LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN069921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.143	412	430	459	rVB	1045656	2382343	4.63%	0.923%
2	3.529	552	574	598	rBV4	167282	561771	1.09%	0.218%
3	3.993	723	747	776	rVB	529625	1439336	2.79%	0.557%
4	4.961	1083	1108	1128	rBV3	190319	631746	1.23%	0.245%
5	5.189	1172	1193	1232	rVB2	888824	3545628	6.88%	1.373%
6	5.374	1236	1262	1309	rVV2	1761363	6248956	12.13%	2.420%
7	5.618	1327	1353	1396	rVB2	1018947	3605548	7.00%	1.397%
8	6.476	1647	1673	1702	rBV5	357294	1347733	2.62%	0.522%
9	6.608	1702	1722	1739	rVV3	212041	648238	1.26%	0.251%
10	6.906	1812	1833	1857	rVV4	264590	755210	1.47%	0.293%
11	7.147	1899	1923	1941	rBV2	1406602	4154596	8.07%	1.609%
12	7.844	2167	2183	2209	rVB2	783552	1918121	3.72%	0.743%
13	8.021	2225	2249	2260	rBV	954891	2311233	4.49%	0.895%
14	8.088	2261	2274	2294	rVV2	2408408	5970544	11.59%	2.313%
15	8.177	2298	2307	2330	rVB5	211640	532682	1.03%	0.206%
16	8.461	2386	2413	2432	rBV	21342977	51502761	100.00%	19.949%
17	8.968	2582	2602	2632	rBV	3008364	6847469	13.30%	2.652%
18	9.244	2697	2705	2725	rVB	286557	589339	1.14%	0.228%
19	9.459	2755	2785	2802	rBV5	452366	1376211	2.67%	0.533%
20	9.971	2960	2976	2987	rBV2	621485	1231891	2.39%	0.477%
21	10.199	3047	3061	3068	rBV	610975	1183358	2.30%	0.458%
22	10.322	3094	3107	3120	rBV	610605	1071217	2.08%	0.415%
23	10.440	3134	3151	3165	rBV	4420391	8329747	16.17%	3.226%
24	10.505	3165	3175	3184	rVV	918380	1707685	3.32%	0.661%
25	10.550	3185	3192	3207	rVB2	535255	947697	1.84%	0.367%
26	10.856	3293	3306	3327	rVV3	334567	705585	1.37%	0.273%
27	11.130	3397	3408	3429	rVB	1189804	2100051	4.08%	0.813%
28	11.615	3570	3589	3618	rVB5	307630	1052626	2.04%	0.408%
29	11.744	3618	3637	3661	rBV	5128661	10001557	19.42%	3.874%
30	11.843	3662	3674	3695	rVV	1896934	3536198	6.87%	1.370%
31	11.948	3697	3713	3740	rVV	9932283	19086635	37.06%	7.393%
32	12.087	3756	3765	3789	rVB5	334712	680850	1.32%	0.264%
33	12.278	3827	3836	3852	rVB	409525	710476	1.38%	0.275%
34	12.578	3935	3948	3963	rVB	3654243	6035097	11.72%	2.338%
35	12.731	3990	4005	4030	rVB	4135700	7420247	14.41%	2.874%
36	12.919	4061	4075	4095	rVB	8459039	14029211	27.24%	5.434%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

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\82N120221W.M
Title : SW846 8260

37	13.058	4119	4127	4143	rVB	406838	716080	1.39%	0.277%
38	13.219	4174	4187	4209	rBV	1479171	2578072	5.01%	0.999%
39	13.364	4232	4241	4257	rVB2	313287	579182	1.12%	0.224%
40	13.498	4276	4291	4304	rVB3	352744	844776	1.64%	0.327%
41	13.672	4342	4356	4386	rBV2	4576959	10026991	19.47%	3.884%
42	13.838	4405	4418	4421	rBV	1821641	2507746	4.87%	0.971%
43	13.876	4421	4432	4467	rVB	16122310	29203030	56.70%	11.311%
44	14.002	4468	4479	4492	rVB2	349951	554322	1.08%	0.215%
45	14.217	4545	4559	4571	rBV	1858948	2962140	5.75%	1.147%
46	14.278	4571	4582	4589	rVV	693691	1162092	2.26%	0.450%
47	14.327	4589	4600	4618	rVB	4103676	6881940	13.36%	2.666%
48	14.538	4666	4679	4701	rBV	1275657	2204076	4.28%	0.854%
49	14.809	4768	4780	4795	rVB	1738860	2838154	5.51%	1.099%
50	14.930	4807	4825	4839	rBV3	2615495	5126266	9.95%	1.986%
51	15.083	4870	4882	4899	rBV2	515164	930603	1.81%	0.360%
52	15.193	4912	4923	4934	rBV4	352798	626271	1.22%	0.243%
53	15.311	4953	4967	4989	rVB3	363017	904778	1.76%	0.350%
54	15.504	5021	5039	5057	rBV	5503957	10512646	20.41%	4.072%
55	16.617	5440	5454	5481	rVB	355621	819287	1.59%	0.317%

