

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
 Data File : VN067456.D
 Acq On : 23 Jun 2021 14:50
 Operator : JC/MD
 Sample : M2802-01
 Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30759

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\82N061421W.M
 Title : SW846 8260

Signal : TIC: VN067456.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.085	1102	1154	1194	rBV3	382188	1838459	1.73%	0.272%
2	6.085	1494	1527	1562	rBV2	629678	1956657	1.85%	0.289%
3	7.125	1896	1915	1937	rVB2	626679	1792964	1.69%	0.265%
4	7.831	2159	2178	2200	rVB2	480728	1239444	1.17%	0.183%
5	8.059	2226	2263	2287	rBV3	4647340	13759084	12.98%	2.035%
6	8.163	2287	2302	2326	rVV	1692123	4322781	4.08%	0.639%
7	8.287	2327	2348	2387	rVV	6120969	14840122	14.00%	2.194%
8	8.448	2388	2408	2427	rVV3	598739	1662906	1.57%	0.246%
9	8.555	2428	2448	2456	rVV5	1156171	2876822	2.71%	0.425%
10	8.609	2458	2468	2490	rVV	2541526	6981346	6.58%	1.032%
11	8.700	2490	2502	2525	rVB2	771133	1811990	1.71%	0.268%
12	8.821	2526	2547	2580	rBV	7125851	14622496	13.79%	2.162%
13	8.965	2582	2601	2632	rBV3	967015	2579778	2.43%	0.381%
14	9.453	2750	2783	2796	rBV	3738045	9276430	8.75%	1.372%
15	9.507	2797	2803	2820	rVB2	939573	1705457	1.61%	0.252%
16	9.636	2841	2851	2865	rVB2	691424	1307663	1.23%	0.193%
17	9.880	2925	2942	2963	rVB3	1732548	3674679	3.47%	0.543%
18	10.014	2980	2992	3005	rVB2	2094698	3936358	3.71%	0.582%
19	10.078	3005	3016	3045	rVB2	1988188	5074562	4.79%	0.750%
20	10.215	3046	3067	3093	rBV2	1821997	4360615	4.11%	0.645%
21	10.368	3113	3124	3136	rVB3	650831	1238824	1.17%	0.183%
