LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

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: VN070658.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	89	101	114	rBV	461255	758534	2.45%	0.339%
2	2.446	157	170	192	rVB	1937965	3091305	9.99%	1.383%
3	3.137	408	428	463	rBV	6904942	16060958	51.92%	7.186%
4	3.513	548	568	603	rBV	1230733	3086821	9.98%	1.381%
5	3.990	723	746	790	rVB3	783839	2158926	6.98%	0.966%
6	4.253	814	844	883	rBV4	426422	1556958	5.03%	0.697%
7	4.958	1076	1107	1125	rBV3	240742	852787	2.76%	0.382%
8	5.079	1127	1152	1161	rBV2	1258608	4108527	13.28%	1.838%
9	5.377	1242	1263	1300	rVB2	368948	1303686	4.21%	0.583%
10	5.618	1321	1353	1398	rBV	2613263	9041906	29.23%	4.046%
11	6.122	1514	1541	1567	rBV2	129744	396469	1.28%	0.177%
12	6.468	1636	1670	1699	rBV3	598468	2097997	6.78%	0.939%
13	6.608	1701	1722	1742	rBV2	467525	1413307	4.57%	0.632%
14	6.796	1772	1792	1812	rBV2	371099	1098759	3.55%	0.492%
15	6.900	1813	1831	1863	rVB6	415014	1270207	4.11%	0.568%
16	7.045	1864	1885	1899	rBV2	298951	855480	2.77%	0.383%
17	7.147	1900	1923	1946	rBV	6060815	17695191	57.20%	7.917%
18	7.844	2169	2183	2203	rVB3	554150	1434107	4.64%	0.642%
19	8.021	2227	2249	2256	rBV	557768	1298964	4.20%	0.581%
20	8.094	2258	2276	2294	rVV2	5291146	13515238	43.69%	6.047%
21	8.174	2295	2306	2332	rVB3	1216824	3203736	10.36%	1.433%
22	8.298	2333	2352	2364	rBV	741626	1712938	5.54%	0.766%
23	8.357	2366	2374	2389	rVB2	283212	584697	1.89%	0.262%
24	8.458	2389	2412	2430	rBV	12974828	30935631	100.00%	13.841%
25	8.539	2431	2442	2448	rBV2	886213	1725768	5.58%	0.772%
26	8.705	2493	2504	2525	rVB2	897707	2041800	6.60%	0.914%
27	8.837	2527	2553	2578	rVB3	365154	1113324	3.60%	0.498%
28	8.968	2581	2602	2628	rBV3	2179503	5510163	17.81%	2.465%
29	9.199	2674	2688	2697	rBV3	226695	471772	1.53%	0.211%
30	9.244	2698	2705	2744	rVB2	229920	490543	1.59%	0.219%
31	9.459	2748	2785	2822	rBV	3826532	10315547	33.35%	4.615%
32	9.639	2841	2852	2867	rVB3	454313	895080	2.89%	0.400%
33	9.797	2897	2911	2918	rBV6	490124	1024233	3.31%	0.458%
34	9.883	2934	2943	2960	rVB	583574	1111714	3.59%	0.497%
35	9.971	2961	2976	2984	rBV	1206846	2279745	7.37%	1.020%
36	10.014	2987	2992	3008	rVB	874912	1461473	4.72%	0.654%

LSC Area Percent Report

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

Instrument :
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ClientSampleId :
MW-24

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	10.202	3046	3062	3068	rBV4	616798	1231007	3.98%	0.551%
38	10.322	3093	3107	3118	rBV3	780497	1497889	4.84%	0.670%
39	10.440	3135	3151	3167	rBV	2840001	5543834	17.92%	2.480%
40	10.542	3179	3189	3205	rVB2	1006810	1977987	6.39%	0.885%
41	10.636	3206	3224	3240	rVB5	381247	986116	3.19%	0.441%
42	10.781	3267	3278	3292	rBV3	164785	310279	1.00%	0.139%
43	10.859	3293	3307	3328	rVB5	548880	1284631	4.15%	0.575%
44	11.057	3361	3381	3388	rBV	225576	458051	1.48%	0.205%
45	11.130	3396	3408	3430	rVB	1415410	2486409	8.04%	1.112%
46	11.460	3518	3531	3543	rBV2	216258	410073	1.33%	0.183%
47	11.586	3568	3578	3588	rBV	247178	448012	1.45%	0.200%
48	11.744	3618	3637	3653	rBV	2518258	4718315	15.25%	2.111%
49	11.843	3656	3674	3696	rVB2	2633880	5604199	18.12%	2.507%
50	11.958	3703	3717	3739	rVB	1477351	2872545	9.29%	1.285%
51	12.050	3740	3751	3761	rBV4	245158	440323	1.42%	0.197%
52	12.278	3813	3836	3854	rBV3	177236	458245	1.48%	0.205%
53	12.500	3905	3919	3936	rBV2	924628	1835464	5.93%	0.821%
54	12.578	3937	3948	3960	rVB	642937	1045199	3.38%	0.468%
55	12.731	3990	4005	4018	rBV	1891395	3300325	10.67%	1.477%
56	12.790	4019	4027	4036	rBV	182363	322920	1.04%	0.144%
57	12.919	4063	4075	4090	rVB	854050	1427756	4.62%	0.639%
58	13.015	4091	4111	4120	rVV	861697	1594436	5.15%	0.713%
59	13.058	4121	4127	4139	rVB2	348887	542158	1.75%	0.243%
60	13.122	4139	4151	4169	rVB	567288	1044101	3.38%	0.467%
61	13.219	4172	4187	4208	rBV	2823695	4739461	15.32%	2.121%
62	13.366	4218	4242	4257	rVB	1908605	3418483	11.05%	1.530%
63	13.675	4342	4357	4364	rBV	1833646	3364769	10.88%	1.505%
64	13.839	4406	4418	4420	rBV	477555	586174	1.89%	0.262%
65	13.876	4421	4432	4466	rVB	4872199	9129561	29.51%	4.085%
66	14.066	4492	4503	4515	rVB	325255	554211	1.79%	0.248%
67	14.131	4516	4527	4533	rBV	300809	518577	1.68%	0.232%
68	14.217	4547	4559	4571	rVB	955171	1493542	4.83%	0.668%
69	14.278	4572	4582	4589	rVV	285807	447190	1.45%	0.200%
70	14.327	4589	4600	4622	rVB2	1306691	2228710	7.20%	0.997%
71	14.458	4638	4649	4662	rBV3	188744	314732	1.02%	0.141%
72	14.539	4664	4679	4687	rBV	501819	878971	2.84%	0.393%
73	14.579	4687	4694	4704	rVB	433521	654938	2.12%	0.293%
74	14.809	4769	4780	4792	rBV2	493918	808871	2.61%	0.362%
75	14.930	4806	4825	4838	rBV3	1048046	2145032	6.93%	0.960%
76	15.083	4870	4882	4898	rBV3	191751	339268	1.10%	0.152%

