

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
 Data File : VN070093.D
 Acq On : 15 Dec 2021 1:12
 Operator : JC/MD
 Sample : M5011-01 10X
 Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HSB-1-(9-9.5)

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: VN070093.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.613	1326	1351	1377	rVB5	37227	128826	1.53%	0.202%
2	7.045	1862	1885	1904	rBV4	46361	139769	1.66%	0.219%
3	7.142	1906	1921	1944	rVB5	29887	90315	1.08%	0.142%
4	8.021	2224	2249	2260	rBV3	837425	2049229	24.39%	3.217%
5	8.083	2261	2272	2292	rVV	1562435	3594919	42.79%	5.644%
6	8.174	2295	2306	2332	rVB3	105671	265020	3.15%	0.416%
7	8.295	2332	2351	2367	rBV3	111213	253609	3.02%	0.398%
8	8.437	2384	2404	2431	rBV	1020986	2376356	28.29%	3.731%
9	8.614	2438	2470	2493	rBV	537563	1433932	17.07%	2.251%
10	8.823	2538	2548	2579	rVB4	69884	183977	2.19%	0.289%
11	8.965	2580	2601	2634	rBV	2544680	5362518	63.84%	8.419%
12	9.456	2754	2784	2795	rBV2	184987	444013	5.29%	0.697%
