

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070014.D
 Acq On : 11 Dec 2021 17:44
 Operator : JC/MD
 Sample : M4873-05 10X
 Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A2-6-6.5

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: VN070014.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	159	168	188	rVB2	155218	258408	1.20%	0.076%
2	3.113	399	419	459	rVB	1877454	4482411	20.79%	1.319%
3	3.494	542	561	595	rBV	1129072	2874443	13.33%	0.846%
4	3.977	720	741	772	rVB2	358868	975846	4.53%	0.287%
5	4.240	812	839	869	rBV4	120363	442238	2.05%	0.130%
6	5.071	1121	1149	1153	rBV3	693409	1862888	8.64%	0.548%
7	5.610	1318	1350	1385	rBV	1279258	4482907	20.79%	1.319%
8	5.927	1443	1468	1497	rBV5	169198	551448	2.56%	0.162%
9	6.114	1509	1538	1574	rBV2	1331933	4105148	19.04%	1.208%
10	6.281	1582	1600	1622	rVB4	84567	245189	1.14%	0.072%
11	6.463	1647	1668	1696	rVB2	481798	1491028	6.91%	0.439%
12	6.603	1697	1720	1742	rBV4	265778	828175	3.84%	0.244%
13	6.898	1805	1830	1858	rBV4	500726	1558575	7.23%	0.459%
14	7.042	1859	1884	1903	rBV2	1365317	4110730	19.06%	1.210%
15	7.144	1904	1922	1942	rVV	1359967	3738756	17.34%	1.100%
16	7.321	1973	1988	2017	rVB3	82494	272715	1.26%	0.080%
17	7.777	2138	2158	2166	rBV4	128502	319737	1.48%	0.094%
18	7.842	2167	2182	2201	rVB2	707940	1713106	7.94%	0.504%
19	8.024	2229	2250	2254	rBV	953759	1953752	9.06%	0.575%
20	8.078	2256	2270	2289	rVV6	3332071	10120176	46.93%	2.978%
21	8.174	2290	2306	2331	rVB2	3714096	9437988	43.77%	2.777%
22	8.295	2332	2351	2369	rBV	2330059	5357287	24.85%	1.577%
23	8.442	2387	2406	2434	rBV3	1271733	3706095	17.19%	1.091%
24	8.617	2435	2471	2494	rVV	7401329	21528836	99.84%	6.335%
25	8.708	2496	2505	2527	rVB2	592987	1457350	6.76%	0.429%
26	8.826	2527	2549	2579	rVB2	2040577	4511855	20.92%	1.328%
27	8.968	2581	2602	2630	rBV2	3807886	9349446	43.36%	2.751%
28	9.126	2649	2661	2675	rVB2	355839	684656	3.18%	0.201%
29	9.199	2675	2688	2695	rVV	213786	410432	1.90%	0.121%
30	9.247	2697	2706	2741	rVB2	372664	984976	4.57%	0.290%
31	9.459	2750	2785	2796	rBV	3855344	9431556	43.74%	2.776%
32	9.510	2797	2804	2821	rVB	1595237	3032374	14.06%	0.892%
33	9.593	2822	2835	2844	rBV	504493	1014272	4.70%	0.298%
34	9.641	2845	2853	2866	rVB	492948	878536	4.07%	0.259%
35	9.732	2867	2887	2902	rBV5	407754	997818	4.63%	0.294%
36	9.826	2904	2922	2924	rBV9	120083	270848	1.26%	0.080%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070014.D
 Acq On : 11 Dec 2021 17:44
 Operator : JC/MD
 Sample : M4873-05 10X
 Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A2-6-6.5

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	9.883	2928	2943	2964	rVB	5344691	10693905	49.60%	3.147%
38	10.017	2965	2993	3007	rBV3	6957078	16119148	74.76%	4.744%
39	10.078	3007	3016	3026	rBV2	1418606	2341742	10.86%	0.689%
40	10.218	3048	3068	3093	rBV2	1880790	4551184	21.11%	1.339%
41	10.322	3094	3107	3112	rBV4	375439	662954	3.07%	0.195%
42	10.371	3113	3125	3138	rVB	3124880	5582538	25.89%	1.643%
43	10.440	3138	3151	3172	rBV	5050243	9853703	45.70%	2.900%
44	10.625	3205	3220	3234	rVB3	2164015	4331149	20.09%	1.275%
45	10.684	3235	3242	3252	rVB2	252475	357641	1.66%	0.105%
46	10.786	3269	3280	3296	rBV5	340943	931366	4.32%	0.274%
47	10.867	3297	3310	3312	rBV2	939950	1457741	6.76%	0.429%
48	10.963	3337	3346	3359	rVB4	427202	783859	3.64%	0.231%
49	11.055	3362	3380	3392	rBV3	443126	927837	4.30%	0.273%
50	11.157	3394	3418	3433	rBV2	721224	2098729	9.73%	0.618%
51	11.221	3435	3442	3447	rBV6	165335	231656	1.07%	0.068%
52	11.457	3521	3530	3538	rBV2	412125	601279	2.79%	0.177%
53	11.527	3546	3556	3582	rVB4	1548102	3655827	16.95%	1.076%
54	11.629	3583	3594	3616	rBV	1206072	2230600	10.34%	0.656%
55	11.744	3620	3637	3652	rVV	5376668	10314601	47.84%	3.035%
56	11.846	3656	3675	3695	rVV	4867942	9753460	45.23%	2.870%
57	11.956	3699	3716	3754	rVB2	7934467	18129538	84.08%	5.335%
58	12.186	3795	3802	3813	rVB5	410224	612778	2.84%	0.180%
59	12.256	3820	3828	3831	rBV6	392004	511452	2.37%	0.151%
60	12.581	3941	3949	3958	rBV	548312	914235	4.24%	0.269%
61	12.731	3992	4005	4016	rVB2	3705953	6727556	31.20%	1.980%
62	12.876	4051	4059	4063	rBV3	300983	433435	2.01%	0.128%
63	12.921	4065	4076	4088	rVV	2705723	4668904	21.65%	1.374%
64	12.983	4089	4099	4104	rVV	2123409	3416290	15.84%	1.005%
65	13.018	4105	4112	4119	rVV	3966858	6545935	30.36%	1.926%
66	13.058	4119	4127	4167	rVB2	5181778	9822756	45.56%	2.891%
67	13.222	4175	4188	4204	rBV	2778240	5021412	23.29%	1.478%
68	13.369	4230	4243	4257	rVB	13354027	21562378	100.00%	6.345%
69	13.608	4326	4332	4339	rBV4	334455	445274	2.07%	0.131%
70	13.675	4346	4357	4364	rBV	4882282	8488397	39.37%	2.498%
71	13.838	4409	4418	4424	rBV	945704	1469438	6.81%	0.432%
72	13.879	4425	4433	4437	rVV	1824469	2838341	13.16%	0.835%
73	13.908	4439	4444	4467	rVB4	3309066	6510072	30.19%	1.916%
74	13.997	4468	4477	4488	rBV5	873051	1362107	6.32%	0.401%
75	14.072	4497	4505	4515	rVB	734758	1082807	5.02%	0.319%
76	14.131	4518	4527	4533	rBV	1504761	2386413	11.07%	0.702%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070014.D
 Acq On : 11 Dec 2021 17:44
 Operator : JC/MD
 Sample : M4873-05 10X
 Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A2-6-6.5

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

77	14.217	4549	4559	4571	rVB	2782915	4264626	19.78%	1.255%
78	14.327	4591	4600	4612	rVB3	1620097	2667410	12.37%	0.785%
79	14.461	4641	4650	4660	rBV3	605067	1022204	4.74%	0.301%
80	14.541	4673	4680	4687	rBV	973404	1334161	6.19%	0.393%
81	14.579	4688	4694	4703	rVB	1710312	2297557	10.66%	0.676%
82	14.622	4704	4710	4718	rVB2	728143	883451	4.10%	0.260%
83	14.764	4756	4763	4771	rBV2	444417	532510	2.47%	0.157%
84	14.812	4771	4781	4789	rBV2	1245439	2151977	9.98%	0.633%
85	14.927	4809	4824	4837	rBV4	1995083	4828396	22.39%	1.421%
86	15.196	4916	4924	4952	rVB6	990374	2645855	12.27%	0.779%
87	15.314	4958	4968	4982	rVB4	755783	1588376	7.37%	0.467%
88	15.507	5031	5040	5053	rVB	1169171	2067977	9.59%	0.609%
89	15.807	5143	5152	5171	rVB	447529	939086	4.36%	0.276%
90	16.617	5441	5454	5485	rVB	1114201	2717186	12.60%	0.800%

