug/l	4091840	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	80
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	Cyclohexanol, 4-methyl-, cis-	114	C7H14O	007731-28-4	38
5	Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
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Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

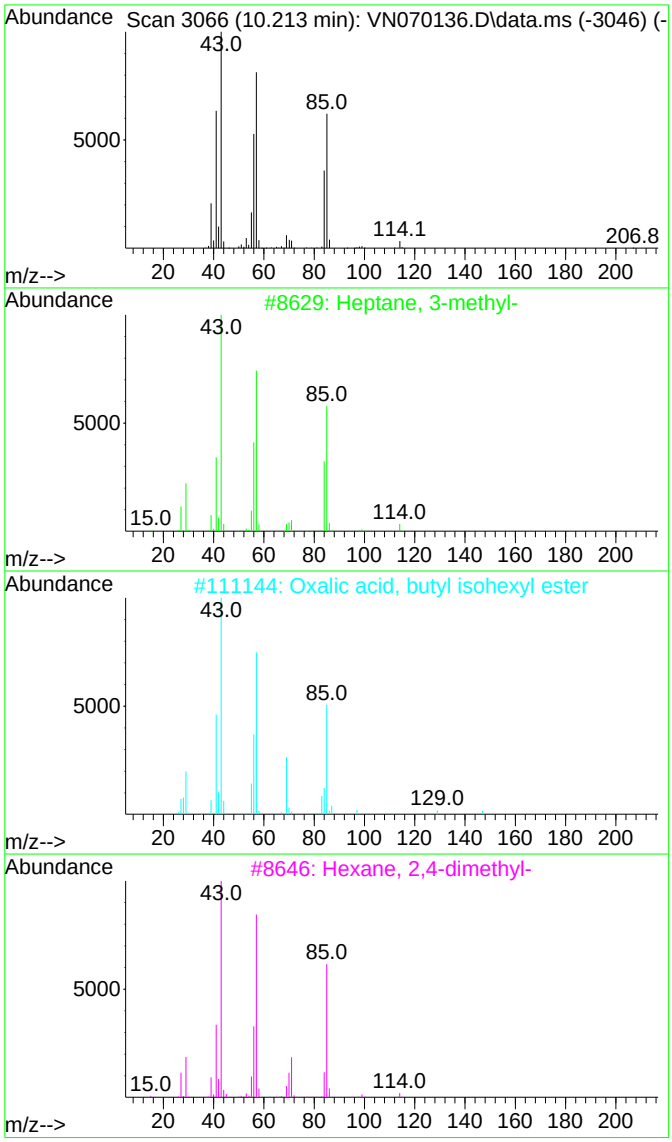
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

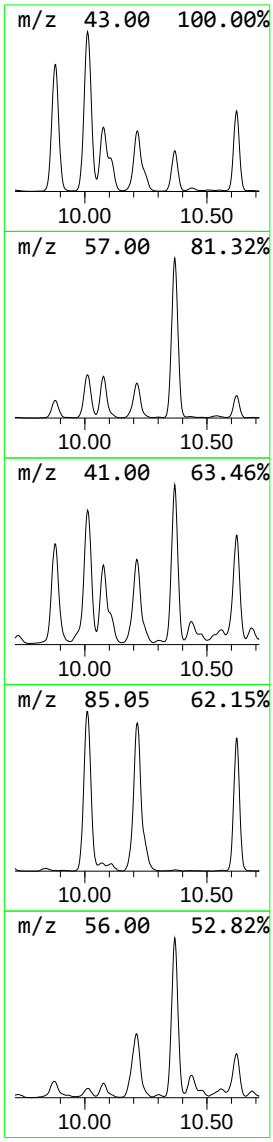
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptane, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.213	30.01 ug/l	3939160	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	78
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4	Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	59
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53





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Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

