LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

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: VN070146.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	80	91	129	rVB3	80047	227842	2.50%	0.128%
2	5.076	1134	1151	1182	rVB4	95918	346958	3.81%	0.195%
3	5.299	1214	1234	1264	rVB2	30555	112753	1.24%	0.064%
4	5.565	1307	1333	1360	rVB4	56022	199228	2.19%	0.112%
5	6.080	1497	1525	1556	rBV6	80774	251339	2.76%	0.142%
6	7.018	1846	1875	1900	rBV3	260912	812934	8.93%	0.458%
7	7.356	1984	2001	2041	rVB	79244	262464	2.88%	0.148%
8	8.021	2224	2249	2257	rBV	885864	2258281	24.80%	1.272%
9	8.078	2260	2270	2287	rVV	1710102	4204181	46.17%	2.368%
10	8.161	2287	2301	2327	rVB3	639610	1601075	17.58%	0.902%
11	8.284	2327	2347	2368	rBV	474086	1098720	12.07%	0.619%
12	8.434	2382	2403	2428	rBV	1110154	2547146	27.97%	1.435%
13	8.606	2432	2467	2494	rBV	1709431	4596978	50.49%	2.589%
14	8.818	2527	2546	2577	rVB2	493179	1054349	11.58%	0.594%
15	8.963	2580	2600	2630	rBV	2755733	5886972	64.65%	3.316%
16	9.260	2698	2711	2736	rVB5	58895	151627	1.67%	0.085%
17	9.453	2753	2783	2793	rBV3	749489	1701007	18.68%	0.958%
18	9.504	2794	2802	2819	rVV	507377	991850	10.89%	0.559%
19	9.588	2819	2833	2843	rVV	119580	253838	2.79%	0.143%
20	9.633	2844	2850	2863	rVV5	67116	123897	1.36%	0.070%
21	9.730	2865	2886	2902	rVB7	121488	319446	3.51%	0.180%
22	9.877	2922	2941	2966	rBV	1249281	2634176	28.93%	1.484%
23	10.014	2968	2992	3005	rVV	1593649	3421018	37.57%	1.927%
24	10.076	3005	3015	3045	rVB2	795857	2034263	22.34%	1.146%
25	10.215	3046	3067	3092	rBV2	764378	1844818	20.26%	1.039%
26	10.368	3108	3124	3137	rBV	1386619	2621116	28.79%	1.476%
27	10.440	3137	3151	3174	rVB	4421608	8380954	92.04%	4.720%
28	10.620	3204	3218	3233	rVB	848472	1627493	17.87%	0.917%
29	10.784	3269	3279	3282	rBV3	76975	105693	1.16%	0.060%
30	10.886	3297	3317	3335	rVB7	347503	922122	10.13%	0.519%
31	10.963	3336	3346	3359	rVB	208277	371624	4.08%	0.209%
32	11.052	3360	3379	3392	rBV2	259692	514829	5.65%	0.290%
33	11.154	3406	3417	3435	rVB	370122	749356	8.23%	0.422%
34	11.454	3520	3529	3537	rBV	210753	328204	3.60%	0.185%
35	11.527	3540	3556	3581	rVB3	1032781	2431400	26.70%	1.369%
36	11.629	3582	3594	3616	rBV	831370	1488235	16.34%	0.838%

LSC Area Percent Report

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ClientSampleId :
HSB-3-(11-11.5)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

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

37	11.747	3619	3638	3653	rBV	4565925	8584360	94.28%	4.835%
38	11.811	3656	3662	3671	rVB	201635	257834	2.83%	0.145%
39	11.958	3707	3717	3725	rBV2	805713	1212035	13.31%	0.683%
40	12.184	3792	3801	3812	rBV6	261913	412661	4.53%	0.232%
41	12.253	3819	3827	3840	rVB4	345536	531183	5.83%	0.299%
42	12.369	3861	3870	3881	rVB	412785	672335	7.38%	0.379%
43	12.734	3994	4006	4028	rVB2	3945482	8541207	93.80%	4.811%
44	12.876	4049	4059	4066	rBV3	283503	529286	5.81%	0.298%
45	12.919	4069	4075	4086	rVB	557060	844932	9.28%	0.476%
46	12.983	4088	4099	4106	rBV	1195388	1968635	21.62%	1.109%
47	13.055	4117	4126	4168	rVB3	2432366	5315616	58.38%	2.994%
48	13.222	4173	4188	4205	rBV2	868990	2007415	22.05%	1.131%
49	13.369	4230	4243	4255	rBV	5144920	8066337	88.59%	4.543%
50	13.608	4324	4332	4338	rBV2	406663	567681	6.23%	0.320%
51	13.675	4346	4357	4379	rBV2	4775485	9105503	100.00%	5.128%
52	13.841	4407	4419	4421	rBV2	1018618	1322174	14.52%	0.745%
53	13.871	4423	4430	4437	rVV2	2719306	4610174	50.63%	2.597%
54	13.911	4438	4445	4466	rVV3	3488903	6949595	76.32%	3.914%
55	13.994	4467	4476	4488	rVV2	1103145	1631245	17.91%	0.919%
56	14.069	4496	4504	4515	rVB	755948	1132304	12.44%	0.638%
57	14.131	4516	4527	4532	rBV	1828055	2824043	31.01%	1.591%
58	14.217	4548	4559	4574	rBV	3322679	5305314	58.26%	2.988%
59	14.327	4589	4600	4612	rVB3	1698026	2802341	30.78%	1.578%
60	14.463	4640	4651	4662	rBV3	781422	1472054	16.17%	0.829%
61	14.541	4671	4680	4687	rBV	1648874	2594310	28.49%	1.461%
62	14.579	4688	4694	4703	rVV	2473857	3461273	38.01%	1.949%
63	14.622	4703	4710	4718	rVV2	1613931	2282229	25.06%	1.285%
64	14.659	4720	4724	4739	rVB2	970073	1314880	14.44%	0.741%
65	14.764	4755	4763	4771	rBV2	831032	1110798	12.20%	0.626%
66	14.812	4771	4781	4788	rBV4	1912830	3247704	35.67%	1.829%
67	14.850	4790	4795	4807	rVB3	1993490	2863284	31.45%	1.613%
68	14.930	4808	4825	4837	rBV5	3072580	7771110	85.35%	4.377%
69	15.086	4875	4883	4899	rVB3	413815	763543	8.39%	0.430%
70	15.196	4903	4924	4952	rVV4	1883881	6155910	67.61%	3.467%
71	15.314	4956	4968	4986	rVB3	1488536	3455581	37.95%	1.946%
72	15.469	5015	5026	5029	rBV7	429777	642209	7.05%	0.362%
73	15.504	5032	5039	5053	rVB	1153282	1993942	21.90%	1.123%
74	15.614	5070	5080	5091	rBV3	662051	1152333	12.66%	0.649%
75	15.807	5137	5152	5168	rBV2	924193	2013338	22.11%	1.134%
76	16.617	5441	5454	5498	rVB2	593956	1582472	17.38%	0.891%

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Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

