LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 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: VN067292.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.291	842	858	891	rVB	48191	138784	2.09%	0.171%
2	4.854	1045	1068	1095	rBV2	155262	480488	7.22%	0.590%
3	7.343	1976	1996	2019	rBV	106469	286312	4.30%	0.352%
4	7.697	2110	2128	2149	rBV3	48982	128426	1.93%	0.158%
5	7.844	2167	2183	2204	rVB2	41400	99371	1.49%	0.122%
6	8.021	2227	2249	2260	rBV	320675	767241	11.53%	0.943%
7	8.086	2260	2273	2299	rVB	595370	1365574	20.52%	1.678%
8	8.440	2385	2405	2430	rBV2	450350	1226172	18.42%	1.507%
9	8.842	2533	2555	2578	rBV2	190479	441219	6.63%	0.542%
10	8.968	2585	2602	2628	rBV2	882104	1862915	27.99%	2.289%
11	9.271	2698	2715	2737	rVB	356096	712089	10.70%	0.875%
12	9.413	2754	2768	2786	rBV	233042	461492	6.93%	0.567%
13	9.558	2811	2822	2838	rVB	55228	99828	1.50%	0.123%
14	9.765	2885	2899	2916	rBV2	58880	109906	1.65%	0.135%
15	9.971	2964	2976	2988	rBV5	42918	78886	1.19%	0.097%
16	10.331	3088	3110	3124	rBV4	40257	98642	1.48%	0.121%
17	10.443	3135	3152	3164	rBV	1394999	2701428	40.59%	3.319%
18	10.508	3164	3176	3207	rVB	2006339	4013189	60.29%	4.931%
19	10.639	3213	3225	3243	rVB6	75314	199112	2.99%	0.245%
20	10.816	3277	3291	3305	rBV	465825	802668	12.06%	0.986%
21	10.977	3341	3351	3366	rVB2	144698	238102	3.58%	0.293%
22	11.090	3374	3393	3406	rVB4	163153	342450	5.15%	0.421%
23	11.521	3546	3554	3575	rVB	111266	203224	3.05%	0.250%
24	11.747	3623	3638	3660	rVB	1287352	2330681	35.02%	2.864%
25	11.846	3662	3675	3689	rVV	1154213	1973958	29.66%	2.425%
26	11.950	3690	3714	3740	rVB2	3178446	6655965	100.00%	8.178%
27	12.103	3765	3771	3779	rVB	60499	71460	1.07%	0.088%
28	12.283	3825	3838	3855	rVB	1557744	2728437	40.99%	3.352%
29	12.355	3856	3865	3874	rBV	113211	178791	2.69%	0.220%
30	12.484	3904	3913	3937	rBV6	130233	359623	5.40%	0.442%
31	12.581	3941	3949	3959	rVV2	134257	231879	3.48%	0.285%
32	12.637	3961	3970	3984	rVB3	189724	341981	5.14%	0.420%
33	12.734	3993	4006	4026	rVB	1177486	2149227	32.29%	2.641%
34	12.921	4067	4076	4088	rBV	476996	759525	11.41%	0.933%
35	12.986	4089	4100	4106	rBV	1066338	1803787	27.10%	2.216%
36	13.222	4173	4188	4204	rBV	726215	1312812	19.72%	1.613%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 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	13.369	4233	4243	4254	rVB	1717281	2694254	40.48%	3.310%
38	13.594	4316	4327	4344	rVB2	1021578	1901604	28.57%	2.337%
39	13.678	4345	4358	4362	rBV	1372765	2260879	33.97%	2.778%
40	13.876	4424	4432	4441	rVB3	640155	939525	14.12%	1.154%
41	13.997	4471	4477	4488	rVB3	326416	457624	6.88%	0.562%
42	14.061	4490	4501	4516	rVB2	685717	1331161	20.00%	1.636%
43	14.134	4519	4528	4532	rBV3	257768	369031	5.54%	0.453%
44	14.217	4550	4559	4570	rVB2	446781	692654	10.41%	0.851%
45	14.329	4592	4601	4624	rVB4	513420	1161923	17.46%	1.428%
46	14.439	4630	4642	4658	rVB7	401578	908846	13.65%	1.117%
47	14.514	4659	4670	4680	rBV	847273	1484505	22.30%	1.824%
48	14.635	4692	4715	4726	rBV2	2414541	6074647	91.27%	7.464%
49	14.815	4771	4782	4808	rVB7	799509	2389433	35.90%	2.936%
50	14.933	4810	4826	4840	rVV4	709633	1924098	28.91%	2.364%
51	14.997	4842	4850	4870	rVB2	896874	1572967	23.63%	1.933%
52	15.086	4872	4883	4901	rVV	872000	1622456	24.38%	1.994%
53	15.456	5001	5021	5030	rBV2	1507735	3776766	56.74%	4.641%
54	15.587	5058	5070	5083	rBV	2714275	4829516	72.56%	5.934%
55	15.673	5095	5102	5112	rBV	577226	794359	11.93%	0.976%
56	16.443	5382	5389	5404	rVB	523781	996285	14.97%	1.224%
57	16.521	5408	5418	5432	rVB2	580222	1237231	18.59%	1.520%
58	16.614	5445	5453	5473	rVB2	1527807	3268106	49.10%	4.016%
59	16.762	5497	5508	5518	rBV4	457361	942503	14.16%	1.158%

