LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-04-060921

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: VN067288.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.856	1051	1069	1092	rVB2	17709	57400	1.91%	0.153%
2	8.021	2229	2249	2260	rBV2	320524	760528	25.26%	2.028%
3	8.086	2261	2273	2298	rVB2	581569	1338305	44.45%	3.569%
4	8.437	2385	2404	2428	rBV2	386917	923682	30.68%	2.463%
5	8.968	2582	2602	2635	rBV	862516	1832823	60.88%	4.887%
6	9.271	2700	2715	2731	rVB3	53426	105632	3.51%	0.282%
7	10.443	3134	3152	3165	rBV	1366940	2551469	84.75%	6.803%
8	10.507	3166	3176	3204	rVB	340736	690719	22.94%	1.842%
9	10.623	3214	3219	3237	rVB7	23625	46191	1.53%	0.123%
10	10.816	3279	3291	3303	rBV2	108894	186584	6.20%	0.498%
11	11.521	3548	3554	3569	rVB2	38135	60729	2.02%	0.162%
12	11.746	3623	3638	3660	rBV	1271479	2264508	75.22%	6.038%
13	11.846	3663	3675	3689	rVV	318103	547742	18.19%	1.461%
14	11.950	3690	3714	3738	rVB2	938153	1952784	64.86%	5.207%
15	12.283	3825	3838	3855	rVB	491272	881574	29.28%	2.351%
16	12.484	3905	3913	3929	rBV5	54932	104353	3.47%	0.278%
17	12.733	3991	4006	4027	rVB	1117752	1993900	66.23%	5.317%
18	12.873	4044	4058	4066	rBV7	66420	140562	4.67%	0.375%
19	12.921	4066	4076	4088	rBV	199732	323524	10.75%	0.863%
20	12.986	4089	4100	4107	rBV	447787	789781	26.23%	2.106%
21	13.222	4177	4188	4203	rVB	290029	498146	16.55%	1.328%
22	13.369	4233	4243	4255	rVB	743567	1182350	39.27%	3.153%
23	13.594	4318	4327	4343	rVB2	302506	561617	18.65%	1.498%
24	13.675	4345	4357	4379	rBV3	1292113	3010710	100.00%	8.028%
25	13.873	4425	4431	4441	rVB2	275321	376171	12.49%	1.003%
26	13.994	4471	4476	4488	rVB4	179721	250968	8.34%	0.669%
27	14.061	4489	4501	4516	rVB3	330026	643518	21.37%	1.716%
28	14.136	4519	4529	4532	rBV3	118211	175176	5.82%	0.467%
29	14.217	4550	4559	4569	rVB2	226876	365058	12.13%	0.973%
30	14.326	4592	4600	4625	rVB4	243426	546850	18.16%	1.458%
31	14.439	4633	4642	4658	rVB7	150938	346219	11.50%	0.923%
32	14.514	4659	4670	4680	rBV2	360642	645528	21.44%	1.721%
33	14.815	4771	4782	4791	rBV4	376179	789464	26.22%	2.105%
34	14.933	4809	4826	4839	rBV4	352807	956554	31.77%	2.551%
35	14.997	4841	4850	4869	rVB2	490179	877732	29.15%	2.340%
36	15.085	4872	4883	4900	rVB	433215	792120	26.31%	2.112%

LSC Area Percent Report

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Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-04-060921

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

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

37	15.453	4999	5020	5029	rBV	740085	1908794	63.40%	5.090%
38	15.587	5058	5070	5083	rBV	1235141	2215445	73.59%	5.907%
39	15.673	5095	5102	5112	rVB2	278901	372980	12.39%	0.995%
40	16.443	5380	5389	5404	rVB3	269470	564266	18.74%	1.505%
41	16.520	5408	5418	5432	rVB2	289721	585983	19.46%	1.562%
42	16.614	5443	5453	5474	rVB3	754862	1755851	58.32%	4.682%
43	16.759	5496	5507	5518	rBV3	241798	528829	17.56%	1.410%