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

Sum of corrected areas: 177549366

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
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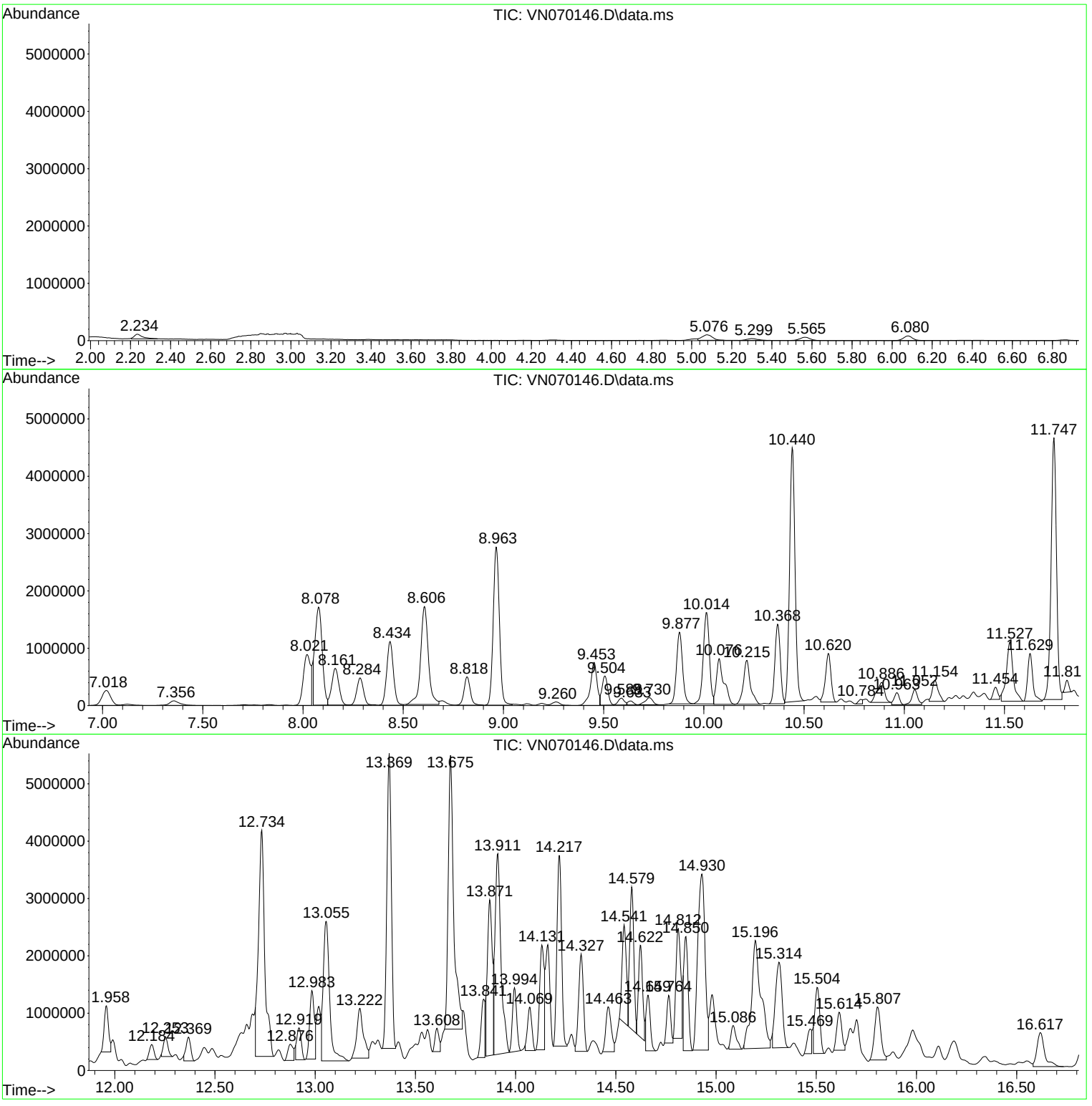
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

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\VN121621\
Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
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Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

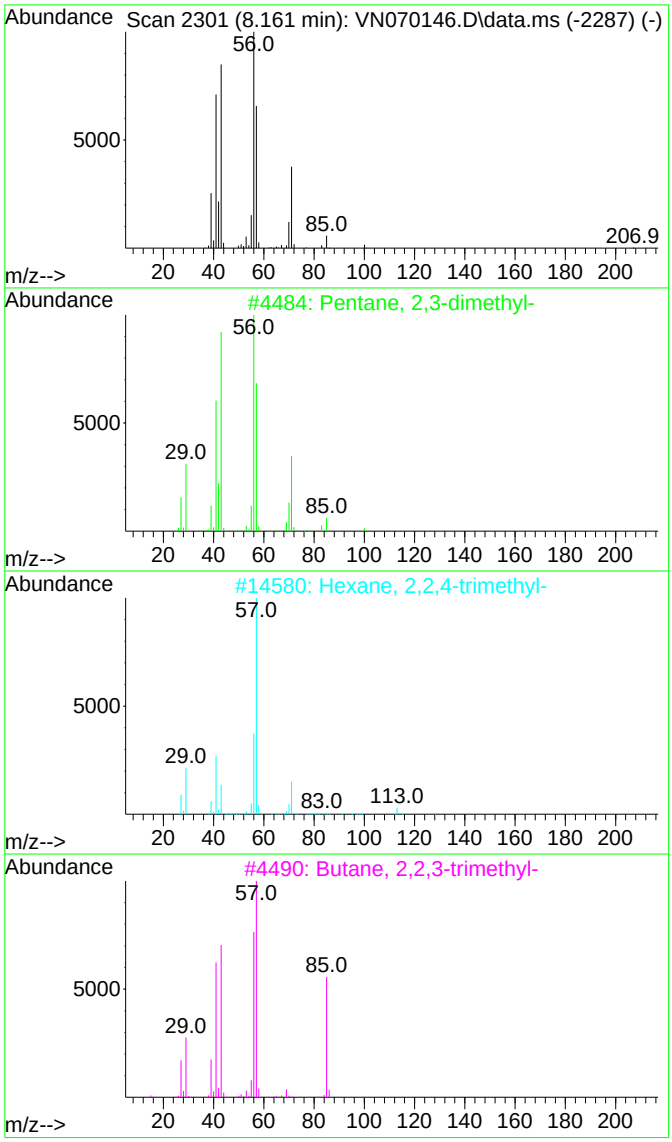
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

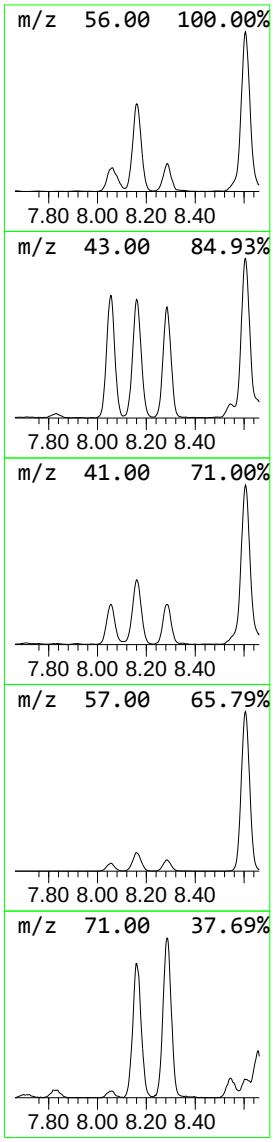
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	19.04 ug/l	1601080	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40
4	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070146.D
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Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

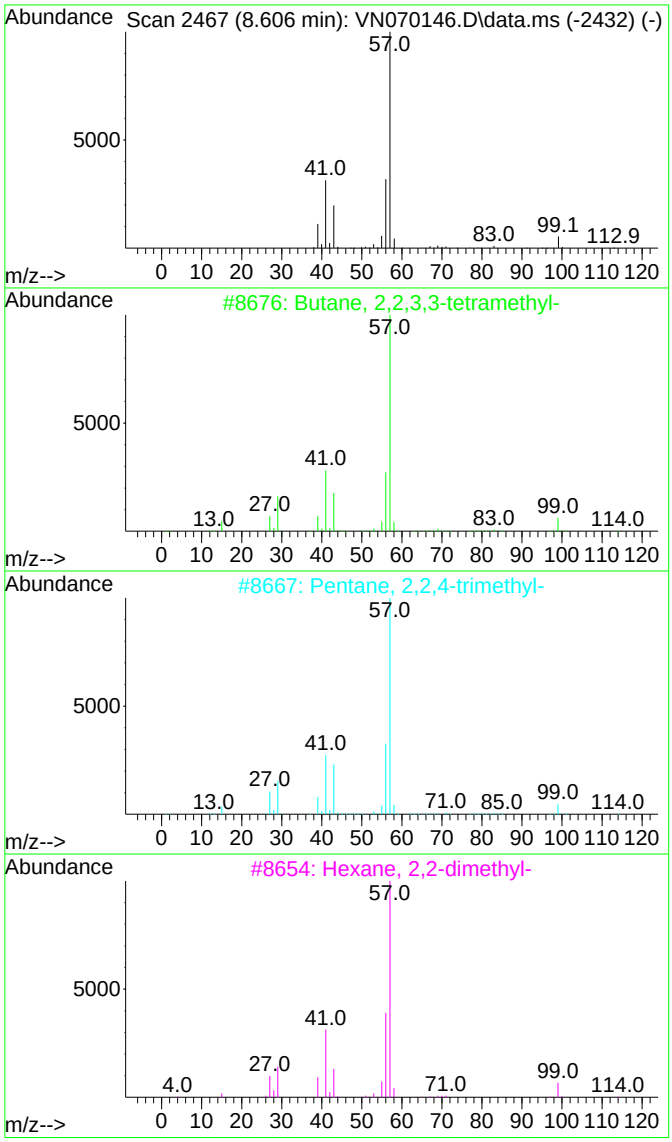
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