Sum of corrected areas: 81386017

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
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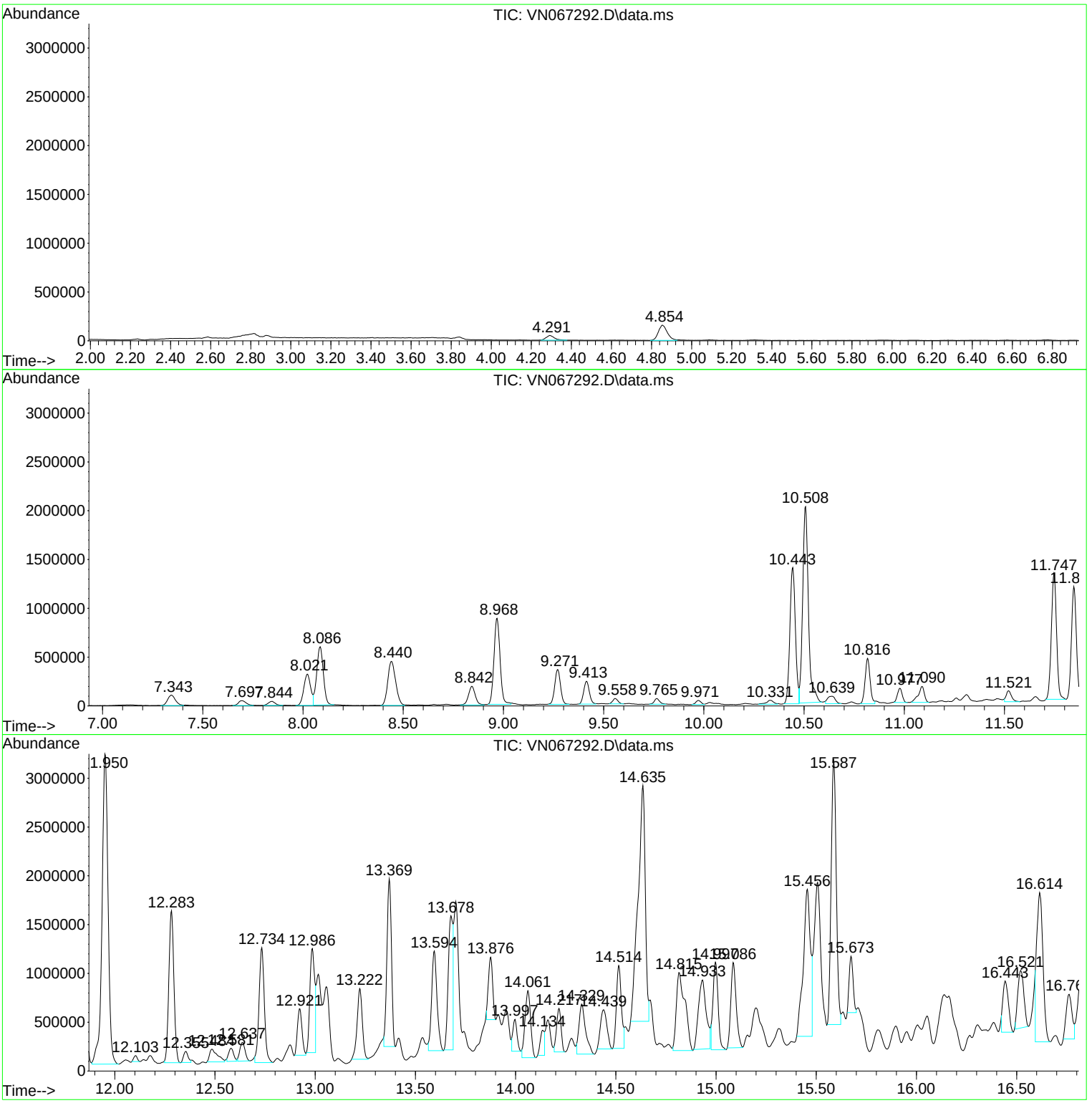
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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 : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
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Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-03-060921

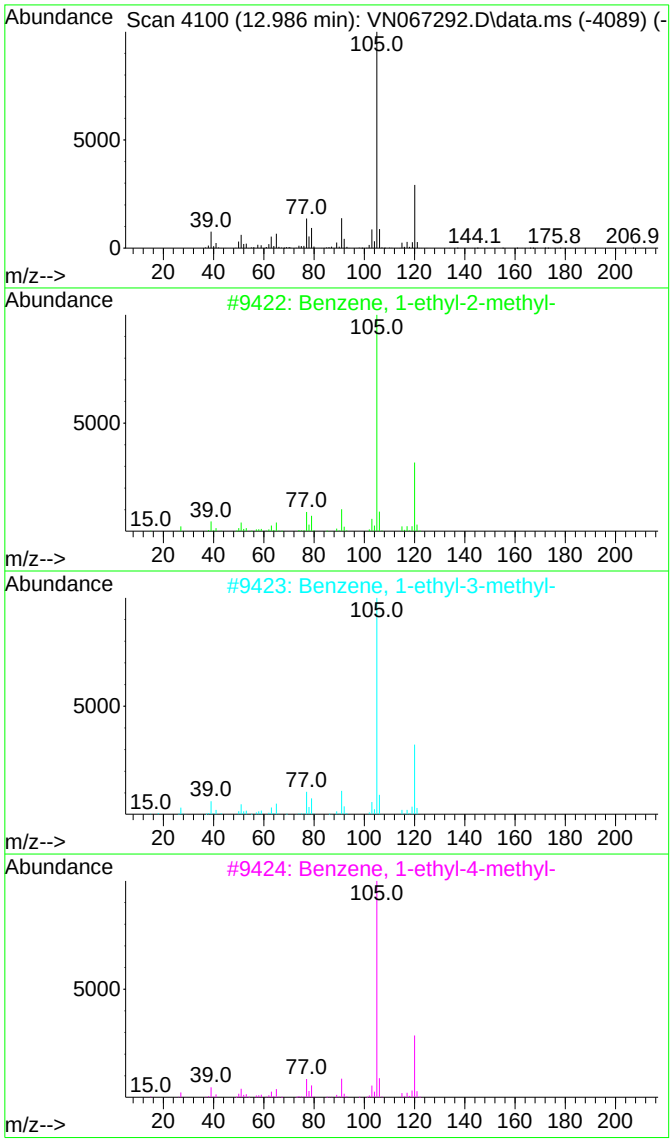
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

