LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	408	426	446	rBV2	340819	802484	9.70%	1.133%
2	4.248	812	842	882	rBV5	122597	553295	6.69%	0.781%
3	5.071	1114	1149	1227	rVB2	397543	1864019	22.52%	2.631%
4	5.382	1235	1265	1318	rBV3	953410	3440406	41.57%	4.856%
5	5.618	1323	1353	1394	rVV2	2345846	8275905	100.00%	11.680%
6	6.503	1657	1683	1705	rVB2	63474	205924	2.49%	0.291%
7	6.884	1802	1825	1844	rBV2	37271	115794	1.40%	0.163%
8	7.045	1863	1885	1905	rBV2	100170	295065	3.57%	0.416%
9	7.842	2145	2182	2206	rBV2	82398	261540	3.16%	0.369%
10	8.021	2220	2249	2260	rBV2	619505	1495682	18.07%	2.111%
11	8.086	2261	2273	2290	rVV	1085810	2523354	30.49%	3.561%
12	8.174	2291	2306	2334	rVB2	413661	1060431	12.81%	1.497%
13	8.357	2360	2374	2387	rVV2	110911	262664	3.17%	0.371%
14	8.440	2387	2405	2426	rVV2	802617	2008271	24.27%	2.834%
15	8.539	2426	2442	2461	rVV4	485477	1295604	15.66%	1.829%
16	8.628	2465	2475	2491	rVV7	142421	443694	5.36%	0.626%
17	8.705	2493	2504	2528	rVB3	175442	409419	4.95%	0.578%
18	8.968	2583	2602	2627	rBV	1729557	3717988	44.93%	5.247%
19	9.059	2630	2636	2651	rVB4	45277	84064	1.02%	0.119%
20	9.201	2674	2689	2699	rBV3	97380	204209	2.47%	0.288%
21	9.424	2753	2772	2796	rBV5	209668	569080	6.88%	0.803%
22	9.732	2863	2887	2901	rBV3	91226	225495	2.72%	0.318%
23	9.877	2927	2941	2963	rVB4	145516	314230	3.80%	0.443%
24	10.014	2965	2992	3004	rBV4	142886	406548	4.91%	0.574%
25	10.121	3020	3032	3046	rVB8	63212	131152	1.58%	0.185%
26	10.202	3047	3062	3068	rBV4	165478	313114	3.78%	0.442%
27	10.365	3112	3123	3134	rVB4	54749	107550	1.30%	0.152%
28	10.441	3134	3151	3180	rBV	2742027	5334107	64.45%	7.528%
29	10.550	3182	3192	3204	rBV2	151920	252159	3.05%	0.356%
30	10.781	3267	3278	3292	rBV3	110118	205153	2.48%	0.290%
31	10.862	3292	3308	3328	rVV5	268360	680372	8.22%	0.960%
32	10.947	3330	3340	3358	rVB6	42710	99108	1.20%	0.140%
33	11.130	3401	3408	3418	rVB3	73501	115078	1.39%	0.162%
34	11.259	3449	3456	3468	rVB4	76493	123178	1.49%	0.174%
35	11.452	3519	3528	3545	rVB4	56101	105617	1.28%	0.149%
36	11.744	3621	3637	3654	rBV	2348453	4292017	51.86%	6.057%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
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Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

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\82N122721W.M
Title : SW846 8260

37	11.841	3665	3673	3696	rVB9	101086	241731	2.92%	0.341%
38	11.959	3707	3717	3724	rBV3	46568	87106	1.05%	0.123%
39	12.731	3988	4005	4026	rBV	2016201	3577004	43.22%	5.048%
40	12.983	4091	4099	4105	rBV	61720	92582	1.12%	0.131%
41	13.058	4122	4127	4140	rVB2	60501	95645	1.16%	0.135%
42	13.222	4178	4188	4200	rBV2	49347	85594	1.03%	0.121%
43	13.367	4233	4242	4258	rVB	215624	370670	4.48%	0.523%
44	13.487	4274	4287	4303	rVB3	114561	273649	3.31%	0.386%
45	13.675	4342	4357	4384	rBV	1807438	3415728	41.27%	4.821%
46	13.839	4405	4418	4425	rBV	1740175	2787833	33.69%	3.935%
47	13.876	4426	4432	4442	rVB	1196017	1793556	21.67%	2.531%
48	14.002	4467	4479	4492	rVB	313243	512381	6.19%	0.723%
49	14.069	4492	4504	4516	rVB	200708	327458	3.96%	0.462%
50	14.150	4518	4534	4547	rBV3	345526	701883	8.48%	0.991%
51	14.217	4548	4559	4569	rBV	252976	402536	4.86%	0.568%
52	14.278	4570	4582	4590	rBV	719175	1208482	14.60%	1.706%
53	14.329	4590	4601	4617	rVB	2954719	4933681	59.62%	6.963%
54	14.463	4642	4651	4661	rVB2	106330	167172	2.02%	0.236%
55	14.539	4668	4679	4688	rBV	303001	477471	5.77%	0.674%
56	14.576	4690	4693	4701	rVV2	92153	98029	1.18%	0.138%
57	14.619	4702	4709	4717	rVV2	124532	157153	1.90%	0.222%
58	14.761	4752	4762	4770	rBV4	140633	222309	2.69%	0.314%
59	14.809	4770	4780	4806	rVB2	549948	1076815	13.01%	1.520%
60	14.933	4809	4826	4838	rBV4	239857	554670	6.70%	0.783%
61	14.997	4840	4850	4863	rVB4	174734	301408	3.64%	0.425%
62	15.083	4873	4882	4899	rBV7	79617	156766	1.89%	0.221%
63	15.196	4910	4924	4934	rBV4	430559	866650	10.47%	1.223%
64	15.311	4953	4967	4985	rVB3	488674	1210678	14.63%	1.709%
65	15.507	5030	5040	5052	rVB	148396	262241	3.17%	0.370%
66	15.614	5072	5080	5093	rBV9	62873	127142	1.54%	0.179%
67	15.804	5137	5151	5170	rBV2	314136	622321	7.52%	0.878%
68	16.108	5255	5264	5278	rBV2	95528	184769	2.23%	0.261%
69	16.193	5282	5296	5311	rVB3	133992	331971	4.01%	0.469%
70	16.620	5441	5455	5484	rVB2	217499	536792	6.49%	0.758%

