LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NWB-1501ME

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N012521W.M
Title : SW846 8260

Signal : TIC: VN065634.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.791	619	638	680	rBV	211736	690486	8.19%	2.131%
2	7.585	1788	1818	1823	rBV3	303194	993988	11.79%	3.068%
3	7.695	1842	1852	1872	rVB2	105506	265982	3.16%	0.821%
4	7.830	1874	1894	1925	rBV	639825	1543023	18.31%	4.763%
5	7.984	1925	1942	1961	rBV	152245	357713	4.24%	1.104%
6	8.103	1962	1979	1993	rBV3	105471	263024	3.12%	0.812%
7	8.392	2049	2069	2090	rBV	1352315	2762482	32.77%	8.527%
8	8.547	2102	2117	2139	rVB	394893	828186	9.83%	2.556%
9	8.859	2192	2214	2229	rVB	54168	119293	1.42%	0.368%
10	9.042	2246	2271	2283	rBV2	189408	465460	5.52%	1.437%
11	9.232	2316	2330	2343	rVB	72633	140300	1.66%	0.433%
12	10.058	2572	2587	2595	rBV	633066	1179539	13.99%	3.641%
13	10.122	2595	2607	2630	rVB	4475313	8428997	100.00%	26.017%
14	11.170	2917	2933	2952	rVB6	51922	124016	1.47%	0.383%
15	11.376	2984	2997	3017	rBV	512433	920124	10.92%	2.840%
16	11.601	3045	3067	3081	rBV5	228203	546172	6.48%	1.686%
17	11.920	3145	3166	3180	rBV3	96291	284358	3.37%	0.878%
18	12.373	3299	3307	3316	rVV	341661	529865	6.29%	1.635%
19	12.415	3316	3320	3329	rVB	75722	101365	1.20%	0.313%
20	12.627	3375	3386	3392	rBV	144953	253825	3.01%	0.783%
21	12.698	3400	3408	3419	rVB2	621833	952521	11.30%	2.940%
22	12.862	3448	3459	3465	rBV	64485	133635	1.59%	0.412%
23	12.932	3474	3481	3493	rVB2	135949	223974	2.66%	0.691%
24	13.010	3494	3505	3515	rBV	283589	471277	5.59%	1.455%
25	13.206	3554	3566	3574	rBV5	117452	229581	2.72%	0.709%
26	13.257	3575	3582	3587	rVV2	118531	172358	2.04%	0.532%
27	13.318	3588	3601	3617	rVV3	539960	1151903	13.67%	3.555%
28	13.395	3618	3625	3627	rVV2	121136	148037	1.76%	0.457%
29	13.421	3628	3633	3647	rVB	251772	401692	4.77%	1.240%
30	13.511	3655	3661	3668	rVB2	103450	128898	1.53%	0.398%
31	13.559	3668	3676	3691	rBV5	140453	394317	4.68%	1.217%
32	13.643	3693	3702	3711	rVB	778834	1137048	13.49%	3.510%
33	13.801	3747	3751	3761	rVB6	132722	185187	2.20%	0.572%
34	13.858	3762	3769	3777	rVB	148113	210507	2.50%	0.650%
35	13.903	3779	3783	3792	rVB4	69882	93533	1.11%	0.289%
36	13.965	3793	3802	3812	rBV2	165963	265502	3.15%	0.819%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NWB-1501ME

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N012521W.M
Title : SW846 8260

37	14.132	3845	3854	3861	rBV8	190348	376100	4.46%	1.161%
38	14.267	3889	3896	3902	rBV2	179212	256782	3.05%	0.793%
39	14.302	3903	3907	3916	rVB3	122392	158230	1.88%	0.488%
40	14.447	3945	3952	3957	rBV	75559	127804	1.52%	0.394%
41	14.492	3959	3966	3975	rVV	611045	861812	10.22%	2.660%
42	14.559	3976	3987	3996	rVV6	284678	609108	7.23%	1.880%
43	14.611	3998	4003	4015	rVB3	179430	295036	3.50%	0.911%
44	14.926	4091	4101	4110	rBV7	120804	251607	2.99%	0.777%
45	15.077	4140	4148	4155	rBV5	110206	201666	2.39%	0.622%
46	15.154	4166	4172	4180	rVB	89142	118448	1.41%	0.366%
47	15.209	4181	4189	4208	rVV8	132658	342655	4.07%	1.058%
48	15.296	4208	4216	4230	rVB4	259612	448990	5.33%	1.386%
49	15.383	4233	4243	4256	rBV6	89836	232440	2.76%	0.717%
50	15.575	4296	4303	4316	rVB	233288	411233	4.88%	1.269%
51	15.868	4383	4394	4404	rBV6	156694	317986	3.77%	0.981%
52	16.058	4444	4453	4463	rVB3	156005	290056	3.44%	0.895%