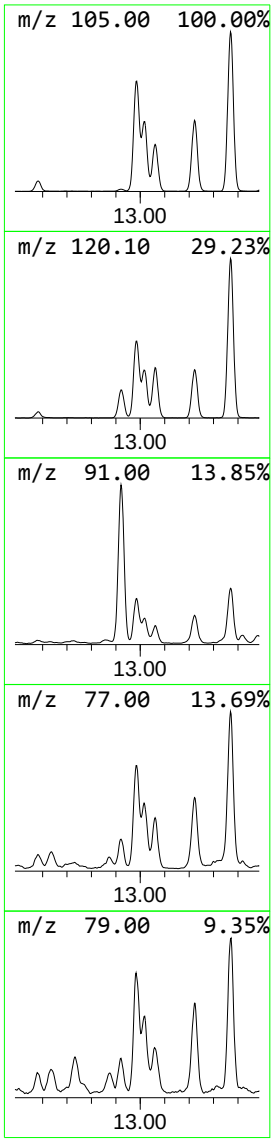
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	39.89 ug/l	1803790	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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

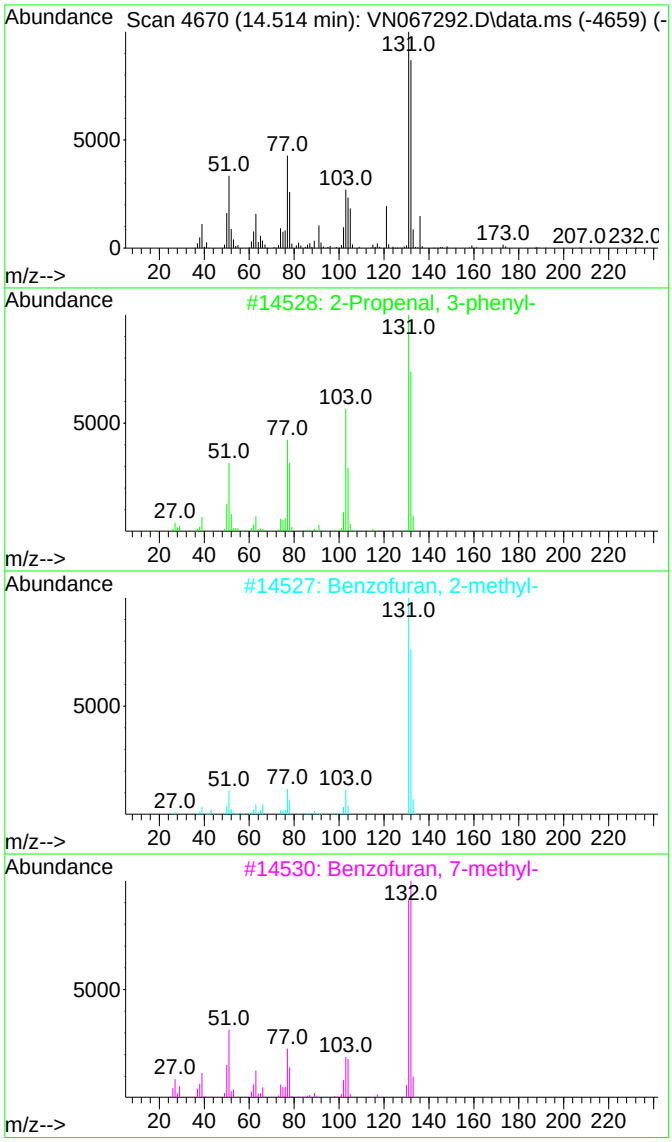
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

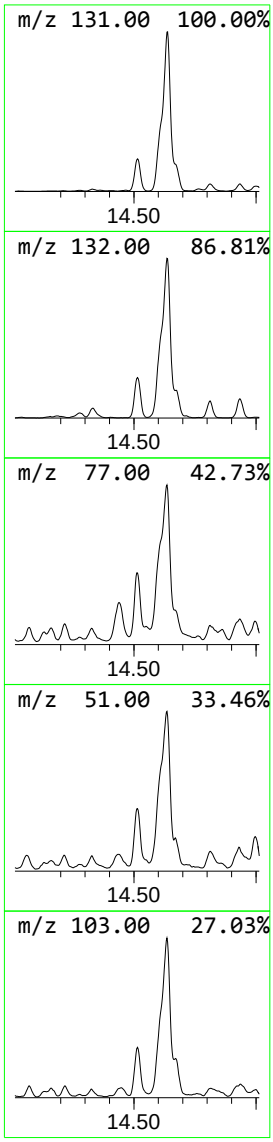
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propenal, 3-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.514	32.83 ug/l	1484510	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	93
2	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	93
3	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	91
4	Benzenemethanol, .alpha.-ethynyl-	132	C9H8O	004187-87-5	90
5	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