13	9.510	2795	2804	2820	rVB3	109333	205713	2.45%	0.323%
14	9.883	2923	2943	2966	rVB	392423	809842	9.64%	1.271%
15	10.014	2966	2992	3007	rVV2	552191	1178335	14.03%	1.850%
16	10.078	3007	3016	3044	rVB5	81456	218651	2.60%	0.343%
17	10.215	3045	3067	3091	rBV5	88665	237838	2.83%	0.373%
18	10.368	3098	3124	3136	rBV	313106	615925	7.33%	0.967%
19	10.440	3136	3151	3173	rVV	4211033	7843453	93.37%	12.314%
20	10.623	3211	3219	3234	rVB5	75844	152286	1.81%	0.239%
21	10.888	3297	3318	3335	rVB6	73769	173935	2.07%	0.273%
22	11.527	3546	3556	3582	rVB6	45255	115784	1.38%	0.182%
23	11.744	3617	3637	3661	rBV	4666850	8400578	100.00%	13.189%
24	11.843	3664	3674	3695	rVV	248326	458246	5.45%	0.719%
25	11.950	3697	3714	3740	rVB2	422778	886299	10.55%	1.391%
26	12.280	3815	3837	3855	rBV3	117203	242650	2.89%	0.381%
27	12.578	3935	3948	3961	rBV	60577	115075	1.37%	0.181%
28	12.731	3988	4005	4031	rVB	3693573	6464925	76.96%	10.150%
29	12.919	4064	4075	4087	rBV	254893	408346	4.86%	0.641%