Sum of corrected areas: 32398121

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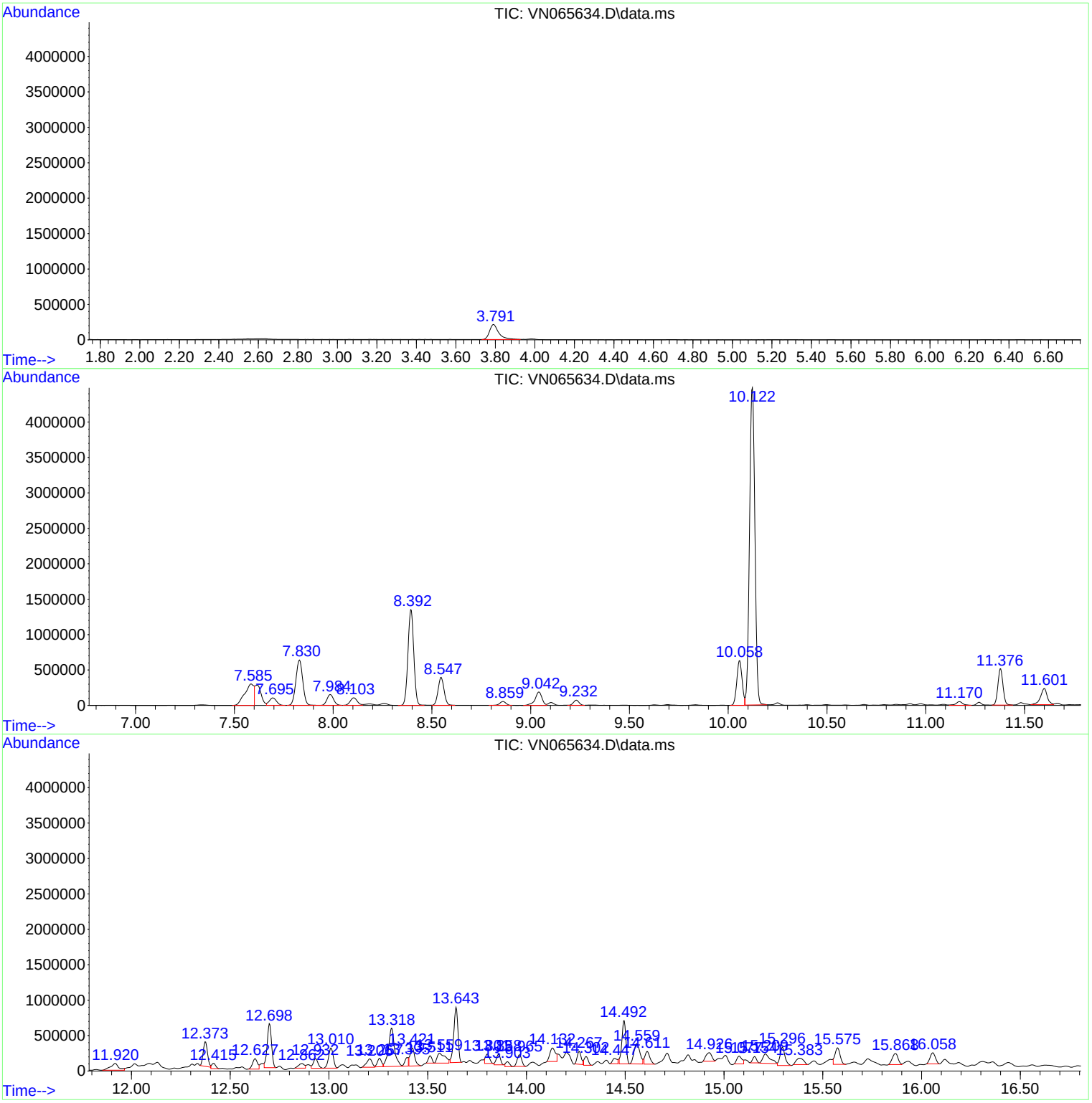
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
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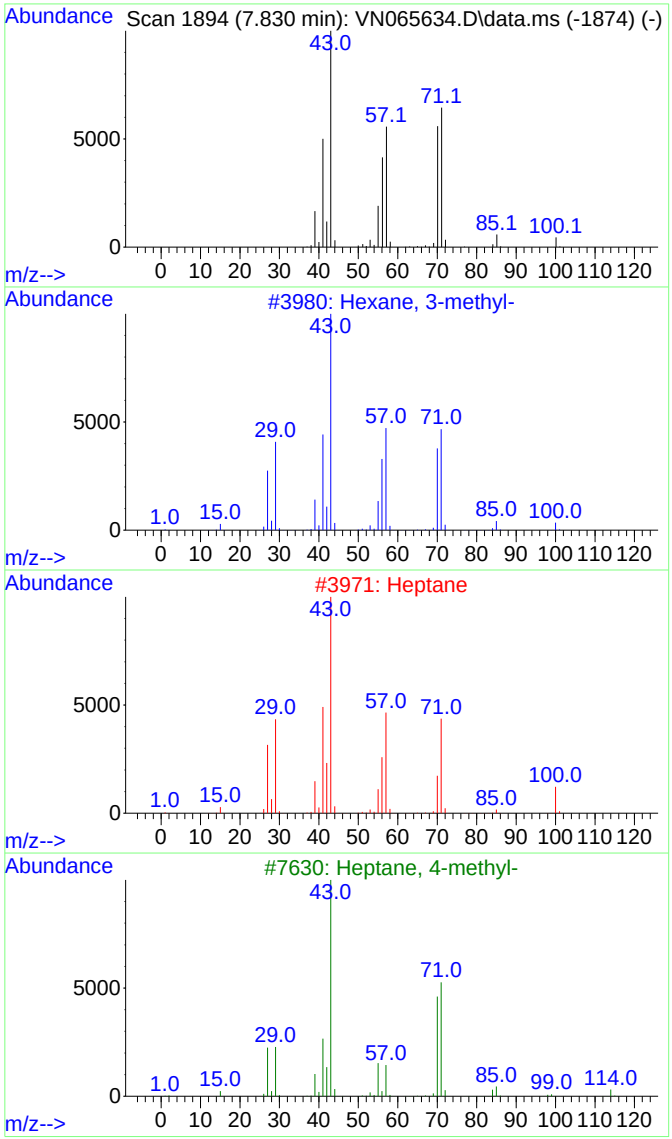
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

