

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
 Data File : VN069800.D
 Acq On : 6 Dec 2021 22:19
 Operator : JC/MD
 Sample : M4932-01 10X
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM1-2DL

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: VN069800.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.112	1508	1537	1567	rBV3	359478	1122968	2.92%	0.264%
2	7.144	1901	1922	1954	rVB3	414986	1233699	3.21%	0.290%
3	8.024	2230	2250	2256	rBV2	943086	2088857	5.44%	0.492%
4	8.083	2259	2272	2292	rVB4	2794272	7468121	19.44%	1.758%
5	8.295	2330	2351	2365	rBV	1403511	3339845	8.70%	0.786%
6	8.437	2388	2404	2430	rVB	1133735	2569087	6.69%	0.605%
7	8.568	2433	2453	2466	rBV4	1081273	2620704	6.82%	0.617%
8	8.641	2468	2480	2491	rVV2	1041194	2378359	6.19%	0.560%
9	8.705	2492	2504	2529	rVB2	1661478	3873328	10.08%	0.912%
10	8.826	2532	2549	2582	rVB	5268565	10923927	28.44%	2.571%
11	8.968	2585	2602	2617	rBV	2838149	5820503	15.15%	1.370%
12	9.459	2752	2785	2801	rBV	8952018	22506861	58.59%	5.298%
13	9.641	2826	2853	2866	rBV2	938858	1956544	5.09%	0.461%
14	9.732	2867	2887	2906	rVB	1430198	3043991	7.92%	0.716%
15	9.874	2923	2940	2960	rBV2	1739751	3485545	9.07%	0.820%
16	10.019	2980	2994	3003	rBV2	633435	1205557	3.14%	0.284%
17	10.078	3003	3016	3047	rVB	5784844	12599452	32.80%	2.966%
18	10.215	3048	3067	3094	rVB4	3098766	7326775	19.07%	1.725%
19	10.338	3095	3113	3115	rBV4	282157	492009	1.28%	0.116%
20	10.440	3134	3151	3162	rBV2	10613543	21384312	55.67%	5.033%
21	10.564	3186	3197	3203	rBV	602746	1026500	2.67%	0.242%
22	10.623	3204	3219	3237	rVB	15131331	27209286	70.84%	6.404%
23	10.741	3254	3263	3268	rBV2	742458	1075379	2.80%	0.253%
24	10.784	3269	3279	3296	rVB	3615332	6689973	17.42%	1.575%
25	10.878	3297	3314	3327	rBV	2262531	5108710	13.30%	1.202%
26	10.966	3338	3347	3359	rVB	953924	1584276	4.12%	0.373%
27	11.052	3359	3379	3392	rBV	2727627	4922634	12.82%	1.159%
28	11.154	3407	3417	3432	rVB	1068966	2008681	5.23%	0.473%
29	11.224	3433	3443	3451	rBV4	1258471	2135443	5.56%	0.503%
30	11.293	3459	3469	3479	rVB	4654267	7140670	18.59%	1.681%
31	11.347	3479	3489	3500	rVV	4339060	7153349	18.62%	1.684%
32	11.395	3501	3507	3517	rVB3	1312522	1976862	5.15%	0.465%
33	11.454	3518	3529	3540	rBV3	3083534	5088443	13.25%	1.198%
34	11.529	3543	3557	3582	rVB5	4460513	12858202	33.48%	3.026%
35	11.629	3582	3594	3606	rBV	4250901	6842926	17.82%	1.611%
36	11.747	3624	3638	3659	rBV	4858304	8849593	23.04%	2.083%

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37	11.840	3660	3673	3681	rBV4	1431797	2714154	7.07%	0.639%
38	11.881	3682	3688	3695	rBV	695114	807541	2.10%	0.190%
39	11.958	3697	3717	3737	rBV2	19411466	36760752	95.70%	8.652%
40	12.092	3758	3767	3773	rBV4	295187	485893	1.26%	0.114%
41	12.259	3811	3829	3833	rBV4	3983827	8017257	20.87%	1.887%
42	12.369	3861	3870	3880	rVB	3778810	5775385	15.04%	1.359%
43	12.457	3881	3903	3909	rBV3	4202317	9184246	23.91%	2.162%
44	12.624	3956	3965	3969	rBV5	1232083	1874578	4.88%	0.441%
45	12.733	3996	4006	4014	rBV	3984791	6411130	16.69%	1.509%
46	12.900	4059	4068	4082	rVB4	2785046	5088012	13.25%	1.198%
47	12.983	4084	4099	4105	rBV7	2138918	4171870	10.86%	0.982%
48	13.047	4113	4123	4139	rVB	22675983	38410999	100.00%	9.041%
49	13.112	4140	4147	4158	rVB2	1916045	2943891	7.66%	0.693%
50	13.222	4172	4188	4203	rBV5	2202100	7156861	18.63%	1.685%
51	13.286	4204	4212	4228	rVB4	4116150	6784853	17.66%	1.597%
52	13.369	4231	4243	4255	rBV	6223872	10419978	27.13%	2.453%
53	13.565	4303	4316	4325	rBV6	3553384	6929801	18.04%	1.631%
54	13.608	4327	4332	4341	rVB3	1360553	1749826	4.56%	0.412%
55	13.675	4348	4357	4363	rBV2	5035081	7622392	19.84%	1.794%
56	13.868	4423	4429	4437	rVB	1439037	1775438	4.62%	0.418%
57	13.914	4439	4446	4463	rVB4	1324976	2074370	5.40%	0.488%
58	13.994	4465	4476	4488	rBV	15104072	22790734	59.33%	5.364%
59	14.217	4552	4559	4570	rVB	1869537	2675860	6.97%	0.630%
60	14.324	4589	4599	4610	rVB3	1283435	2077424	5.41%	0.489%
61	14.622	4703	4710	4719	rVB3	926241	1179514	3.07%	0.278%
62	14.670	4720	4728	4742	rVB5	777964	1364944	3.55%	0.321%
63	14.847	4786	4794	4807	rVB4	1741979	2775007	7.22%	0.653%
64	14.917	4809	4820	4837	rVB3	1633079	3445827	8.97%	0.811%
65	15.201	4917	4926	4954	rVB5	387511	1058798	2.76%	0.249%
66	15.303	4955	4964	4984	rVB4	274492	569756	1.48%	0.134%
67	15.507	5029	5040	5062	rVB2	326469	648576	1.69%	0.153%