30	12.983	4087	4099	4106	rBV	719209	1201670	14.30%	1.887%
31	13.058	4119	4127	4141	rVB	527562	854540	10.17%	1.342%
32	13.222	4171	4188	4205	rBV	285675	510239	6.07%	0.801%
33	13.366	4228	4242	4273	rVB	1516743	2621492	31.21%	4.116%
34	13.498	4273	4291	4303	rBV4	71738	194508	2.32%	0.305%
35	13.560	4307	4314	4324	rVV	68976	107312	1.28%	0.168%
36	13.613	4324	4334	4341	rVV2	61676	106655	1.27%	0.167%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
 Data File : VN070093.D
 Acq On : 15 Dec 2021 1:12
 Operator : JC/MD
 Sample : M5011-01 10X
 Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HSB-1-(9-9.5)

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

37	13.675	4342	4357	4398	rVB	4072085	7680335	91.43%	12.058%
38	13.838	4404	4418	4422	rBV	247800	374528	4.46%	0.588%
39	13.871	4423	4430	4436	rVV3	375212	600760	7.15%	0.943%
40	13.908	4437	4444	4467	rVB4	550113	1154300	13.74%	1.812%
41	13.997	4467	4477	4491	rVB7	54245	101794	1.21%	0.160%
42	14.069	4492	4504	4514	rBV2	99986	165751	1.97%	0.260%
