

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
 Data File : VN069784.D
 Acq On : 6 Dec 2021 15:27
 Operator : JC/MD
 Sample : M4932-01
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM1-2

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: VN069784.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.079	1100	1152	1188	rBV2	836254	3319031	1.13%	0.097%
2	6.077	1494	1524	1559	rBV	3905979	12039617	4.10%	0.351%
3	7.120	1892	1913	1947	rVB	3658297	10885663	3.71%	0.318%
4	8.061	2232	2264	2287	rBV5	13571291	47469718	16.17%	1.385%
5	8.161	2289	2301	2325	rVB	3719567	9807068	3.34%	0.286%
6	8.284	2326	2347	2362	rBV	14357807	34362094	11.70%	1.003%
7	8.560	2428	2450	2464	rBV2	10151196	24428513	8.32%	0.713%
8	8.633	2464	2477	2488	rVV	9677246	22300226	7.59%	0.651%
9	8.700	2489	2502	2526	rVV	15353456	35723536	12.17%	1.043%
10	8.820	2527	2547	2582	rVV2	53808327	112438610	38.29%	3.282%
11	8.965	2584	2601	2612	rVV	3324611	7218634	2.46%	0.211%
12	9.016	2613	2620	2636	rVB	1806592	3248060	1.11%	0.095%
13	9.456	2750	2784	2799	rBV4	80092722	207010419	70.49%	6.042%
14	9.636	2826	2851	2865	rBV	9152500	18612888	6.34%	0.543%
15	9.727	2866	2885	2904	rVB	14482198	31453926	10.71%	0.918%
16	9.869	2922	2938	2969	rVB2	17917285	38001769	12.94%	1.109%
17	10.017	2979	2993	3002	rBV	6932366	13090148	4.46%	0.382%
18	10.078	3002	3016	3046	rVB2	59372115	133273658	45.38%	3.890%
19	10.215	3047	3067	3093	rVB4	33117766	79750811	27.16%	2.328%
20	10.333	3095	3111	3113	rBV4	3026385	4604376	1.57%	0.134%
21	10.438	3133	3150	3159	rBV4	64375638	129014592	43.93%	3.765%
22	10.564	3185	3197	3203	rBV	6793561	11853850	4.04%	0.346%
23	10.625	3203	3220	3237	rVB5	134119430	270877531	92.24%	7.906%
24	10.741	3239	3263	3269	rBV2	11813540	23019420	7.84%	0.672%
25	10.784	3269	3279	3296	rVB	37085957	71098899	24.21%	2.075%
26	10.878	3298	3314	3327	rBV2	24629382	54855158	18.68%	1.601%
27	10.963	3338	3346	3358	rVB	10033381	16360731	5.57%	0.477%
28	11.052	3358	3379	3392	rBV	26746594	48395471	16.48%	1.412%
29	11.154	3407	3417	3432	rVB	10695472	20229354	6.89%	0.590%
30	11.224	3433	3443	3451	rBV3	13951166	23544480	8.02%	0.687%
31	11.293	3460	3469	3479	rVB2	45588248	70636943	24.05%	2.062%
32	11.347	3479	3489	3500	rVV3	45961987	76456735	26.04%	2.231%
33	11.395	3501	3507	3517	rVB4	15267157	22852059	7.78%	0.667%
34	11.454	3518	3529	3541	rBV4	31751247	53042019	18.06%	1.548%
35	11.532	3543	3558	3582	rVB7	42567195	128434284	43.74%	3.748%
36	11.629	3582	3594	3606	rBV2	39226503	64401123	21.93%	1.880%

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37	11.747	3628	3638	3647	rBV	6097172	10746143	3.66%	0.314%
38	11.840	3661	3673	3680	rBV4	14814224	26567057	9.05%	0.775%
39	11.881	3682	3688	3695	rVV	9349774	12104883	4.12%	0.353%
40	11.961	3697	3718	3738	rVV9	124102160	293656468	100.00%	8.570%
41	12.095	3759	3768	3773	rBV3	2867940	4563014	1.55%	0.133%
42	12.259	3811	3829	3834	rBV4	37906355	80756445	27.50%	2.357%
43	12.369	3863	3870	3880	rVB	23351095	33980080	11.57%	0.992%
44	12.420	3880	3889	3891	rBV2	8444053	9898588	3.37%	0.289%
45	12.457	3893	3903	3910	rBV	31822638	56904639	19.38%	1.661%
46	12.733	3998	4006	4013	rBV4	7775524	12362352	4.21%	0.361%
47	12.900	4059	4068	4082	rVB4	28047608	51437471	17.52%	1.501%
48	12.983	4089	4099	4105	rBV4	15938897	27148585	9.25%	0.792%
49	13.050	4115	4124	4139	rVB6	110201368	204010024	69.47%	5.954%
50	13.112	4140	4147	4159	rVB2	17359688	26569857	9.05%	0.775%
51	13.224	4173	4189	4204	rBV3	19524934	53725224	18.30%	1.568%
52	13.286	4206	4212	4230	rVB4	17278354	30945575	10.54%	0.903%
53	13.372	4232	4244	4266	rBV2	54656925	97572595	33.23%	2.848%
54	13.565	4304	4316	4326	rBV4	29003405	51917199	17.68%	1.515%
55	13.707	4351	4369	4380	rVB3	37490823	67727359	23.06%	1.977%
56	13.868	4423	4429	4438	rVB	15036874	19157637	6.52%	0.559%
57	13.914	4438	4446	4464	rVB4	16407873	30712679	10.46%	0.896%
58	13.997	4466	4477	4489	rBV2	54774733	84722508	28.85%	2.473%
59	14.133	4520	4528	4532	rBV	9688424	12661420	4.31%	0.370%
60	14.217	4551	4559	4575	rVB	20794879	32218531	10.97%	0.940%
61	14.324	4589	4599	4610	rVB3	12937795	21424368	7.30%	0.625%
62	14.509	4661	4668	4675	rBV4	6758543	8634766	2.94%	0.252%
63	14.579	4689	4694	4703	rVB	9400226	11757780	4.00%	0.343%
64	14.622	4703	4710	4719	rVB2	7540385	9562899	3.26%	0.279%
65	14.670	4719	4728	4742	rVB3	7368268	13755734	4.68%	0.401%
66	14.850	4773	4795	4807	rVB6	9440361	25625214	8.73%	0.748%
67	14.917	4808	4820	4837	rVV3	17319011	37748627	12.85%	1.102%
68	14.984	4838	4845	4860	rVB2	3722913	6583532	2.24%	0.192%
69	15.198	4917	4925	4954	rVB4	4614829	13010934	4.43%	0.380%
70	15.303	4955	4964	4984	rVB3	3132431	6346360	2.16%	0.185%
71	15.507	5029	5040	5054	rVB	3185279	5736247	1.95%	0.167%