22	10.440	3137	3151	3160	rBV3	2244520	4479488	4.22%	0.662%
23	10.510	3161	3177	3204	rVV3	53648894	106029991	100.00%	15.679%
24	10.623	3206	3219	3235	rVB	4107524	7703539	7.27%	1.139%
25	10.784	3268	3279	3296	rVB2	681422	1329912	1.25%	0.197%
26	10.878	3296	3314	3336	rBV8	1004951	2642874	2.49%	0.391%
27	11.052	3360	3379	3392	rBV2	1003824	1829711	1.73%	0.271%
28	11.154	3407	3417	3433	rVB	799341	1533809	1.45%	0.227%
29	11.224	3434	3443	3451	rBV4	663890	1131347	1.07%	0.167%
30	11.293	3461	3469	3479	rVB	1272092	1962693	1.85%	0.290%
31	11.347	3479	3489	3502	rVB	1425776	2553301	2.41%	0.378%
32	11.454	3518	3529	3538	rBV4	1088080	1808549	1.71%	0.267%
33	11.529	3539	3557	3582	rVB6	4557975	11717321	11.05%	1.733%
34	11.629	3582	3594	3607	rBV	3863115	6373293	6.01%	0.942%
35	11.749	3628	3639	3650	rBV	925551	1581616	1.49%	0.234%
36	11.848	3663	3676	3695	rBV	4484894	8986905	8.48%	1.329%

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37	11.956	3696	3716	3738	rBV4	27852338	56335046	53.13%	8.331%
38	12.178	3788	3799	3811	rVB4	1288818	2438707	2.30%	0.361%
39	12.283	3812	3838	3855	rBV3	8776155	25088101	23.66%	3.710%
40	12.369	3862	3870	3881	rVB	3848254	6037321	5.69%	0.893%
41	12.455	3881	3902	3906	rBV8	2595923	5771317	5.44%	0.853%
42	12.583	3941	3950	3954	rBV3	1294526	2035105	1.92%	0.301%
43	12.739	4001	4008	4011	rBV5	1072056	1284157	1.21%	0.190%
44	12.768	4012	4019	4030	rVB	4576915	6586988	6.21%	0.974%
45	12.921	4062	4076	4086	rVB	3688694	7763506	7.32%	1.148%
46	12.986	4087	4100	4108	rBV	12138016	21635465	20.41%	3.199%
47	13.053	4115	4125	4140	rVB2	36443959	61573695	58.07%	9.105%