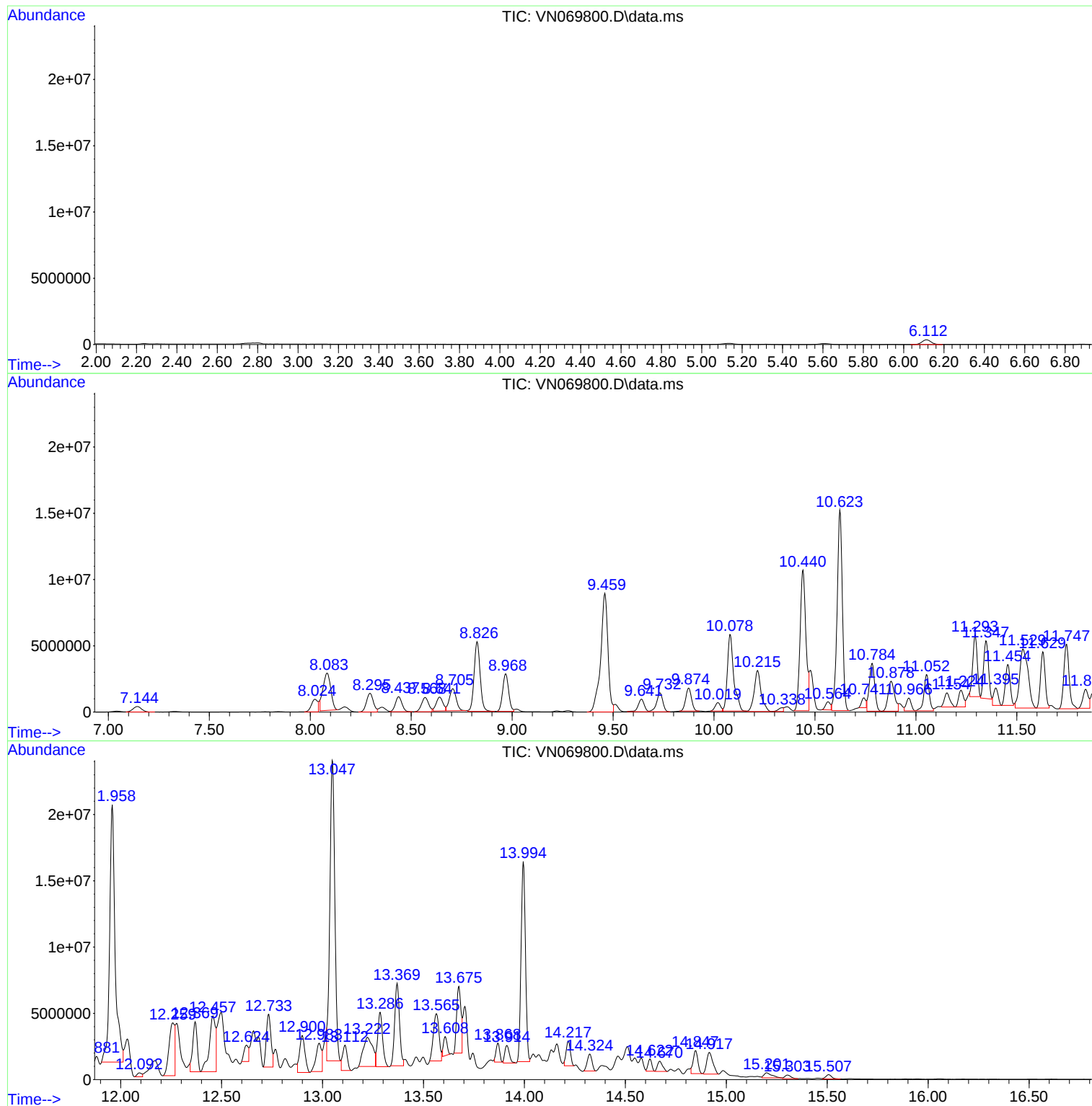
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Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

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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Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

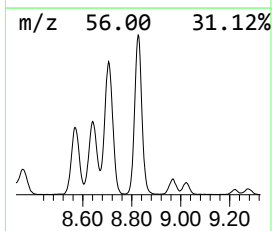
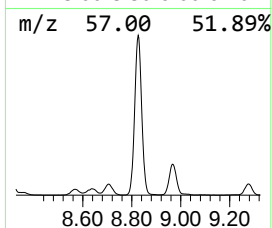
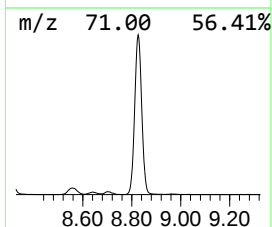
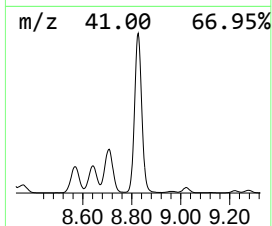
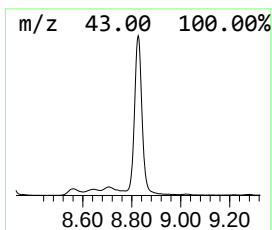
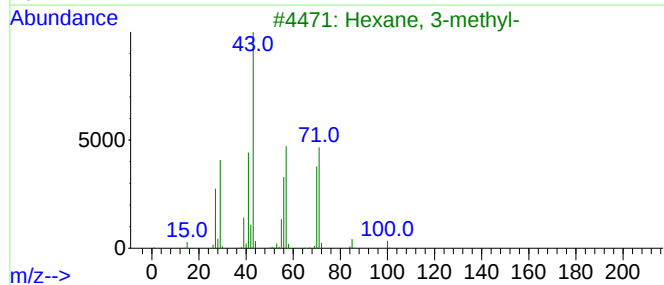
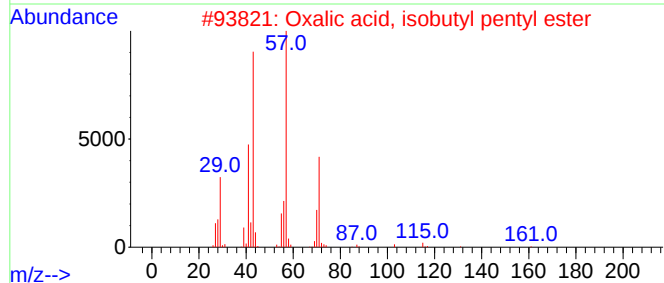
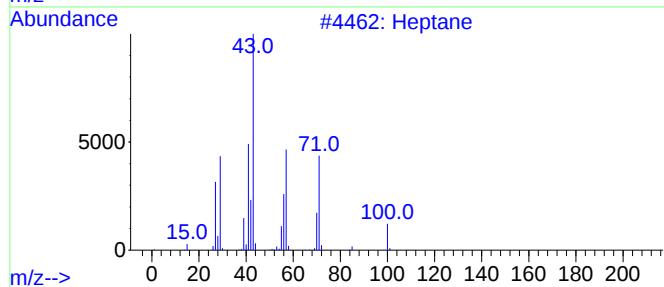
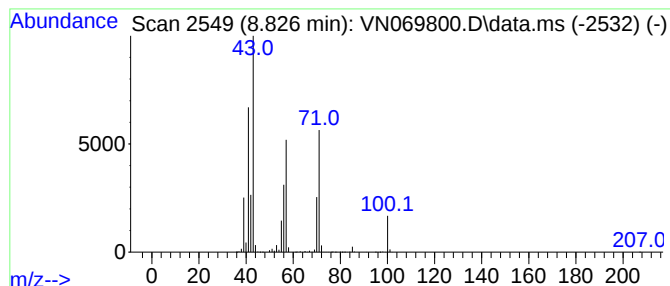
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	93.84 ug/l	10923900	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, 3-methyl-	100	C7H16	000589-34-4	42
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38