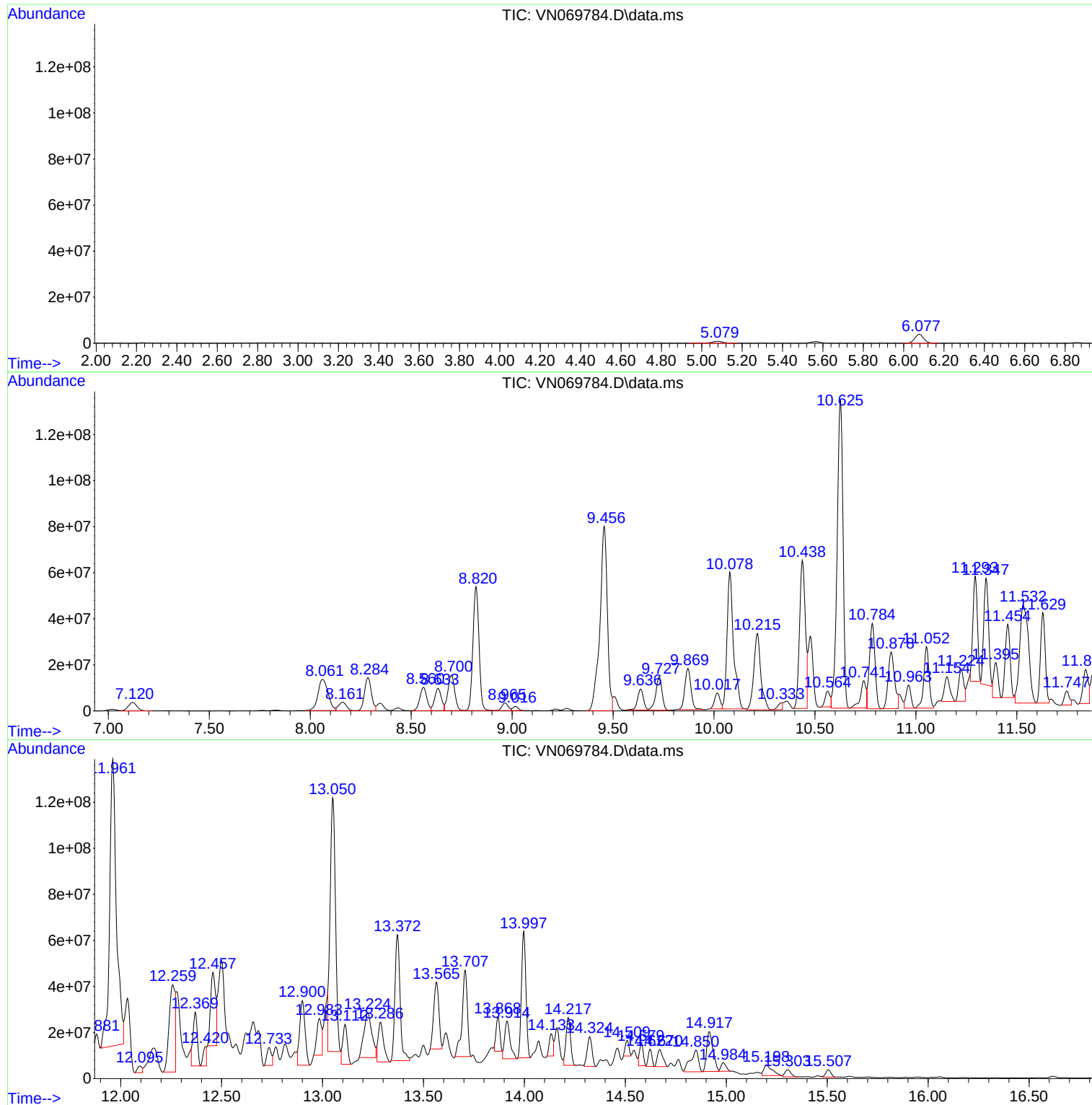
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MSVOA_N
ClientSampleId :
DRUM1-2

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

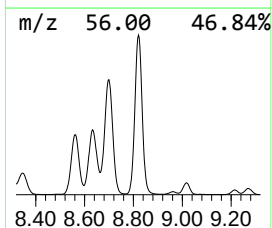
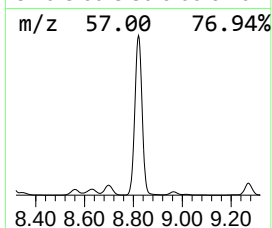
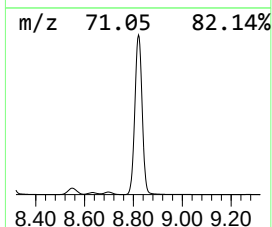
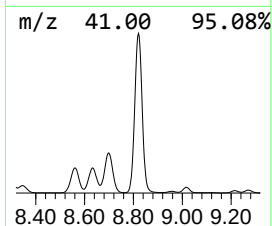
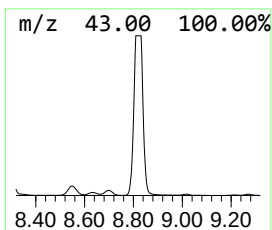
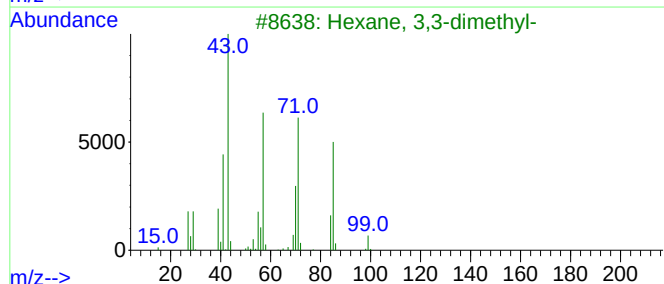
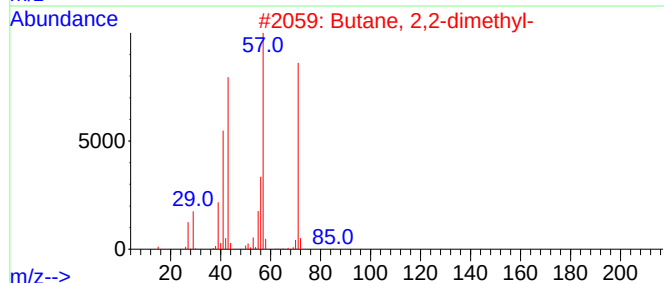
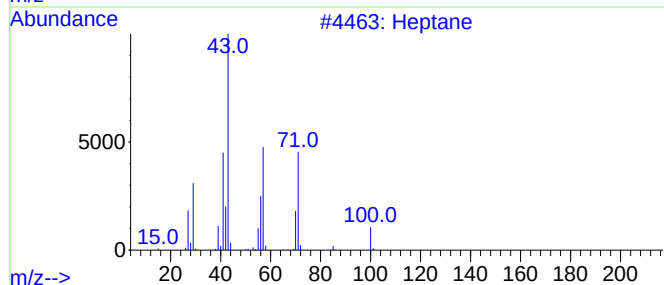
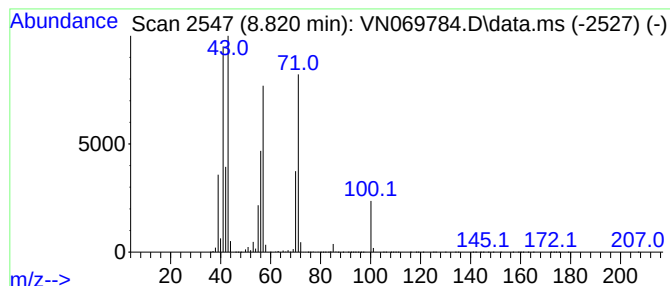
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.820	778.81 ug/l	112439000	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	90
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	42