Sum of corrected areas: 258178045

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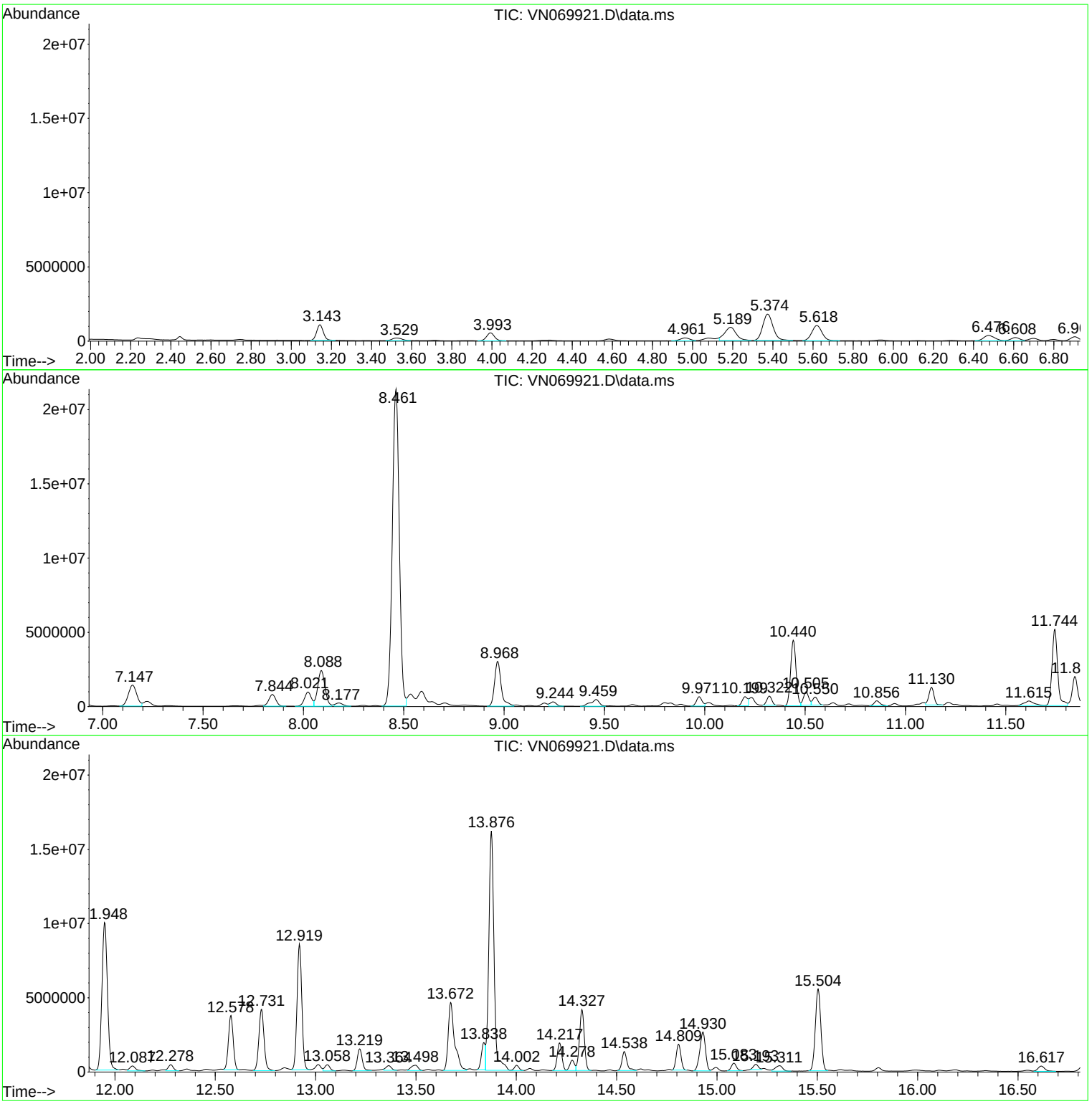
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

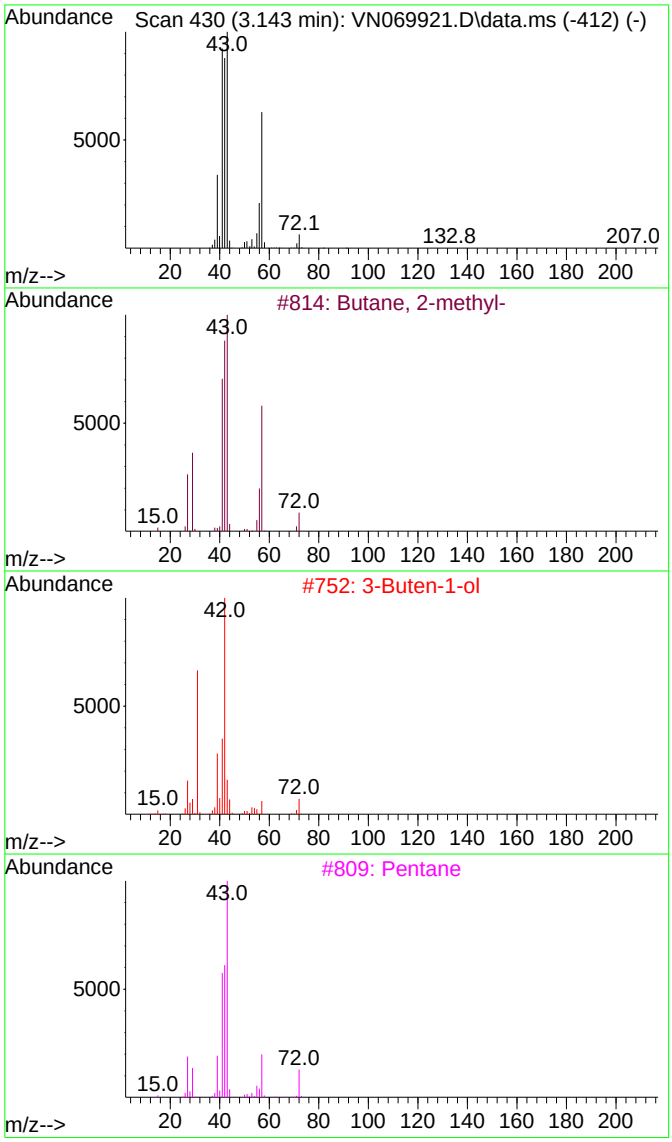
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