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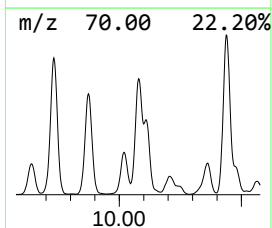
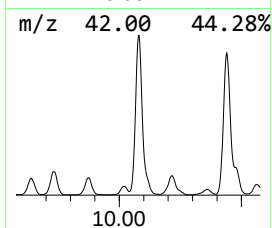
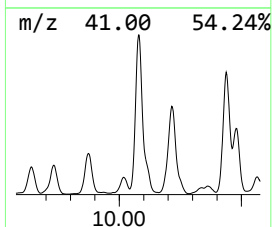
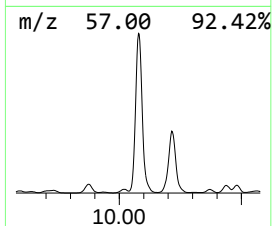
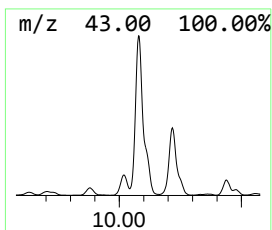
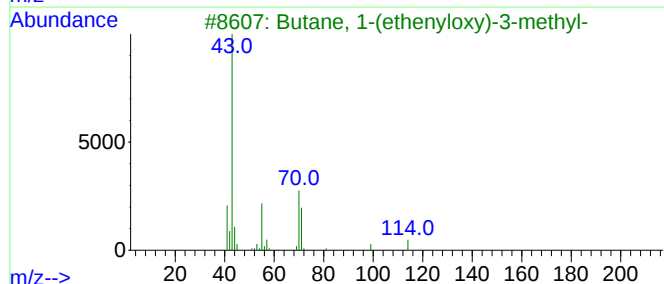
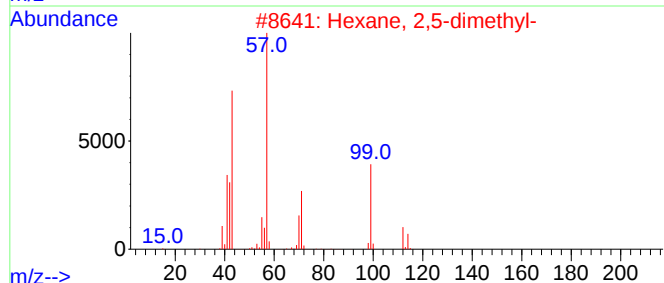
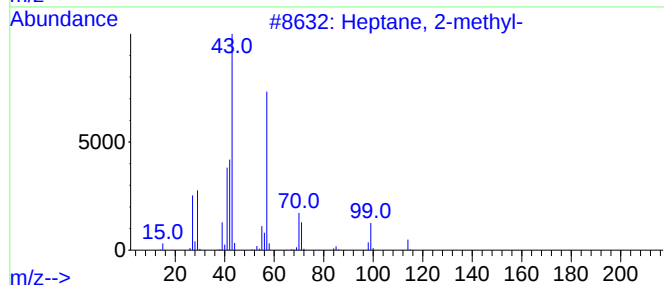
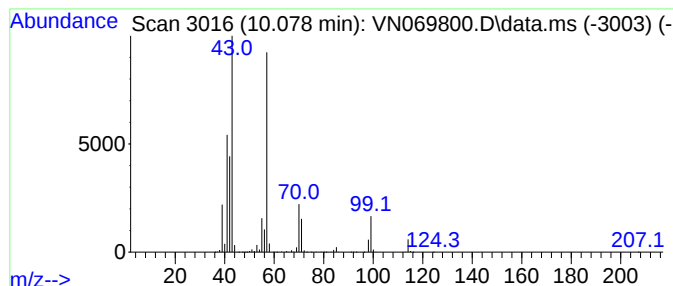
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.078	108.23 ug/l	12599500	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	95
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	83
3			Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	38
4			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	38
5			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	35