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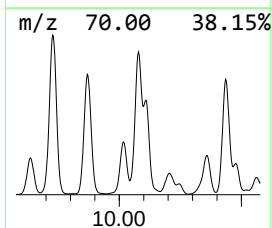
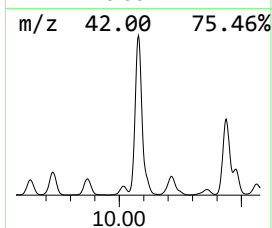
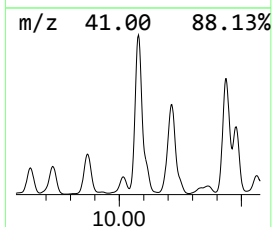
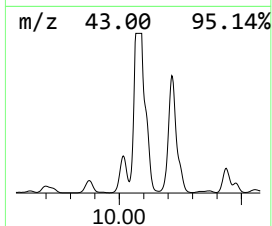
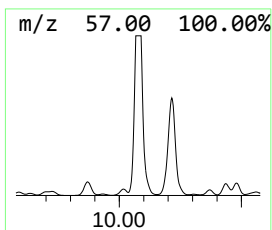
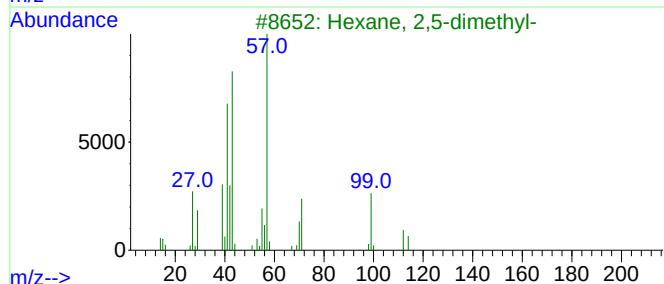
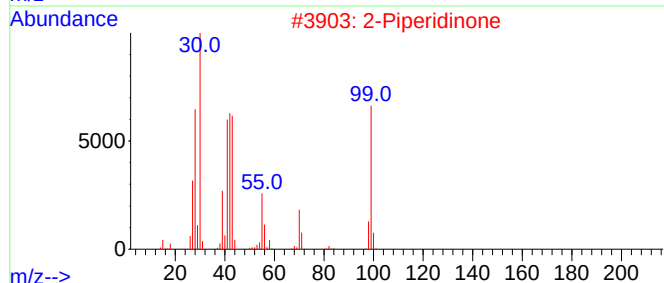
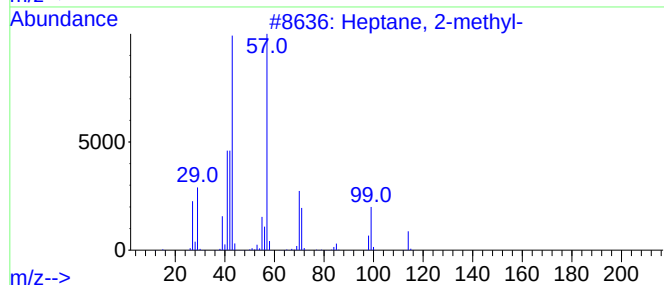
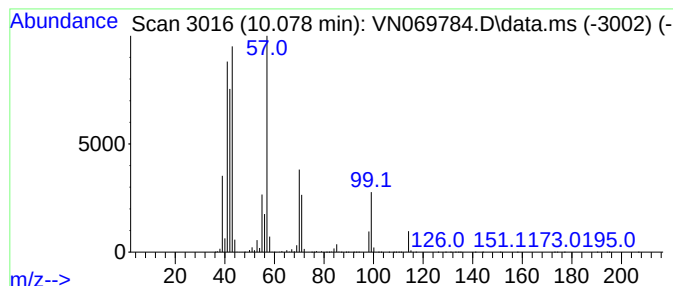
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.078	923.12 ug/l	133274000	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	81
2			2-Piperidinone	99	C5H9NO	000675-20-7	59
3			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	55
4			1-Pentene	70	C5H10	000109-67-1	43
5			Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	35