Sum of corrected areas: 37503119

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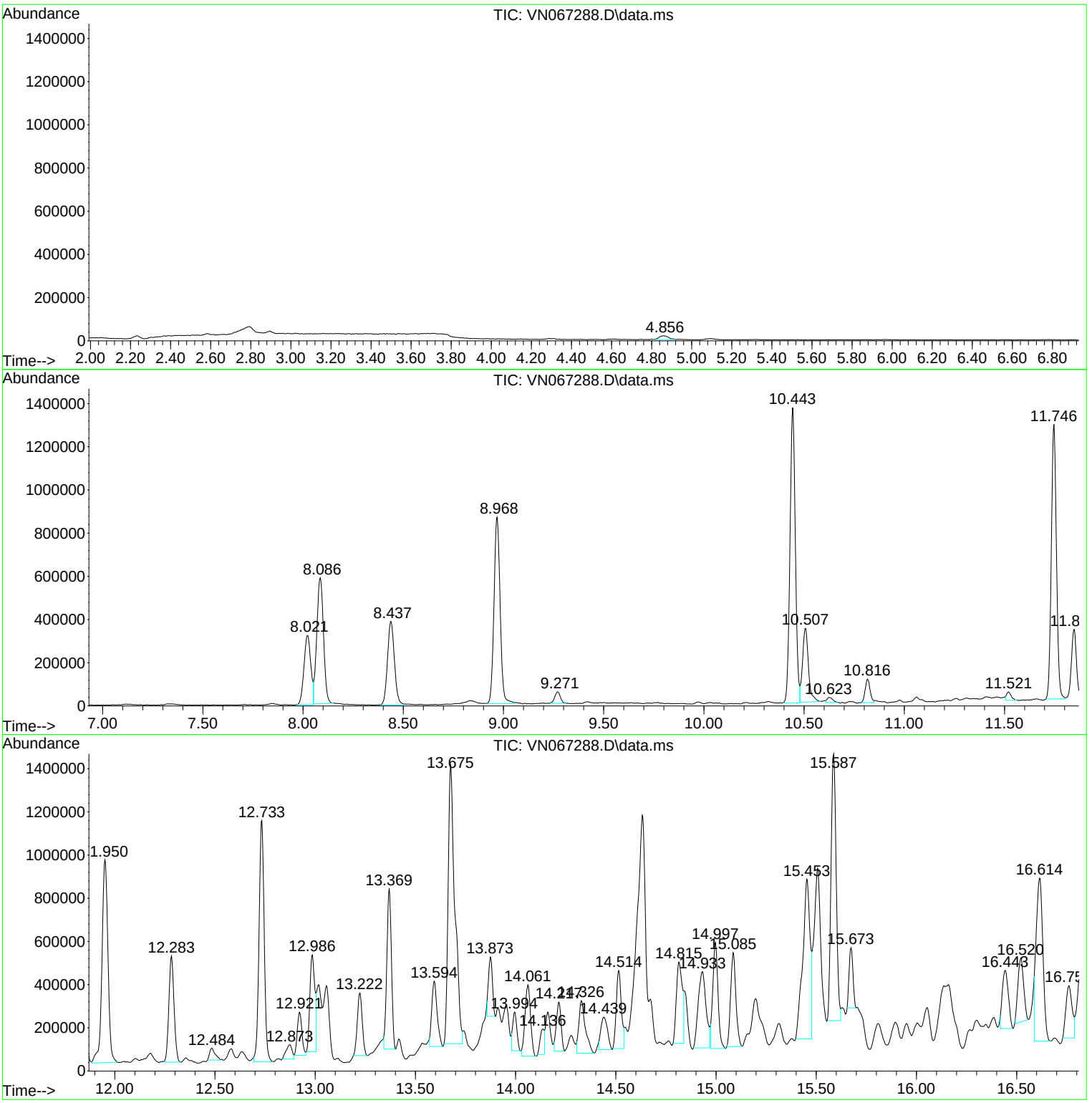
Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

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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Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

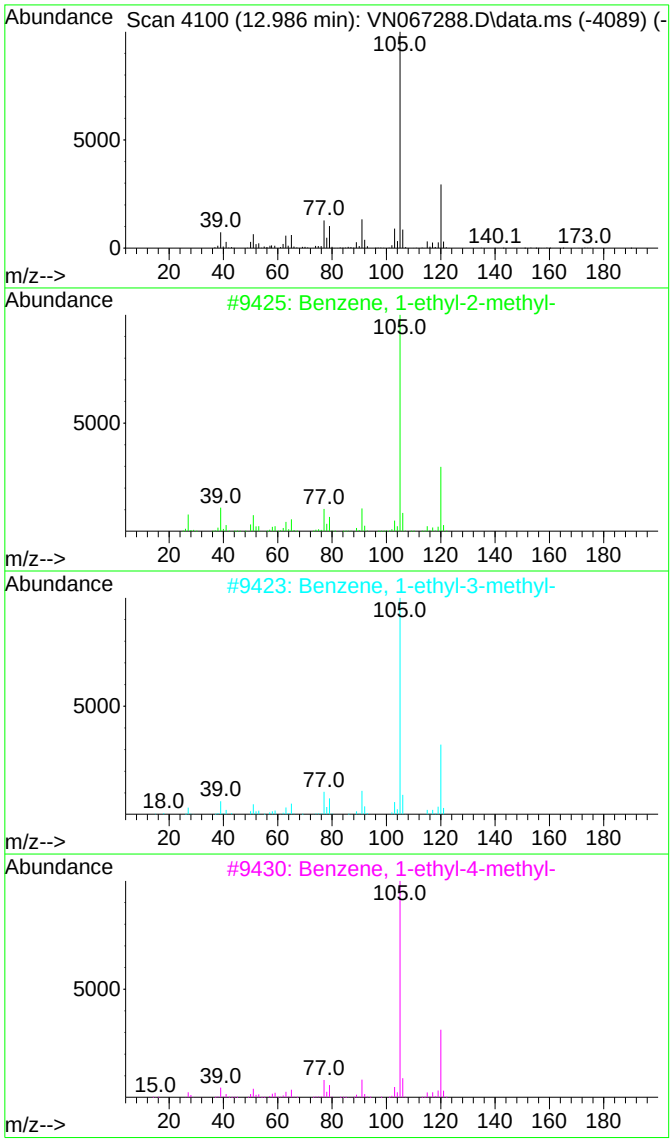
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

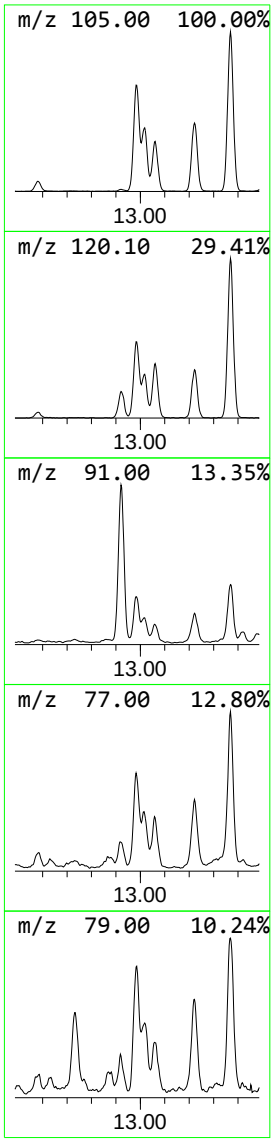
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	13.12 ug/l	789781	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	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Data File : VN067288.D
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Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