43	14.128	4514	4526	4532	rBV	231430	380096	4.52%	0.597%
44	14.217	4547	4559	4573	rVB	505379	815600	9.71%	1.280%
45	14.324	4586	4599	4611	rVB4	103022	177253	2.11%	0.278%
46	14.458	4637	4649	4660	rVB	71747	113661	1.35%	0.178%
47	14.538	4661	4679	4686	rVV2	158617	276878	3.30%	0.435%
48	14.579	4686	4694	4703	rVV	226023	371450	4.42%	0.583%
49	14.622	4703	4710	4718	rVV2	88836	142138	1.69%	0.223%
50	14.807	4770	4779	4789	rBV2	70061	121310	1.44%	0.190%
51	14.922	4806	4822	4836	rBV4	153378	384742	4.58%	0.604%
52	15.196	4913	4924	4940	rBV5	39672	86960	1.04%	0.137%
53	15.507	5024	5040	5058	rVB	105900	211206	2.51%	0.332%
54	15.700	5102	5112	5125	rVB4	47750	89266	1.06%	0.140%

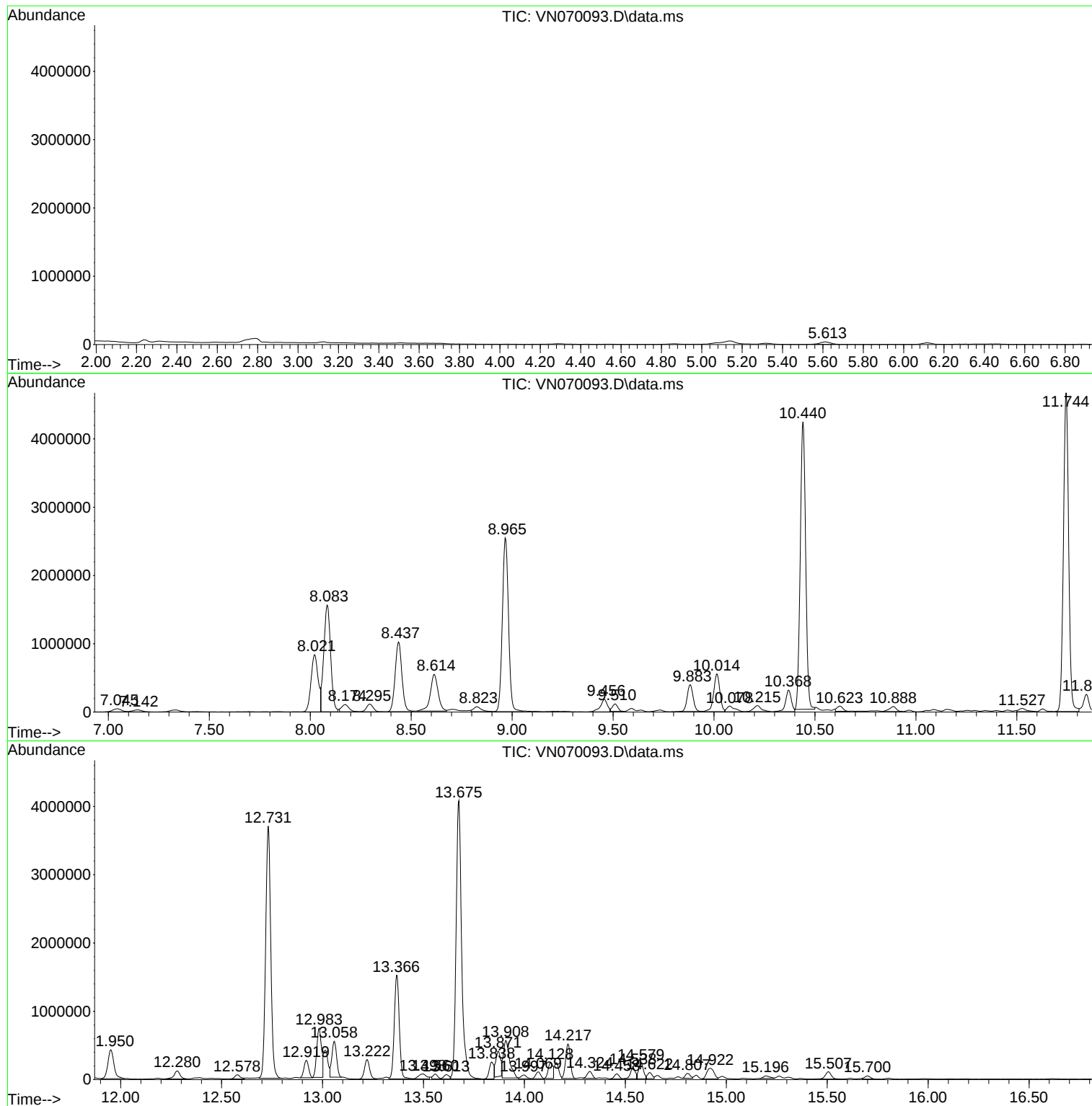
Sum of corrected areas: 63694808

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

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\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

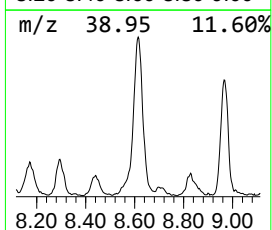
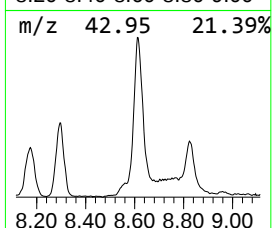
