LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

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: VN070635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	160	168	186	rVB2	84533	136501	1.00%	0.098%
2	3.129	409	425	456	rVB	382467	899435	6.62%	0.648%
3	4.291	818	858	884	rBV2	98046	333502	2.46%	0.240%
4	5.076	1125	1151	1161	rBV4	52595	183711	1.35%	0.132%
5	5.382	1233	1265	1311	rBV	1168504	4175521	30.74%	3.006%
6	5.618	1321	1353	1408	rVB	3708150	13137104	96.71%	9.458%
7	7.147	1898	1923	1945	rBV3	158667	478854	3.53%	0.345%
8	7.345	1973	1997	2019	rBV2	52253	151514	1.12%	0.109%
9	7.842	2170	2182	2202	rVB3	54488	136130	1.00%	0.098%
10	8.021	2224	2249	2260	rBV2	680646	1681412	12.38%	1.211%
11	8.086	2261	2273	2294	rVB	1164920	2668912	19.65%	1.921%
12	8.442	2384	2406	2424	rBV3	1006533	2793642	20.57%	2.011%
13	8.536	2424	2441	2472	rVV	6022766	13584020	100.00%	9.780%
14	8.968	2582	2602	2629	rBV	1941884	4222649	31.09%	3.040%
15	9.129	2649	2662	2675	rVB2	95074	182569	1.34%	0.131%
16	9.461	2779	2786	2802	rVB6	73500	146865	1.08%	0.106%
17	9.971	2953	2976	2989	rBV4	296659	704503	5.19%	0.507%
18	10.237	3045	3075	3101	rBV	3367710	8697077	64.02%	6.261%
19	10.440	3136	3151	3164	rBV	2977228	5519986	40.64%	3.974%
20	10.505	3165	3175	3182	rVV	1027926	1868165	13.75%	1.345%
21	10.550	3182	3192	3213	rVB	3240582	6026332	44.36%	4.339%
22	10.810	3273	3289	3300	rBV3	86553	173103	1.27%	0.125%
23	11.089	3376	3393	3420	rBV	1196069	2270149	16.71%	1.634%
24	11.213	3428	3439	3448	rBV2	150569	279865	2.06%	0.201%
25	11.615	3572	3589	3618	rBV2	2006926	4718398	34.73%	3.397%
26	11.744	3619	3637	3661	rVV	7079241	13467409	99.14%	9.696%
27	11.846	3662	3675	3698	rVV	1481961	2958933	21.78%	2.130%
28	11.953	3699	3715	3740	rVV2	2213554	4951062	36.45%	3.565%
29	12.044	3742	3749	3773	rVB6	77768	164563	1.21%	0.118%
30	12.280	3819	3837	3851	rBV	1248008	2296297	16.90%	1.653%
31	12.355	3852	3865	3875	rVV	681554	1290434	9.50%	0.929%
32	12.398	3877	3881	3891	rVV	269258	381049	2.81%	0.274%
33	12.535	3920	3932	3939	rBV5	158968	299886	2.21%	0.216%
34	12.581	3940	3949	3967	rVB	297598	527849	3.89%	0.380%
35	12.656	3969	3977	3987	rVB2	154847	227072	1.67%	0.163%
36	12.731	3987	4005	4031	rVB5	3372116	6534795	48.11%	4.705%

LSC Area Percent Report

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Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

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	12.841	4032	4046	4058	rBV	1340034	2511551	18.49%	1.808%
38	12.892	4059	4065	4070	rBV2	160296	200571	1.48%	0.144%
39	12.983	4088	4099	4105	rBV	559296	910560	6.70%	0.656%
40	13.058	4118	4127	4146	rVB	965085	1723490	12.69%	1.241%
41	13.222	4172	4188	4199	rBV	687539	1197574	8.82%	0.862%
42	13.366	4221	4242	4257	rBV	1871902	3366503	24.78%	2.424%
43	13.450	4258	4273	4286	rBV4	206482	512540	3.77%	0.369%
44	13.672	4342	4356	4391	rVV2	2102992	4905013	36.11%	3.531%
45	13.801	4394	4404	4409	rVV2	327605	512495	3.77%	0.369%
46	13.836	4411	4417	4421	rVV	511549	691875	5.09%	0.498%
47	13.876	4422	4432	4466	rVB	2864022	5508733	40.55%	3.966%
48	14.066	4490	4503	4515	rVB2	93621	193781	1.43%	0.140%
49	14.133	4516	4528	4535	rBV2	155559	301142	2.22%	0.217%
50	14.217	4547	4559	4572	rVB	489956	800810	5.90%	0.577%
51	14.278	4572	4582	4590	rVV	143494	240000	1.77%	0.173%
52	14.329	4590	4601	4621	rVB	596440	1043613	7.68%	0.751%
53	14.538	4662	4679	4686	rBV	193293	341299	2.51%	0.246%
54	14.579	4686	4694	4706	rVB	302791	471464	3.47%	0.339%
55	14.807	4768	4779	4793	rBV2	248950	414798	3.05%	0.299%
56	14.930	4808	4825	4839	rBV3	561316	1061176	7.81%	0.764%
57	15.083	4870	4882	4900	rBV4	117200	218193	1.61%	0.157%
58	15.305	4953	4965	4986	rVB4	61302	145925	1.07%	0.105%
59	15.507	5022	5040	5061	rVV	1324573	2578904	18.98%	1.857%
60	15.606	5065	5077	5091	rVB	92709	178984	1.32%	0.129%
61	16.620	5439	5455	5482	rVB	247755	598893	4.41%	0.431%