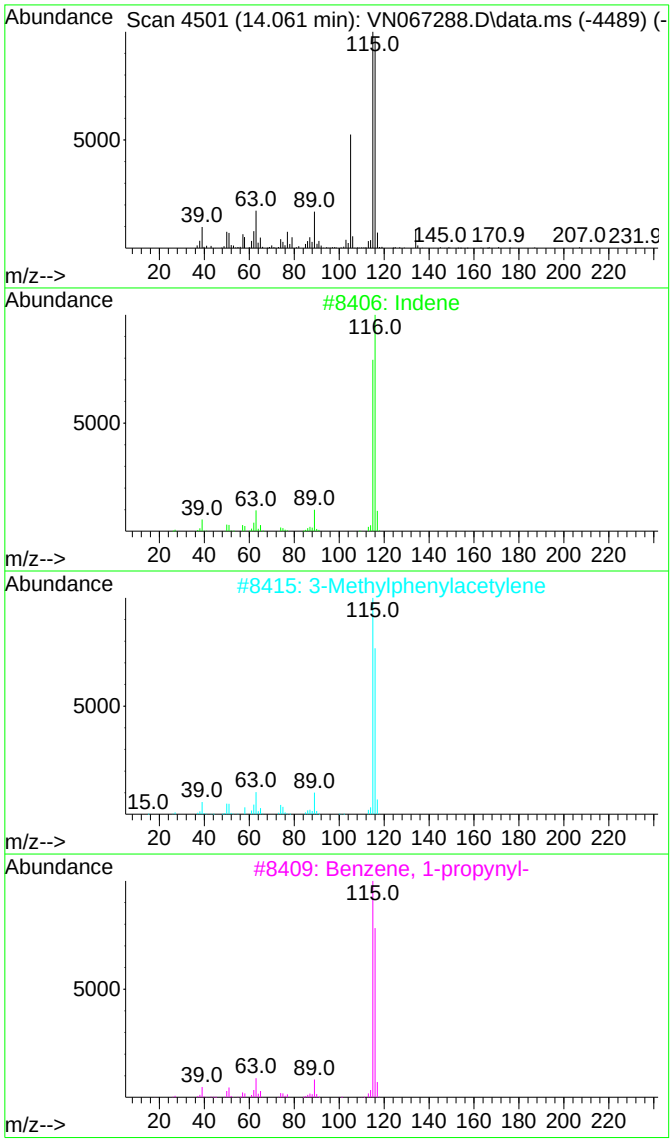
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

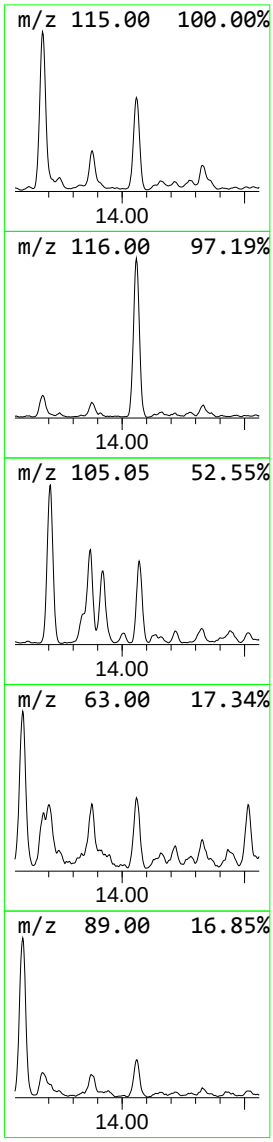
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Indene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.061	10.69 ug/l	643518	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	92
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	87
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	87
4	2-Methylphenylacetylene	116	C9H8	000766-47-2	83
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

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

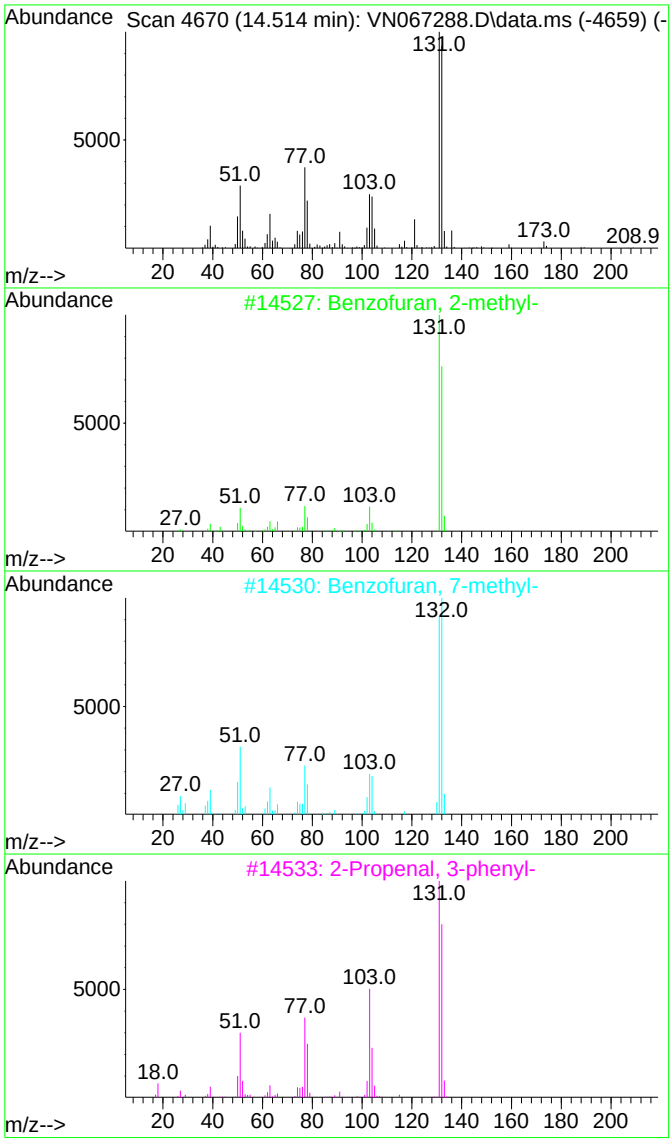
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