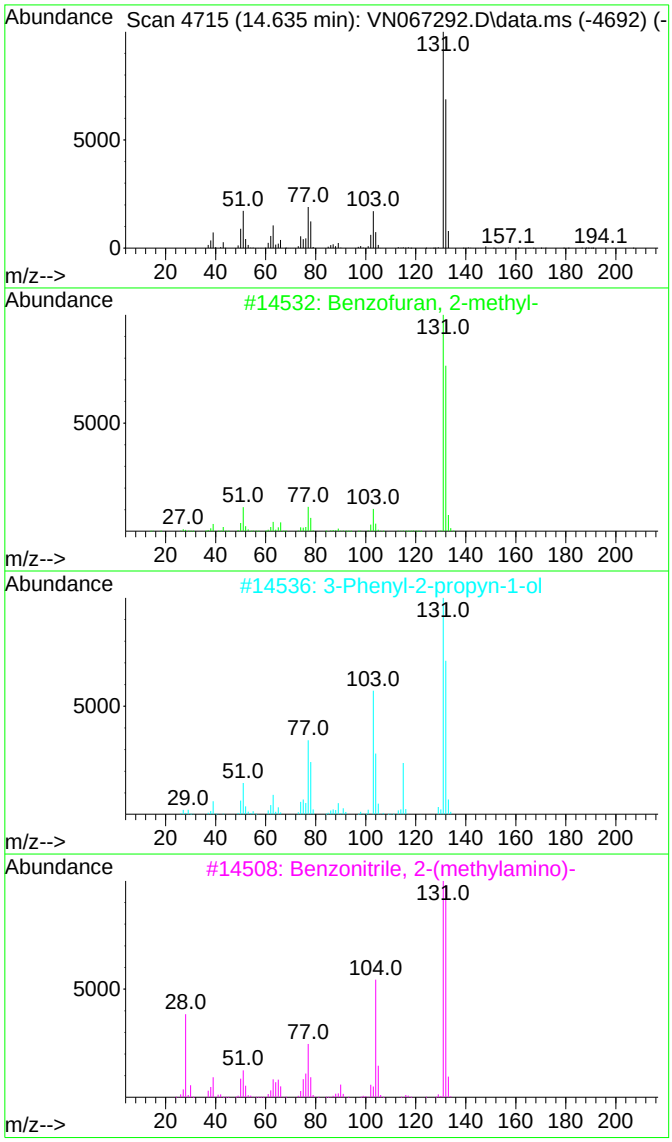
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

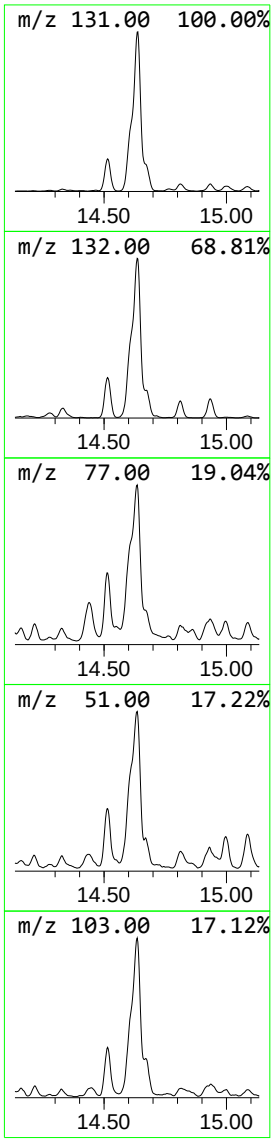
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	134.34 ug/l	6074650	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	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
3	Benzonitrile, 2-(methylamino)-	132	C8H8N2	017583-40-3	87
4	4-Aminobenzyl cyanide	132	C8H8N2	003544-25-0	86
5	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

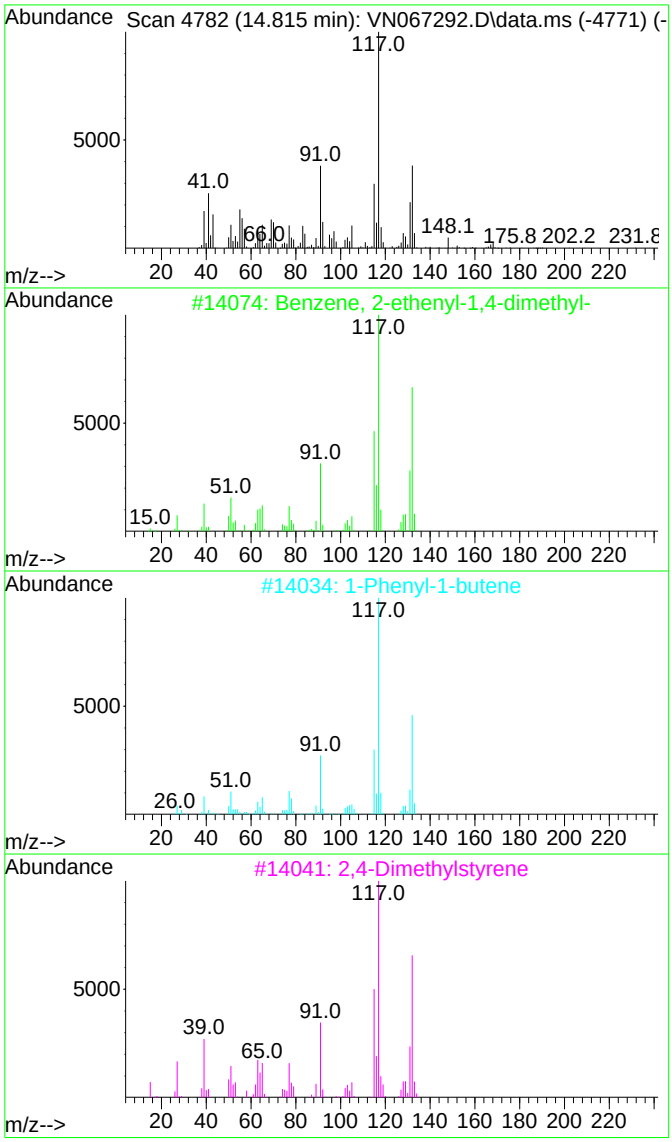
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

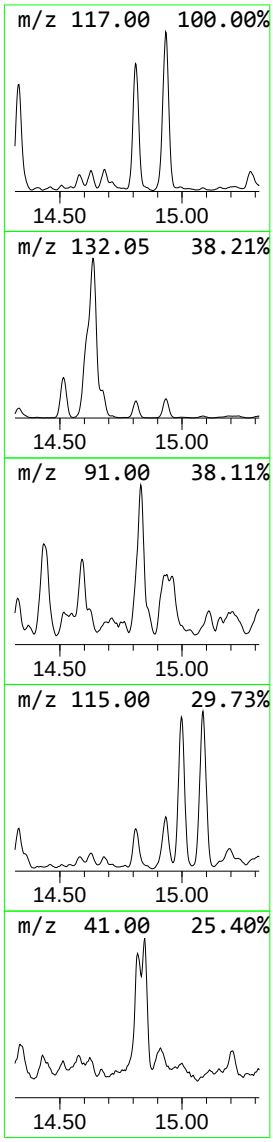
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	52.84 ug/l	2389430	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	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3	2,4-Dimethylstyrene	132	C10H12	002234-20-0	93
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	93





