LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067295.D
Acq On : 11 Jun 2021 17:56
Operator : JC/MD
Sample : M2674-05
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-05-060921

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\82N061021W.M
Title : SW846 8260

Signal : TIC: VN067295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.848	1040	1066	1093	rBV2	154453	487972	4.19%	0.611%
2	8.016	2227	2247	2258	rBV3	288589	694306	5.96%	0.869%
3	8.080	2259	2271	2298	rVB2	544474	1255303	10.78%	1.572%
4	8.434	2385	2403	2427	rBV	371256	857601	7.36%	1.074%
5	8.965	2584	2601	2624	rBV	784956	1669725	14.34%	2.091%
6	10.443	3138	3152	3165	rBV	1222814	2297218	19.72%	2.876%
7	10.505	3167	3175	3190	rVB	280459	491489	4.22%	0.615%
8	11.746	3626	3638	3657	rVB	1172365	2133509	18.32%	2.671%
9	11.846	3666	3675	3687	rBV2	365387	588296	5.05%	0.737%
10	11.953	3704	3715	3737	rVB4	1360507	2636126	22.63%	3.300%
11	12.283	3828	3838	3852	rBV	680829	1172805	10.07%	1.468%
12	12.484	3905	3913	3934	rVB2	371403	617106	5.30%	0.773%
13	12.733	3996	4006	4027	rVB2	1243744	2229643	19.14%	2.792%
14	12.985	4091	4100	4116	rBV2	856034	2434008	20.90%	3.047%
15	13.224	4180	4189	4203	rVB	693428	1113235	9.56%	1.394%
16	13.369	4234	4243	4256	rVB	1696018	2674058	22.96%	3.348%
17	13.677	4348	4358	4364	rBV	1262620	2184542	18.76%	2.735%
18	13.994	4470	4476	4488	rVB	1248113	1788798	15.36%	2.240%
19	14.216	4552	4559	4570	rVB2	764795	1102778	9.47%	1.381%
20	14.326	4593	4600	4623	rVB4	830286	1468090	12.61%	1.838%
21	14.514	4661	4670	4687	rBV2	1016987	2057140	17.66%	2.576%
22	14.820	4773	4784	4789	rBV5	1998388	3519617	30.22%	4.407%
23	14.935	4810	4827	4839	rBV3	1454557	3909887	33.57%	4.895%
24	15.085	4874	4883	4899	rVB	1221050	2065846	17.74%	2.586%
25	15.453	5001	5020	5031	rBV2	3555451	9476172	81.36%	11.864%
26	15.587	5059	5070	5092	rBV	6239071	11646586	100.00%	14.582%
27	15.675	5095	5103	5110	rBV	1868297	2775897	23.83%	3.475%
28	16.445	5380	5390	5404	rVB3	2116261	4521381	38.82%	5.661%
29	16.523	5407	5419	5433	rBV	2419358	5667868	48.67%	7.096%
30	16.762	5496	5508	5518	rBV2	2023556	4334128	37.21%	5.426%

Sum of corrected areas: 79871130

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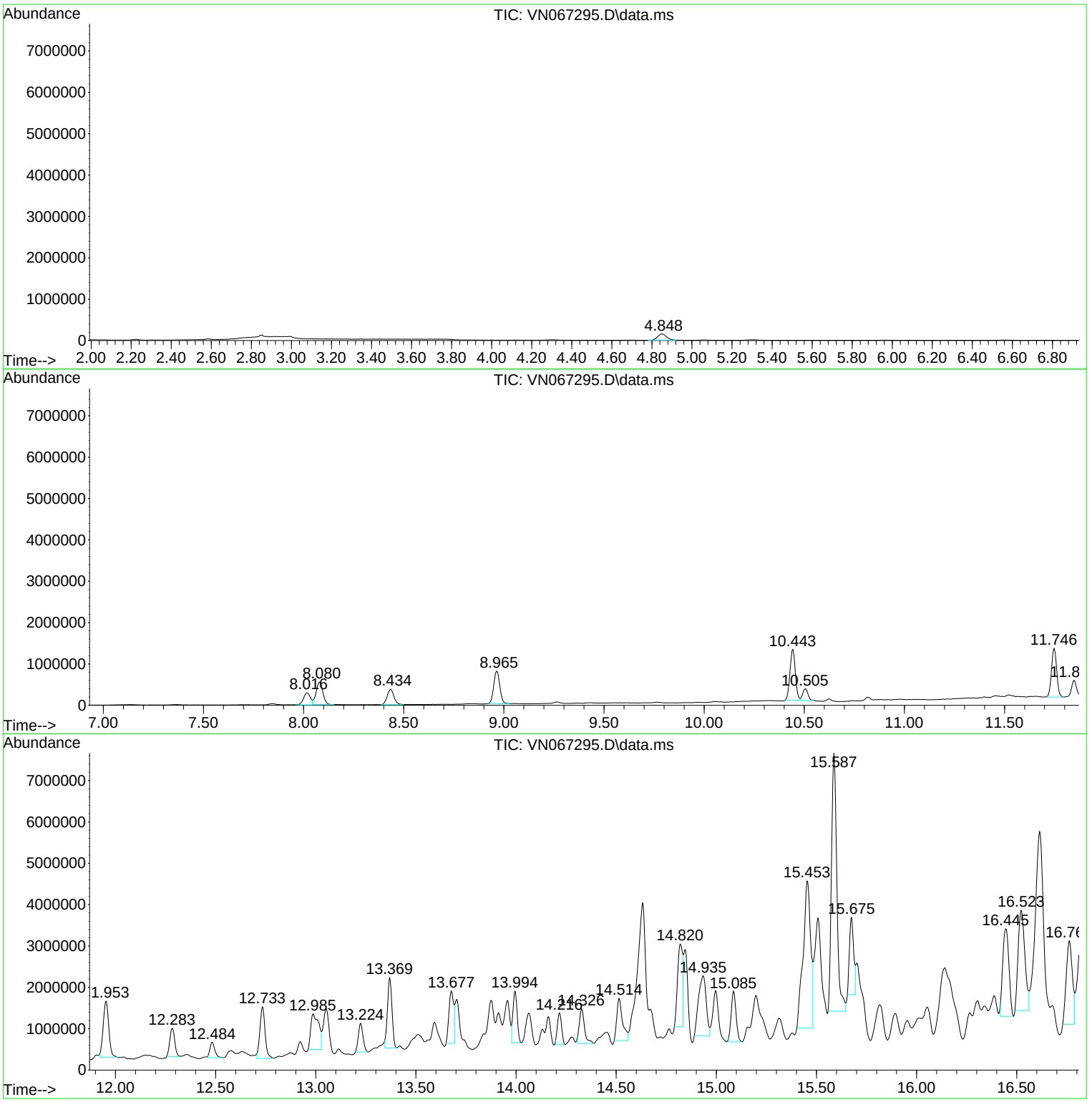
Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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