LSC Area Percent Report

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Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

77	15.193	4912	4923	4933	rBV6	184192	361158	1.17%	0.162%
78	15.311	4953	4967	4985	rVB4	229645	552731	1.79%	0.247%
79	15.507	5026	5040	5055	rVB	422644	795881	2.57%	0.356%
80	16.620	5440	5455	5473	rVB2	150322	352999	1.14%	0.158%

Sum of corrected areas: 223499824

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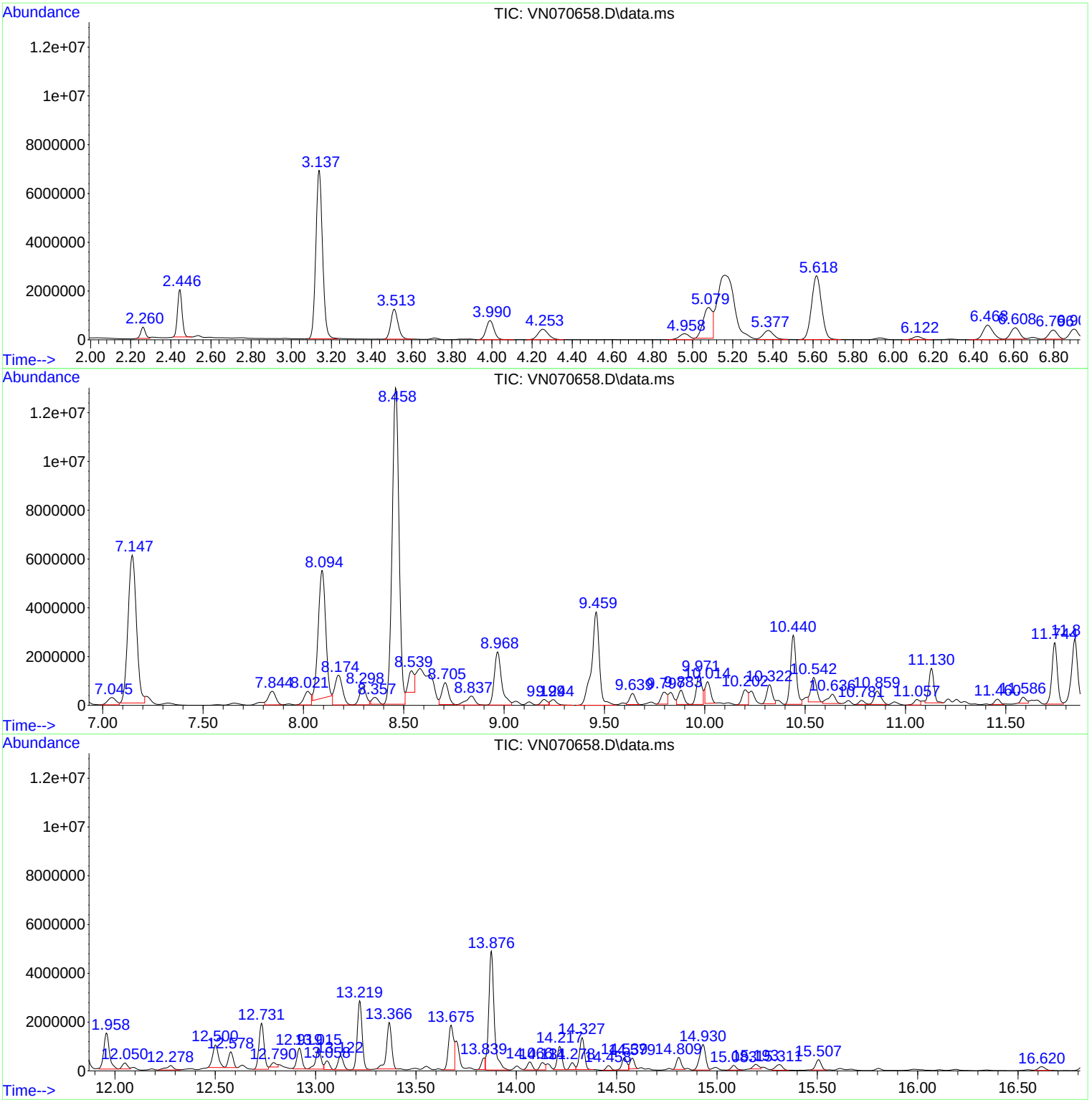
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

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



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Data File : VN070658.D
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Operator : JC/MD
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ALS Vial : 20 Sample Multiplier: 1