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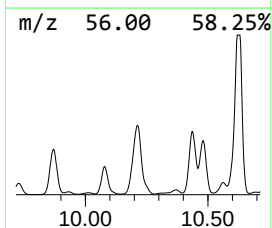
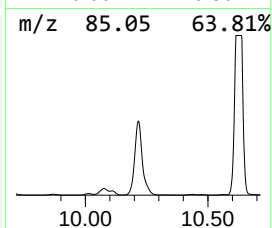
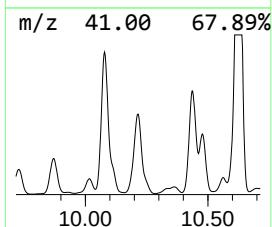
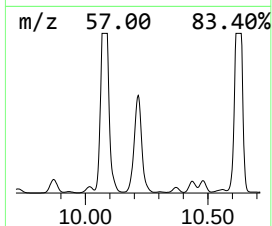
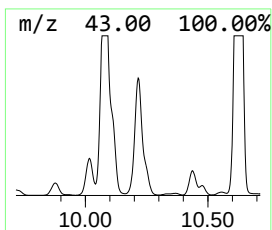
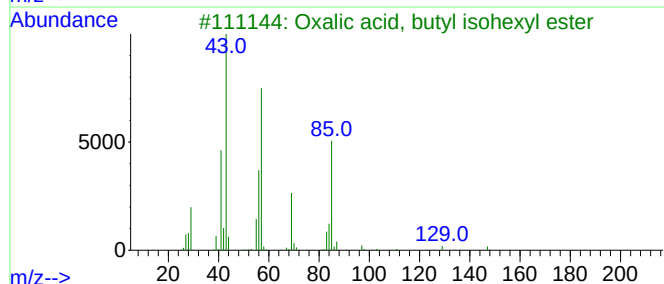
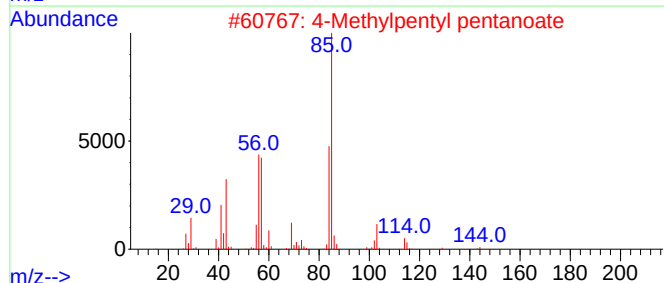
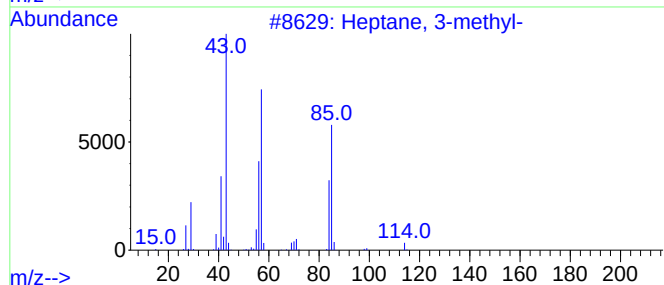
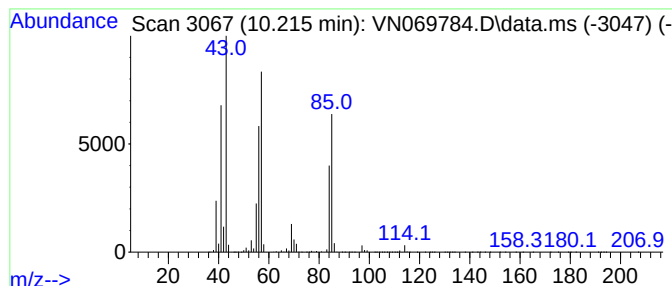
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heptane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	552.39 ug/l	79750800	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2			4-Methylpentyl pentanoate	186	C11H22O2	035852-47-2	64
3			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	58
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53



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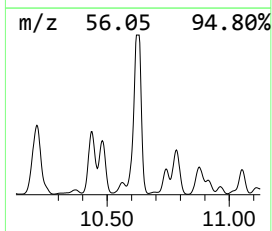
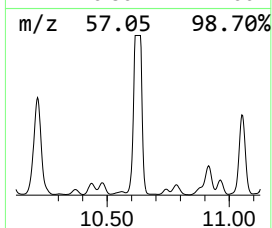
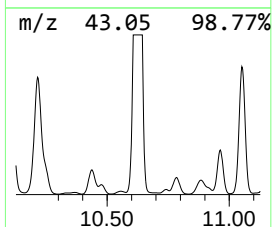
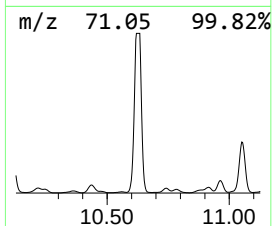
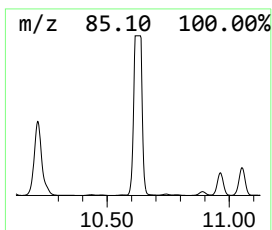
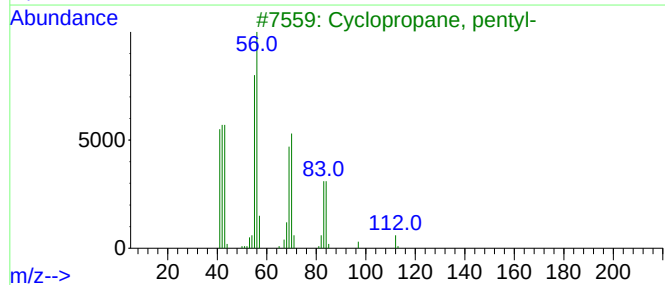
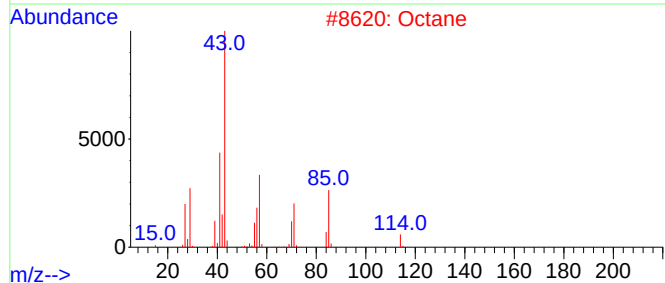
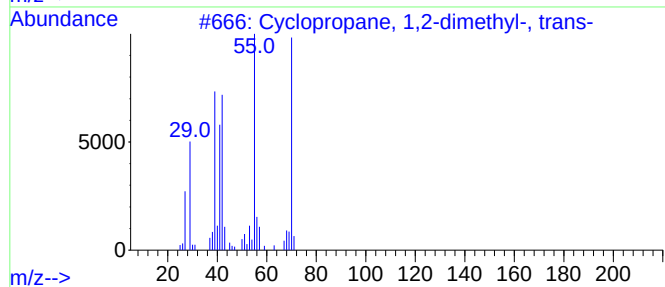
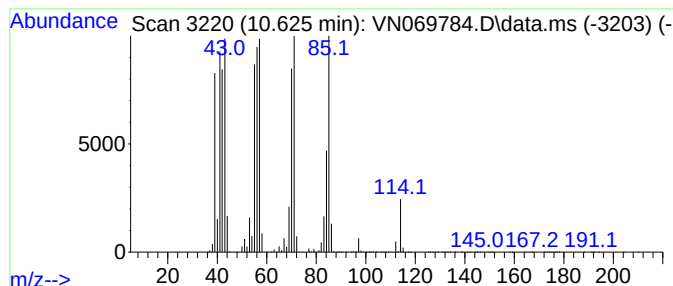
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown10.626 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.626	1260.35 ug/l	270878000	Chlorobenzene-d5	11.746	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	49
2	Octane	114	C8H18	000111-65-9	43
3	Cyclopropane, pentyl-	112	C8H16	002511-91-3	38
4	2H-Pyran-2-one, tetrahydro-4-met...	114	C6H10O2	001121-84-2	25
5	Octane, 4-methyl-	128	C9H20	002216-34-4	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