Sum of corrected areas: 70855646

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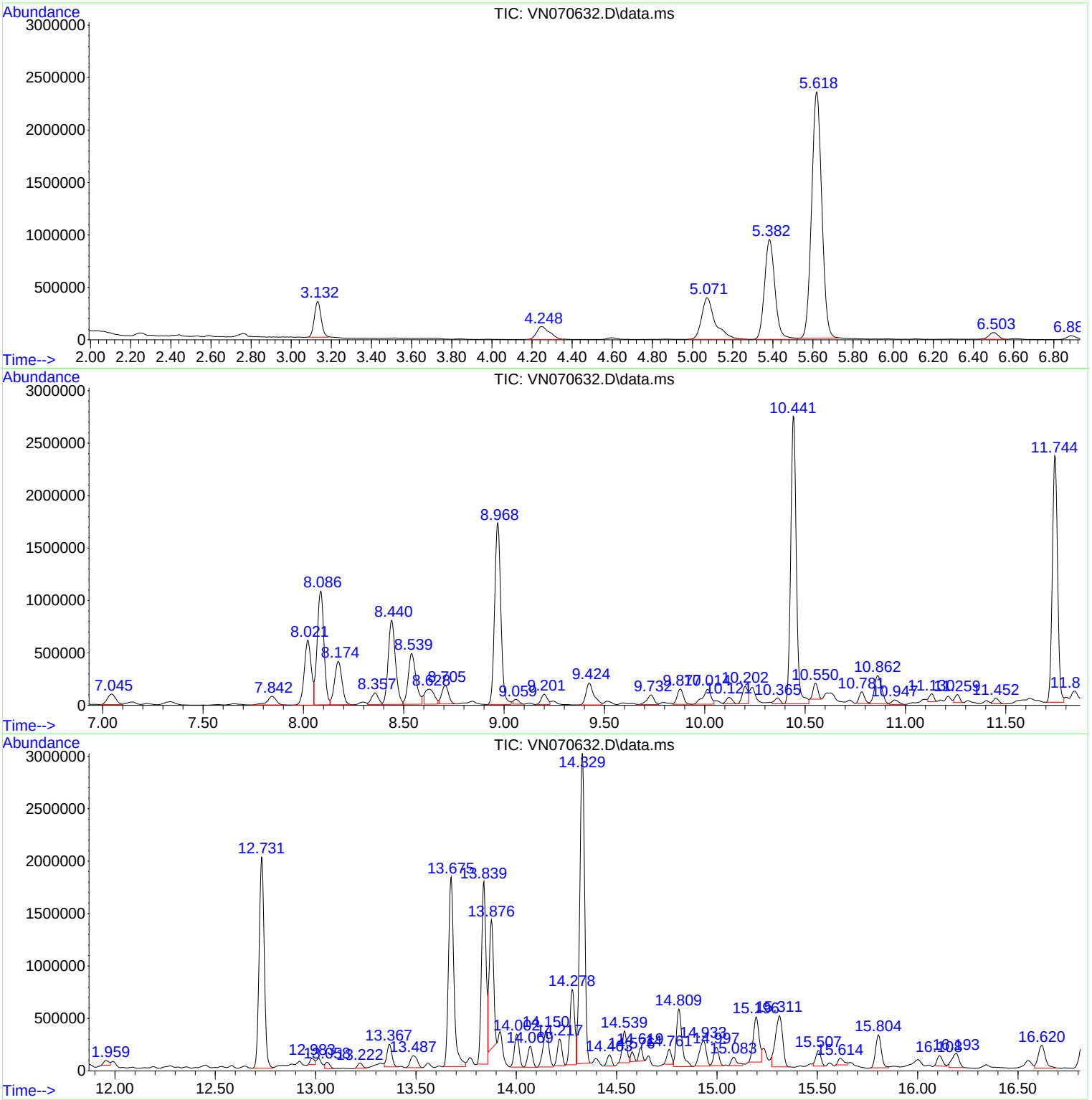
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
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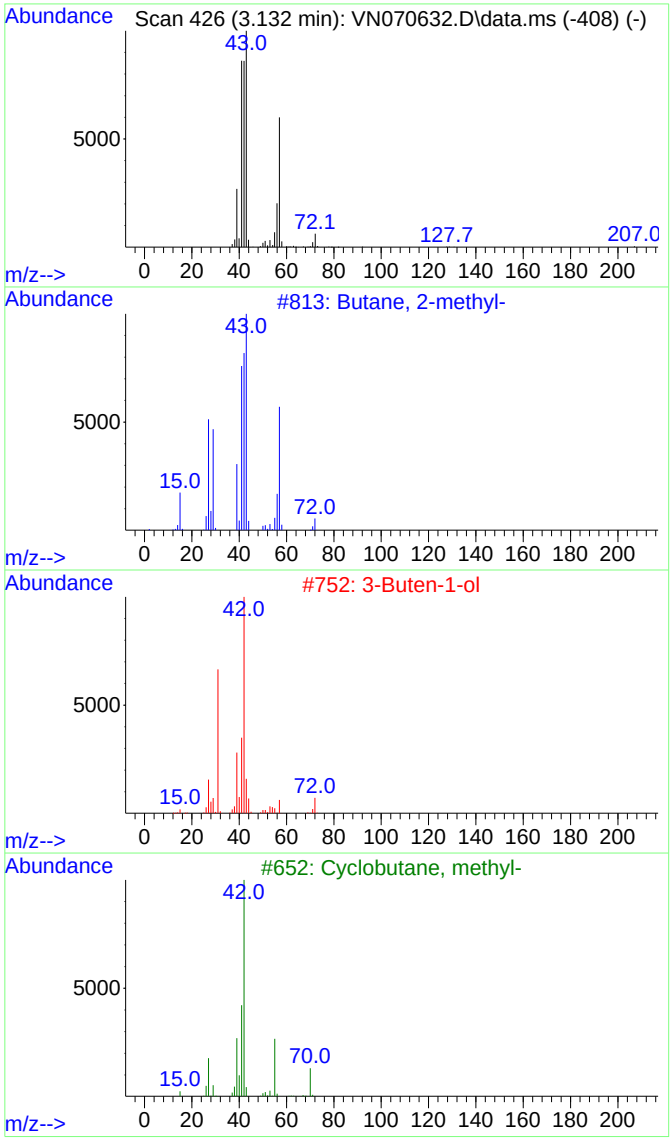
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