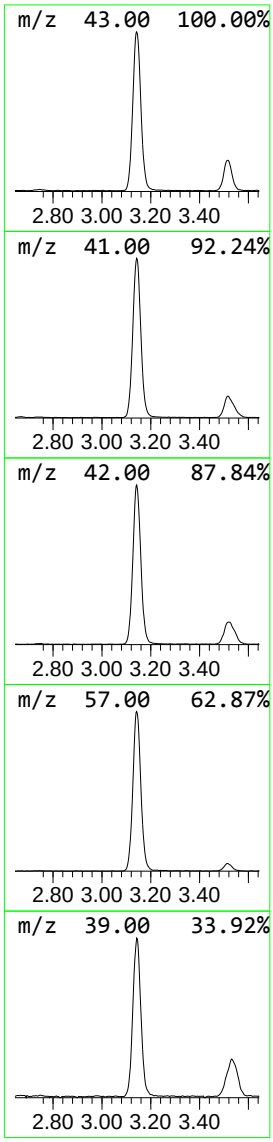
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	19.95 ug/l	2382340	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	47
3	Pentane	72	C5H12	000109-66-0	36
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5	1-Butene	56	C4H8	000106-98-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

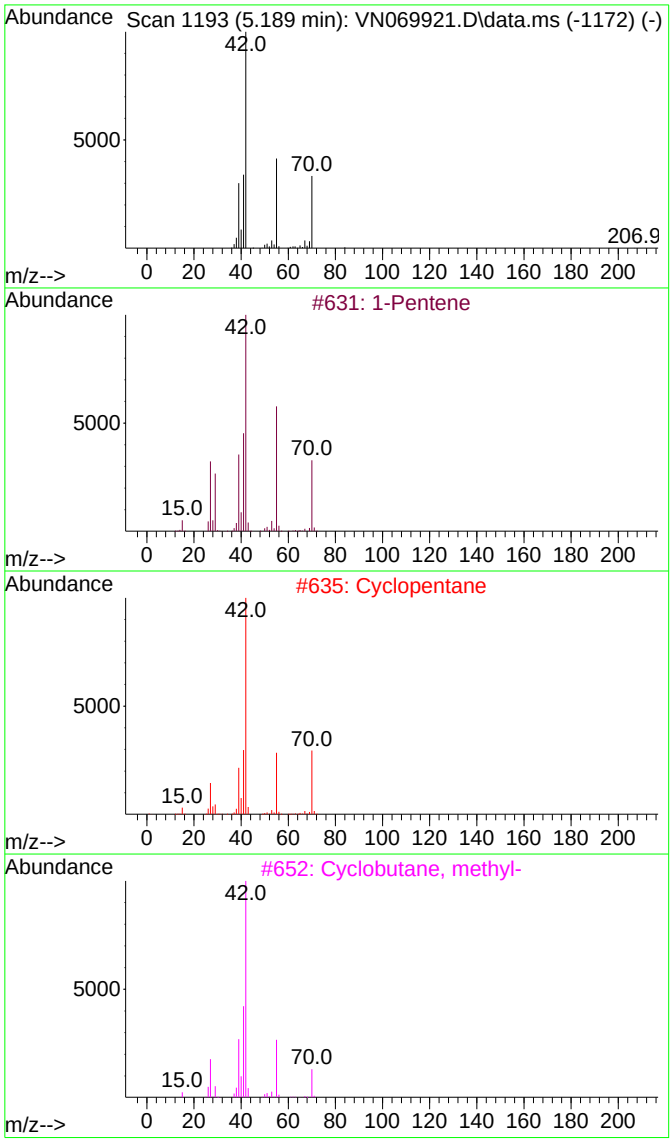
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

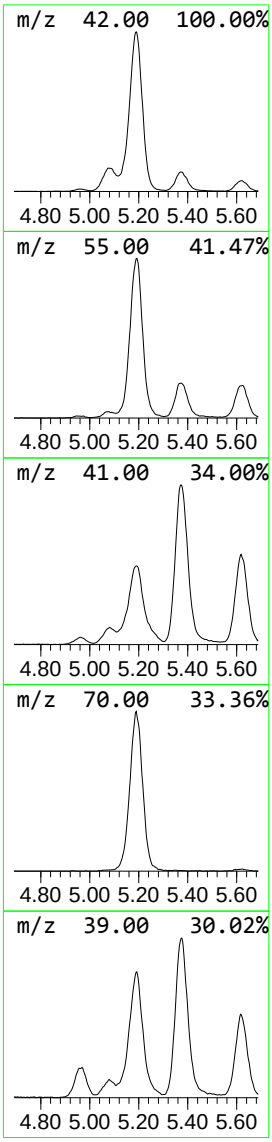
****

Peak Number 2 1-Pentene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.189	29.69 ug/l	3545630	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	86
2	Cyclopentane	70	C5H10	000287-92-3	78
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	53
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5	Cyclobutanone	70	C4H6O	001191-95-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