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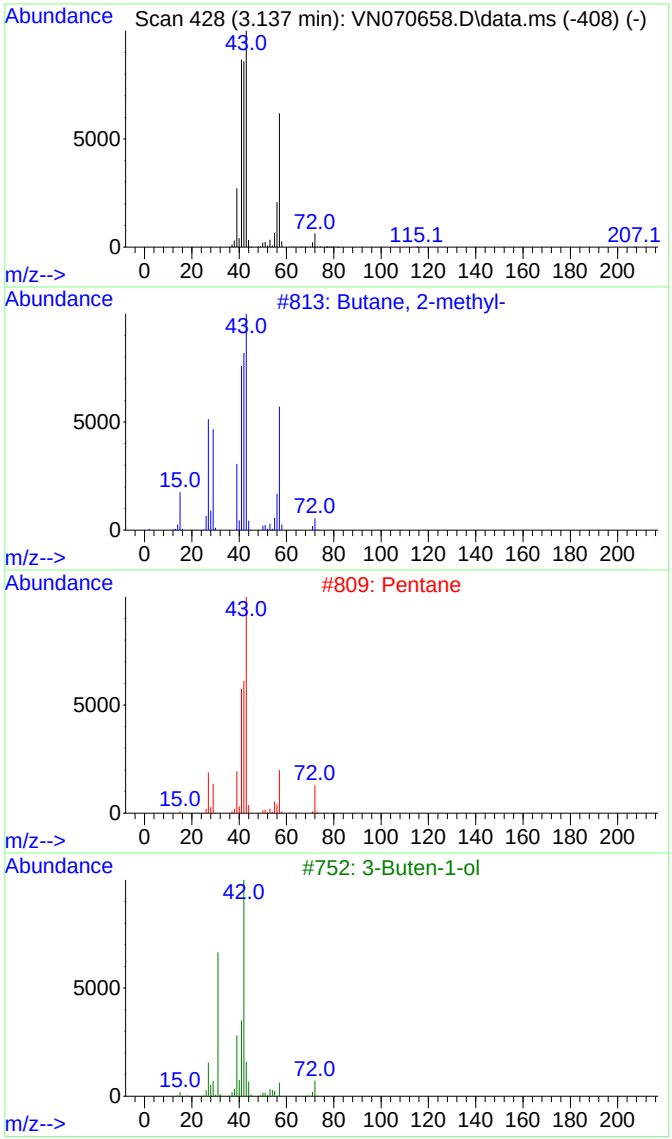
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

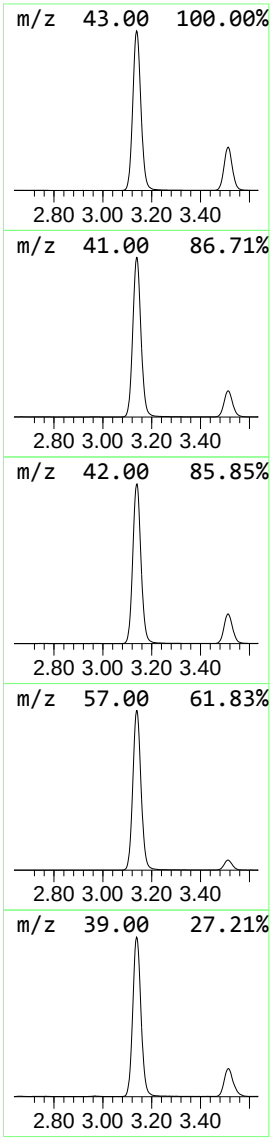
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.137	59.42 ug/l	16061000	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
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Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

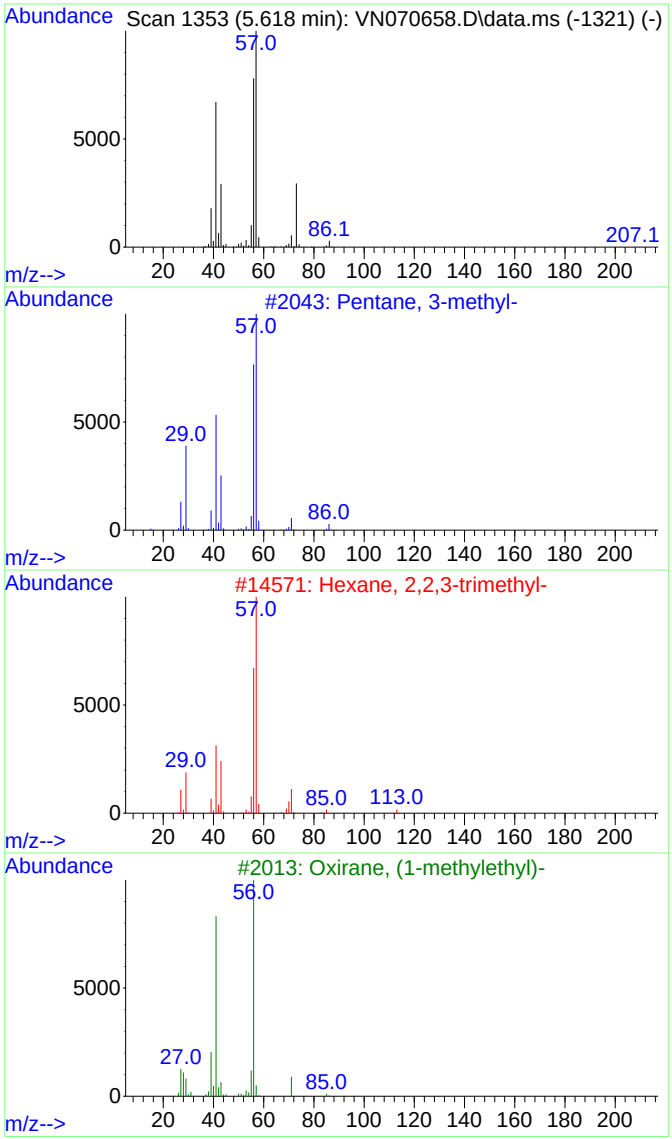
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

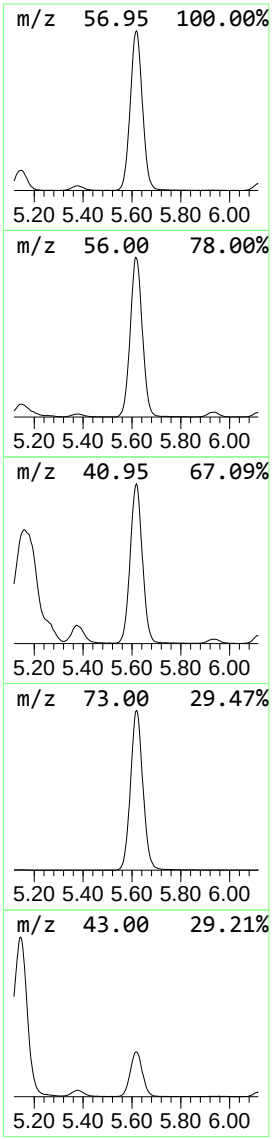
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.618	33.45 ug/l	9041910	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	40
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	38
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	38