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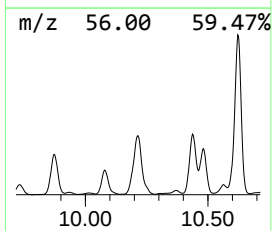
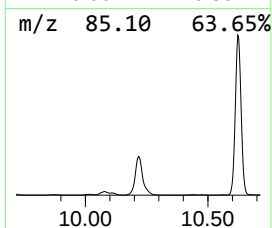
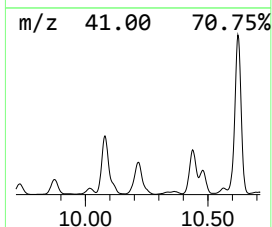
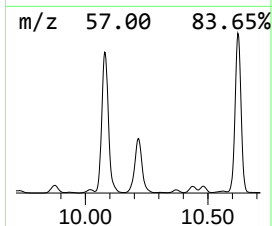
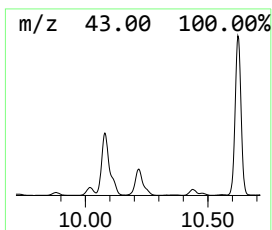
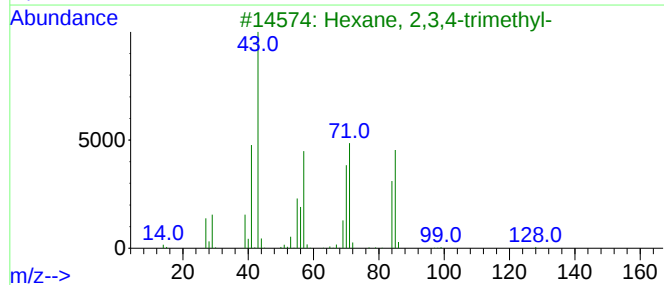
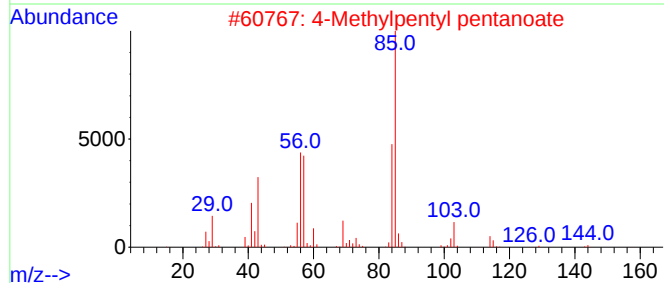
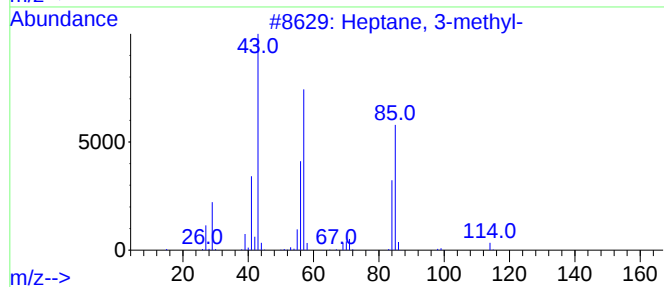
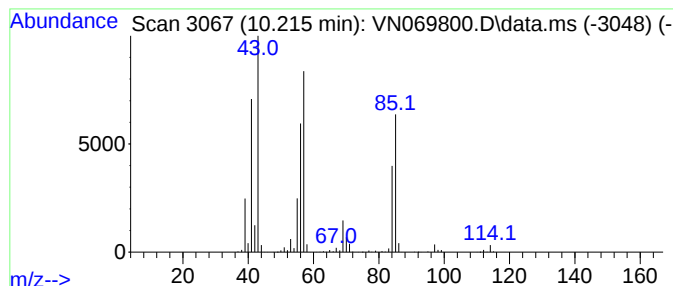
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	62.94 ug/l	7326780	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	86
2			4-Methylpentyl pentanoate	186	C11H22O2	035852-47-2	64
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	52
5			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	50



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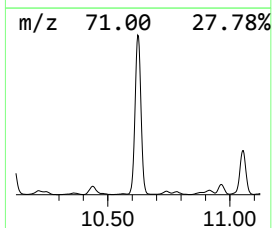
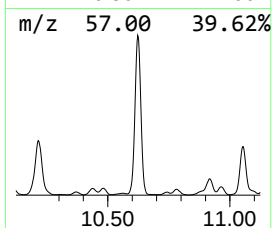
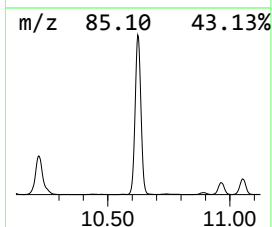
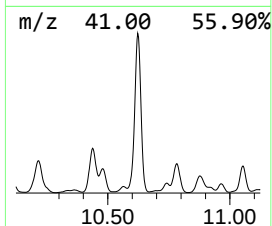
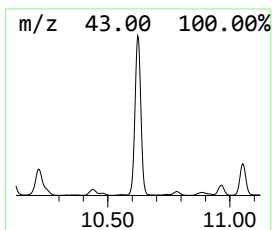
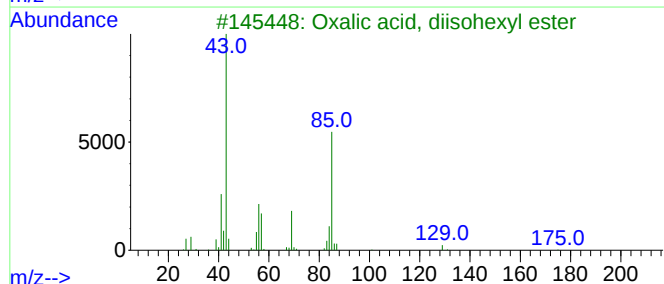
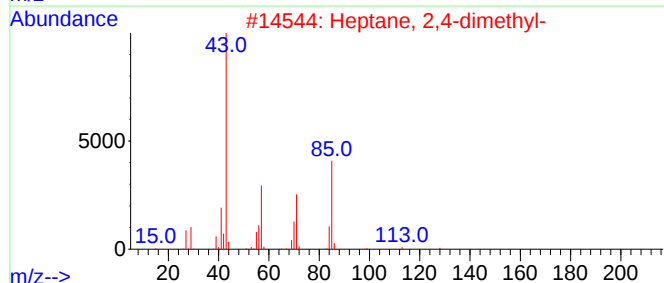
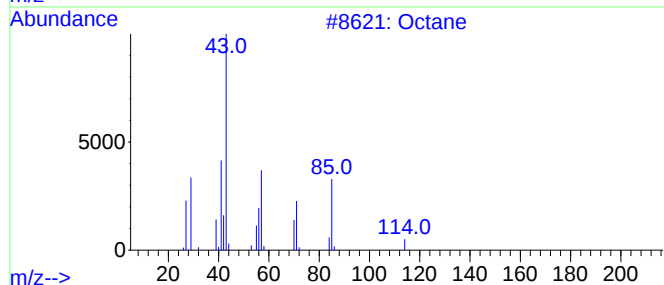
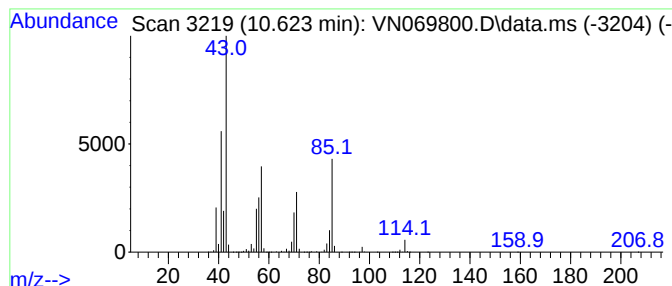
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 Octane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.623	153.73 ug/l	27209300	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	94
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
3			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	59
4			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53
5			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