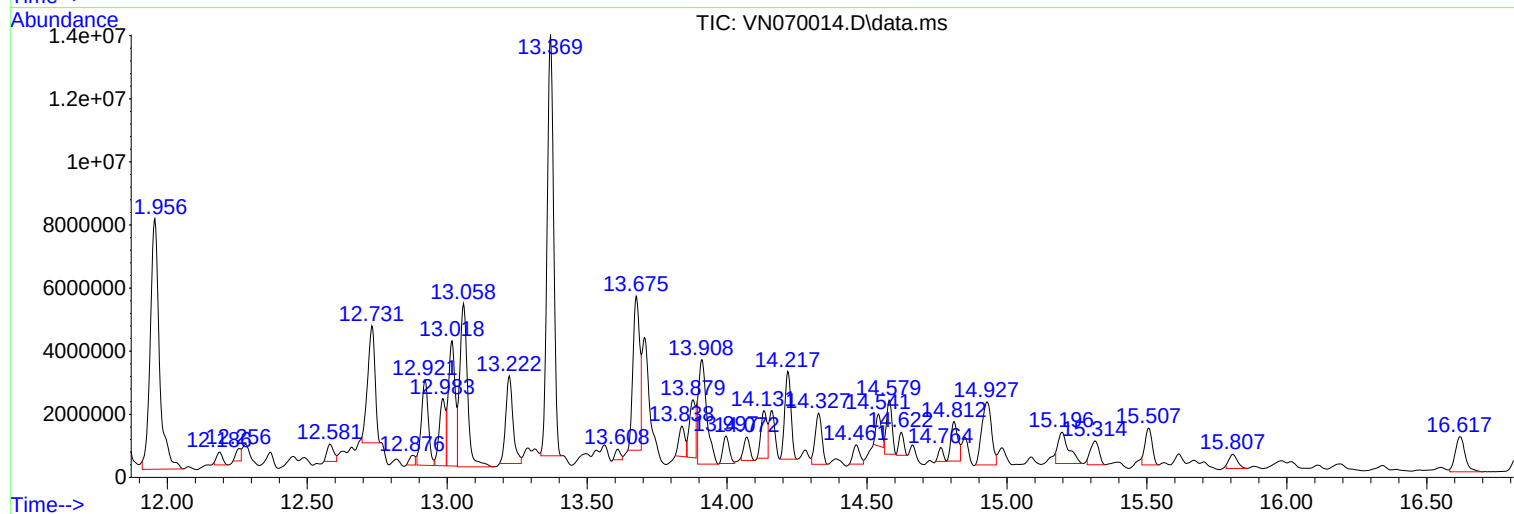
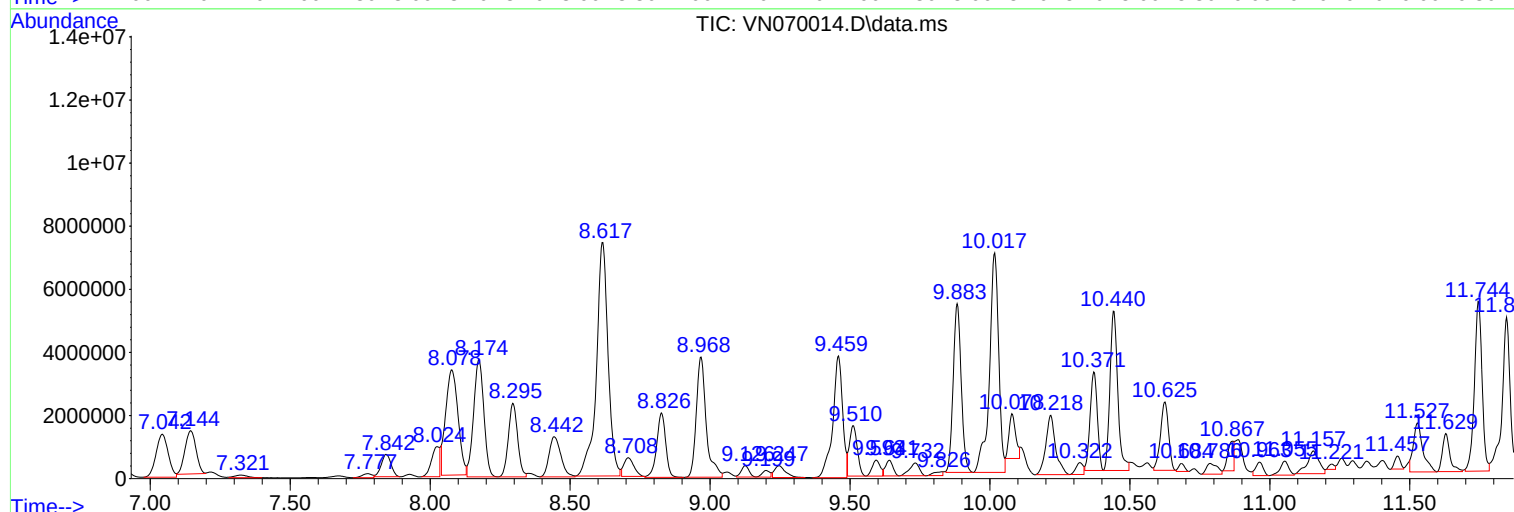
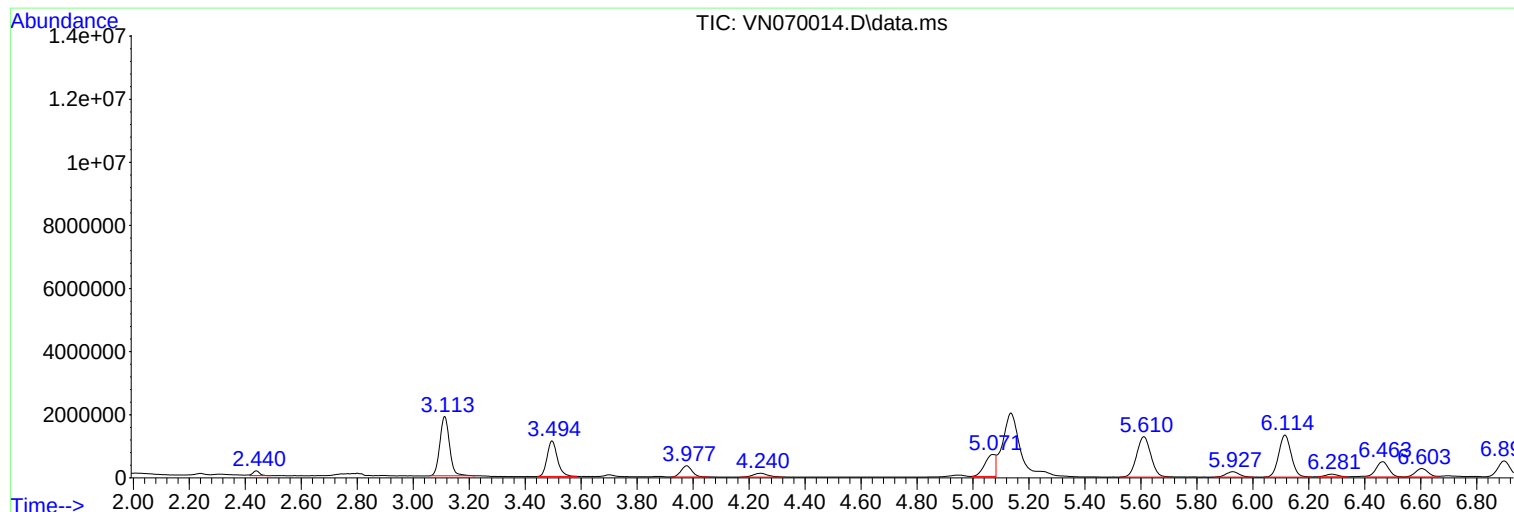
Sum of corrected areas: 339813210

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

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\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

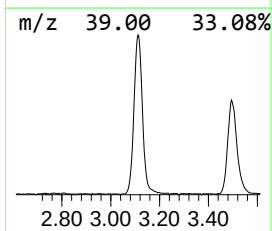
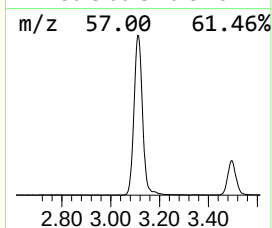
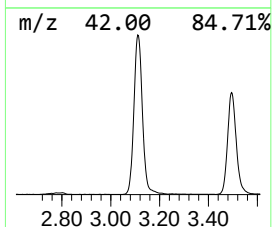
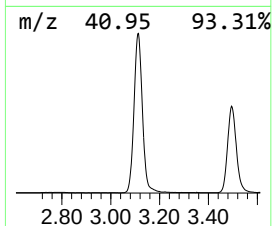
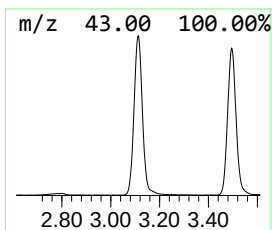
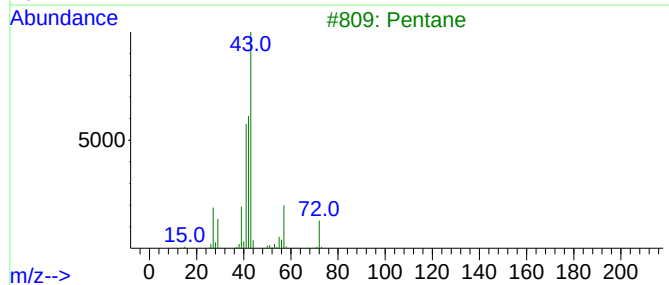
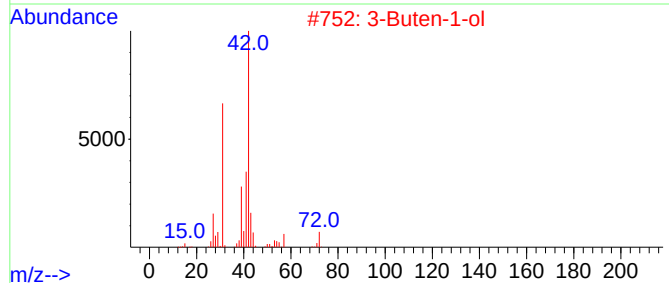
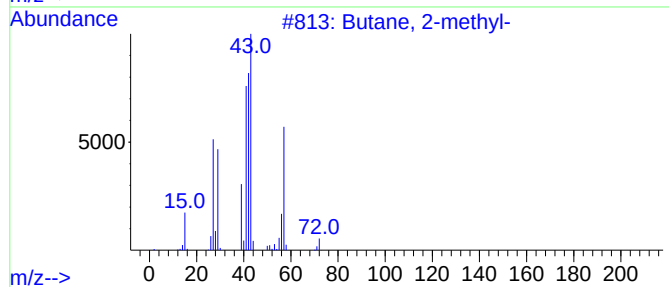
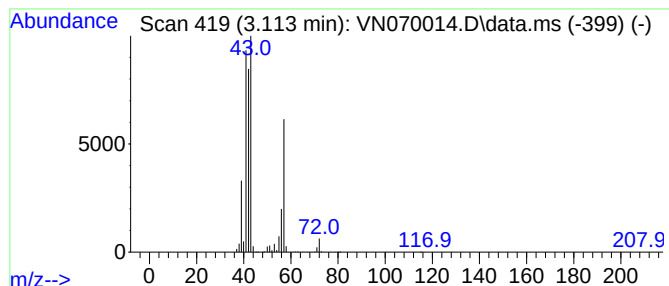
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.113	22.15 ug/l	4482410	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5			Azetidine	57	C3H7N	000503-29-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

