

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
 Data File : VN069666.D
 Acq On : 29 Nov 2021 16:11
 Operator : JC/MD
 Sample : M4852-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N110921W.M
 Title : SW846 8260

Signal : TIC: VN069666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.152	1126	1179	1222	rBV5	469040	2471488	2.07%	0.361%
2	5.621	1320	1354	1389	rBV2	449235	1581428	1.33%	0.231%
3	6.122	1512	1541	1576	rBV2	671772	2047837	1.72%	0.299%
4	7.147	1899	1923	1965	rVB2	2670961	7863597	6.60%	1.148%
5	8.024	2224	2250	2256	rBV	997279	2179823	1.83%	0.318%
6	8.094	2258	2276	2296	rVV3	8758041	24201401	20.32%	3.534%
7	8.174	2298	2306	2331	rVV2	575854	1368275	1.15%	0.200%
8	8.298	2333	2352	2364	rVV2	1589754	3703860	3.11%	0.541%
9	8.357	2365	2374	2390	rVV2	935617	2179979	1.83%	0.318%
10	8.440	2390	2405	2432	rVV2	1243200	3205586	2.69%	0.468%
11	8.571	2432	2454	2467	rVV3	1938580	4714162	3.96%	0.688%
12	8.641	2468	2480	2492	rVV	1821229	4099469	3.44%	0.599%
13	8.708	2492	2505	2531	rVB	2813497	6474288	5.44%	0.945%
14	8.826	2531	2549	2581	rVB	1742058	3550480	2.98%	0.518%
15	8.968	2582	2602	2634	rBV	2967434	6353225	5.33%	0.928%
16	9.459	2744	2785	2829	rBV	19610204	45873941	38.51%	6.699%
17	9.641	2837	2853	2867	rBV	1260076	2449990	2.06%	0.358%
18	9.730	2868	2886	2902	rVB	766313	1675777	1.41%	0.245%
19	9.872	2926	2939	2963	rVB2	974592	1992924	1.67%	0.291%
20	10.078	3004	3016	3026	rBV	1092208	2096863	1.76%	0.306%
21	10.212	3046	3066	3093	rVB5	1314916	3365728	2.83%	0.492%
22	10.440	3133	3151	3182	rBV2	8429157	19232171	16.15%	2.809%
23	10.617	3202	3217	3237	rVB6	2265855	5462928	4.59%	0.798%
24	10.781	3265	3278	3295	rVB2	2657230	5015514	4.21%	0.732%
25	10.875	3296	3313	3337	rBV3	1501658	3261748	2.74%	0.476%
26	11.291	3449	3468	3479	rBV	2937815	5746081	4.82%	0.839%
27	11.347	3479	3489	3501	rVB	1439512	2499530	2.10%	0.365%
28	11.527	3540	3556	3582	rVB6	861349	2960596	2.49%	0.432%
29	11.629	3582	3594	3604	rBV	846846	1472263	1.24%	0.215%
30	11.744	3622	3637	3653	rBV	4533236	8362335	7.02%	1.221%
31	11.840	3660	3673	3695	rVB2	4154465	7581956	6.37%	1.107%
32	11.956	3696	3716	3739	rBV	8308402	18790598	15.78%	2.744%
33	12.154	3780	3790	3810	rVB6	493363	1218485	1.02%	0.178%
34	12.253	3811	3827	3842	rBV3	1441494	3930797	3.30%	0.574%
35	12.455	3879	3902	3910	rBV2	2219756	5172843	4.34%	0.755%
36	12.578	3936	3948	3970	rBV	9012785	14910948	12.52%	2.178%

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Peak Location: TOP

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37	12.731	3993	4005	4025	rBV2	3730060	6648851	5.58%	0.971%
38	12.811	4026	4035	4046	rVB4	729218	1209588	1.02%	0.177%
39	12.919	4058	4075	4087	rBV	9574312	16741019	14.05%	2.445%
40	12.980	4087	4098	4105	rBV	6962515	11092327	9.31%	1.620%
41	13.058	4116	4127	4142	rVB	29231570	48031336	40.32%	7.014%
42	13.219	4171	4187	4202	rBV	7060905	12980818	10.90%	1.896%
43	13.286	4203	4212	4217	rVV4	1416664	2285126	1.92%	0.334%
44	13.321	4220	4225	4229	rVV	2223224	2818339	2.37%	0.412%
45	13.366	4230	4242	4269	rVB3	67621880	119114892	100.00%	17.395%
46	13.498	4275	4291	4302	rVB2	3393825	6999605	5.88%	1.022%
47	13.560	4302	4314	4325	rBV	4984309	8290000	6.96%	1.211%
48	13.611	4325	4333	4345	rVB2	1281022	1943496	1.63%	0.284%
49	13.704	4346	4368	4383	rBV3	35540958	65905195	55.33%	9.625%
50	13.771	4385	4393	4404	rVB	1830857	2797171	2.35%	0.408%
51	13.836	4405	4417	4421	rBV	4643531	6544605	5.49%	0.956%
52	13.871	4423	4430	4438	rBV3	7193780	10434139	8.76%	1.524%
53	13.999	4466	4478	4490	rBV4	3455946	5883655	4.94%	0.859%
54	14.066	4493	4503	4514	rBV	3788031	5725987	4.81%	0.836%
55	14.128	4515	4526	4532	rBV	5608744	9080510	7.62%	1.326%
56	14.214	4548	4558	4571	rVB	9584407	14667683	12.31%	2.142%
57	14.278	4572	4582	4588	rBV	2347102	3591642	3.02%	0.525%
58	14.324	4589	4599	4612	rVB3	10221438	17256682	14.49%	2.520%
59	14.458	4637	4649	4660	rBV3	3952567	6660040	5.59%	0.973%
60	14.538	4661	4679	4686	rVV	5028343	9040933	7.59%	1.320%
61	14.576	4686	4693	4704	rVV	5470912	8323071	6.99%	1.215%
62	14.809	4770	4780	4790	rBV3	1450669	2448564	2.06%	0.358%
63	14.917	4806	4820	4838	rBV3	10965591	22715834	19.07%	3.317%
64	15.083	4870	4882	4898	rVB	2415718	4045255	3.40%	0.591%
65	15.308	4955	4966	4982	rVB3	977215	2245046	1.88%	0.328%
66	15.504	5025	5039	5055	rVB	5523066	10172191	8.54%	1.486%