48	13.112	4142	4147	4157	rVB2	2588748	3496740	3.30%	0.517%
49	13.157	4158	4164	4172	rBV3	1311798	1710548	1.61%	0.253%
50	13.224	4174	4189	4204	rBV2	4559757	11804027	11.13%	1.746%
51	13.286	4206	4212	4228	rVB4	4728142	7791175	7.35%	1.152%
52	13.372	4231	4244	4256	rBV	22081429	36525576	34.45%	5.401%
53	13.565	4305	4316	4326	rBV5	5755587	10593526	9.99%	1.567%
54	13.608	4327	4332	4340	rVB3	2717889	3309317	3.12%	0.489%
55	13.675	4351	4357	4362	rBV2	2513089	3269884	3.08%	0.484%
56	13.707	4363	4369	4378	rVV	5938156	8805987	8.31%	1.302%
57	13.747	4380	4384	4396	rVB2	3310127	3999487	3.77%	0.591%
58	13.873	4423	4431	4439	rBV3	6093464	9043931	8.53%	1.337%
59	13.914	4440	4446	4466	rVB5	6607033	14094944	13.29%	2.084%
60	13.997	4466	4477	4489	rBV2	19705221	31110411	29.34%	4.600%
61	14.219	4552	4560	4571	rVB	6202446	9613119	9.07%	1.422%
62	14.329	4590	4601	4612	rVB3	5401342	8978124	8.47%	1.328%
63	14.512	4660	4669	4676	rBV6	4744270	7359384	6.94%	1.088%
64	14.581	4689	4695	4703	rVB	4235111	5539945	5.22%	0.819%
65	14.624	4704	4711	4717	rBV2	2591565	3609428	3.40%	0.534%
66	14.726	4743	4749	4756	rBV6	1284472	1883303	1.78%	0.278%
67	14.815	4773	4782	4787	rBV3	3219383	5346521	5.04%	0.791%
68	14.930	4810	4825	4837	rBV5	6502839	16229767	15.31%	2.400%
69	15.088	4877	4884	4898	rVB2	2537653	4225823	3.99%	0.625%
70	16.338	5338	5350	5369	rVB5	1650616	4166977	3.93%	0.616%
71	16.620	5444	5455	5489	rVB	1809977	4667750	4.40%	0.690%

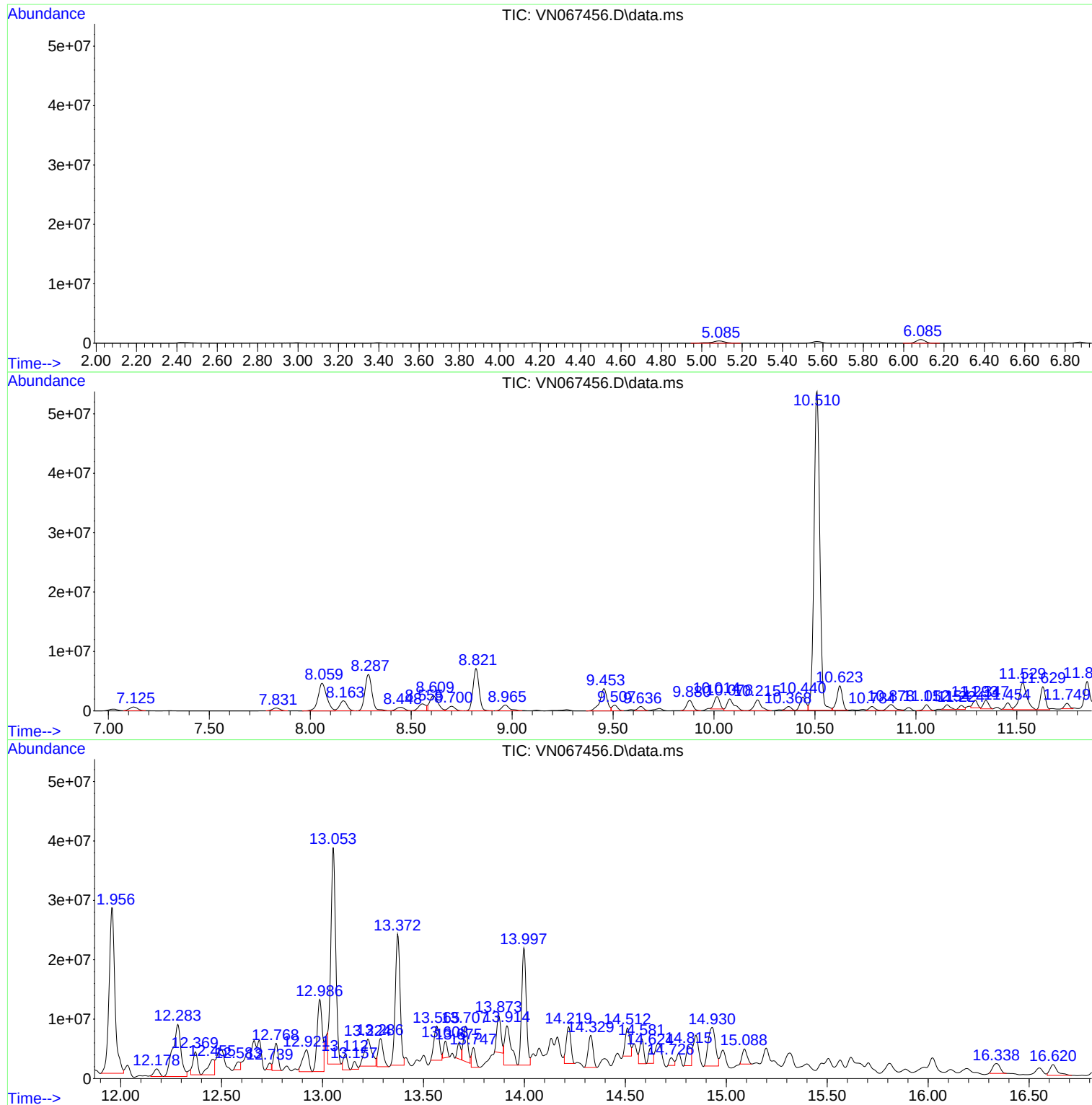
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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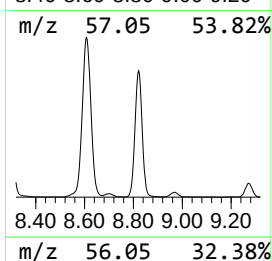