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Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

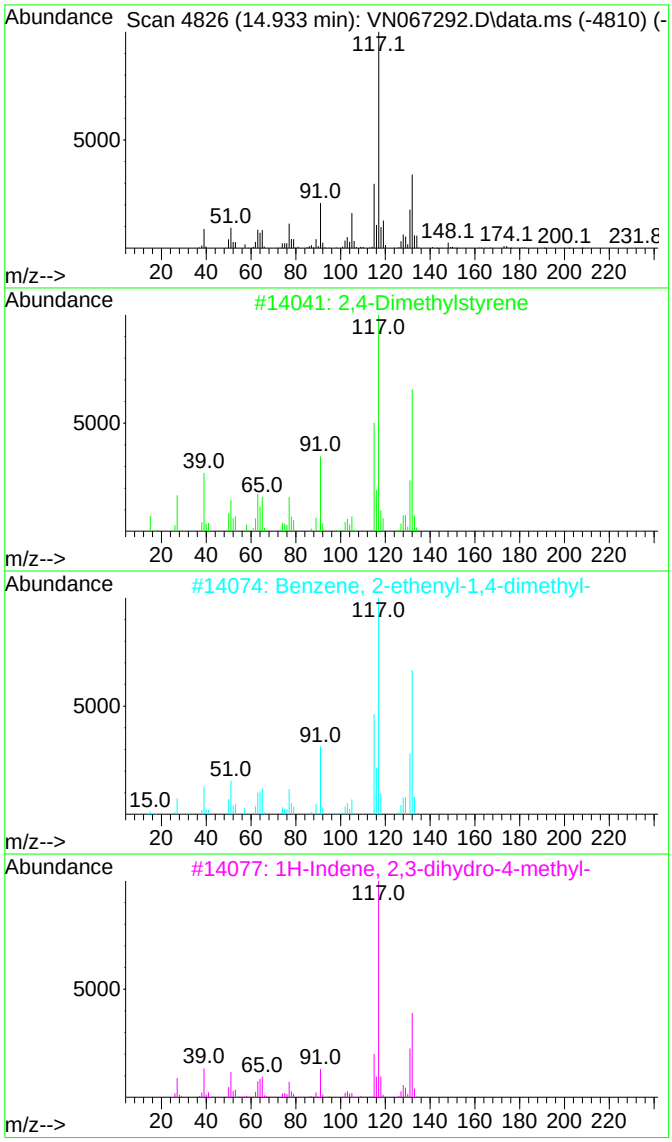
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

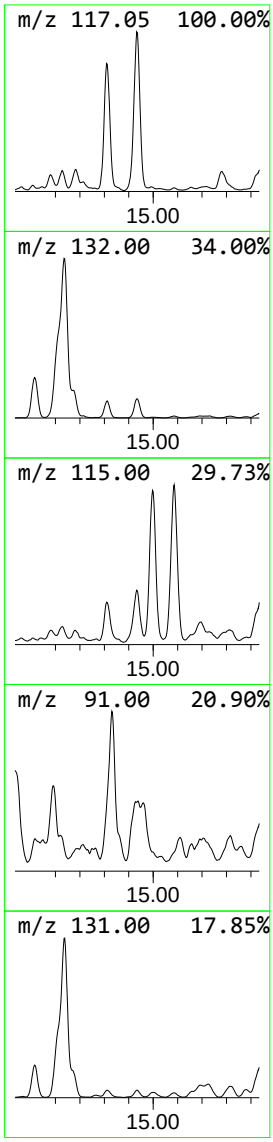
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4-Dimethylstyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	42.55 ug/l	1924100	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	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





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Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

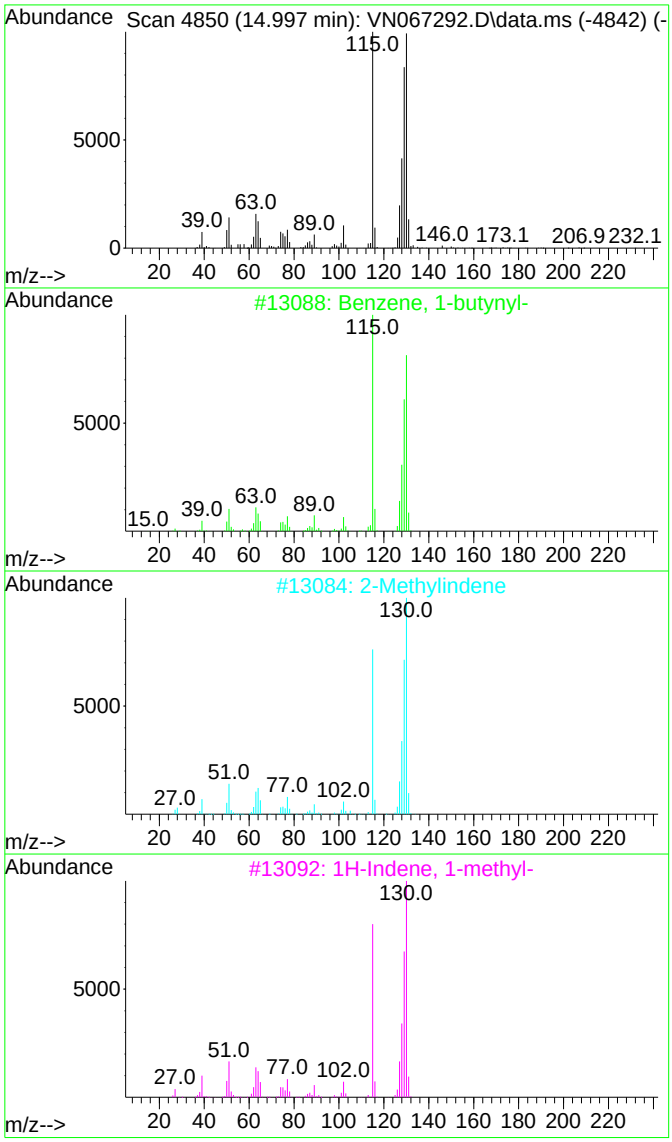
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