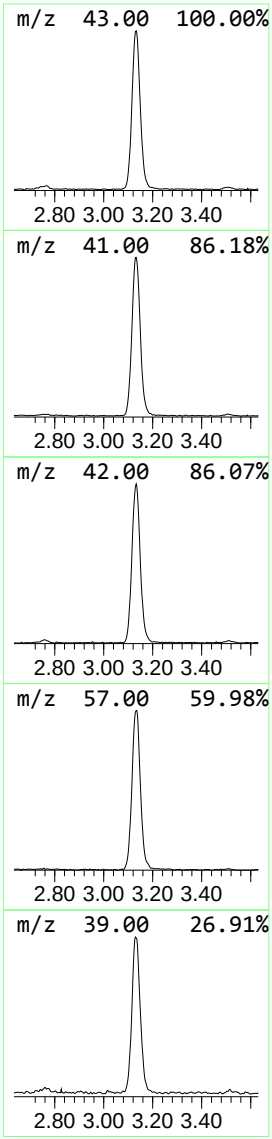
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.132	15.90 ug/l	802484	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	37
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5	Pentane	72	C5H12	000109-66-0	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

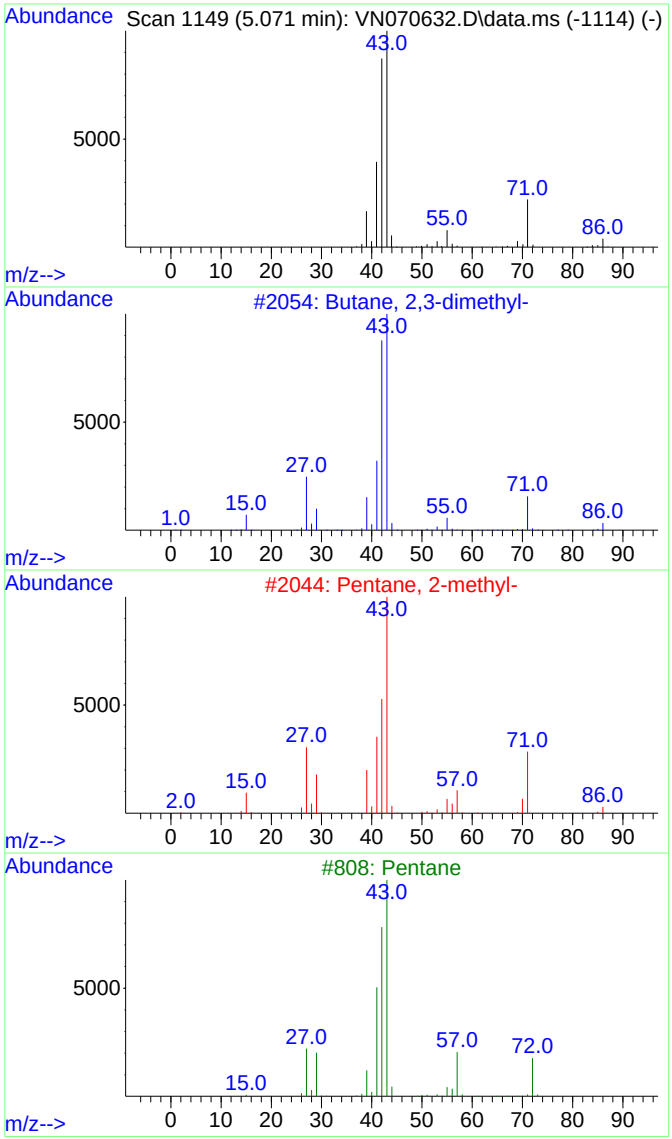
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

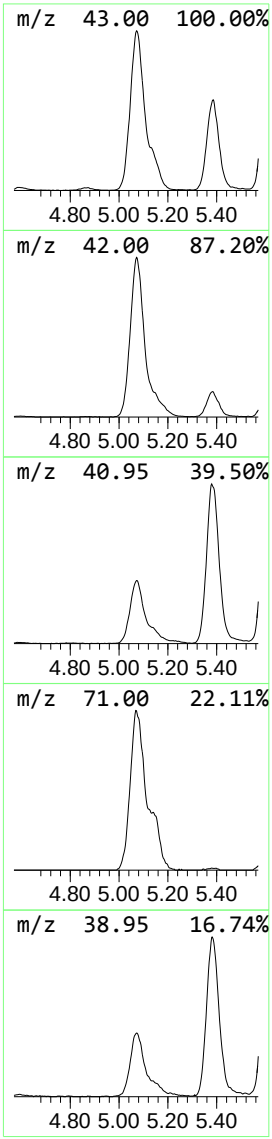
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.071	36.94 ug/l	1864020	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pentane	72	C5H12	000109-66-0	38
4	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	27
5	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