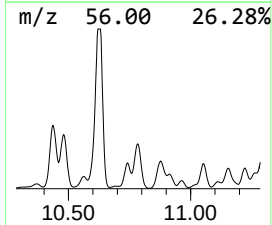
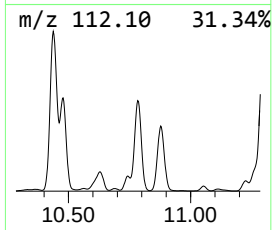
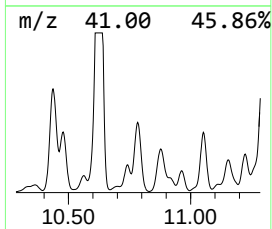
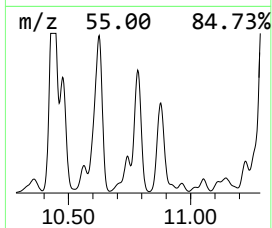
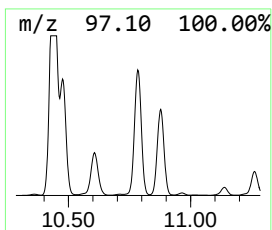
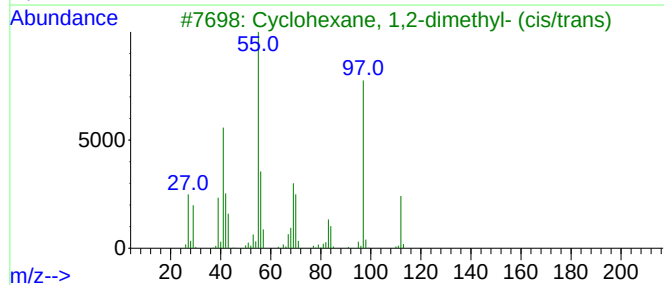
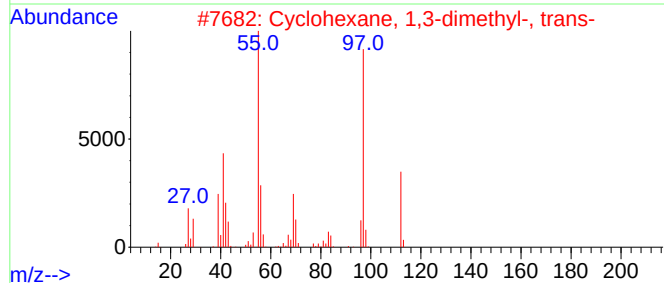
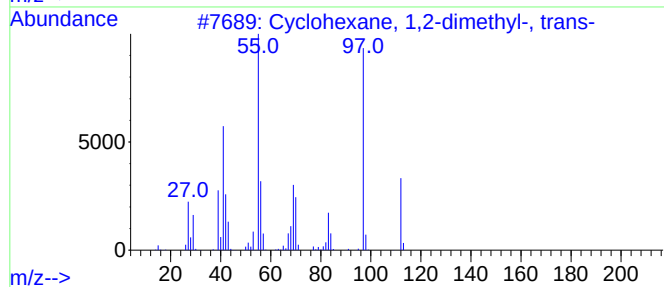
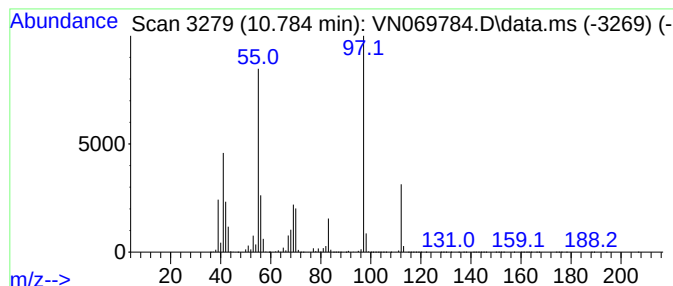
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.784	330.81 ug/l	71098900	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	94
2			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	90
3			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	90
4			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	83
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