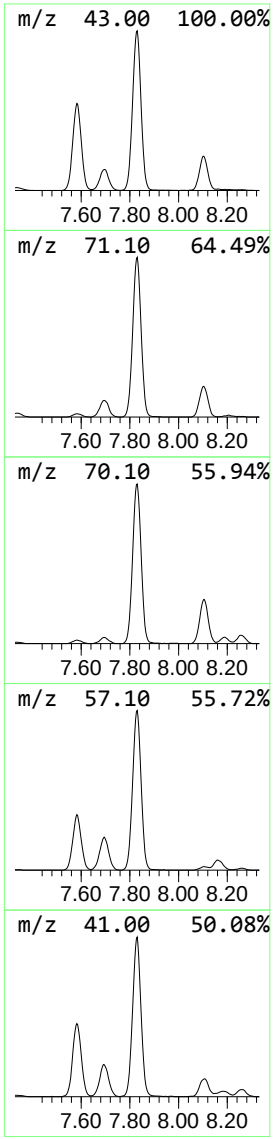
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.830	77.62 ug/l	1543020	Pentafluorobenzene	7.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	74
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

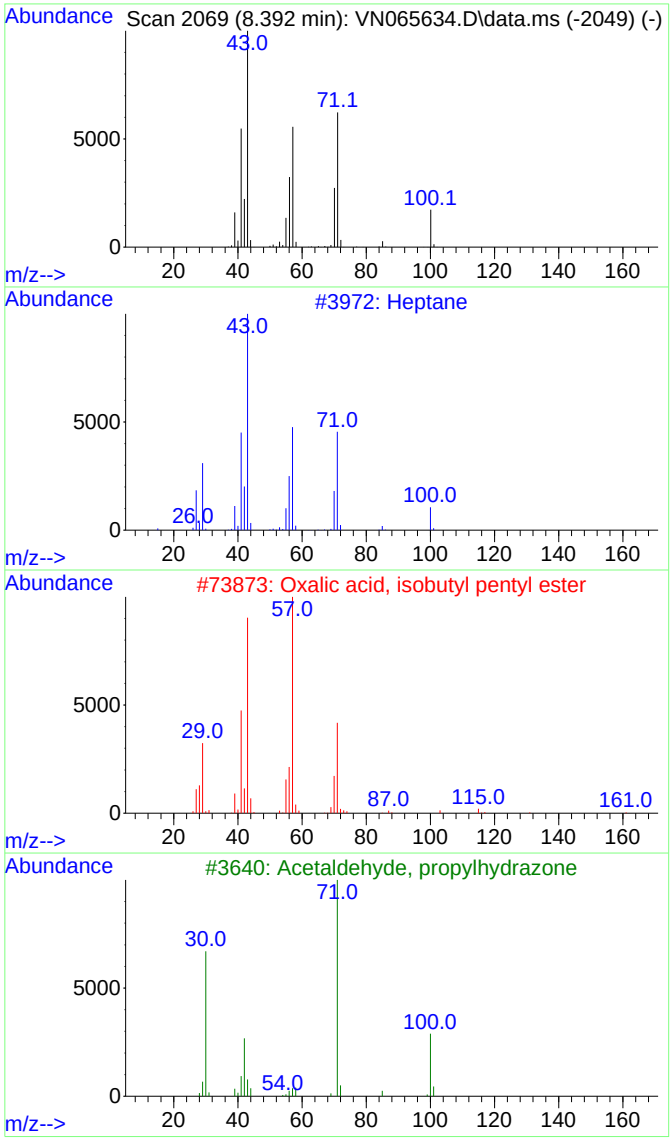
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

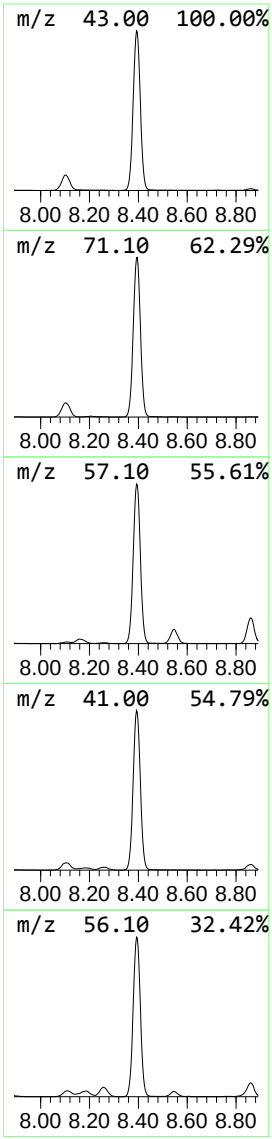
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.392	166.78 ug/l	2762480	1,4-Difluorobenzene	8.547

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	46
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

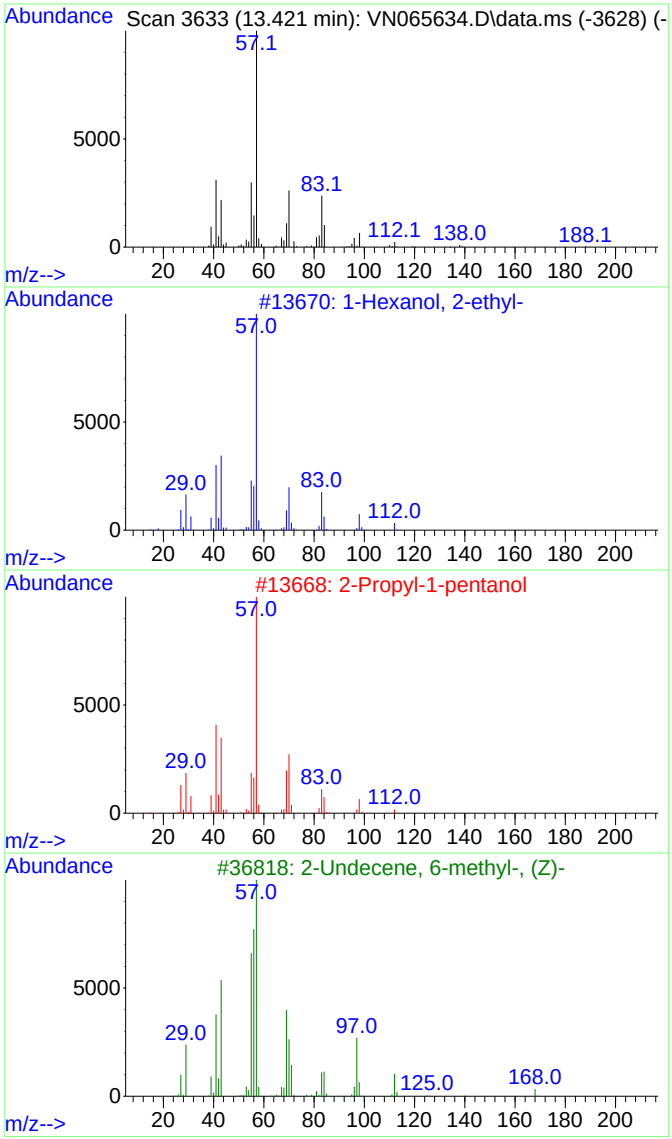
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