Sum of corrected areas: 138899155

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Data File : VN070635.D
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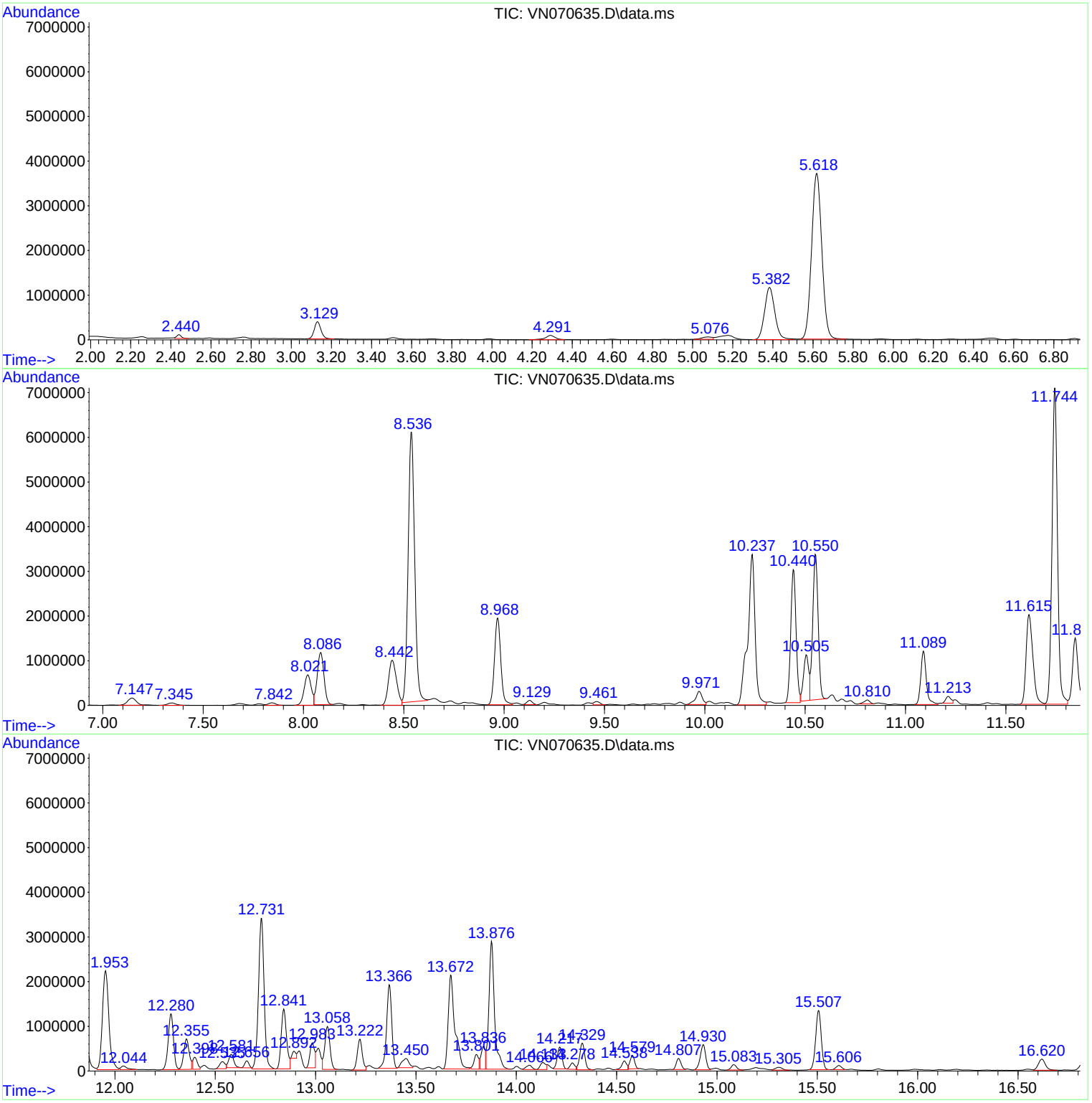
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

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 : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

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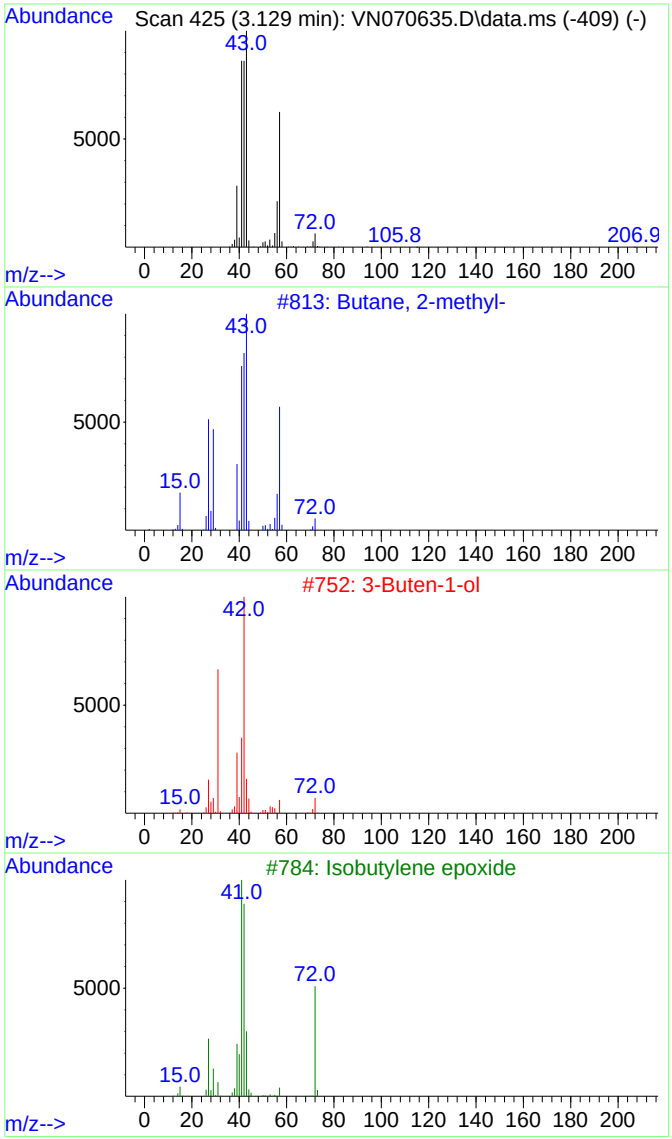
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

