

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
 Data File : VN070702.D
 Acq On : 19 Jan 2022 16:12
 Operator : JC/MD
 Sample : N1145-08
 Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A3-8-5.5

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
 Title : SW846 8260

Signal : TIC: VN070702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	365	381	408	rVB2	2964008	5784274	7.05%	0.500%
2	3.419	511	533	570	rVB	2682255	6738295	8.22%	0.582%
3	3.926	699	722	750	rBV2	407757	1105014	1.35%	0.095%
4	4.194	790	822	846	rBV3	292550	1007172	1.23%	0.087%
5	5.039	1104	1137	1138	rBV2	1857186	4331408	5.28%	0.374%
6	5.583	1307	1340	1382	rBV2	4090222	14273389	17.41%	1.234%
7	5.905	1434	1460	1490	rVB3	293065	962278	1.17%	0.083%
8	6.093	1500	1530	1568	rBV	4331948	13352365	16.28%	1.154%
9	6.444	1636	1661	1689	rVB2	1009831	3058635	3.73%	0.264%
10	6.584	1689	1713	1738	rBV3	518126	1631851	1.99%	0.141%
11	6.882	1797	1824	1851	rBV4	1106356	3501014	4.27%	0.303%
12	7.026	1852	1878	1898	rBV	5072584	15460379	18.85%	1.336%
13	7.131	1899	1917	1939	rVB	4466472	12646478	15.42%	1.093%
14	7.831	2163	2178	2198	rVB	1733953	4223399	5.15%	0.365%
15	8.059	2225	2263	2285	rBV3	11363336	33934791	41.39%	2.933%
16	8.164	2286	2302	2327	rVB2	11927692	30422956	37.10%	2.629%
17	8.287	2328	2348	2368	rBV	11539955	26837213	32.73%	2.319%
18	8.434	2387	2403	2420	rBV	766873	1925111	2.35%	0.166%