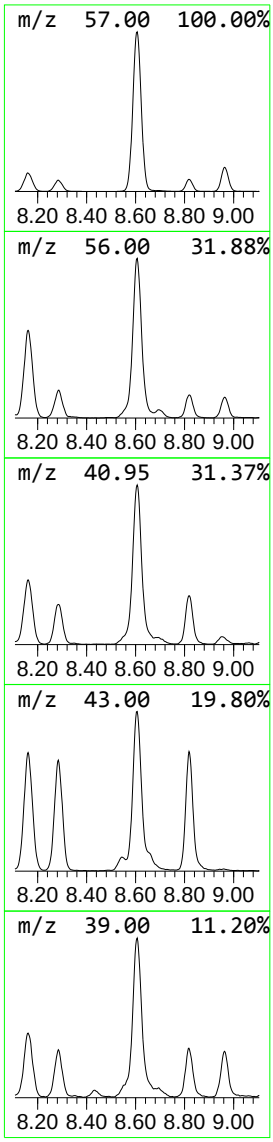
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.606	39.04 ug/l	4596980	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59





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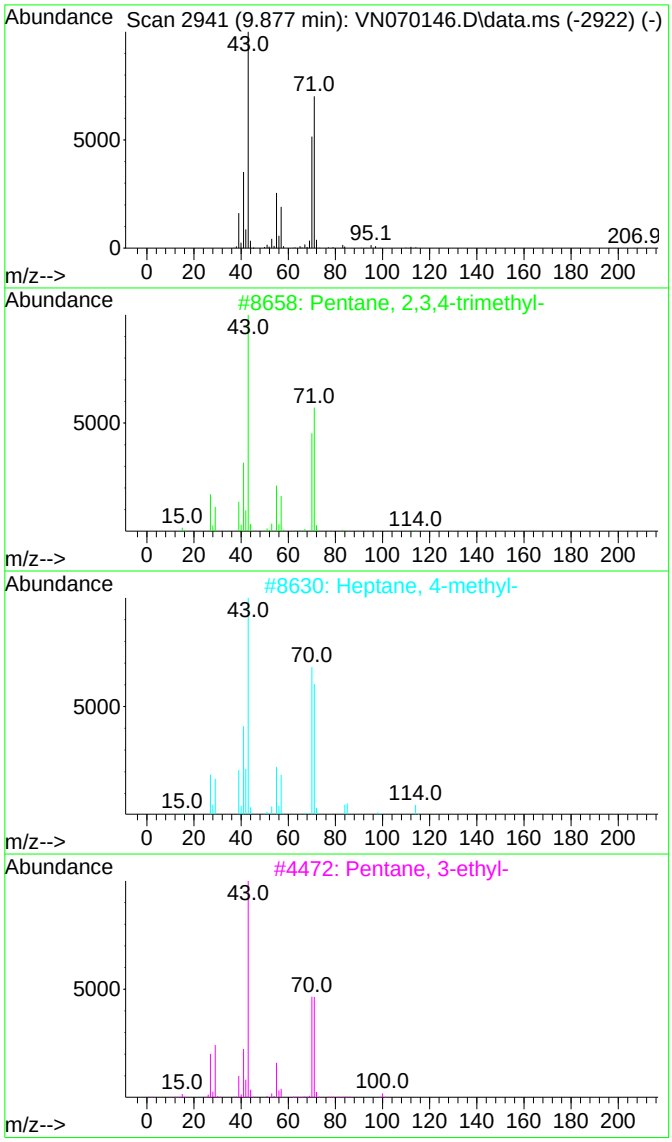
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

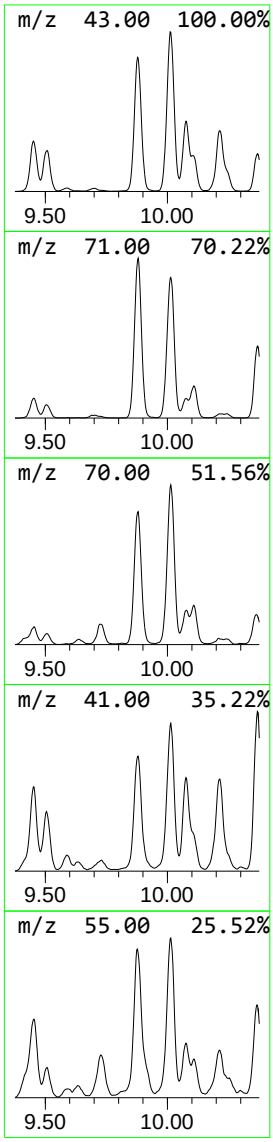
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	22.37 ug/l	2634180	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	59





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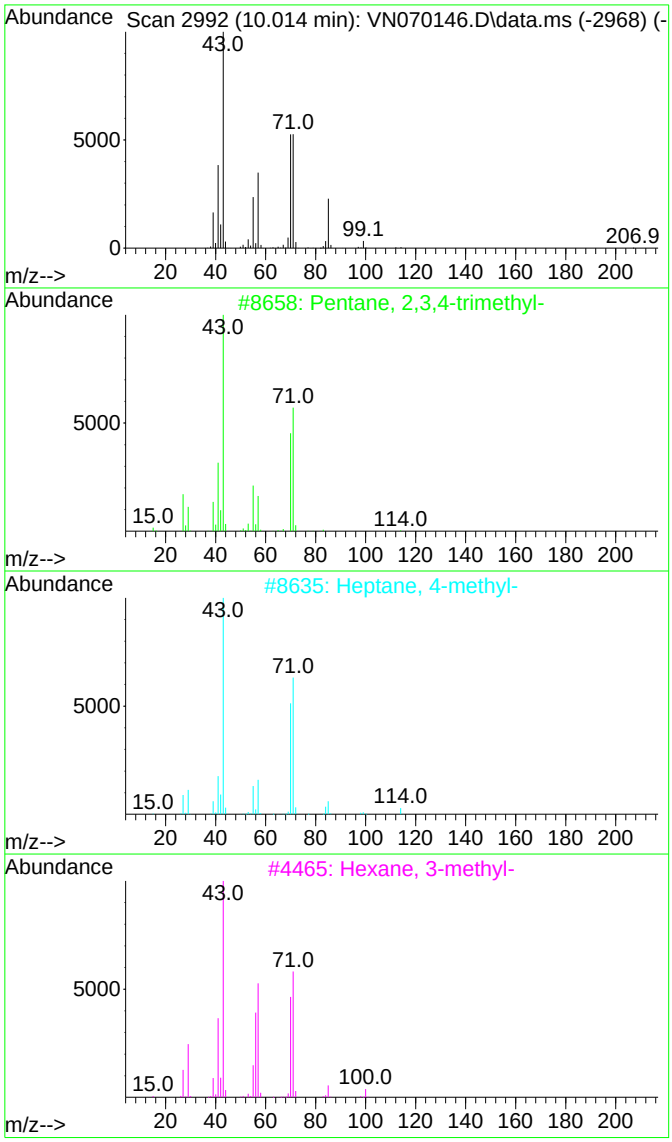
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

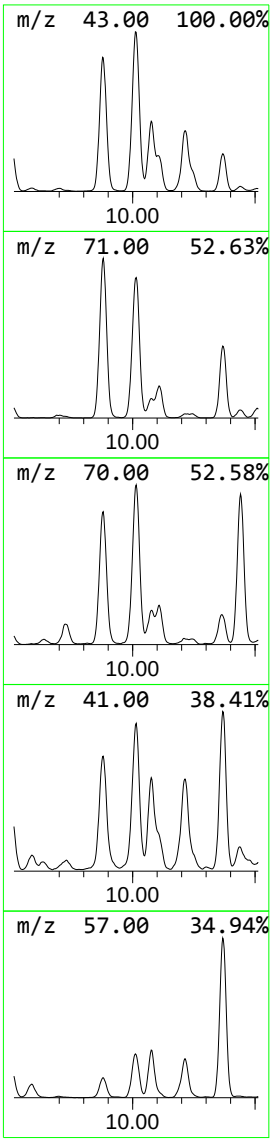
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	29.06 ug/l	3421020	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	74
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47