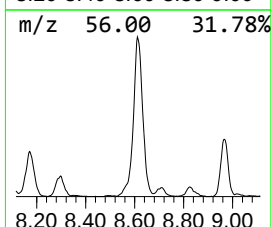
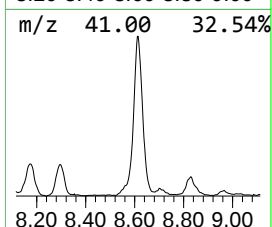
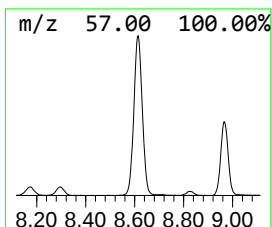
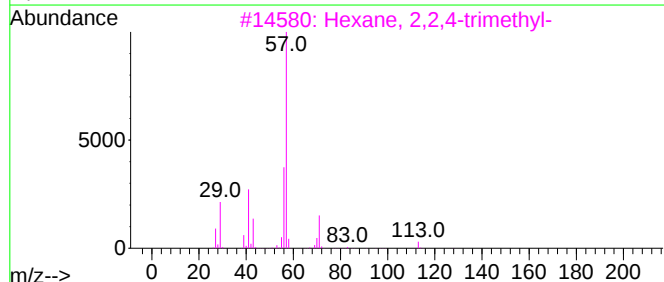
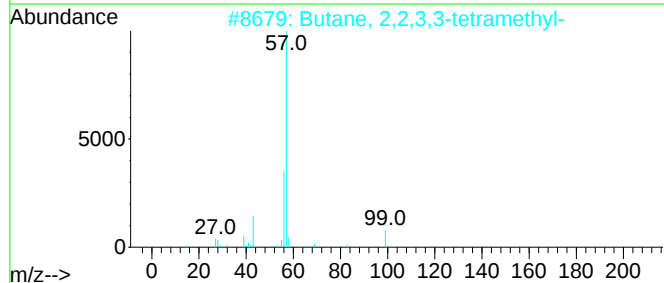
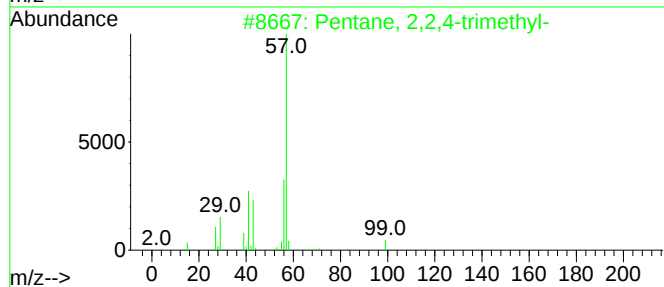
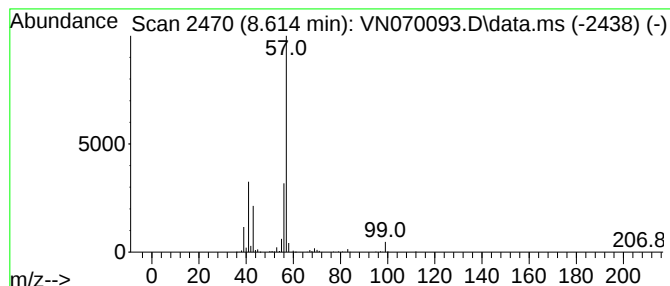
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	13.37 ug/l	1433930	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

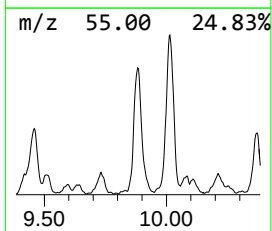
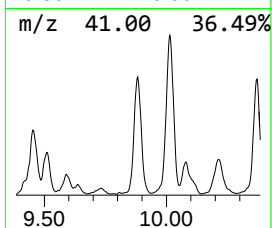
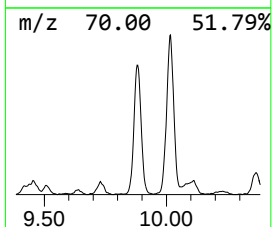
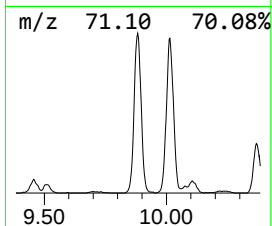
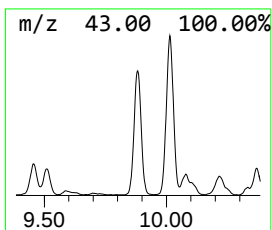
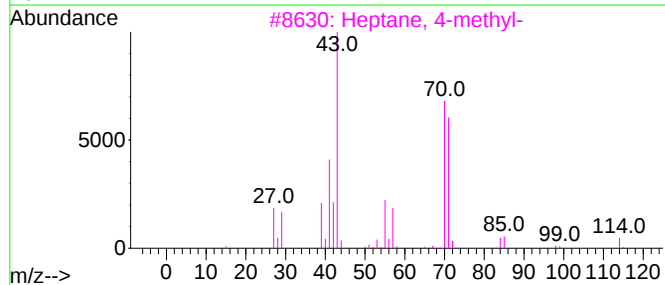
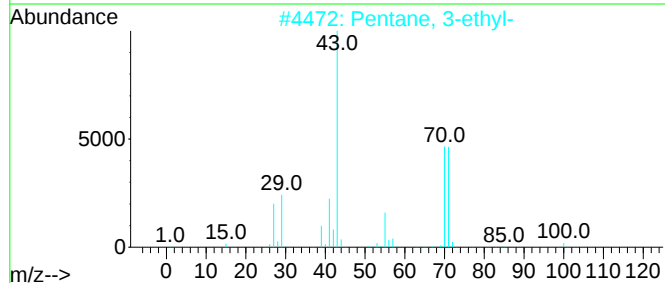
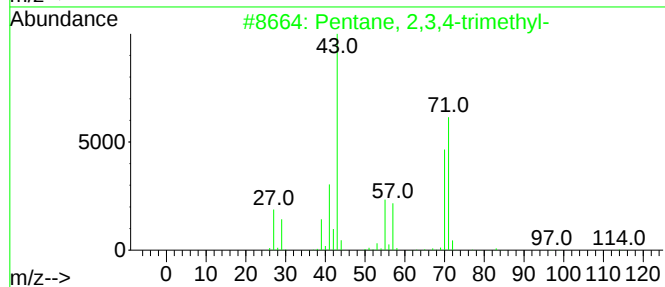
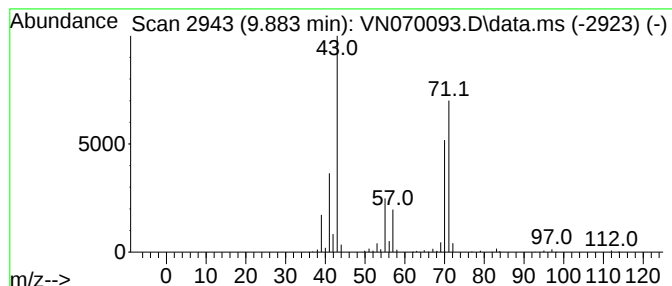
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	7.55 ug/l	809842	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		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	78