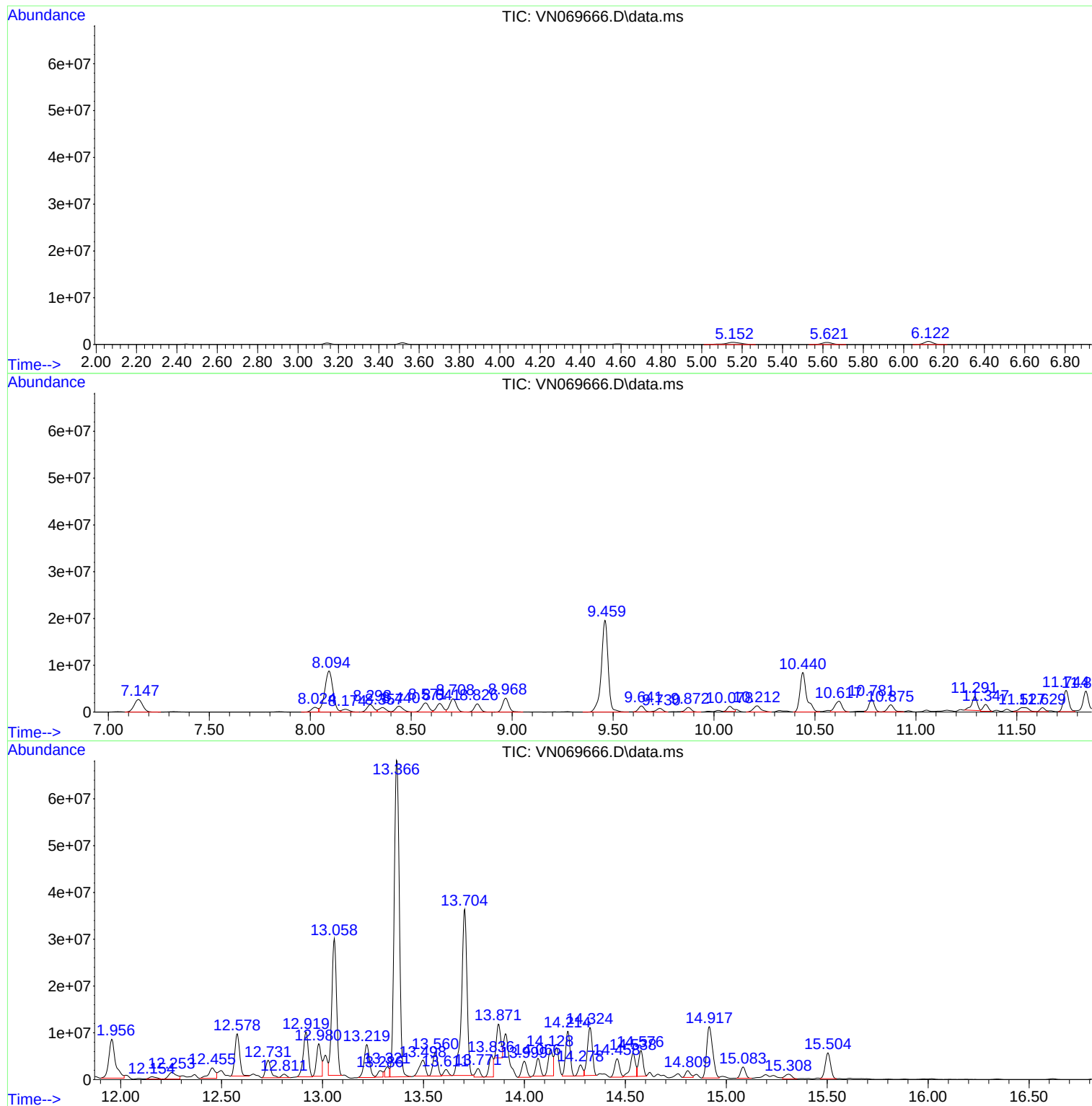
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Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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



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Acq On : 29 Nov 2021 16:11
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

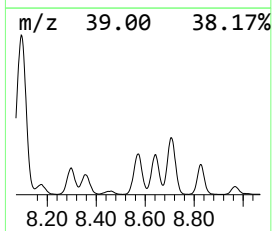
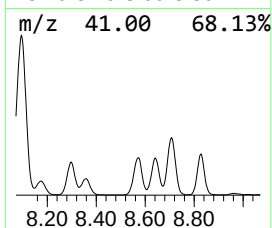
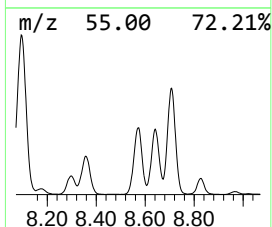
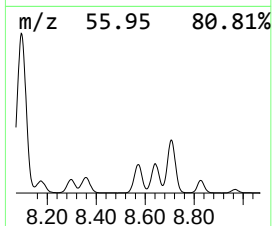
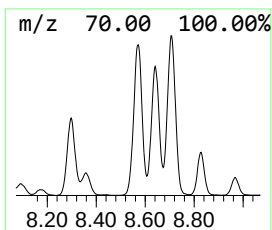
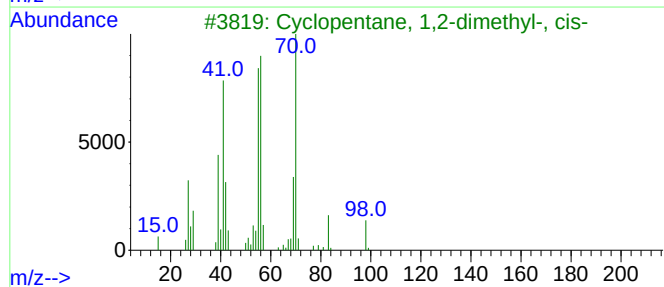
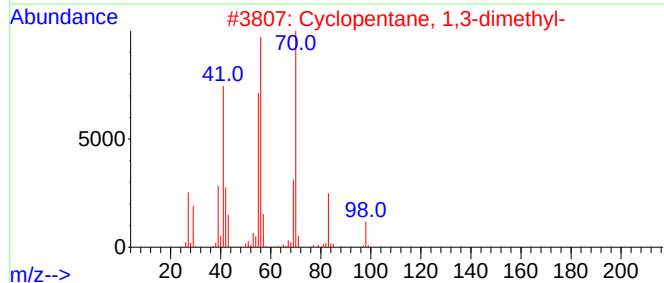
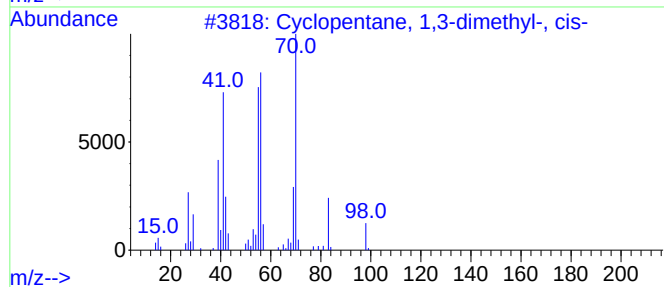
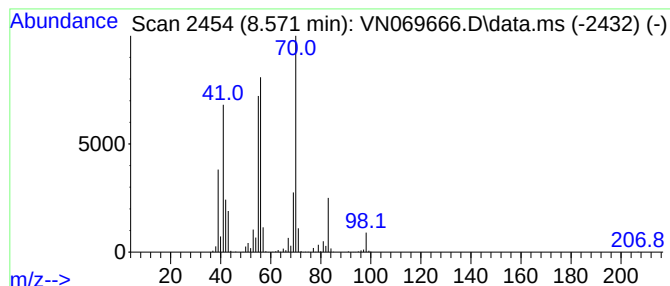
Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, 1,3-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.571	37.10 ug/l	4714160	1,4-Difluorobenzene	8.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	97
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	94
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	81
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	81
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	59