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MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

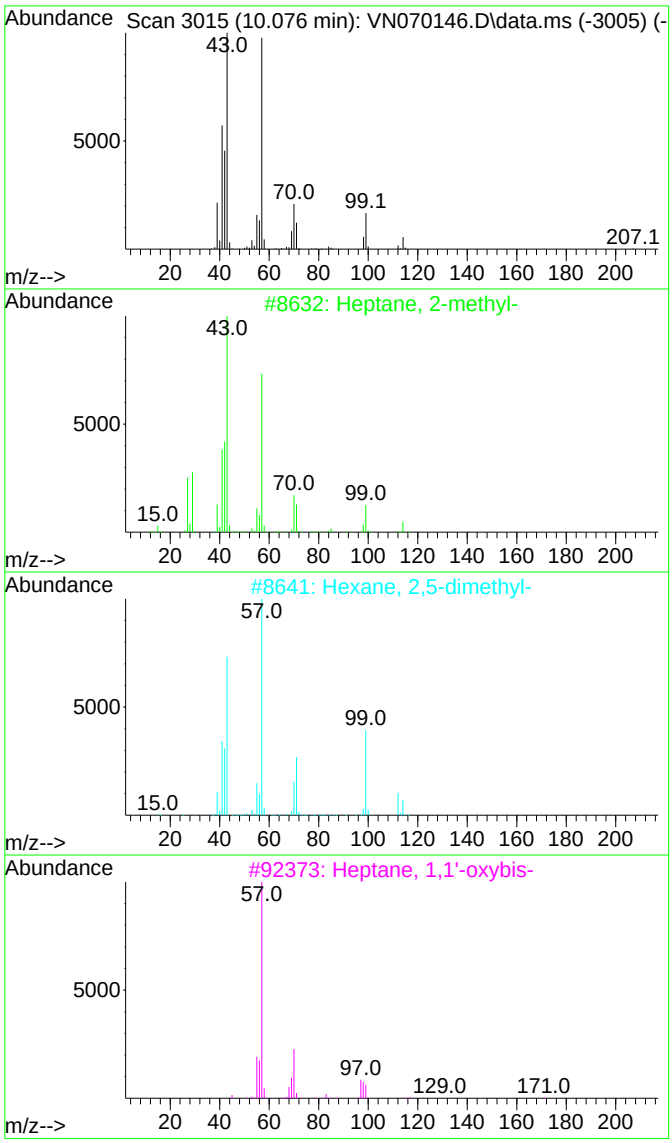
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

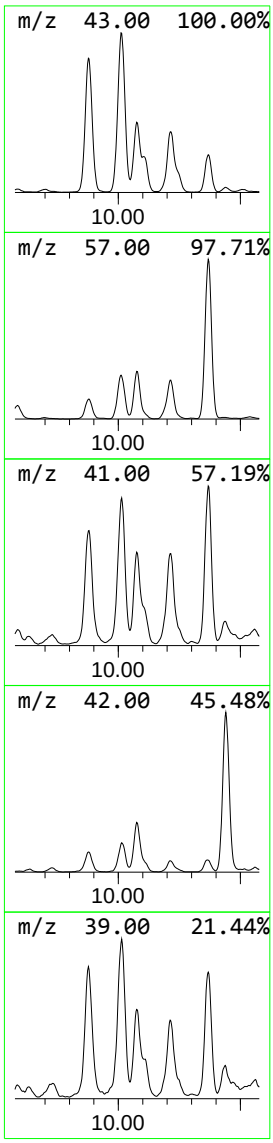
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.076	17.28 ug/l	2034260	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	38
5	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070146.D
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Operator : JC/MD
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Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

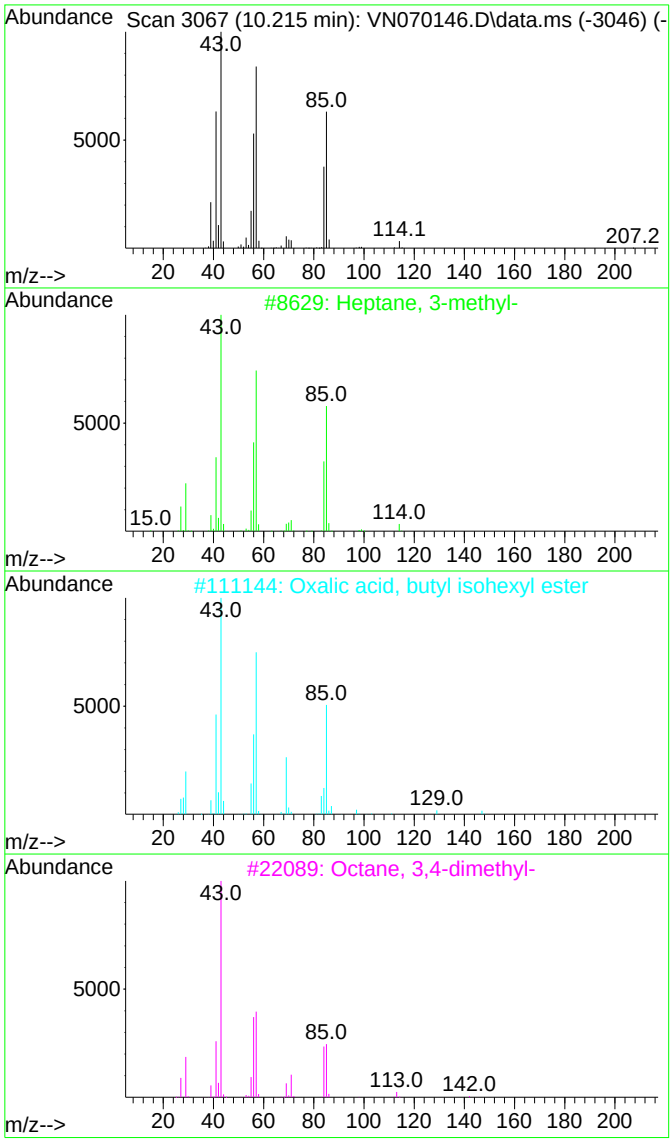
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

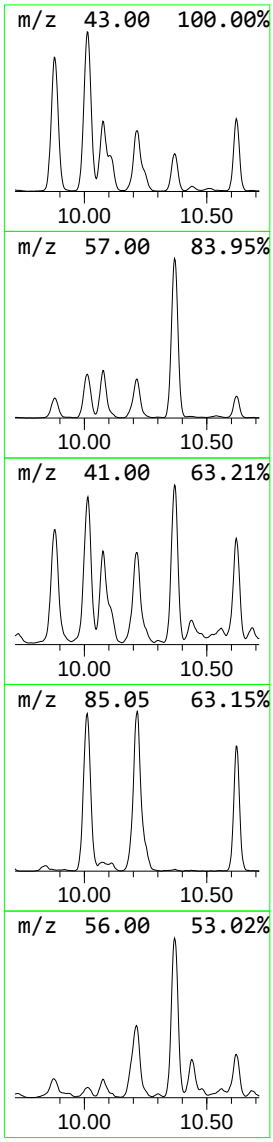
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	15.67 ug/l	1844820	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	78
3	Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	72
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
5	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	50





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Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