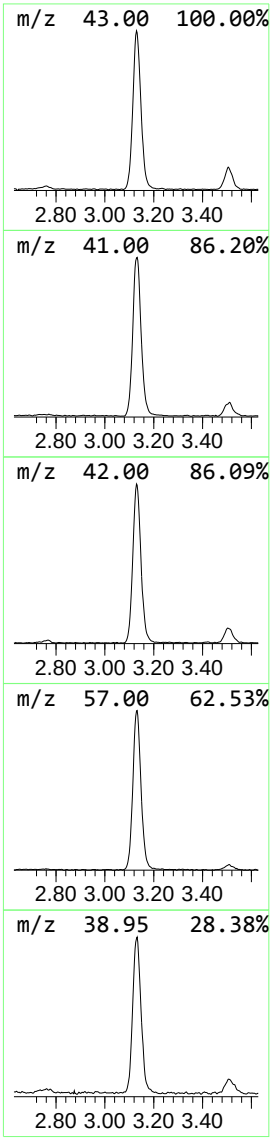
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.129	16.85 ug/l	899435	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Isobutylene epoxide	72	C4H8O	000558-30-5	42
4	Pentane	72	C5H12	000109-66-0	39
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

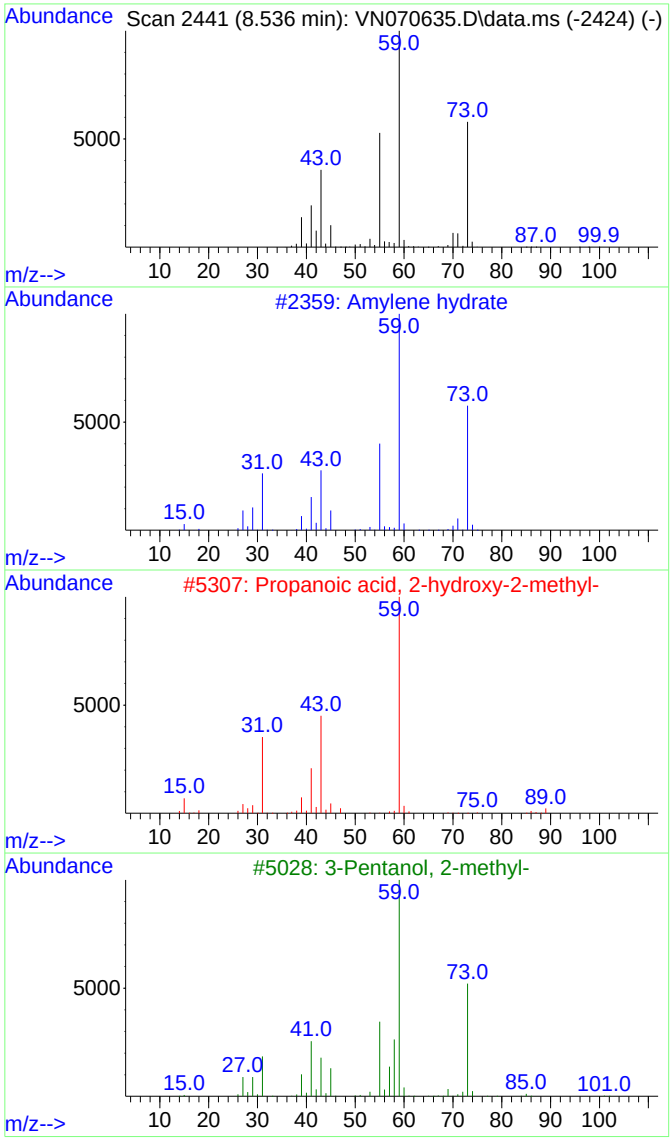
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

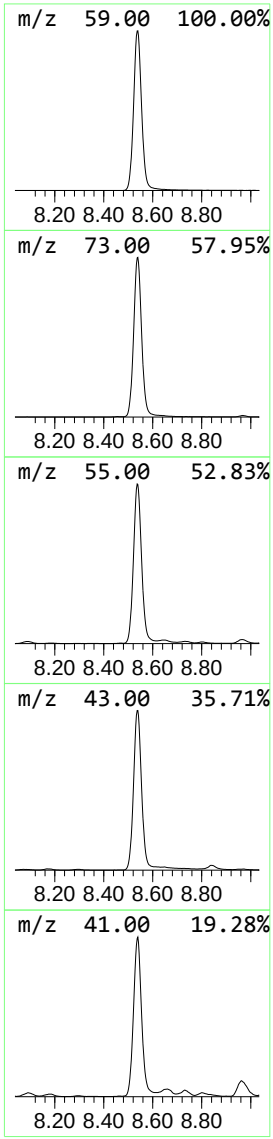
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.536	160.85 ug/l	13584000	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	40
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
4	Butanamide	87	C4H9NO	000541-35-5	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