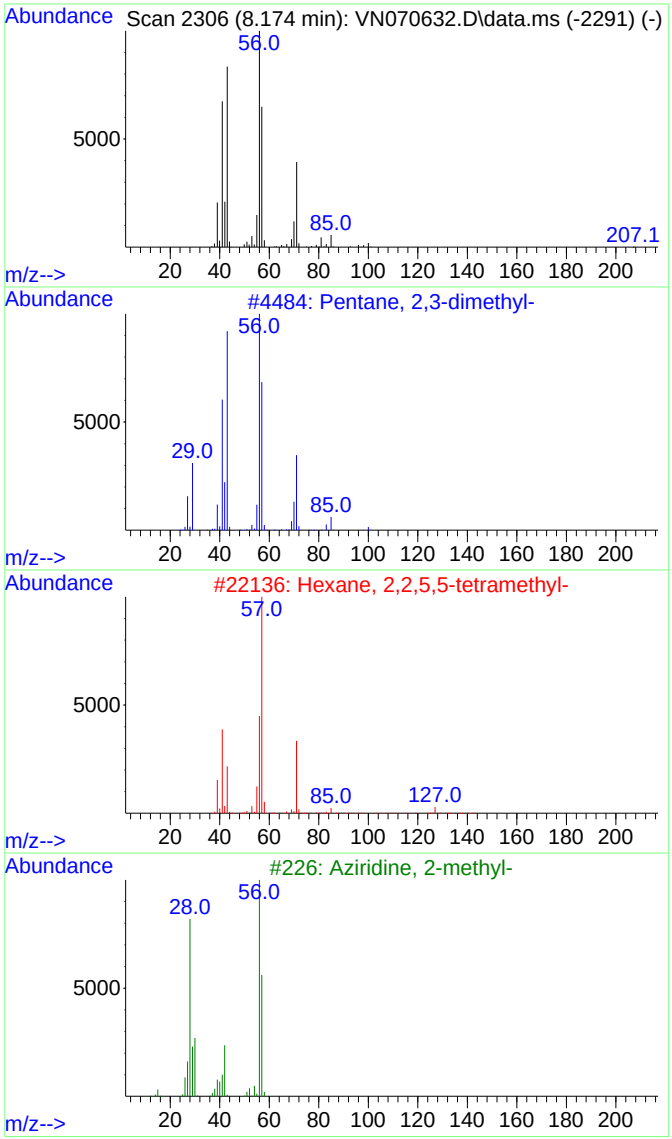
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

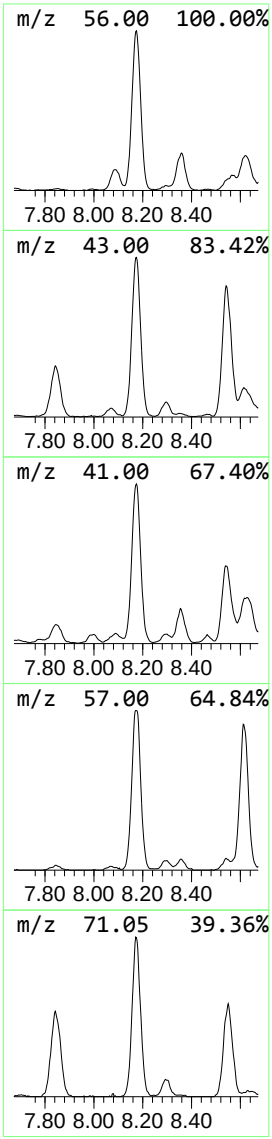
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	21.01 ug/l	1060430	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

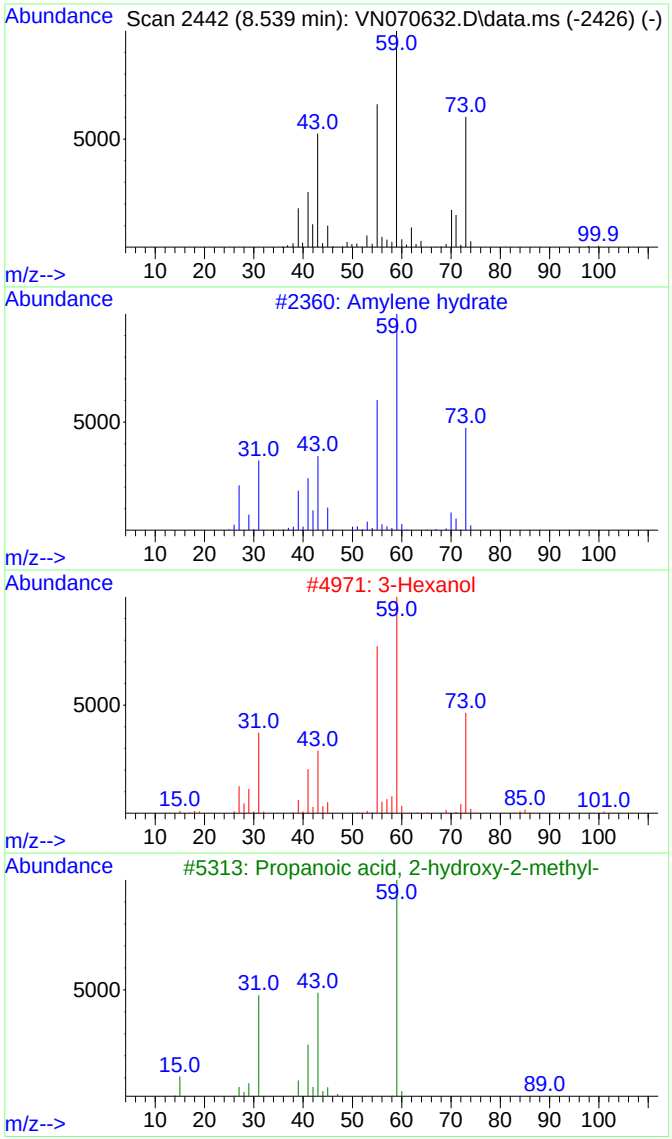
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