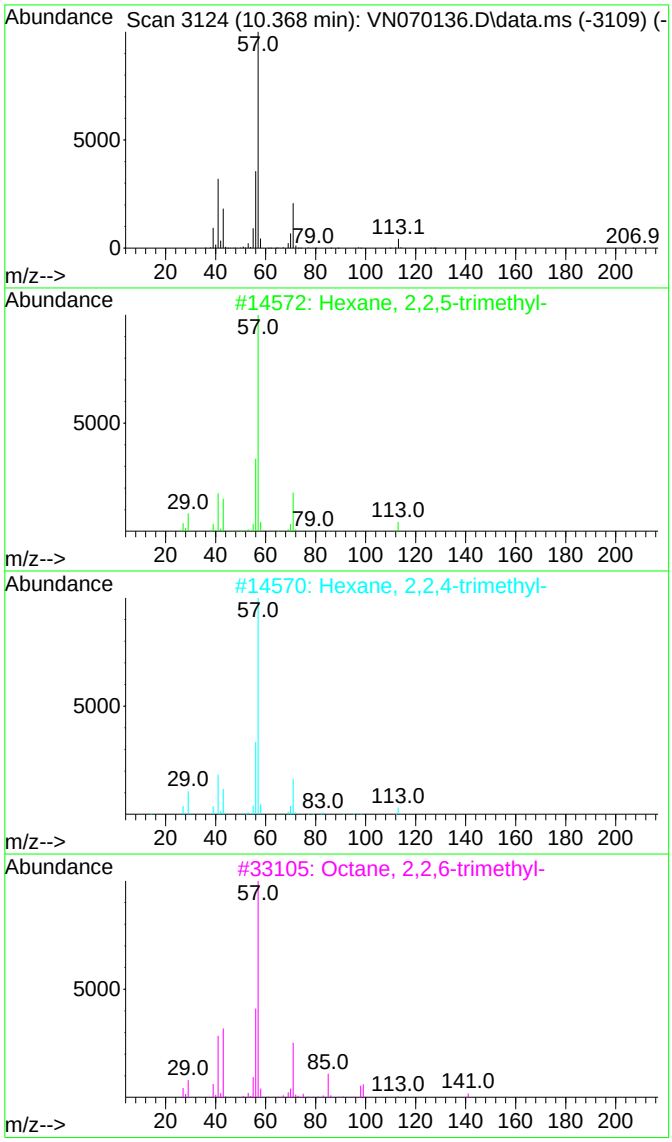
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

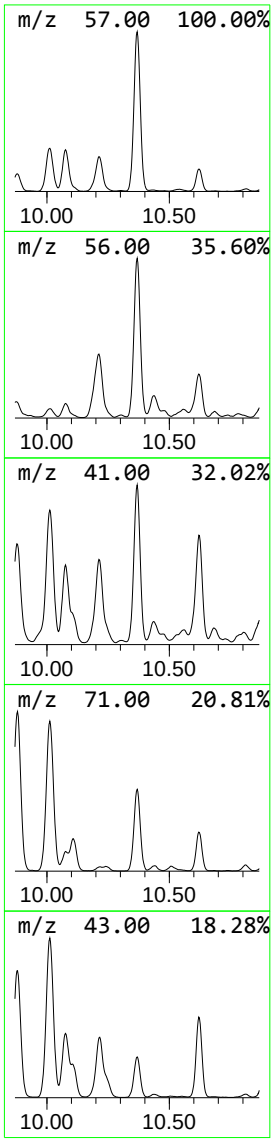
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexane, 2,2,5-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	31.87 ug/l	5680540	Chlorobenzene-d5	11.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	83
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	83
3	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
4	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