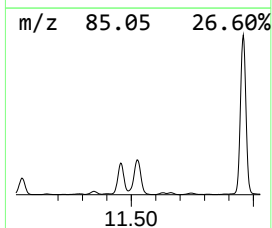
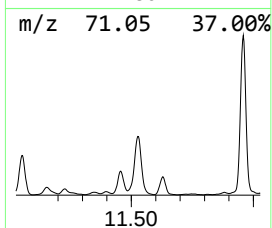
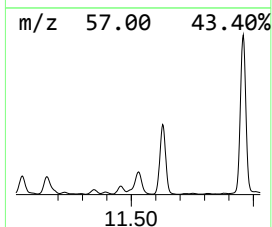
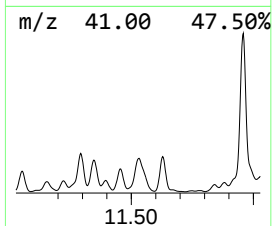
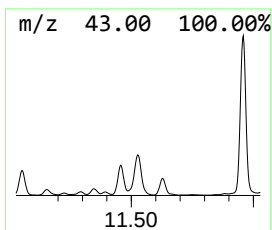
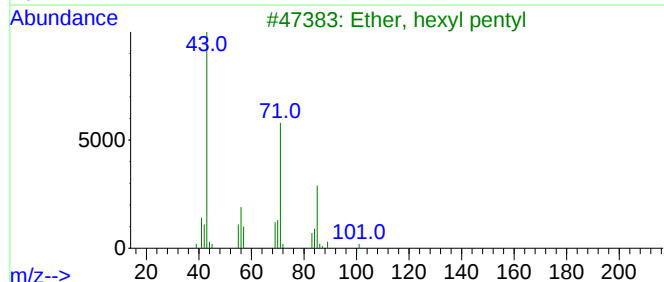
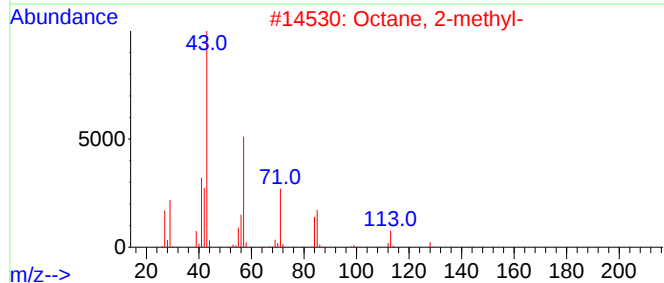
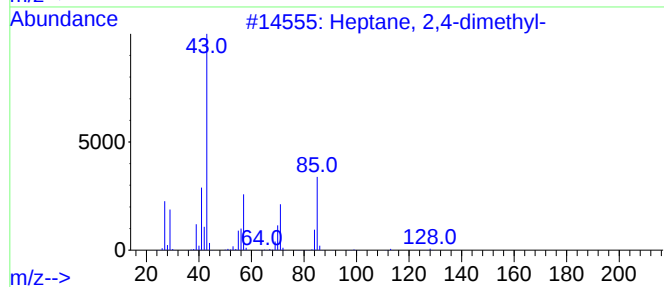
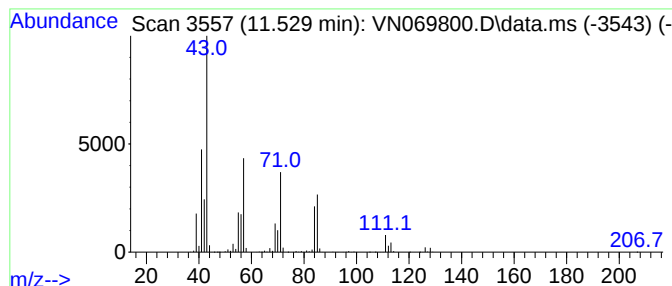
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Quant Title : SW846 8260

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

Peak Number 5 Heptane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	72.65 ug/l	12858200	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	58
2			Octane, 2-methyl-	128	C9H20	003221-61-2	58
3			Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
5			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

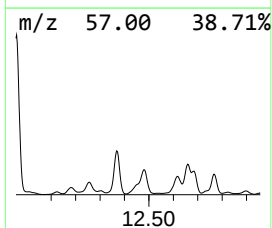
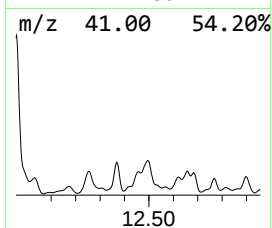
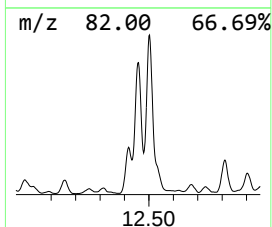
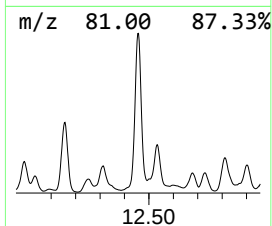
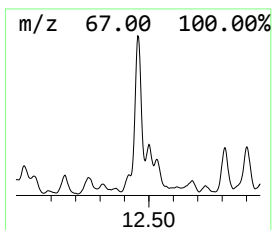
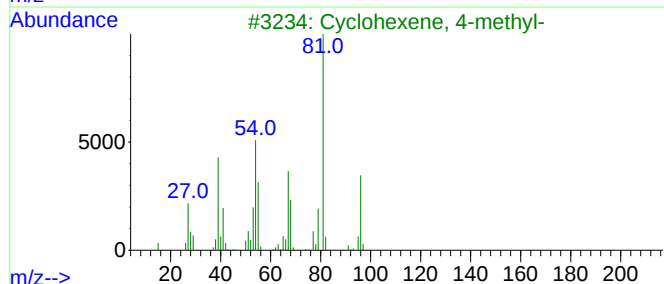
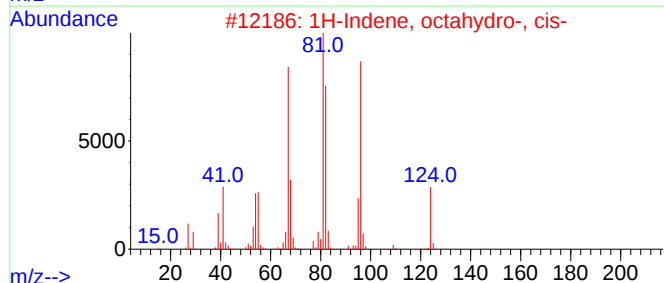
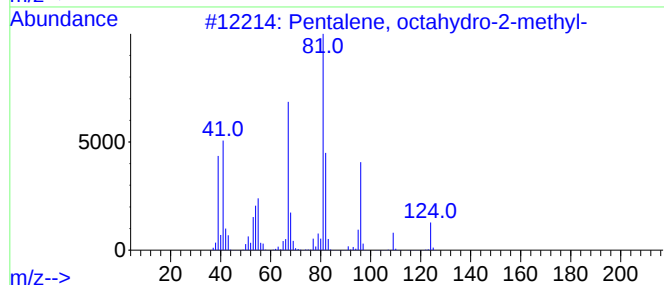
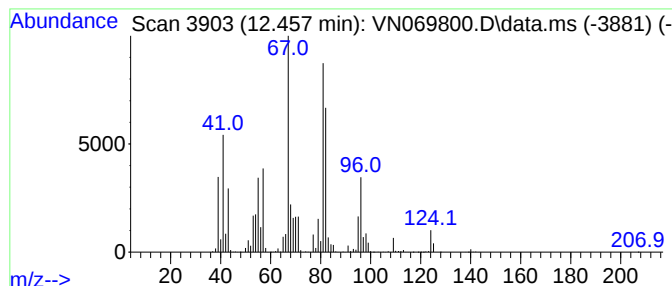
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ClientSampleId :
DRUM1-2DL