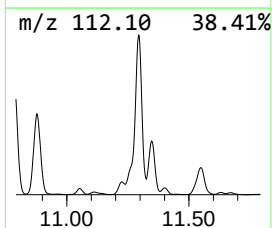
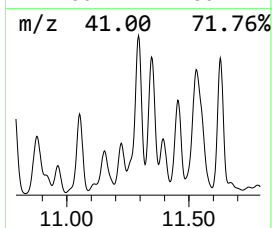
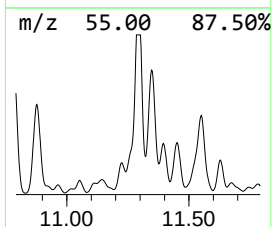
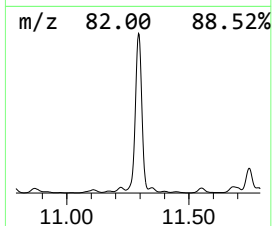
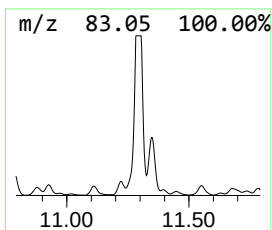
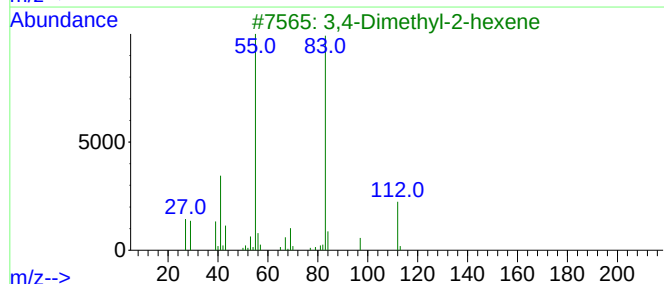
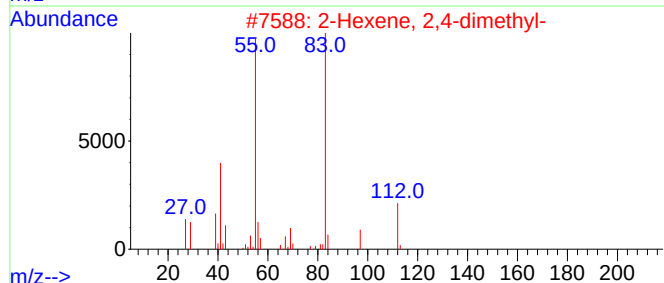
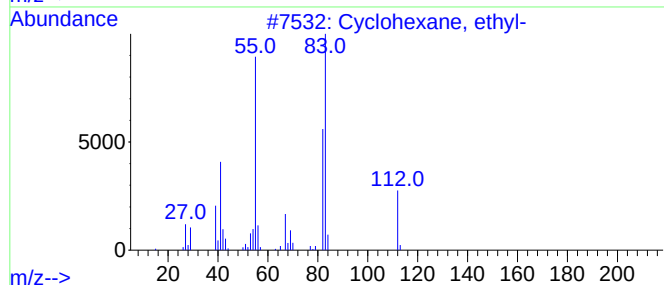
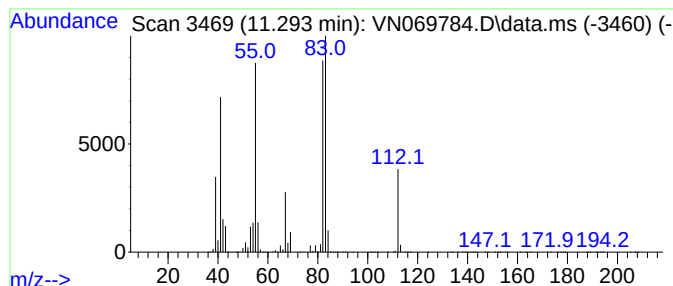
Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

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 Cyclohexane, ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.293	328.66 ug/l	70636900	Chlorobenzene-d5			11.746
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-		112	C8H16	001678-91-7	81
2	2-Hexene, 2,4-dimethyl-		112	C8H16	014255-23-3	52
3	3,4-Dimethyl-2-hexene		112	C8H16	002213-37-8	52
4	3-Heptene, 3-methyl-		112	C8H16	007300-03-0	50
5	trans-3,4-Dimethyl-2-hexene		112	C8H16	019550-82-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

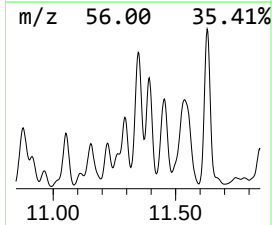
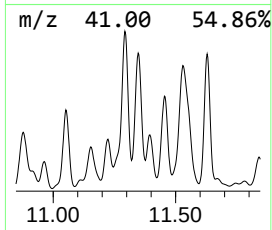
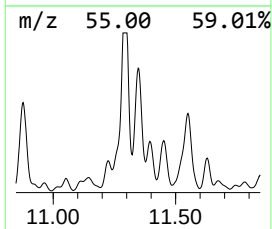
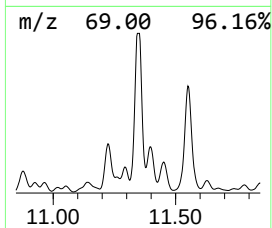
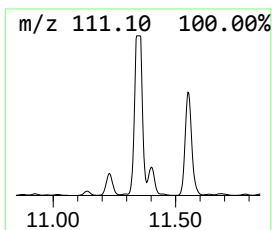
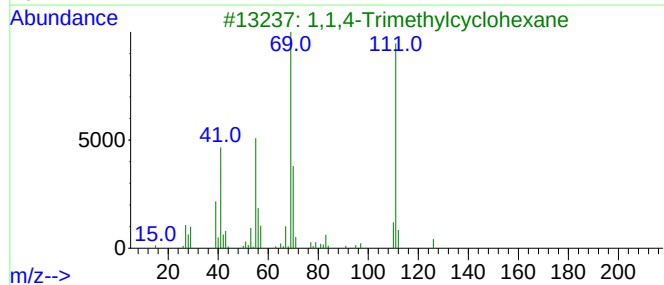
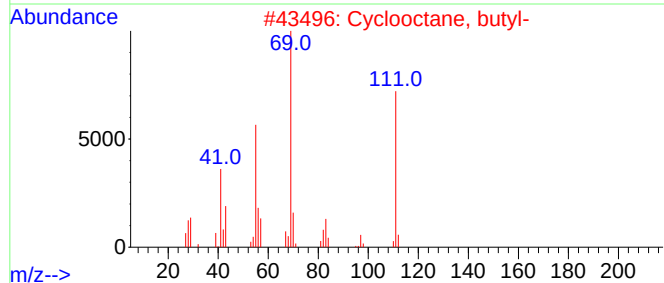
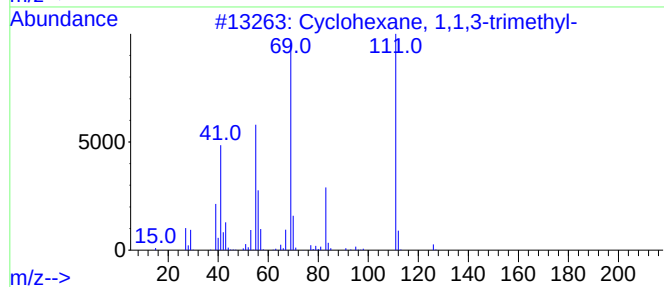
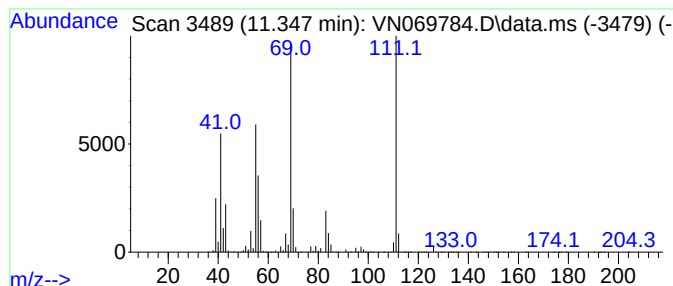
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.347	355.74 ug/l	76456700	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
2			Cyclooctane, butyl-	168	C12H24	016538-93-5	78
3			1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	59
4			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	59
5			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