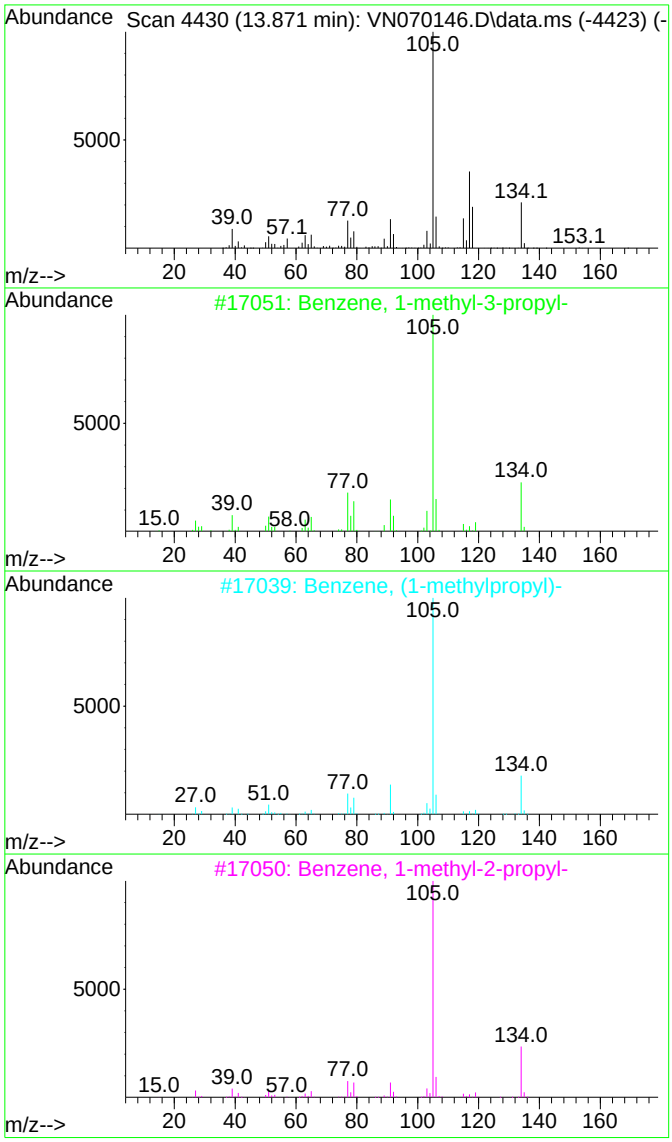
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

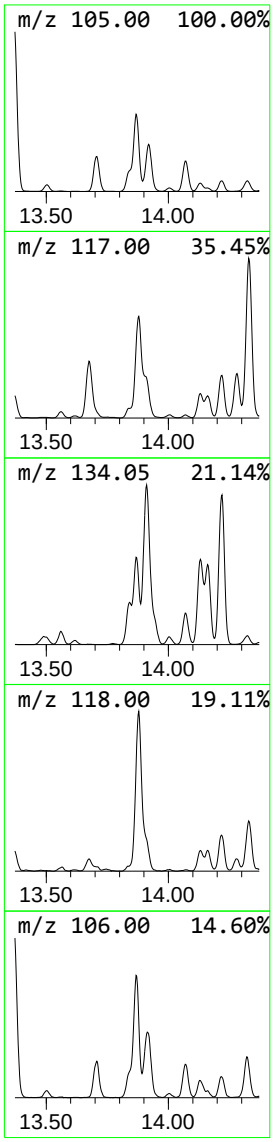
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-methyl-3-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	25.32 ug/l	4610170	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	55
2	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	55
3	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	46
4	2-Tolyloxirane	134	C9H10O	002783-26-8	45
5	2-Indanol	134	C9H10O	004254-29-9	43





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Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

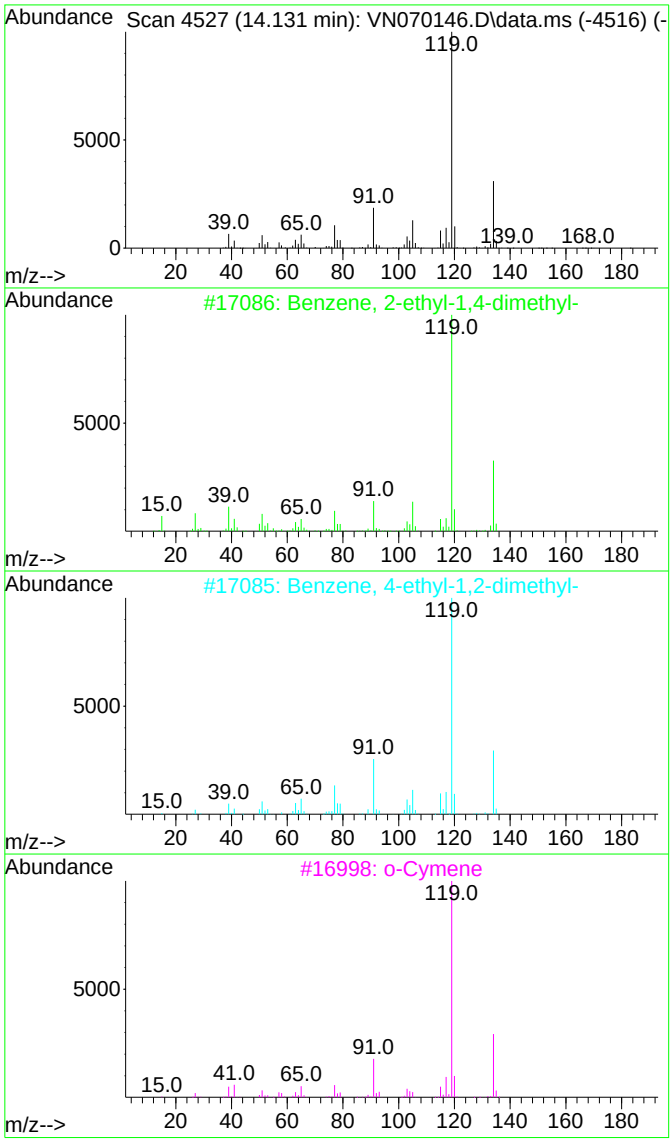
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

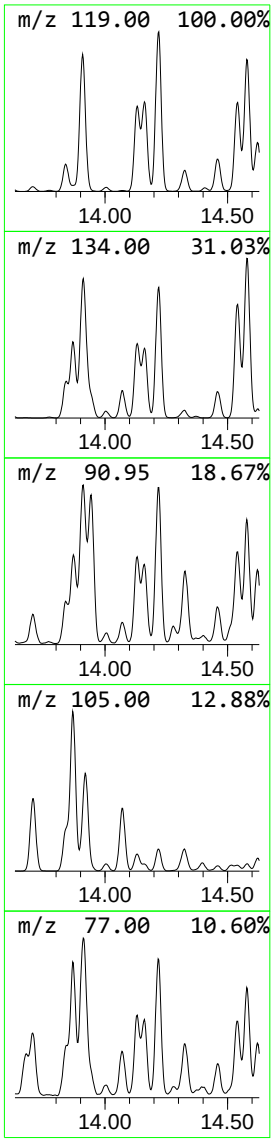
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.131	15.51 ug/l	2824040	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	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





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Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

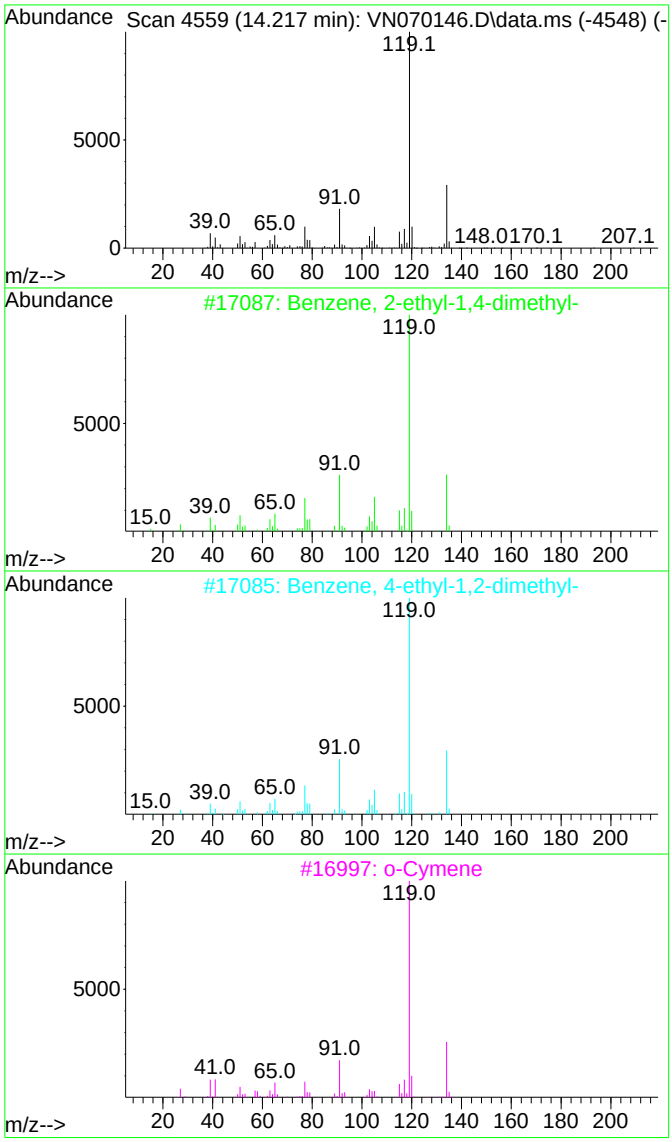
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