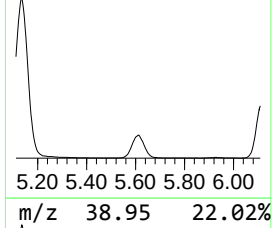
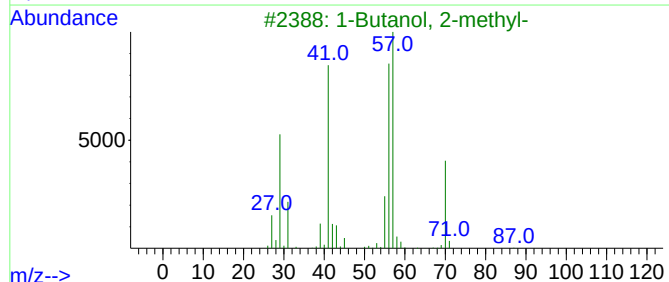
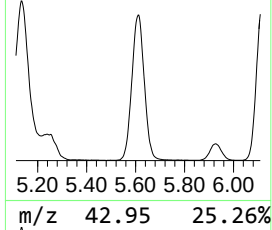
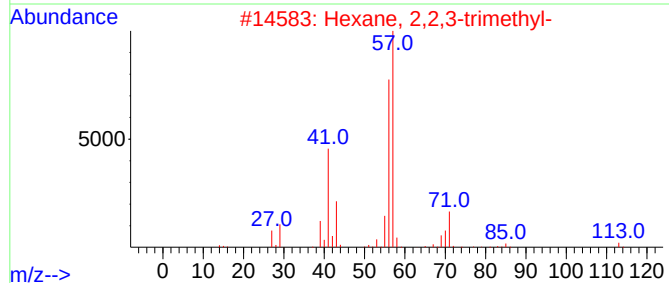
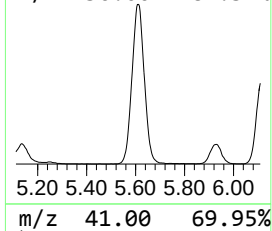
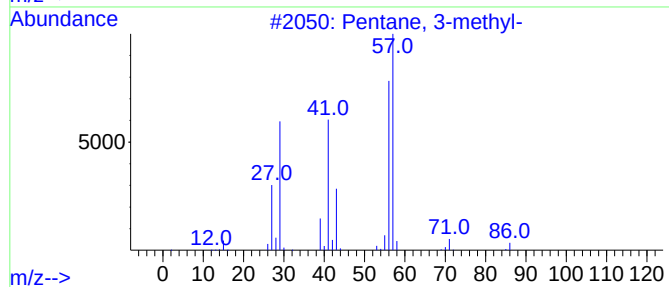
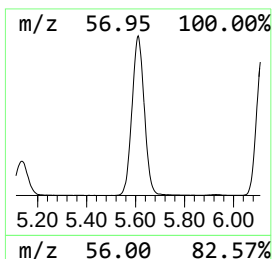
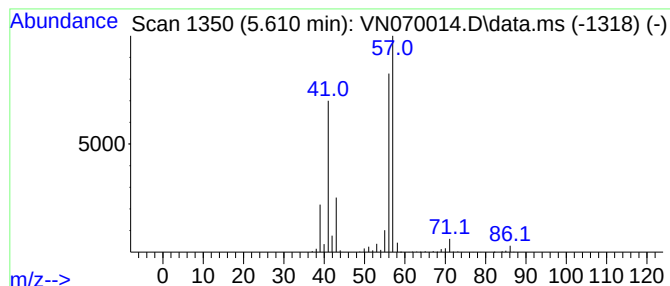
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.610	22.15 ug/l	4482910	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	43
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

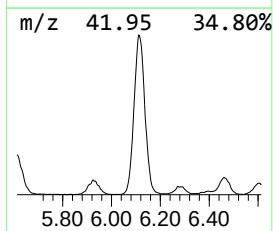
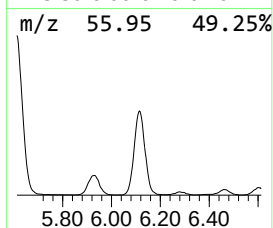
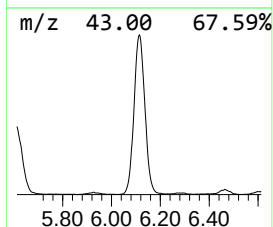
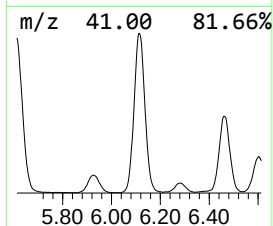
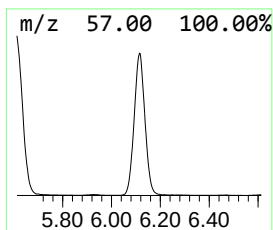
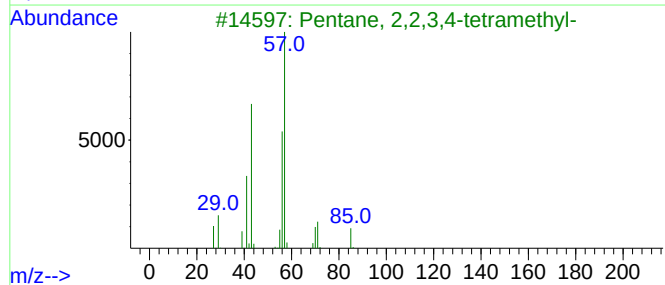
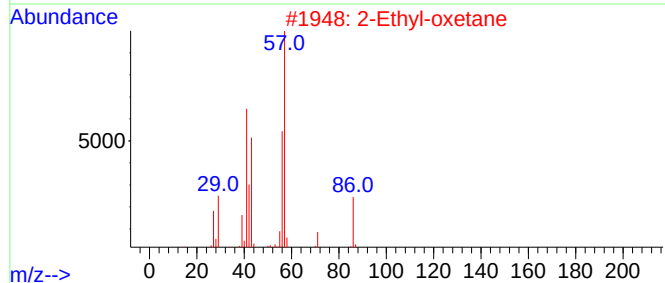
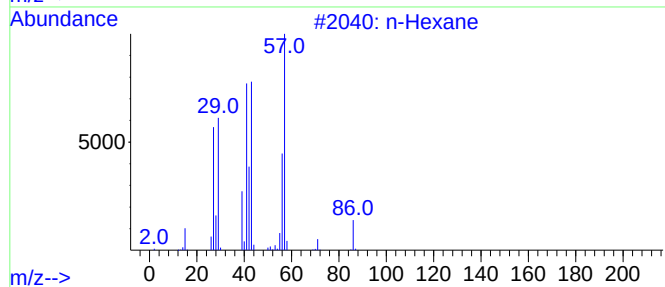
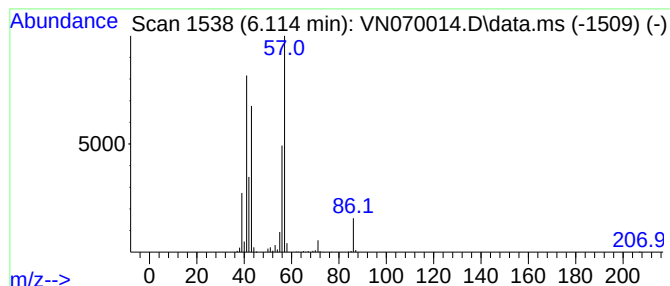
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 n-Hexane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.114	20.28 ug/l	4105150	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	83
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