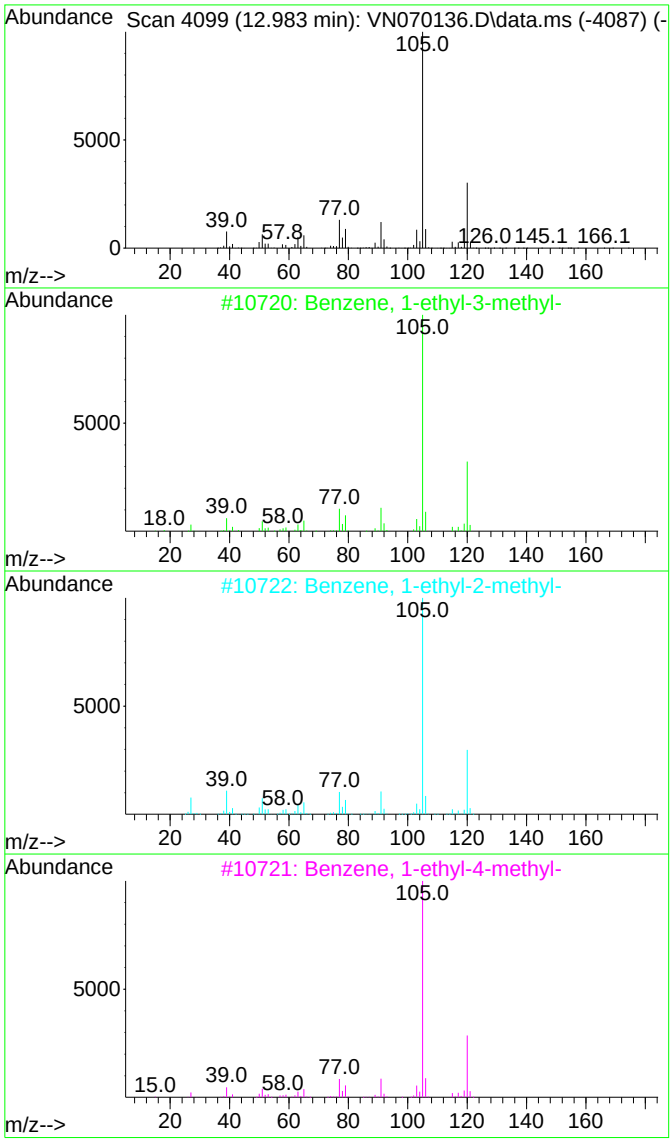
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

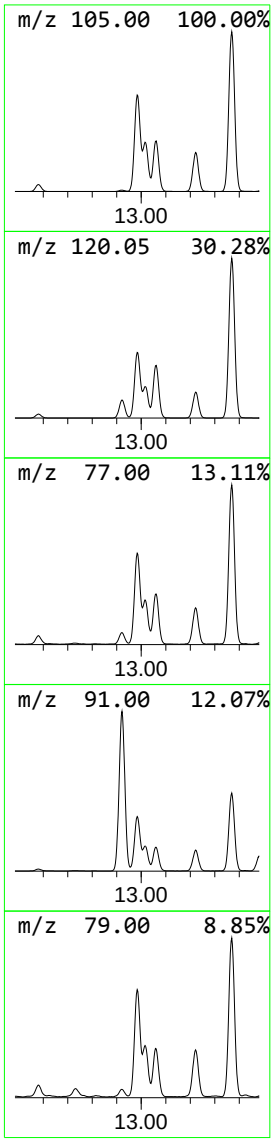
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	108.97 ug/l	17824600	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

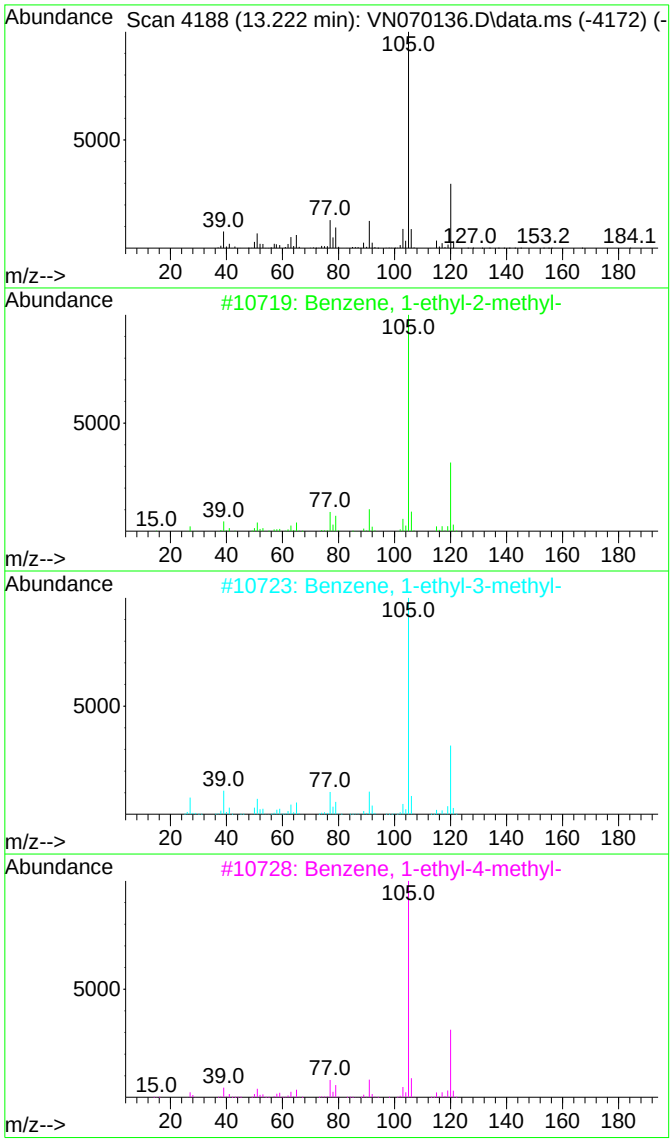
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