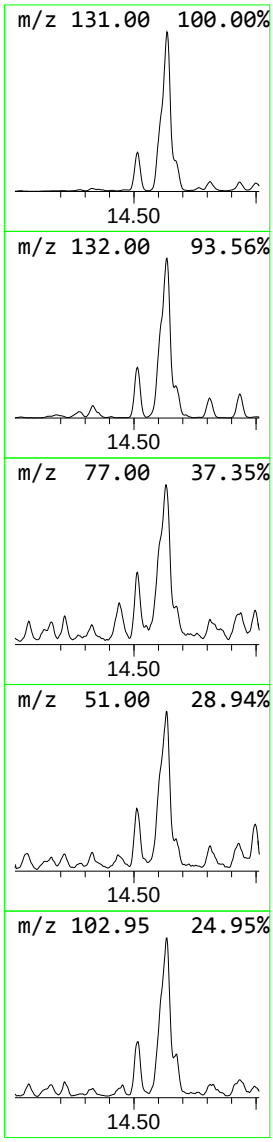
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.514	10.72 ug/l	645528	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	94
3	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	93
4	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	87
5	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	74





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Data File : VN067288.D
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Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

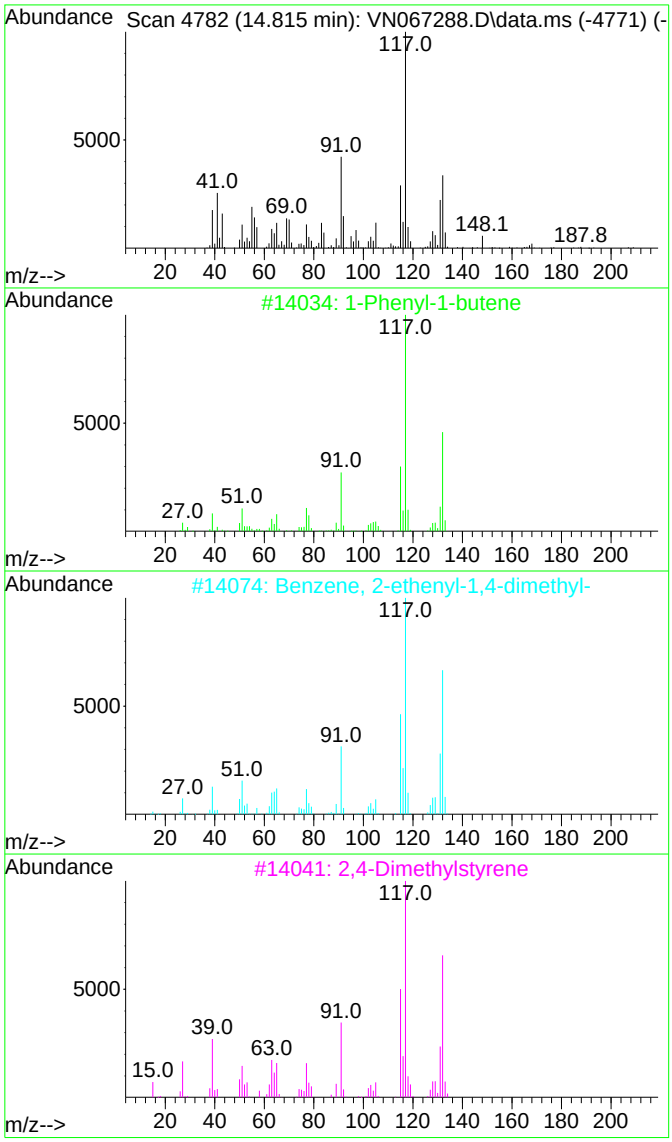
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

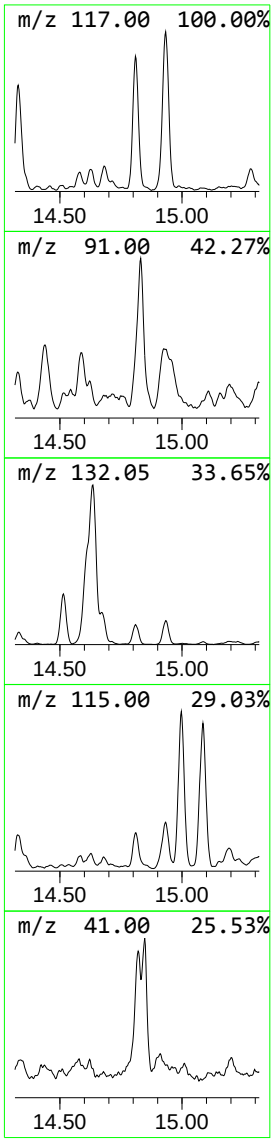
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	13.11 ug/l	789464	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3	2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90