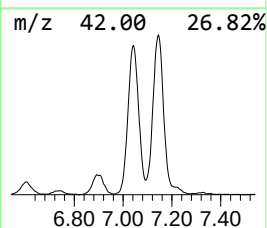
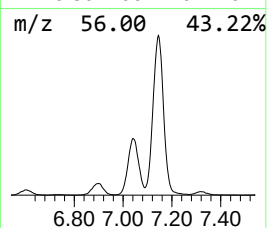
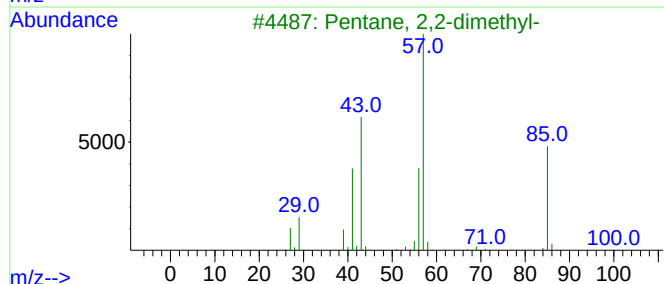
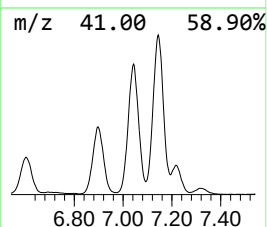
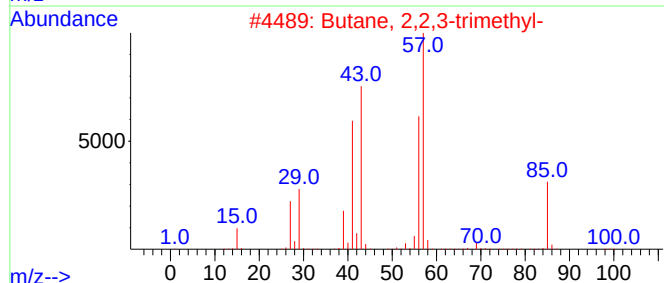
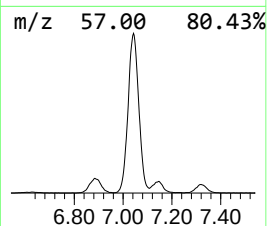
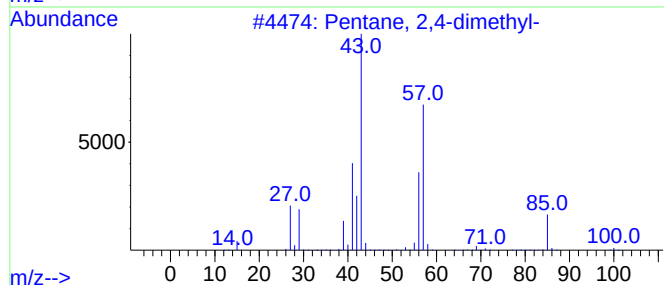
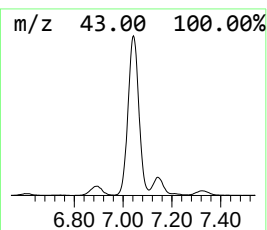
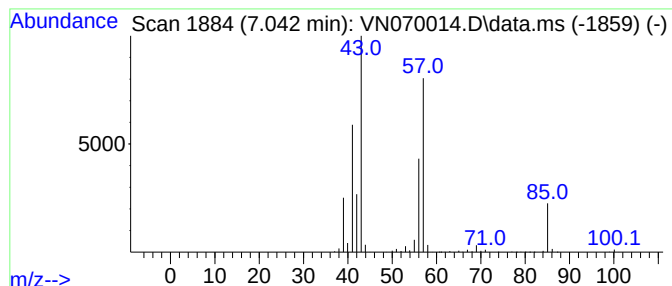
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,4-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.042	20.31 ug/l	4110730	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	56
4			n-Hexane	86	C6H14	000110-54-3	53
5			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

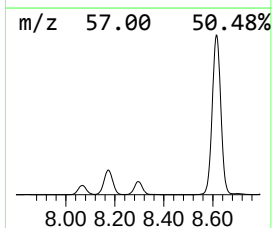
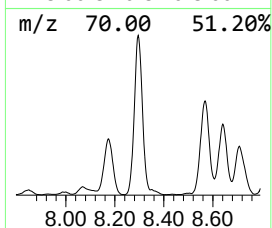
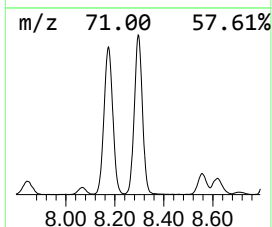
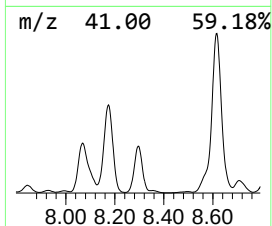
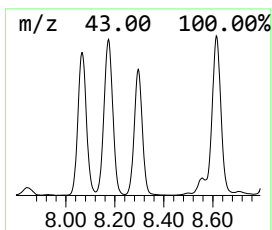
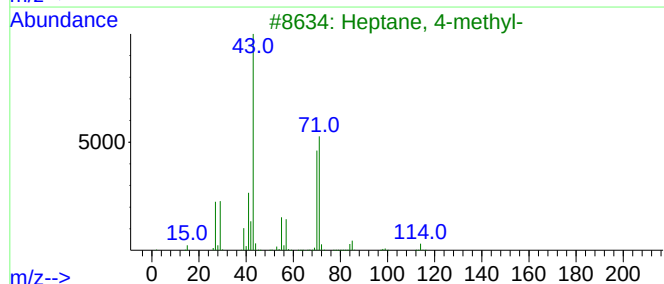
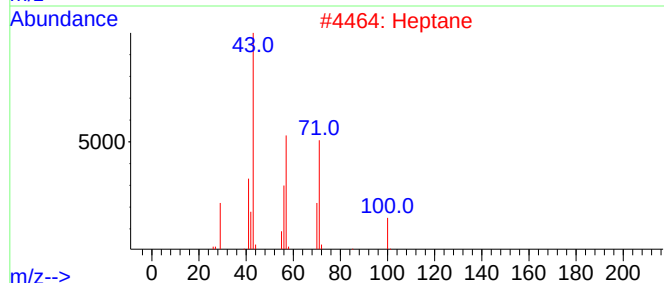
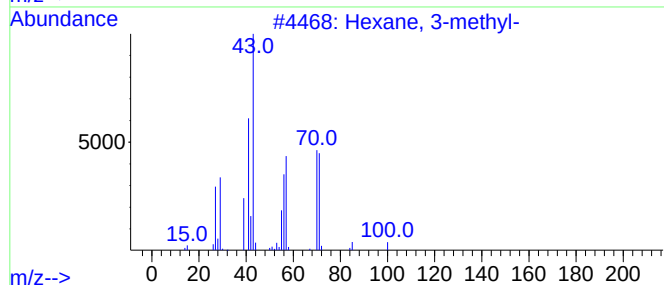
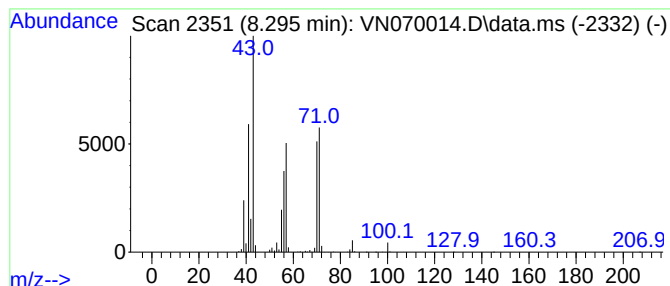
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.295	26.47 ug/l	5357290	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane	100	C7H16	000142-82-5	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

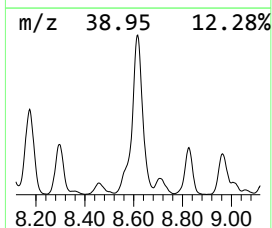
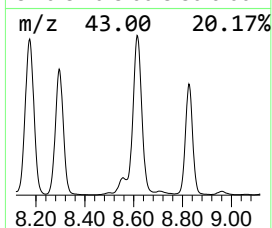
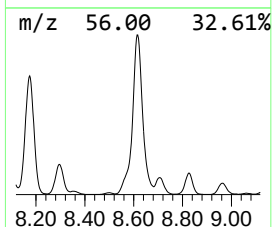
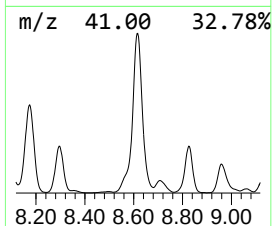
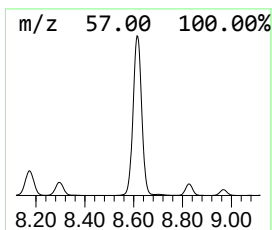
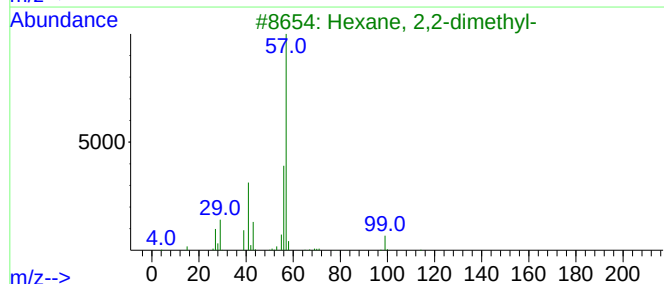
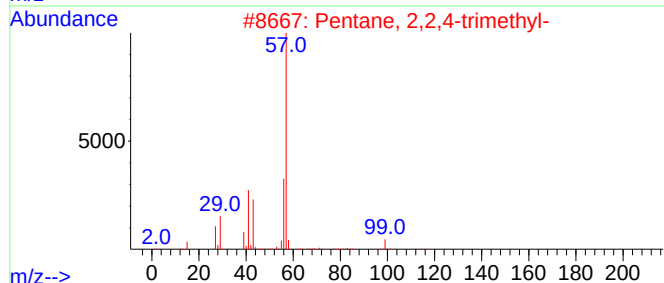
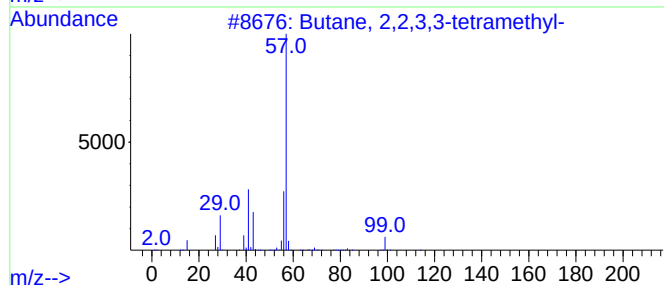
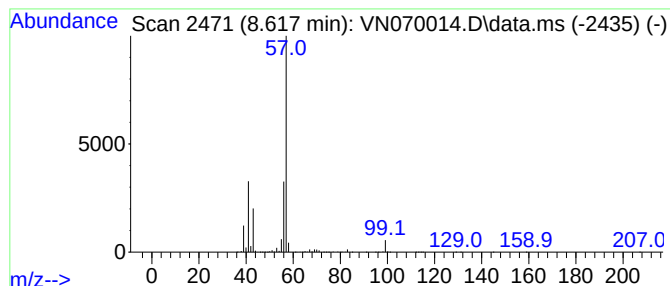
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	115.13 ug/l	21528800	1,4-Difluorobenzene	8.968