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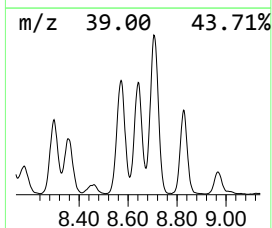
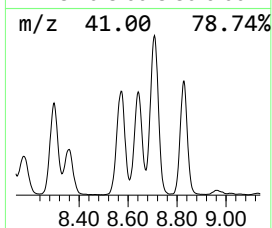
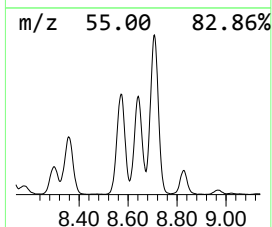
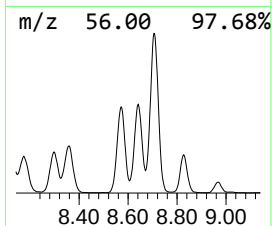
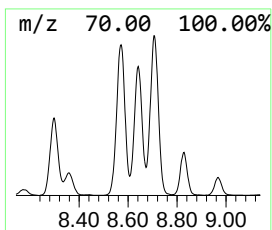
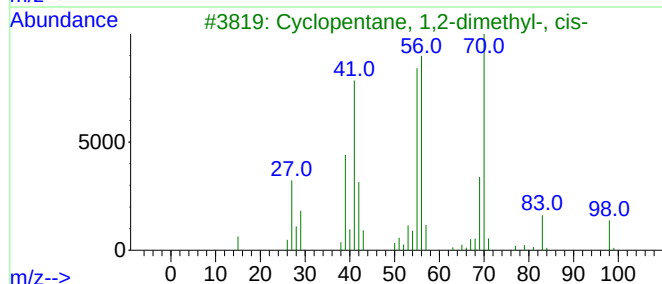
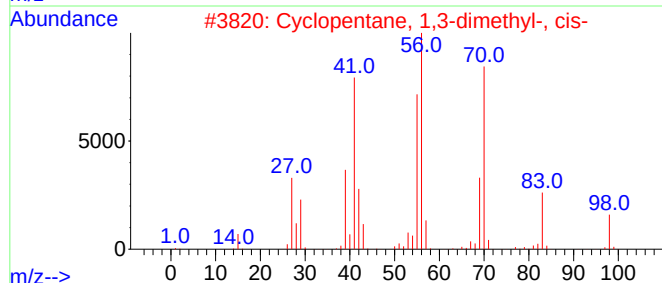
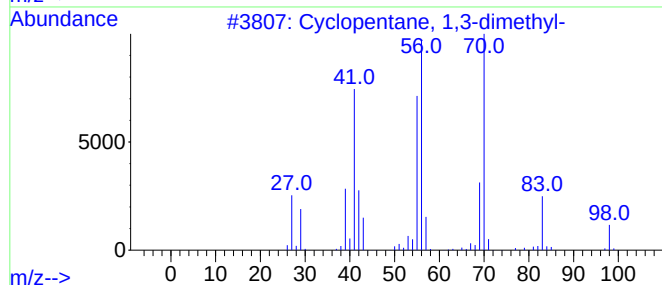
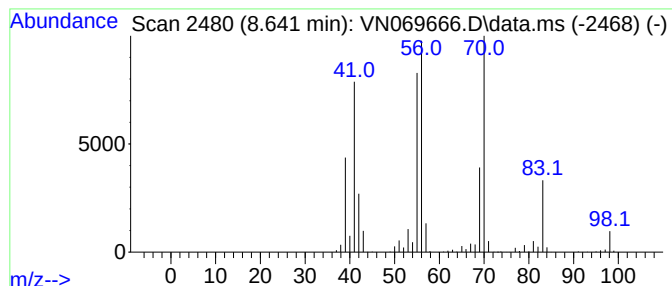
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.641	32.26 ug/l	4099470	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	93
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	93
3			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
4			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	81
5			1-Pentene, 3,4-dimethyl-	98	C7H14	007385-78-6	59