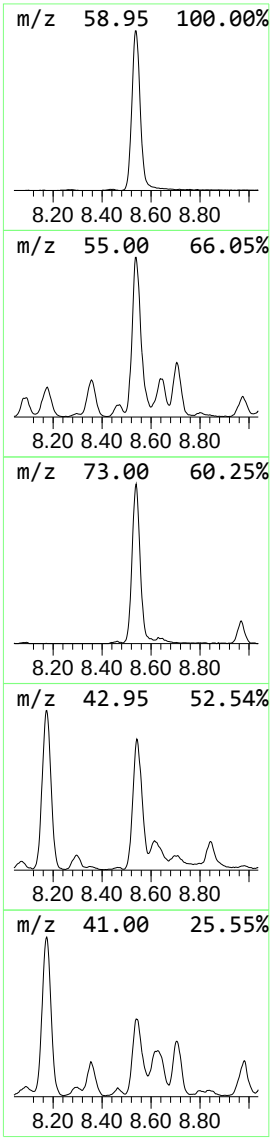
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Amylene hydrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	17.42 ug/l	1295600	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	53
2	3-Hexanol	102	C6H14O	000623-37-0	38
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	38
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	35
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	33





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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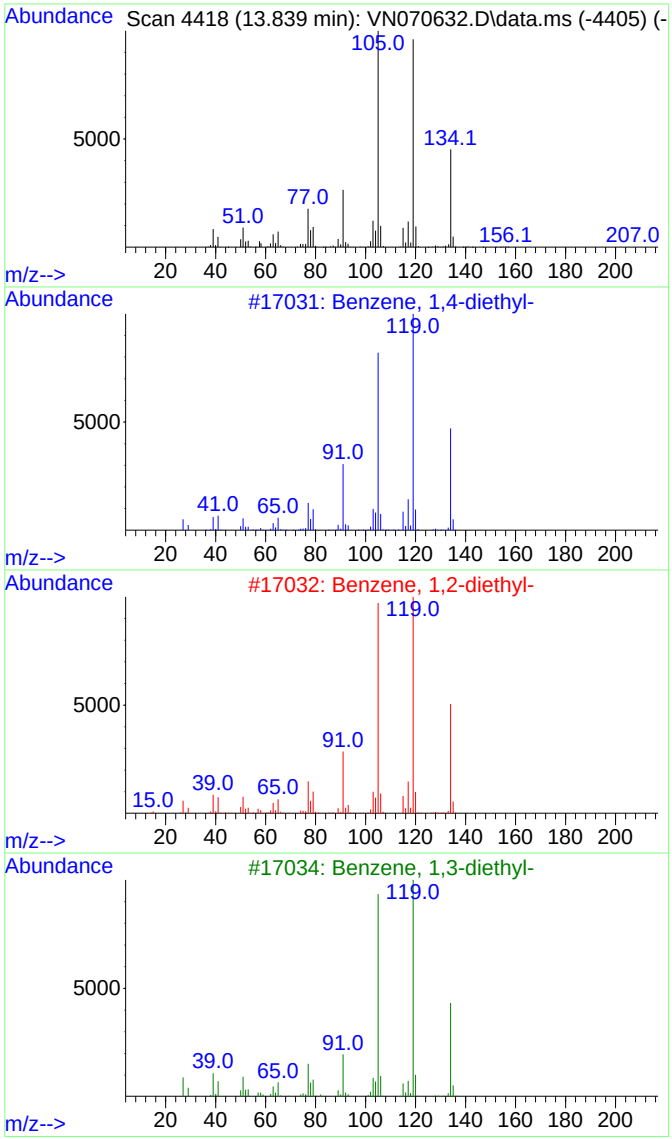
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

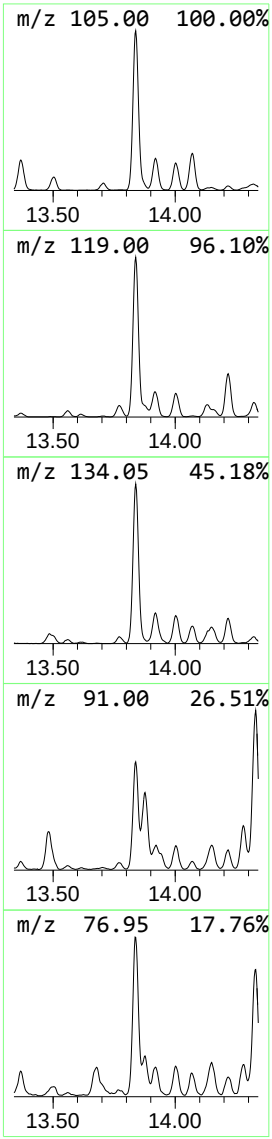
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,4-diethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	40.81 ug/l	2787830	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	83





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

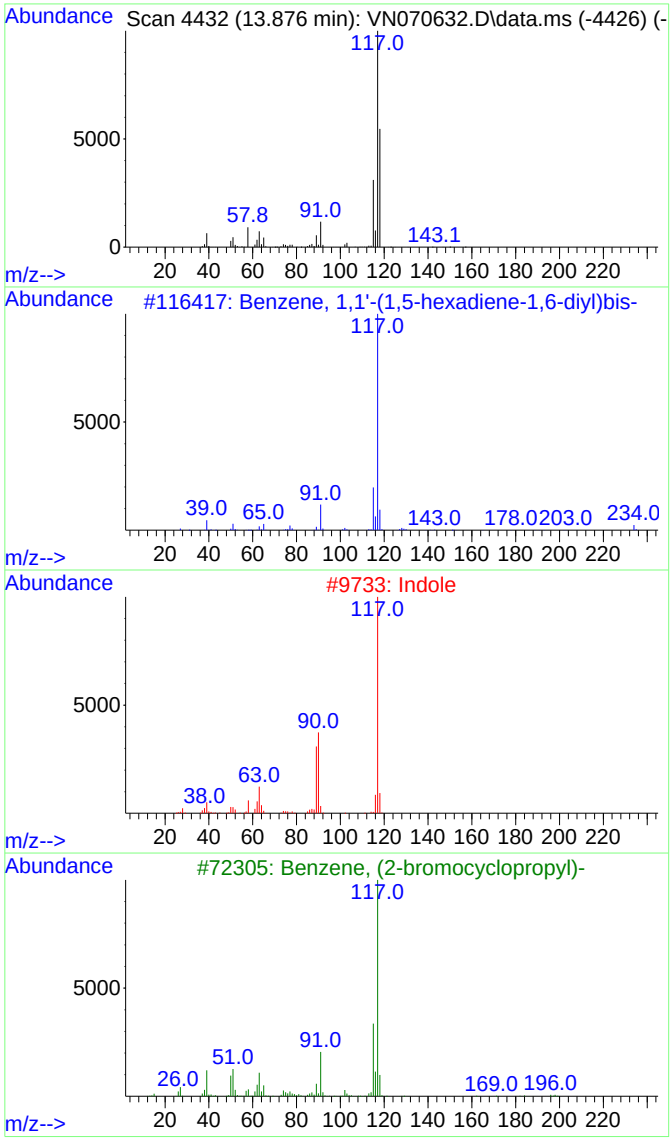
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