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ALS Vial : 20 Sample Multiplier: 1

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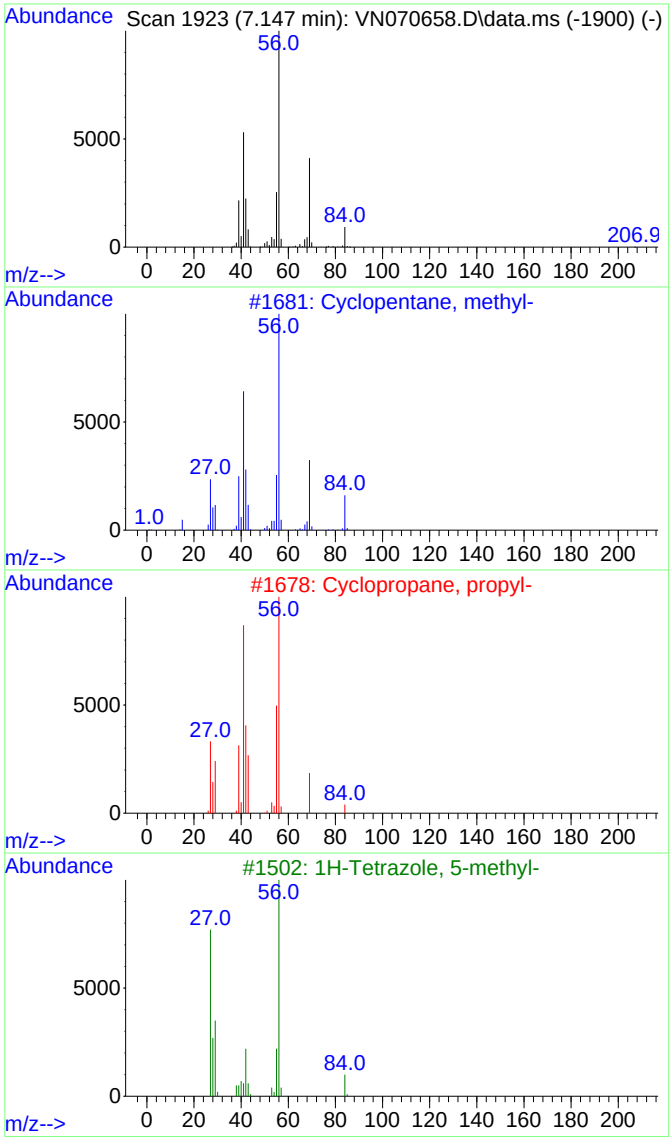
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

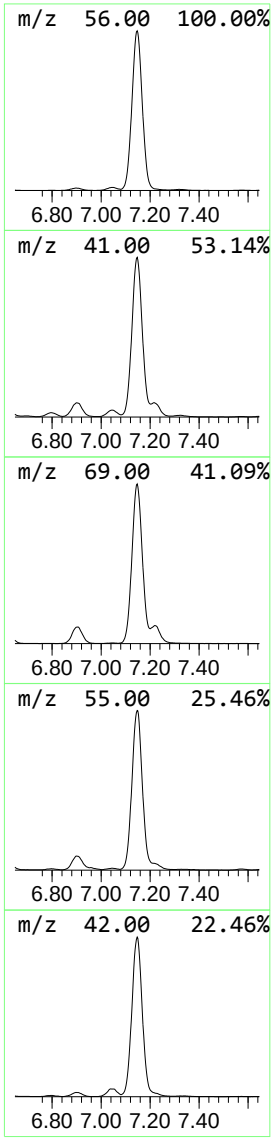
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	65.46 ug/l	17695200	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64





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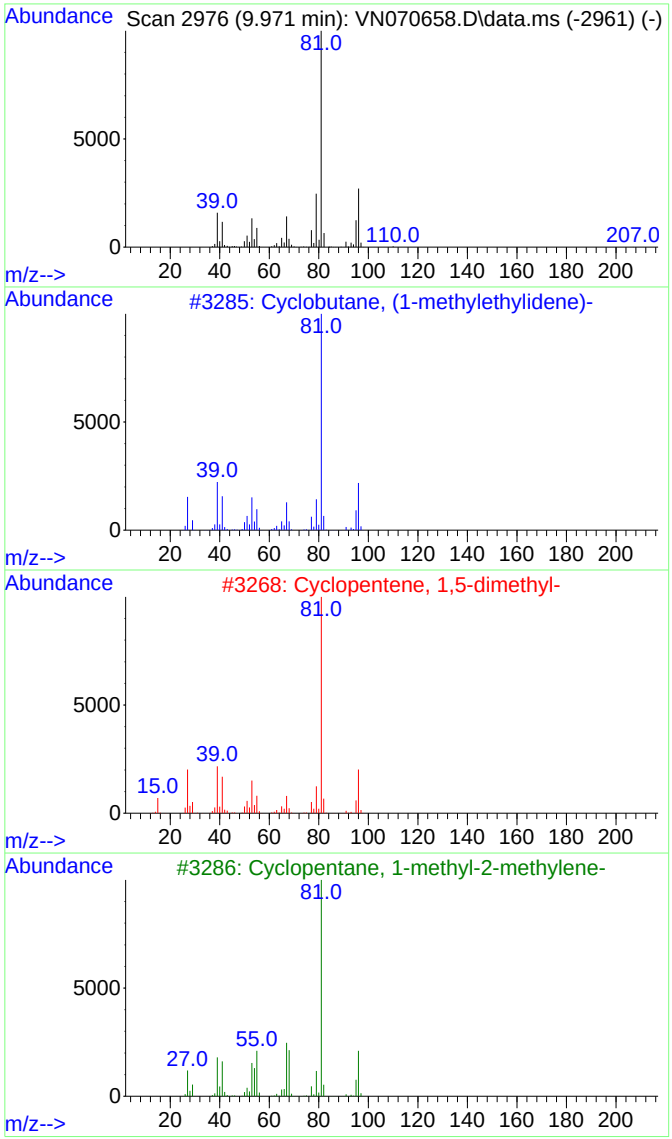
Quant Title : SW846 8260