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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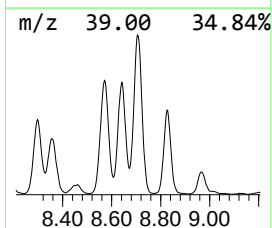
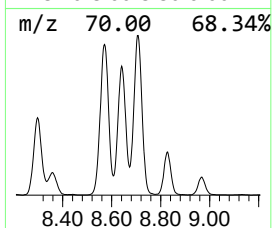
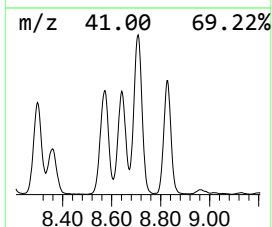
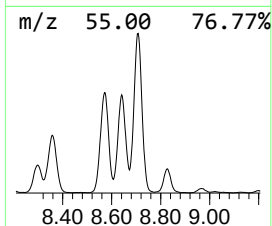
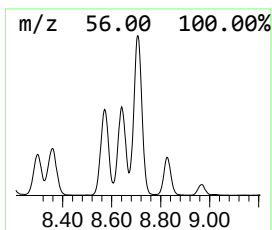
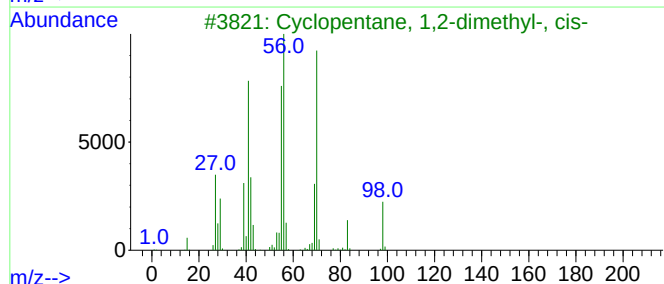
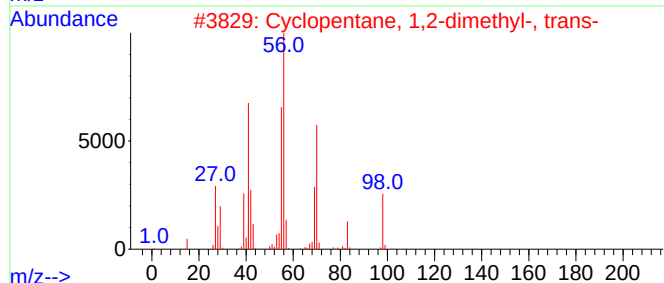
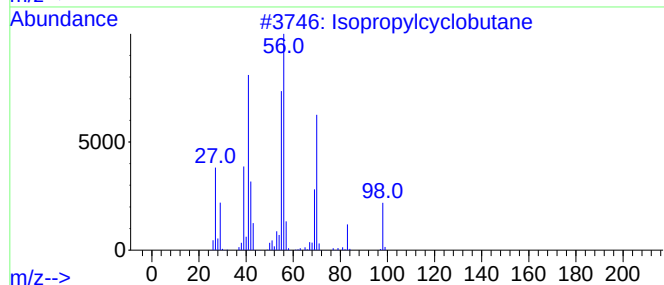
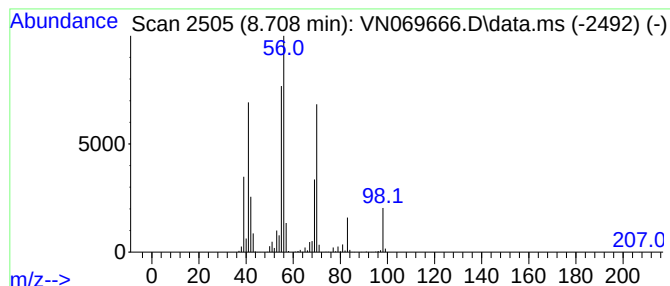
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropylcyclobutane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.708	50.95 ug/l	6474290	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropylcyclobutane	98	C7H14	000872-56-0	97
2			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
3			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
4			1-Heptene	98	C7H14	000592-76-7	86
5			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	80



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ClientSampleId :
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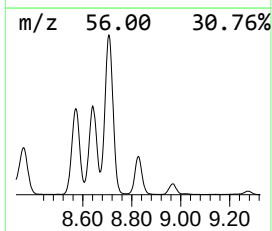
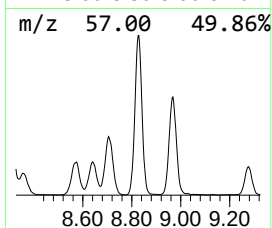
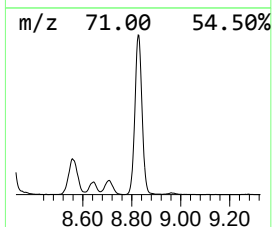
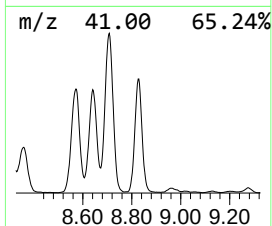
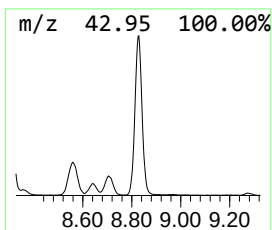
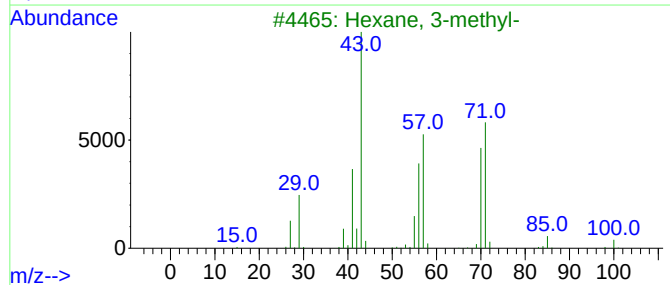
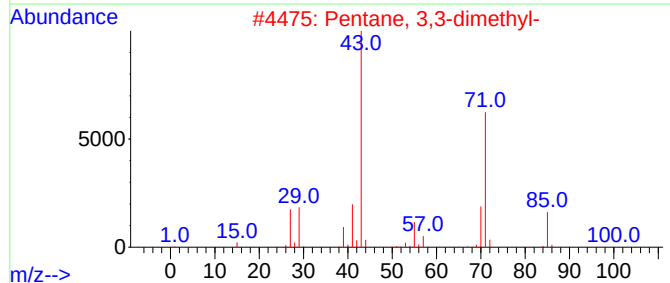
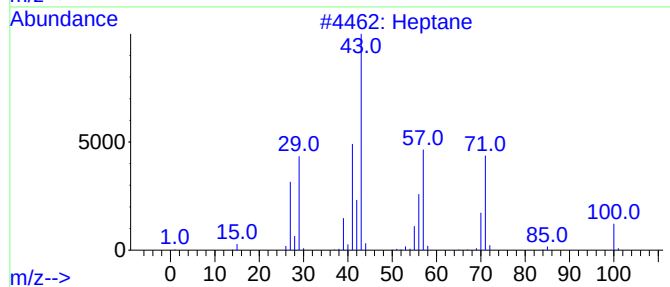
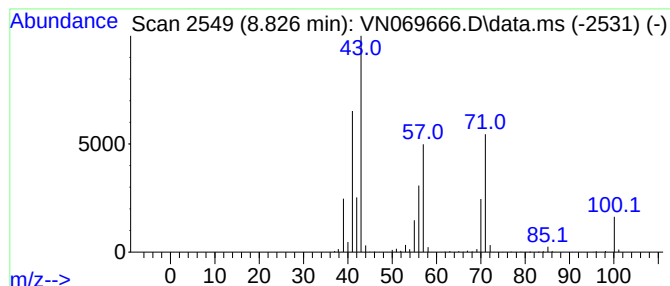
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 4 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	27.94 ug/l	3550480	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	94
2			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	47
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

