LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

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: VN069919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.260	82	101	113	rBV	302990	685920	1.83%	0.149%
2	2.443	151	169	190	rVB	1685767	2892499	7.73%	0.627%
3	3.143	410	430	462	rBV	7234024	16447303	43.97%	3.567%
4	3.516	548	569	606	rBV3	2705474	6996844	18.71%	1.518%
5	3.717	629	644	661	rVB2	187643	454905	1.22%	0.099%
6	3.993	726	747	779	rVB3	1018147	2779897	7.43%	0.603%
7	4.253	817	844	881	rBV6	208650	808076	2.16%	0.175%
8	4.958	1067	1107	1126	rBV7	222126	874438	2.34%	0.190%
9	5.079	1127	1152	1162	rBV2	1037689	3435450	9.18%	0.745%
10	5.374	1240	1262	1310	rVB2	1088034	3884316	10.38%	0.843%
11	5.618	1326	1353	1389	rVB2	1760085	6077853	16.25%	1.318%
12	5.935	1445	1471	1504	rVB2	448269	1456422	3.89%	0.316%
13	6.122	1516	1541	1568	rBV4	561027	1690627	4.52%	0.367%
14	6.289	1577	1603	1624	rBV3	186705	576535	1.54%	0.125%
15	6.471	1648	1671	1700	rVB3	1427914	4661270	12.46%	1.011%
16	6.608	1701	1722	1743	rBV3	778275	2320556	6.20%	0.503%
17	6.903	1810	1832	1865	rBV2	1119334	3357691	8.98%	0.728%
18	7.048	1868	1886	1901	rBV3	261622	715588	1.91%	0.155%
19	7.147	1902	1923	1942	rBV	2794606	8132989	21.74%	1.764%
20	7.675	2095	2120	2139	rBV6	125216	413716	1.11%	0.090%
21	7.780	2139	2159	2168	rBV5	286045	721473	1.93%	0.156%
22	7.844	2169	2183	2203	rVV2	1100802	2684366	7.18%	0.582%
23	8.021	2227	2249	2259	rVV2	964221	2474128	6.61%	0.537%
24	8.088	2261	2274	2292	rVV3	2600649	6915059	18.49%	1.500%
25	8.177	2294	2307	2332	rVB4	1170059	3181363	8.51%	0.690%
26	8.295	2334	2351	2366	rBV2	429749	999093	2.67%	0.217%
27	8.461	2387	2413	2435	rBV	15509359	37404731	100.00%	8.113%
28	8.708	2496	2505	2526	rVB6	445227	1113311	2.98%	0.241%
29	8.802	2528	2540	2575	rVB6	313568	1024714	2.74%	0.222%
30	8.968	2580	2602	2630	rBV3	4249439	11005350	29.42%	2.387%
31	9.126	2649	2661	2674	rVB2	345792	650822	1.74%	0.141%
32	9.199	2674	2688	2697	rVV2	735436	1517813	4.06%	0.329%
33	9.244	2698	2705	2729	rVB	701251	1393094	3.72%	0.302%
34	9.459	2753	2785	2801	rBV2	1453825	4295547	11.48%	0.932%
35	9.641	2842	2853	2868	rVB3	321594	635068	1.70%	0.138%
36	9.802	2899	2913	2918	rBV4	346534	676076	1.81%	0.147%

LSC Area Percent Report

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

37	9.883	2933	2943	2960	rVB4	561277	1131021	3.02%	0.245%
38	9.971	2961	2976	2986	rBV	2026752	3975461	10.63%	0.862%
39	10.202	3048	3062	3092	rBV9	271399	932572	2.49%	0.202%
40	10.322	3093	3107	3119	rBV	1027764	1898636	5.08%	0.412%
41	10.440	3135	3151	3164	rBV	4508112	8412475	22.49%	1.825%
42	10.505	3164	3175	3203	rVB	1829704	3687533	9.86%	0.800%
43	10.636	3215	3224	3236	rVB4	333759	601086	1.61%	0.130%
44	10.856	3293	3306	3328	rVB3	802194	1713482	4.58%	0.372%
45	11.130	3397	3408	3419	rBV	758130	1212317	3.24%	0.263%
46	11.744	3621	3637	3660	rBV	4784841	9071023	24.25%	1.968%
47	11.843	3660	3674	3696	rVV	15409874	26834417	71.74%	5.820%
48	11.950	3698	3714	3741	rVB	11442523	22667608	60.60%	4.917%
49	12.087	3756	3765	3791	rVB6	236701	483966	1.29%	0.105%
50	12.280	3822	3837	3858	rVB	4114537	6982060	18.67%	1.514%
51	12.578	3934	3948	3963	rBV	2873180	4741734	12.68%	1.029%
52	12.731	3990	4005	4028	rVB	3911423	6853468	18.32%	1.487%
53	12.919	4060	4075	4088	rBV	7503612	12374962	33.08%	2.684%
54	12.983	4088	4099	4103	rVV	3007732	4613695	12.33%	1.001%
55	13.015	4104	4111	4118	rVV	5880052	9148006	24.46%	1.984%
56	13.058	4118	4127	4149	rVB	9490118	15869558	42.43%	3.442%
57	13.219	4170	4187	4211	rBV	10764577	18295373	48.91%	3.968%
58	13.366	4227	4242	4271	rVB	13439096	22355854	59.77%	4.849%
59	13.498	4273	4291	4303	rBV4	478821	1148179	3.07%	0.249%
60	13.559	4303	4314	4325	rBV	589558	910919	2.44%	0.198%
61	13.675	4342	4357	4362	rBV	4843977	8154647	21.80%	1.769%
62	13.838	4404	4418	4422	rBV	2593381	3863115	10.33%	0.838%
63	13.876	4422	4432	4468	rVB2	13139022	28990865	77.51%	6.288%
64	14.002	4468	4479	4491	rBV	583455	927720	2.48%	0.201%
65	14.066	4491	4503	4515	rVB2	756581	1252659	3.35%	0.272%
66	14.131	4515	4527	4535	rBV	1309340	2247068	6.01%	0.487%
67	14.217	4546	4559	4571	rBV	7453495	11557368	30.90%	2.507%
68	14.278	4571	4582	4589	rVV	1638131	2542662	6.80%	0.552%
69	14.327	4589	4600	4620	rVB2	6245442	10490522	28.05%	2.275%
70	14.458	4637	4649	4661	rBV2	566856	929570	2.49%	0.202%
71	14.538	4663	4679	4687	rBV	4079835	6877954	18.39%	1.492%
72	14.576	4687	4693	4705	rVV	3086183	4825794	12.90%	1.047%
73	14.809	4767	4780	4792	rVV	4744667	7636249	20.42%	1.656%
74	14.930	4806	4825	4839	rBV3	8530830	17088381	45.69%	3.707%
75	14.994	4839	4849	4866	rVB4	544965	1070599	2.86%	0.232%
76	15.083	4868	4882	4899	rBV	1265914	2279547	6.09%	0.494%