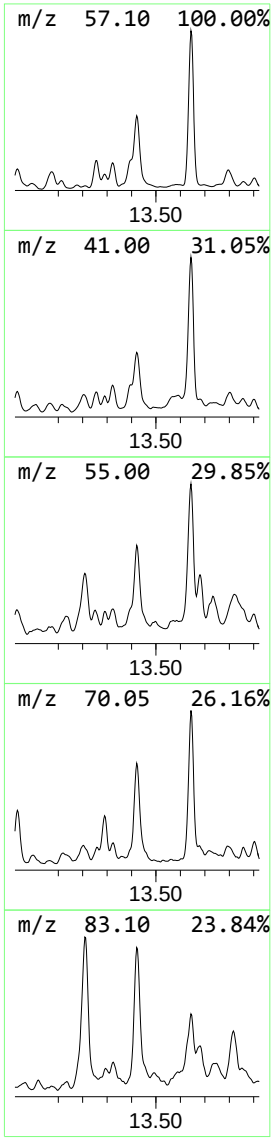
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	17.44 ug/l	401692	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42
3	2-Undecene, 6-methyl-, (Z)-	168	C12H24	074630-43-6	42
4	Trichloroacetic acid, 2-ethylhex...	274	C10H17Cl3O2	016397-79-8	42
5	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

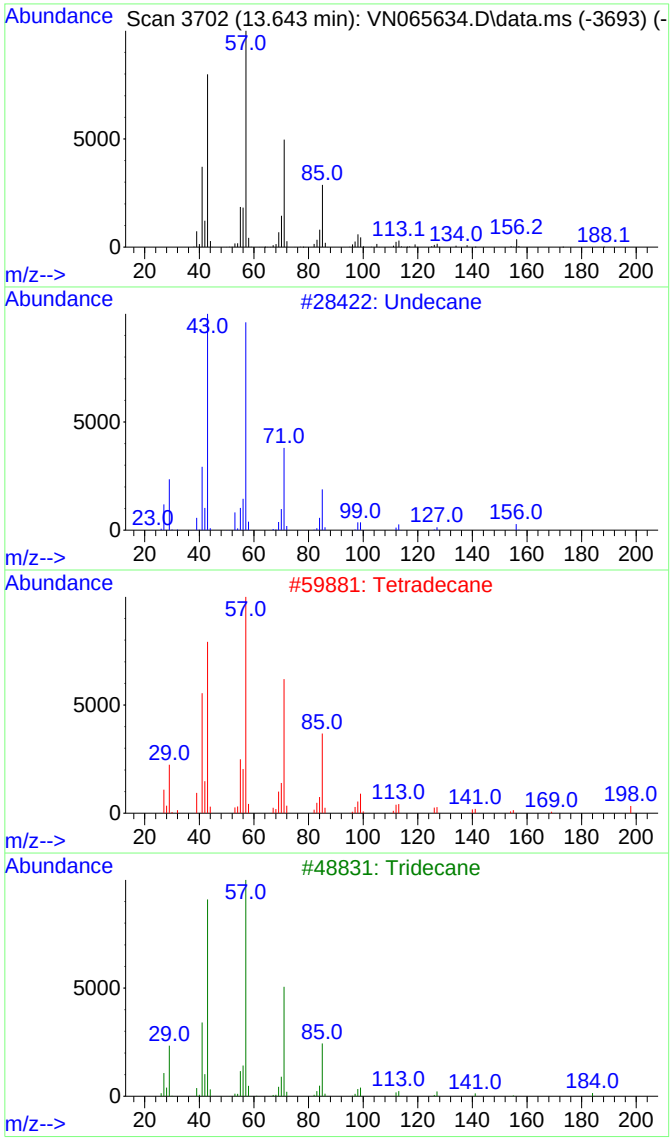
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

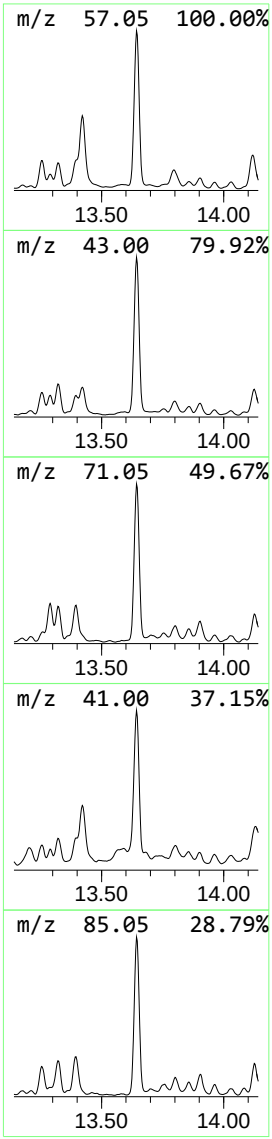
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.643	49.36 ug/l	1137050	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Tridecane	184	C13H28	000629-50-5	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