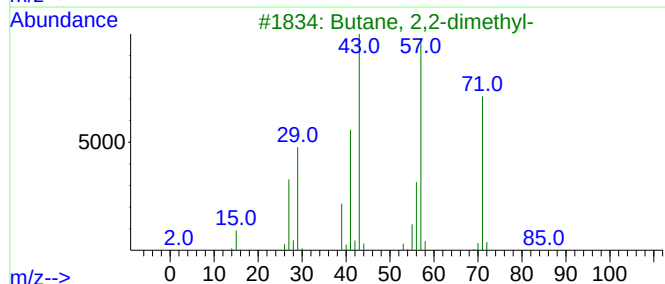
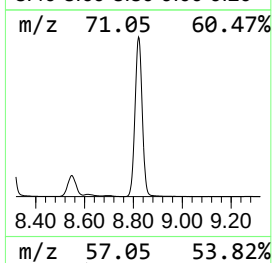
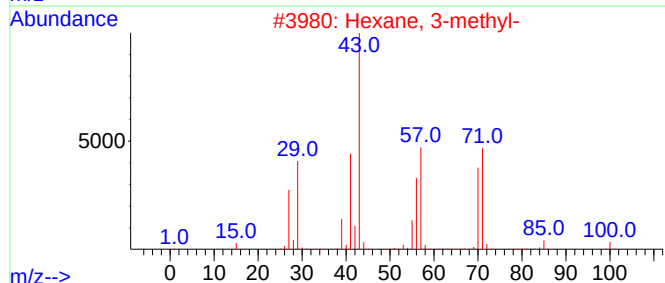
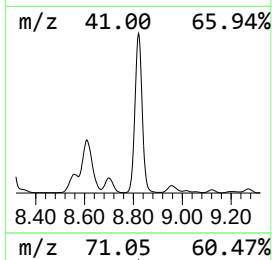
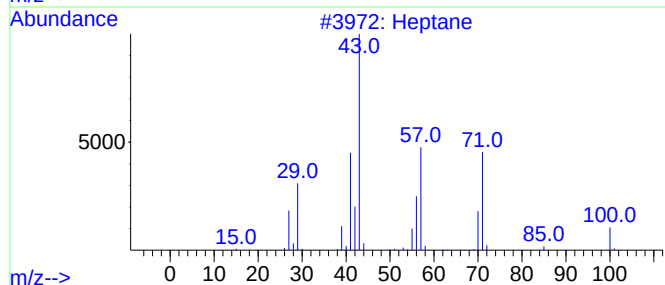
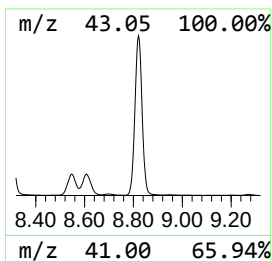
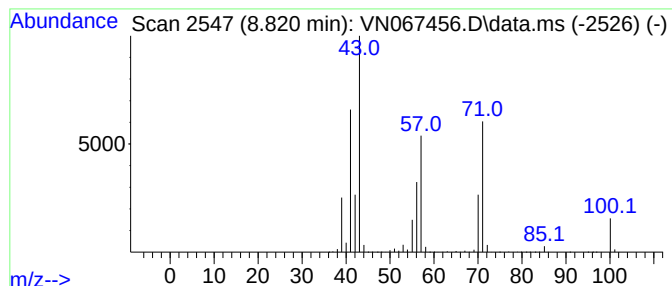
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.820	283.41 ug/l	14622500	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	94
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	42
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5			3-Hexanone	100	C6H12O	000589-38-8	35



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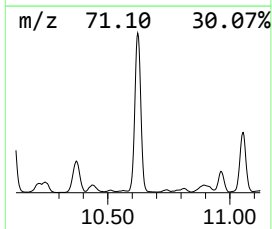
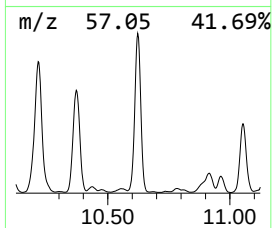
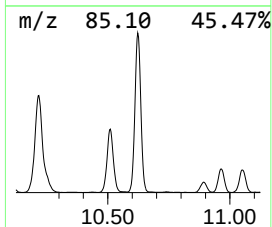
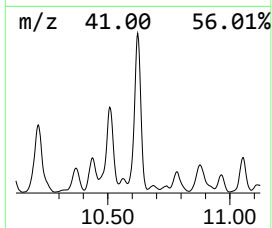
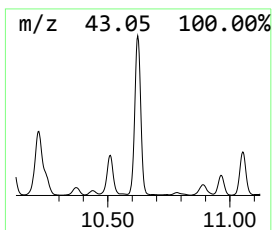
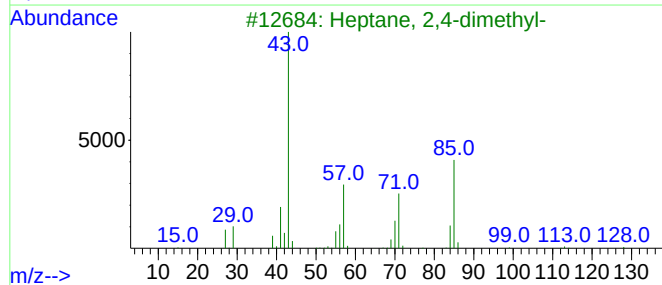
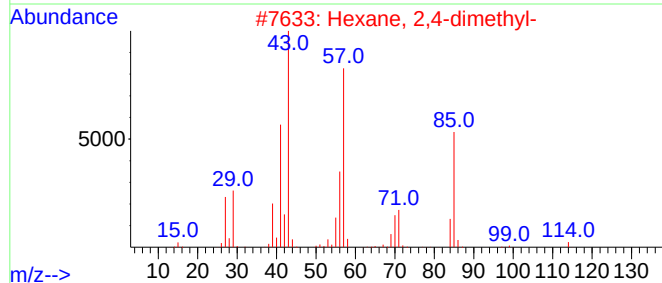
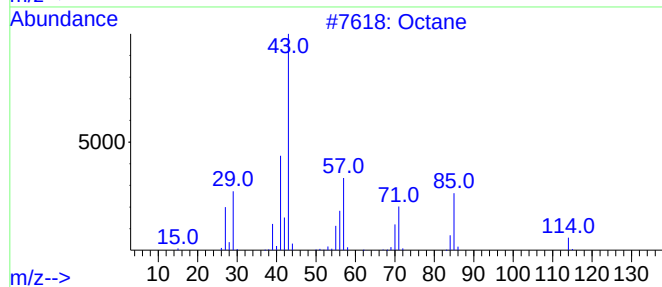
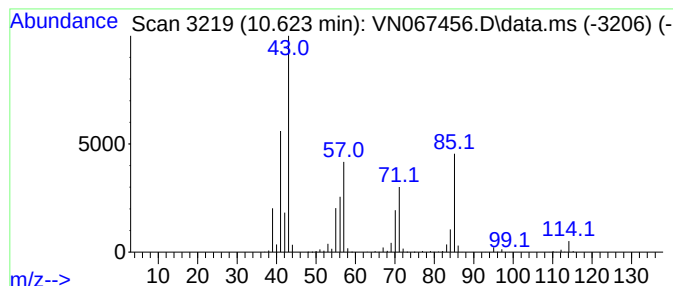
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.623	243.53 ug/l	7703540	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	94
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
4			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	72
5			Hexane, 3-ethyl-	114	C8H18	000619-99-8	59



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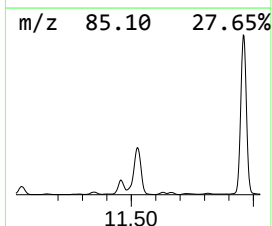
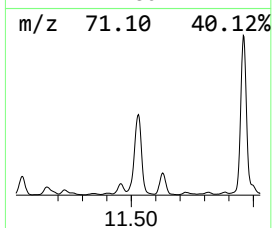
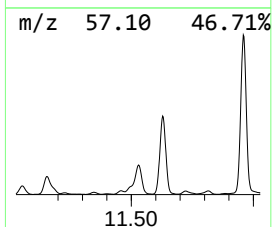
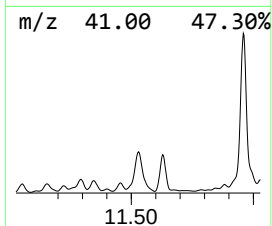
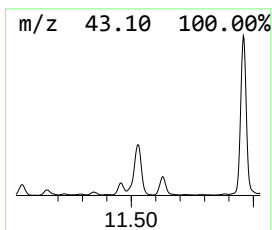
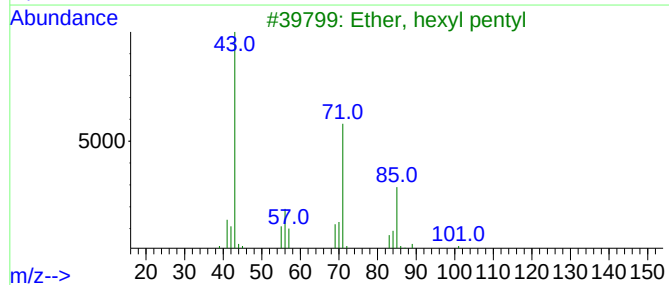