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Quant Title : SW846 8260

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

Peak Number 6 Pentalene, octahydro-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.457	51.89 ug/l	9184250	Chlorobenzene-d5			11.746
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-		124	C9H16	003868-64-2	70
2	1H-Indene, octahydro-, cis-		124	C9H16	004551-51-3	58
3	Cyclohexene, 4-methyl-		96	C7H12	000591-47-9	55
4	1H-Indene, octahydro-		124	C9H16	000496-10-6	53
5	Cyclohexene,3-propyl-		124	C9H16	003983-06-0	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

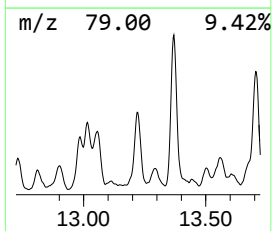
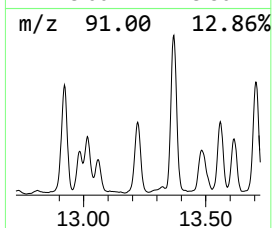
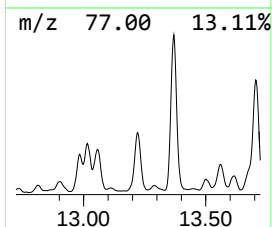
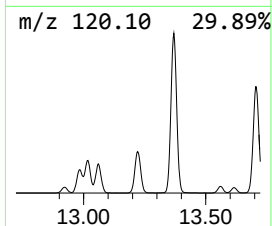
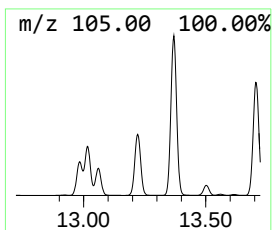
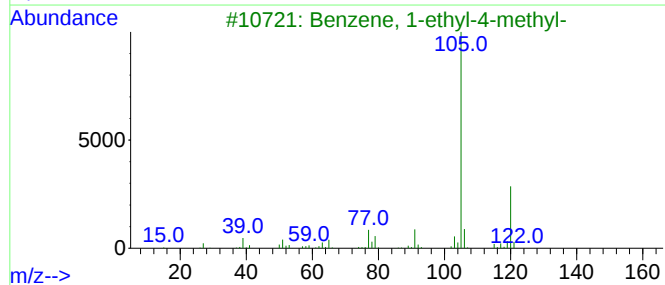
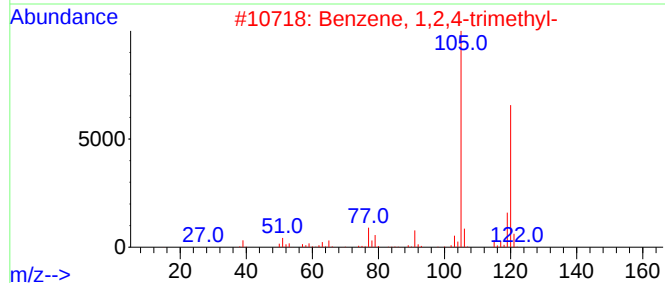
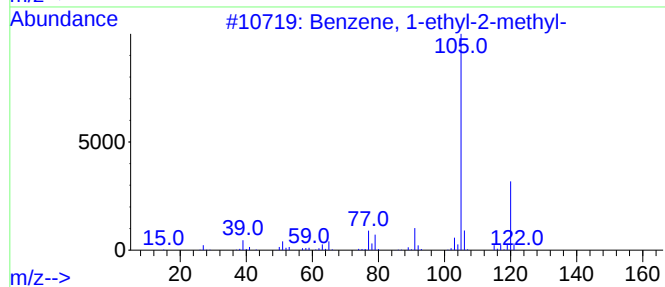
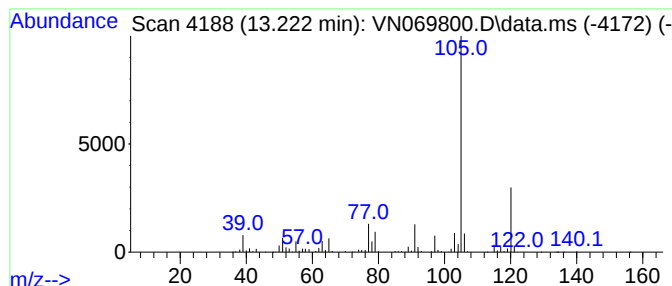
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	46.95 ug/l	7156860	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