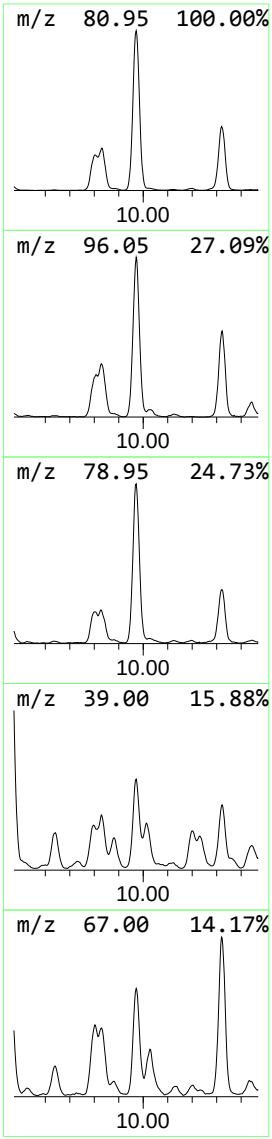
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, (1-methylethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.971	20.69 ug/l	2279750	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	90
3	Cyclopentane, 1-methyl-2-methylene-	96	C7H12	041158-41-2	78
4	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	72
5	2,3-Diazabicyclo[2.2.1]hept-2-en...	124	C7H12N2	071312-54-4	64





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ALS Vial : 20 Sample Multiplier: 1

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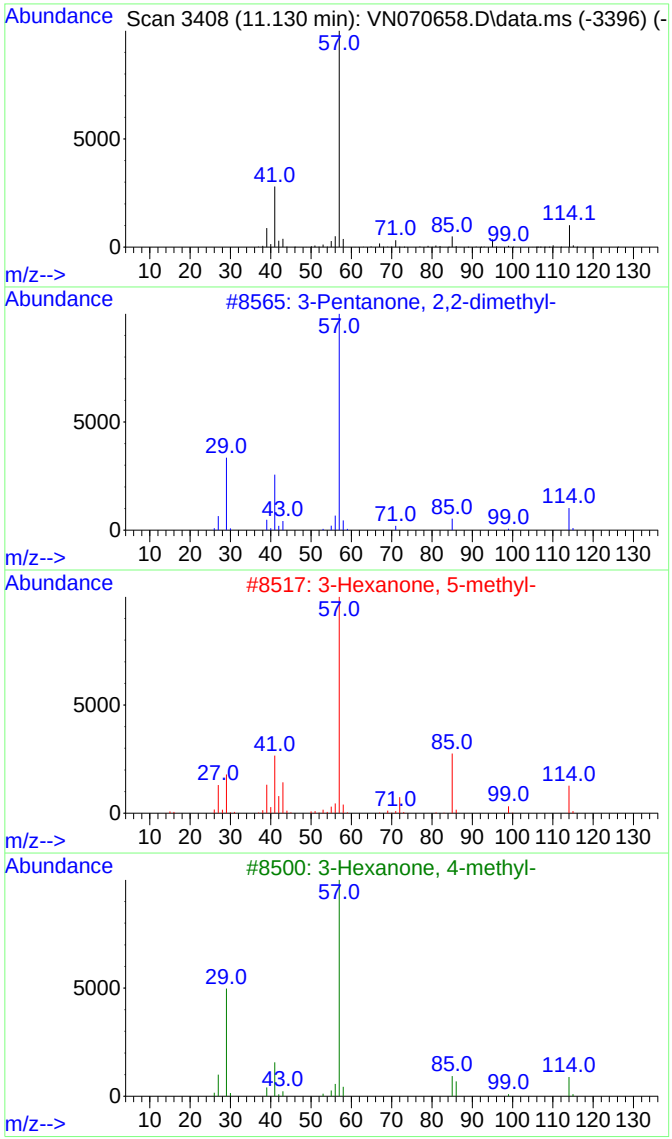
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

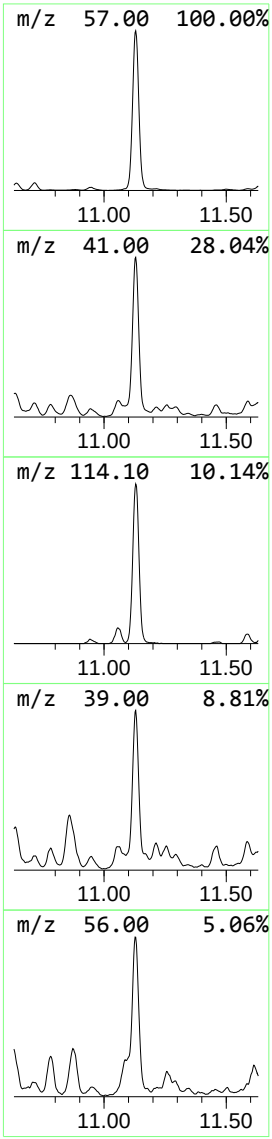
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanone, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.130	26.35 ug/l	2486410	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	72
2	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	50
3	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	47
4	3,4-Hexanedione	114	C6H10O2	004437-51-8	46
5	3-Heptanone	114	C7H14O	000106-35-4	43





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Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