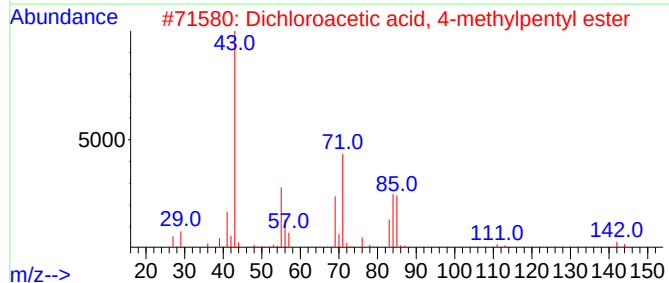
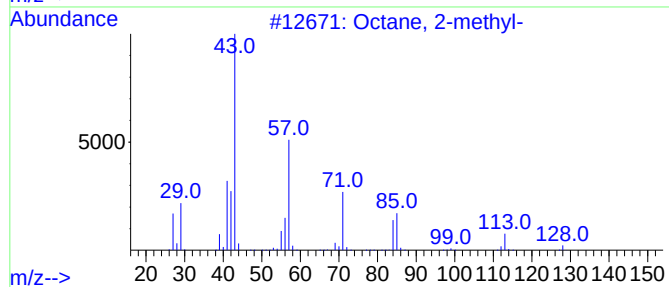
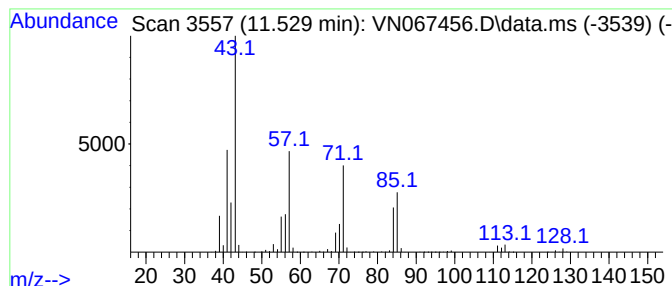
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Peak Number 3 Octane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	370.42 ug/l	11717300	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	72
2			Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	59
3			Ether, hexyl pentyl	172	C11H24O	032357-83-8	59
4			Octane, 4-methyl-	128	C9H20	002216-34-4	59
5			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	59



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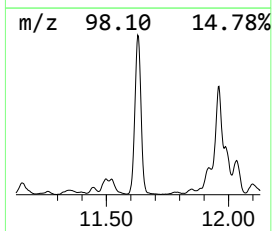
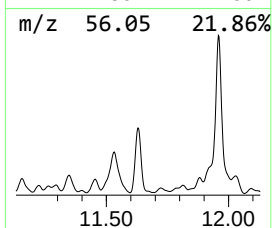
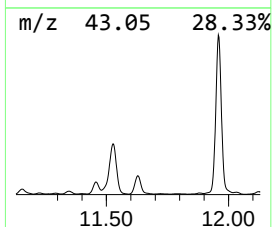
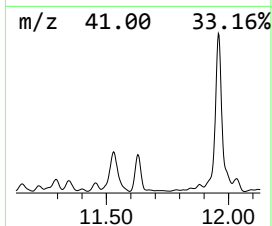
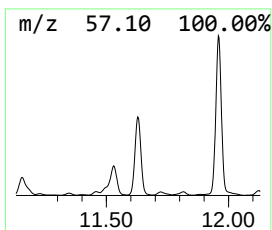
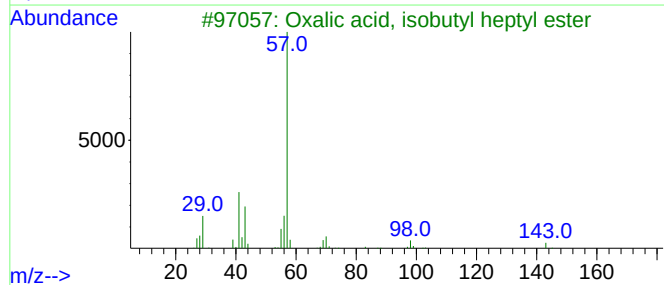
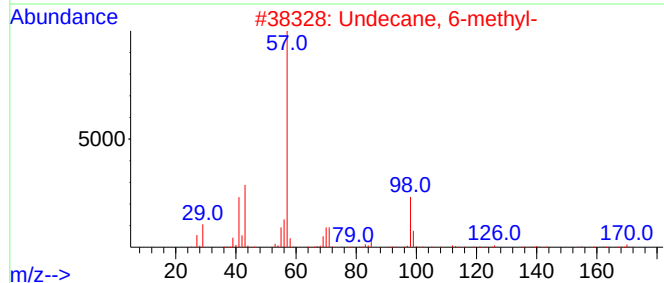
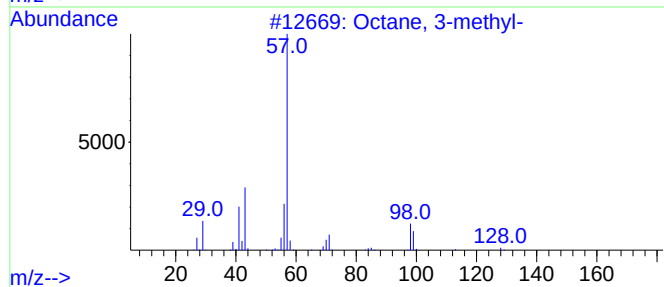
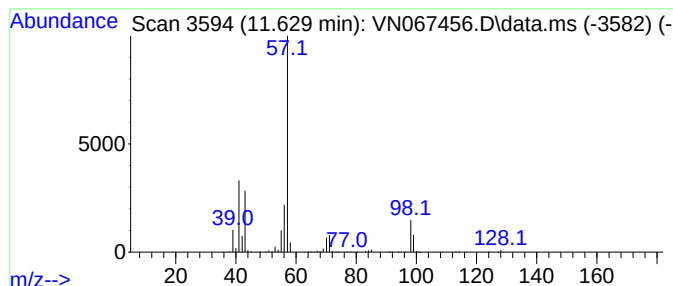
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Peak Number 4 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.629	201.48 ug/l	6373290	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	90
2			Undecane, 6-methyl-	170	C12H26	017302-33-9	64
3			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
4			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	58
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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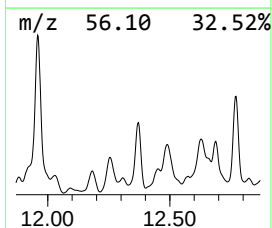
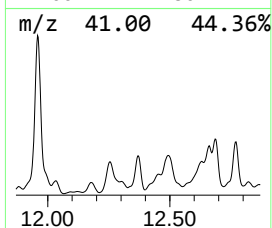
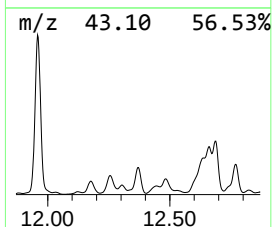