19	8.609	2431	2468	2491	rBV2	27574265	81996671	100.00%	7.086%
20	8.700	2493	2502	2524	rVB3	2066330	5025096	6.13%	0.434%
21	8.821	2525	2547	2577	rVB	8657267	18431301	22.48%	1.593%
22	8.960	2578	2599	2627	rBV4	4804901	13708113	16.72%	1.185%
23	9.118	2646	2658	2673	rVB	929337	1800298	2.20%	0.156%
24	9.193	2673	2686	2693	rVV	450791	890490	1.09%	0.077%
25	9.242	2694	2704	2742	rVB3	954558	2995478	3.65%	0.259%
26	9.454	2748	2783	2794	rBV2	13467658	33971951	41.43%	2.936%
27	9.507	2794	2803	2820	rVB	7924912	15324119	18.69%	1.324%
28	9.588	2820	2833	2841	rBV	1454527	2835311	3.46%	0.245%
29	9.636	2842	2851	2864	rVB	2131611	3954117	4.82%	0.342%
30	9.727	2864	2885	2901	rVB3	1857183	4851698	5.92%	0.419%
31	9.880	2902	2942	2963	rBV	16830958	36421162	44.42%	3.148%
32	10.011	2964	2991	3004	rBV2	20635745	46460539	56.66%	4.015%
33	10.076	3005	3015	3025	rBV	9980816	17909455	21.84%	1.548%
34	10.215	3045	3067	3092	rBV	13233069	30838788	37.61%	2.665%
35	10.317	3093	3105	3110	rBV4	841965	1459145	1.78%	0.126%
36	10.365	3111	3123	3137	rVB	8998155	16342147	19.93%	1.412%

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37	10.438	3137	3150	3174	rBV3	5904399	13614418	16.60%	1.177%
38	10.620	3204	3218	3232	rVB	11528856	22152364	27.02%	1.914%
39	10.682	3233	3241	3251	rVB2	901720	1335388	1.63%	0.115%
40	10.781	3268	3278	3296	rBV6	1096974	2961237	3.61%	0.256%
41	10.878	3296	3314	3334	rBV8	3611139	10607094	12.94%	0.917%
