LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-03-060921

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: VN067287.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	1047	1069	1090	rBV2	63797	196436	6.16%	0.482%
2	7.345	1979	1997	2021	rBV2	41165	111790	3.51%	0.274%
3	7.702	2113	2130	2145	rBV2	22154	56075	1.76%	0.138%
4	7.844	2167	2183	2194	rBV6	17502	40857	1.28%	0.100%
5	8.021	2223	2249	2260	rBV	318284	773843	24.27%	1.898%
6	8.086	2261	2273	2306	rVB2	594815	1389859	43.60%	3.409%
7	8.440	2385	2405	2431	rBV3	416654	1045229	32.79%	2.564%
8	8.842	2536	2555	2577	rBV2	80486	192210	6.03%	0.471%
9	8.968	2583	2602	2646	rVB	871965	1883101	59.07%	4.619%
10	9.271	2698	2715	2732	rBV	155813	310494	9.74%	0.762%
11	9.416	2754	2769	2794	rBV	99589	198876	6.24%	0.488%
12	9.558	2813	2822	2835	rVB	21499	40132	1.26%	0.098%
13	9.974	2962	2977	2988	rBV4	19780	37554	1.18%	0.092%
14	10.328	3101	3109	3127	rVB7	17221	32673	1.02%	0.080%
15	10.443	3131	3152	3165	rBV	1380404	2636156	82.69%	6.466%
16	10.507	3165	3176	3207	rVB	866246	1743737	54.70%	4.277%
17	10.636	3216	3224	3244	rVB9	35912	83592	2.62%	0.205%
18	10.816	3278	3291	3307	rBV2	198721	350360	10.99%	0.859%
19	10.979	3340	3352	3363	rVB	60885	100996	3.17%	0.248%
20	11.087	3372	3392	3407	rVB3	65882	152722	4.79%	0.375%
21	11.518	3546	3553	3571	rVB4	45969	86840	2.72%	0.213%
22	11.746	3622	3638	3661	rVV	1288770	2327694	73.02%	5.710%
23	11.846	3662	3675	3689	rVV	497384	864433	27.12%	2.120%
24	11.950	3691	3714	3739	rVB3	1310930	2801992	87.90%	6.873%
25	12.100	3764	3770	3780	rBV3	24694	33665	1.06%	0.083%
26	12.283	3825	3838	3855	rVB	654201	1162978	36.48%	2.853%
27	12.353	3856	3864	3887	rVB4	52465	114436	3.59%	0.281%
28	12.484	3904	3913	3937	rBV7	52790	143788	4.51%	0.353%
29	12.581	3940	3949	3959	rVV3	59375	105154	3.30%	0.258%
30	12.637	3962	3970	3984	rVB4	78829	140573	4.41%	0.345%
31	12.733	3992	4006	4027	rVB	1068198	1922151	60.30%	4.715%
32	12.921	4067	4076	4088	rBV	199235	315691	9.90%	0.774%
33	12.986	4089	4100	4107	rBV	460420	808422	25.36%	1.983%
34	13.222	4172	4188	4204	rBV	318151	578880	18.16%	1.420%
35	13.369	4232	4243	4255	rVB	719748	1154997	36.23%	2.833%
36	13.592	4316	4326	4343	rVB2	433102	797648	25.02%	1.957%

LSC Area Percent Report

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Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-03-060921

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

37	13.677	4344	4358	4380	rBV3	1262315	3187859	100.00%	7.819%
38	13.876	4424	4432	4441	rVB3	257395	380420	11.93%	0.933%
39	13.994	4471	4476	4488	rVB2	134491	190458	5.97%	0.467%
40	14.061	4490	4501	4516	rVB4	284119	558116	17.51%	1.369%
41	14.133	4519	4528	4531	rBV2	95076	123981	3.89%	0.304%
42	14.217	4550	4559	4571	rVB2	187168	296859	9.31%	0.728%
43	14.329	4592	4601	4625	rVB4	221155	485650	15.23%	1.191%
44	14.439	4628	4642	4658	rBV5	190294	452231	14.19%	1.109%
45	14.514	4659	4670	4680	rBV	353205	628074	19.70%	1.541%
46	14.635	4694	4715	4726	rBV2	896320	2150456	67.46%	5.275%
47	14.815	4771	4782	4807	rVB7	323052	934039	29.30%	2.291%
48	14.933	4809	4826	4840	rVV5	304682	811142	25.44%	1.990%
49	14.997	4841	4850	4869	rVB2	370338	653022	20.48%	1.602%
50	15.086	4872	4883	4900	rVB2	348365	647239	20.30%	1.588%
51	15.456	5000	5021	5030	rBV2	608492	1578230	49.51%	3.871%
52	15.587	5058	5070	5084	rBV	1047474	1856893	58.25%	4.555%
53	15.673	5095	5102	5112	rVB	228614	312197	9.79%	0.766%
54	16.443	5380	5389	5404	rVB3	209620	428133	13.43%	1.050%
55	16.762	5497	5508	5518	rBV4	168765	357251	11.21%	0.876%