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Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
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TIC Library : C:\DATABASE\NIST11.L
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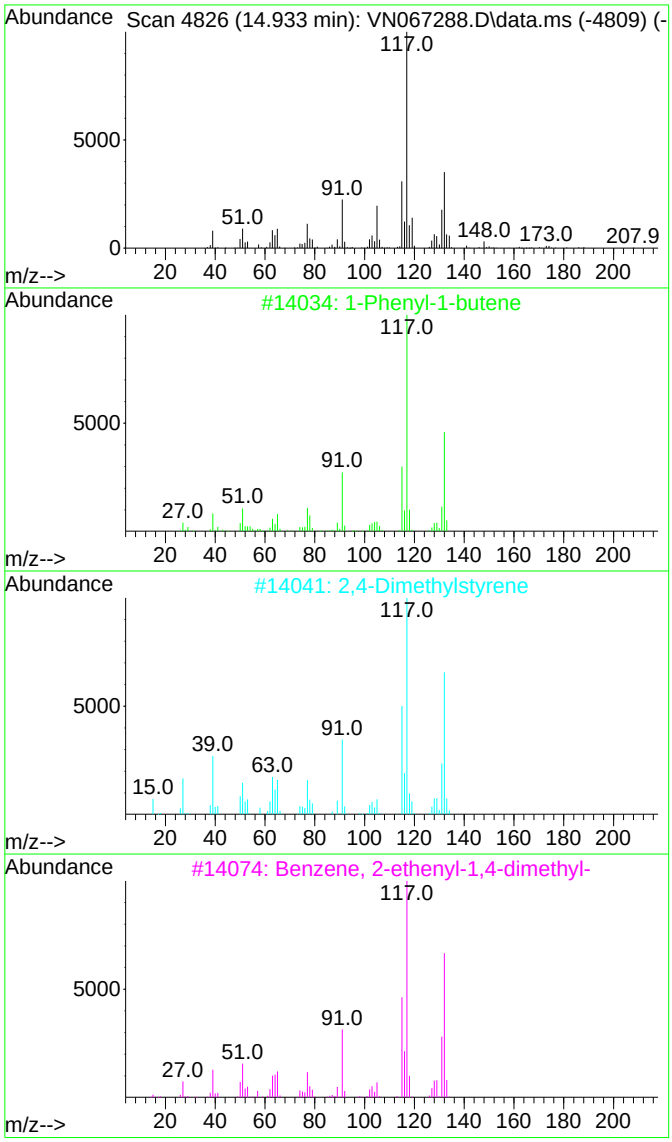
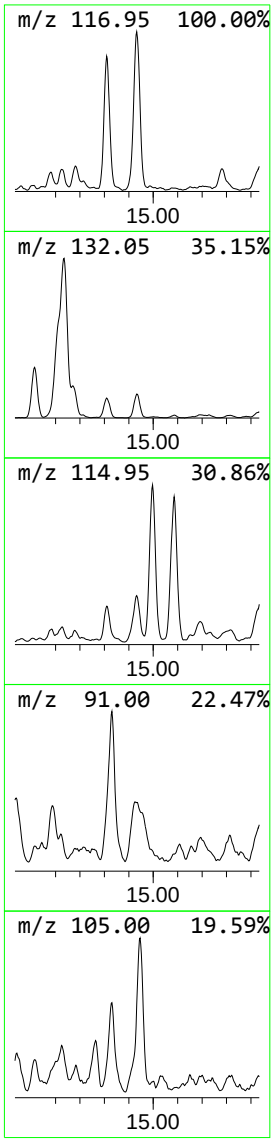
****
Peak Number 5 2,4-Dimethylstyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	15.89 ug/l	956554	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	96
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	93
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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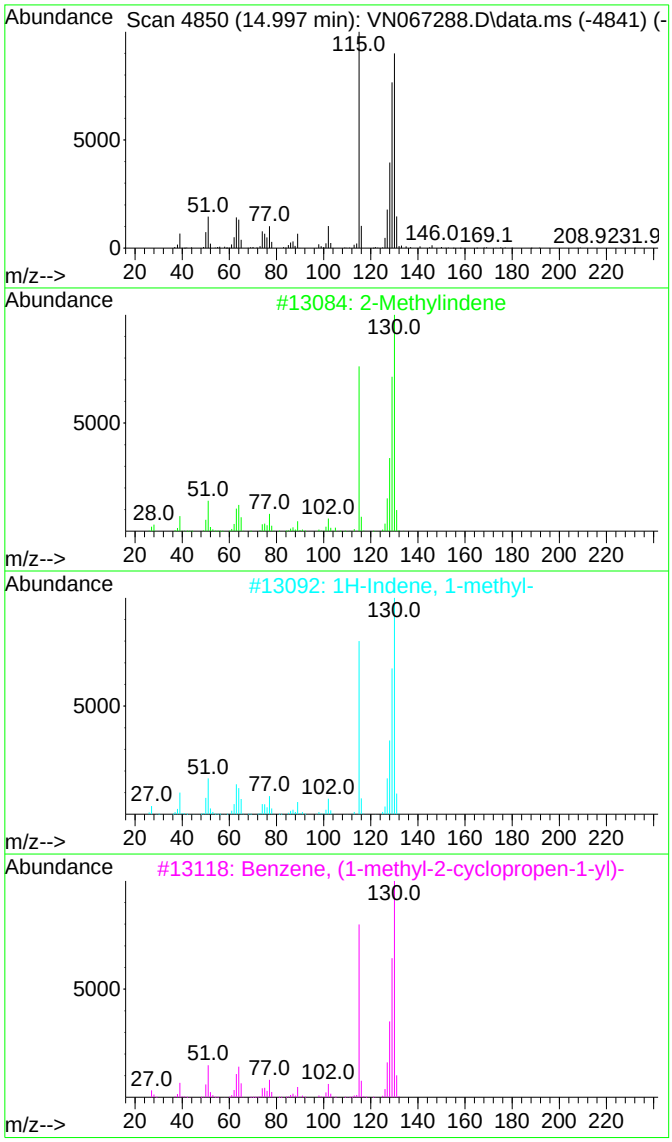
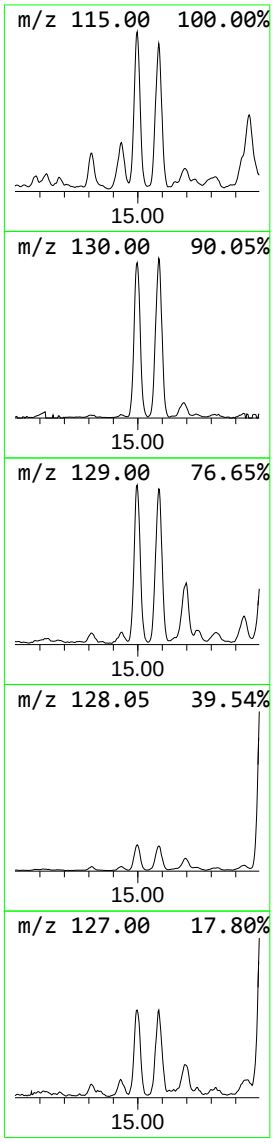
****
Peak Number 6 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	14.58 ug/l	877732	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	97
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
4	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	92