42	10.961	3335	3345	3359	rVB	2782382	4930540	6.01%	0.426%
43	11.052	3359	3379	3391	rBV2	2788849	5575613	6.80%	0.482%
44	11.111	3392	3401	3404	rBV2	727911	963172	1.17%	0.083%
45	11.151	3406	3416	3433	rVB	4371520	8611765	10.50%	0.744%
46	11.221	3435	3442	3448	rBV5	885773	1263121	1.54%	0.109%
47	11.344	3479	3488	3499	rBV2	1114834	1946779	2.37%	0.168%
48	11.454	3519	3529	3536	rBV2	2342936	3768201	4.60%	0.326%
49	11.524	3537	3555	3580	rVB3	12789419	29080756	35.47%	2.513%
50	11.626	3580	3593	3616	rBV	9739459	16981131	20.71%	1.468%
51	11.741	3618	3636	3648	rBV3	3409941	8656016	10.56%	0.748%
52	11.843	3653	3674	3694	rVB2	23888298	45445859	55.42%	3.927%
53	11.956	3704	3716	3726	rBV	9235752	15803418	19.27%	1.366%
54	12.181	3772	3800	3811	rBV5	2286030	5664721	6.91%	0.490%
55	12.251	3816	3826	3840	rBV5	2824348	5300859	6.46%	0.458%
56	12.363	3860	3868	3880	rVB	3053843	4935473	6.02%	0.427%
57	12.444	3888	3898	3906	rBV4	1477800	2678595	3.27%	0.231%
58	12.581	3938	3949	3958	rBV	4158707	8036843	9.80%	0.695%
59	12.766	4012	4018	4027	rVB	4291135	5761573	7.03%	0.498%
60	12.873	4049	4058	4063	rBV2	1579112	2470050	3.01%	0.213%
61	12.919	4064	4075	4091	rVB	16226095	26876080	32.78%	2.323%
62	13.015	4100	4111	4117	rBV	6512109	10421800	12.71%	0.901%
63	13.055	4117	4126	4168	rVB2	13230838	28567487	34.84%	2.469%
64	13.219	4170	4187	4204	rBV	8341513	17735972	21.63%	1.533%
65	13.367	4232	4242	4252	rVB	4725708	7700247	9.39%	0.665%