Sum of corrected areas: 40768284

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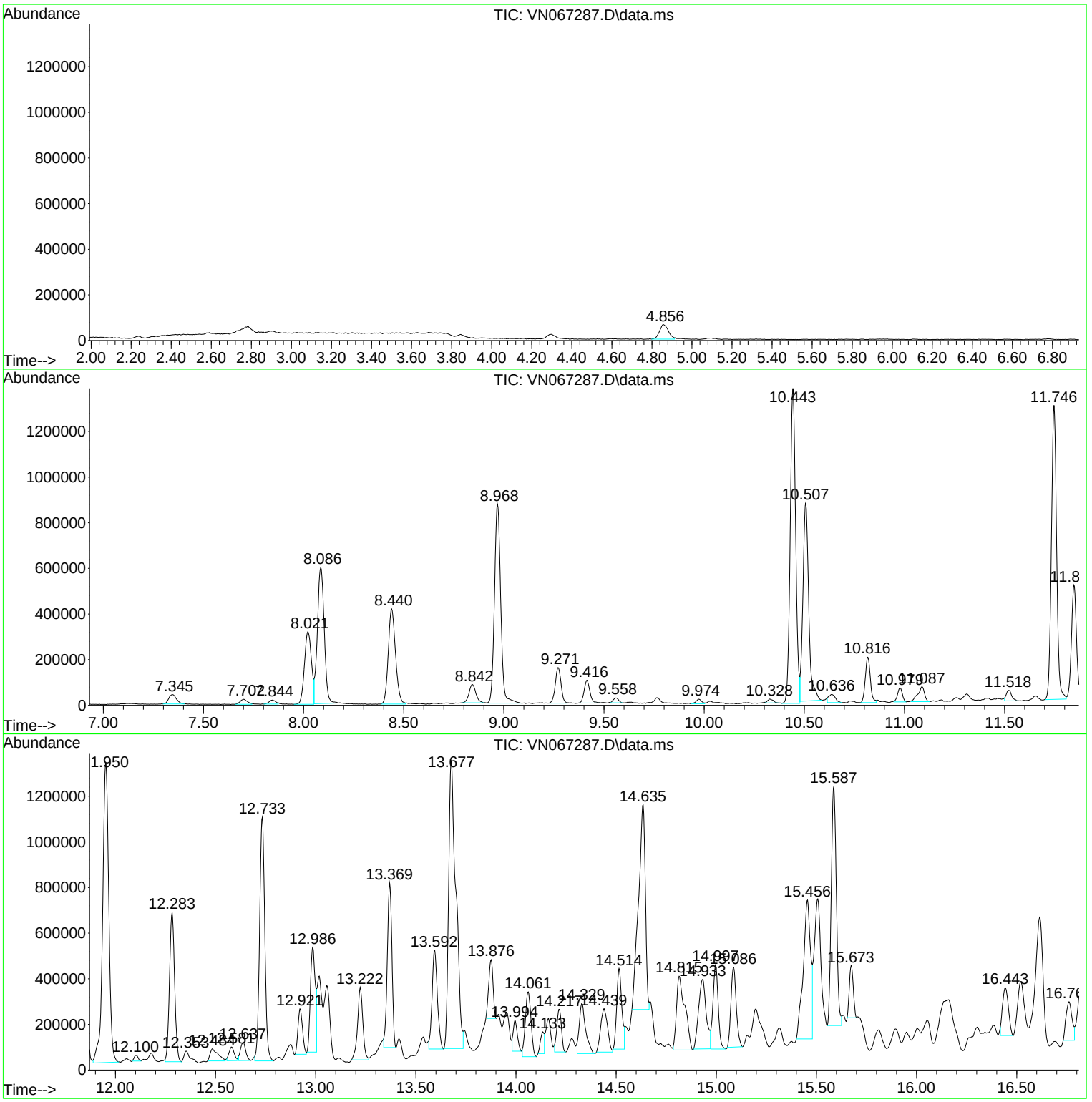
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
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MSVOA_N
ClientSampleId :
TMR-DS-03-060921

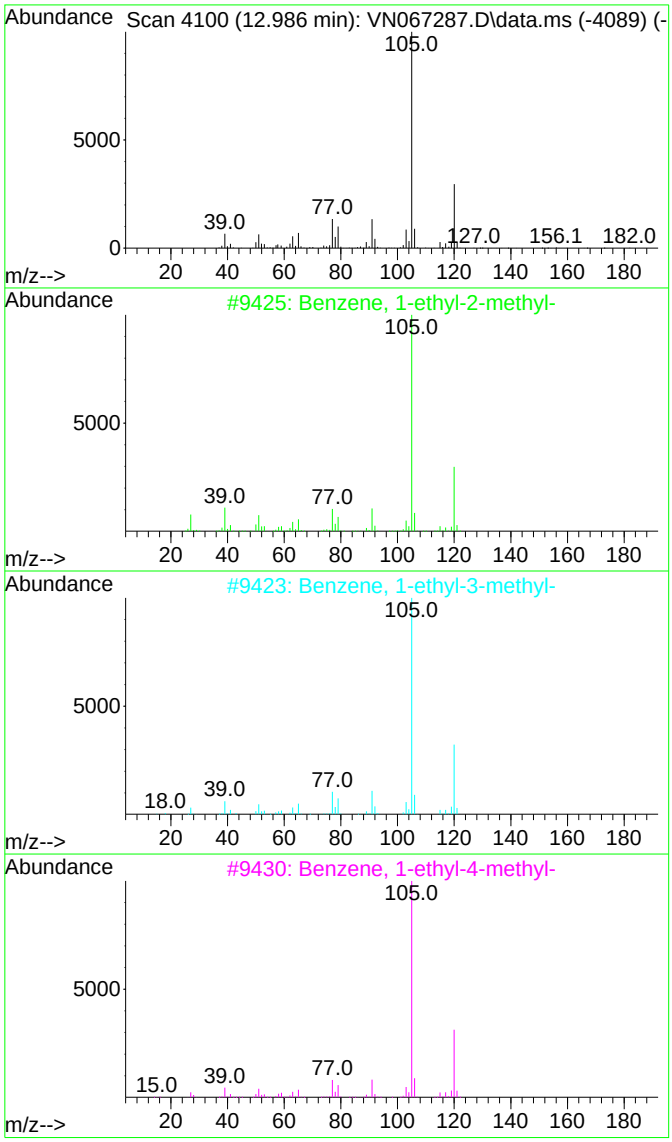
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