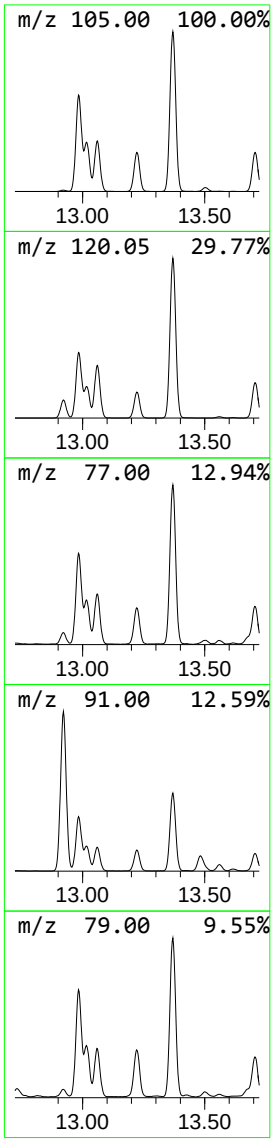
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	48.16 ug/l	7878200	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	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

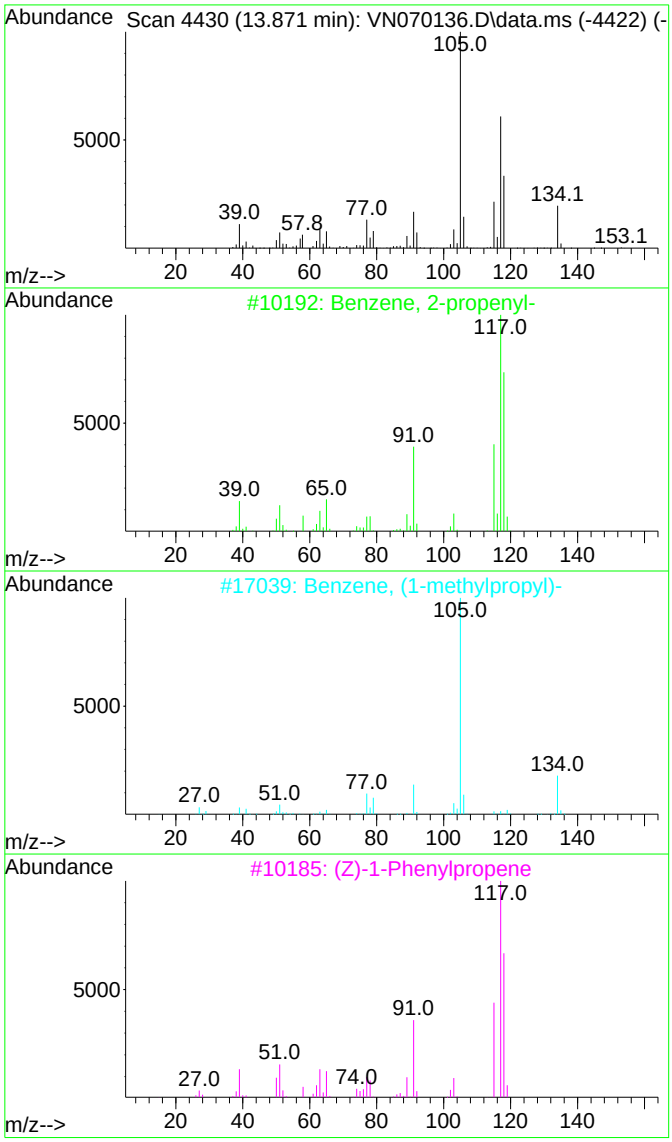
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