66	13.412	4253	4259	4270	rVB2	1380396	2075179	2.53%	0.179%
67	13.493	4272	4289	4298	rBV3	2781893	7769657	9.48%	0.671%
68	13.608	4324	4332	4338	rBV2	2150081	3188420	3.89%	0.276%
69	13.704	4349	4368	4400	rVB2	14622224	38476883	46.92%	3.325%
70	13.839	4405	4418	4423	rBV	8030948	12636345	15.41%	1.092%
71	13.876	4424	4432	4439	rBV2	10031679	14655347	17.87%	1.267%
72	13.994	4467	4476	4489	rBV3	3716494	5687707	6.94%	0.492%
73	14.069	4493	4504	4515	rVB	5198825	8245987	10.06%	0.713%
74	14.136	4516	4529	4546	rVB5	5754073	14655972	17.87%	1.267%
75	14.217	4546	4559	4572	rBV	18858192	30014028	36.60%	2.594%
76	14.276	4575	4581	4588	rVV	1719602	2509866	3.06%	0.217%

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77	14.324	4589	4599	4612	rVB3	8938442	15203227	18.54%	1.314%
78	14.407	4621	4630	4640	rVB2	2912800	4574961	5.58%	0.395%
79	14.458	4641	4649	4660	rVB	3084037	4592144	5.60%	0.397%
80	14.539	4663	4679	4687	rBV	9255714	15829775	19.31%	1.368%
81	14.579	4688	4694	4702	rVB	5459961	6965082	8.49%	0.602%
82	14.622	4702	4710	4718	rBV2	4457927	5921024	7.22%	0.512%
83	14.761	4755	4762	4770	rBV	2314518	2904109	3.54%	0.251%
84	14.809	4770	4780	4789	rBV2	8356980	14115375	17.21%	1.220%
85	14.927	4807	4824	4836	rBV4	12445520	29833174	36.38%	2.578%
86	14.981	4837	4844	4859	rVB2	3574781	6412517	7.82%	0.554%
87	15.083	4874	4882	4899	rVB2	2711642	5007682	6.11%	0.433%
88	15.196	4901	4924	4952	rVV5	5874548	17874270	21.80%	1.545%