4		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

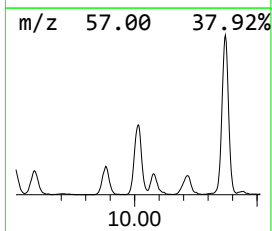
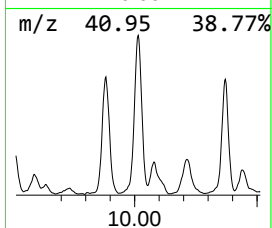
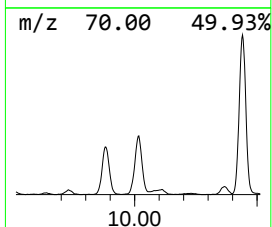
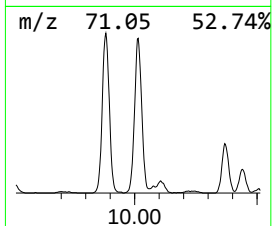
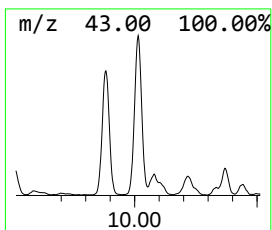
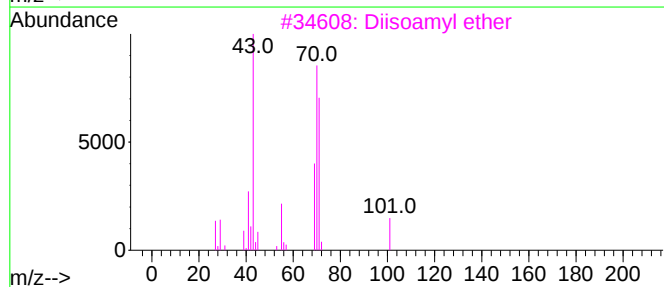
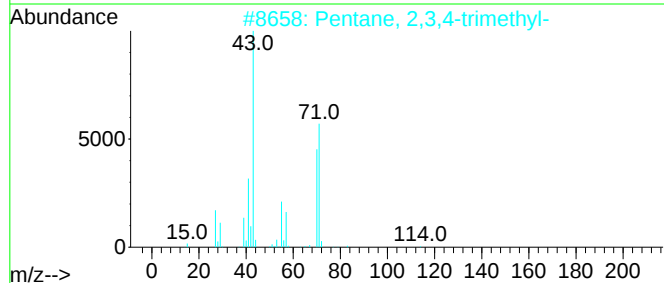
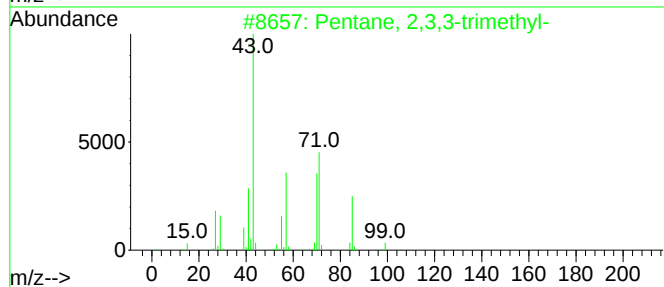
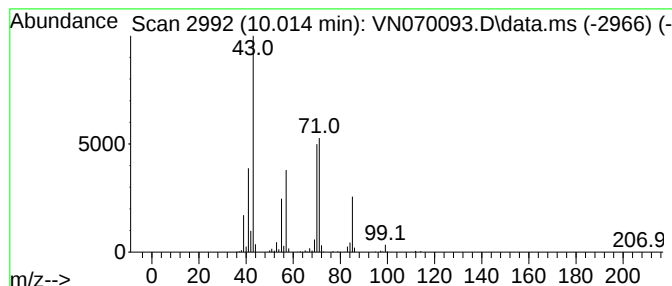
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	10.99 ug/l	1178340	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	76
3			Diisoamyl ether	158	C10H22O	000544-01-4	59
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

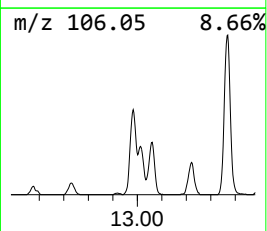
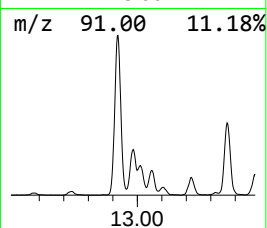
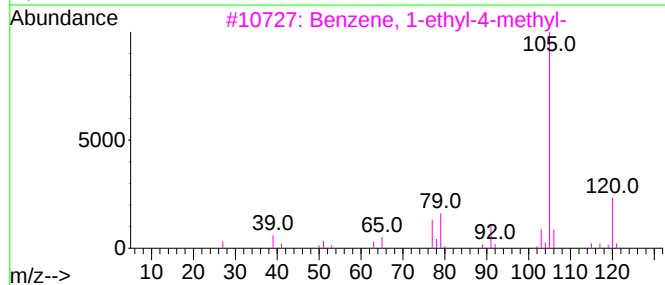
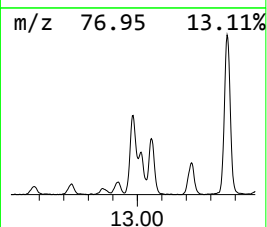
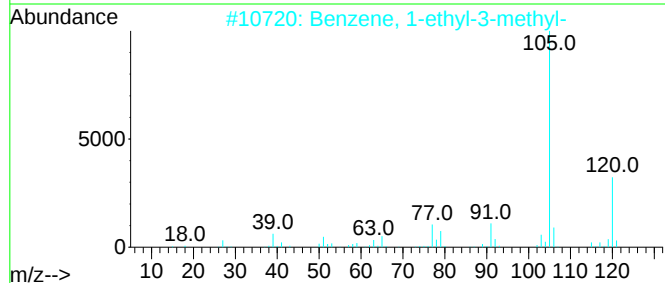
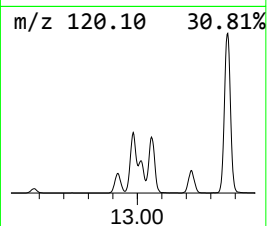
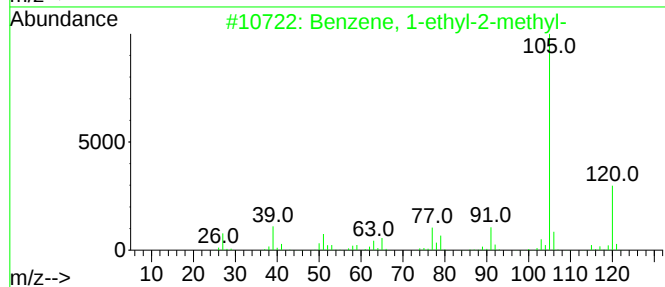
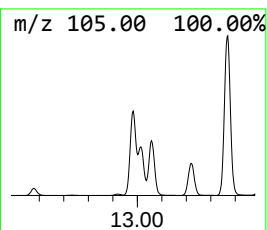
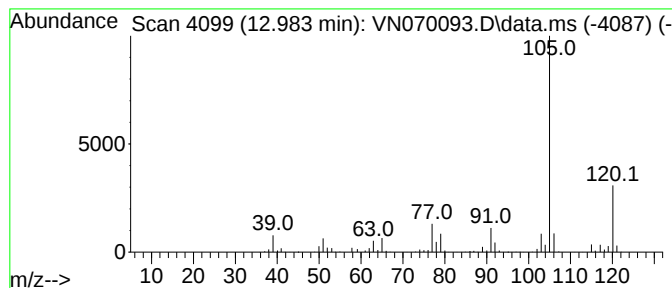