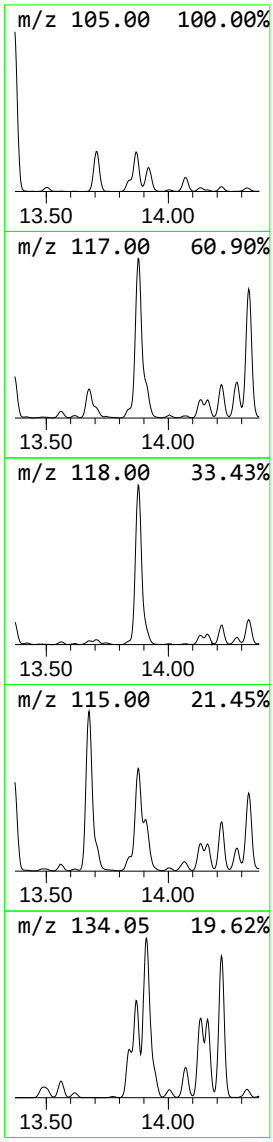
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 2-propenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	65.43 ug/l	10702200	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	50
2	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	46
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	45
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	45
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	43





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Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

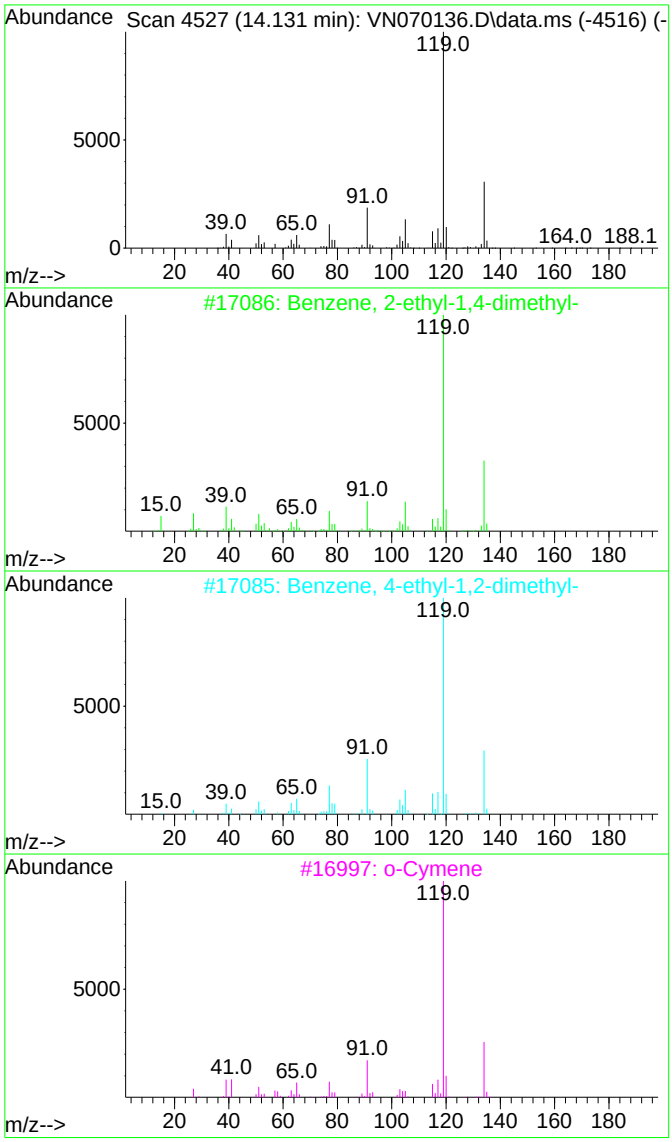
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

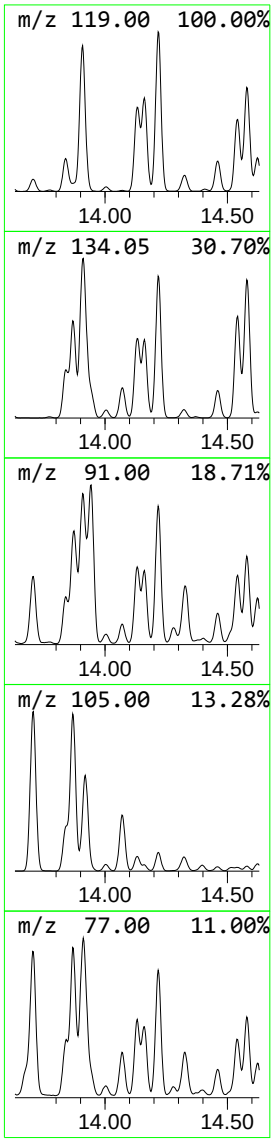
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.131	29.30 ug/l	4791980	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	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93