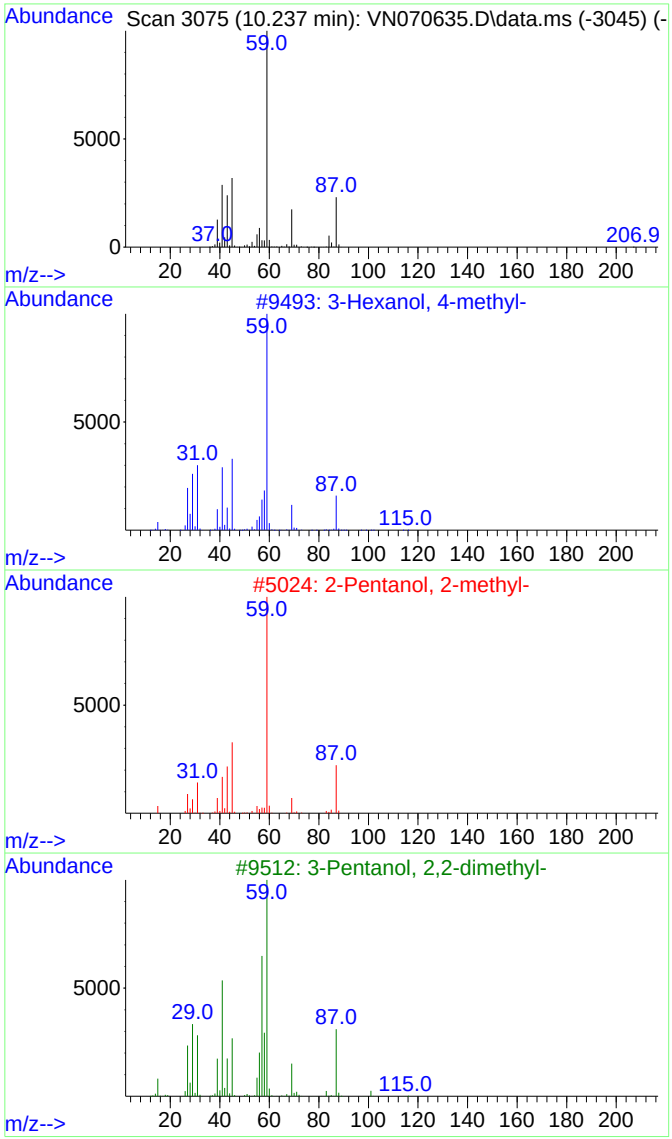
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

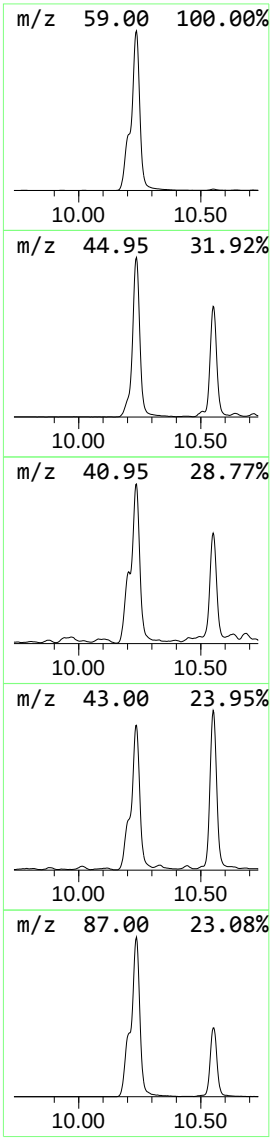
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Hexanol, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.236	102.98 ug/l	8697080	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	72
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

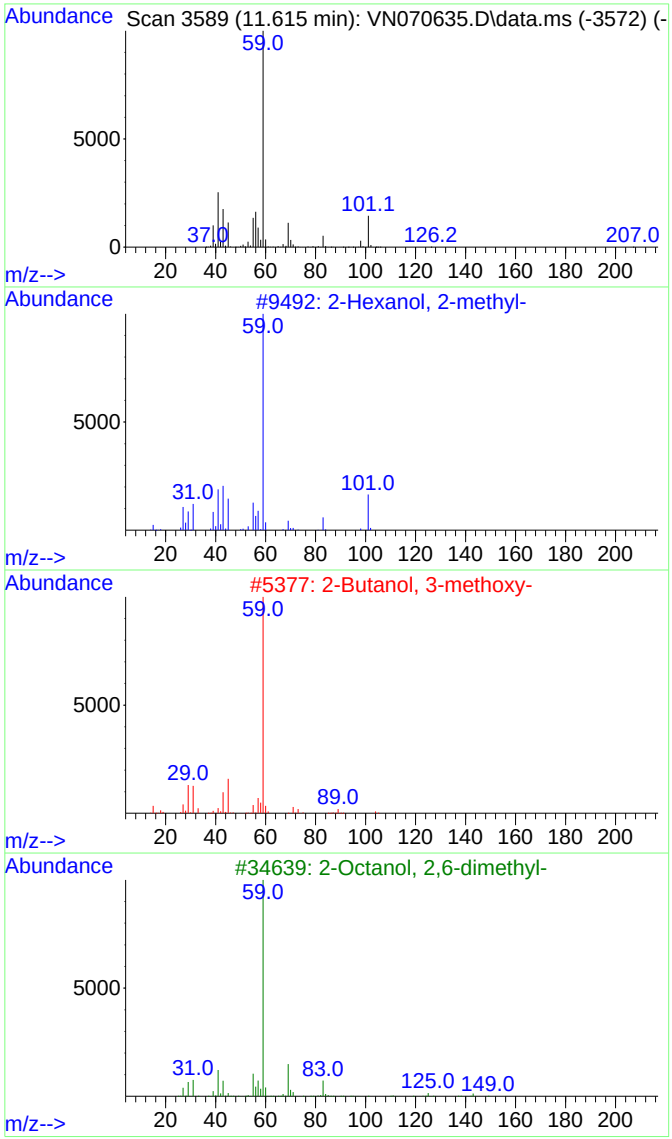
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

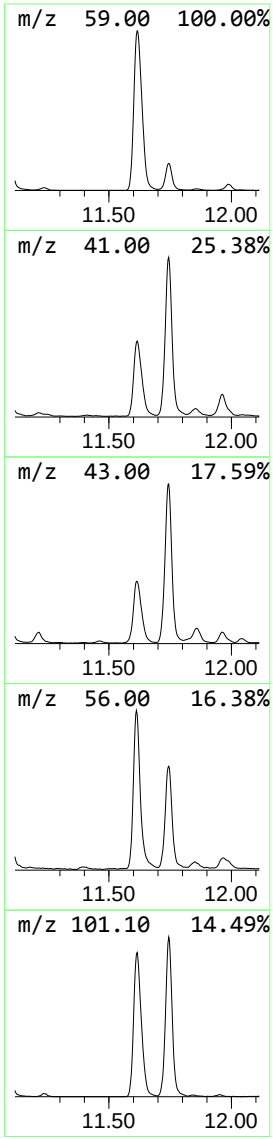
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Hexanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	17.52 ug/l	4718400	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	78
2	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	64
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	59
4	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	56
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	50