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	7.82 ug/l	1201670	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

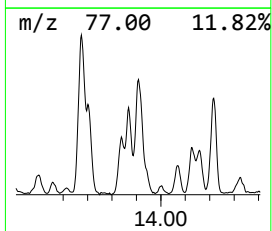
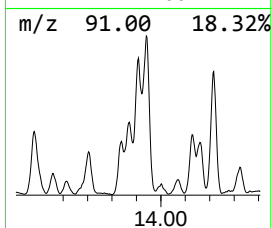
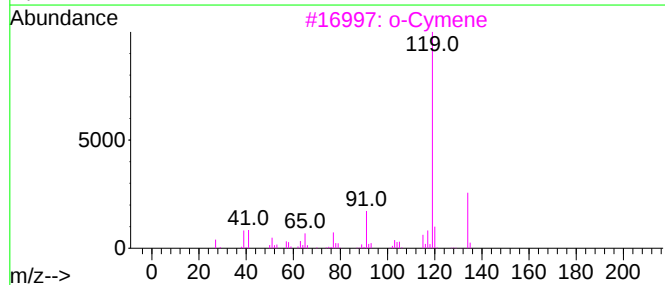
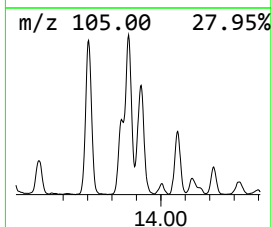
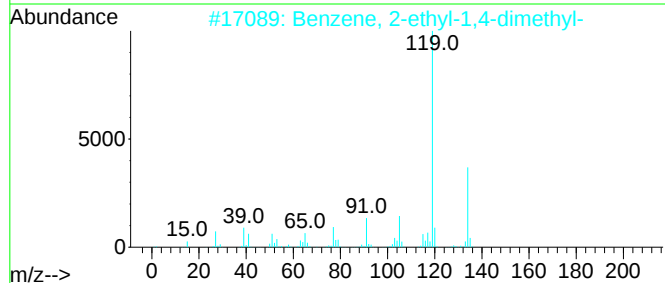
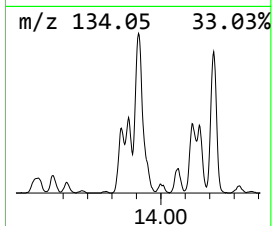
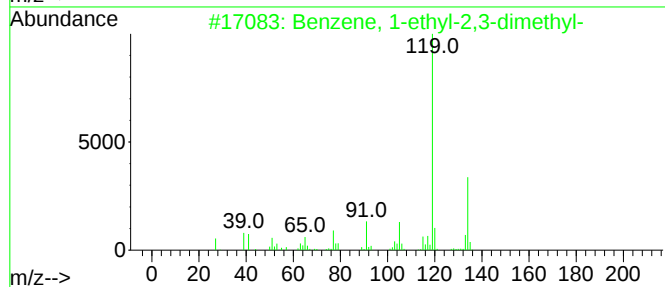
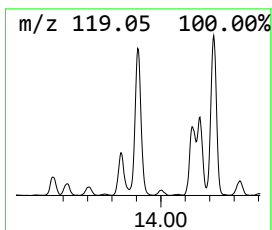
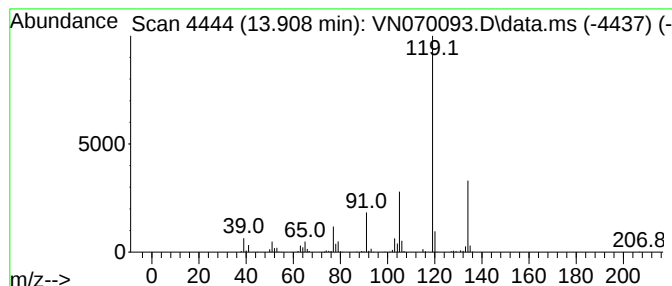
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.908	7.51 ug/l	1154300	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	90
3			o-Cymene	134	C10H14	000527-84-4	83
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	80
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

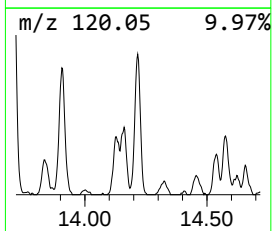
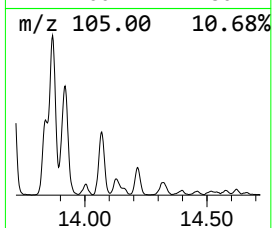
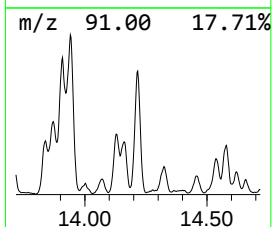
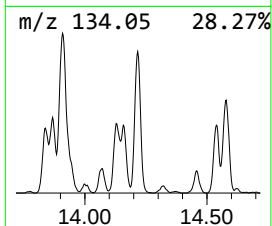
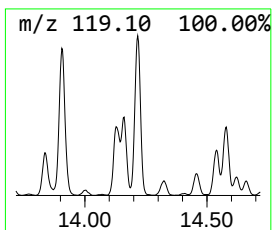