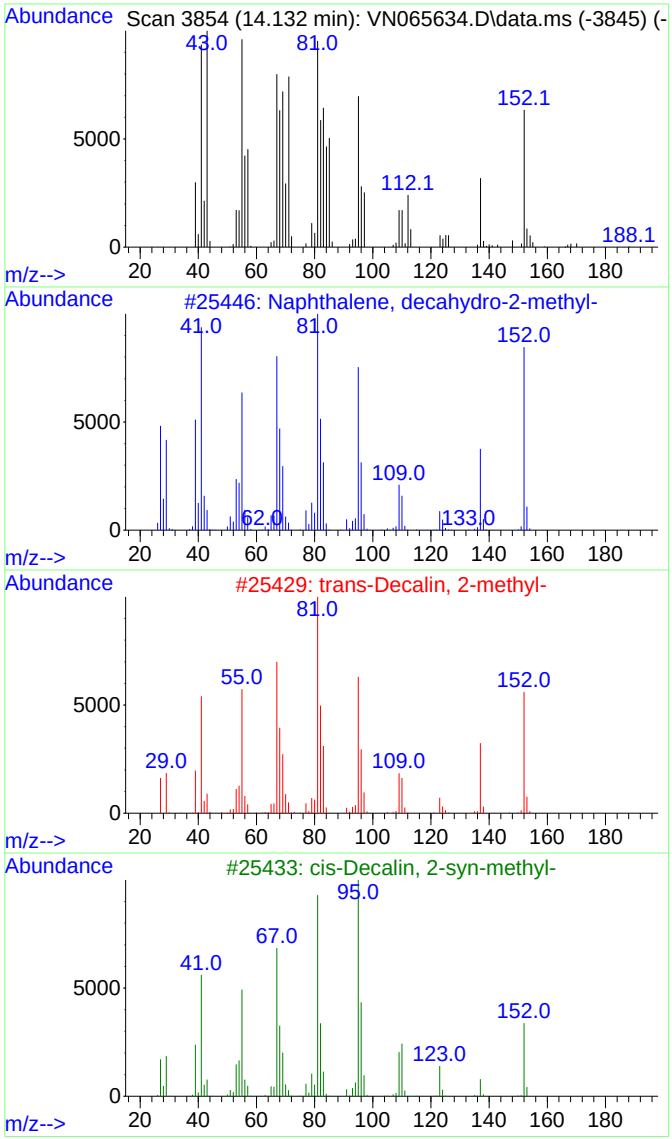
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

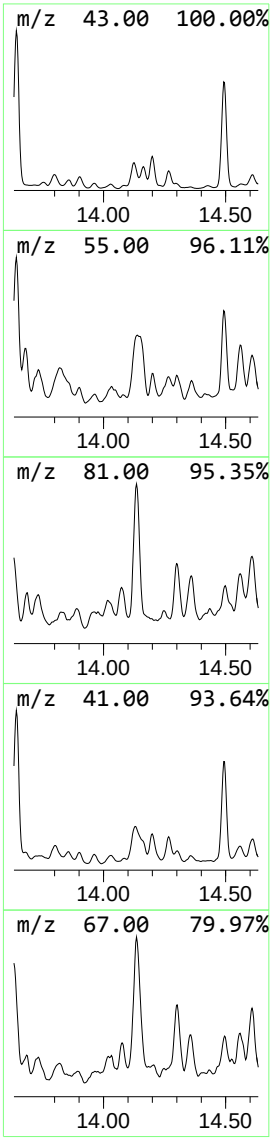
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, decahydro-2-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.132	16.33 ug/l	376100	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	95
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
3	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	55
4	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	55
5	Pulegone	152	C10H16O	000089-82-7	50





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Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

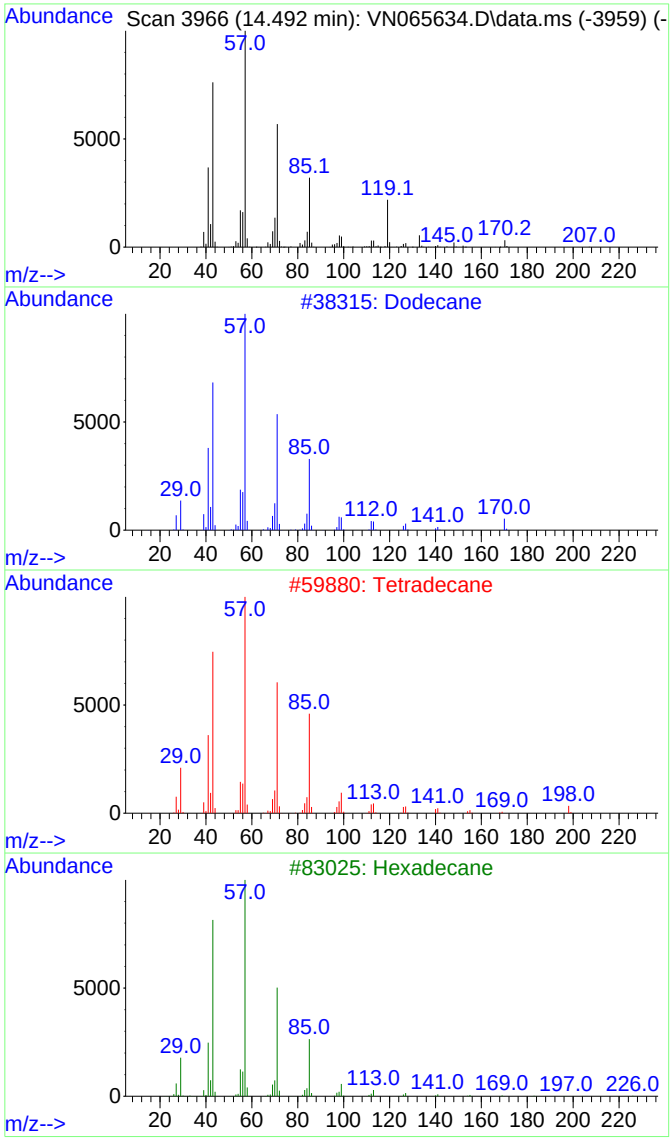
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