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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
MW-2

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
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Peak separation: 5

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

77	15.193	4901	4923	4933	rBV5	1014667	2498858	6.68%	0.542%
78	15.311	4952	4967	4984	rVB4	950736	2290848	6.12%	0.497%
79	15.504	5023	5039	5056	rVB	4879719	9067891	24.24%	1.967%
80	15.611	5068	5079	5090	rBV4	268788	538333	1.44%	0.117%
81	15.668	5093	5100	5124	rVB3	256010	506721	1.35%	0.110%
82	15.804	5136	5151	5167	rBV	430481	846545	2.26%	0.184%
83	15.981	5199	5217	5243	rBV4	236486	783766	2.10%	0.170%
84	16.614	5438	5453	5484	rVB	1076737	2495448	6.67%	0.541%

Sum of corrected areas: 461033438

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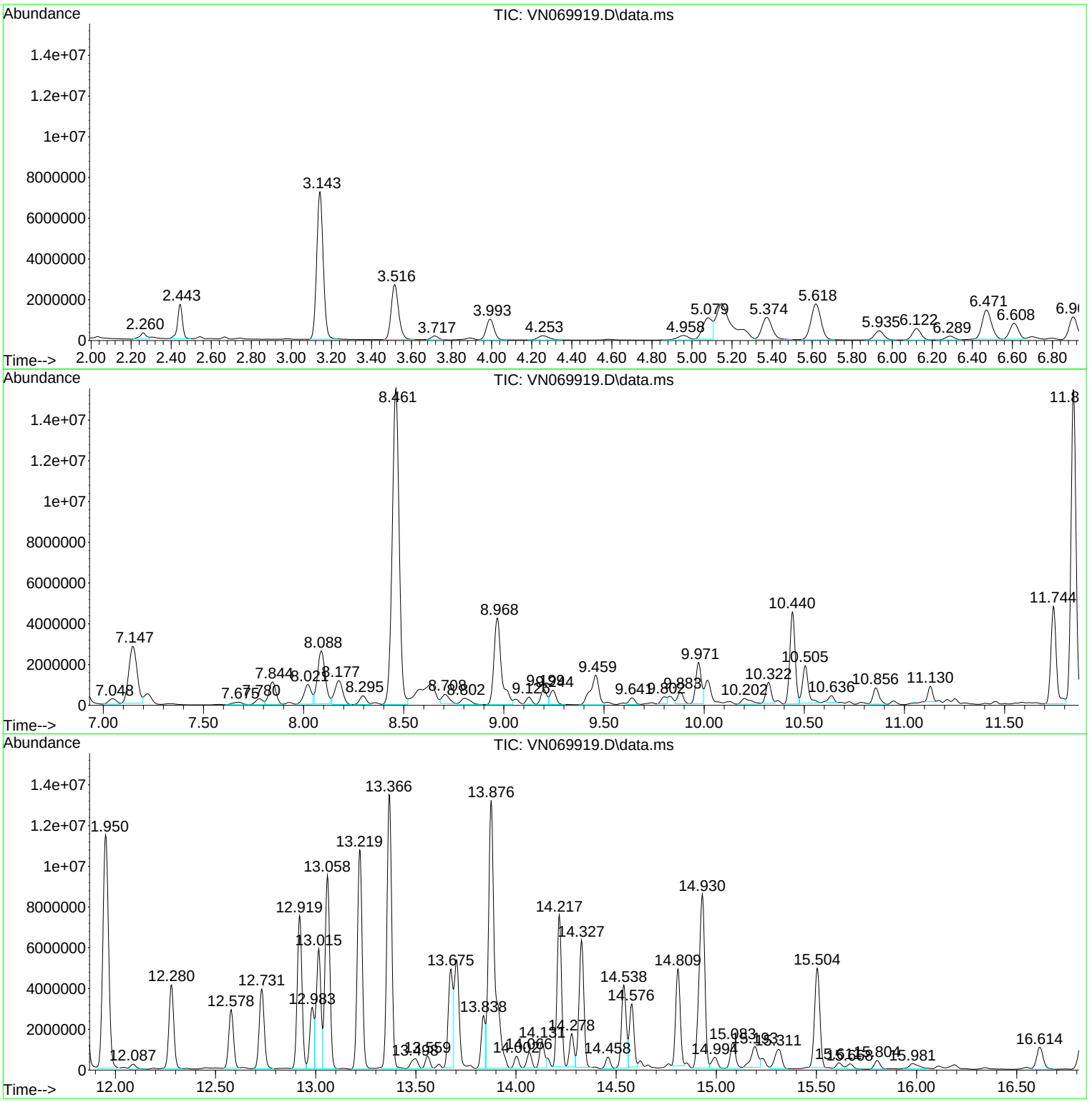
MW-2

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 : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-2