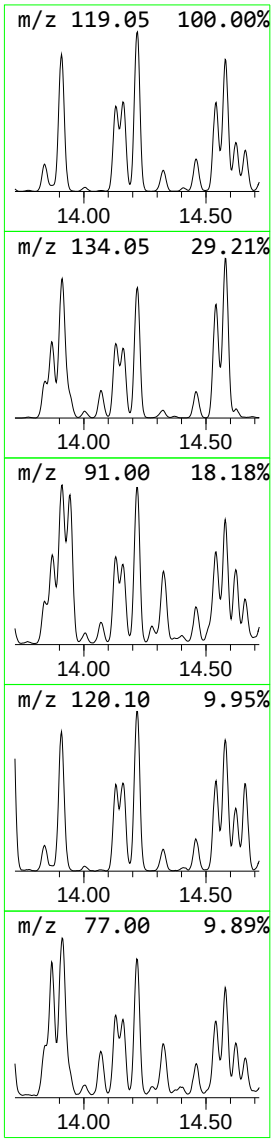
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	29.13 ug/l	5305310	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	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





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Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

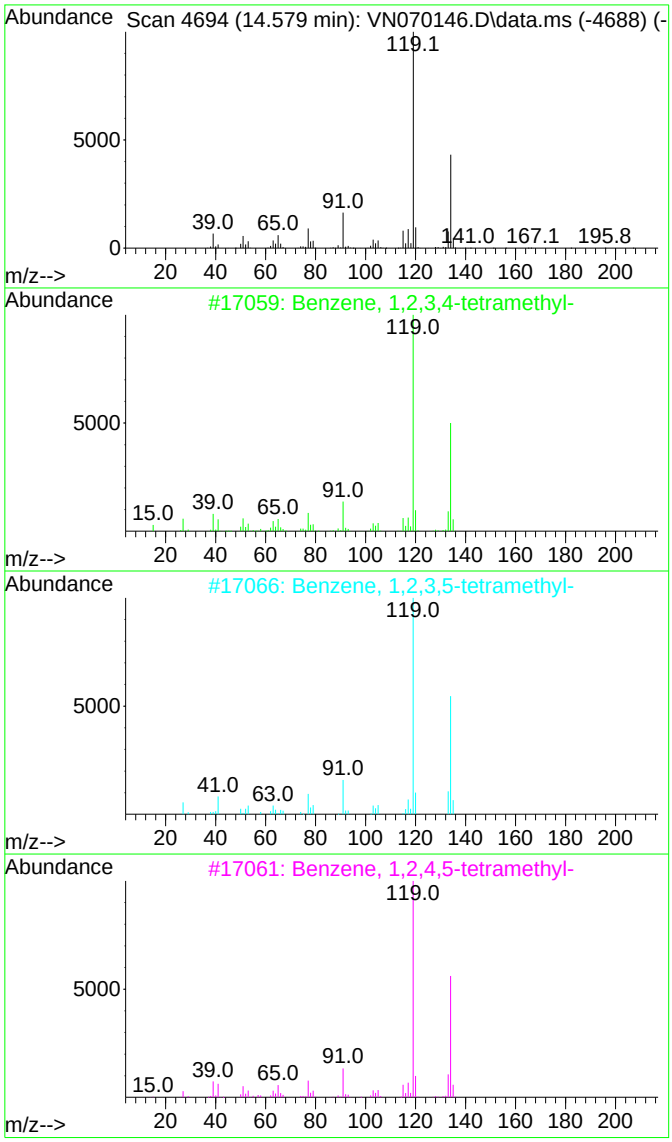
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

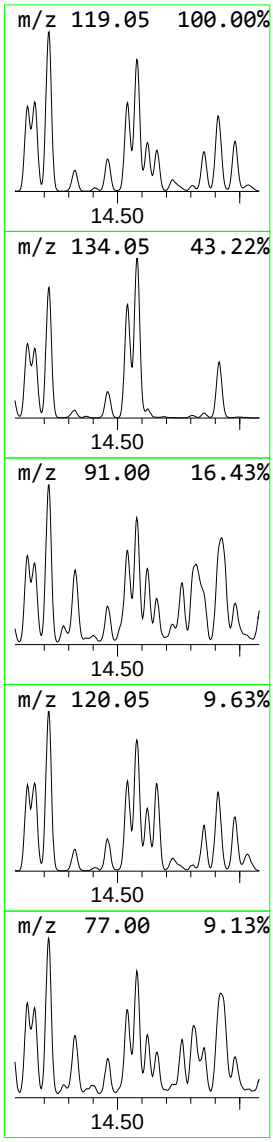
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.579	19.01 ug/l	3461270	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	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





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Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

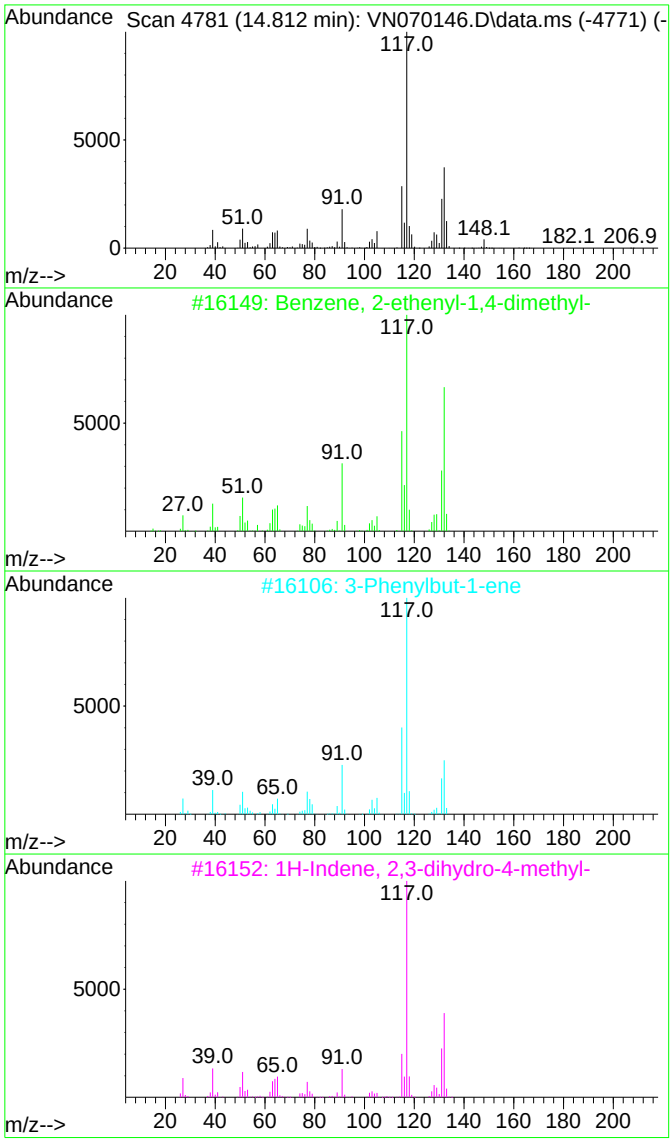
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

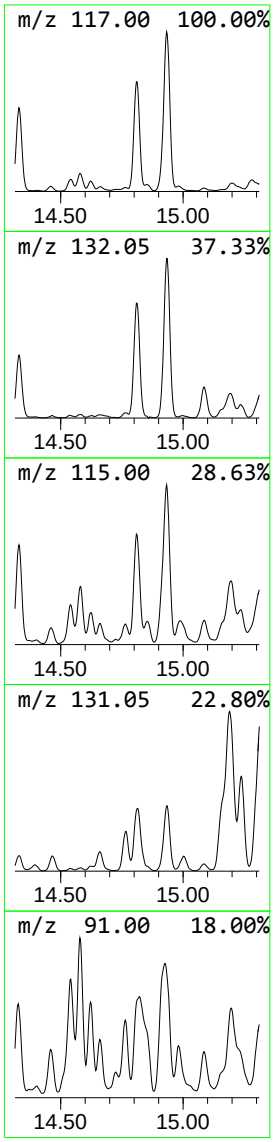
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 3-Phenylbut-1-ene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.812	17.83 ug/l	3247700	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	95
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
5	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	87