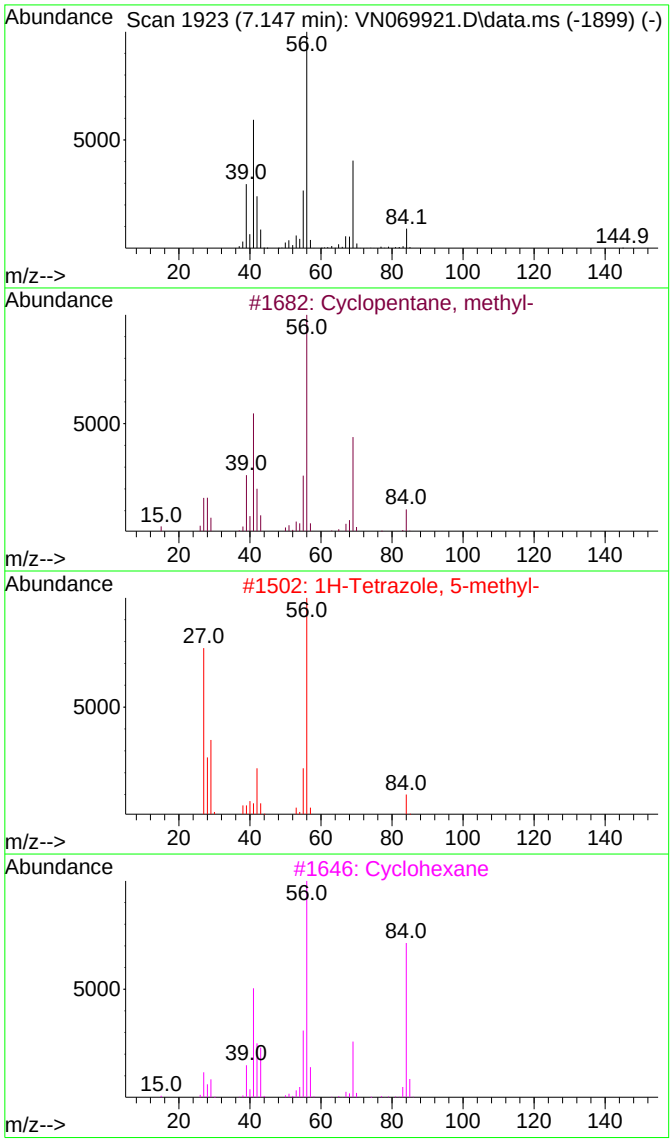
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

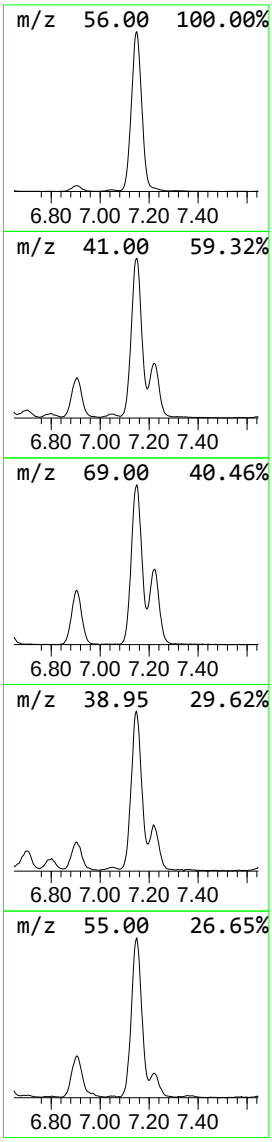
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	34.79 ug/l	4154600	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclohexane	84	C6H12	000110-82-7	64
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclobutane	56	C4H8	000287-23-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

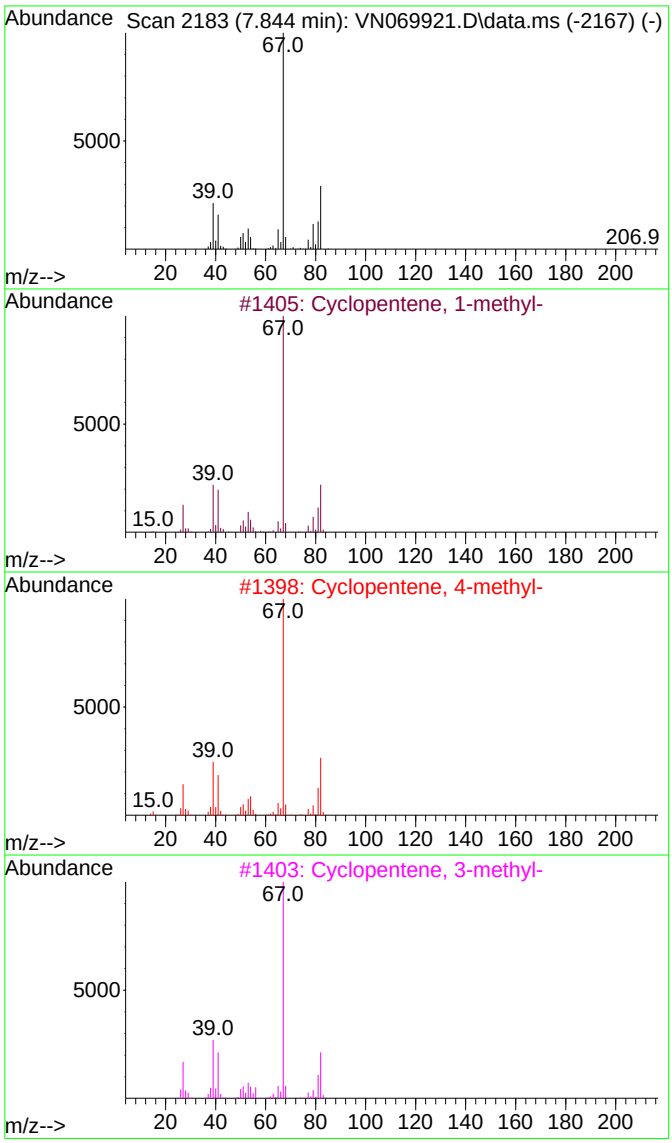
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

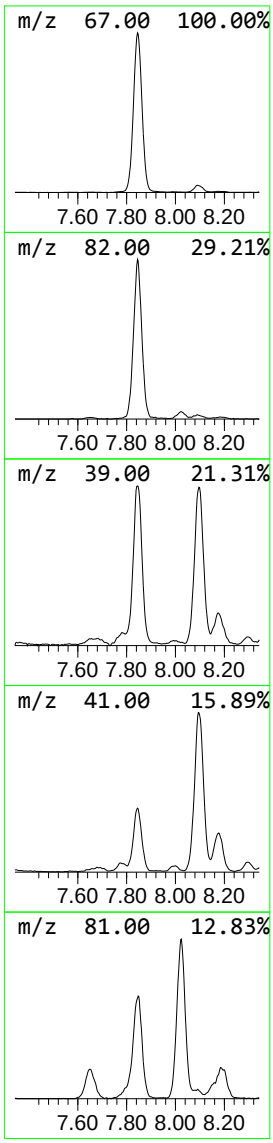
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.844	16.06 ug/l	1918120	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	87
3	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4	1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	86
5	Cyclopentane, methylene-	82	C6H10	001528-30-9	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