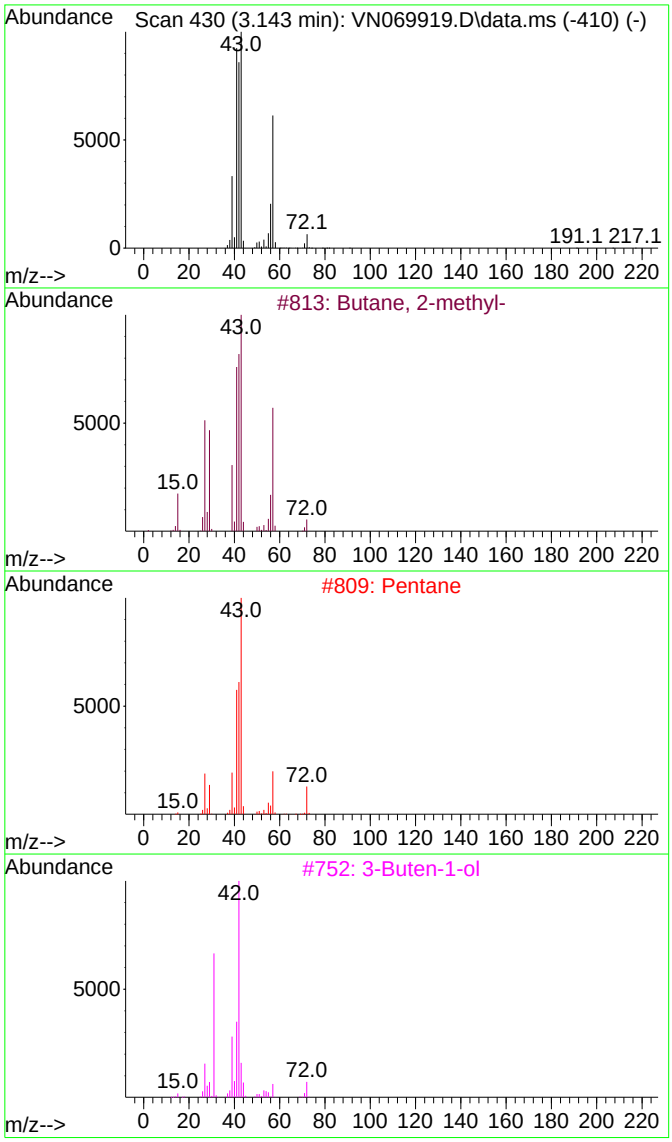
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

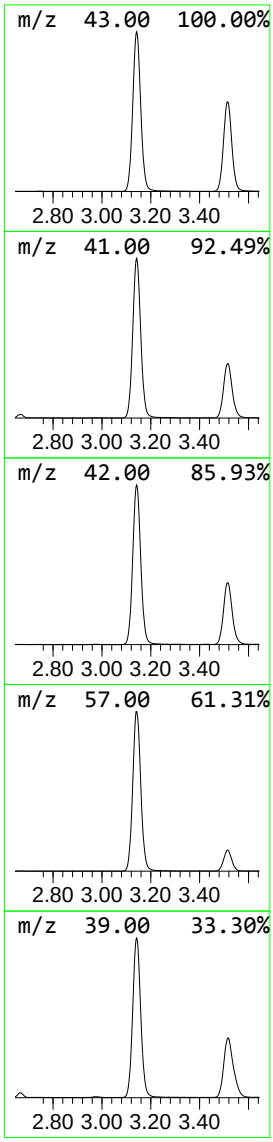
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	118.92 ug/l	16447300	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	33
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





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Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

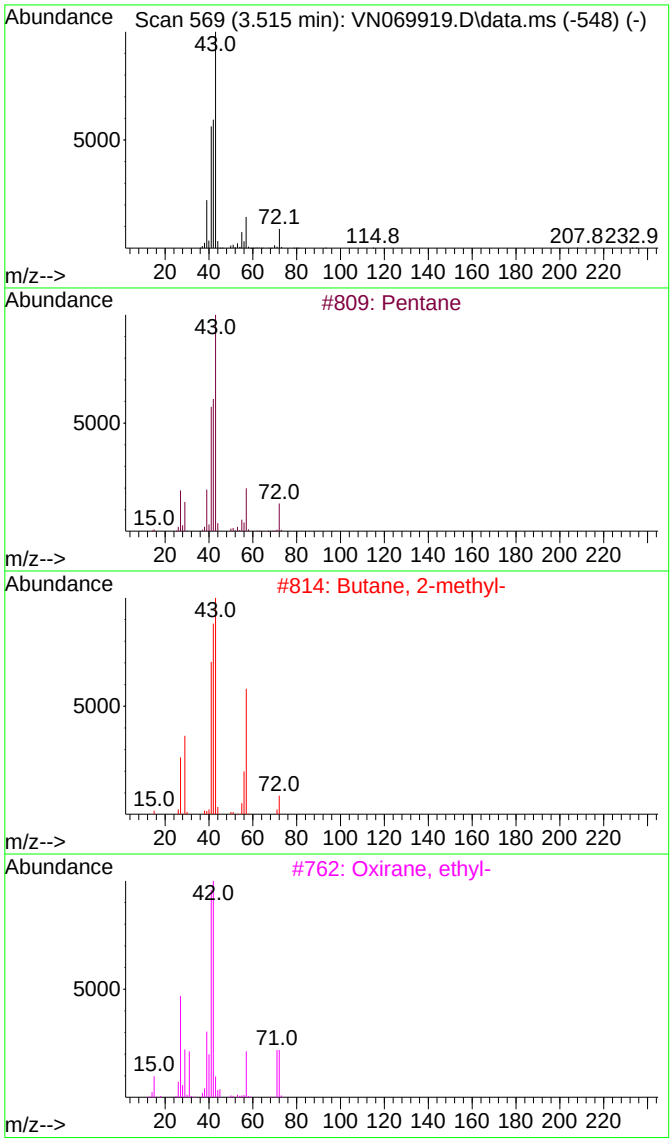
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

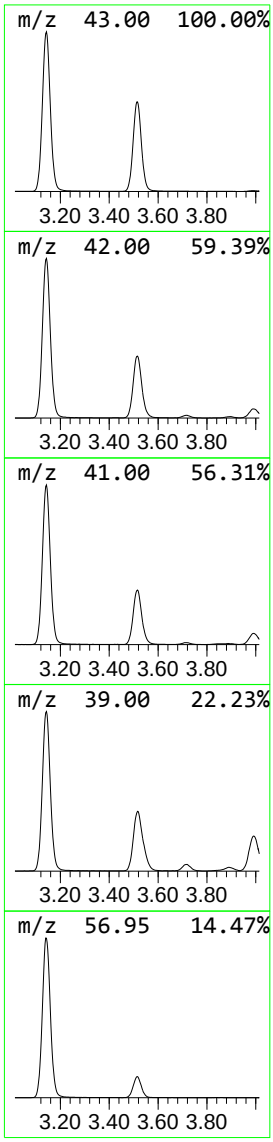
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.515	50.59 ug/l	6996840	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4	Methyl glyoxal	72	C3H4O2	000078-98-8	9
5	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