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Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

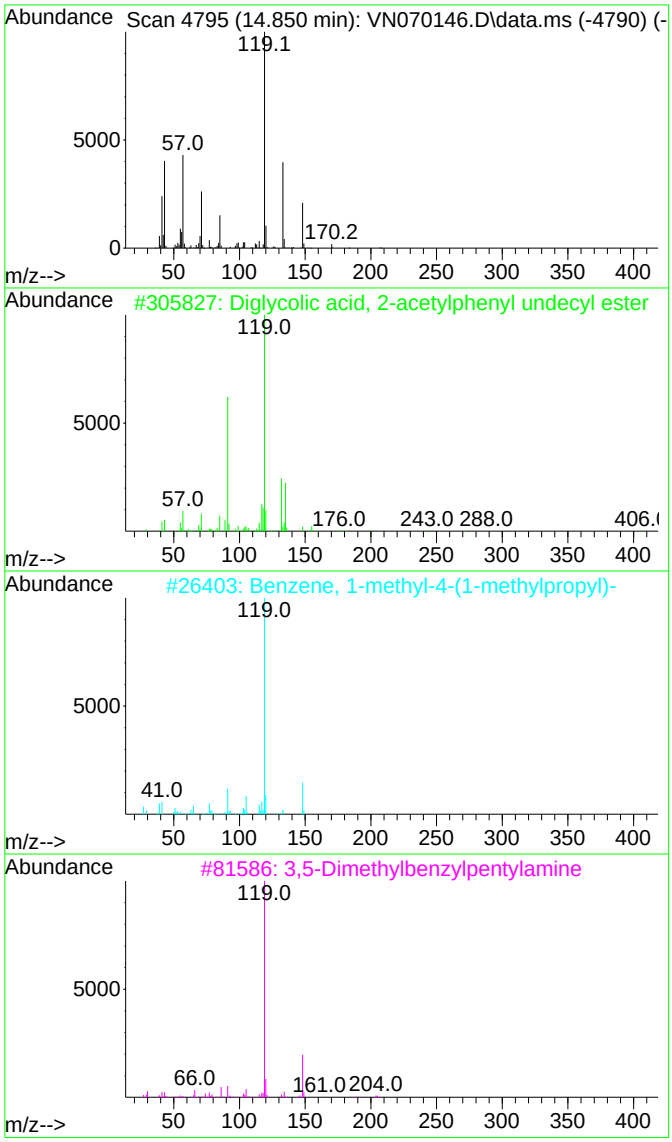
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

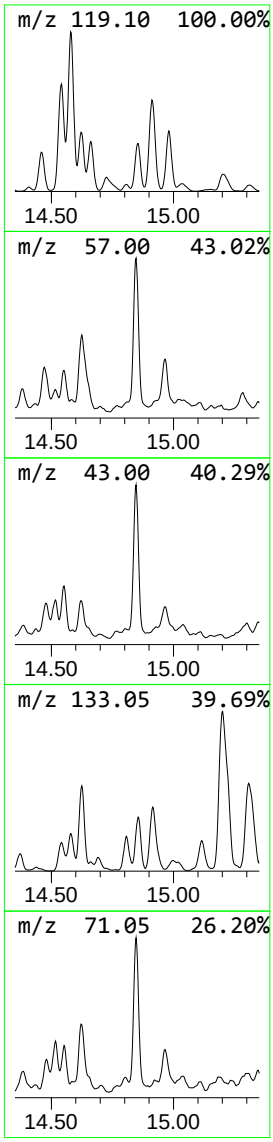
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 unknown14.850 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.850	15.72 ug/l	2863280	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diglycolic acid, 2-acetylphenyl ...	406	C23H34O6	1000382-72-7	47
2	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	43
3	3,5-Dimethylbenzylpentylamine	205	C14H23N	1000491-60-8	43
4	Diglycolic acid, 2-acetylphenyl ...	392	C22H32O6	1000382-72-6	38
5	2-Propenal, 3-(2-pyridinylamino)-	148	C8H8N2O	068970-82-1	37





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Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

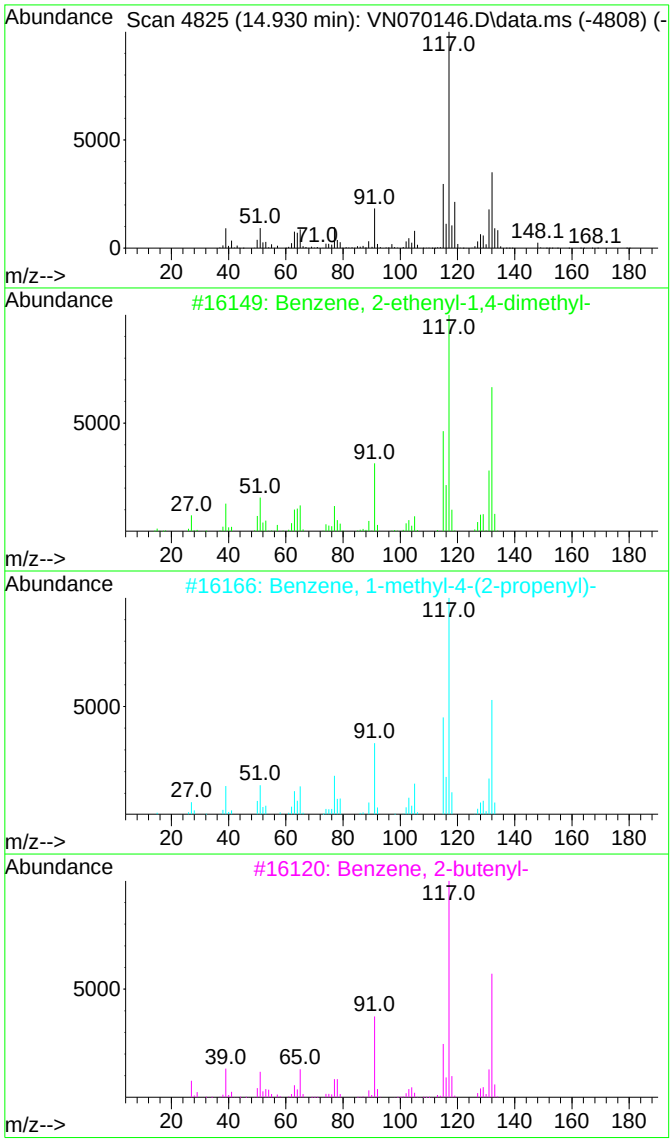
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

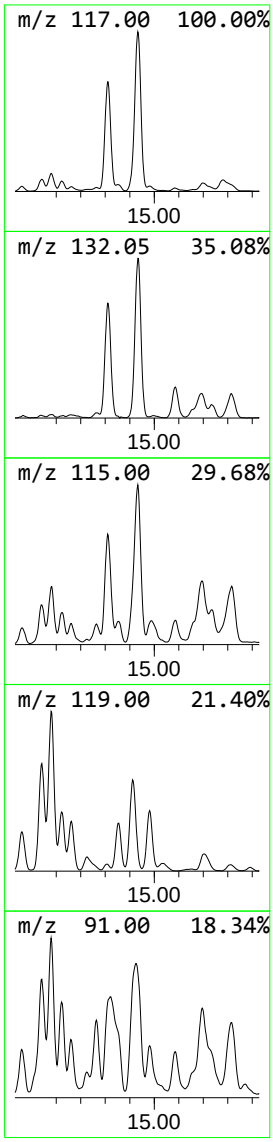
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	42.67 ug/l	7771110	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	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81





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Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