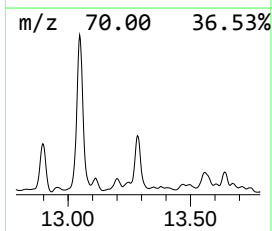
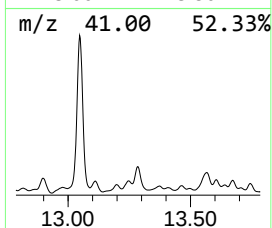
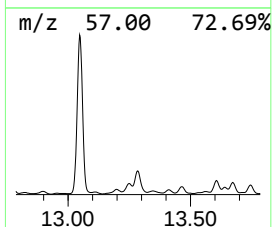
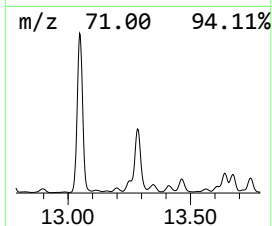
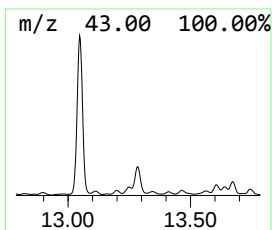
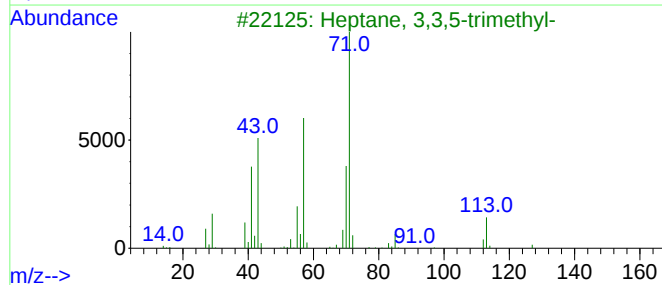
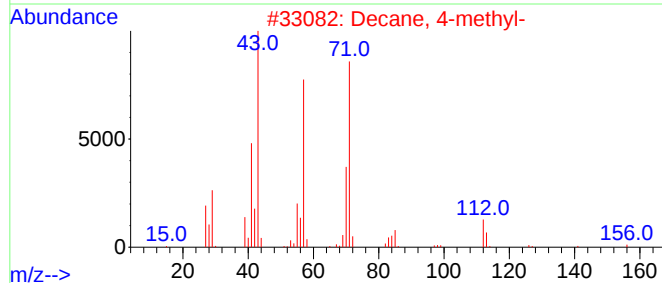
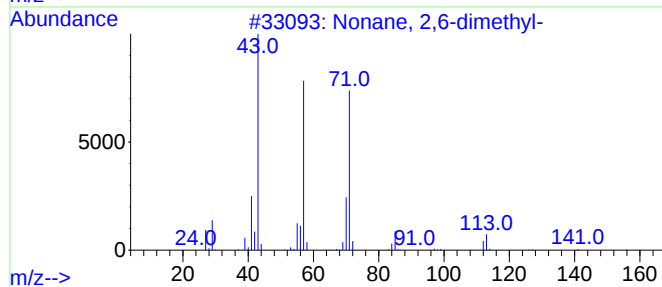
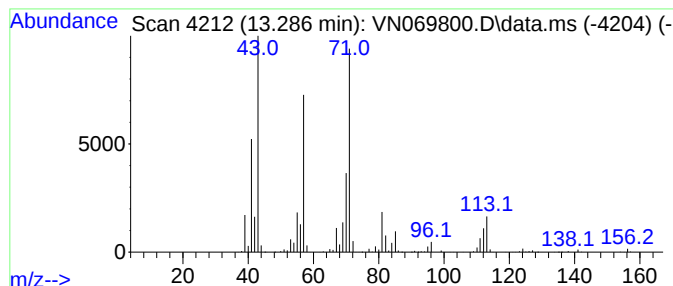
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Quant Title : SW846 8260

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

Peak Number 8 Nonane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	44.51 ug/l	6784850	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	90
2			Decane, 4-methyl-	156	C11H24	002847-72-5	87
3			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	64
4			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	64
5			Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

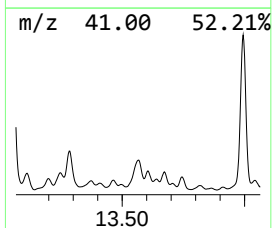
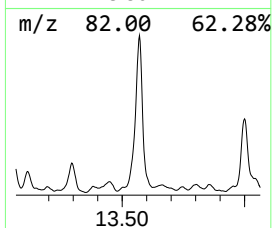
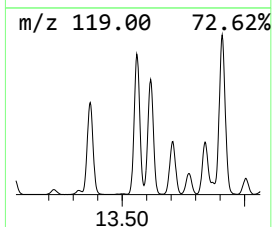
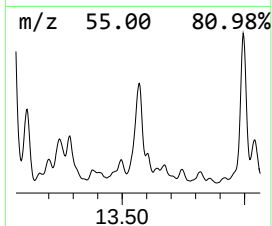
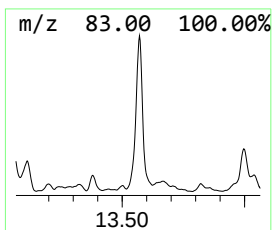
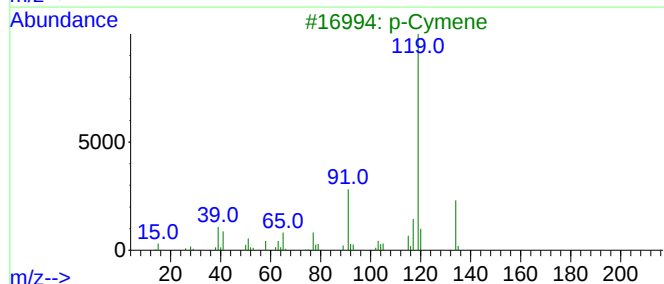
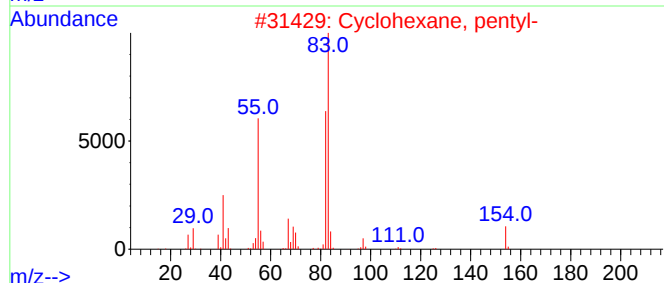
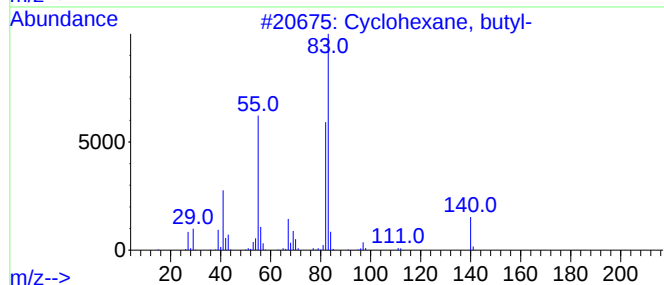
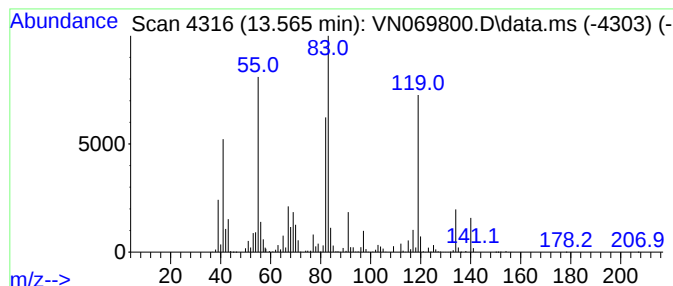
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.565	45.46 ug/l	6929800	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	70
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
3			p-Cymene	134	C10H14	000099-87-6	59
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	56
5			1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