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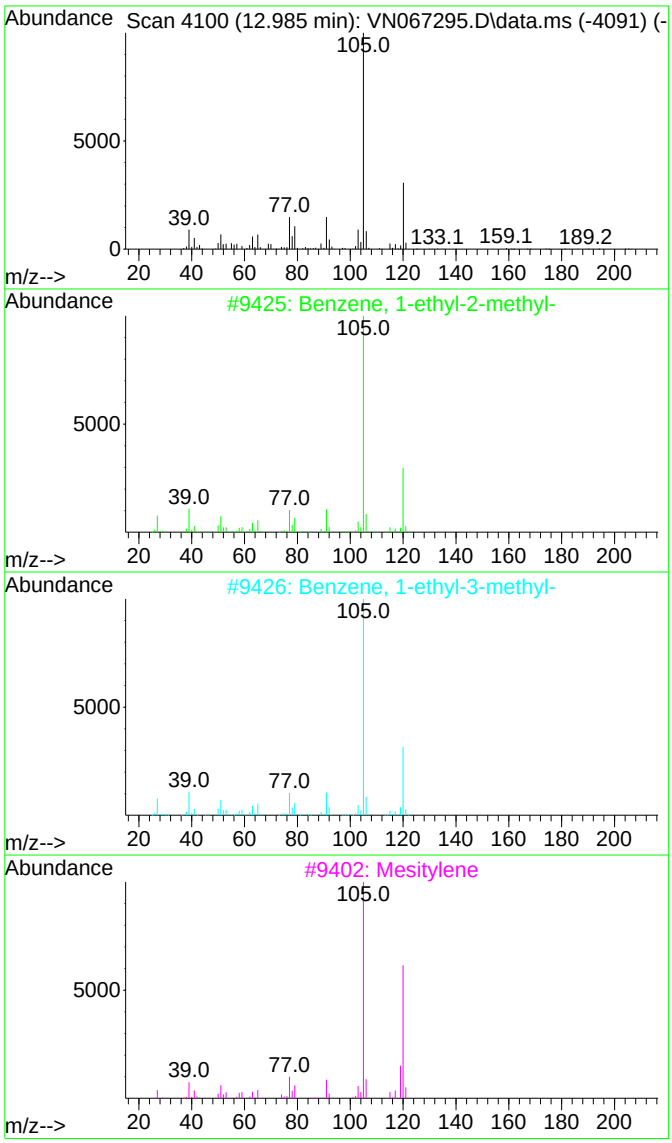
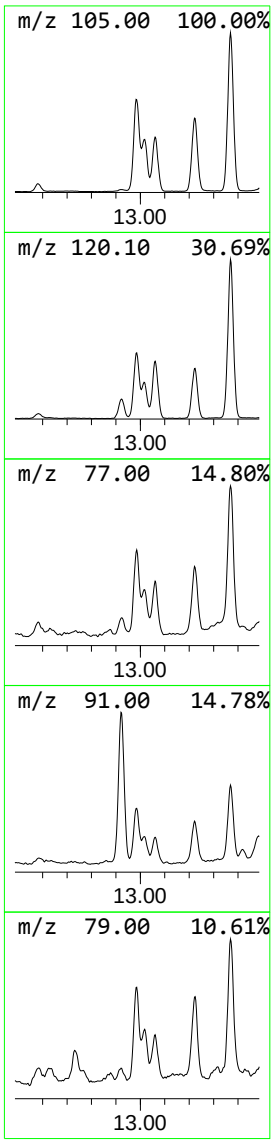
****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	55.71 ug/l	2434010	1,4-Dichlorobenzene-d4	13.677