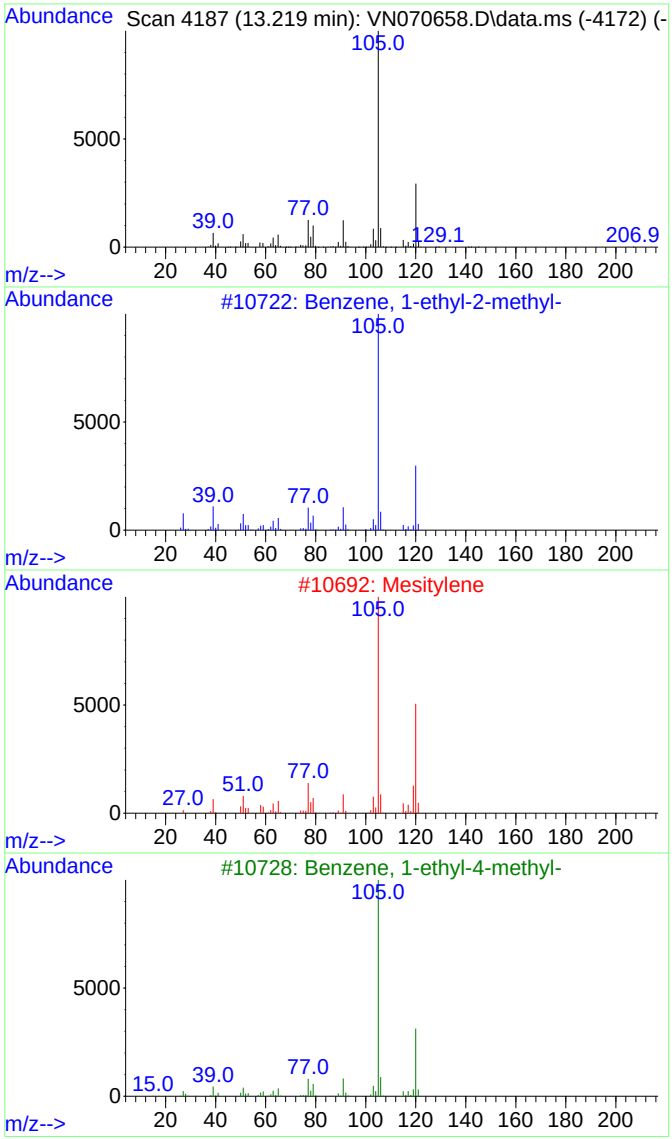
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

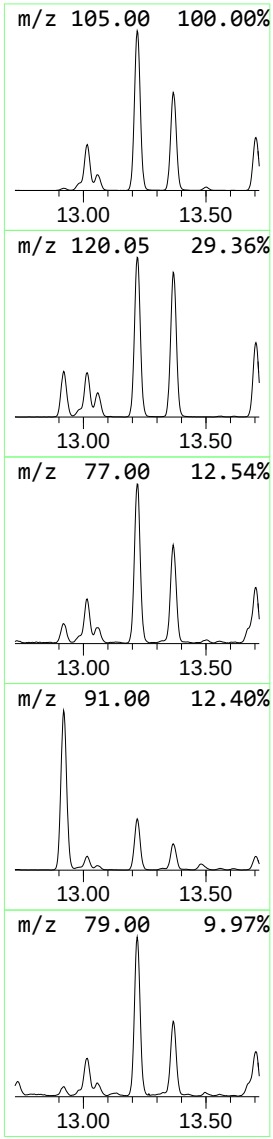
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	70.43 ug/l	4739460	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

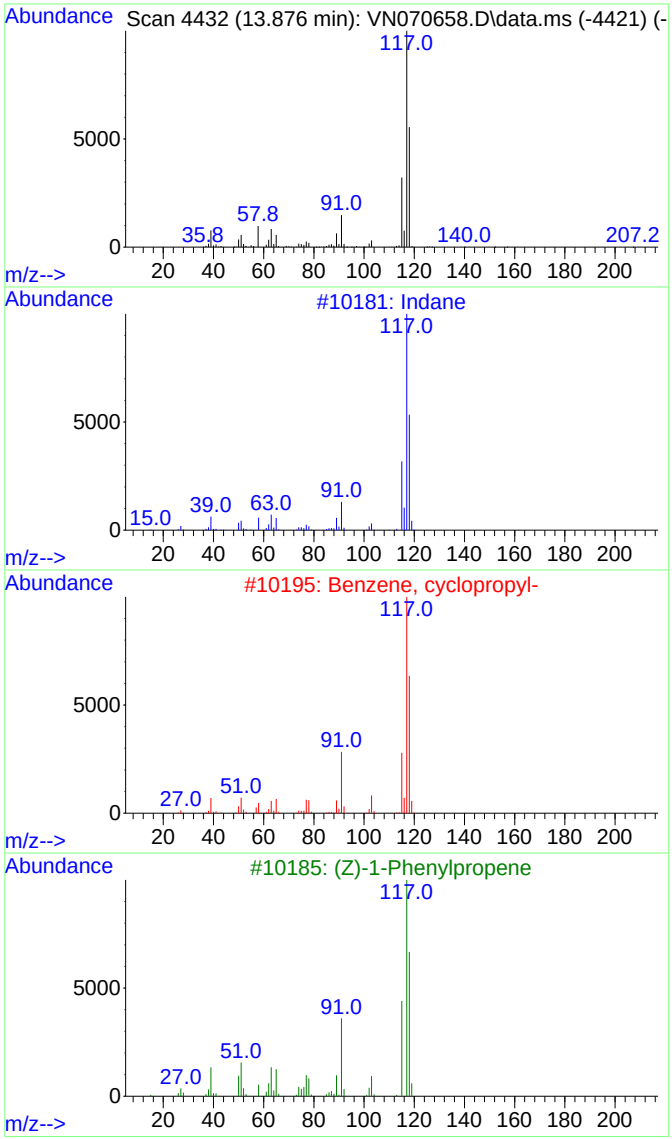
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

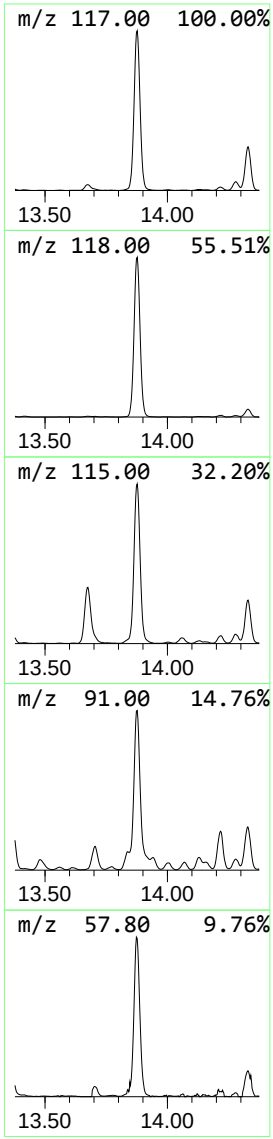
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	135.66 ug/l	9129560	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	59
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