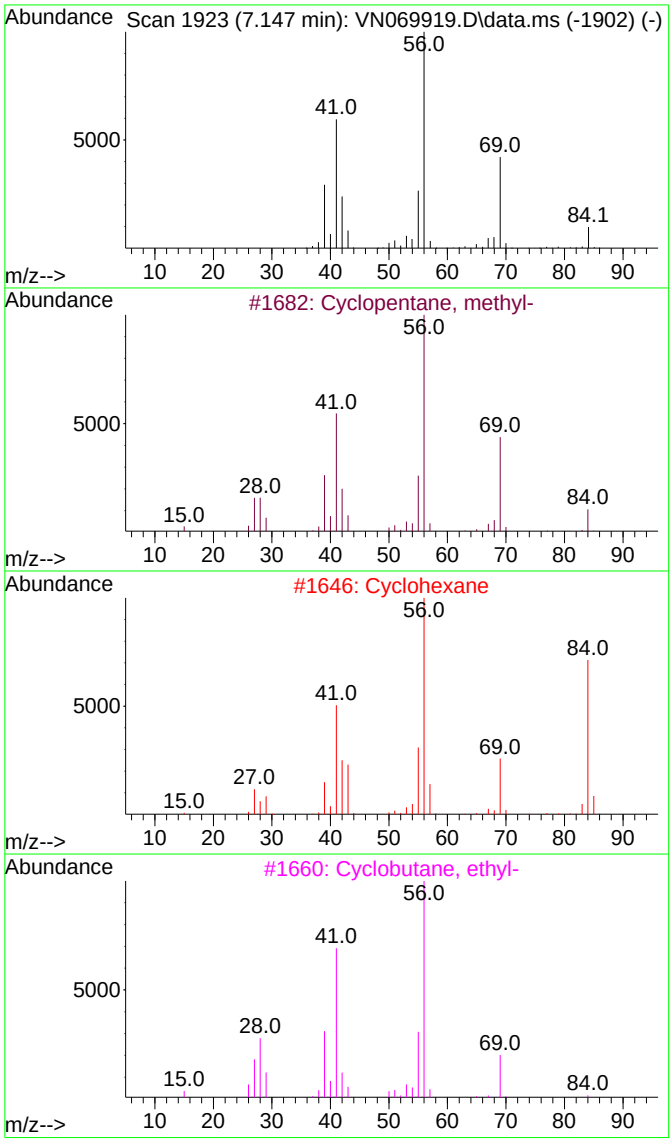
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

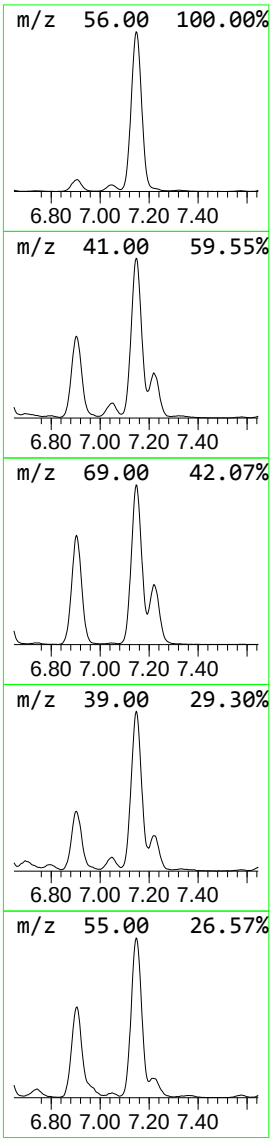
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	58.81 ug/l	8132990	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclobutane	56	C4H8	000287-23-0	50
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





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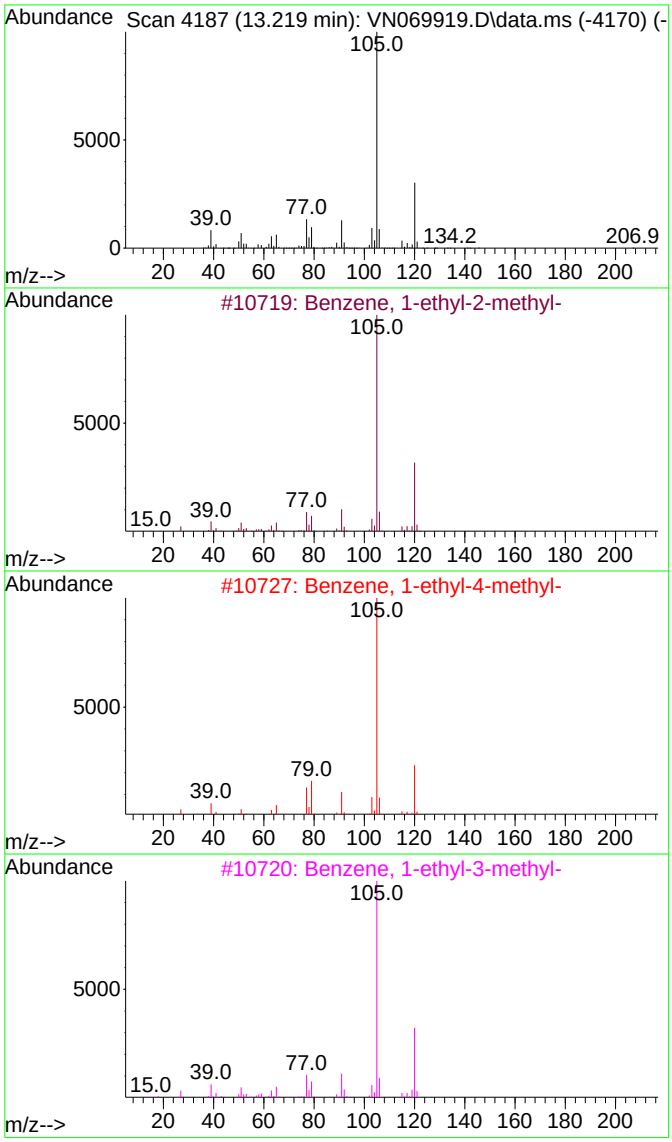
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