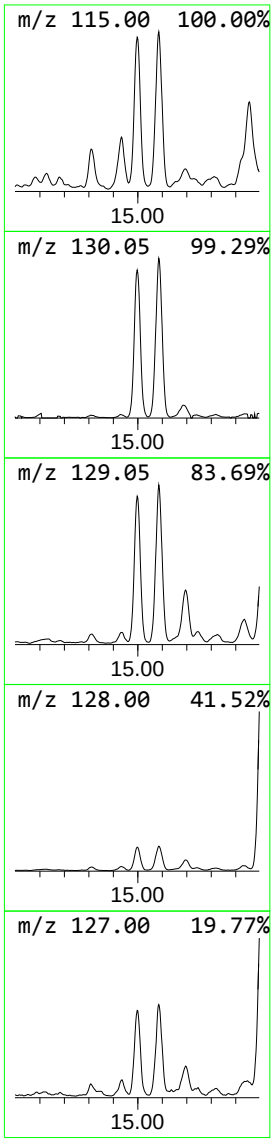
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-butynyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	34.79 ug/l	1572970	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-butynyl-	130	C10H10	000622-76-4	97
2	2-Methylindene	130	C10H10	002177-47-1	96
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
5	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

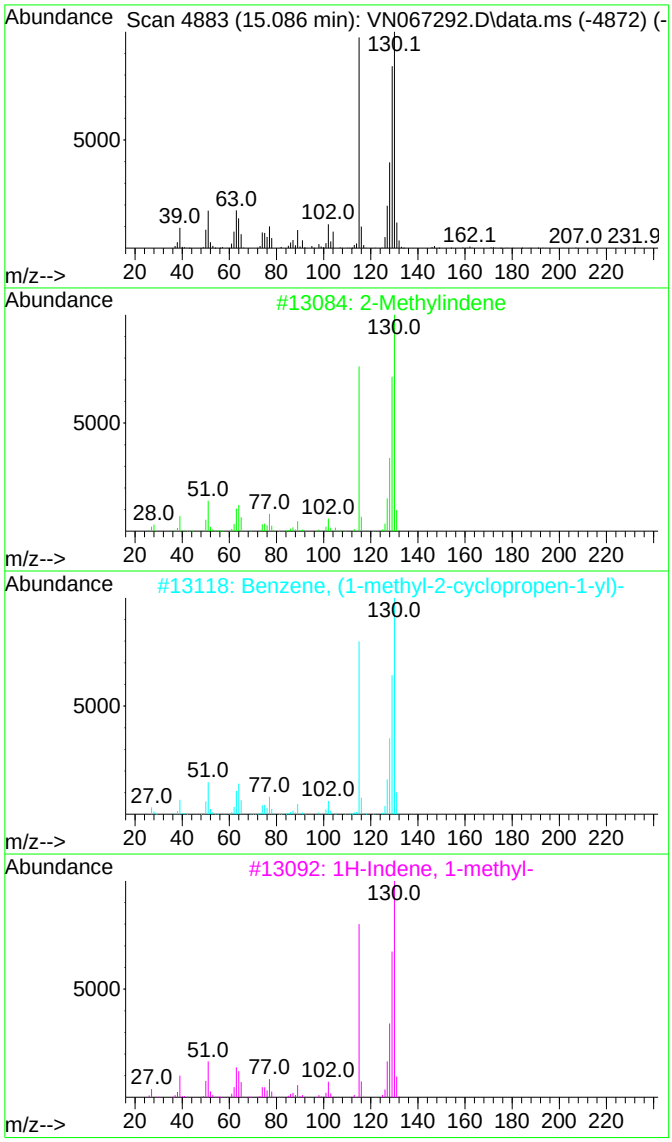
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

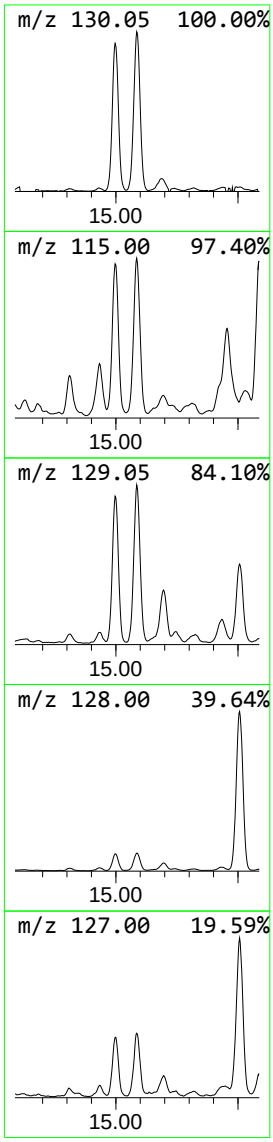
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Methylindene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	35.88 ug/l	1622460	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	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	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 : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