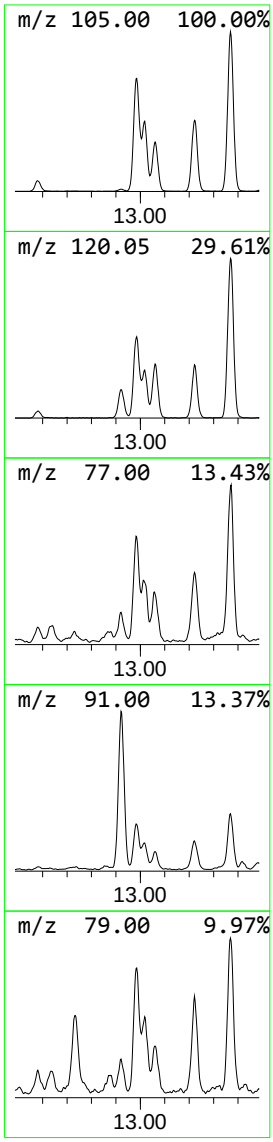
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	12.68 ug/l	808422	1,4-Dichlorobenzene-d4	13.678

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

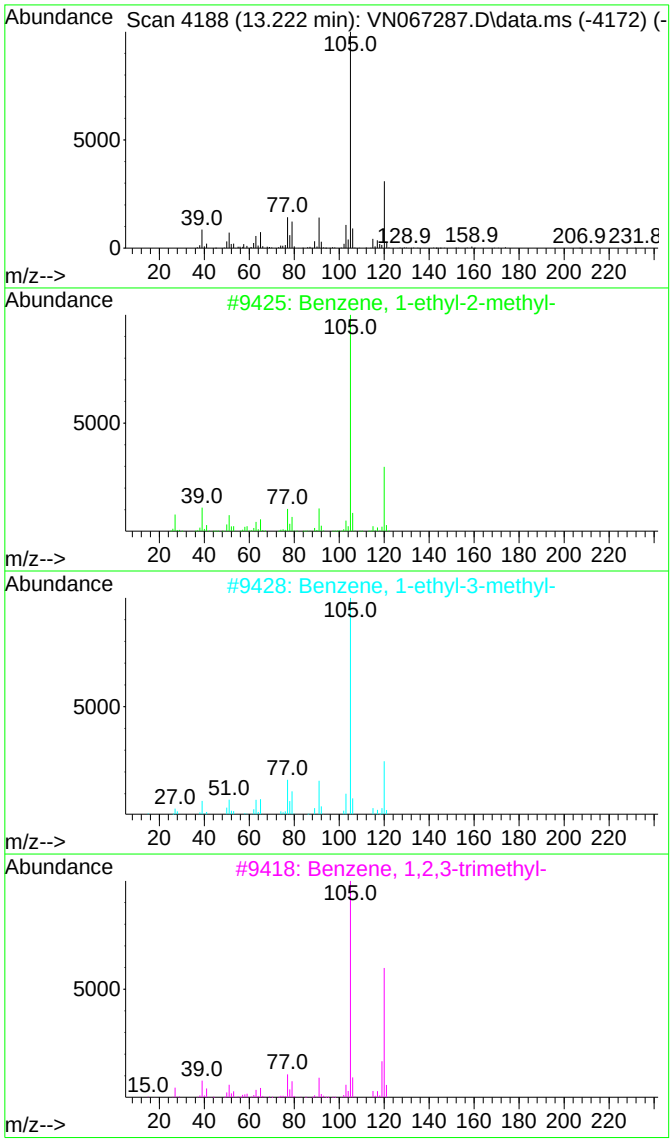
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

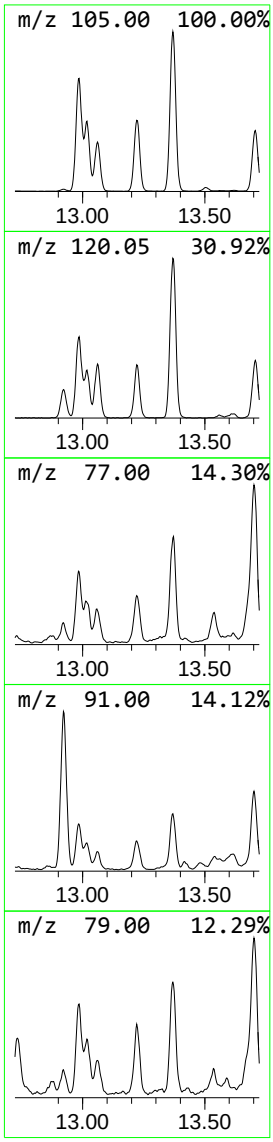
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	9.08 ug/l	578880	1,4-Dichlorobenzene-d4	13.678

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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

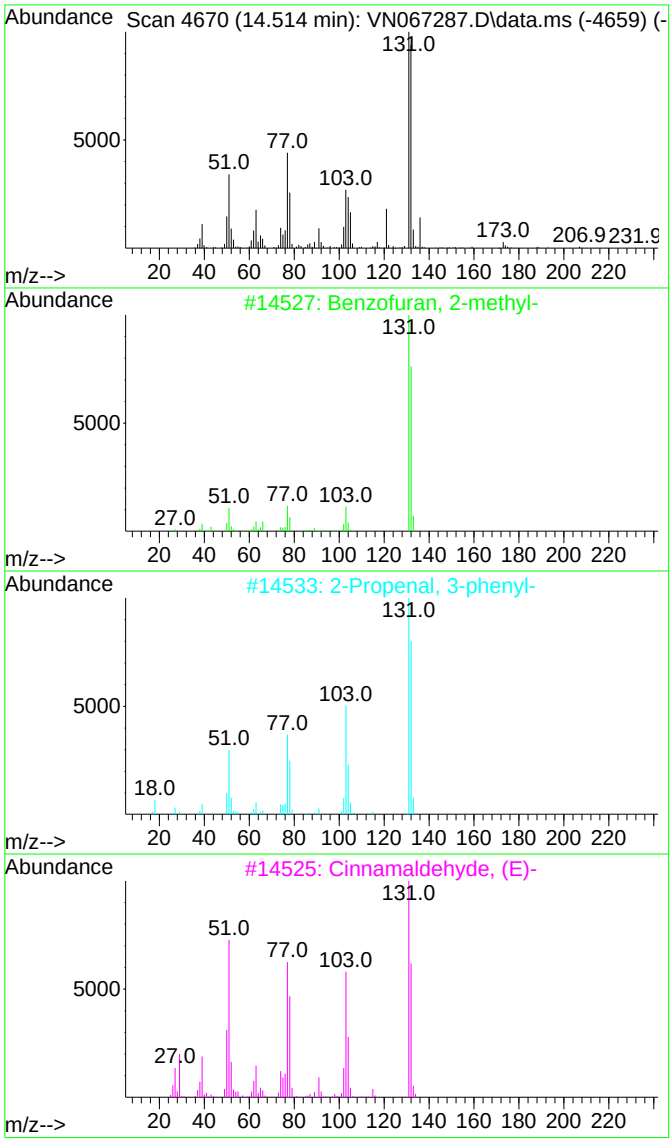
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