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Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

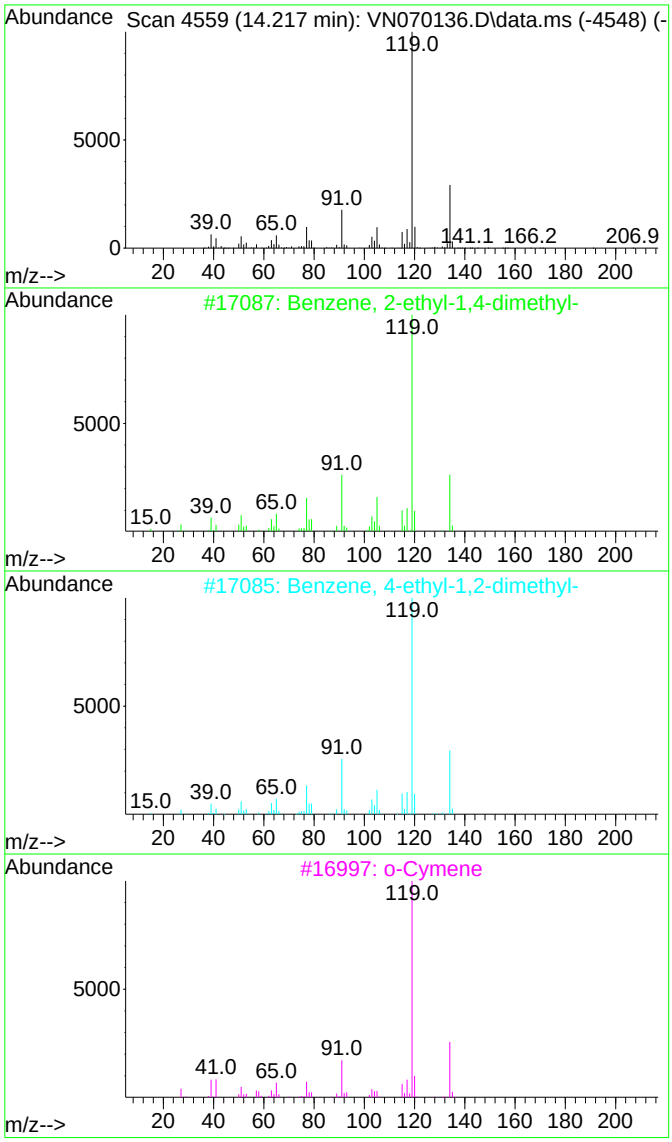
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

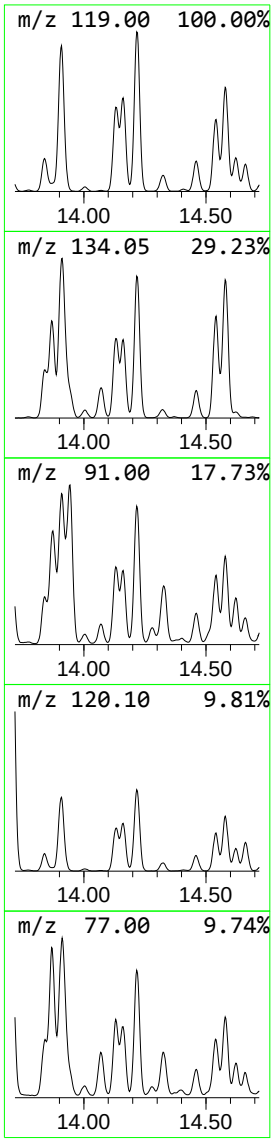
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	50.92 ug/l	8329030	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	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