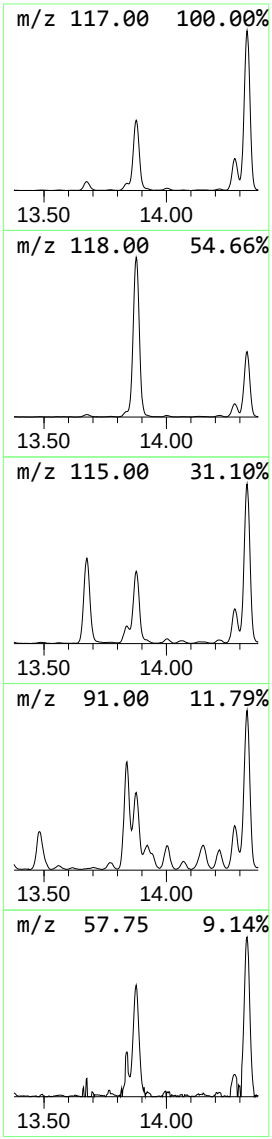
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	26.25 ug/l	1793560	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	Indole	117	C8H7N	000120-72-9	47
3	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	40
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	40
5	Benzyl nitrile	117	C8H7N	000140-29-4	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

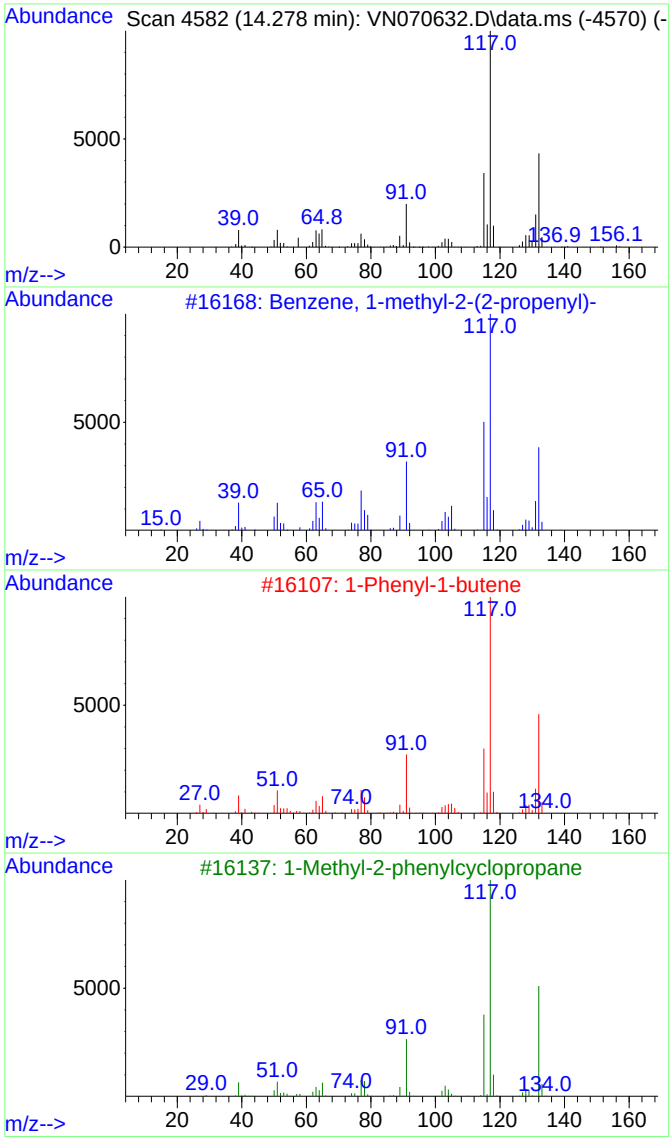
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

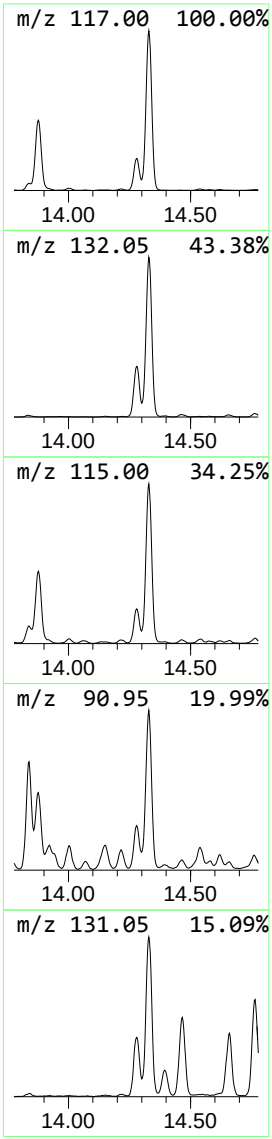
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.278	17.69 ug/l	1208480	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	93
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	93
5	Indan, 1-methyl-	132	C10H12	000767-58-8	91