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

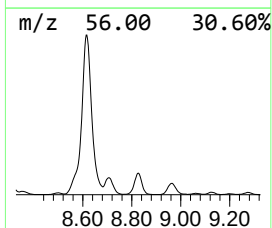
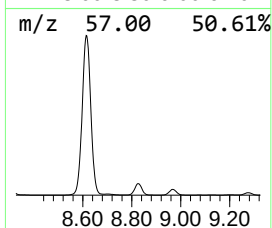
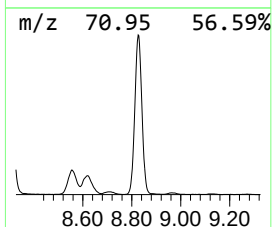
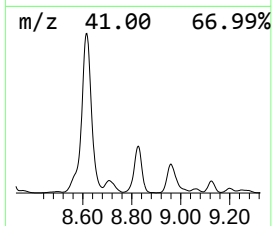
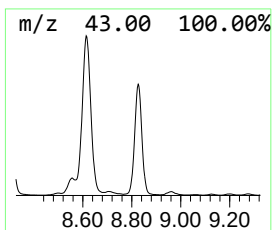
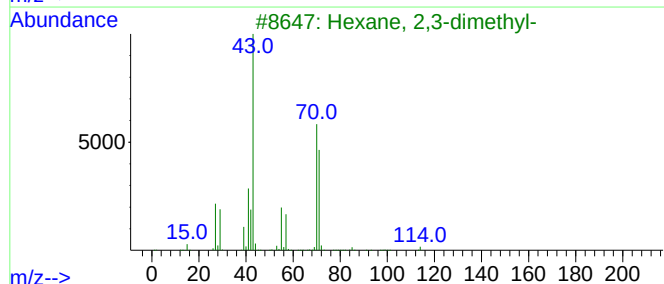
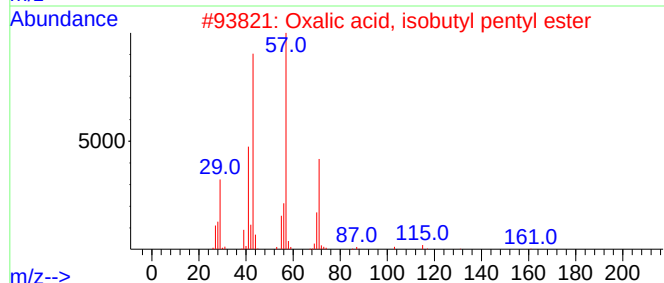
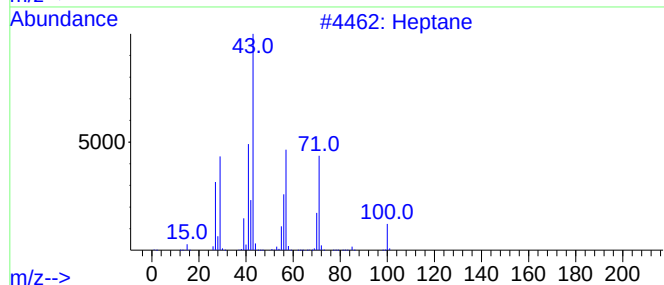
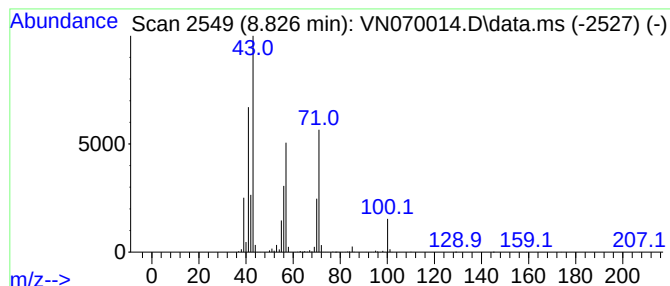
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 7 Heptane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	24.13 ug/l	4511860	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	94
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	45
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
4			Isobutyl 3-methylbutan-2-yl carb...	188	C10H20O3	1000372-77-0	38
5			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

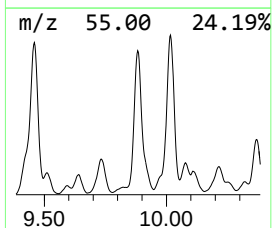
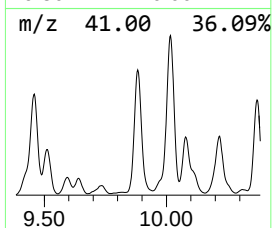
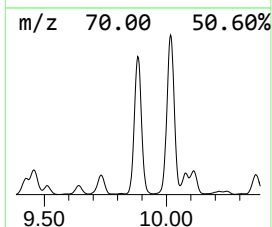
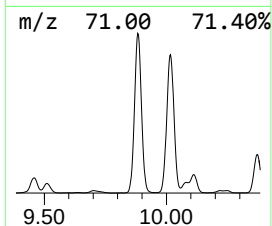
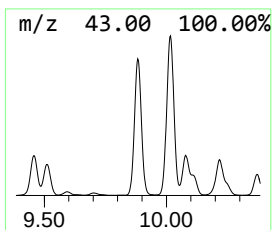
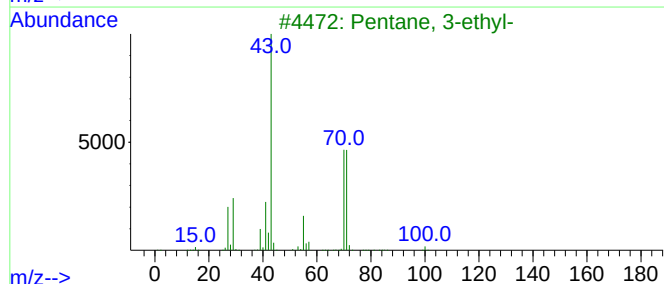
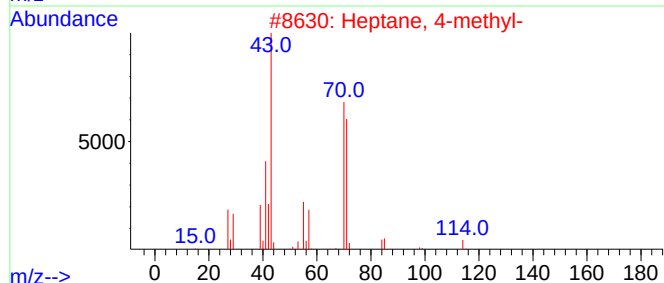
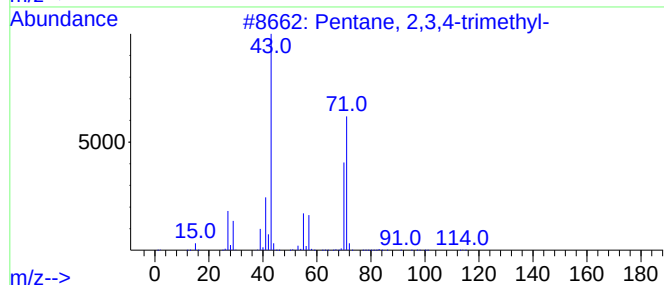
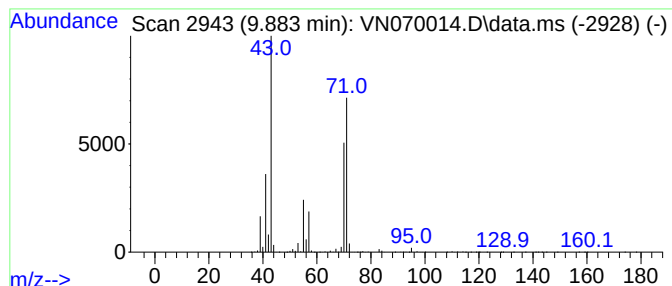
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	57.19 ug/l	10693900	1,4-Difluorobenzene	8.968

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	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