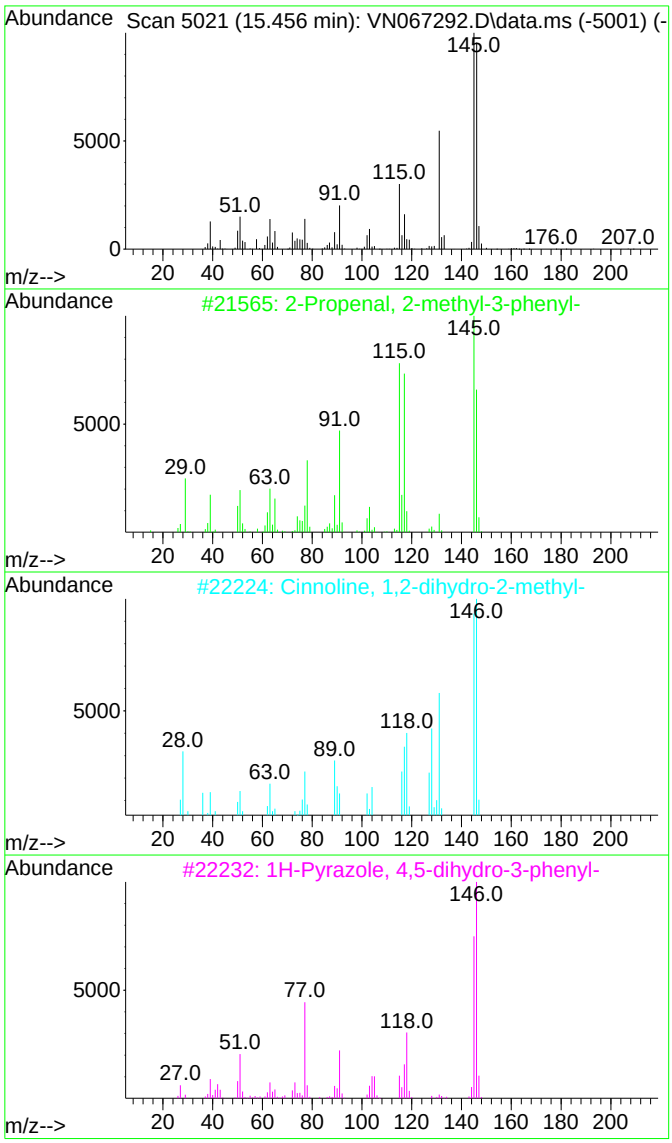
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

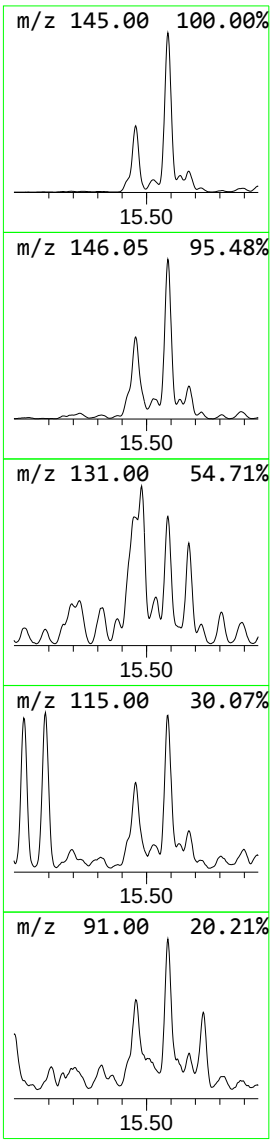
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Propenal, 2-methyl-3-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	83.52 ug/l	3776770	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	76
2	Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	64
3	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	64
4	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	52
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

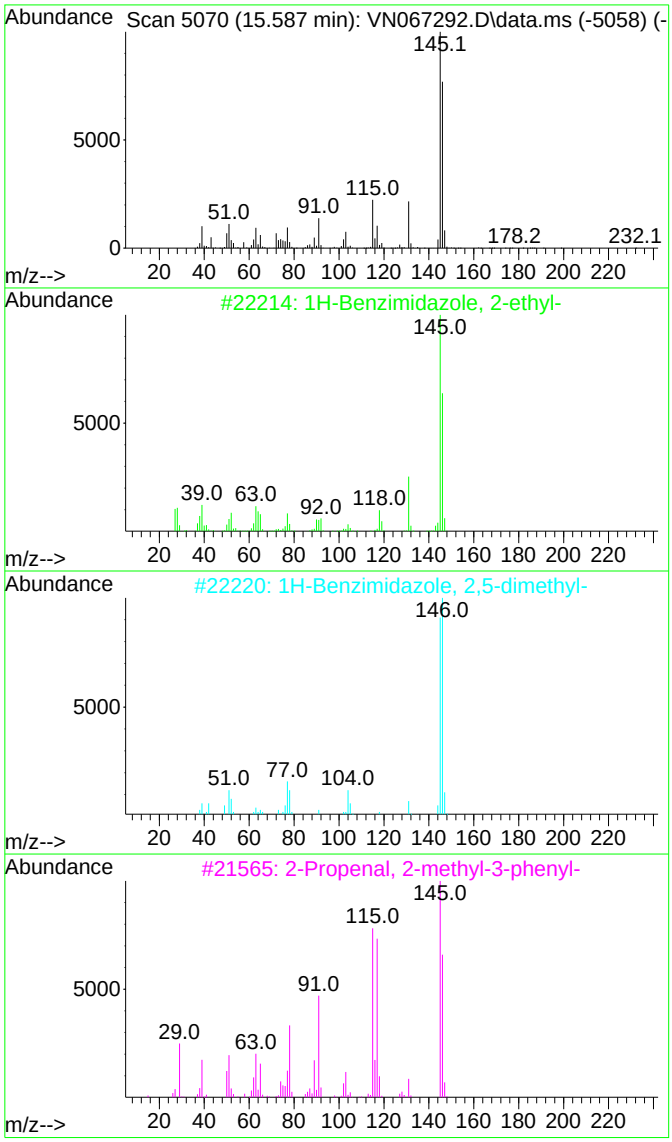
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