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Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

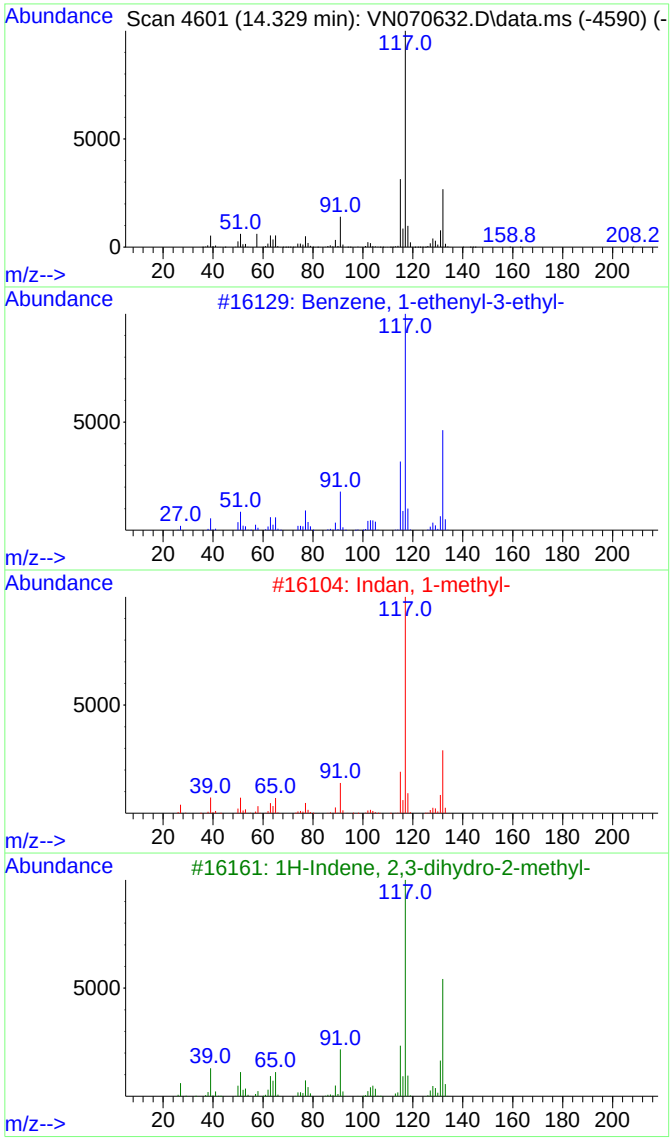
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

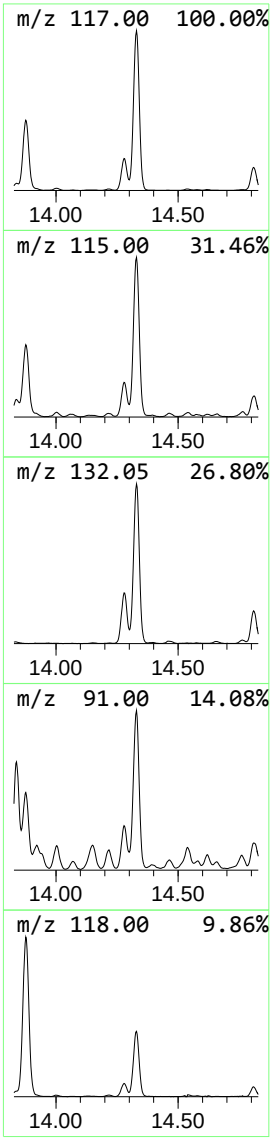
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	72.22 ug/l	4933680	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	86
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

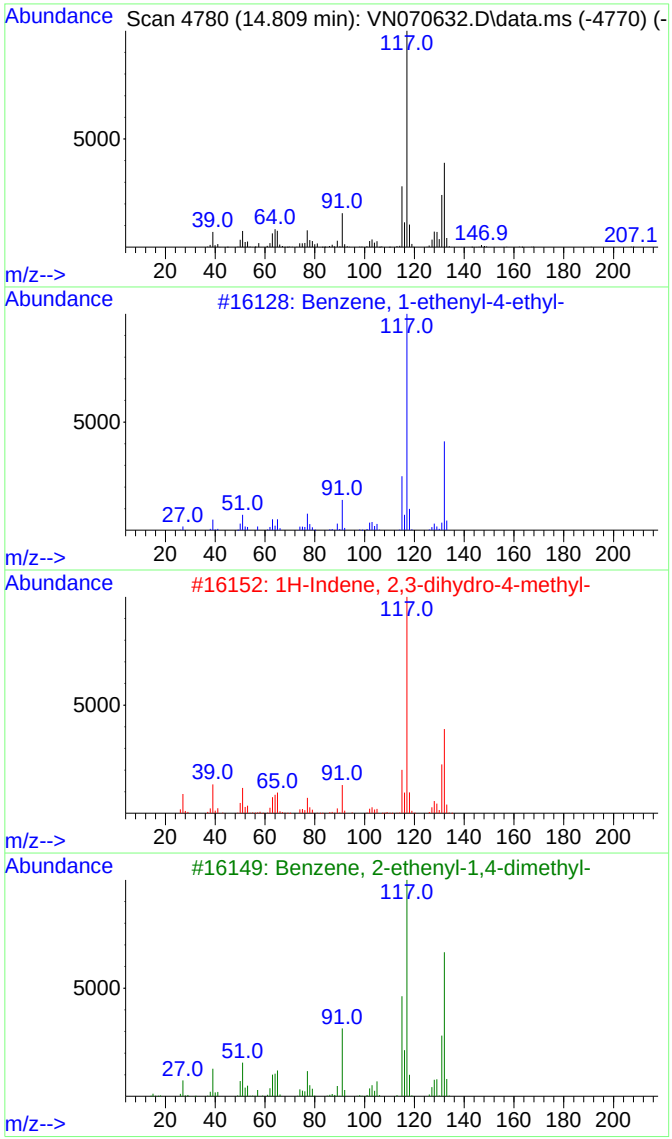
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