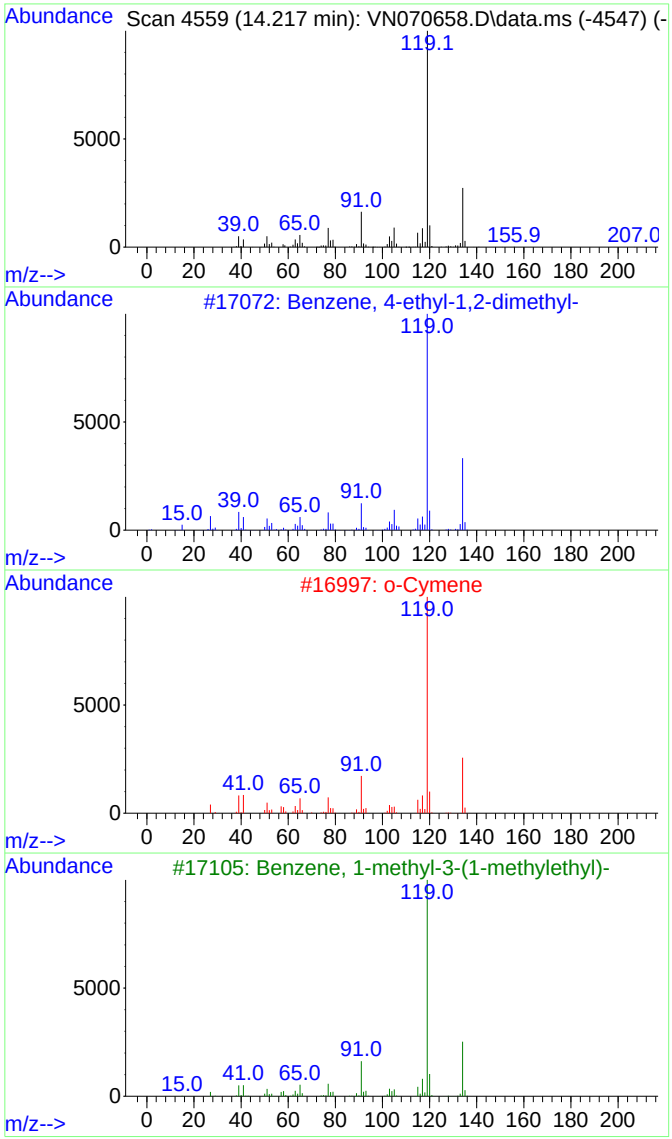
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

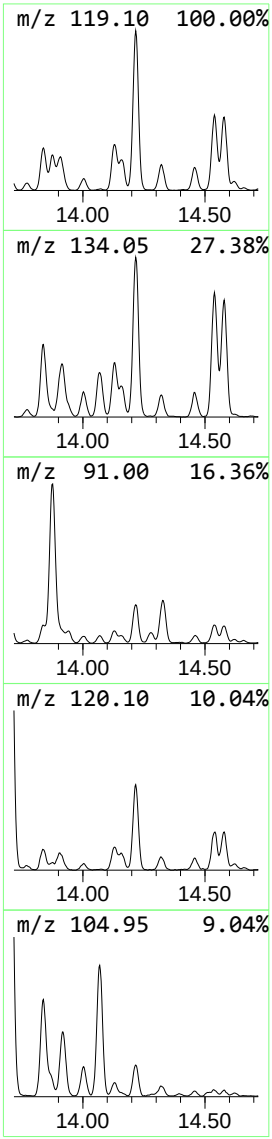
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	22.19 ug/l	1493540	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	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

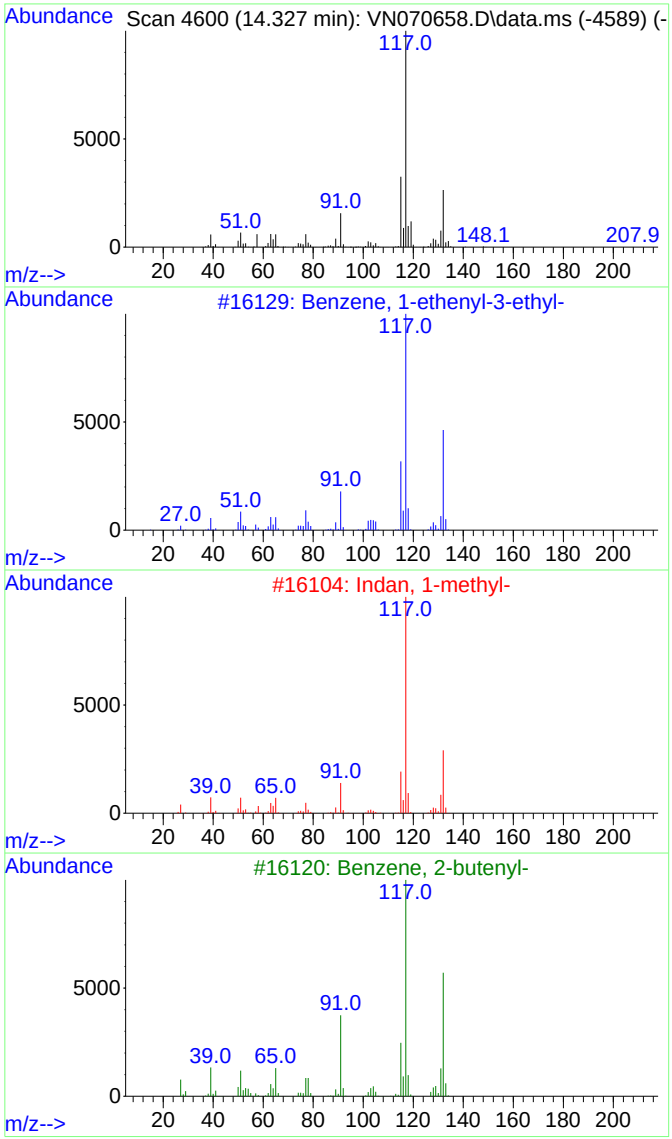
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