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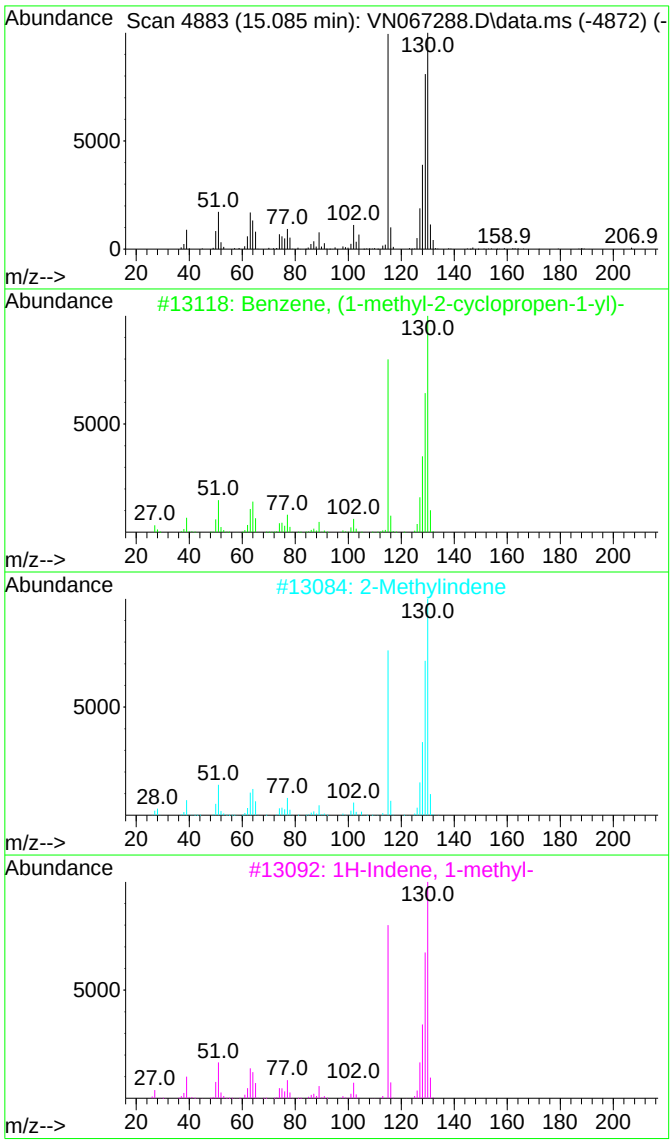
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

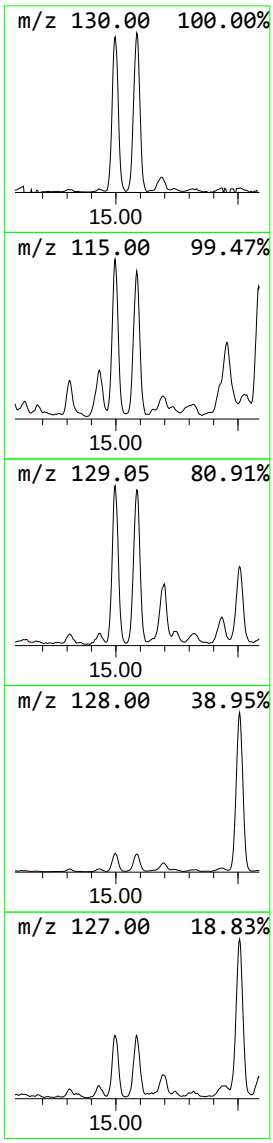
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (1-methyl-2-cyclop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	13.15 ug/l	792120	1,4-Dichlorobenzene-d4	13.675

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
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Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