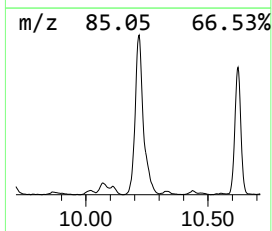
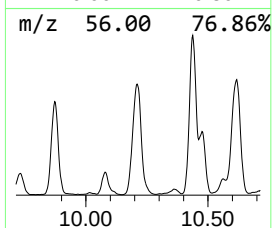
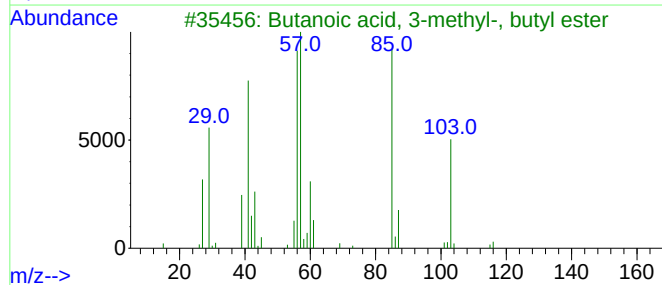
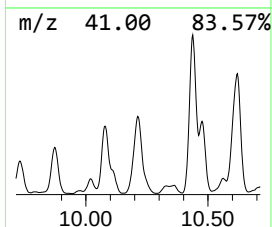
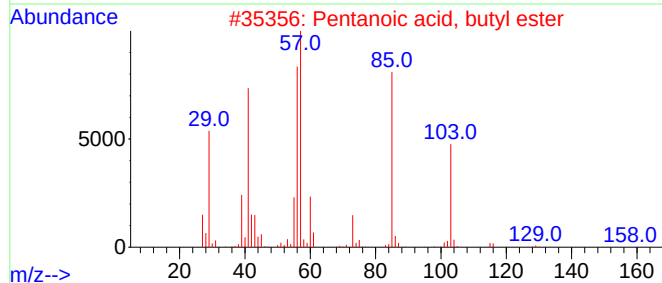
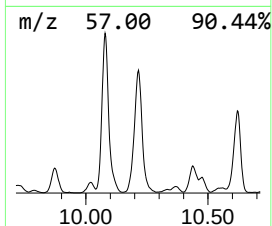
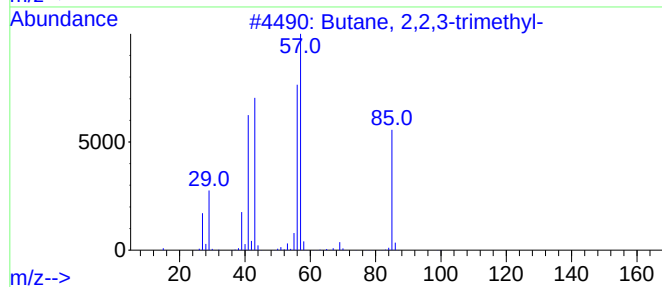
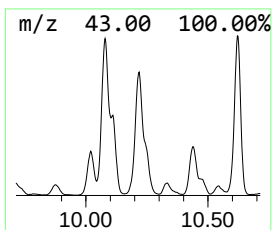
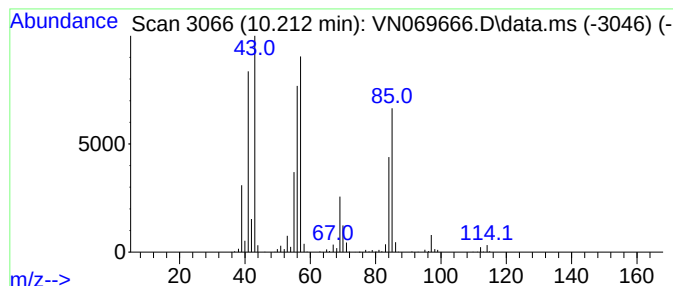
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Quant Title : SW846 8260

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

Peak Number 5 Butane, 2,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.213	26.49 ug/l	3365730	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
2			Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	50
3			Butanoic acid, 3-methyl-, butyl ...	158	C9H18O2	000109-19-3	50
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	49
5			Heptane, 3-methyl-	114	C8H18	000589-81-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