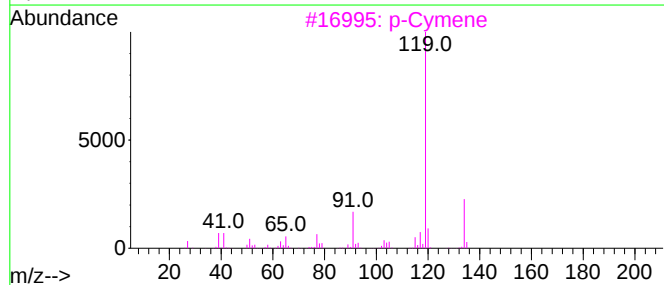
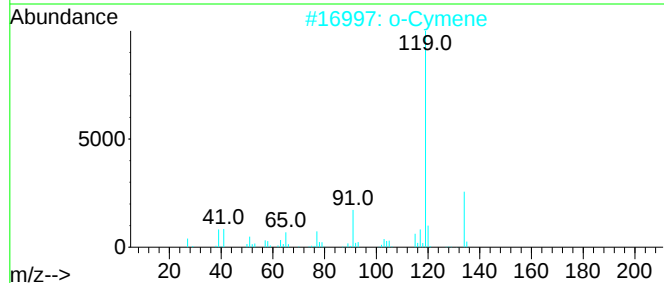
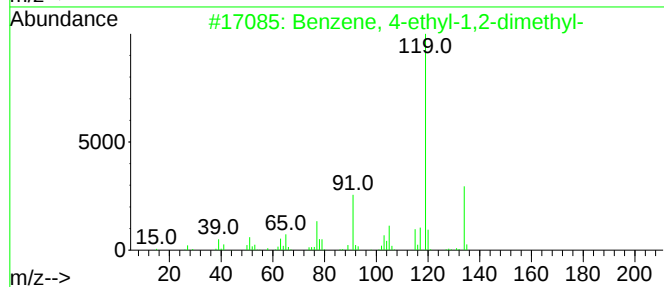
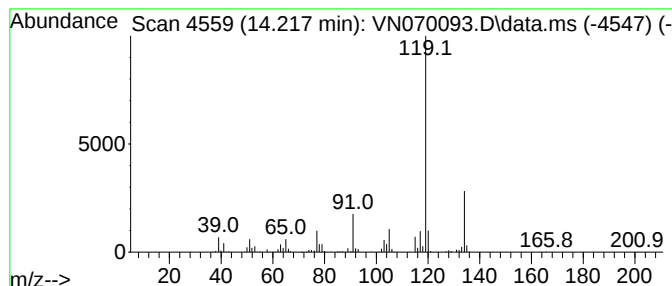
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	5.31 ug/l	815600	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			o-Cymene	134	C10H14	000527-84-4	95
3			p-Cymene	134	C10H14	000099-87-6	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070093.D
Acq On : 15 Dec 2021 1:12
Operator : JC/MD
Sample : M5011-01 10X
Misc : 5.81g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HSB-1-(9-9.5)

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,4-...	8.614	13.4	ug/l	1433930	2	8.965	5362520	50.0
Pentane, 2,3,4-...	9.883	7.5	ug/l	809842	2	8.965	5362520	50.0
Pentane, 2,3,3-...	10.014	11.0	ug/l	1178340	2	8.965	5362520	50.0
Benzene, 1-ethy...	12.983	7.8	ug/l	1201670	4	13.675	7680340	50.0
Benzene, 1-ethy...	13.908	7.5	ug/l	1154300	4	13.675	7680340	50.0
Benzene, 4-ethy...	14.217	5.3	ug/l	815600	4	13.675	7680340	50.0