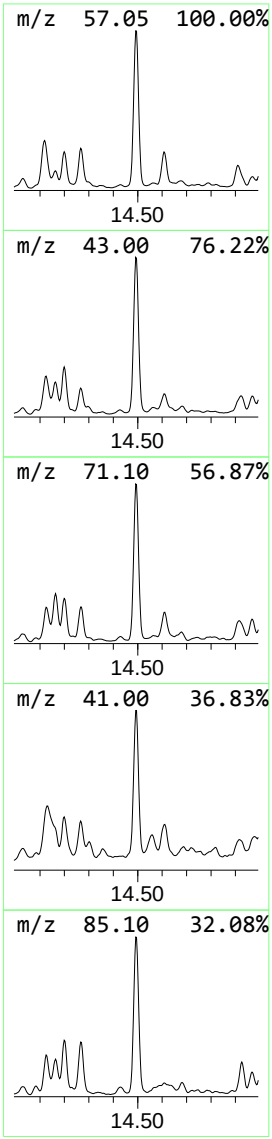
****

Peak Number 6 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	37.41 ug/l	861812	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	93
2	Tetradecane	198	C14H30	000629-59-4	72
3	Hexadecane	226	C16H34	000544-76-3	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64





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Data File : VN065634.D
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Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NWB-1501ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

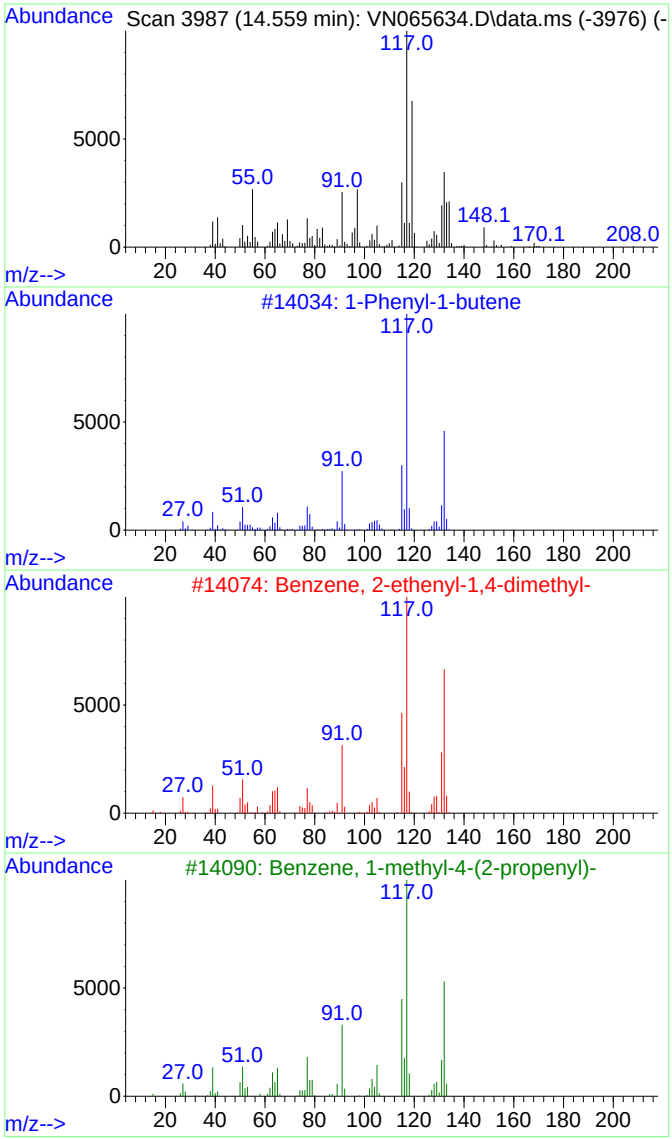
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