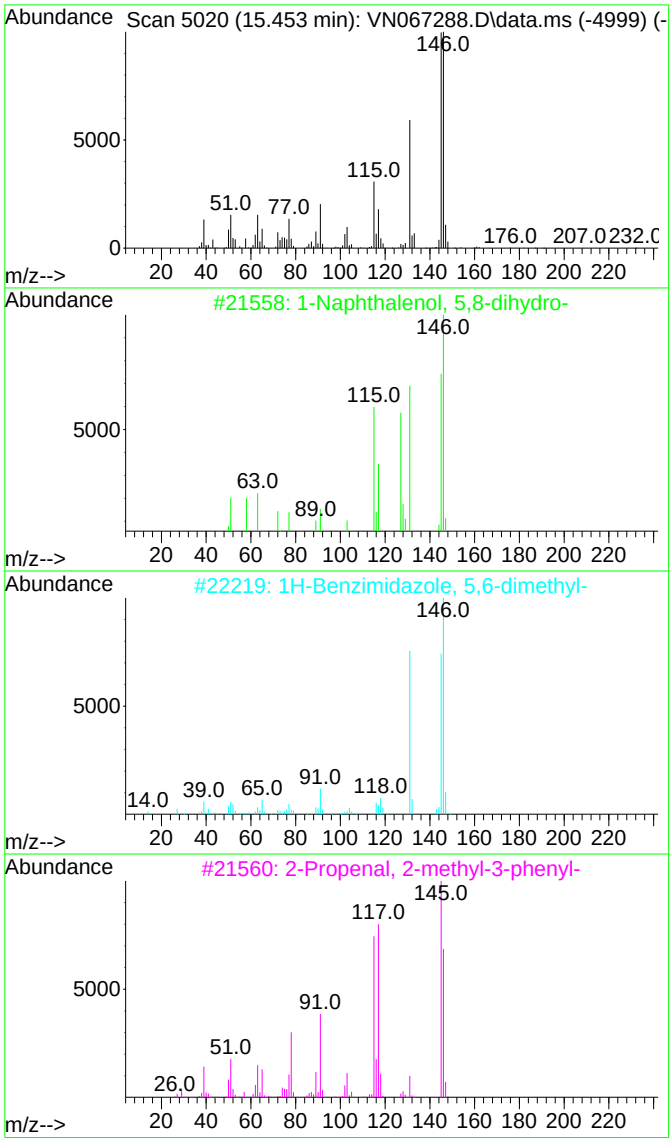
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

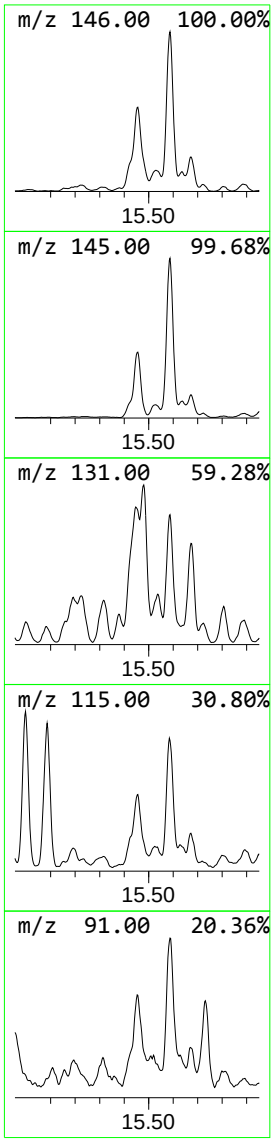
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	31.70 ug/l	1908790	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, 5,8-dihydro-	146	C10H10O	027673-48-9	87
2	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	83
3	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	64
4	Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	64
5	3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	53





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Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

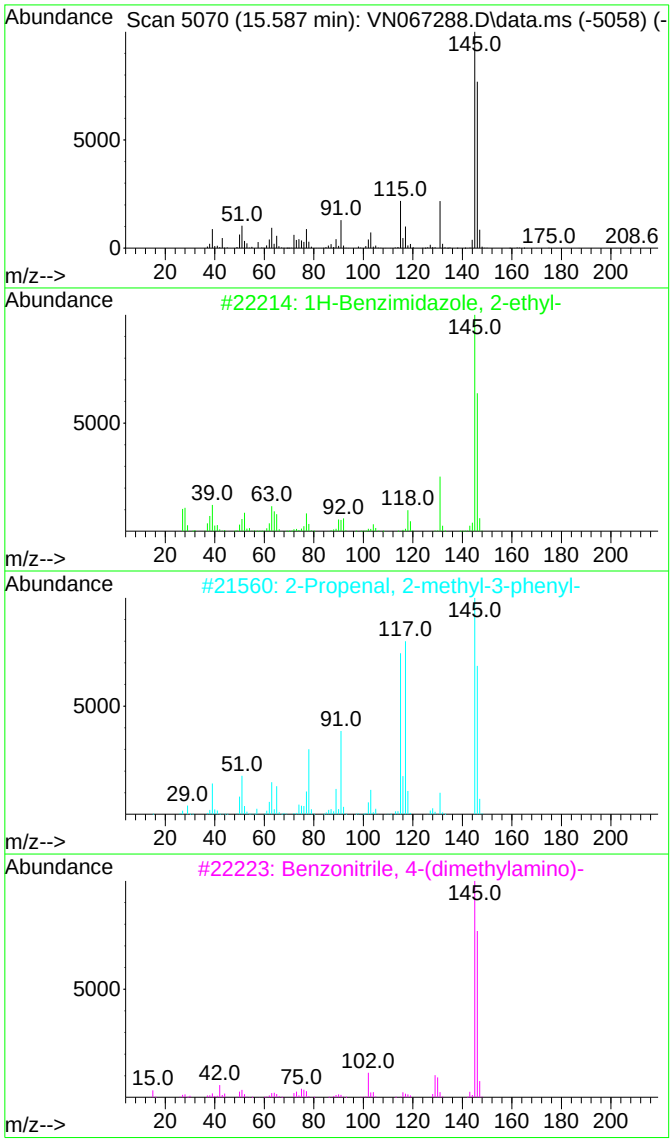
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