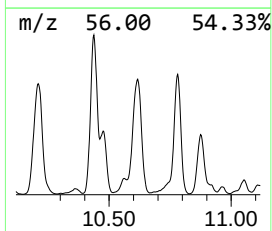
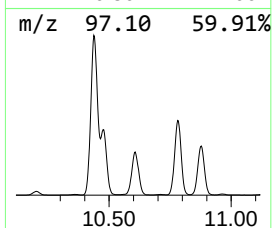
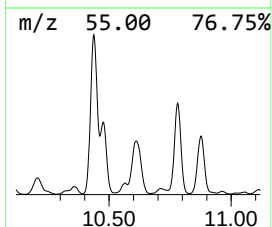
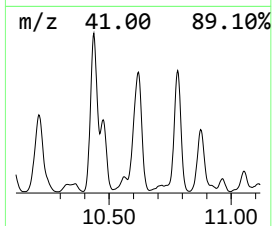
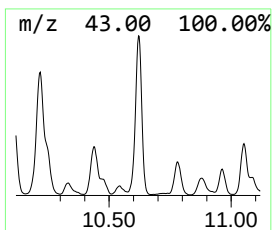
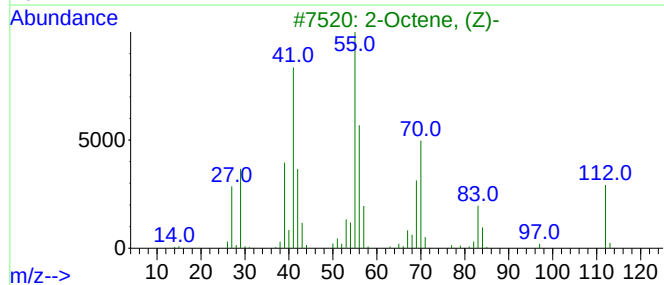
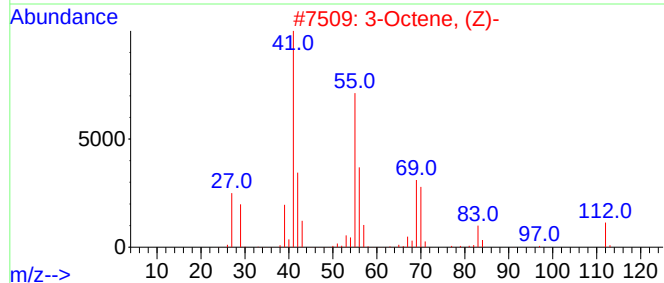
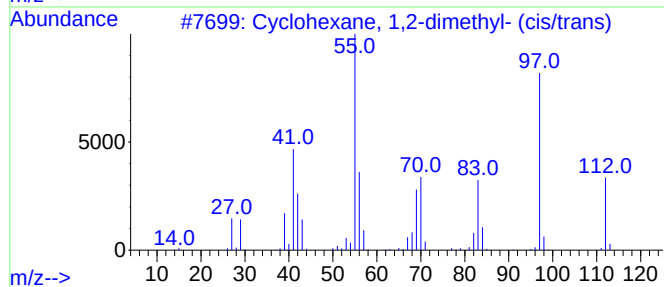
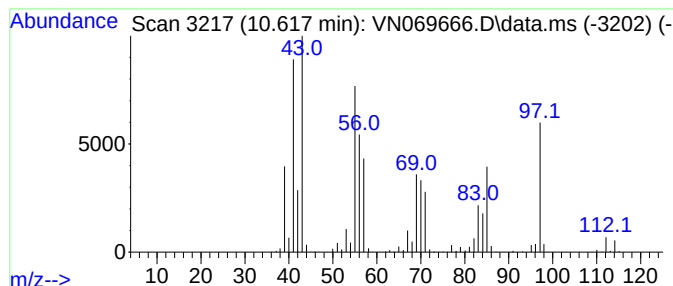
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Quant Title : SW846 8260

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

Peak Number 6 unknown10.618 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.618	32.66 ug/l	5462930	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	43
2			3-Octene, (Z)-	112	C8H16	014850-22-7	43
3			2-Octene, (Z)-	112	C8H16	007642-04-8	43
4			Cyclooctane	112	C8H16	000292-64-8	43
5			2-Octene	112	C8H16	000111-67-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

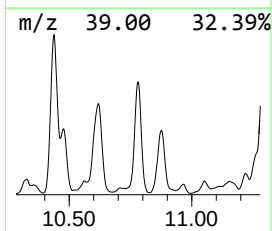
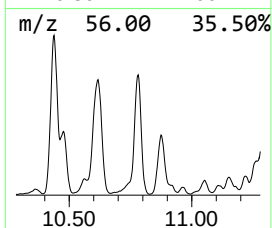
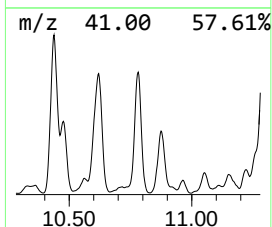
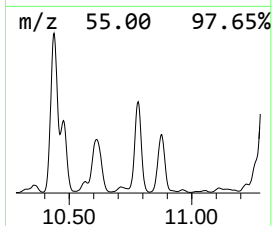
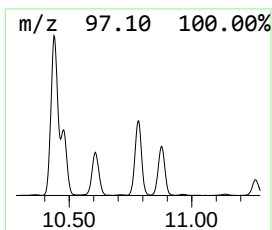
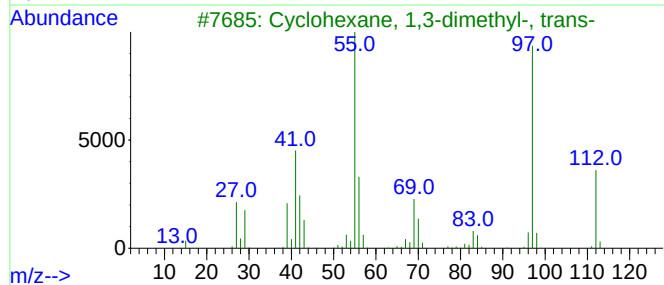
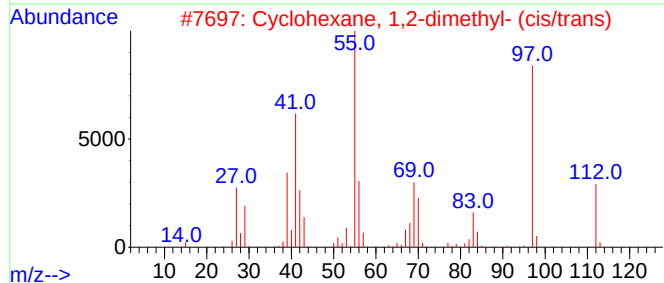
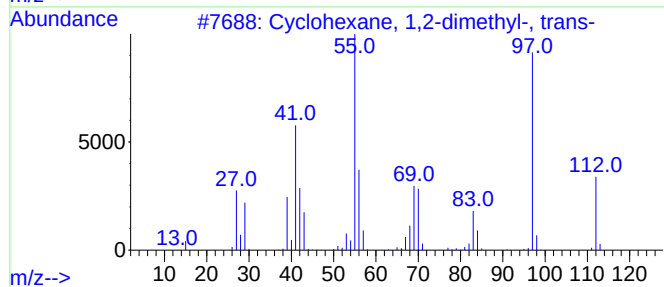
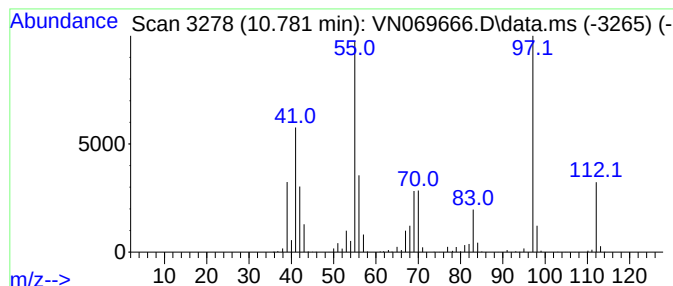
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	29.99 ug/l	5015510	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	94
2			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	94
3			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	81
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	72
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