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Sample : N1148-08
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

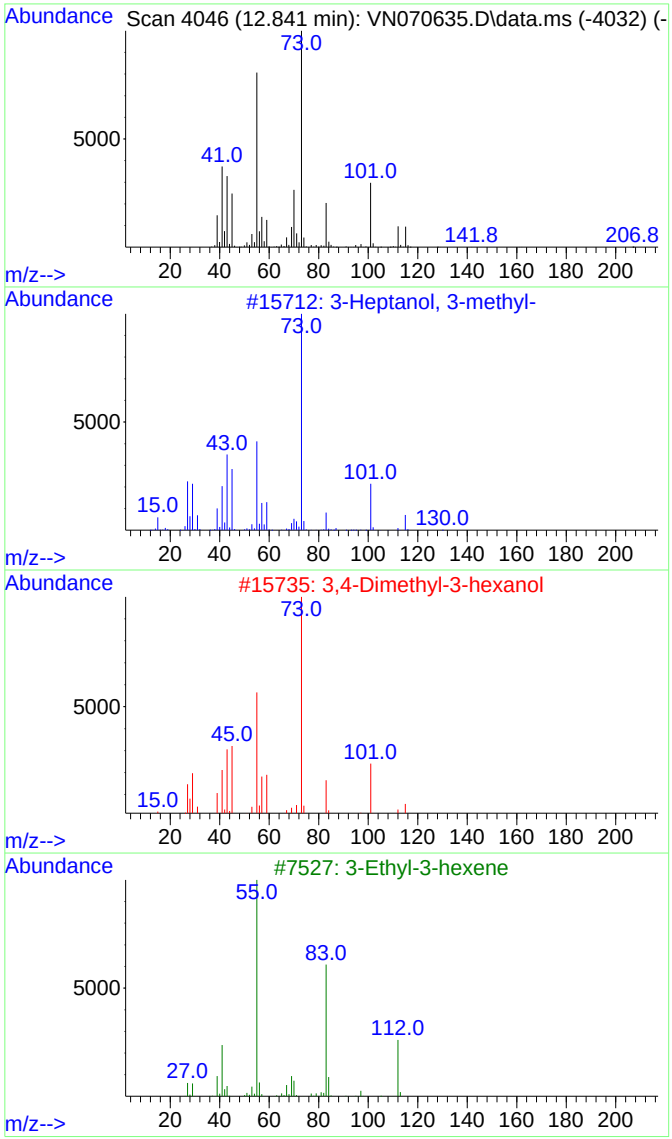
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

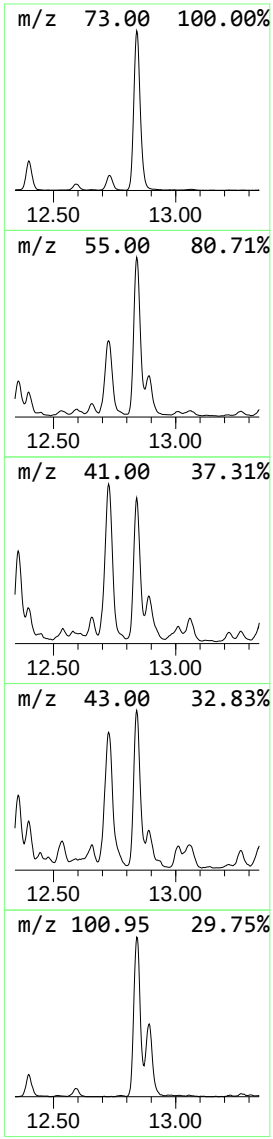
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown12.841 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	25.60 ug/l	2511550	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	38
2	3,4-Dimethyl-3-hexanol	130	C8H18O	019550-08-4	35
3	3-Ethyl-3-hexene	112	C8H16	016789-51-8	22
4	3-Heptene, 3-methyl-	112	C8H16	007300-03-0	18
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	14





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

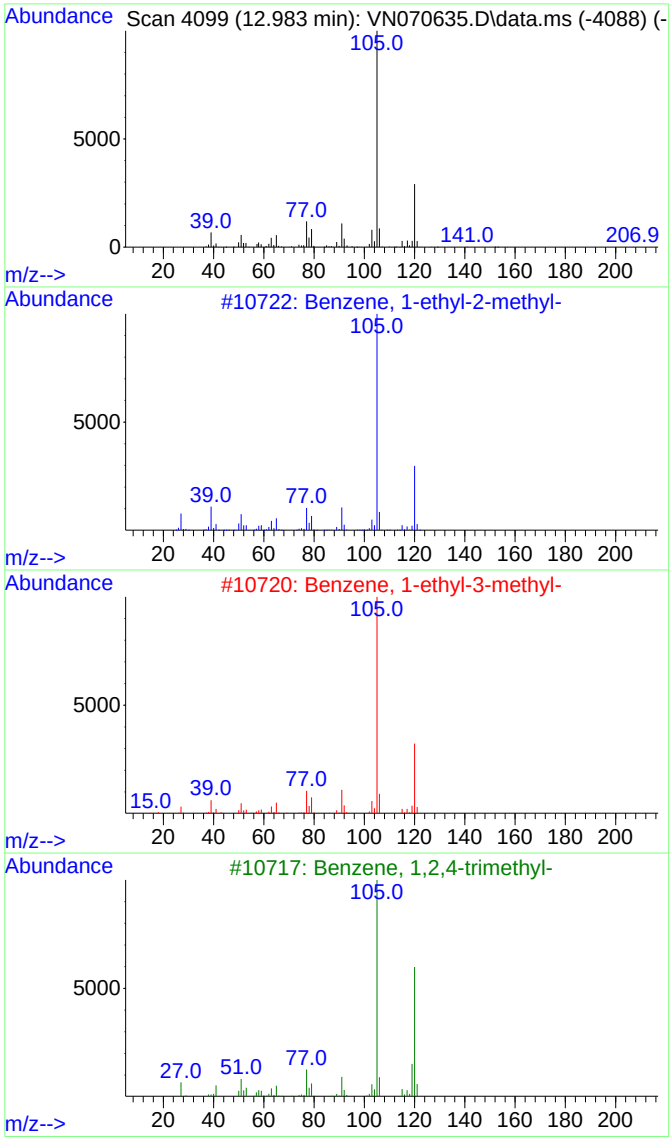
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