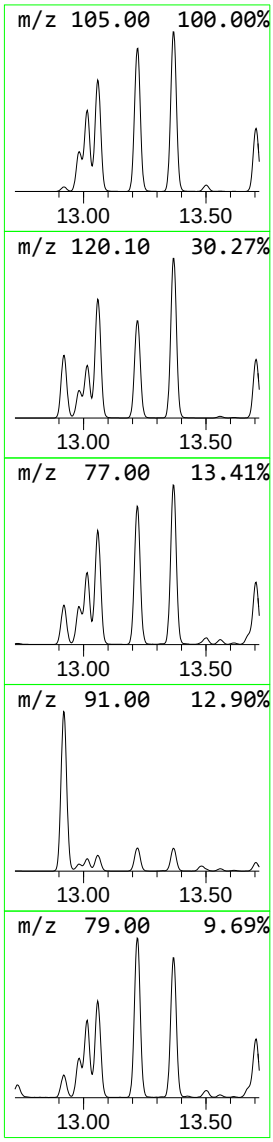
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	112.18 ug/l	18295400	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	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

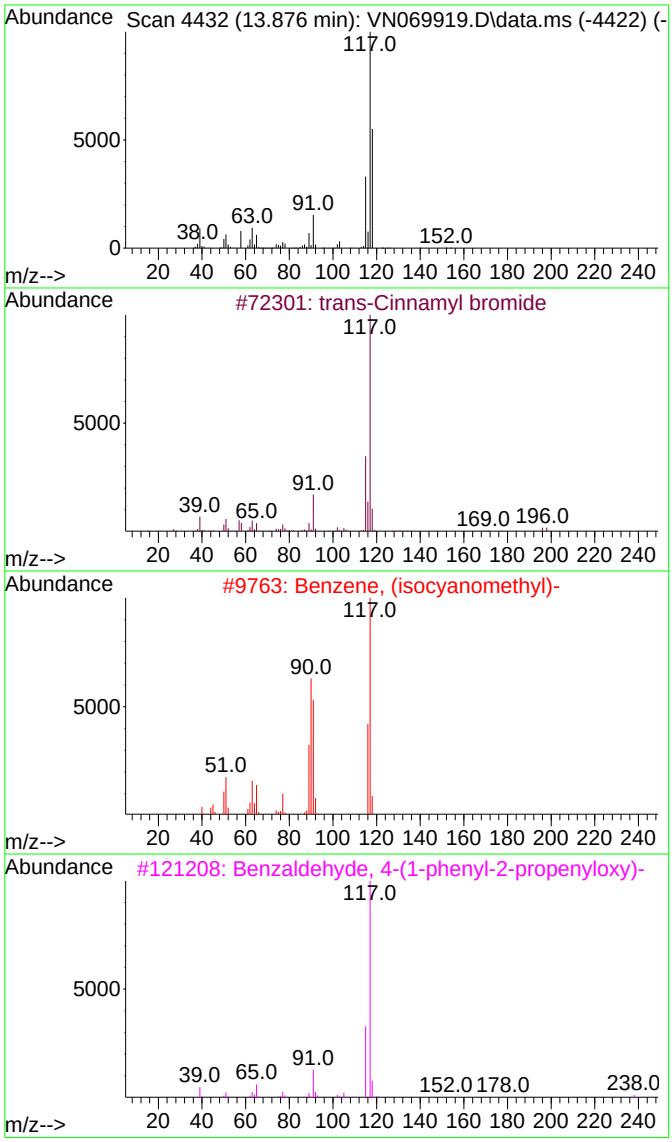
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

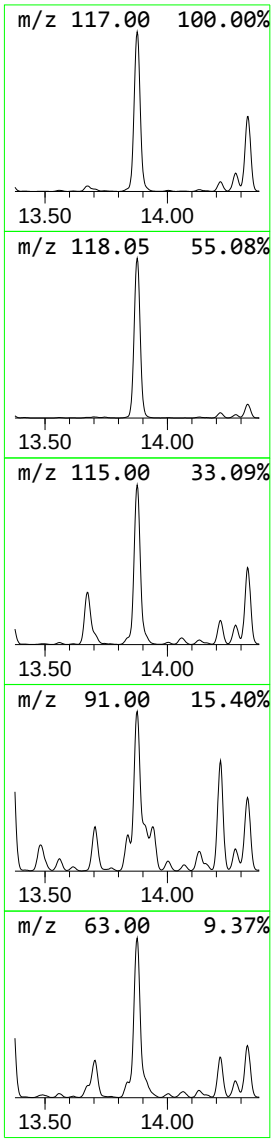
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 trans-Cinnamyl bromide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	177.76 ug/l	28990900	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	Benzene, (isocyanomethyl)-	117	C8H7N	010340-91-7	50
3	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
4	4-Ethynylaniline	117	C8H7N	014235-81-5	47
5	Indole	117	C8H7N	000120-72-9	47





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Acq On : 9 Dec 2021 18:28
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