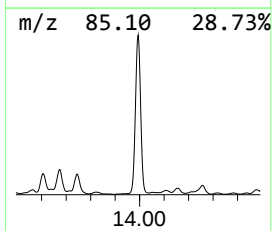
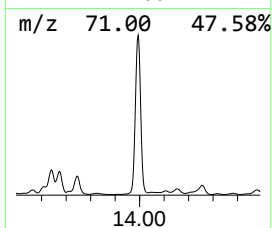
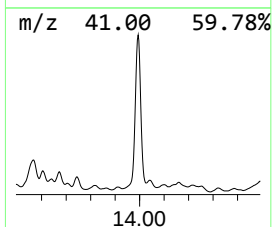
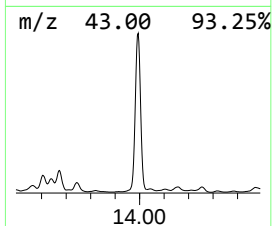
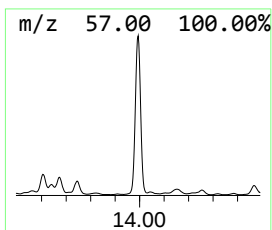
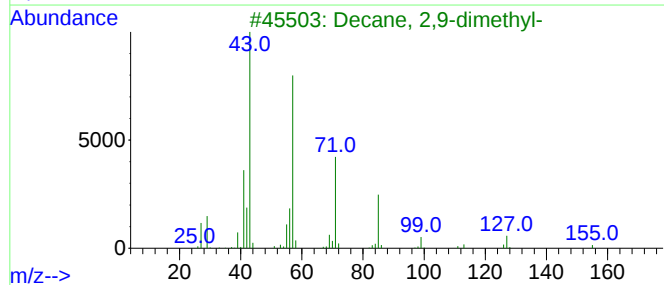
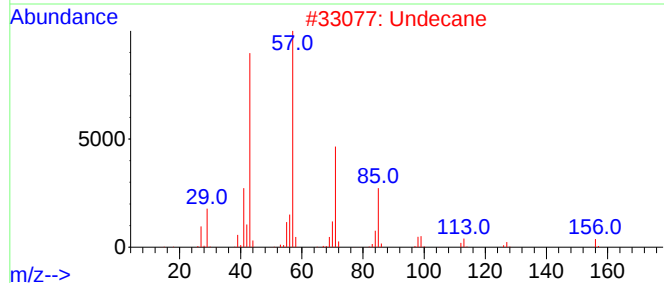
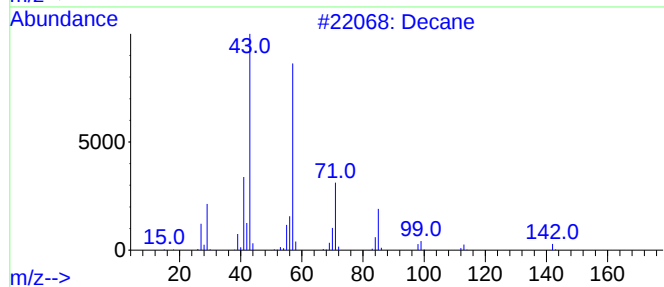
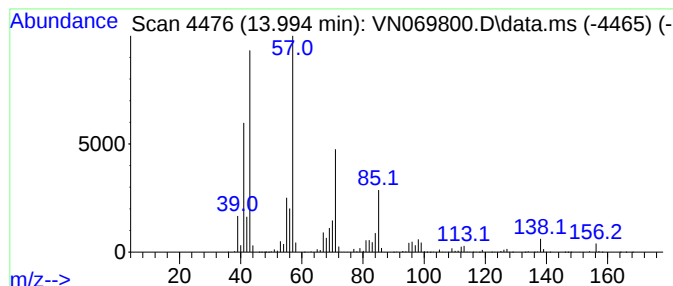
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Quant Title : SW846 8260

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

Peak Number 10 Decane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	149.50 ug/l	22790700	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	80
2			Undecane	156	C11H24	001120-21-4	80
3			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
4			Tridecane	184	C13H28	000629-50-5	59
5			Heptadecane	240	C17H36	000629-78-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069800.D
Acq On : 6 Dec 2021 22:19
Operator : JC/MD
Sample : M4932-01 10X
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM1-2DL

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
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Heptane, 2-methyl-	10.078	108.2	ug/l	12599500	2	8.968	5820500	50.0
Heptane, 3-methyl-	10.215	62.9	ug/l	7326780	2	8.968	5820500	50.0
Octane	10.623	153.7	ug/l	27209300	3	11.746	8849590	50.0
Heptane, 2,4-di...	11.529	72.7	ug/l	12858200	3	11.746	8849590	50.0
Pentalene, octa...	12.457	51.9	ug/l	9184250	3	11.746	8849590	50.0
Benzene, 1-ethy...	13.222	47.0	ug/l	7156860	4	13.675	7622390	50.0
Nonane, 2,6-dim...	13.286	44.5	ug/l	6784850	4	13.675	7622390	50.0
Cyclohexane, bu...	13.565	45.5	ug/l	6929800	4	13.675	7622390	50.0
Decane	13.994	149.5	ug/l	22790700	4	13.675	7622390	50.0