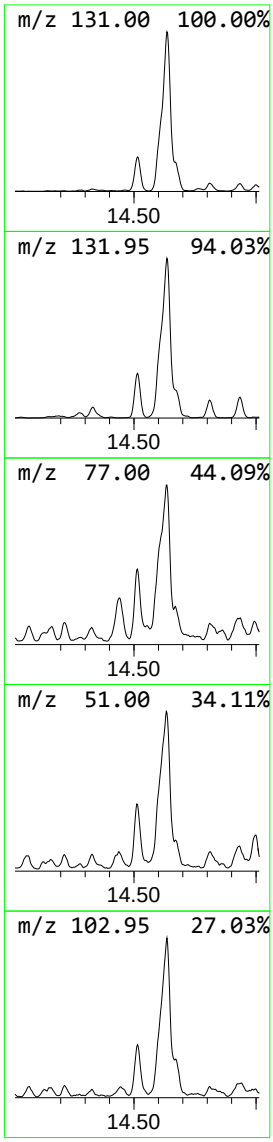
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.514	9.85 ug/l	628074	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	93
2	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	91
3	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	90
4	Benzenemethanol, .alpha.-ethynyl-	132	C9H8O	004187-87-5	87
5	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

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

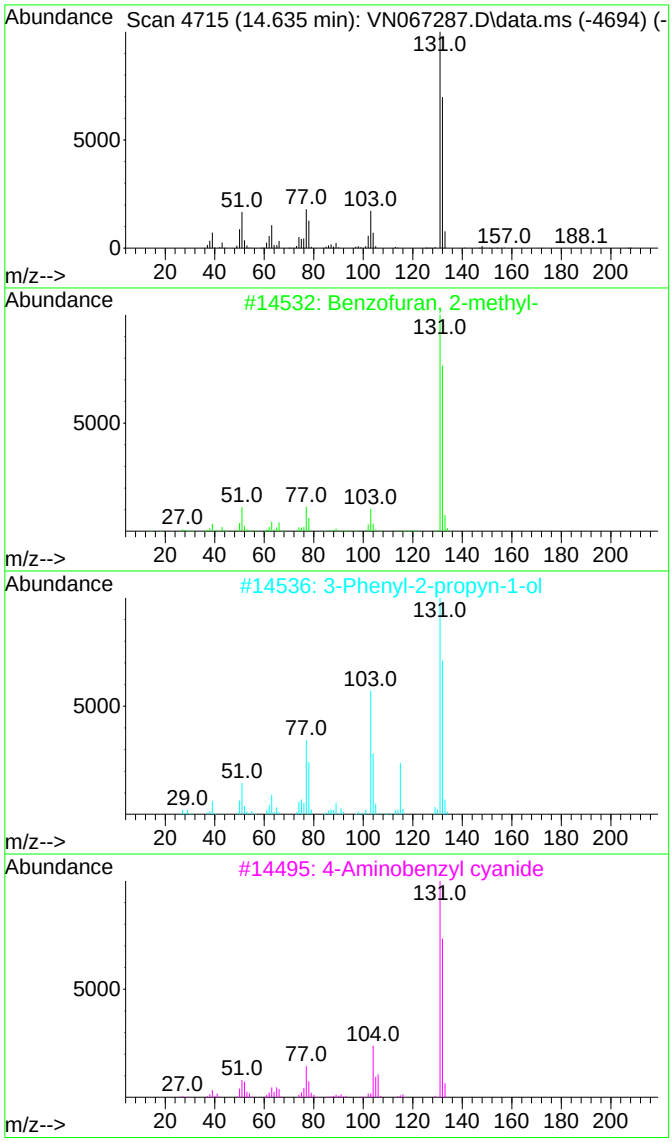
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

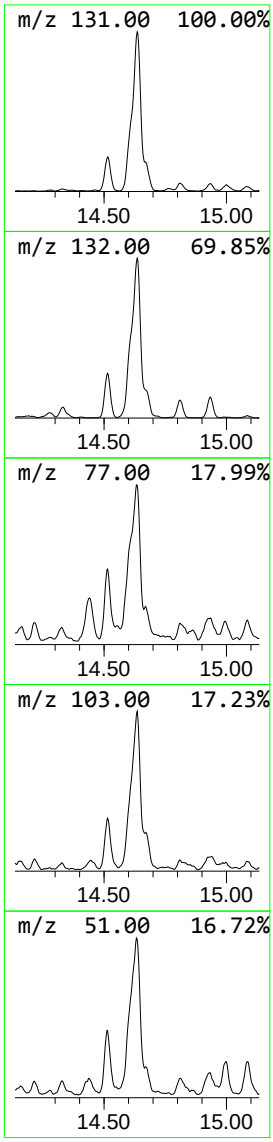
****

Peak Number 4 3-Phenyl-2-propyn-1-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	33.73 ug/l	2150460	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
3	4-Aminobenzyl cyanide	132	C8H8N2	003544-25-0	80
4	5-Methylbenzimidazole	132	C8H8N2	000614-97-1	80
5	Benzopyrimidine, 3,4-dihydro-	132	C8H8N2	001904-64-9	80