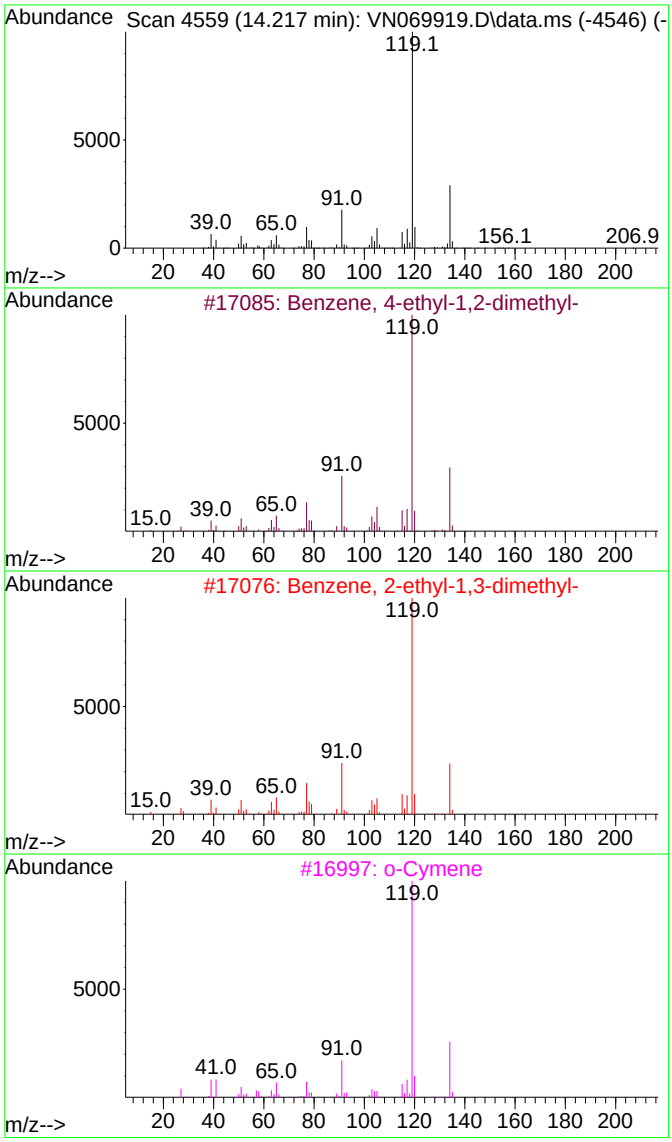
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

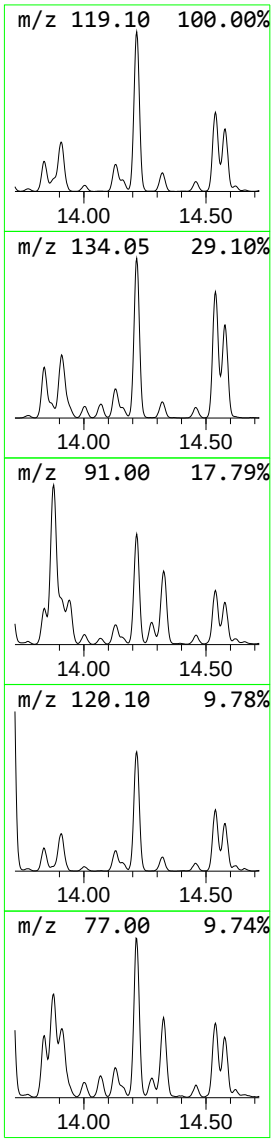
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	70.86 ug/l	11557400	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

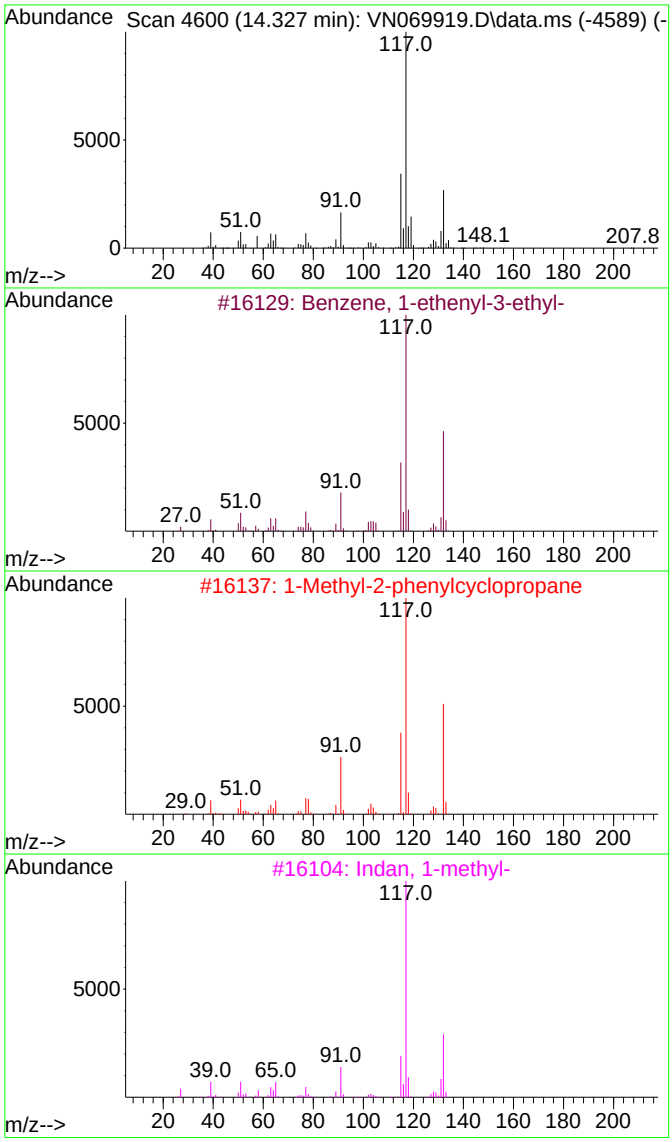
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

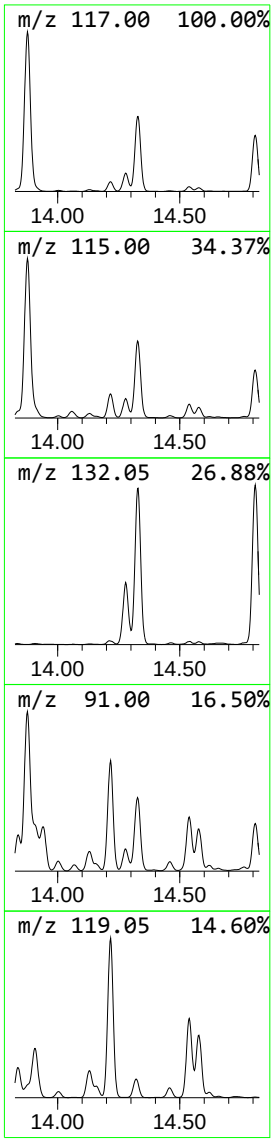
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.326	64.32 ug/l	10490500	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	83
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
3	Indan, 1-methyl-	132	C10H12	000767-58-8	81
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