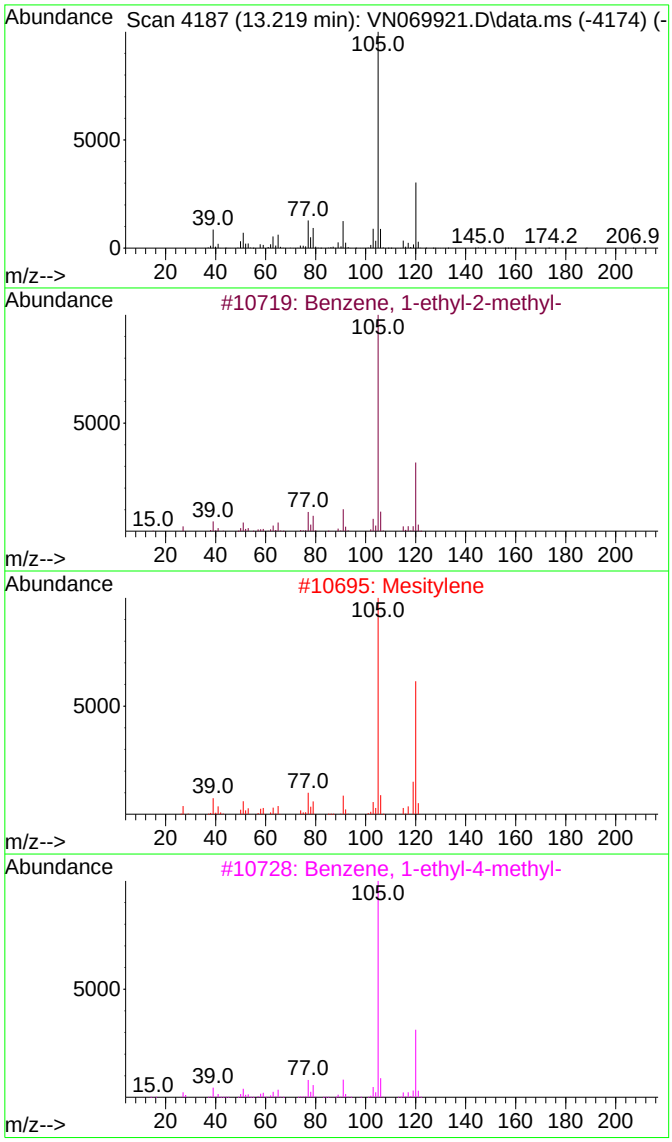
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

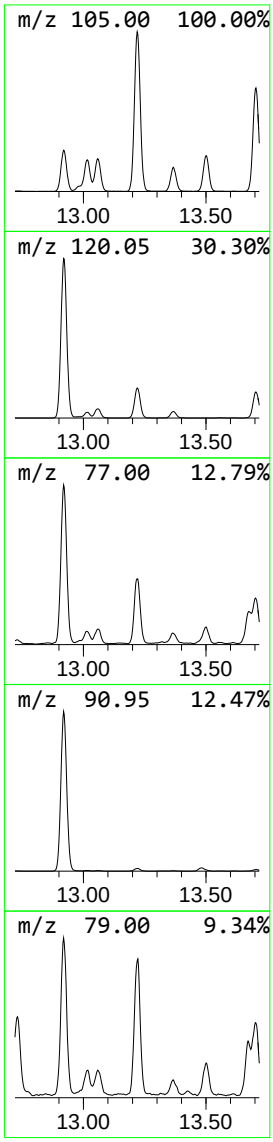
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	12.86 ug/l	2578070	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	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
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Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

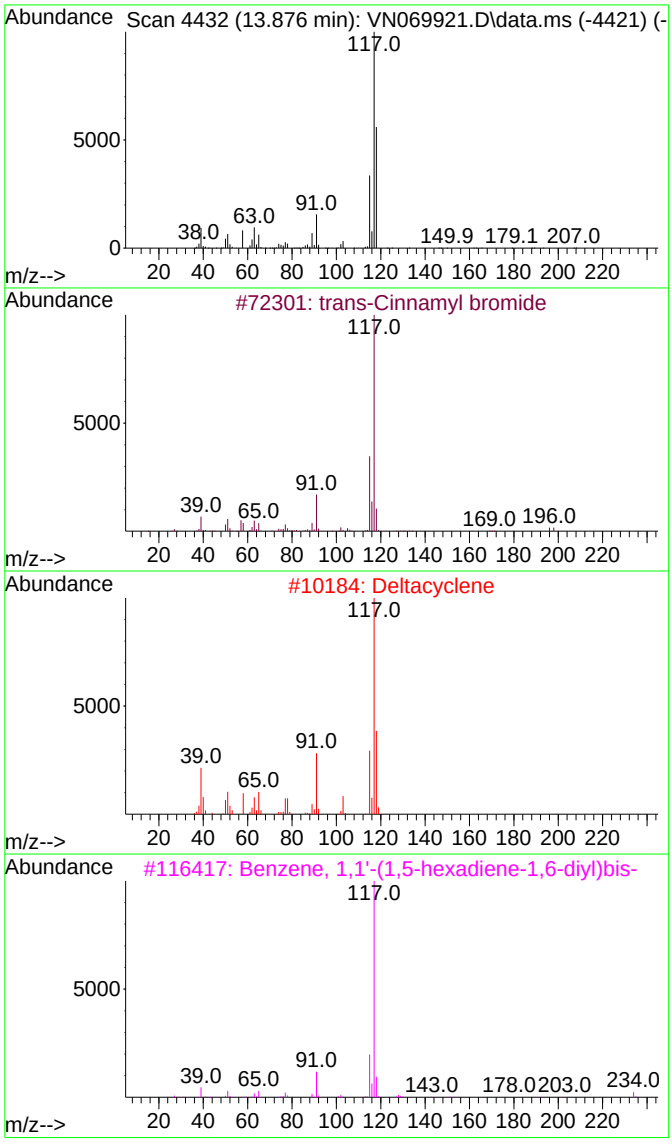
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