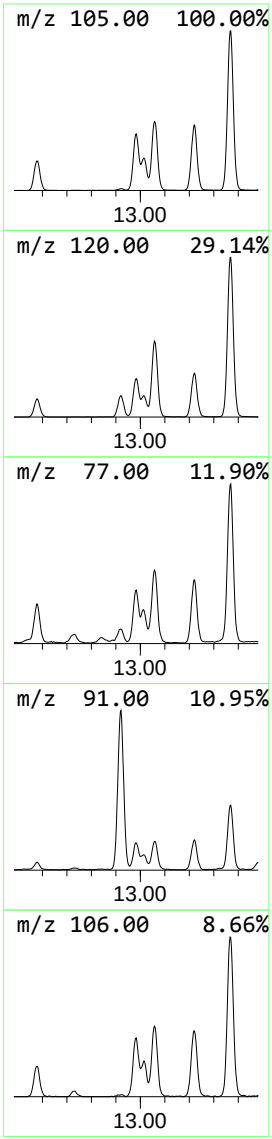
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	9.28 ug/l	910560	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	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

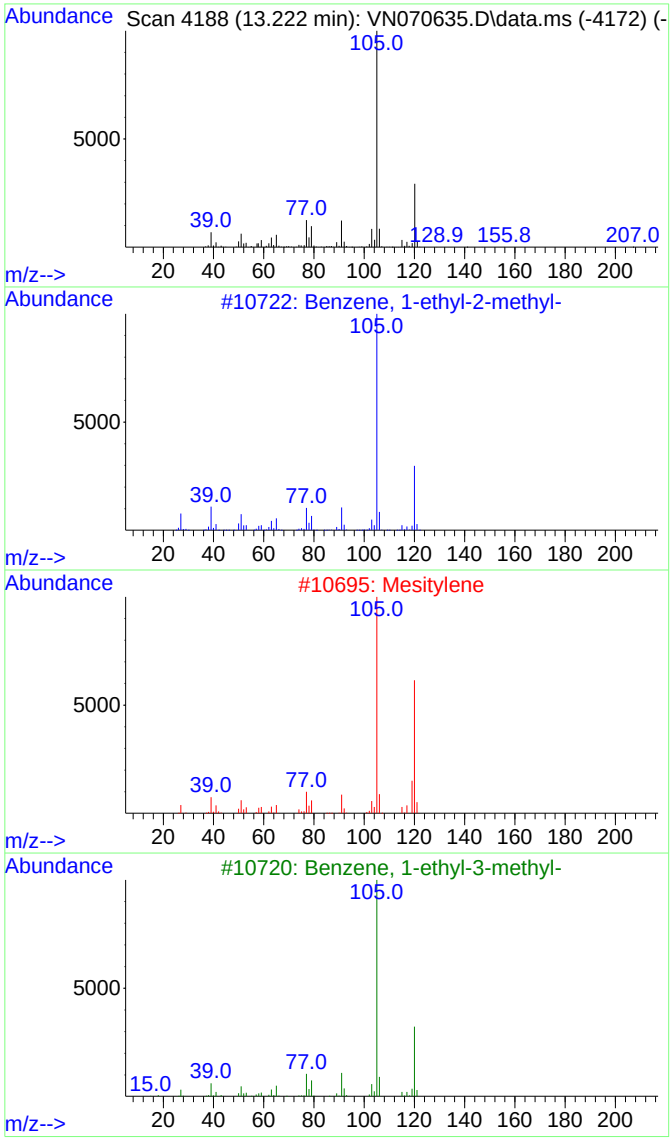
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

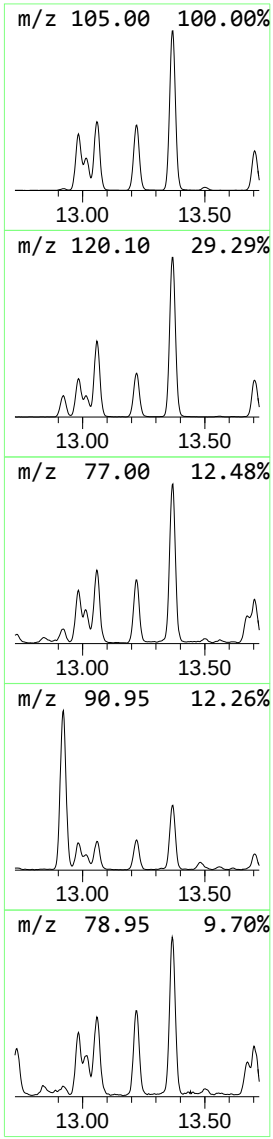
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	12.21 ug/l	1197570	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	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