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	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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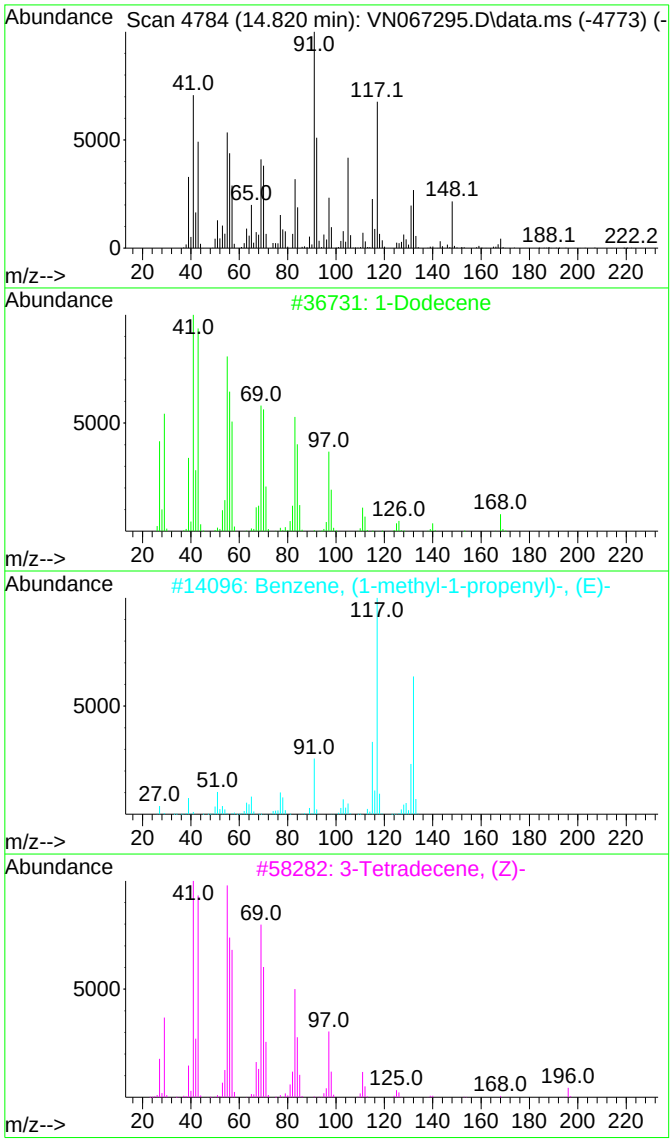
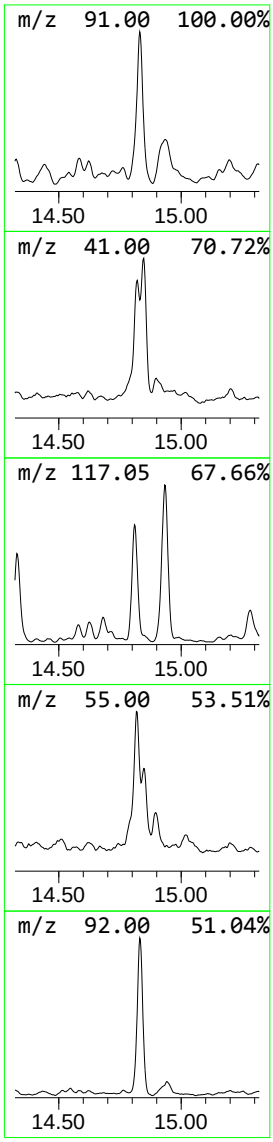
****
Peak Number 2 1-Dodecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.820	80.56 ug/l	3519620	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecene	168	C12H24	000112-41-4	50
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	47
3	3-Tetradecene, (Z)-	196	C14H28	041446-67-7	42
4	4-Dodecene, (E)-	168	C12H24	007206-15-7	38
5	6-Tridecene, (Z)-	182	C13H26	006508-77-6	38





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MSVOA_N
ClientSampleId :
TMR-DS-05-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

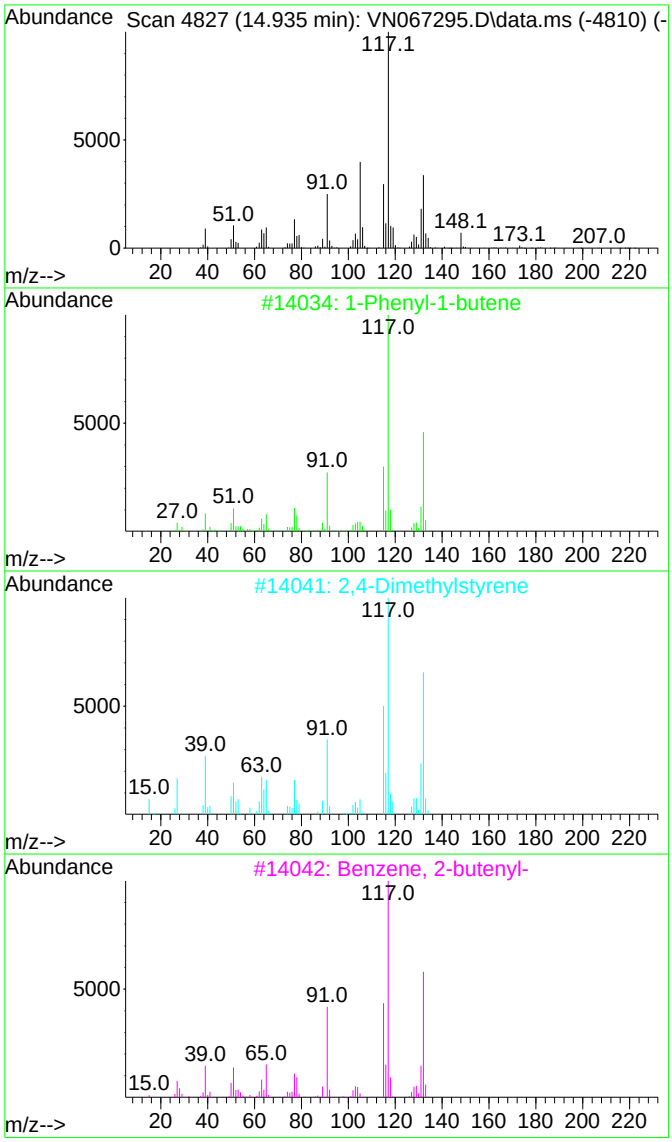
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