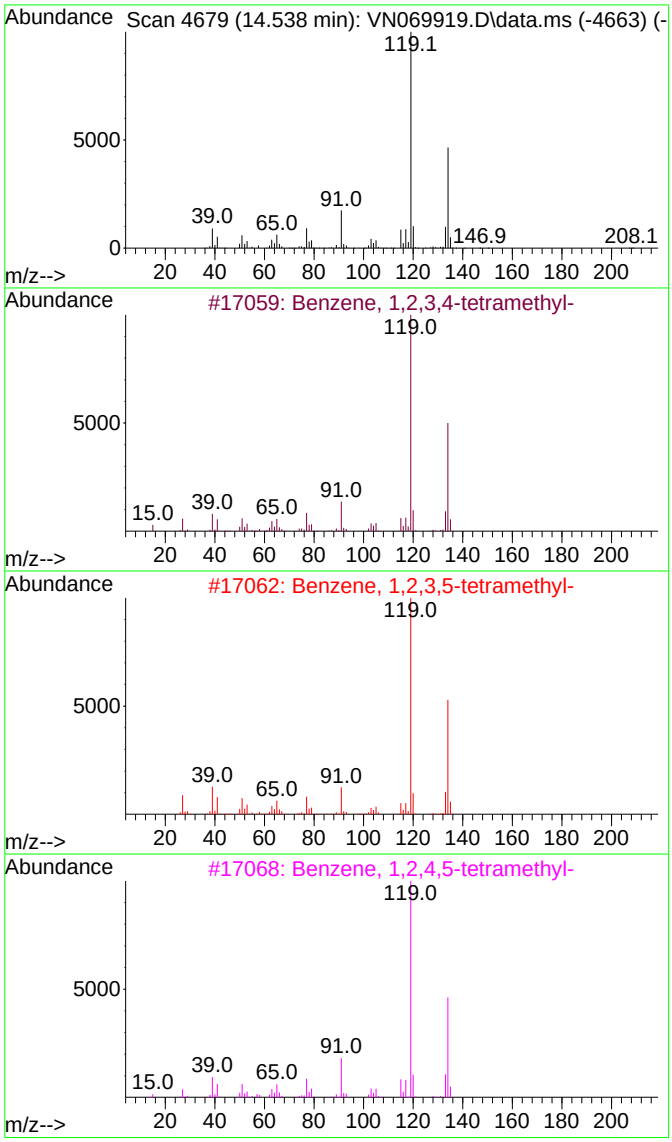
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

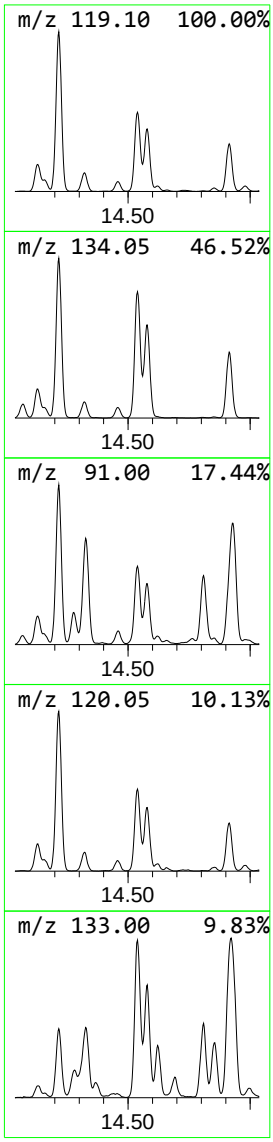
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.538	42.17 ug/l	6877950	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

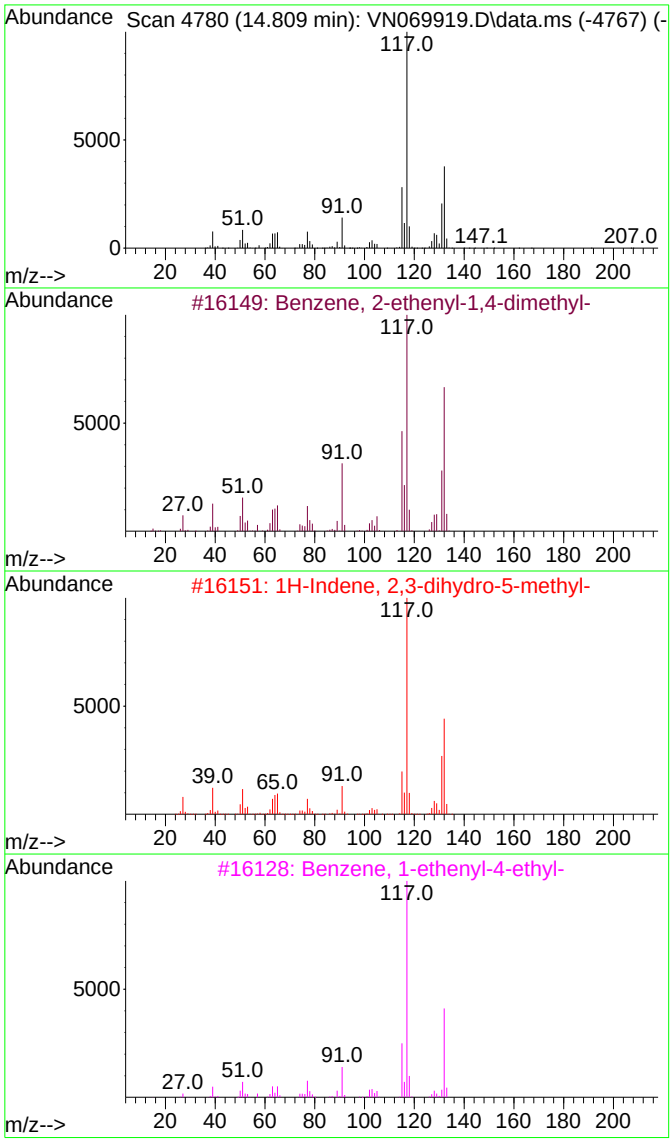
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