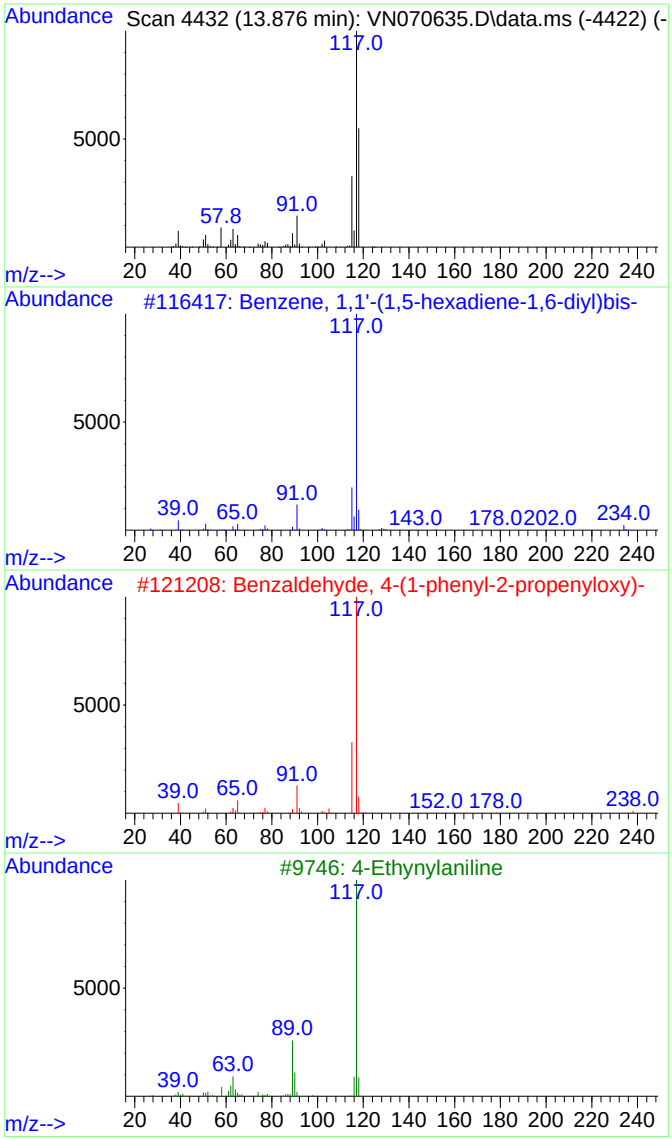
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

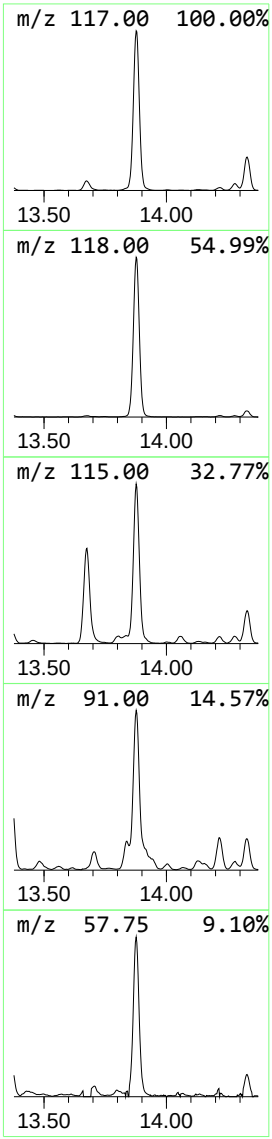
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	56.15 ug/l	5508730	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	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
3	4-Ethynylaniline	117	C8H7N	014235-81-5	47
4	Indole	117	C8H7N	000120-72-9	46
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43





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Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

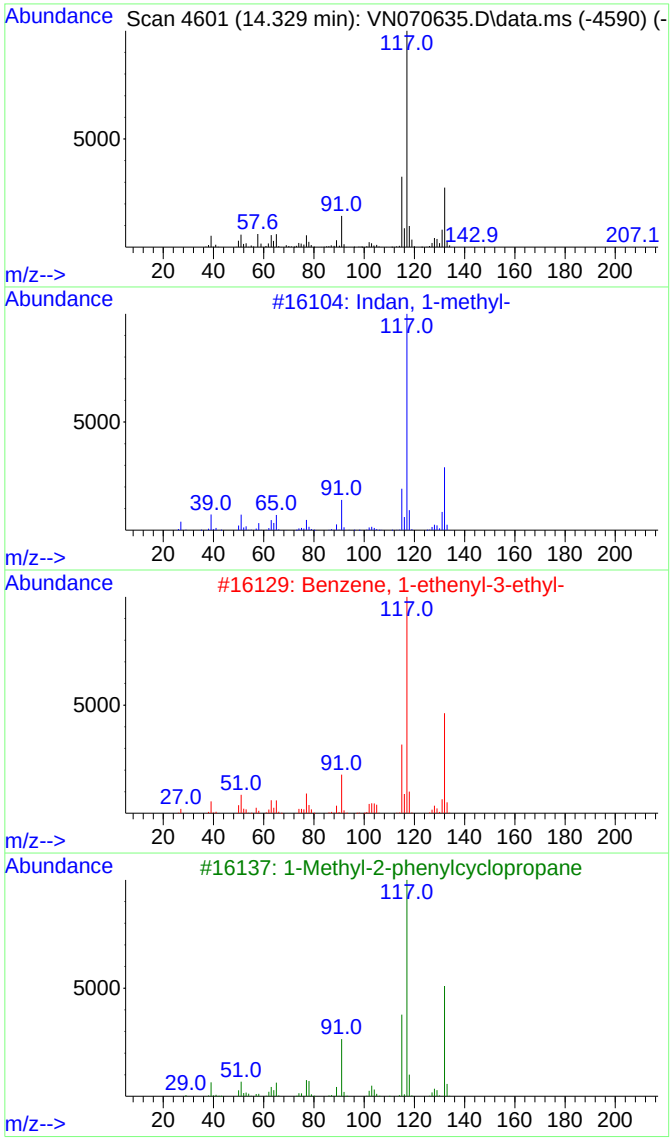
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