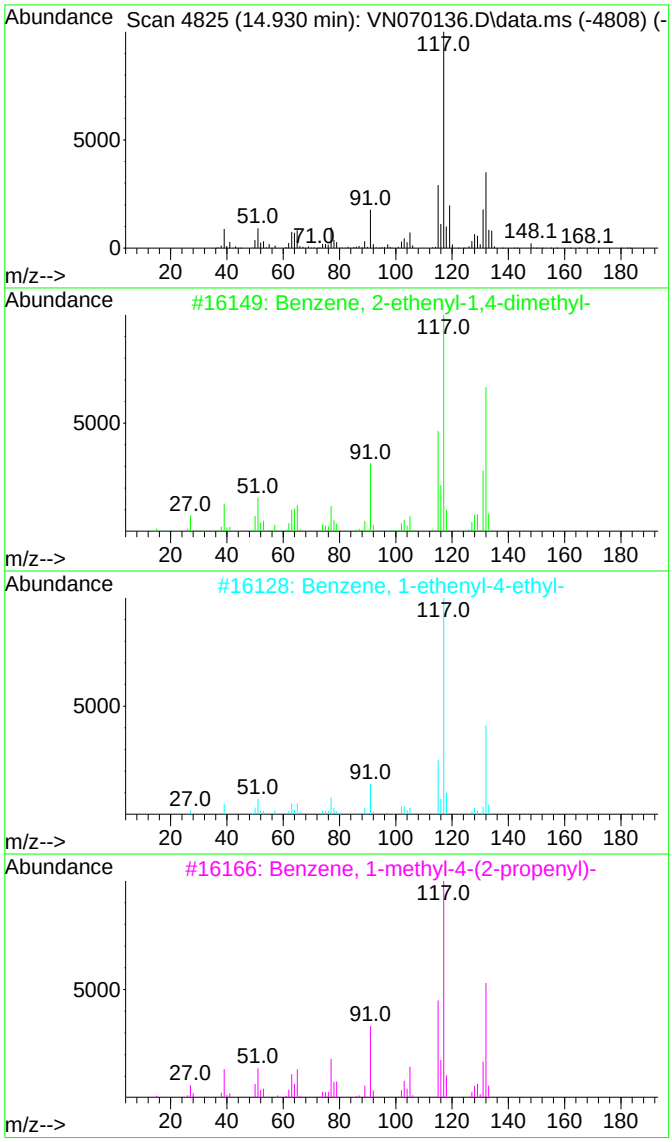
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

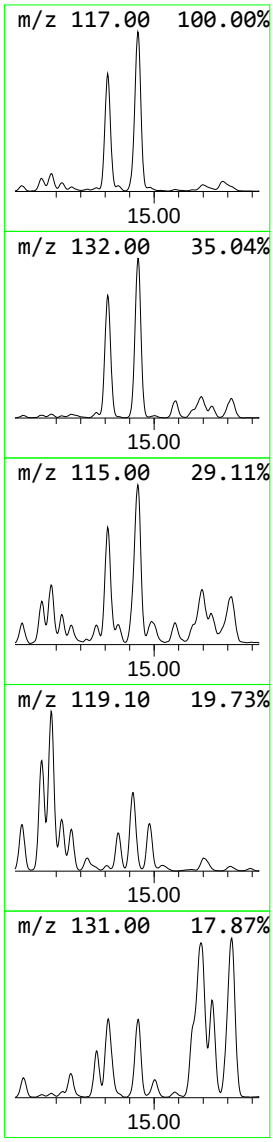
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	55.43 ug/l	9065930	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





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Acq On : 16 Dec 2021 14:31
Operator : JC/MD
Sample : M5011-03
Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-2-(9-9.5)