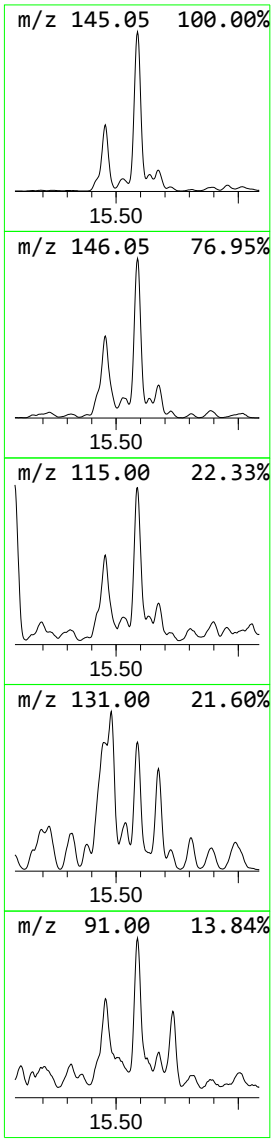
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	106.81 ug/l	4829520	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	1H-Benzimidazole, 2,5-dimethyl-	146	C9H10N2	001792-41-2	64
3	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	64
4	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
5	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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

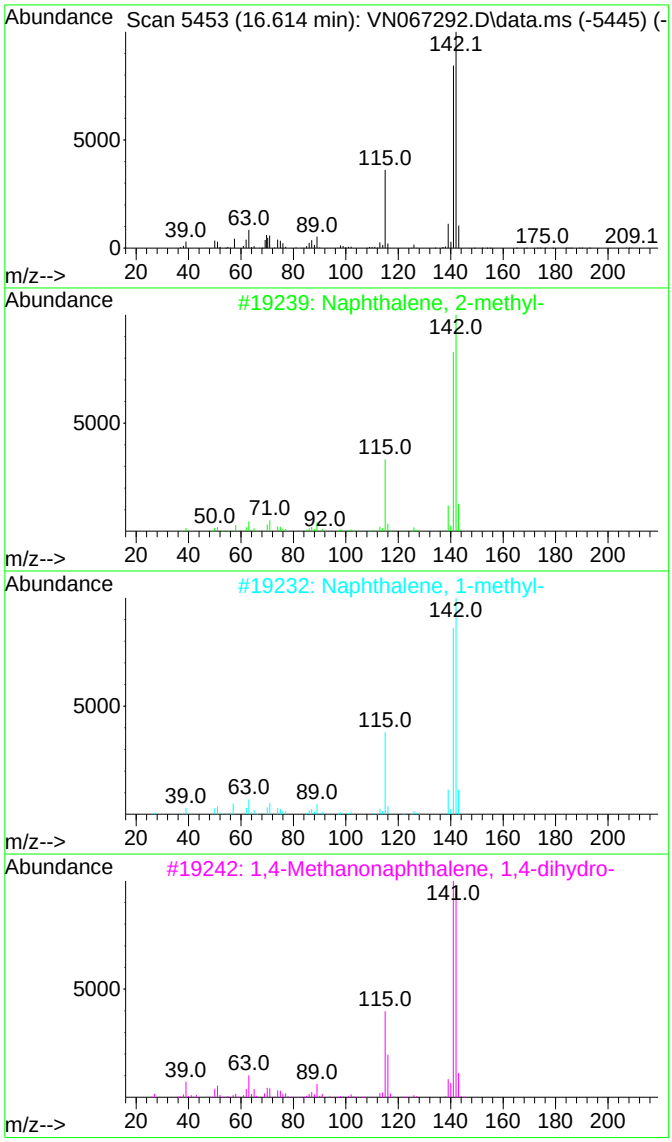
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

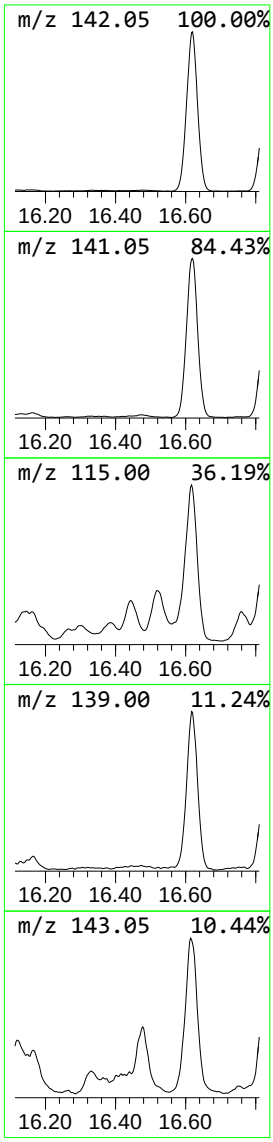
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	72.28 ug/l	3268110	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	93
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	93
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067292.D
Acq On : 11 Jun 2021 16:43
Operator : JC/MD
Sample : M2674-03 5X
Misc : 5.41g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 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	39.9	ug/l	1803790	4	13.675	2260880	50.0
2-Propenal, 3-p...	14.514	32.8	ug/l	1484510	4	13.675	2260880	50.0
Benzofuran, 2-m...	14.635	134.3	ug/l	6074650	4	13.675	2260880	50.0
Benzene, 2-ethe...	14.815	52.8	ug/l	2389430	4	13.675	2260880	50.0
2,4-Dimethylsty...	14.933	42.5	ug/l	1924100	4	13.675	2260880	50.0
Benzene, 1-buty...	14.997	34.8	ug/l	1572970	4	13.675	2260880	50.0
2-Methylindene	15.086	35.9	ug/l	1622460	4	13.675	2260880	50.0
2-Propenal, 2-m...	15.456	83.5	ug/l	3776770	4	13.675	2260880	50.0
1H-Benzimidazol...	15.587	106.8	ug/l	4829520	4	13.675	2260880	50.0
Naphthalene, 1-...	16.614	72.3	ug/l	3268110	4	13.675	2260880	50.0