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

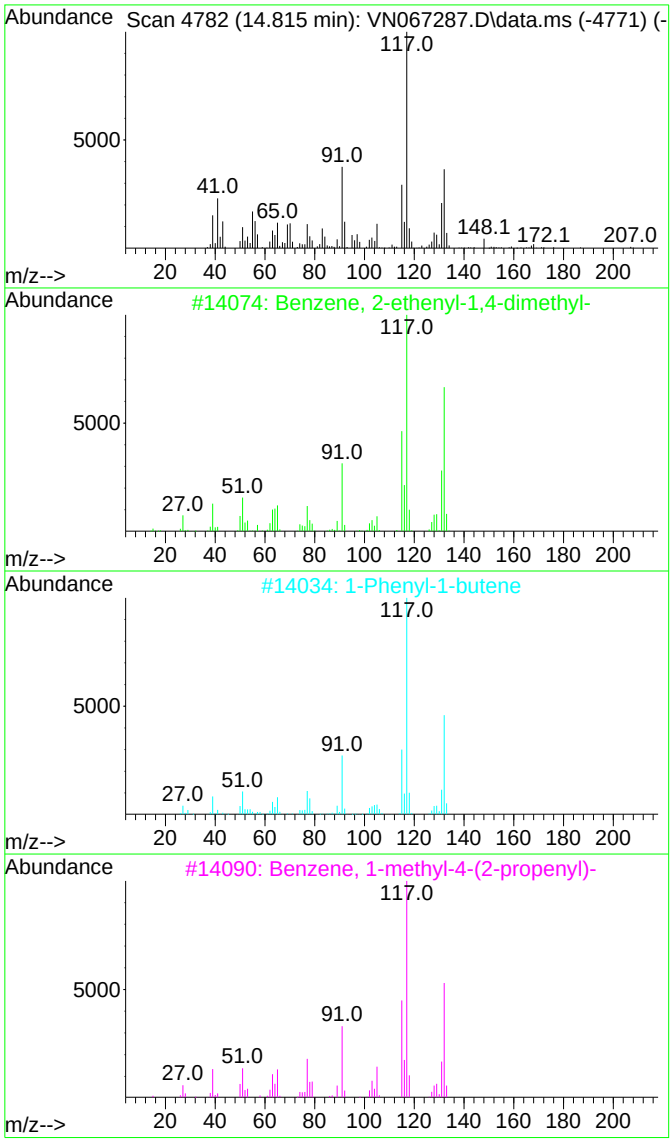
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

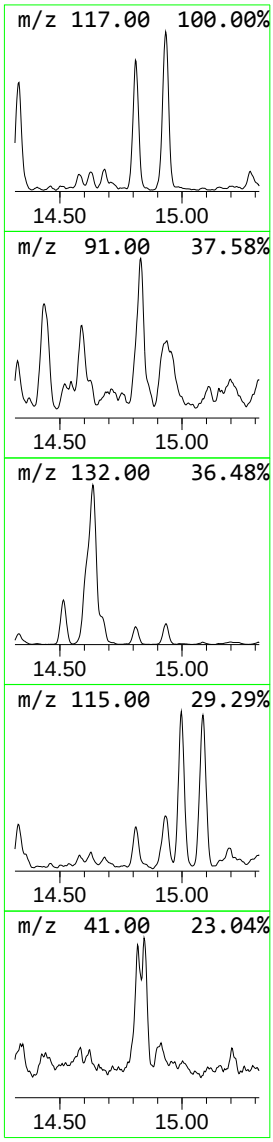
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	14.65 ug/l	934039	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

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

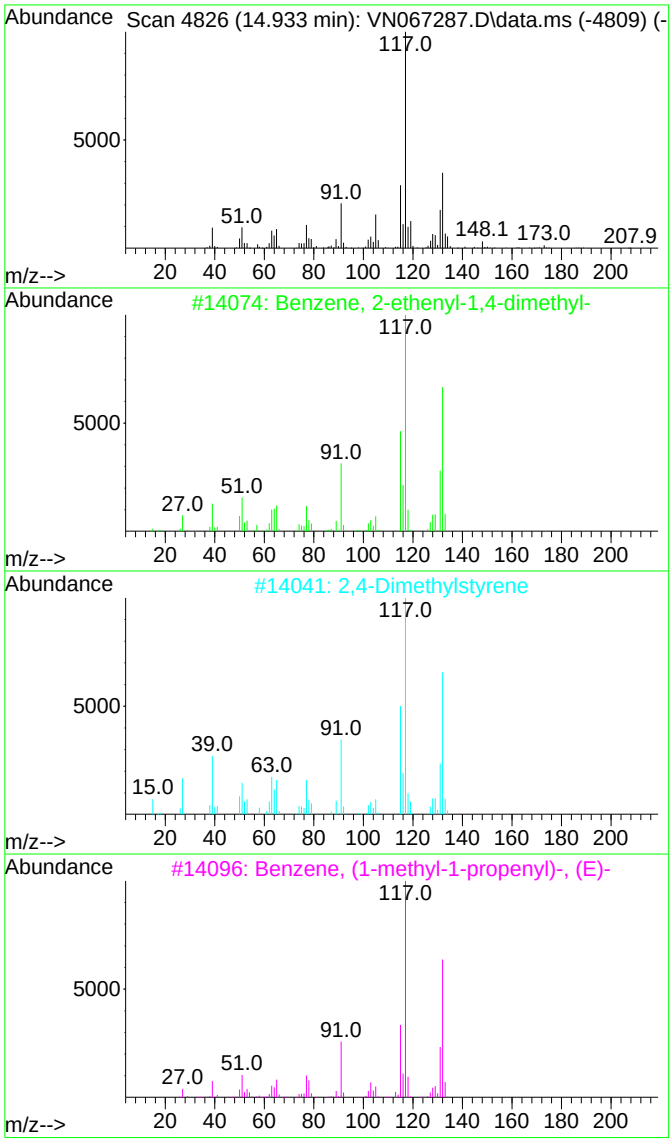
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