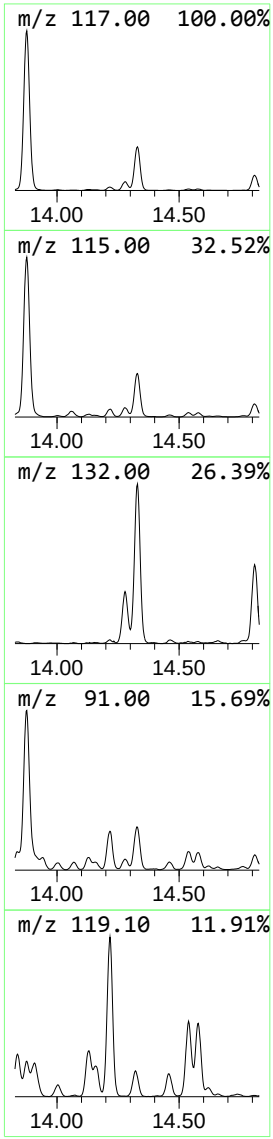
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	33.12 ug/l	2228710	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	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

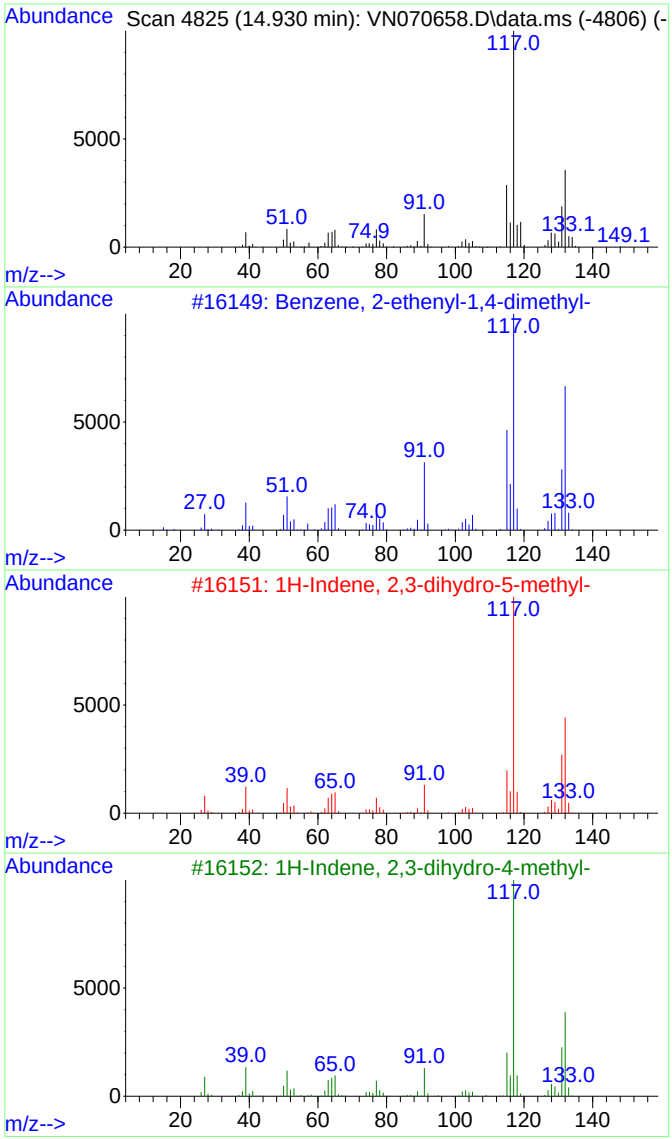
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

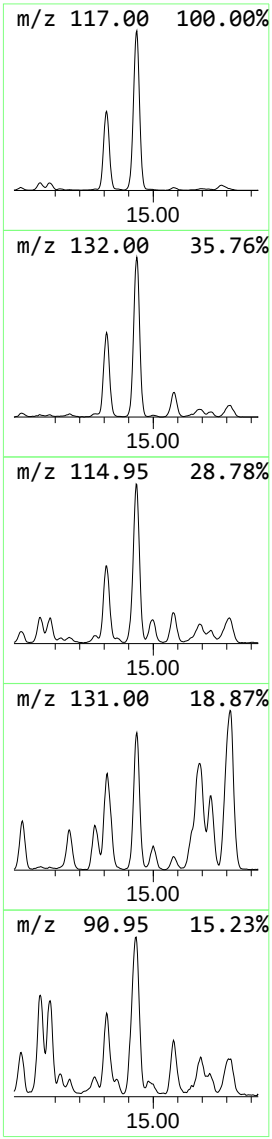
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	31.87 ug/l	2145030	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	93
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
Data File : VN070658.D
Acq On : 17 Jan 2022 20:43
Operator : JC/MD
Sample : N1148-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-24

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-	3.137	59.4	ug/l	16061000	1	8.086	13515200	50.0
Pentane, 3-methyl-	5.618	33.5	ug/l	9041910	1	8.086	13515200	50.0
Cyclopentane, m...	7.147	65.5	ug/l	17695200	1	8.086	13515200	50.0
Cyclobutane, (1...	9.971	20.7	ug/l	2279750	2	8.968	5510160	50.0
3-Pentanone, 2,...	11.130	26.4	ug/l	2486410	3	11.744	4718320	50.0
Benzene, 1-ethy...	13.219	70.4	ug/l	4739460	4	13.675	3364770	50.0
Indane	13.876	135.7	ug/l	9129560	4	13.675	3364770	50.0
Benzene, 4-ethy...	14.217	22.2	ug/l	1493540	4	13.675	3364770	50.0
Benzene, 1-ethe...	14.327	33.1	ug/l	2228710	4	13.675	3364770	50.0
Benzene, 2-ethe...	14.930	31.9	ug/l	2145030	4	13.675	3364770	50.0