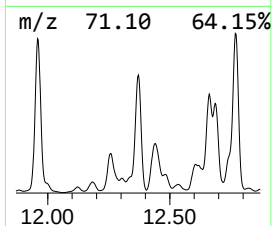
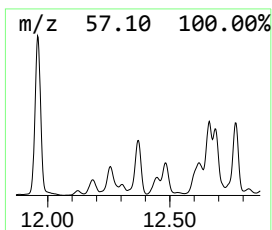
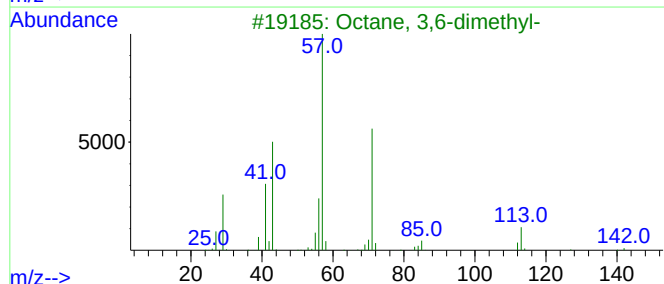
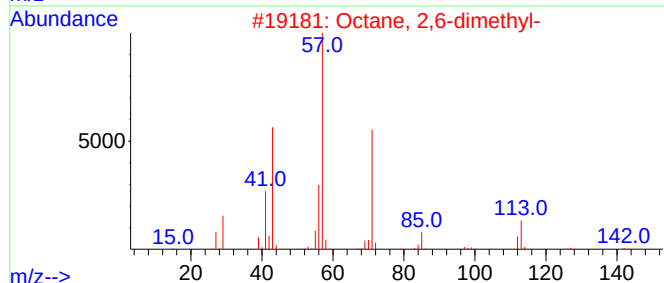
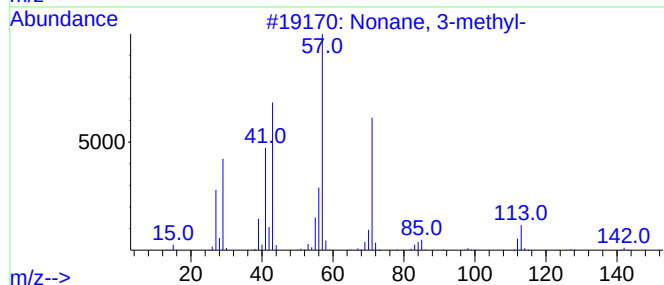
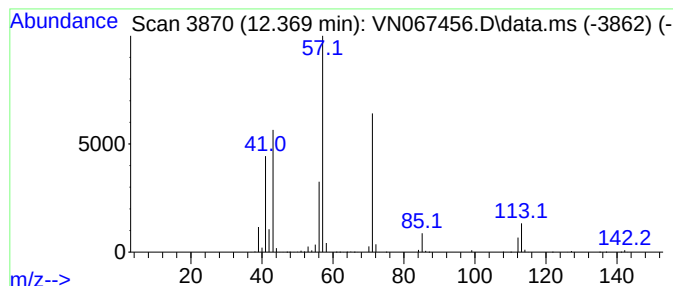
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	190.86 ug/l	6037320	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-	142	C10H22	005911-04-6	90
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	86
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	78
5			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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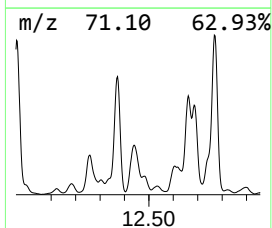
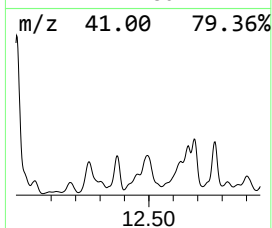
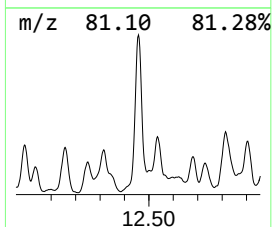
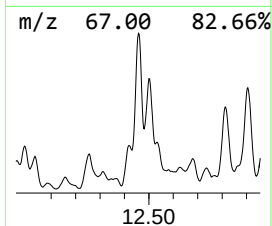
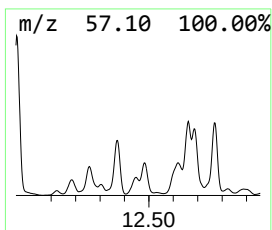
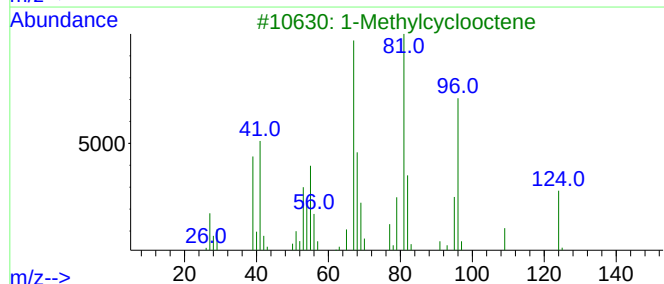
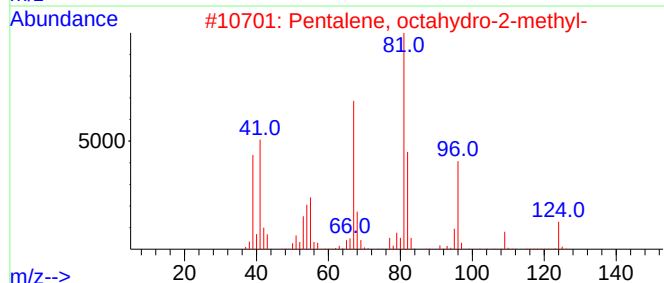
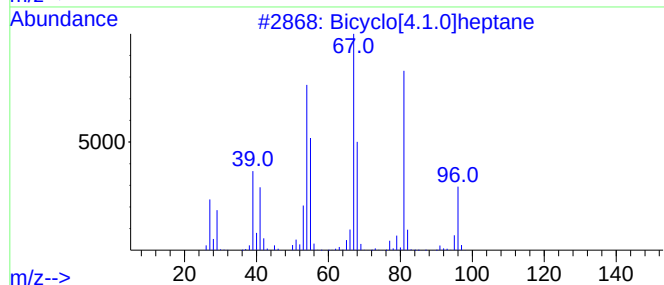
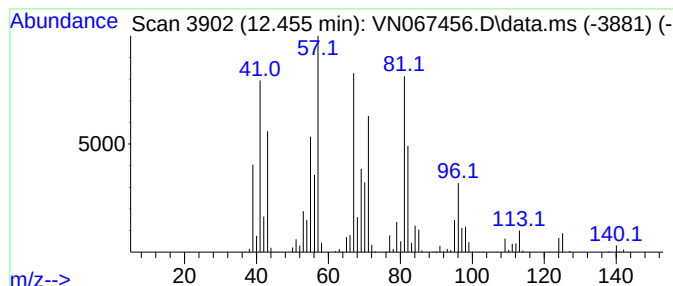
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown12.455 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	182.45 ug/l	5771320	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane	96	C7H12	000286-08-8	49
2			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	43
3			1-Methylcyclooctene	124	C9H16	000933-11-9	42
4			Cyclohexane, isocyanato-	125	C7H11NO	003173-53-3	41
5			1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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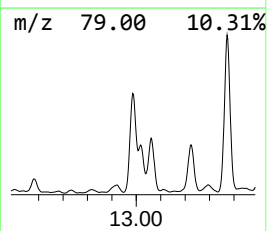
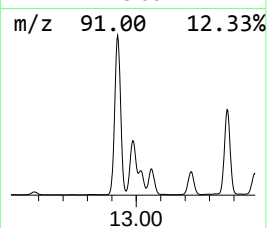