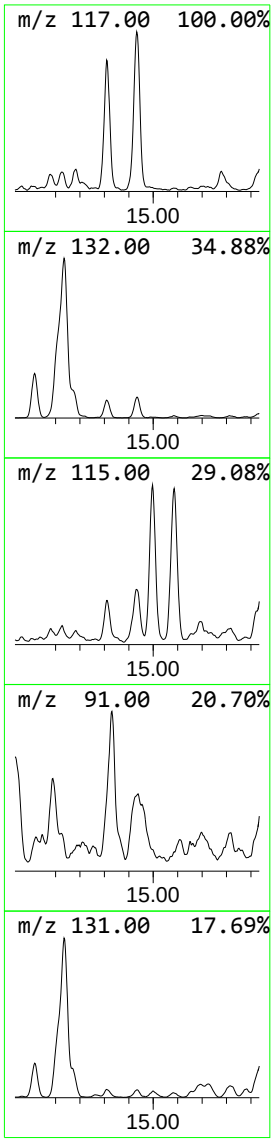
****

Peak Number 6 2,4-Dimethylstyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	12.72 ug/l	811142	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	93
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	92
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

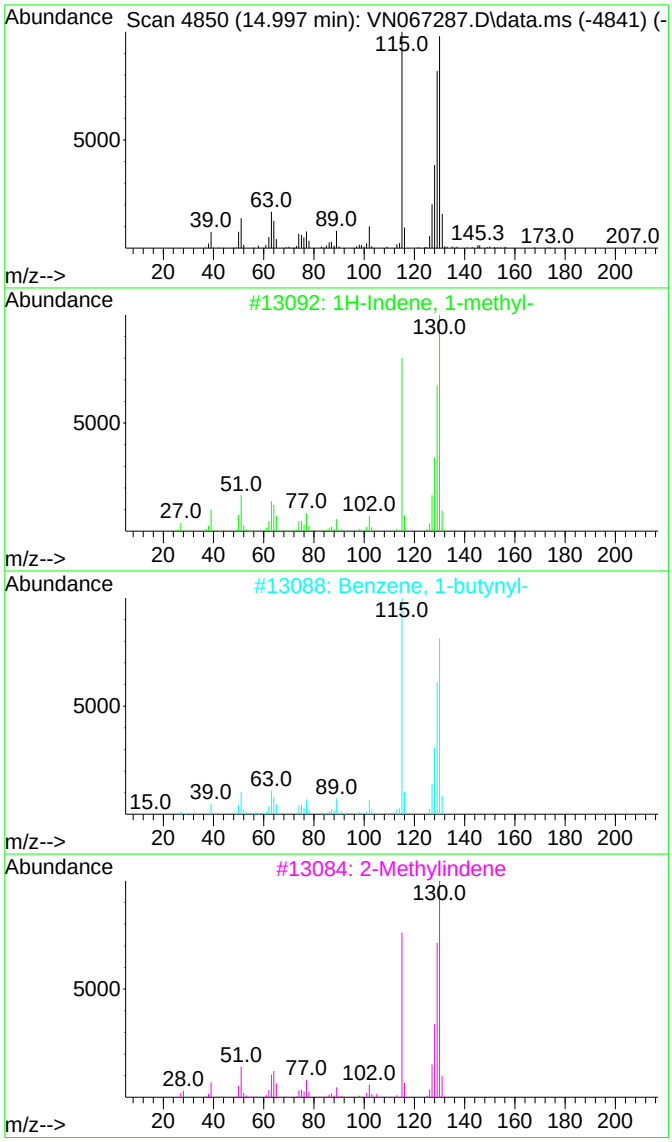
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

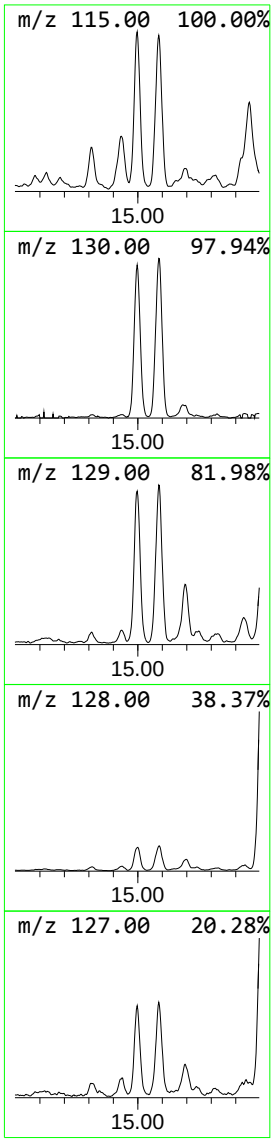
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	10.24 ug/l	653022	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
2	Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
3	2-Methylindene	130	C10H10	002177-47-1	94
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