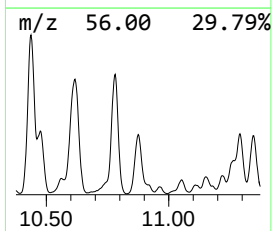
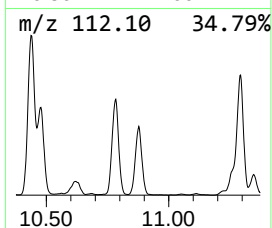
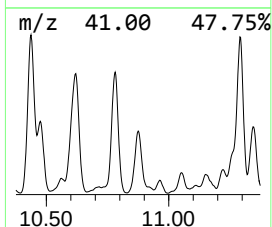
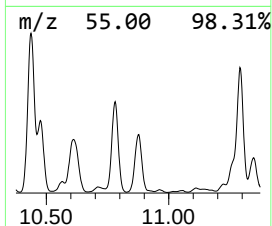
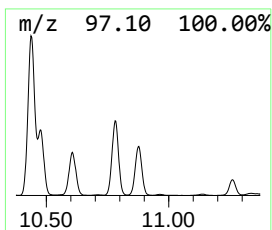
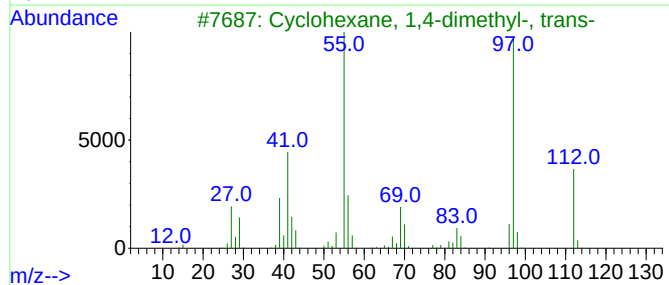
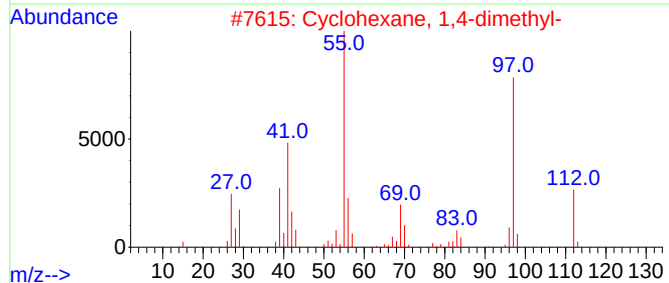
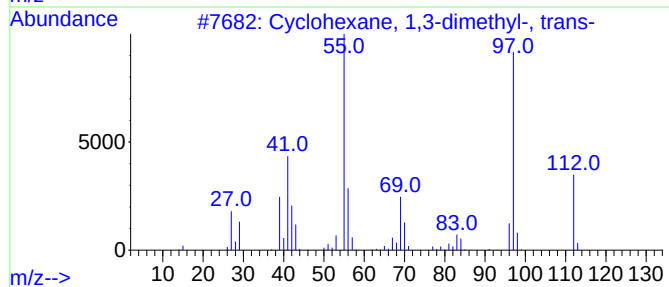
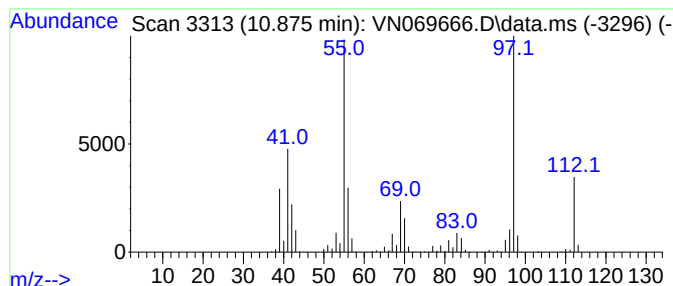
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	19.50 ug/l	3261750	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	96
2			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	94
3			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	93
4			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	91
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

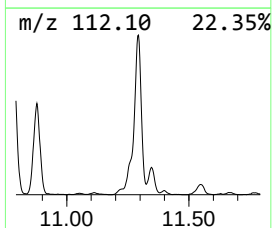
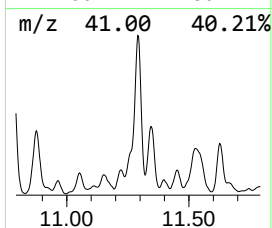
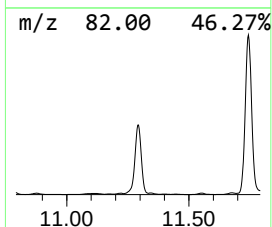
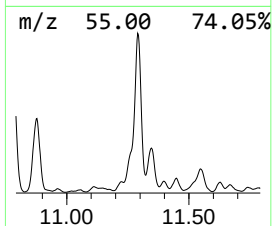
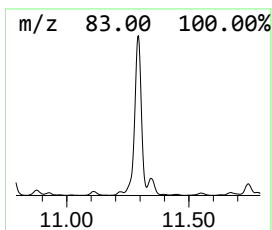
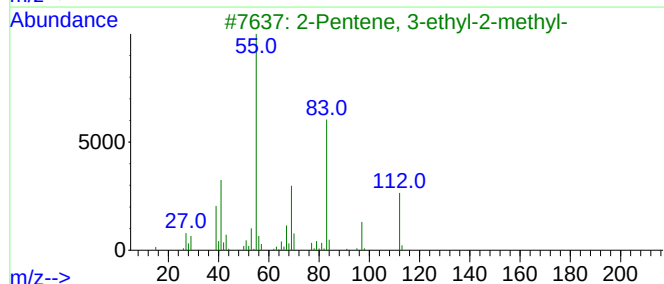
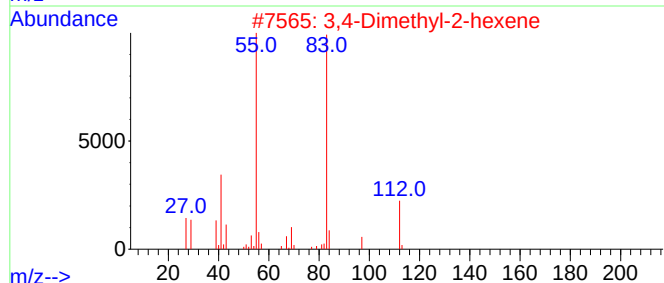
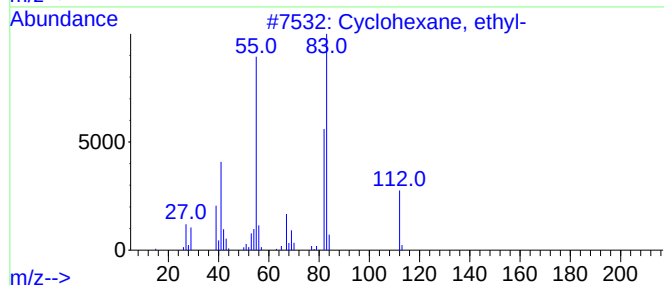
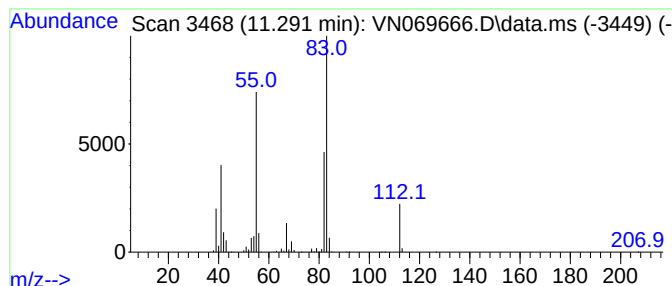
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	34.36 ug/l	5746080	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethyl-	112	C8H16	001678-91-7	91
2			3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	58
3			2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	53
4			2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	53
5			Oxalic acid, cyclohexyl octyl ester	284	C16H28O4	1000309-31-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