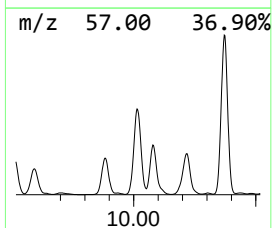
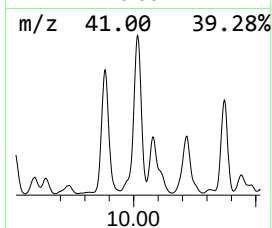
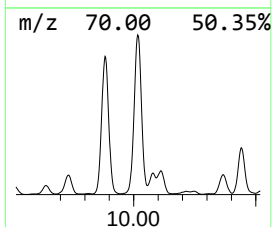
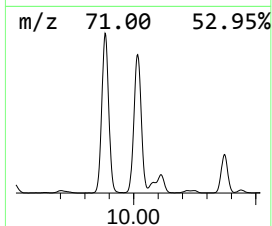
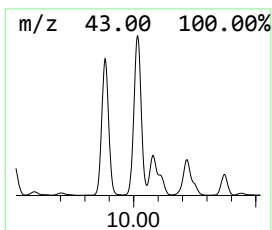
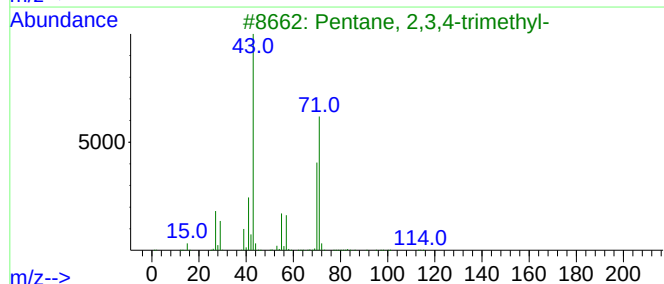
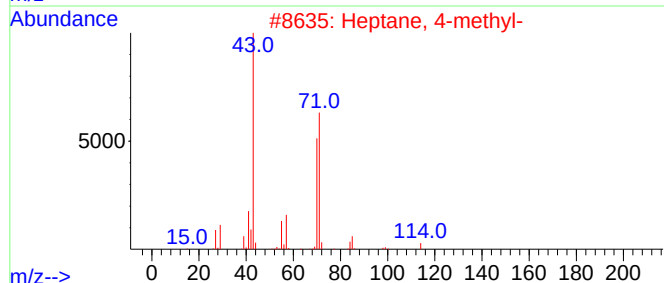
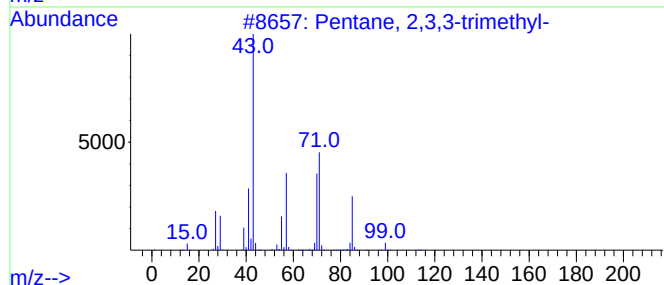
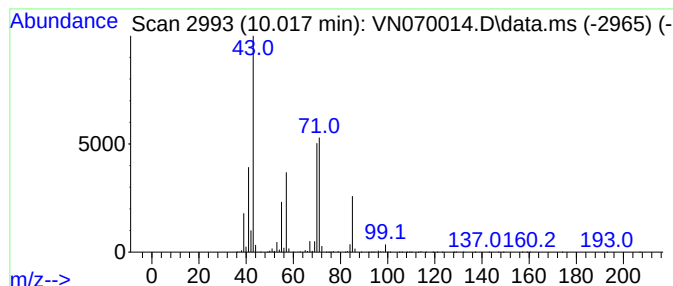
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.017	86.20 ug/l	16119100	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56
5			Pyrrolidine	71	C4H9N	000123-75-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

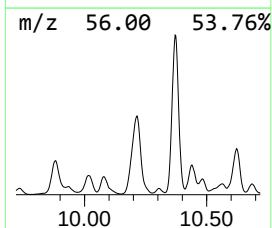
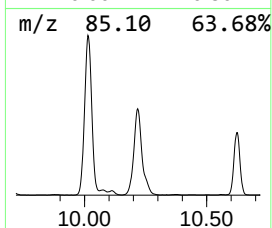
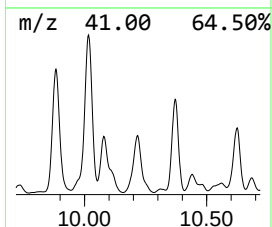
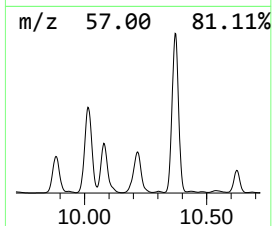
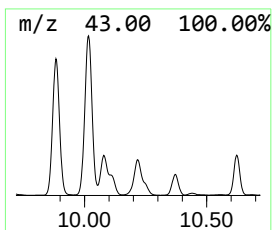
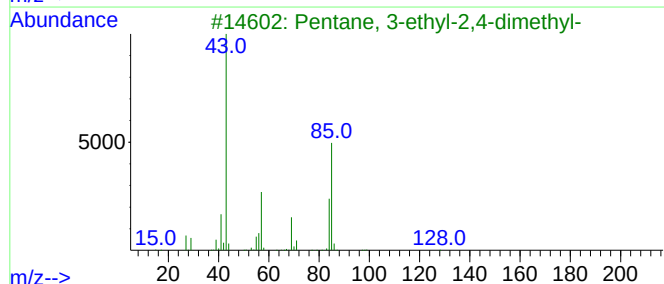
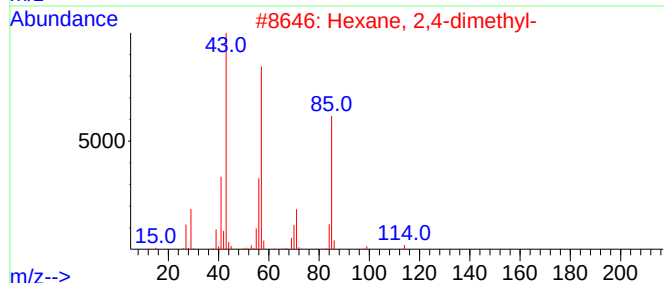
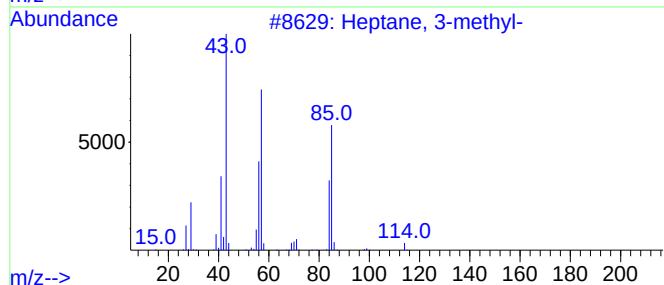
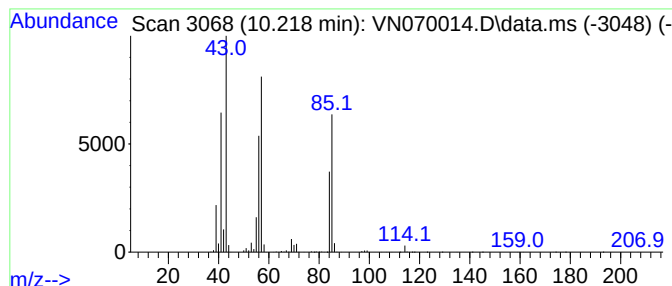
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 10 Heptane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.218	24.34 ug/l	4551180	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
3			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
5			Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

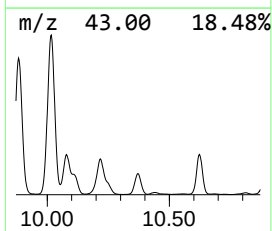
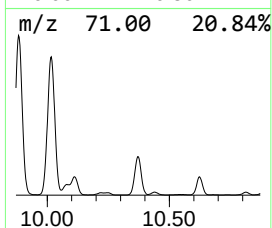
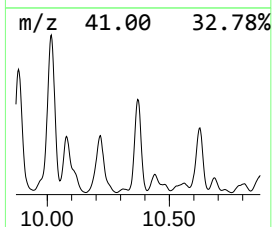
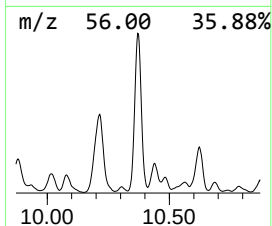
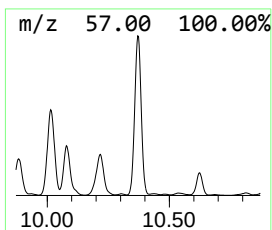
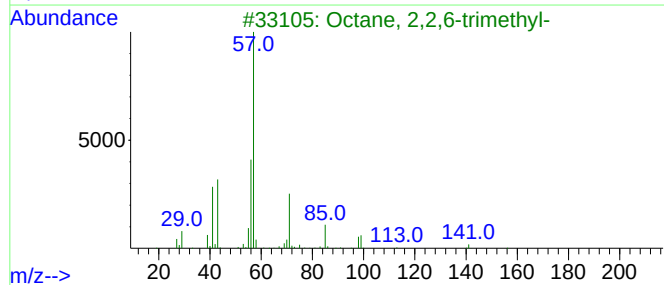
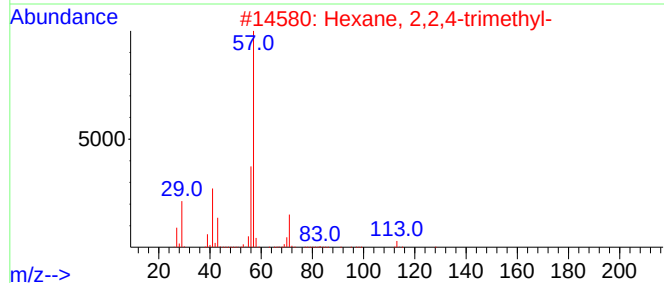
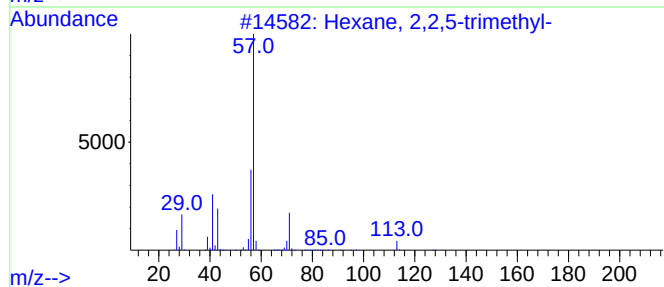
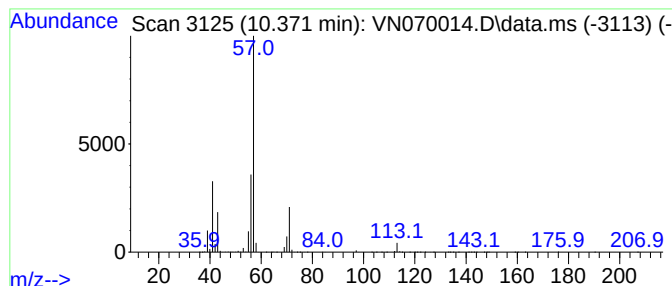
Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