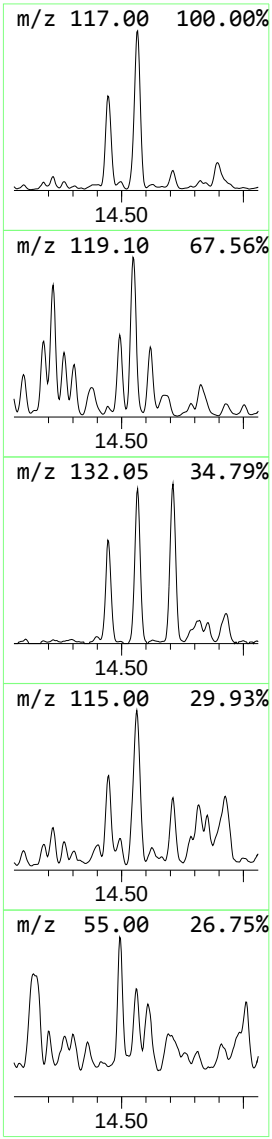
****

Peak Number 7 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.559	26.44 ug/l	609108	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	86
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	83
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	70
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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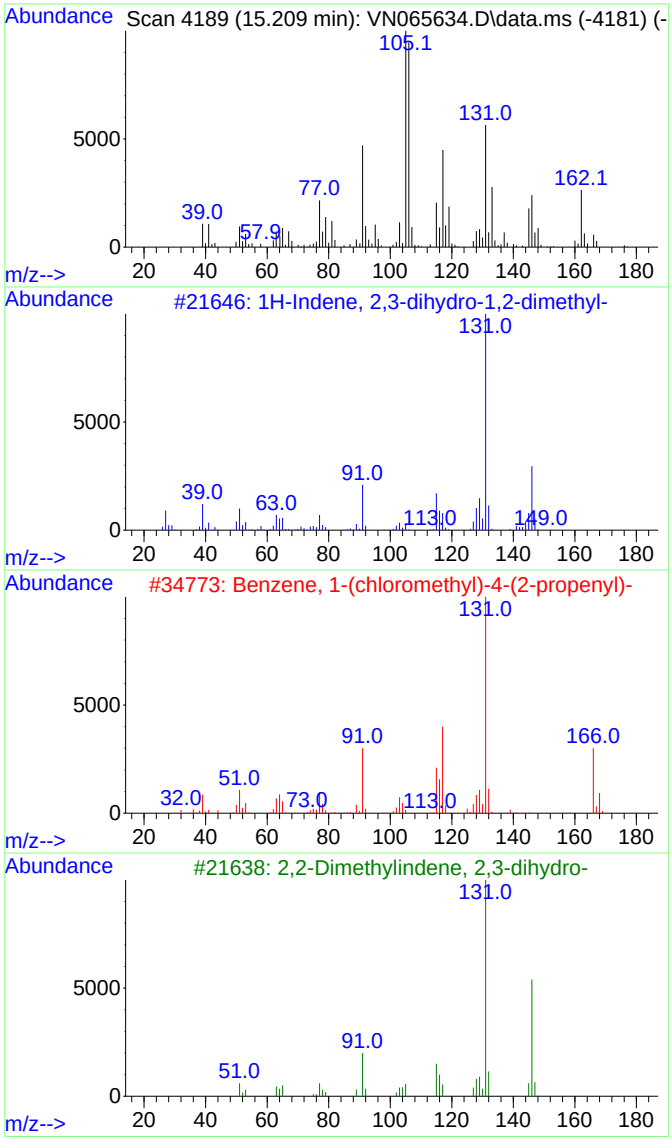
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

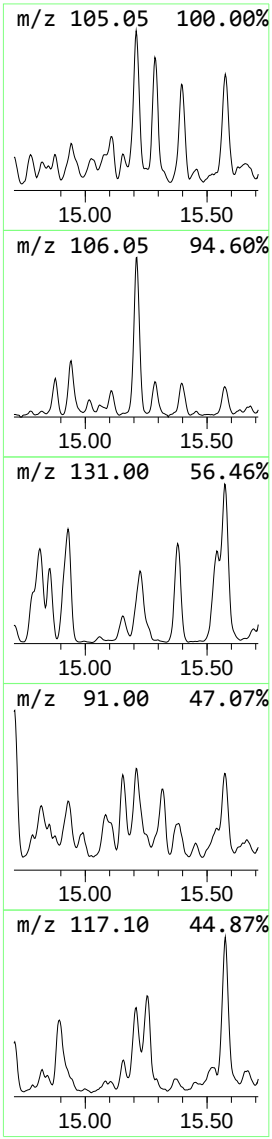
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.209	14.87 ug/l	342655	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	35
2	Benzene, 1-(chloromethyl)-4-(2-p...	166	C10H11Cl	036875-10-2	35
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	35
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	35
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	30





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Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

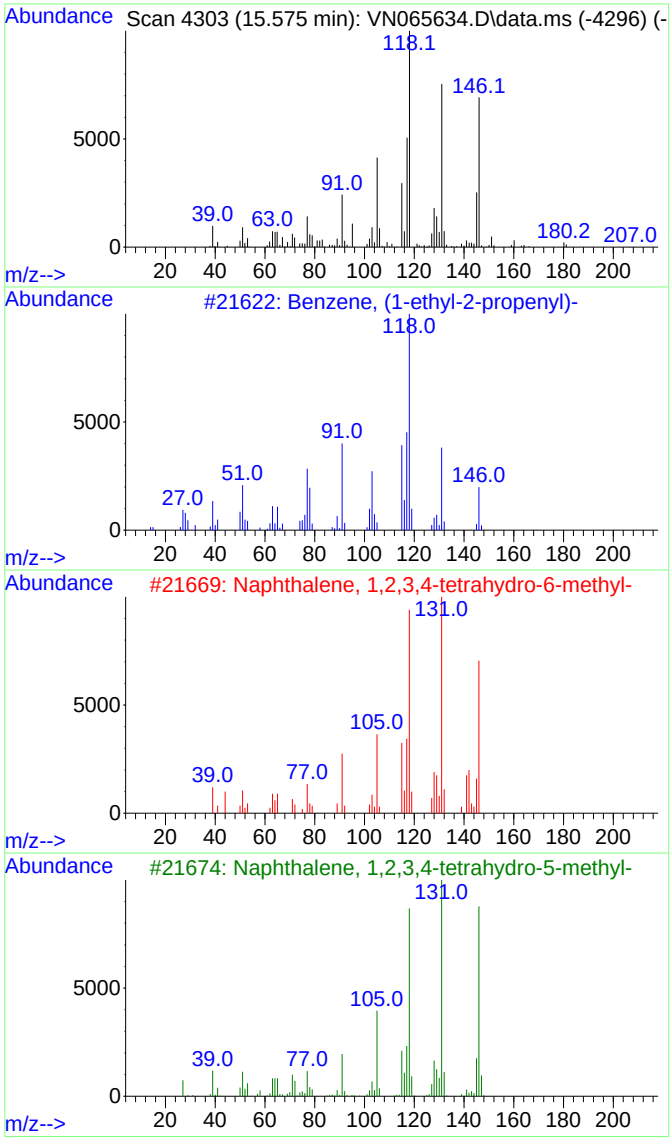
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