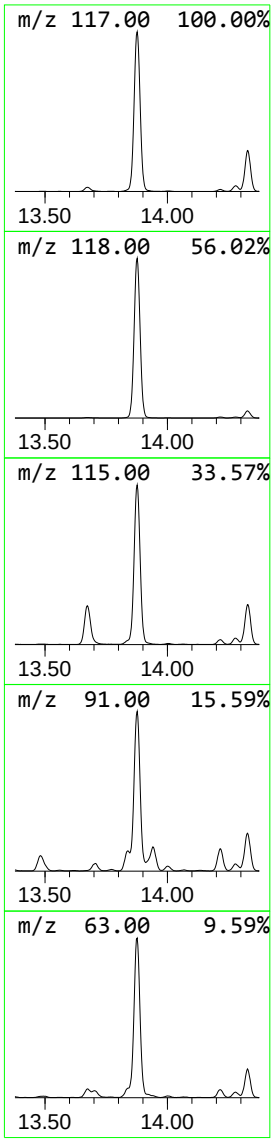
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 trans-Cinnamyl bromide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	145.62 ug/l	29203000	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2	Deltacyclene	118	C9H10	007785-10-6	53
3	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	50
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50





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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

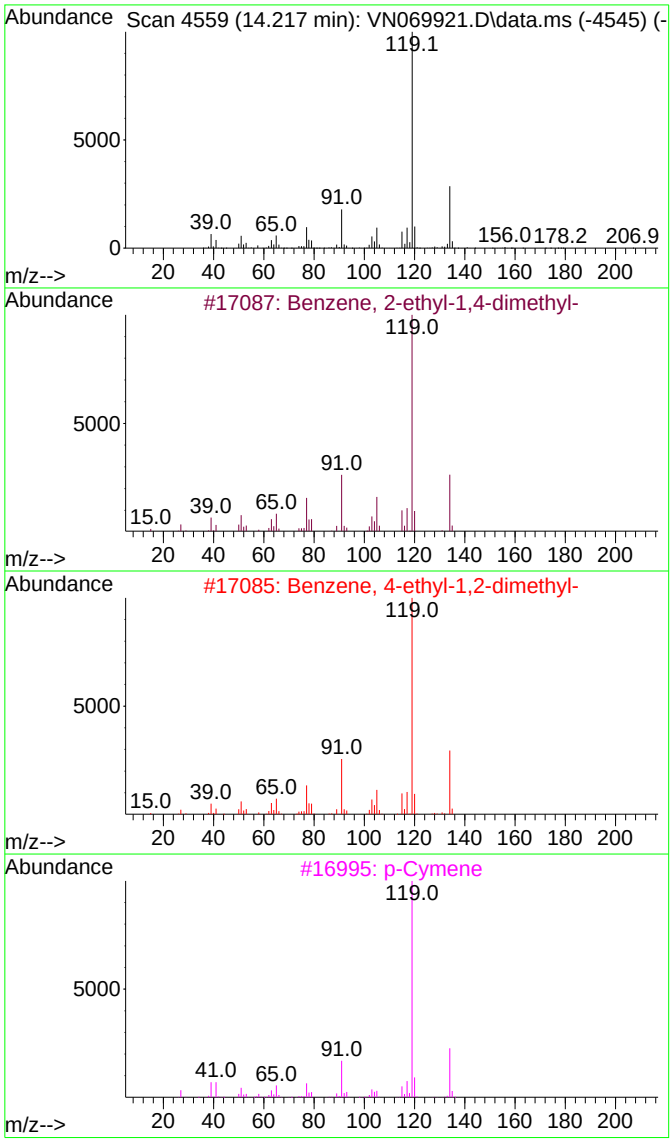
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

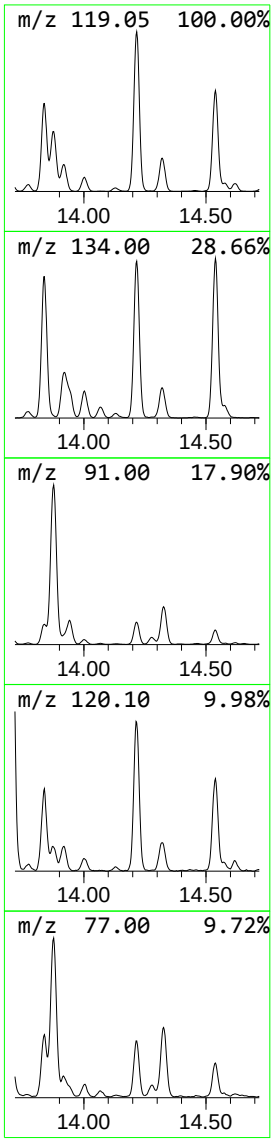
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	14.77 ug/l	2962140	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	p-Cymene	134	C10H14	000099-87-6	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