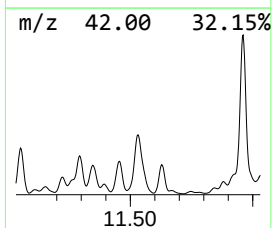
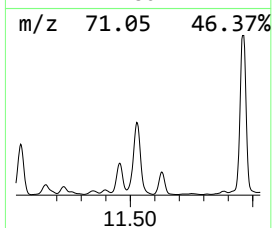
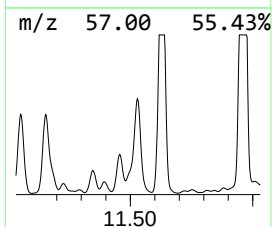
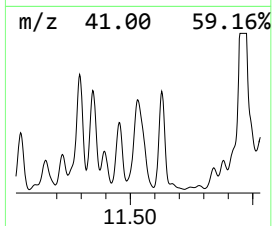
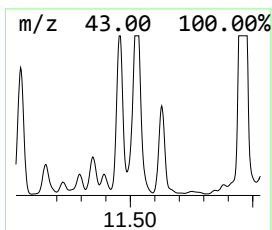
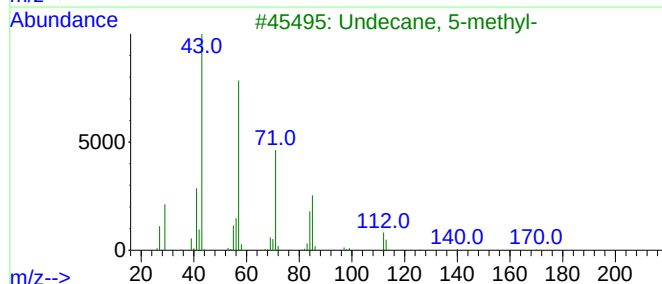
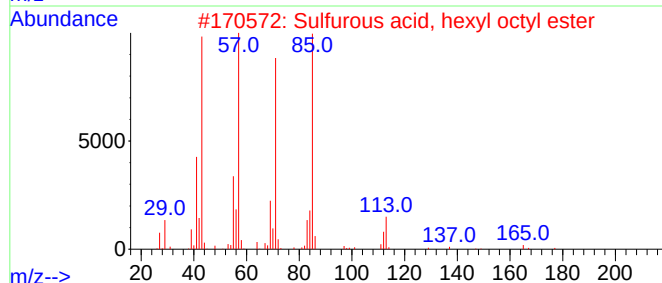
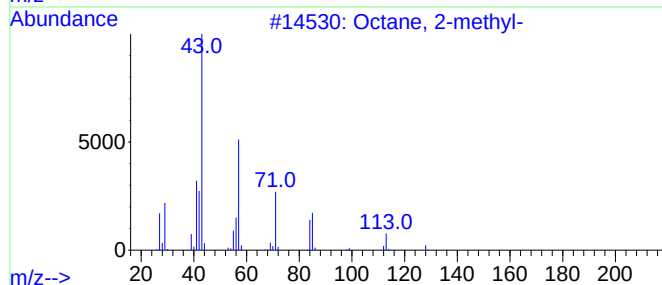
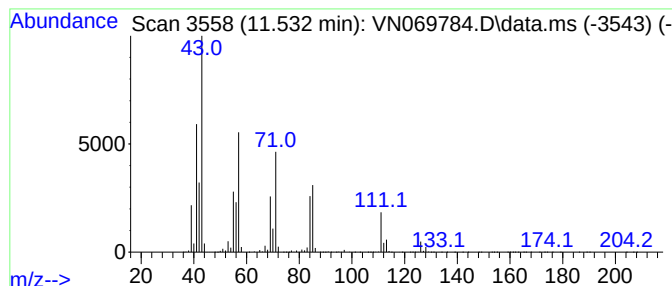
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Quant Title : SW846 8260

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

Peak Number 8 Octane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.532	597.58 ug/l	128434000	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	72
2			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	50
3			Undecane, 5-methyl-	170	C12H26	001632-70-8	50
4			Tridecane	184	C13H28	000629-50-5	50
5			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

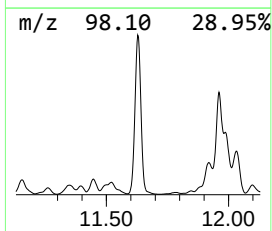
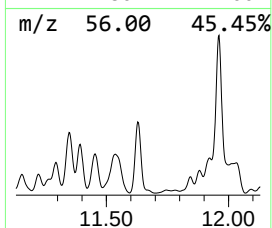
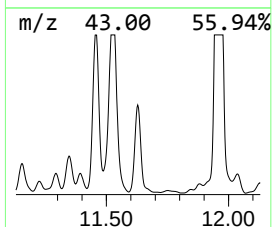
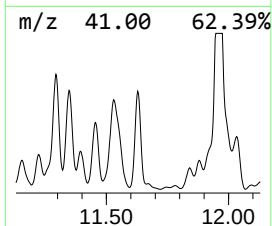
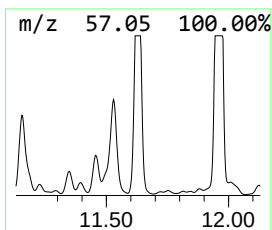
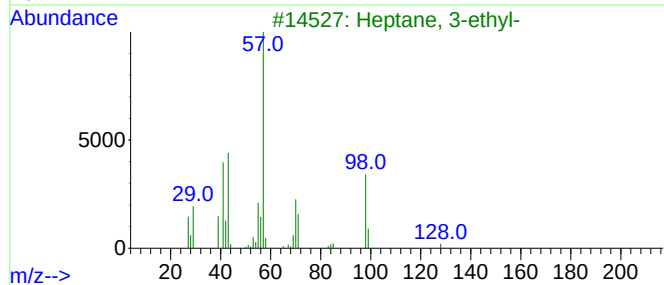
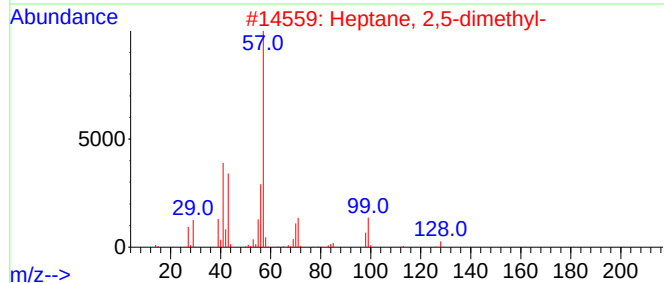
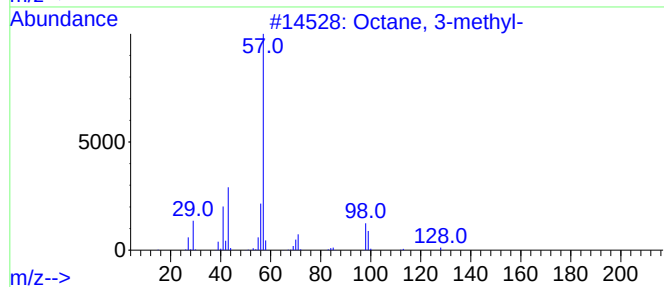
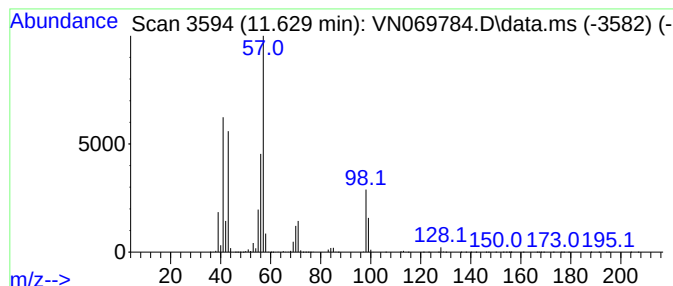
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.629	299.65 ug/l	64401100	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	74
2			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	58
3			Heptane, 3-ethyl-	128	C9H20	015869-80-4	58
4			Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	53
5			Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