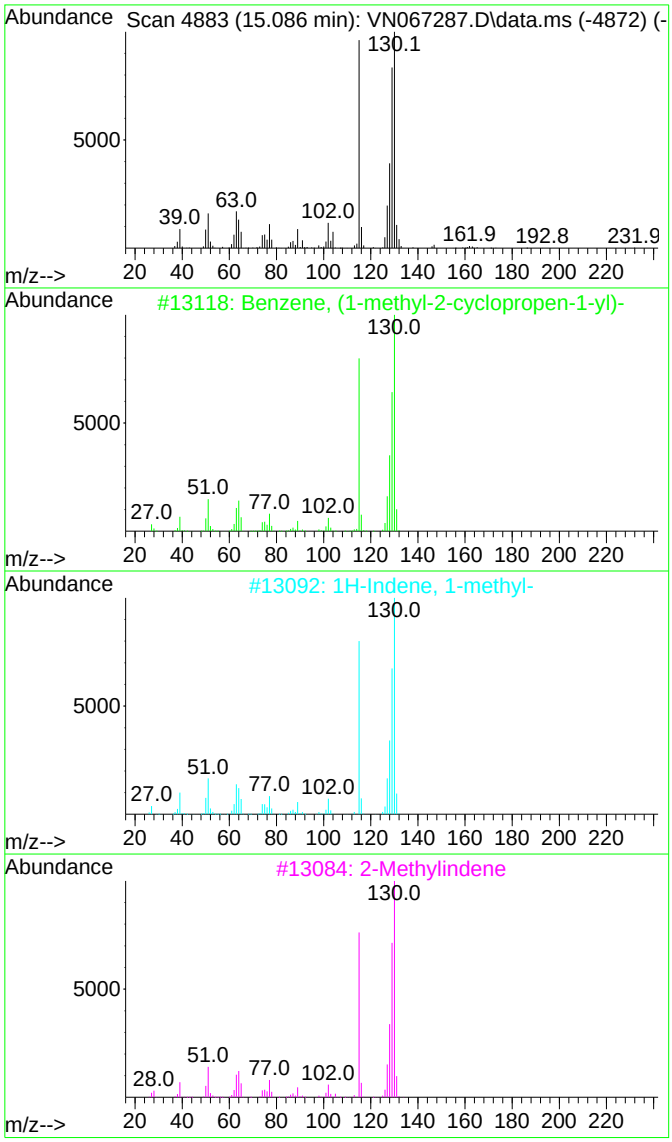
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

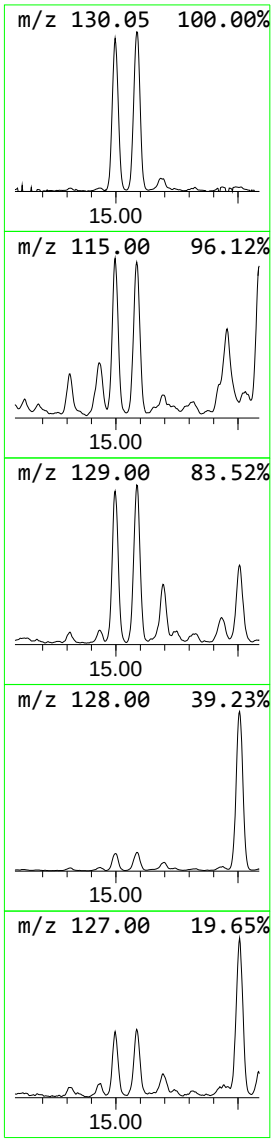
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (1-methyl-2-cyclop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	10.15 ug/l	647239	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	2-Methylindene	130	C10H10	002177-47-1	96
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

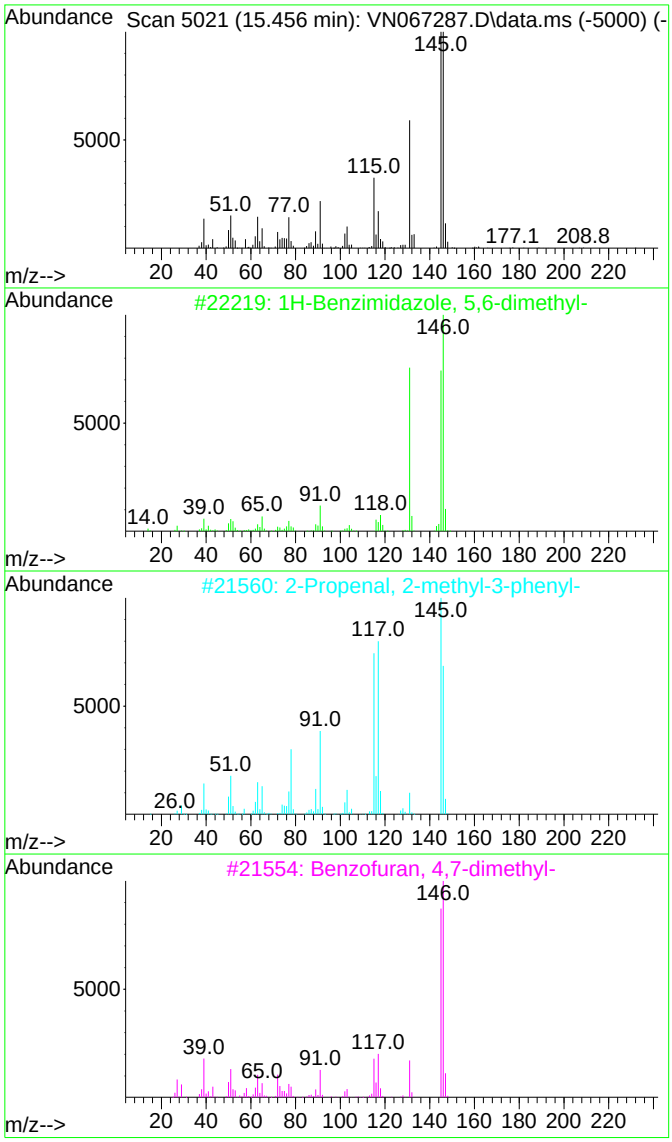
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