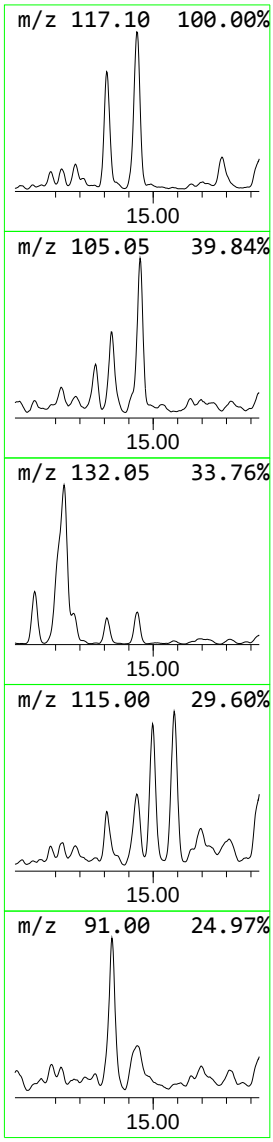
****

Peak Number 3 1-Phenyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	89.49 ug/l	3909890	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	92
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	90





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Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

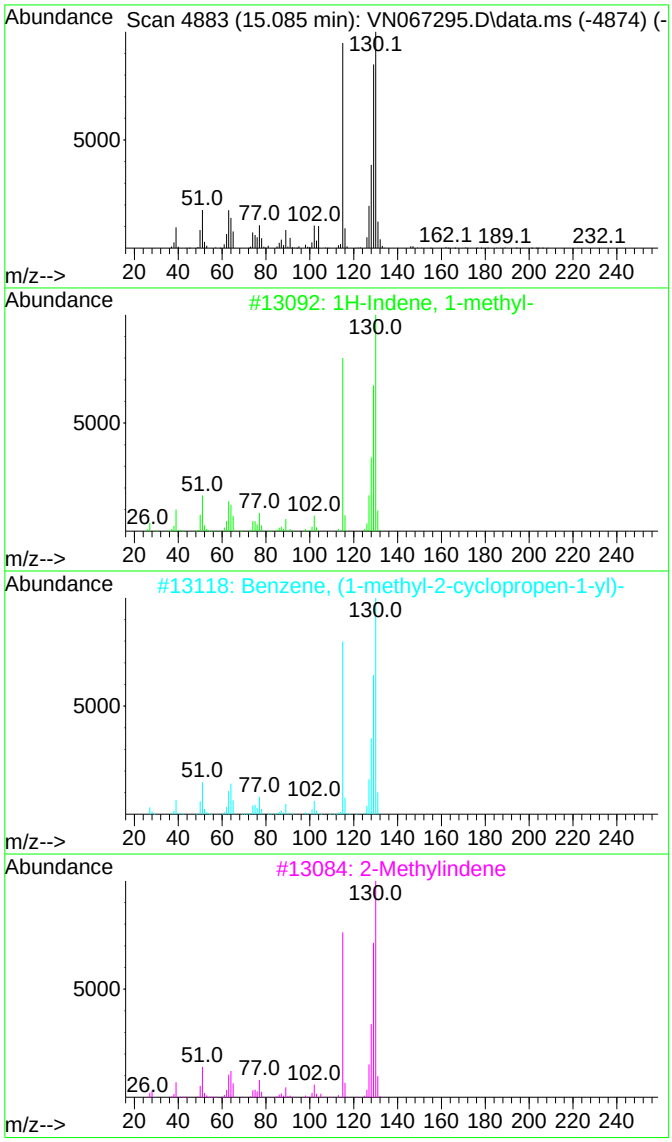
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

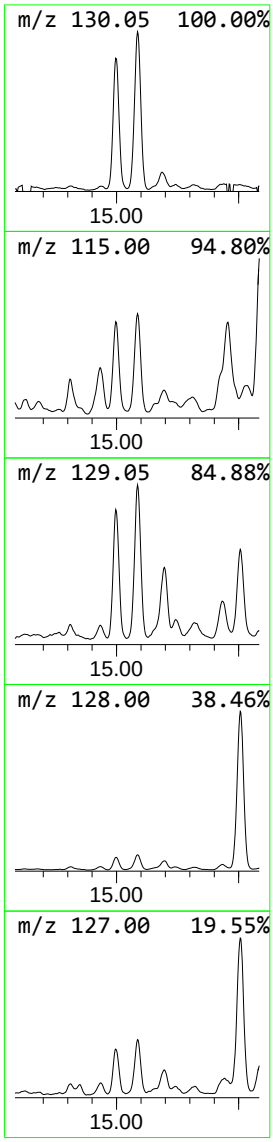
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.085	47.28 ug/l	2065850	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3	2-Methylindene	130	C10H10	002177-47-1	95
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93