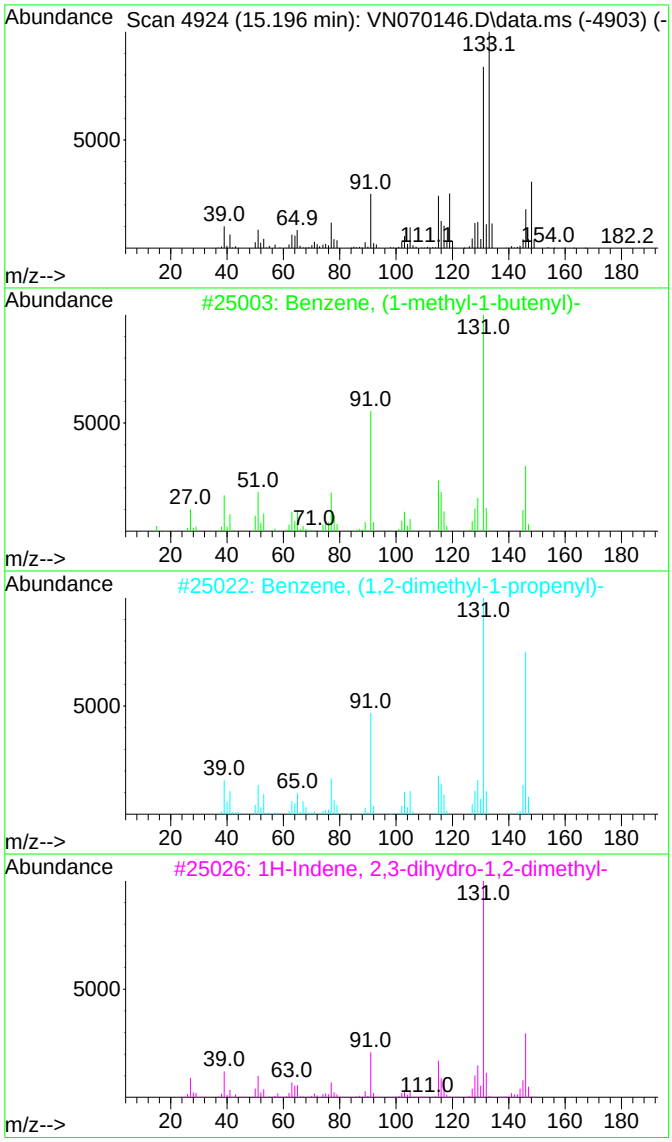
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

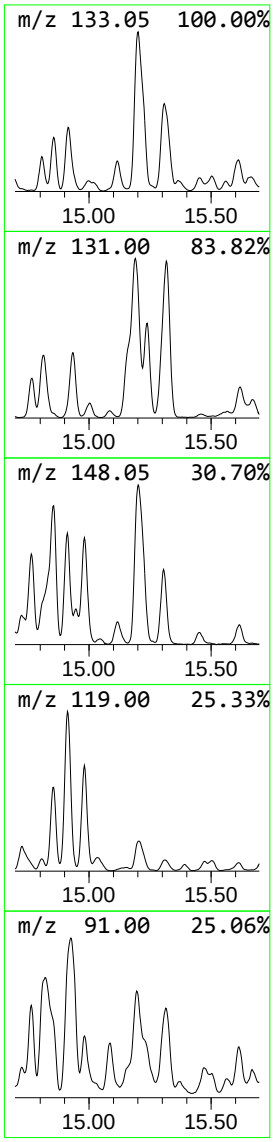
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, (1-methyl-1-butenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	33.80 ug/l	6155910	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	89
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	64
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	62





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Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

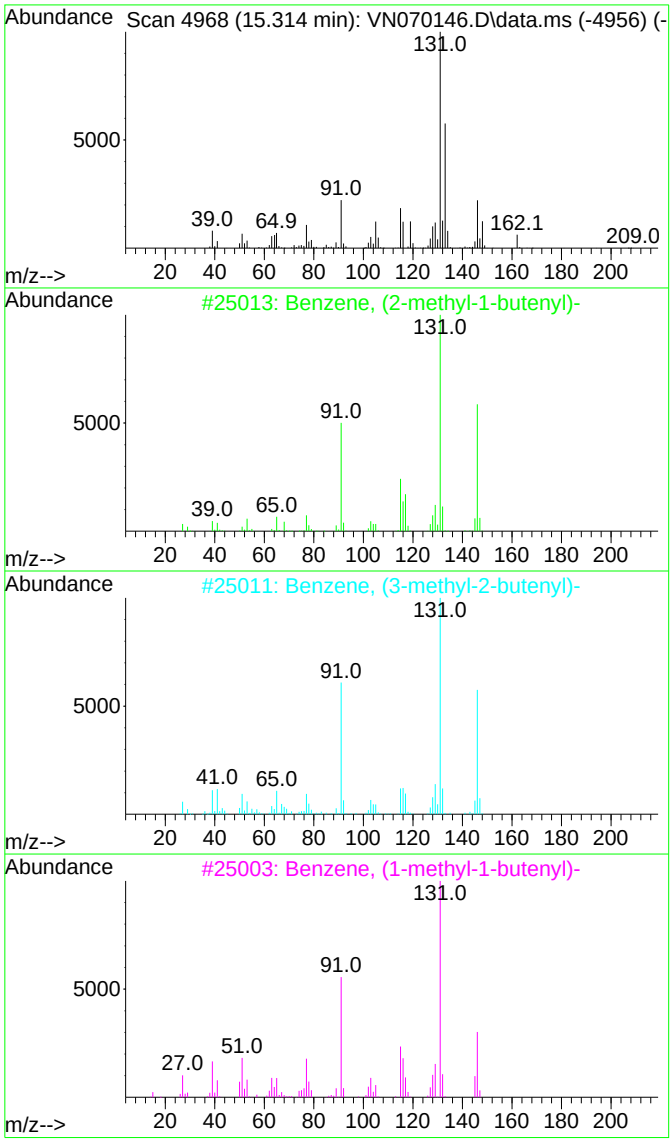
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

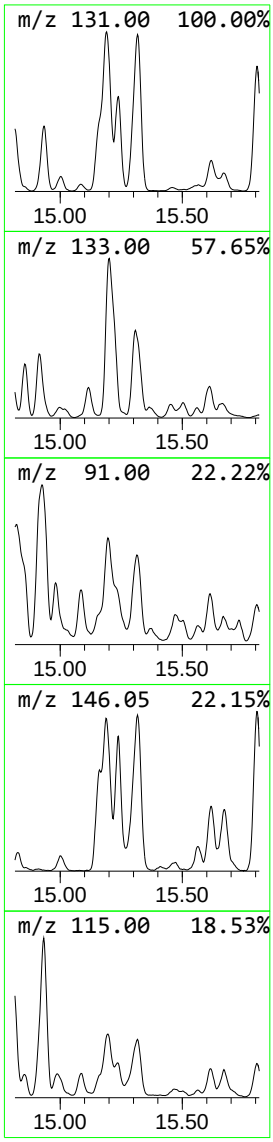
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, (2-methyl-1-butenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.314	18.98 ug/l	3455580	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	91
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	83
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	83
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	83
5	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121621\
Data File : VN070146.D
Acq On : 16 Dec 2021 18:48
Operator : JC/MD
Sample : M5011-06
Misc : 2.37g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-3-(11-11.5)

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
Pentane, 2,3-di...	8.161	19.0	ug/l	1601080	1	8.080	4204180	50.0
Butane, 2,2,3,3...	8.606	39.0	ug/l	4596980	2	8.965	5886970	50.0
Pentane, 2,3,4-...	9.877	22.4	ug/l	2634180	2	8.965	5886970	50.0
Heptane, 4-methyl-	10.014	29.1	ug/l	3421020	2	8.965	5886970	50.0
Heptane, 2-methyl-	10.076	17.3	ug/l	2034260	2	8.965	5886970	50.0
Heptane, 3-methyl-	10.215	15.7	ug/l	1844820	2	8.965	5886970	50.0
Benzene, 1-meth...	13.871	25.3	ug/l	4610170	4	13.675	9105500	50.0
Benzene, 2-ethy...	14.131	15.5	ug/l	2824040	4	13.675	9105500	50.0
Benzene, 4-ethy...	14.217	29.1	ug/l	5305310	4	13.675	9105500	50.0
Benzene, 1,2,3,...	14.579	19.0	ug/l	3461270	4	13.675	9105500	50.0
3-Phenylbut-1-ene	14.812	17.8	ug/l	3247700	4	13.675	9105500	50.0
unknown14.850	14.850	15.7	ug/l	2863280	4	13.675	9105500	50.0
Benzene, 2-ethe...	14.930	42.7	ug/l	7771110	4	13.675	9105500	50.0
Benzene, (1-met...	15.196	33.8	ug/l	6155910	4	13.675	9105500	50.0
Benzene, (2-met...	15.314	19.0	ug/l	3455580	4	13.675	9105500	50.0