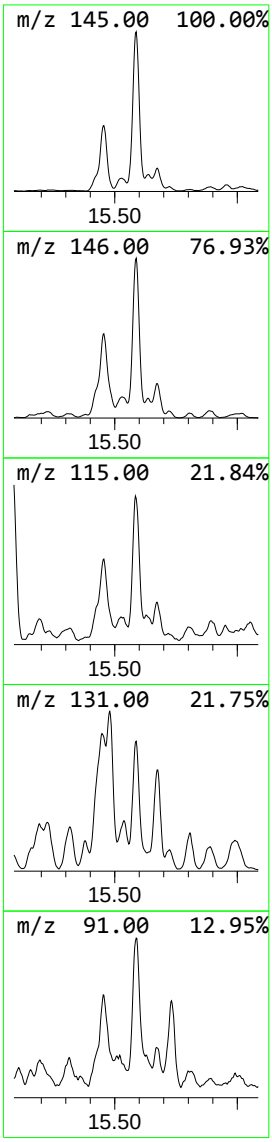
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Benzimidazole, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	36.79 ug/l	2215450	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	72
2	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	72
3	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
4	1H-Benzimidazole, 2,5-dimethyl-	146	C9H10N2	001792-41-2	47
5	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

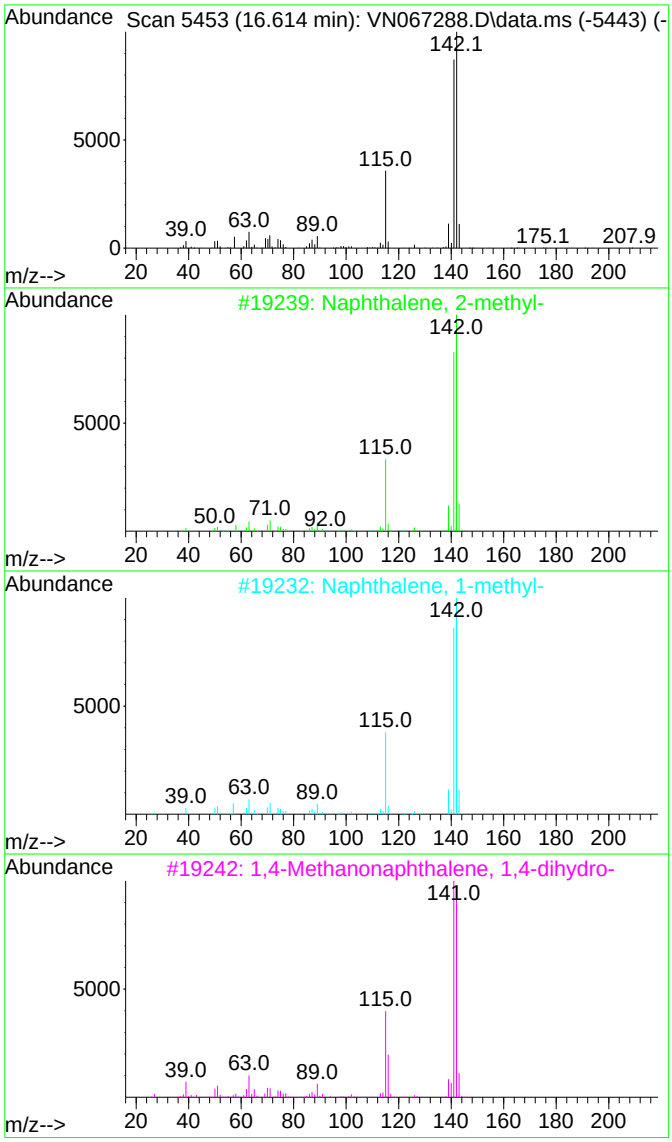
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

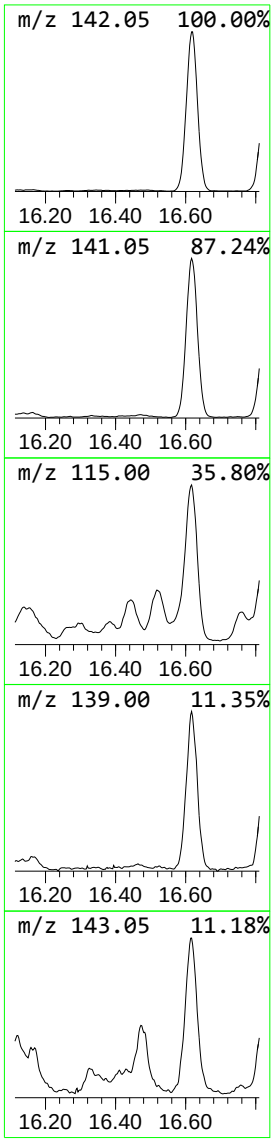
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	29.16 ug/l	1755850	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067288.D
Acq On : 11 Jun 2021 15:06
Operator : JC/MD
Sample : M2674-04 10X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-04-060921

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	13.1	ug/l	789781	4	13.675	3010710	50.0
Indene	14.061	10.7	ug/l	643518	4	13.675	3010710	50.0
Benzofuran, 2-m...	14.514	10.7	ug/l	645528	4	13.675	3010710	50.0
1-Phenyl-1-butene	14.815	13.1	ug/l	789464	4	13.675	3010710	50.0
2,4-Dimethylsty...	14.933	15.9	ug/l	956554	4	13.675	3010710	50.0
2-Methylindene	14.997	14.6	ug/l	877732	4	13.675	3010710	50.0
Benzene, (1-met...	15.086	13.2	ug/l	792120	4	13.675	3010710	50.0
1-Naphthalenol,...	15.453	31.7	ug/l	1908790	4	13.675	3010710	50.0
1H-Benzimidazol...	15.587	36.8	ug/l	2215450	4	13.675	3010710	50.0
Naphthalene, 1-...	16.614	29.2	ug/l	1755850	4	13.675	3010710	50.0