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Instrument :
MSVOA_N
ClientSampleId :
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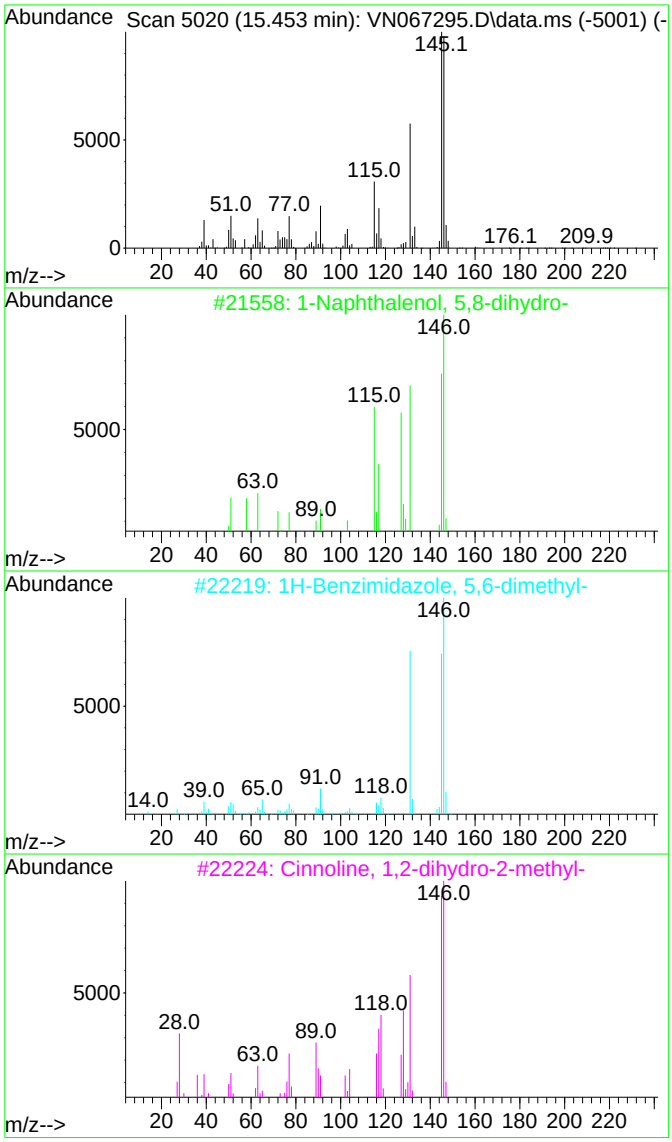
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

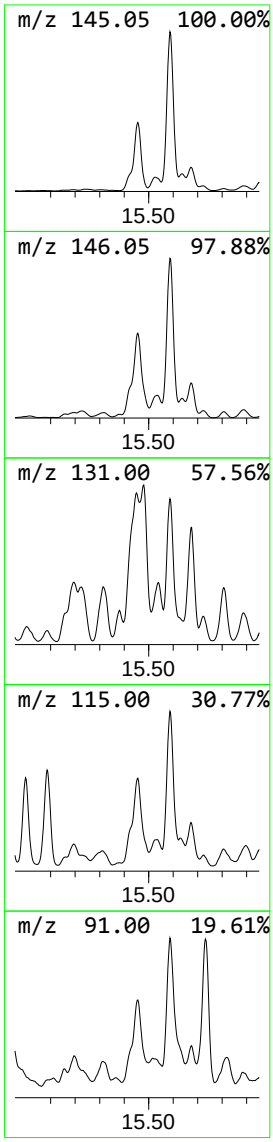
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Naphthalenol, 5,8-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	216.89 ug/l	9476170	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, 5,8-dihydro-	146	C10H10O	027673-48-9	76
2	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	72
3	Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	64
4	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	59
5	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	50





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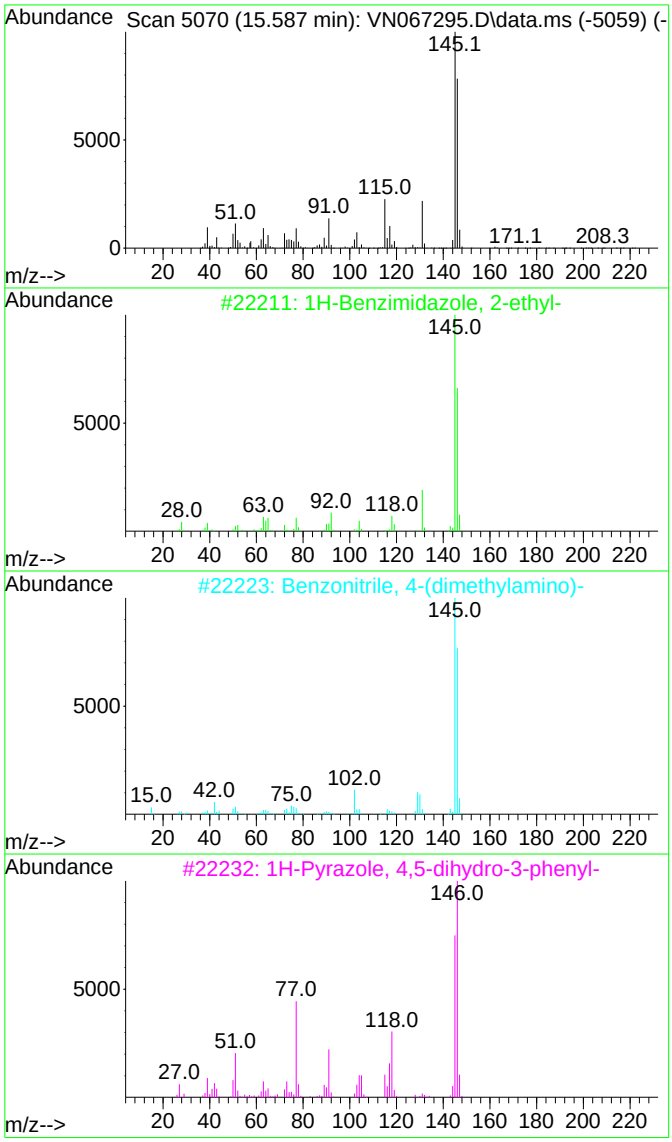
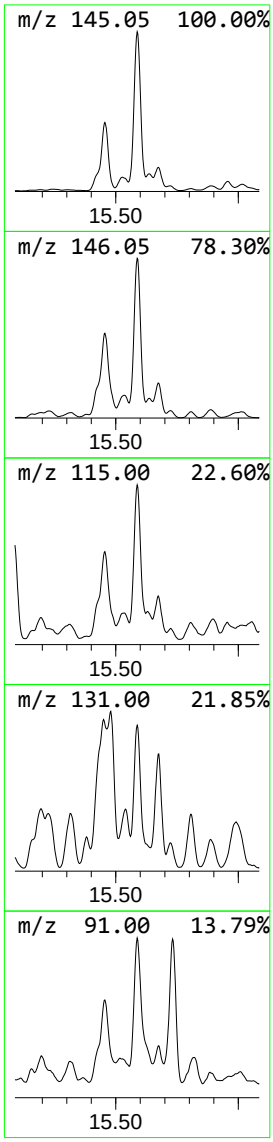
****
Peak Number 6 1H-Benzimidazole, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	266.57 ug/l	11646600	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	72
2	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
3	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	50
4	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	50
5	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	47