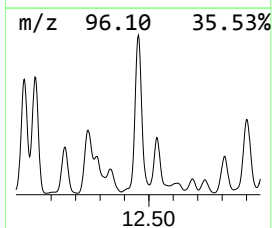
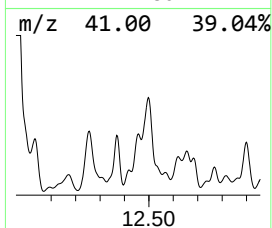
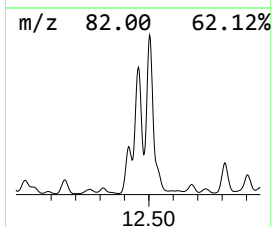
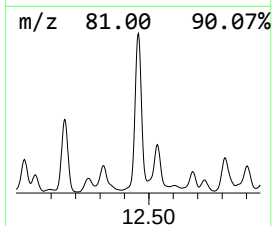
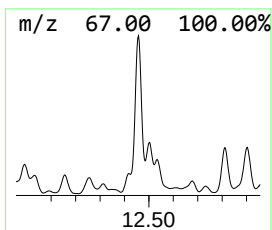
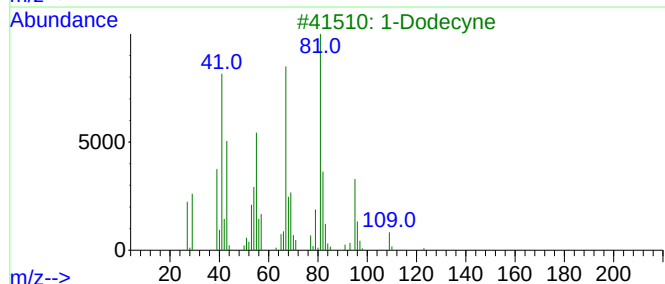
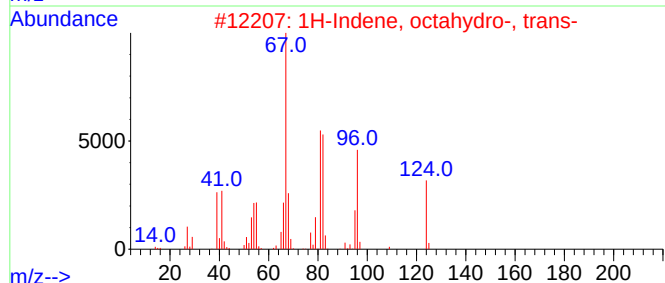
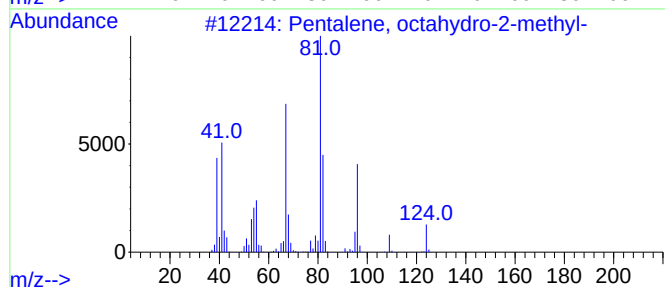
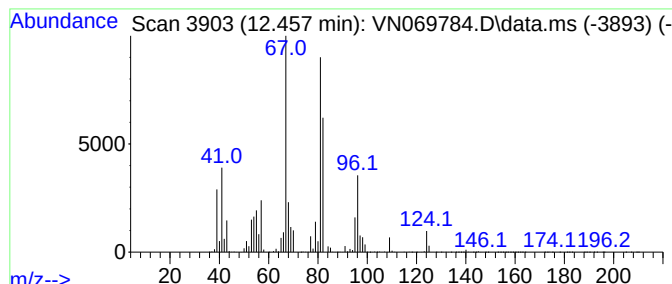
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 10 Pentalene, octahydro-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	264.77 ug/l	56904600	Chlorobenzene-d5	11.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	58
2		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	58
3		1-Dodecyne	166	C12H22	000765-03-7	50
4		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	46
5		1H-Indene, octahydro-	124	C9H16	000496-10-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069784.D
Acq On : 6 Dec 2021 15:27
Operator : JC/MD
Sample : M4932-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Heptane, 2-methyl-	10.078	923.1	ug/l	133274000	2	8.965	7218630	50.0
Heptane, 3-methyl-	10.215	552.4	ug/l	79750800	2	8.965	7218630	50.0
unknown10.626	10.626	1260.3	ug/l	270878000	3	11.746	10746100	50.0
Cyclohexane, 1,...	10.784	330.8	ug/l	71098900	3	11.746	10746100	50.0
Cyclohexane, et...	11.293	328.7	ug/l	70636900	3	11.746	10746100	50.0
Cyclohexane, 1,...	11.347	355.7	ug/l	76456700	3	11.746	10746100	50.0
Octane, 2-methyl-	11.532	597.6	ug/l	128434000	3	11.746	10746100	50.0
Octane, 3-methyl-	11.629	299.6	ug/l	64401100	3	11.746	10746100	50.0
Pentalene, octa...	12.457	264.8	ug/l	56904600	3	11.746	10746100	50.0