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 Hexane, 2,2,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.371	27.06 ug/l	5582540	Chlorobenzene-d5			11.746
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5-trimethyl-		128	C9H20	003522-94-9	83
2	Hexane, 2,2,4-trimethyl-		128	C9H20	016747-26-5	83
3	Octane, 2,2,6-trimethyl-		156	C11H24	062016-28-8	64
4	Heptane, 2,2-dimethyl-		128	C9H20	001071-26-7	59
5	Pentane, 2,2,4,4-tetramethyl-		128	C9H20	001070-87-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

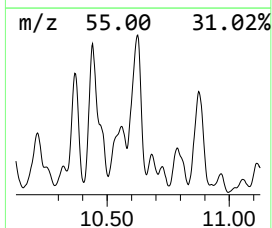
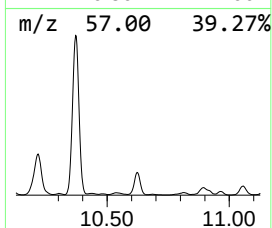
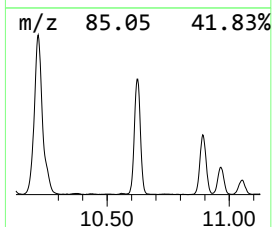
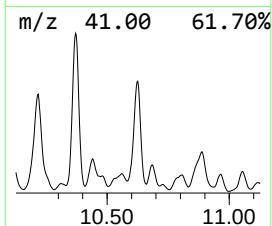
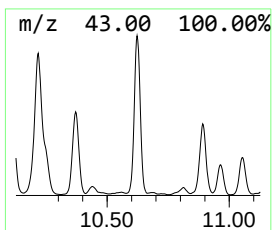
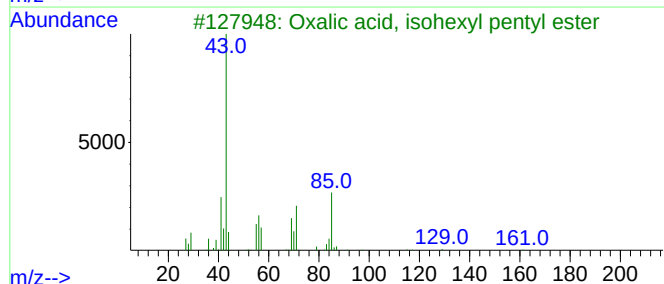
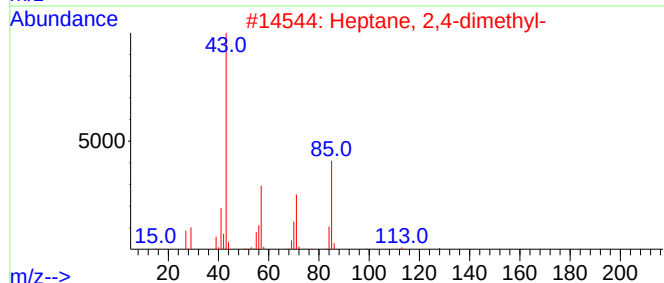
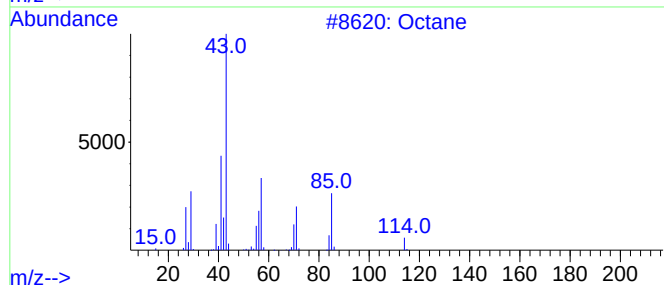
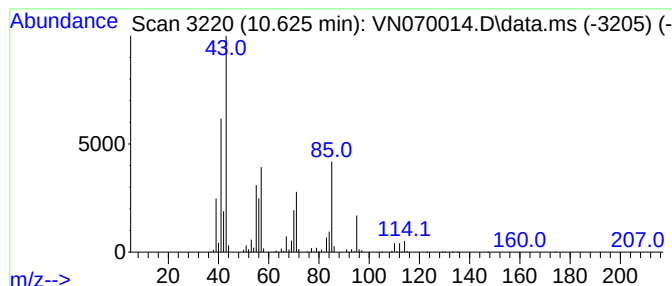
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 12 Octane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.626	21.00 ug/l	4331150	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	87
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
3			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	59
4			Hexane, 3-ethyl-	114	C8H18	000619-99-8	52
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

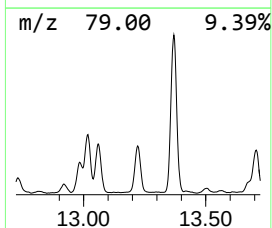
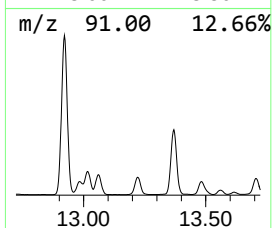
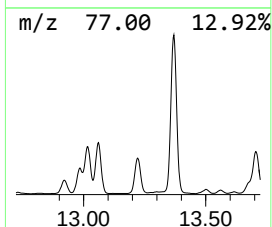
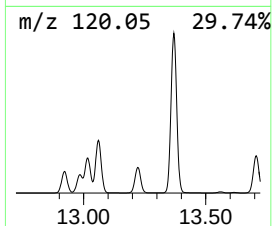
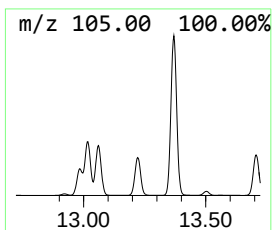
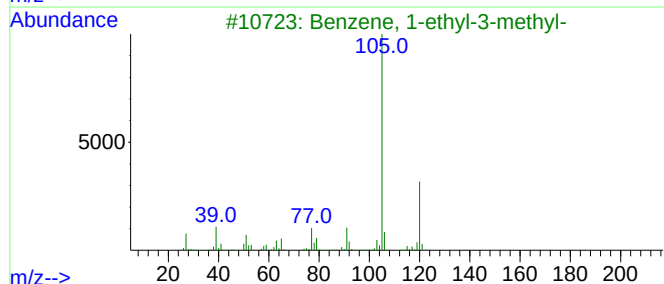
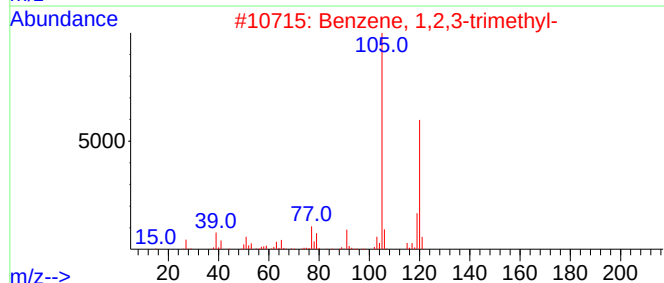
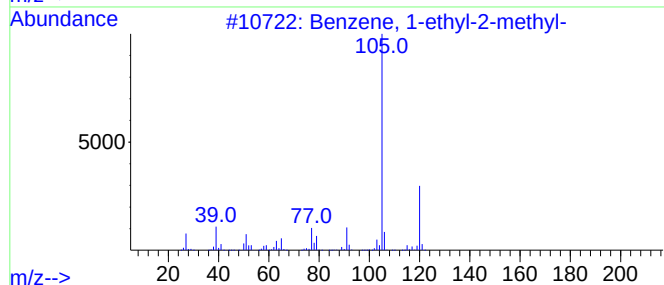
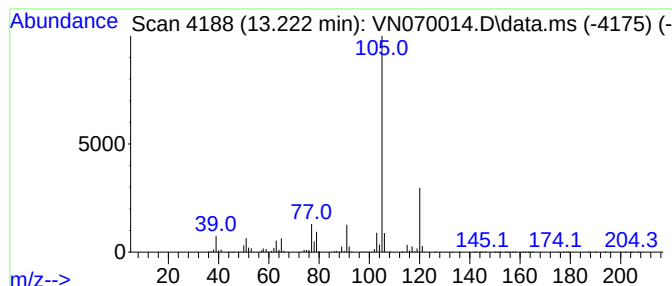
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 13 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	29.58 ug/l	5021410	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