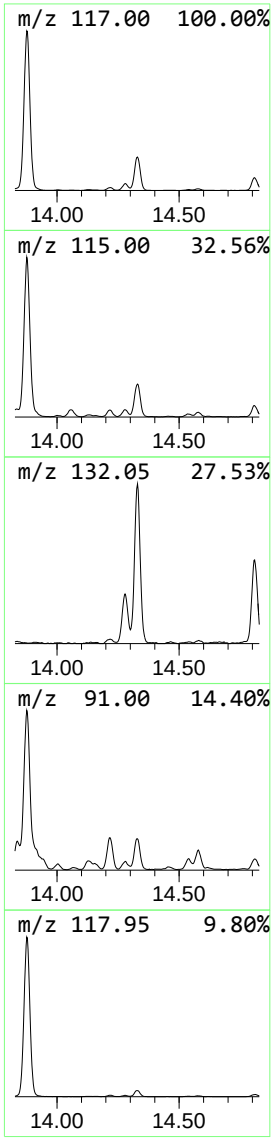
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	10.64 ug/l	1043610	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
Operator : JC/MD
Sample : N1148-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

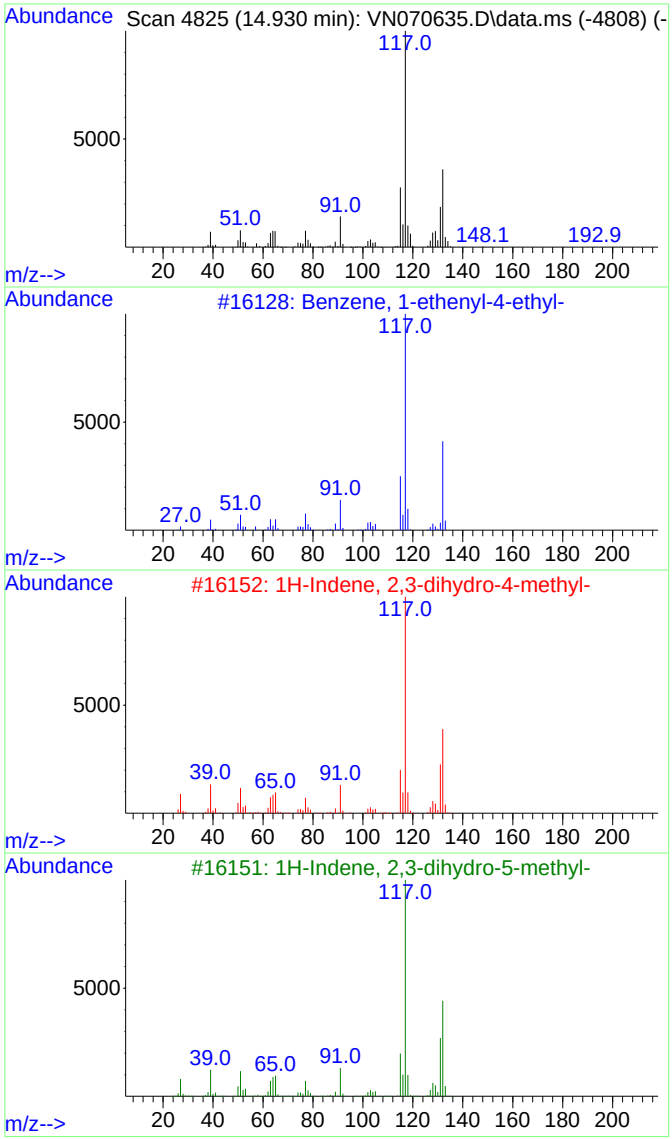
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

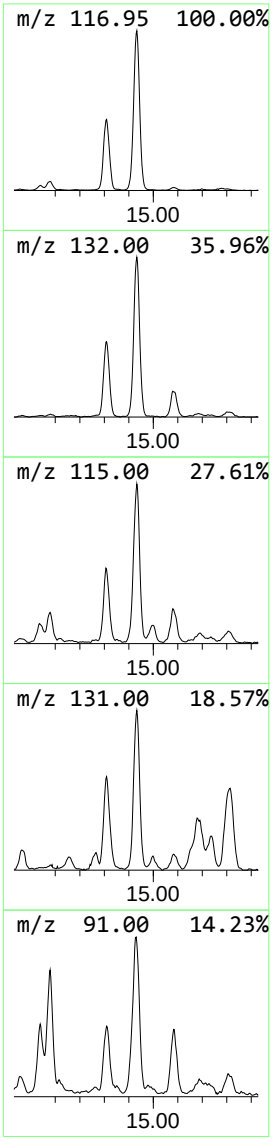
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	10.82 ug/l	1061180	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	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070635.D
Acq On : 14 Jan 2022 20:19
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

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-	3.129	16.9	ug/l	899435	1	8.086	2668910	50.0
Amylene hydrate	8.536	160.8	ug/l	13584000	2	8.968	4222650	50.0
3-Hexanol, 4-me...	10.236	103.0	ug/l	8697080	2	8.968	4222650	50.0
2-Hexanol, 2-me...	11.615	17.5	ug/l	4718400	3	11.744	13467400	50.0
unknown12.841	12.841	25.6	ug/l	2511550	4	13.675	4905010	50.0
Benzene, 1-ethy...	12.983	9.3	ug/l	910560	4	13.675	4905010	50.0
Benzene, 1-ethy...	13.222	12.2	ug/l	1197570	4	13.675	4905010	50.0
Benzene, 1,1'-(...	13.876	56.1	ug/l	5508730	4	13.675	4905010	50.0
Indan, 1-methyl-	14.329	10.6	ug/l	1043610	4	13.675	4905010	50.0
Benzene, 1-ethe...	14.930	10.8	ug/l	1061180	4	13.675	4905010	50.0