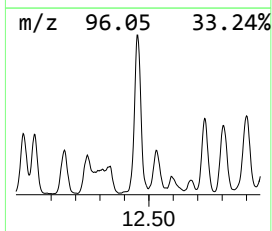
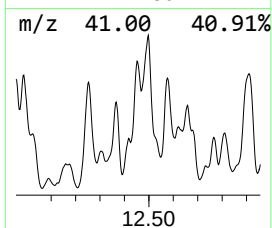
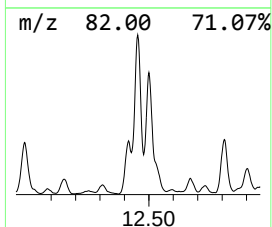
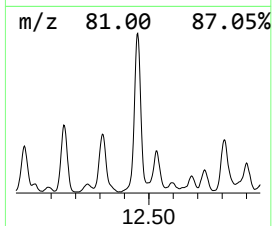
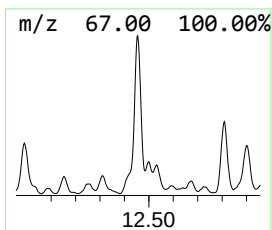
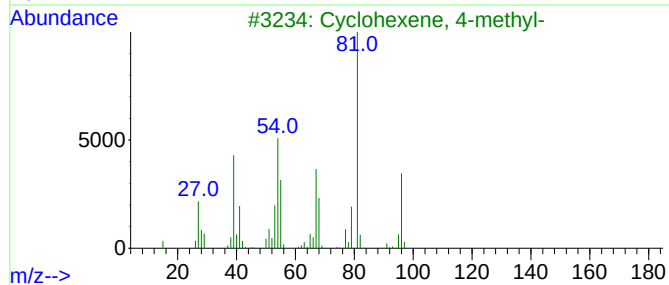
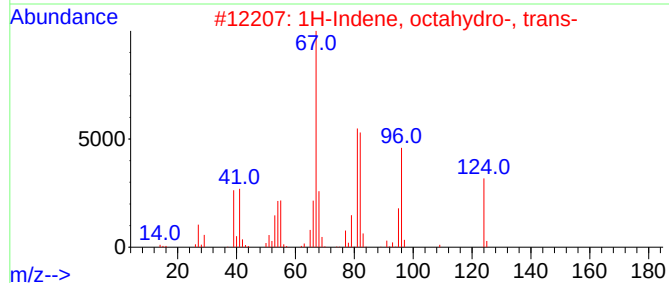
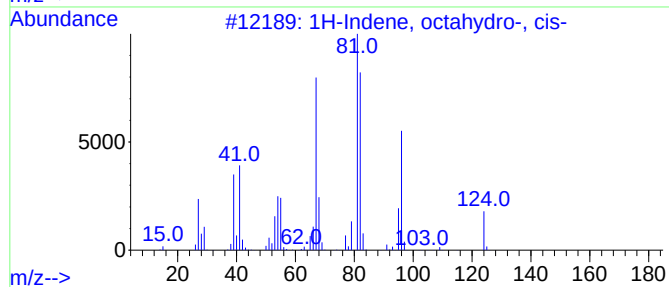
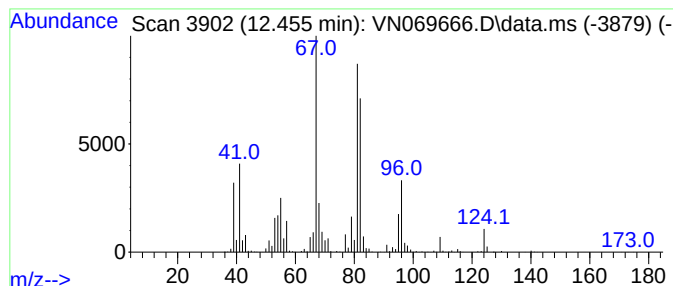
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, octahydro-, cis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	30.93 ug/l	5172840	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	74
2			1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	62
3			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	55
4			1H-Indene, octahydro-	124	C9H16	000496-10-6	49
5			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069666.D
Acq On : 29 Nov 2021 16:11
Operator : JC/MD
Sample : M4852-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.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
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Cyclopentane, 1...	8.641	32.3	ug/l	4099470	2	8.968	6353230	50.0
Isopropylcyclob...	8.708	51.0	ug/l	6474290	2	8.968	6353230	50.0
Heptane	8.826	27.9	ug/l	3550480	2	8.968	6353230	50.0
Butane, 2,2,3-t...	10.213	26.5	ug/l	3365730	2	8.968	6353230	50.0
unknown10.618	10.618	32.7	ug/l	5462930	3	11.744	8362340	50.0
Cyclohexane, 1,...	10.781	30.0	ug/l	5015510	3	11.744	8362340	50.0
Cyclohexane, 1,...	10.875	19.5	ug/l	3261750	3	11.744	8362340	50.0
Cyclohexane, et...	11.291	34.4	ug/l	5746080	3	11.744	8362340	50.0
1H-Indene, octa...	12.455	30.9	ug/l	5172840	3	11.744	8362340	50.0