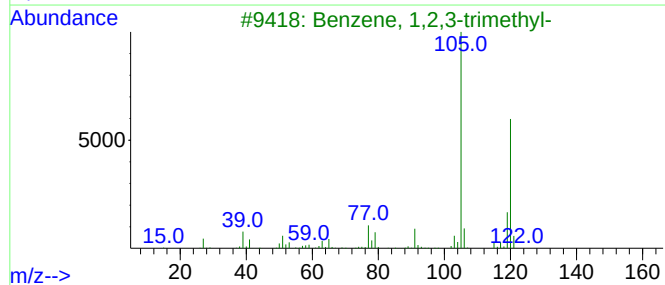
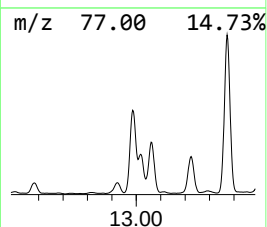
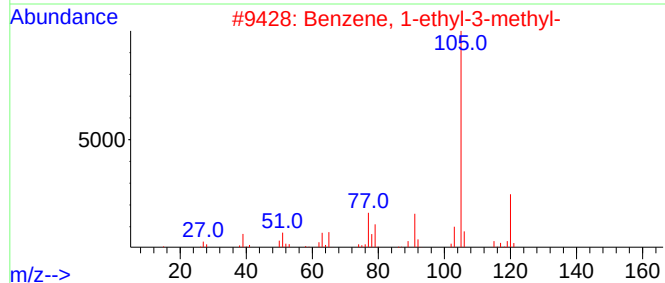
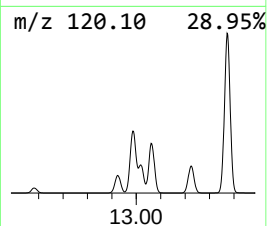
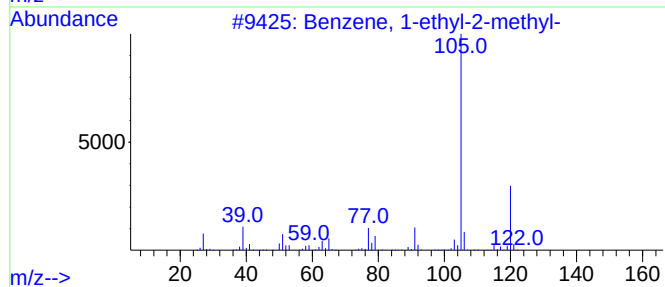
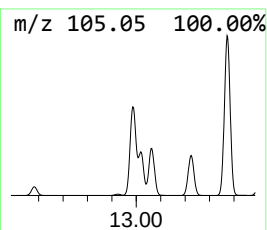
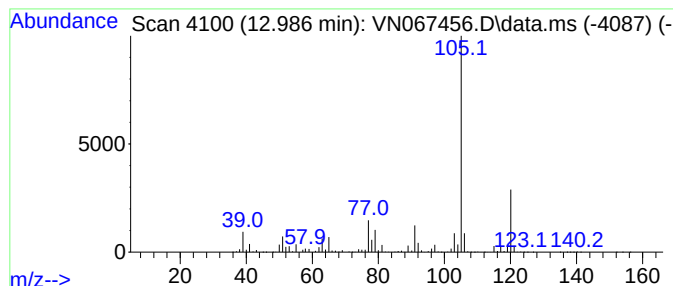
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	330.83 ug/l	21635500	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	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\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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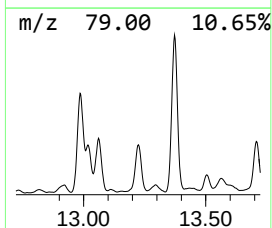
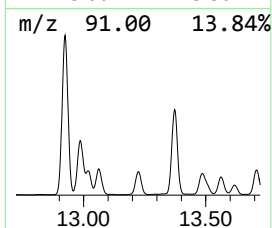
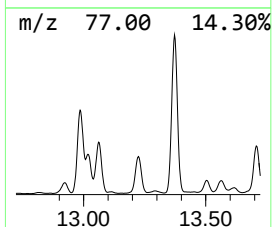
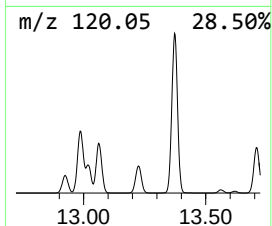
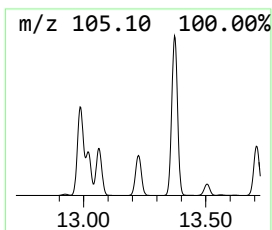
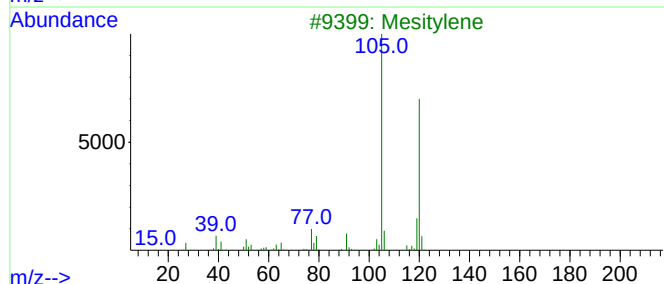
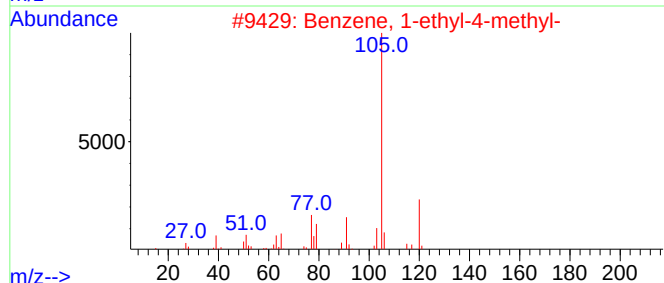
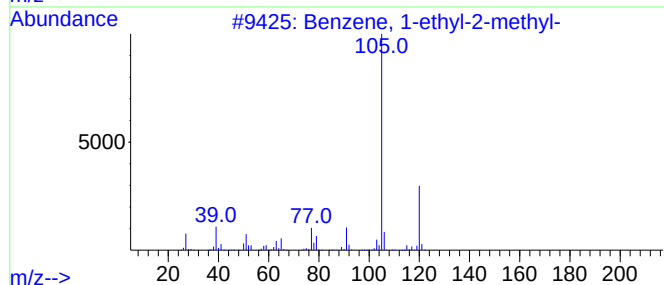
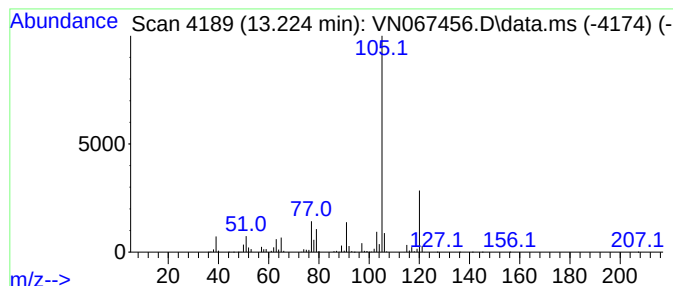
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	180.50 ug/l	11804000	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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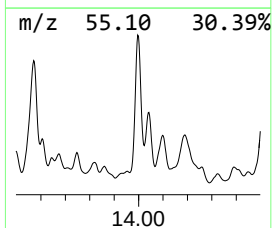
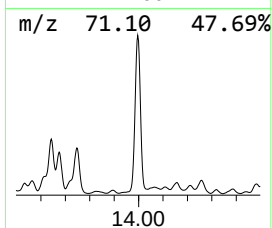
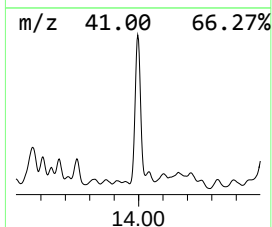
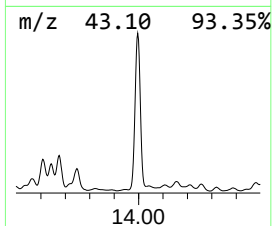
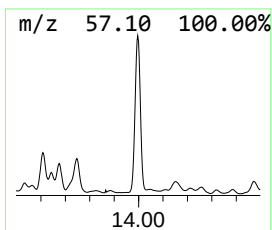
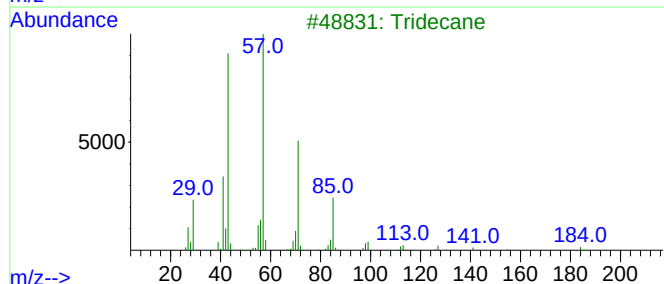
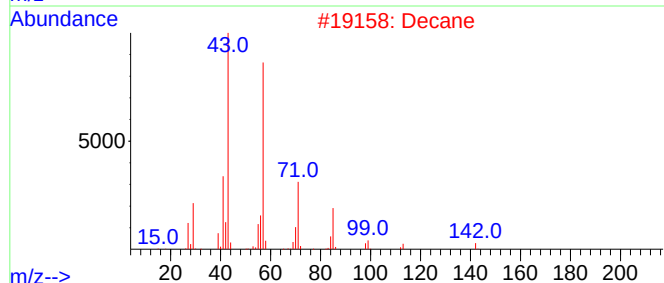
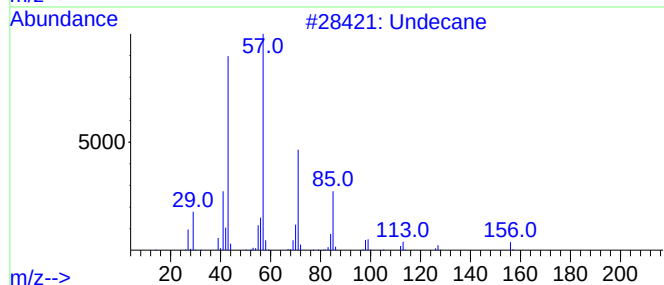
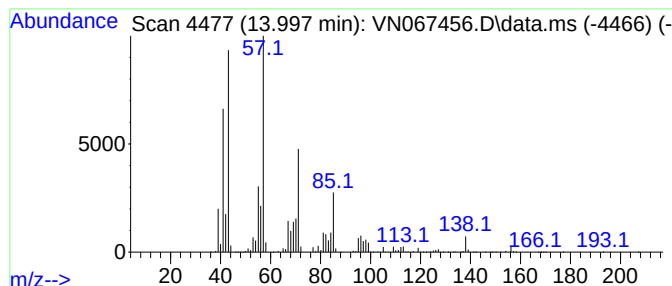
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	475.71 ug/l	31110400	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	81