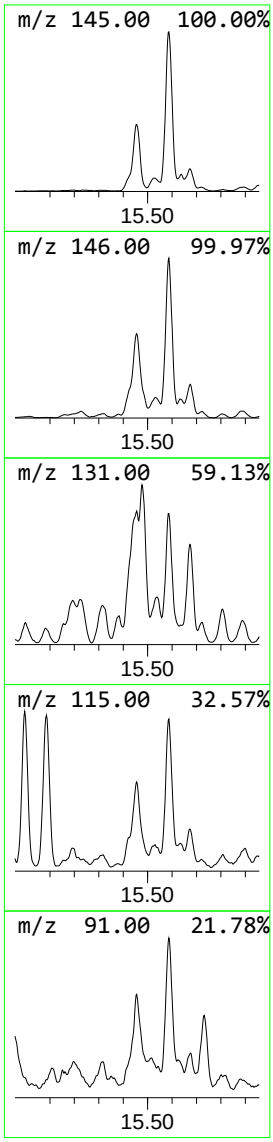
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Benzimidazole, 5,6-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	24.75 ug/l	1578230	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	74
2	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	64
3	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	59
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	58
5	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

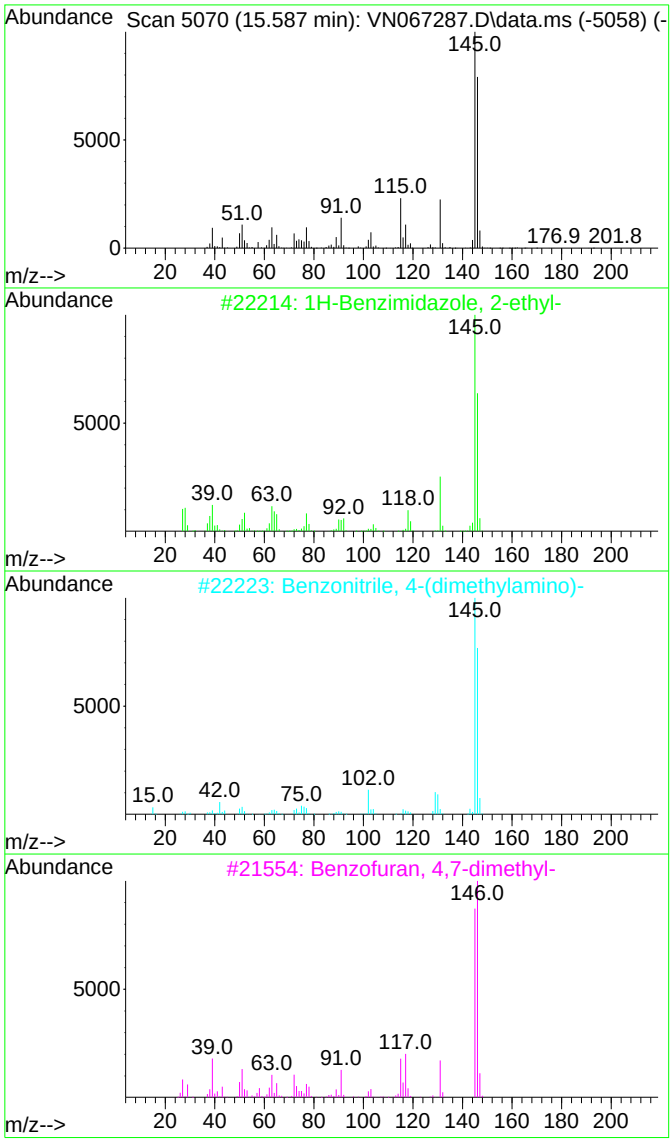
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

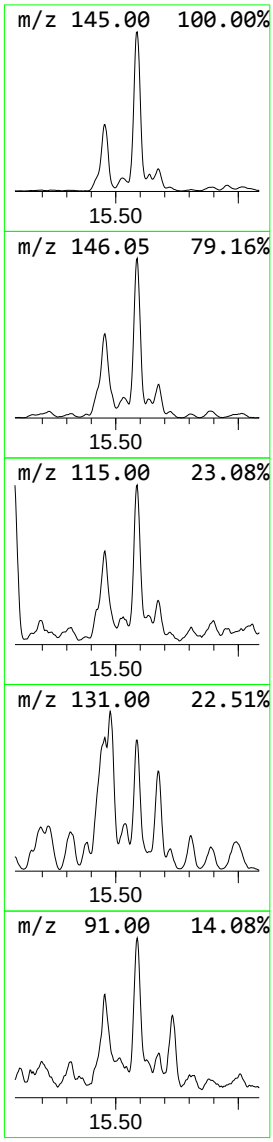
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Benzimidazole, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	29.12 ug/l	1856890	1,4-Dichlorobenzene-d4	13.678

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	59
3	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	58
4	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	52
5	1H-Benzimidazole, 2,5-dimethyl-	146	C9H10N2	001792-41-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067287.D
Acq On : 11 Jun 2021 14:41
Operator : JC/MD
Sample : M2674-03 10X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-03-060921

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	12.7	ug/l	808422	4	13.678	3187860	50.0
Benzene, 1-ethy...	13.222	9.1	ug/l	578880	4	13.678	3187860	50.0
Benzofuran, 2-m...	14.514	9.8	ug/l	628074	4	13.678	3187860	50.0
3-Phenyl-2-prop...	14.635	33.7	ug/l	2150460	4	13.678	3187860	50.0
Benzene, 2-ethe...	14.815	14.7	ug/l	934039	4	13.678	3187860	50.0
2,4-Dimethylsty...	14.933	12.7	ug/l	811142	4	13.678	3187860	50.0
1H-Indene, 1-me...	14.997	10.2	ug/l	653022	4	13.678	3187860	50.0
Benzene, (1-met...	15.086	10.2	ug/l	647239	4	13.678	3187860	50.0
1H-Benzimidazol...	15.456	24.8	ug/l	1578230	4	13.678	3187860	50.0
1H-Benzimidazol...	15.587	29.1	ug/l	1856890	4	13.678	3187860	50.0