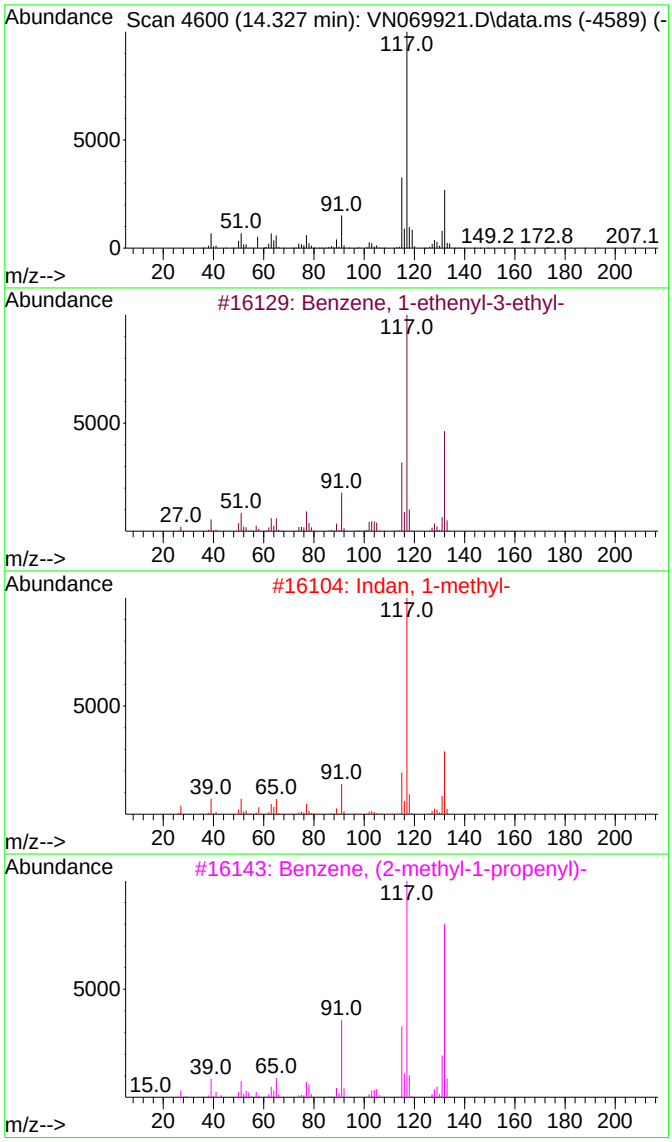
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

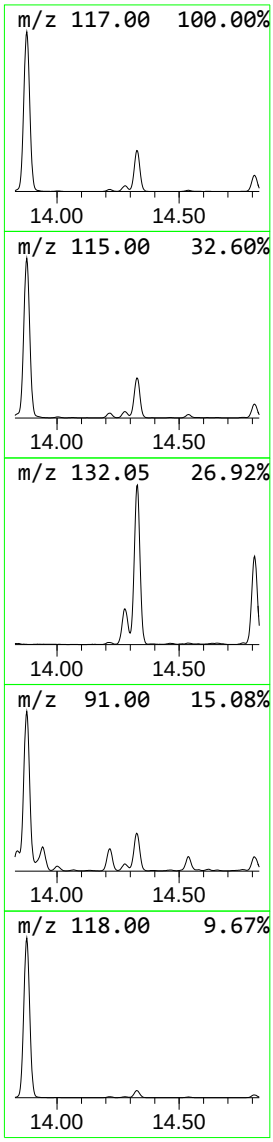
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	34.32 ug/l	6881940	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	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

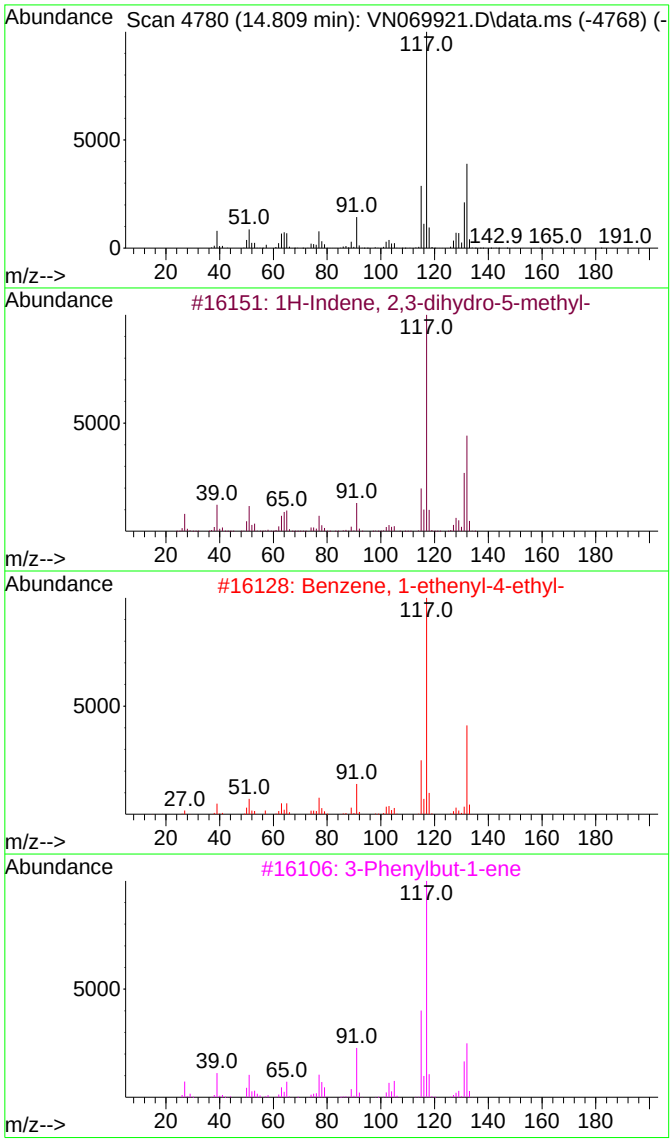
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