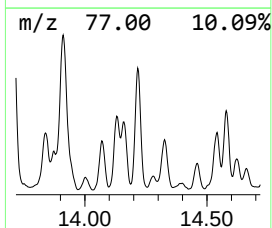
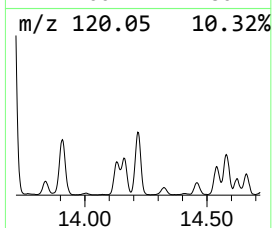
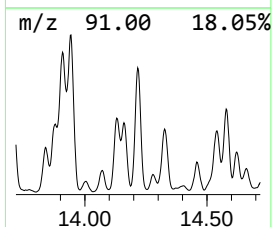
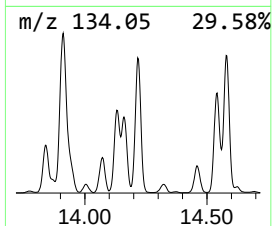
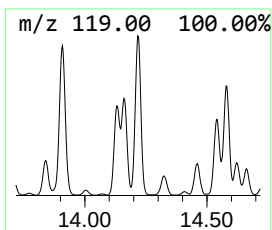
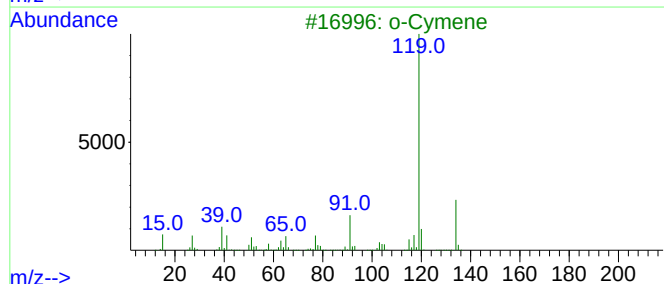
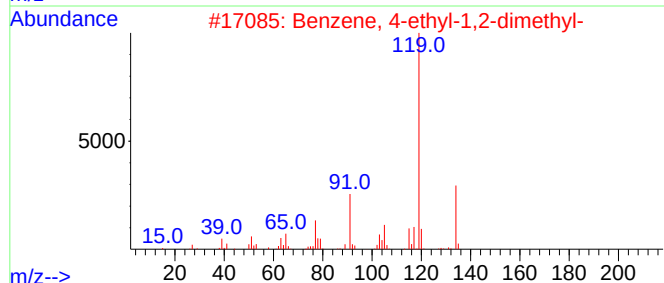
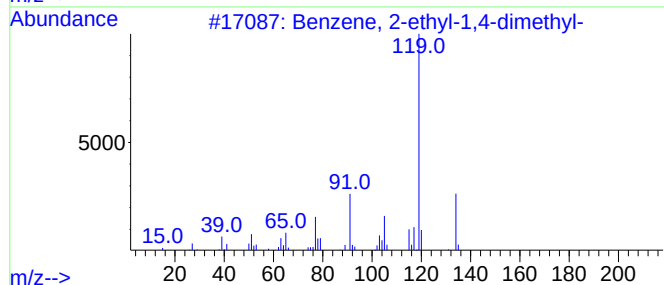
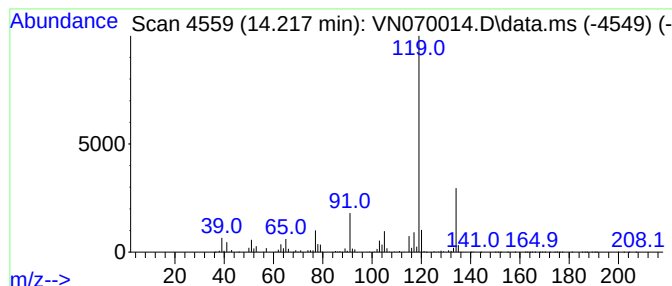
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 14 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	25.12 ug/l	4264630	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-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

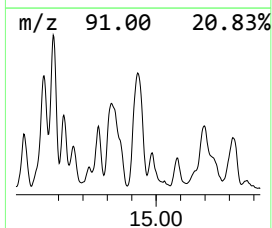
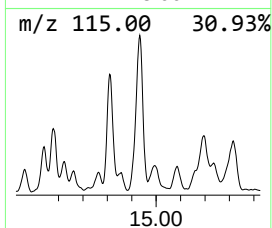
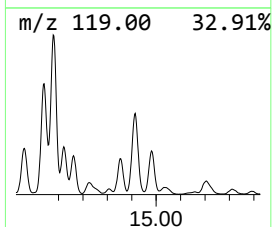
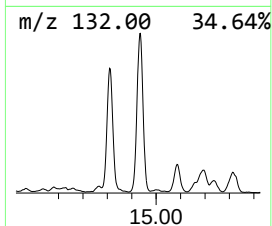
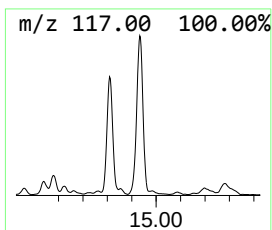
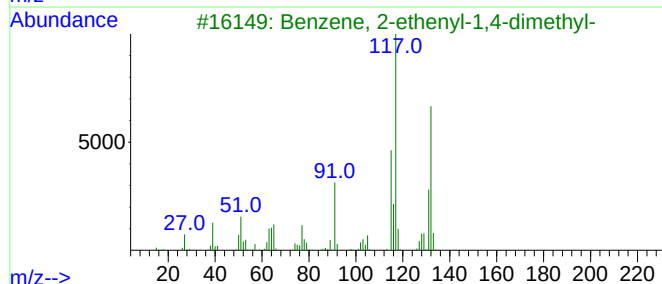
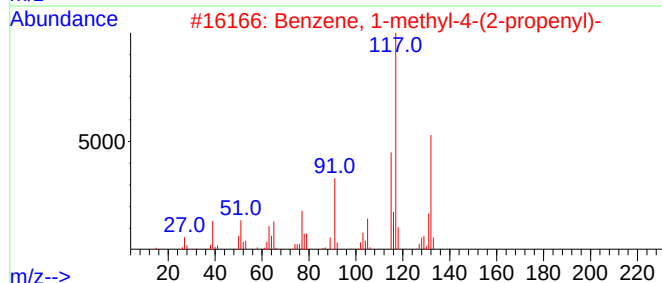
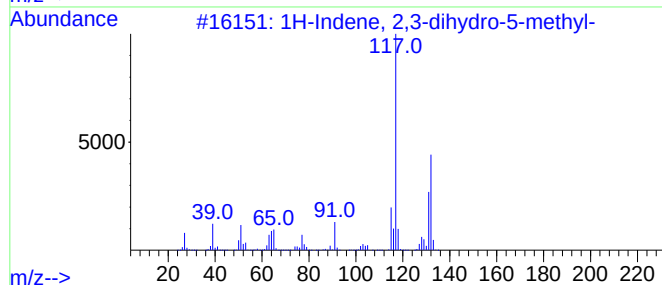
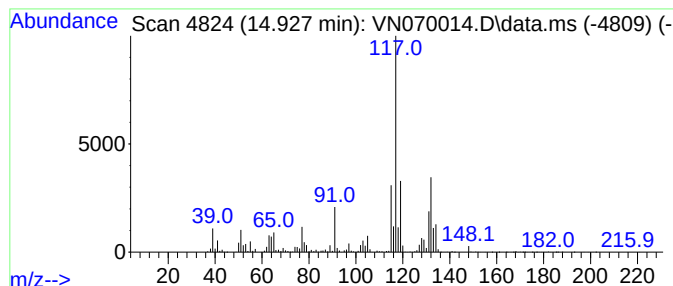
Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

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 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.927	28.44 ug/l	4828400	1,4-Dichlorobenzene-d4			13.675
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-		132	C10H12	000874-35-1	93
2	Benzene, 1-methyl-4-(2-propenyl)-		132	C10H12	003333-13-9	91
3	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	90
4	Benzene, 2-butenyl-		132	C10H12	001560-06-1	81
5	1-Phenyl-1-butene		132	C10H12	000824-90-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070014.D
Acq On : 11 Dec 2021 17:44
Operator : JC/MD
Sample : M4873-05 10X
Misc : 5.86g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-6-6.5

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
Butane, 2-methyl-	3.113	22.1	ug/l	4482410	1	8.086	10120200	50.0
Pentane, 3-methyl-	5.610	22.1	ug/l	4482910	1	8.086	10120200	50.0
n-Hexane	6.114	20.3	ug/l	4105150	1	8.086	10120200	50.0
Pentane, 2,4-di...	7.042	20.3	ug/l	4110730	1	8.086	10120200	50.0
Hexane, 3-methyl-	8.295	26.5	ug/l	5357290	1	8.086	10120200	50.0
Butane, 2,2,3,3...	8.617	115.1	ug/l	21528800	2	8.968	9349450	50.0
Heptane	8.826	24.1	ug/l	4511860	2	8.968	9349450	50.0
Pentane, 2,3,4-...	9.883	57.2	ug/l	10693900	2	8.968	9349450	50.0
Pentane, 2,3,3-...	10.017	86.2	ug/l	16119100	2	8.968	9349450	50.0
Heptane, 3-methyl-	10.218	24.3	ug/l	4551180	2	8.968	9349450	50.0
Hexane, 2,2,5-t...	10.371	27.1	ug/l	5582540	3	11.746	10314600	50.0
Octane	10.626	21.0	ug/l	4331150	3	11.746	10314600	50.0
Benzene, 1-ethy...	13.222	29.6	ug/l	5021410	4	13.675	8488400	50.0
Benzene, 2-ethy...	14.217	25.1	ug/l	4264630	4	13.675	8488400	50.0
1H-Indene, 2,3-...	14.927	28.4	ug/l	4828400	4	13.675	8488400	50.0