2	Decane			142	C10H22	000124-18-5	80
3	Tridecane			184	C13H28	000629-50-5	64
4	Decane, 2,9-dimethyl-			170	C12H26	001002-17-1	64
5	Decane, 2,3,5-trimethyl-			184	C13H28	062238-11-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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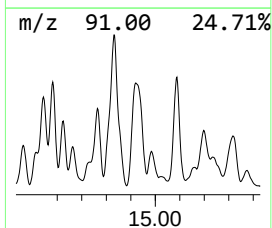
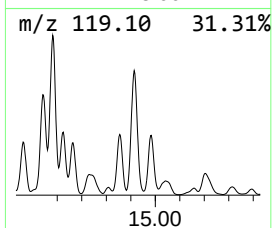
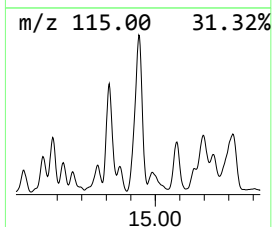
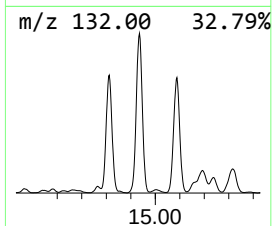
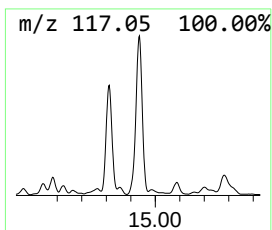
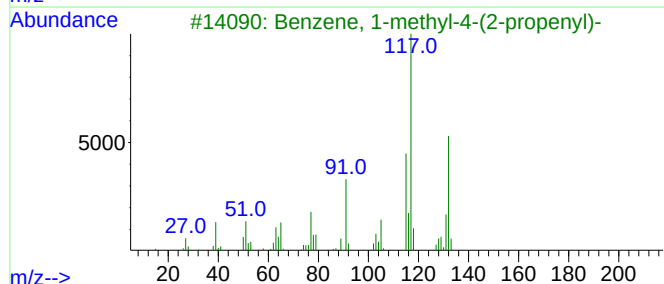
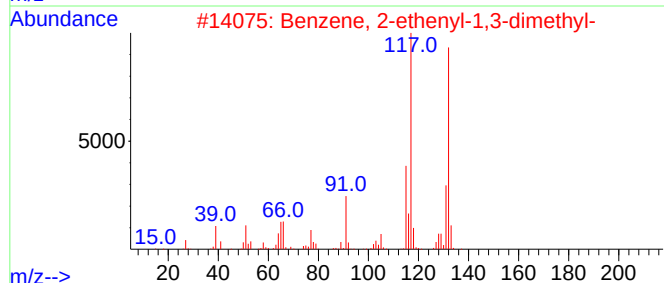
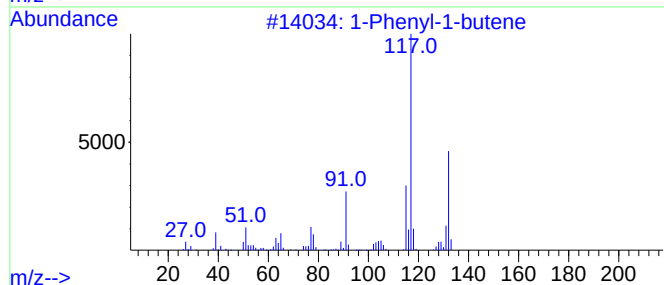
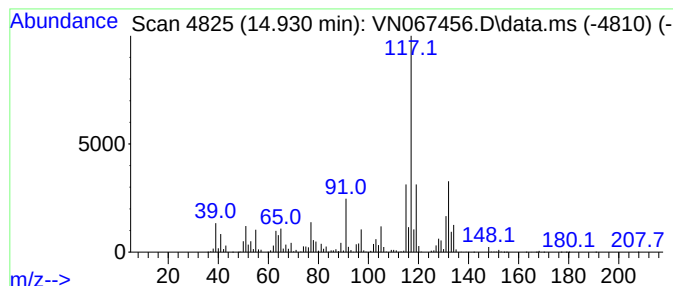
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	248.17 ug/l	16229800	1,4-Dichlorobenzene-d4	13.678

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	89
3		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067456.D
Acq On : 23 Jun 2021 14:50
Operator : JC/MD
Sample : M2802-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Octane	10.623	243.5	ug/l	7703540	3	11.749	1581620	50.0
Octane, 2-methyl-	11.529	370.4	ug/l	11717300	3	11.749	1581620	50.0
Octane, 3-methyl-	11.629	201.5	ug/l	6373290	3	11.749	1581620	50.0
Nonane, 3-methyl-	12.369	190.9	ug/l	6037320	3	11.749	1581620	50.0
unknown12.455	12.455	182.4	ug/l	5771320	3	11.749	1581620	50.0
Benzene, 1-ethy...	12.986	330.8	ug/l	21635500	4	13.678	3269880	50.0
Benzene, 1-ethy...	13.224	180.5	ug/l	11804000	4	13.678	3269880	50.0
Undecane	13.997	475.7	ug/l	31110400	4	13.678	3269880	50.0
1-Phenyl-1-butene	14.930	248.2	ug/l	16229800	4	13.678	3269880	50.0