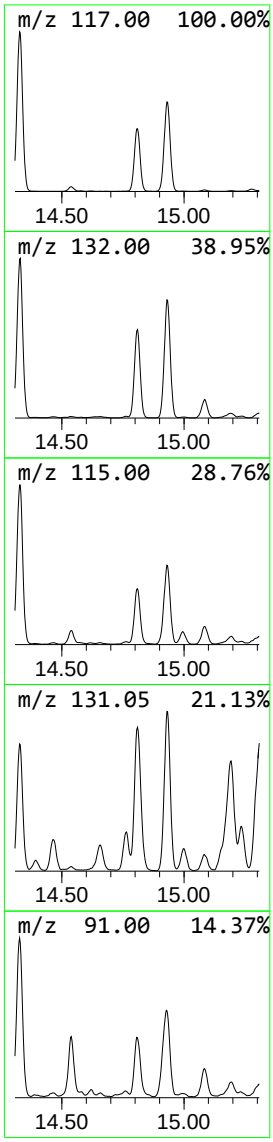
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	14.15 ug/l	2838150	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

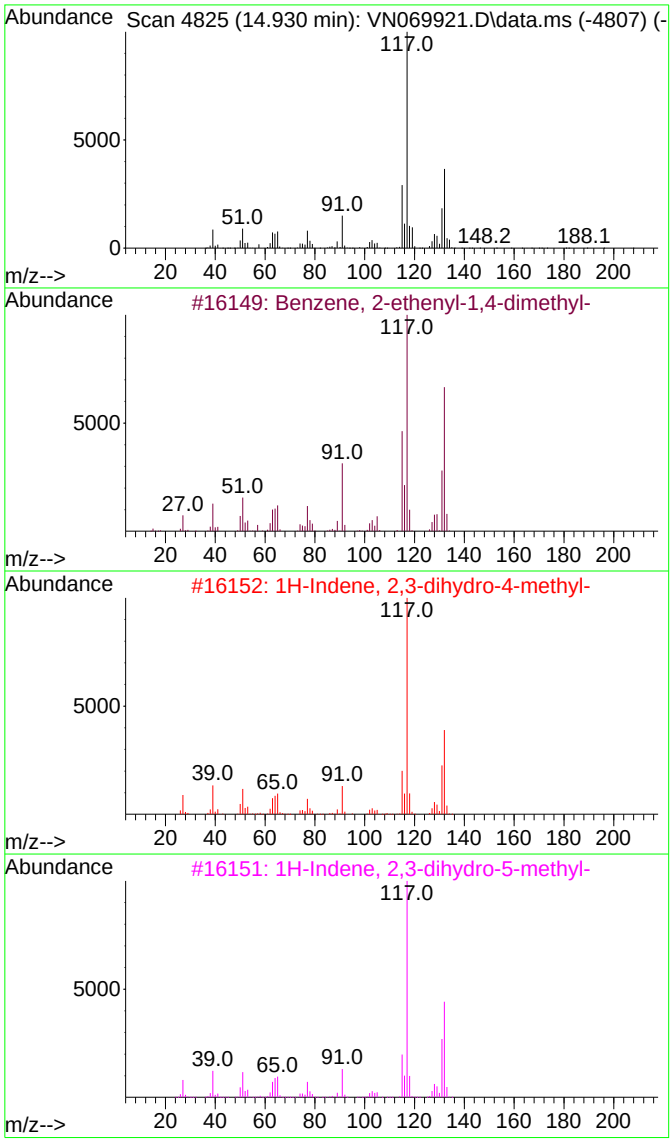
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

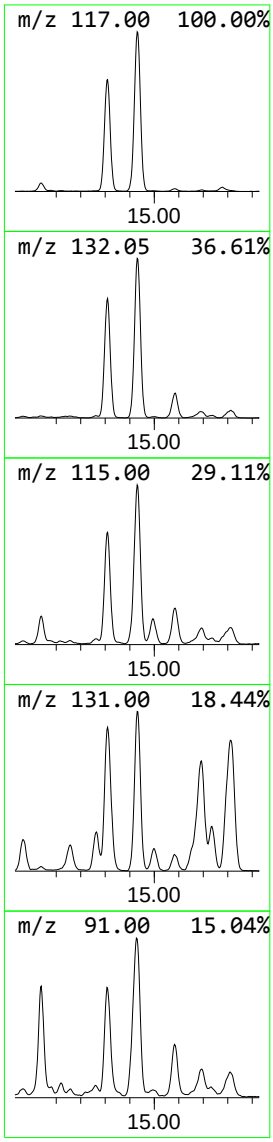
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	25.56 ug/l	5126270	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	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069921.D
Acq On : 9 Dec 2021 19:19
Operator : JC/MD
Sample : M4969-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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-	3.143	19.9	ug/l	2382340	1	8.086	5970540	50.0
1-Pentene	5.189	29.7	ug/l	3545630	1	8.086	5970540	50.0
Cyclopentane, m...	7.147	34.8	ug/l	4154600	1	8.086	5970540	50.0
Cyclopentene, 1...	7.844	16.1	ug/l	1918120	1	8.086	5970540	50.0
Benzene, 1-ethy...	13.219	12.9	ug/l	2578070	4	13.675	10027000	50.0
trans-Cinnamyl ...	13.876	145.6	ug/l	29203000	4	13.675	10027000	50.0
Benzene, 2-ethy...	14.217	14.8	ug/l	2962140	4	13.675	10027000	50.0
Benzene, 1-ethe...	14.327	34.3	ug/l	6881940	4	13.675	10027000	50.0
1H-Indene, 2,3-...	14.809	14.2	ug/l	2838150	4	13.675	10027000	50.0
Benzene, 2-ethe...	14.930	25.6	ug/l	5126270	4	13.675	10027000	50.0