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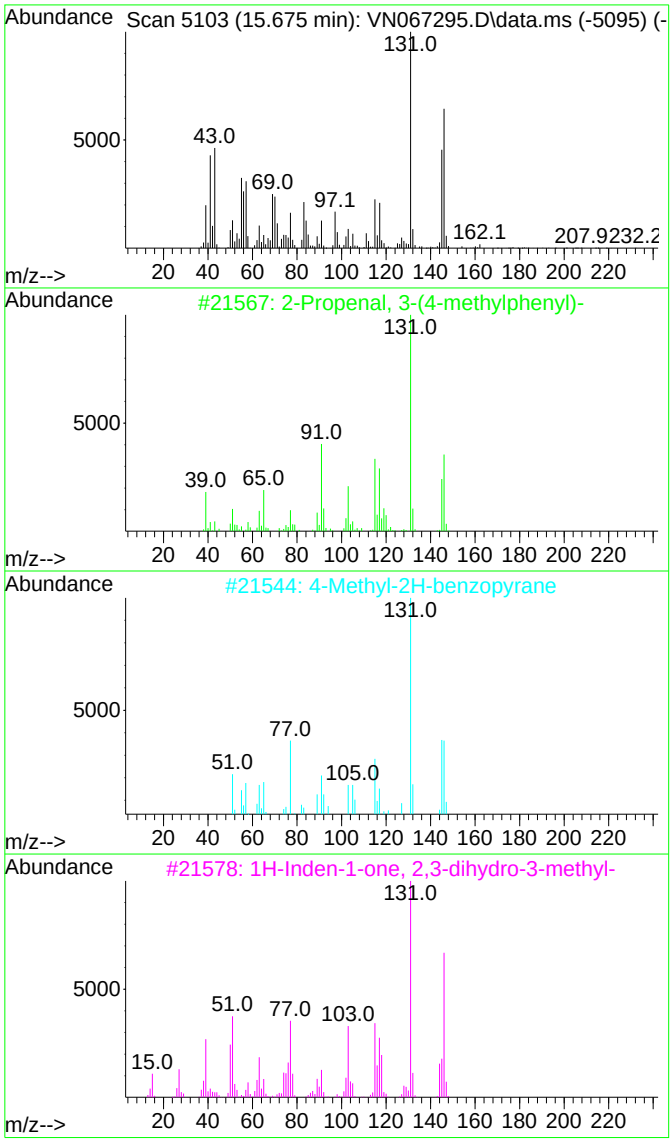
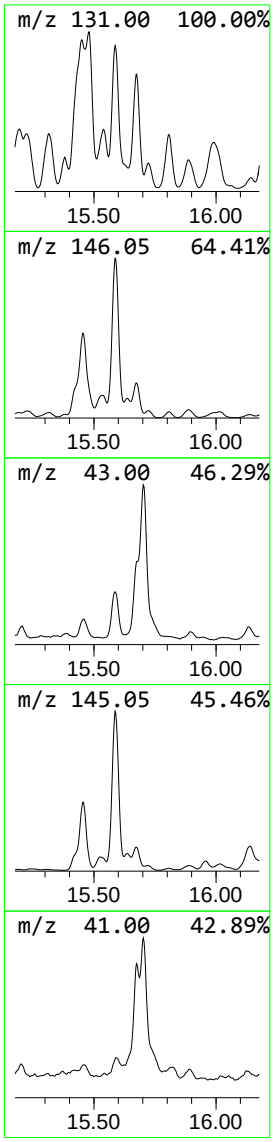
****
Peak Number 7 2-Propenal, 3-(4-methylphen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.676	63.53 ug/l	2775900	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	52
2	4-Methyl-2H-benzopyrane	146	C10H10O	021776-94-3	52
3	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	49
4	3-Buten-2-one, 4-phenyl-	146	C10H10O	000122-57-6	46
5	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	46