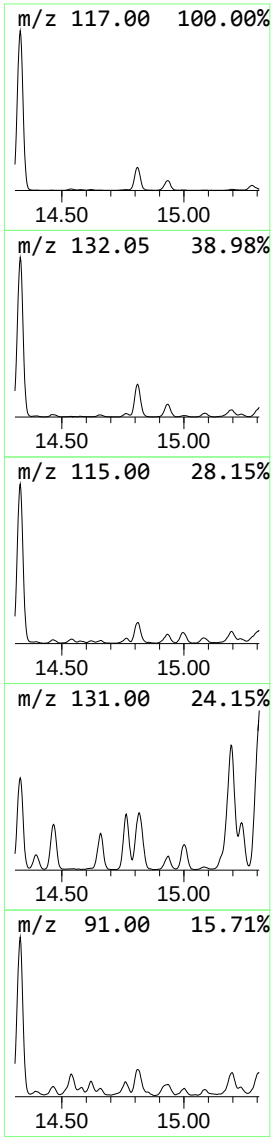
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	15.76 ug/l	1076820	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

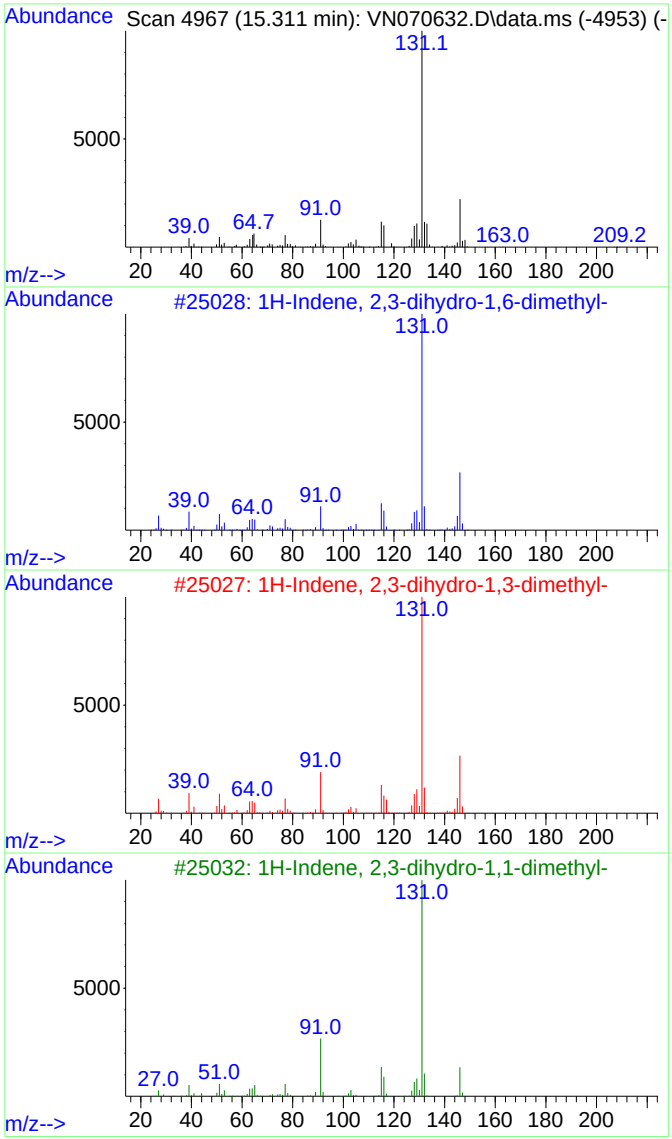
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

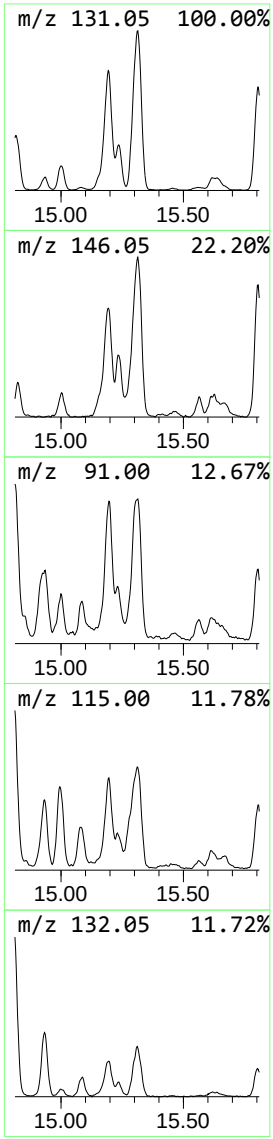
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.311	17.72 ug/l	1210680	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
2	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91
3	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	91
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070632.D
Acq On : 14 Jan 2022 19:03
Operator : JC/MD
Sample : N1148-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	3.132	15.9	ug/l	802484	1	8.086	2523350	50.0
Butane, 2,3-dim...	5.071	36.9	ug/l	1864020	1	8.086	2523350	50.0
Pentane, 2,3-di...	8.174	21.0	ug/l	1060430	1	8.086	2523350	50.0
Amylene hydrate	8.539	17.4	ug/l	1295600	2	8.968	3717990	50.0
Benzene, 1,4-di...	13.839	40.8	ug/l	2787830	4	13.675	3415730	50.0
Benzene, 1,1'-(...	13.876	26.3	ug/l	1793560	4	13.675	3415730	50.0
Benzene, 1-meth...	14.278	17.7	ug/l	1208480	4	13.675	3415730	50.0
Benzene, 1-ethe...	14.329	72.2	ug/l	4933680	4	13.675	3415730	50.0
Benzene, 1-ethe...	14.809	15.8	ug/l	1076820	4	13.675	3415730	50.0
1H-Indene, 2,3-...	15.311	17.7	ug/l	1210680	4	13.675	3415730	50.0