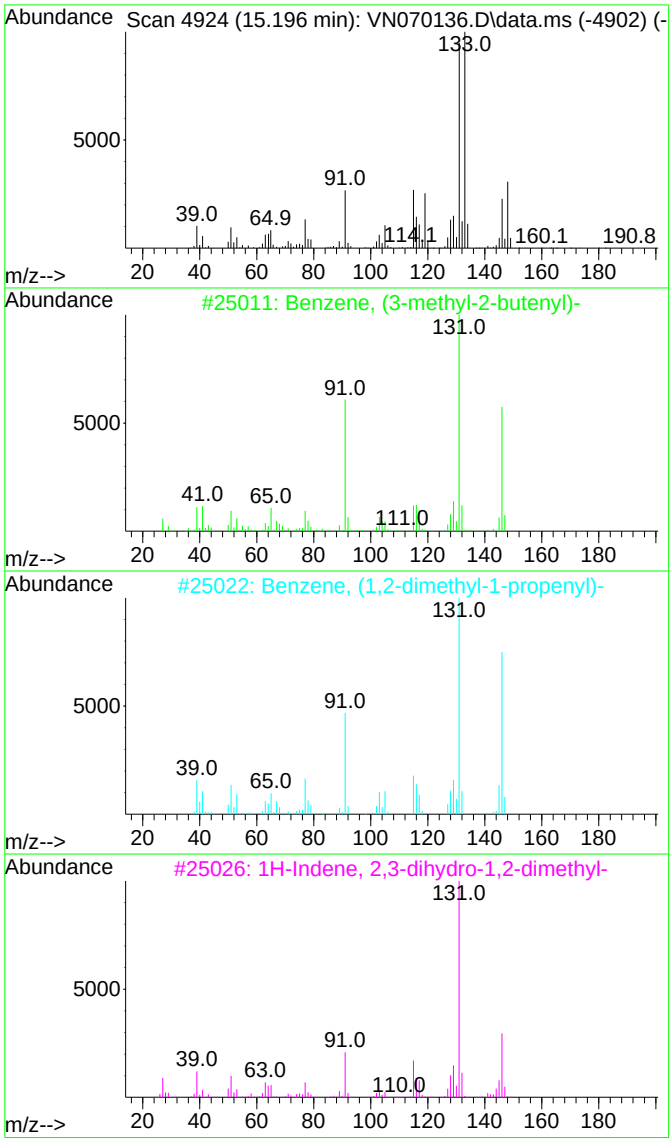
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

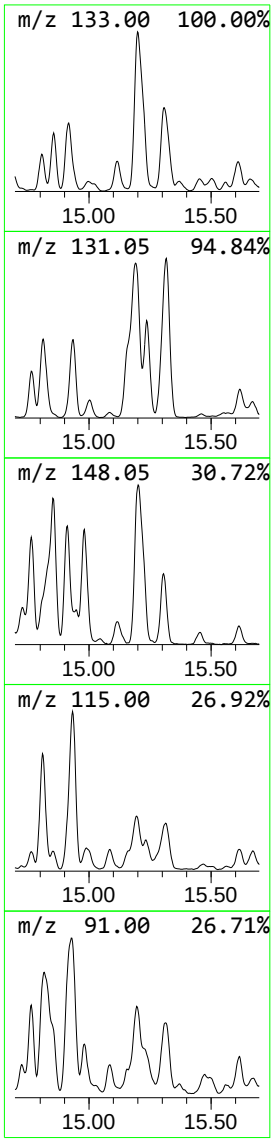
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, (3-methyl-2-butenyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	28.95 ug/l	4735140	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	89
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	86
4	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	83
5	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	50





Tentatively Identified Compound (LSC) summary

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Data File : VN070136.D
Acq On : 16 Dec 2021 14:31
Operator : JC/MD
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Misc : 3.72g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
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ClientSampleId :
HSB-2-(9-9.5)

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, 2,3-di...	8.161	36.2	ug/l	1619960	1	8.080	2239050	50.0
Hexane, 3-methyl-	8.284	40.6	ug/l	1816150	1	8.080	2239050	50.0
Butane, 2,2,3,3...	8.606	60.0	ug/l	7880400	2	8.963	6562030	50.0
Pentane, 2,3,4-...	9.877	43.4	ug/l	5695310	2	8.963	6562030	50.0
Pentane, 2,3,3-...	10.011	64.0	ug/l	8401200	2	8.963	6562030	50.0
Heptane, 2-methyl-	10.076	31.2	ug/l	4091840	2	8.963	6562030	50.0
Heptane, 3-methyl-	10.213	30.0	ug/l	3939160	2	8.963	6562030	50.0
Hexane, 2,2,5-t...	10.368	31.9	ug/l	5680540	3	11.747	8913170	50.0
Benzene, 1-ethy...	12.983	109.0	ug/l	17824600	4	13.675	8178540	50.0
Benzene, 1-ethy...	13.222	48.2	ug/l	7878200	4	13.675	8178540	50.0
Benzene, 2-prop...	13.871	65.4	ug/l	10702200	4	13.675	8178540	50.0
Benzene, 2-ethy...	14.131	29.3	ug/l	4791980	4	13.675	8178540	50.0
Benzene, 4-ethy...	14.217	50.9	ug/l	8329030	4	13.675	8178540	50.0
Benzene, 2-ethe...	14.930	55.4	ug/l	9065930	4	13.675	8178540	50.0
Benzene, (3-met...	15.196	28.9	ug/l	4735140	4	13.675	8178540	50.0