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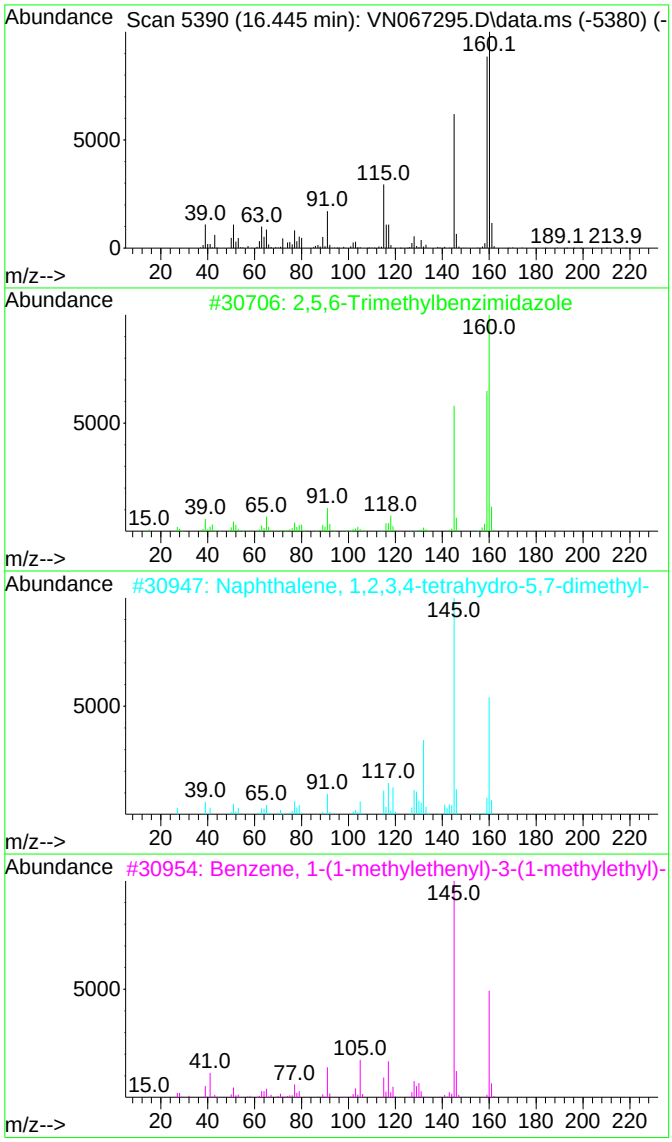
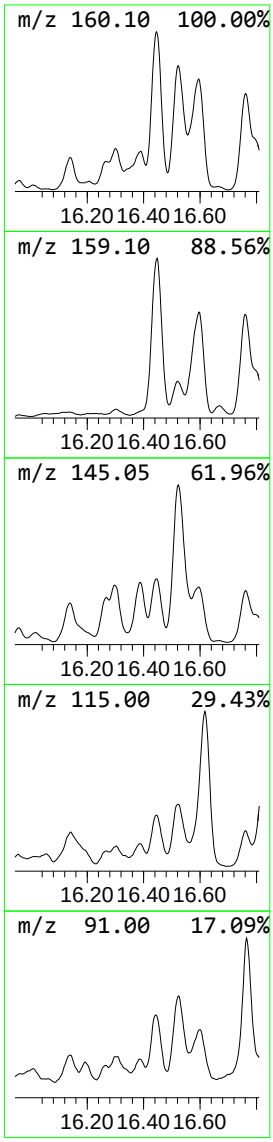
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,5,6-Trimethylbenzimidazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	103.49 ug/l	4521380	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,6-Trimethylbenzimidazole	160	C10H12N2	003363-56-2	72
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	49
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	43
4	Thiophene, 3-phenyl-	160	C10H8S	002404-87-7	38
5	Benzene, 1-(1-methylethenyl)-4-(...	160	C12H16	002388-14-9	38





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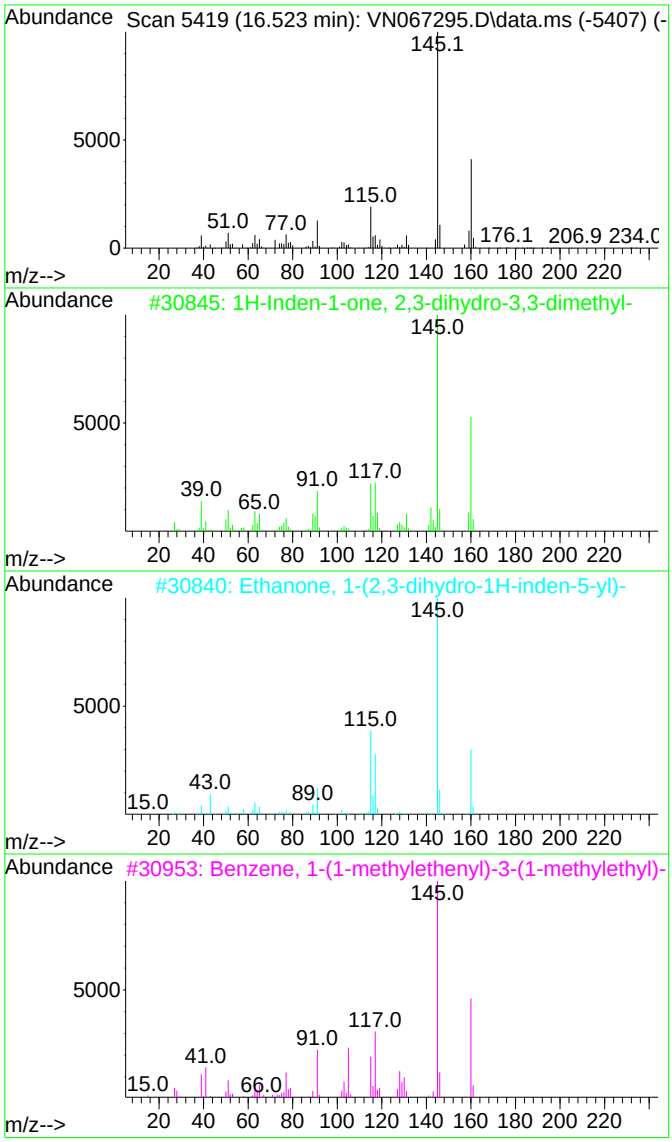
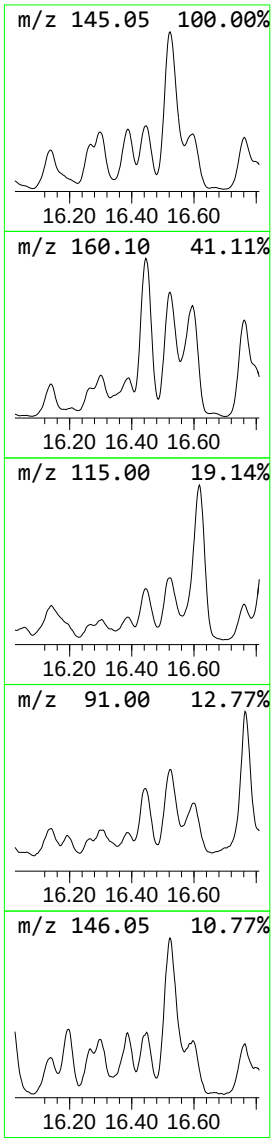
****
Peak Number 9 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.523	129.73 ug/l	5667870	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	90
2	Ethanone, 1-(2,3-dihydro-1H-inde...	160	C11H12O	004228-10-8	87
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	86
4	1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	80
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067295.D
Acq On : 11 Jun 2021 17:56
Operator : JC/MD
Sample : M2674-05
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