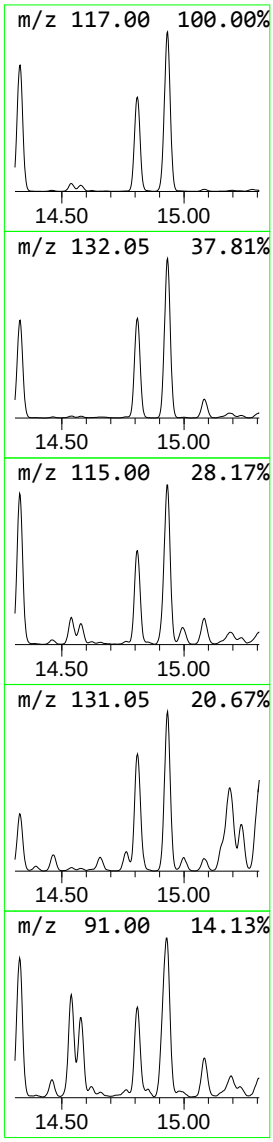
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	46.82 ug/l	7636250	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-5-methyl-	132	C10H12	000874-35-1	94
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

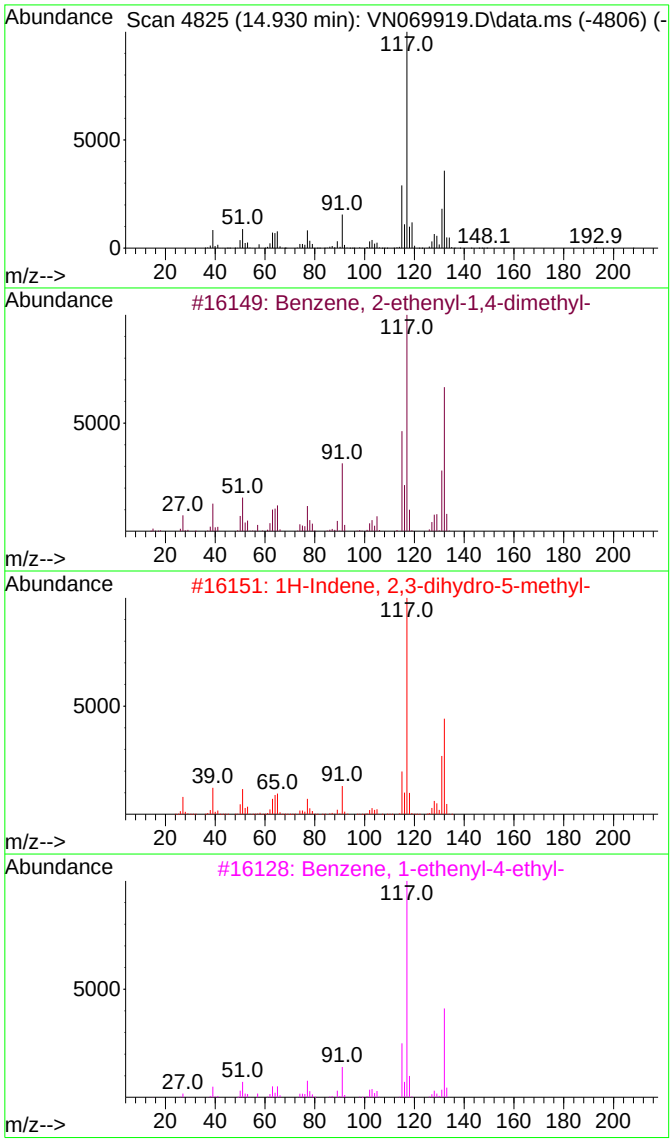
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

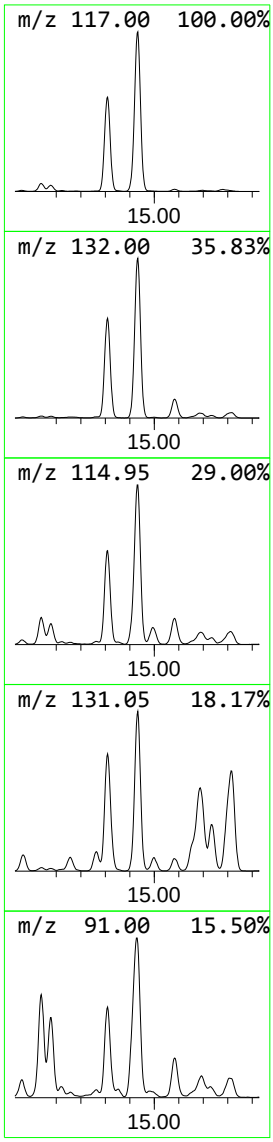
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	104.78 ug/l	17088400	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-5-methyl-	132	C10H12	000874-35-1	95
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
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 : VN069919.D
Acq On : 9 Dec 2021 18:28
Operator : JC/MD
Sample : M4969-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

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	118.9	ug/l	16447300	1	8.086	6915060	50.0
Pentane	3.515	50.6	ug/l	6996840	1	8.086	6915060	50.0
Cyclopentane, m...	7.147	58.8	ug/l	8132990	1	8.086	6915060	50.0
Benzene, 1-ethy...	13.219	112.2	ug/l	18295400	4	13.675	8154650	50.0
trans-Cinnamyl ...	13.876	177.8	ug/l	28990900	4	13.675	8154650	50.0
Benzene, 4-ethy...	14.217	70.9	ug/l	11557400	4	13.675	8154650	50.0
Benzene, 1-ethe...	14.326	64.3	ug/l	10490500	4	13.675	8154650	50.0
Benzene, 1,2,3,...	14.538	42.2	ug/l	6877950	4	13.675	8154650	50.0
Benzene, 2-ethe...	14.809	46.8	ug/l	7636250	4	13.675	8154650	50.0
1H-Indene, 2,3-...	14.930	104.8	ug/l	17088400	4	13.675	8154650	50.0