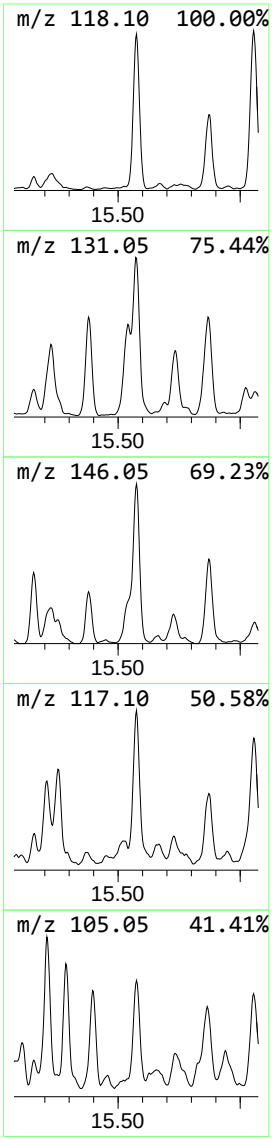
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-ethyl-2-propenyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.575	17.85 ug/l	411233	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	87
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	49
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NWB-1501ME

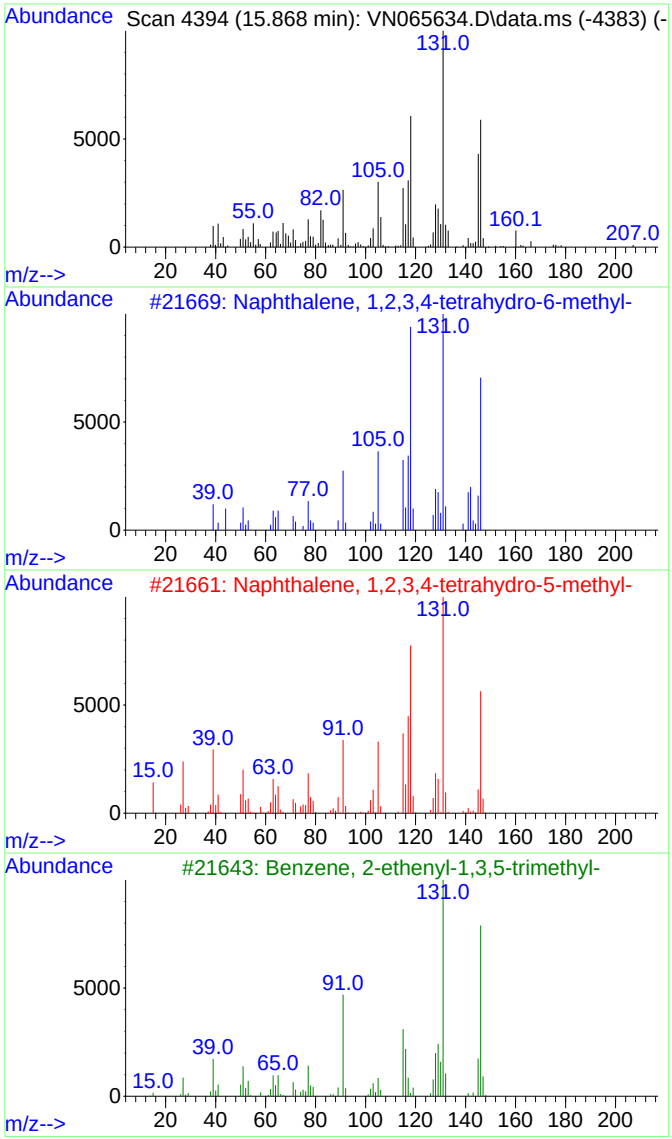
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

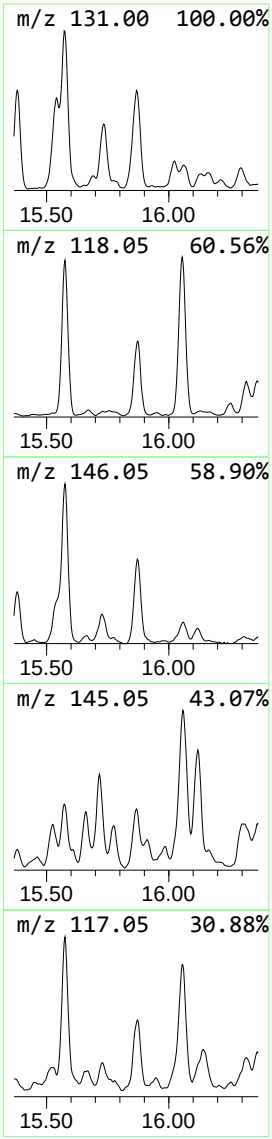
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	13.80 ug/l	317986	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	83
4	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	70
5	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065634.D
Acq On : 27 Jan 2021 17:01
Operator : JC/MD
Sample : M1230-01ME
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NWB-1501ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 3-methyl-	7.830	77.6	ug/l	1543020	1	7.621	993988	50.0
Heptane	8.392	166.8	ug/l	2762480	2	8.547	828186	50.0
1-Hexanol, 2-et...	13.421	17.4	ug/l	401692	4	13.315	1151900	50.0
Undecane	13.643	49.4	ug/l	1137050	4	13.315	1151900	50.0
Naphthalene, de...	14.132	16.3	ug/l	376100	4	13.315	1151900	50.0
Dodecane	14.492	37.4	ug/l	861812	4	13.315	1151900	50.0
1-Phenyl-1-butene	14.559	26.4	ug/l	609108	4	13.315	1151900	50.0
1H-Indene, 2,3-...	15.209	14.9	ug/l	342655	4	13.315	1151900	50.0
Benzene, (1-eth...	15.575	17.9	ug/l	411233	4	13.315	1151900	50.0
Naphthalene, 1,...	15.868	13.8	ug/l	317986	4	13.315	1151900	50.0