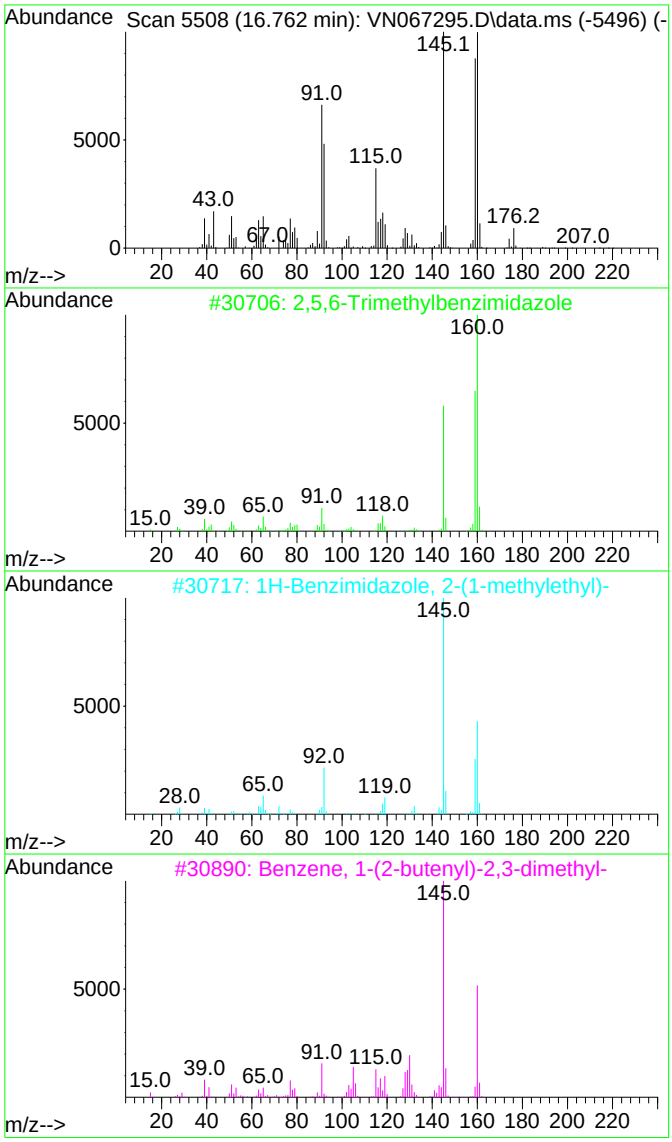
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

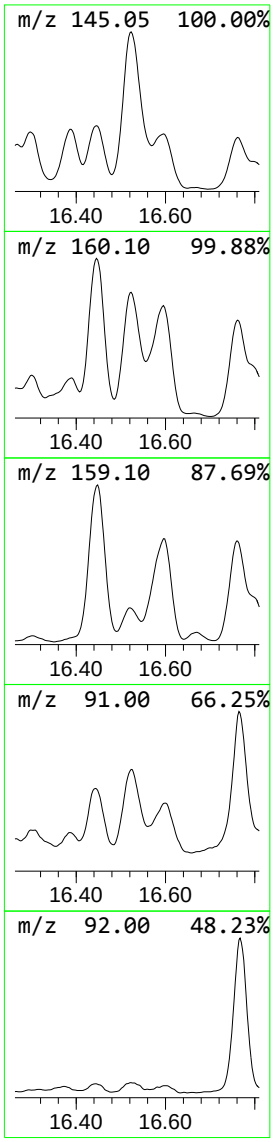
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Benzimidazole, 2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	99.20 ug/l	4334130	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,6-Trimethylbenzimidazole	160	C10H12N2	003363-56-2	90
2	1H-Benzimidazole, 2-(1-methyleth...	160	C10H12N2	005851-43-4	64
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	60
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	60
5	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067295.D
Acq On : 11 Jun 2021 17:56
Operator : JC/MD
Sample : M2674-05
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-05-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.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
Benzene, 1-ethy...	12.986	55.7	ug/l	2434010	4	13.677	2184540	50.0
1-Dodecene	14.820	80.6	ug/l	3519620	4	13.677	2184540	50.0
1-Phenyl-1-butene	14.935	89.5	ug/l	3909890	4	13.677	2184540	50.0
1H-Indene, 1-me...	15.085	47.3	ug/l	2065850	4	13.677	2184540	50.0
1-Naphthalenol,...	15.453	216.9	ug/l	9476170	4	13.677	2184540	50.0
1H-Benzimidazol...	15.587	266.6	ug/l	11646600	4	13.677	2184540	50.0
2-Propenal, 3-(...	15.676	63.5	ug/l	2775900	4	13.677	2184540	50.0
2,5,6-Trimethyl...	16.445	103.5	ug/l	4521380	4	13.677	2184540	50.0
1H-Inden-1-one,...	16.523	129.7	ug/l	5667870	4	13.677	2184540	50.0
1H-Benzimidazol...	16.762	99.2	ug/l	4334130	4	13.677	2184540	50.0