89	15.308	4954	4966	4983	rVB5	3843010	8669681	10.57%	0.749%
90	15.504	5014	5039	5053	rBV	7973337	16065288	19.59%	1.388%
91	15.611	5068	5079	5090	rBV3	1911585	3507789	4.28%	0.303%
92	15.804	5135	5151	5167	rBV	2506983	5451767	6.65%	0.471%
93	16.107	5255	5264	5276	rVB2	930417	1659678	2.02%	0.143%
94	16.185	5280	5293	5330	rVB6	1267116	3966416	4.84%	0.343%
95	16.614	5438	5453	5495	rVB	5350338	12406967	15.13%	1.072%

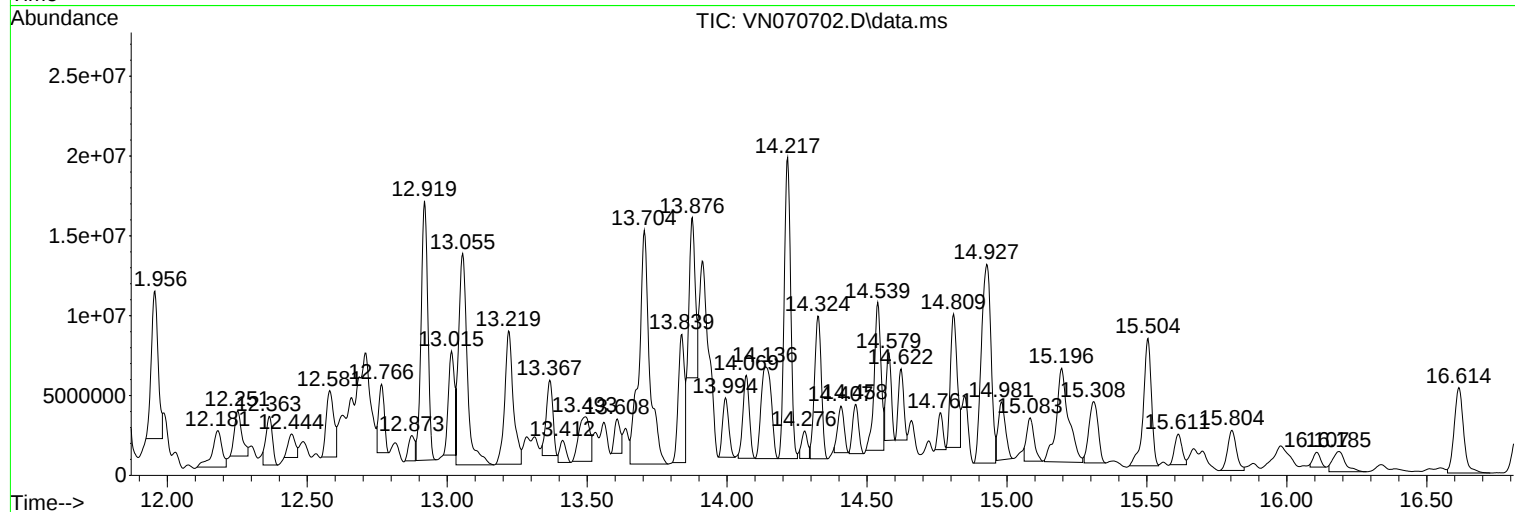
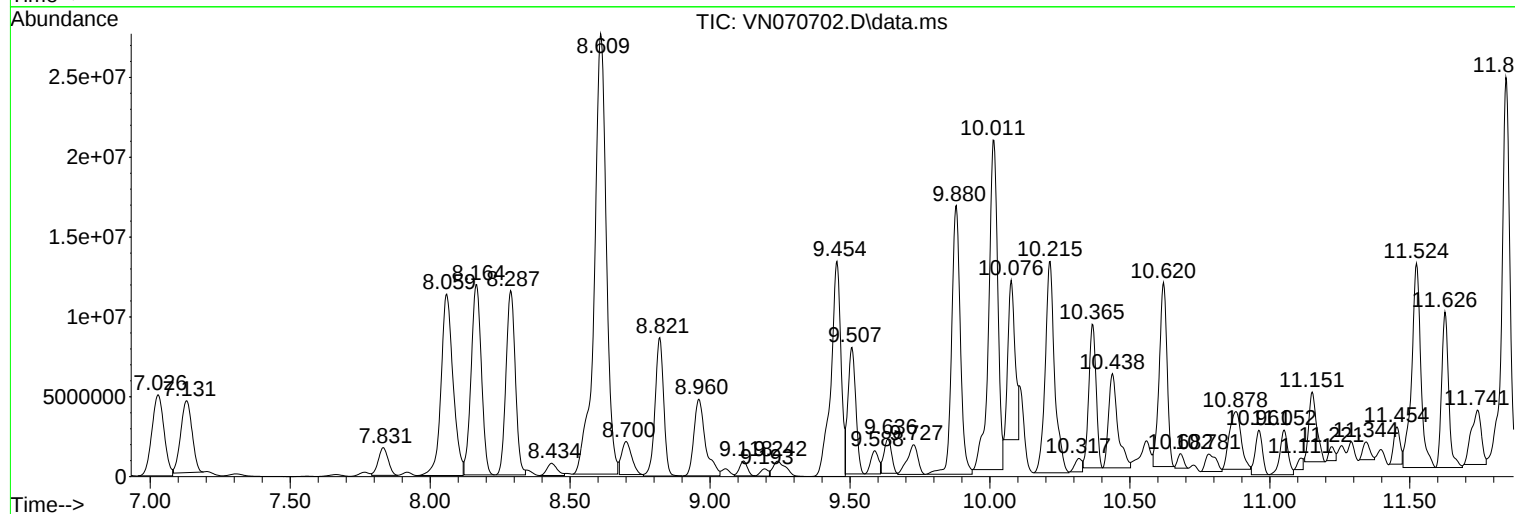
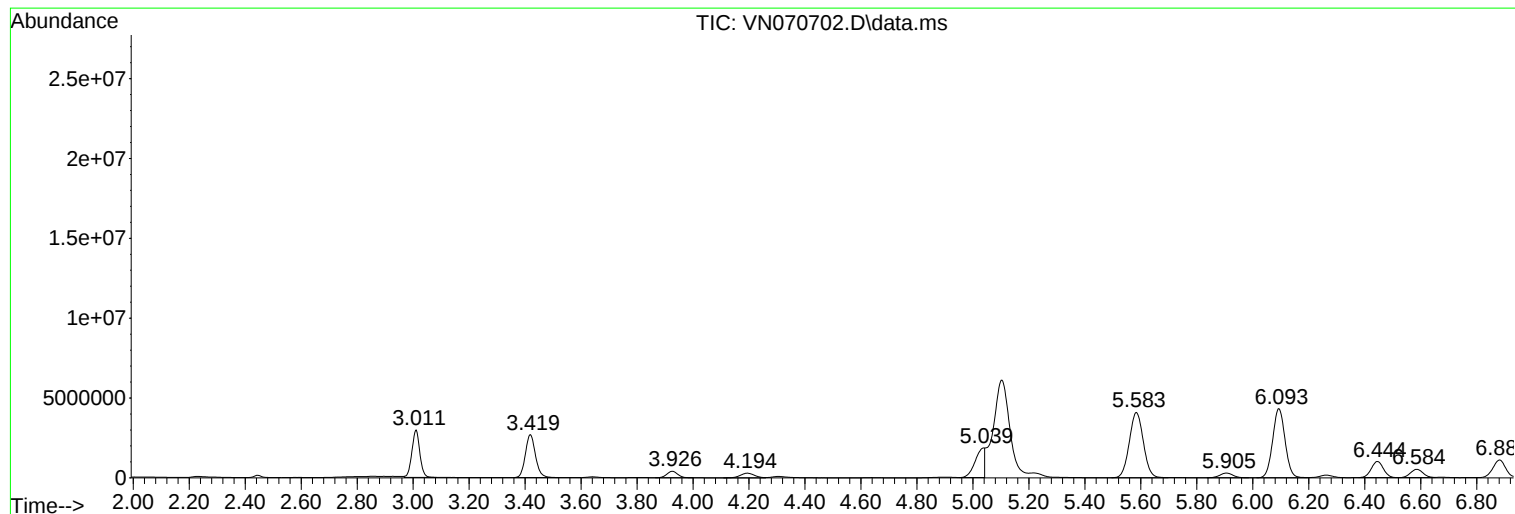
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

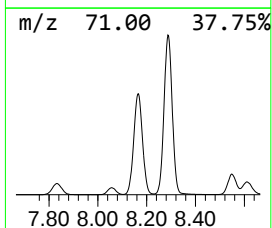
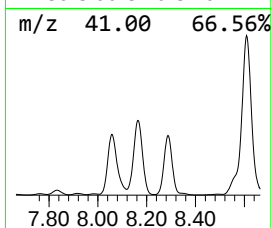
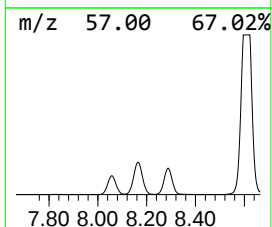
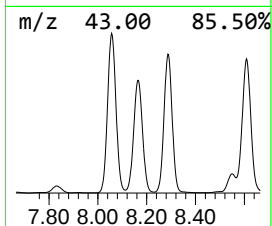
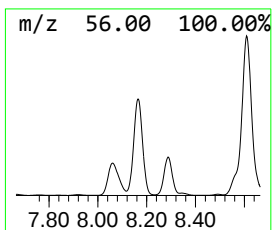
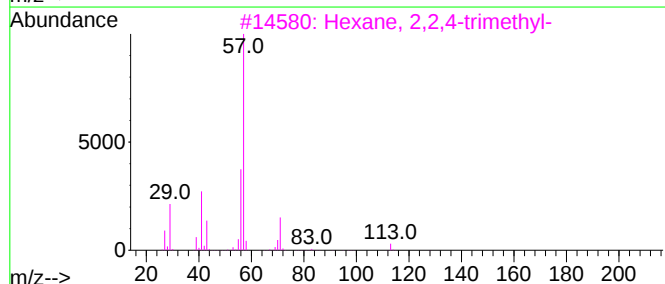
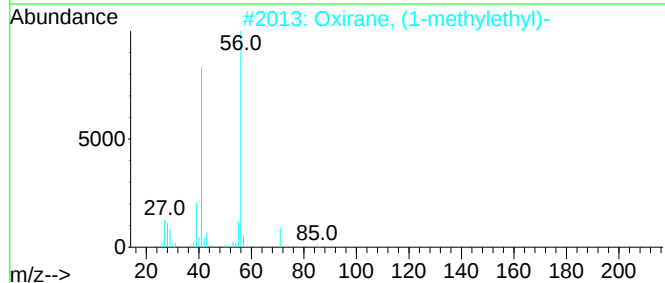
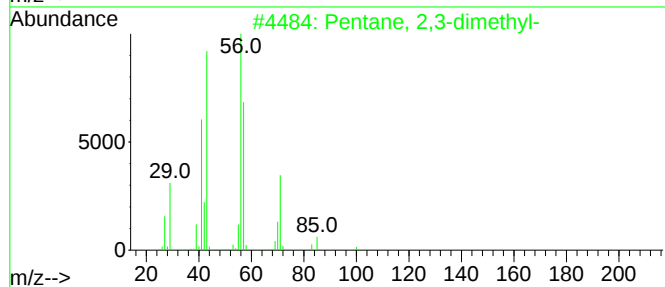
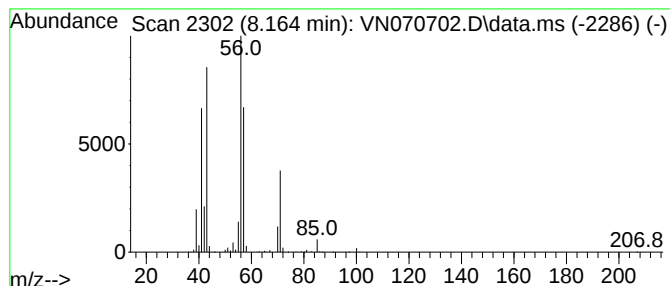
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.164	44.83 ug/l	30423000	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40



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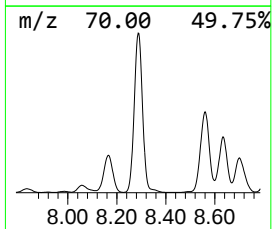
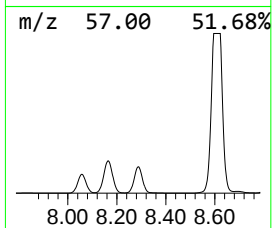
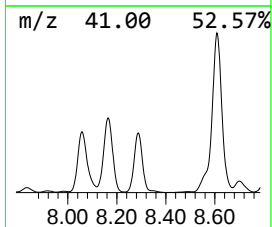
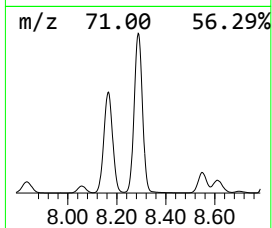
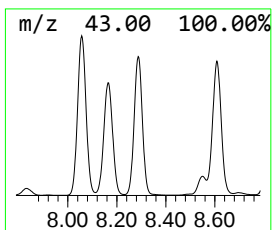
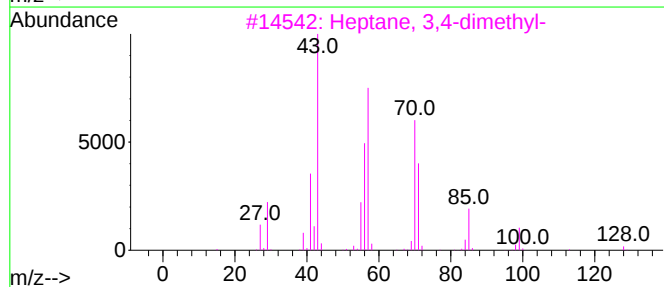
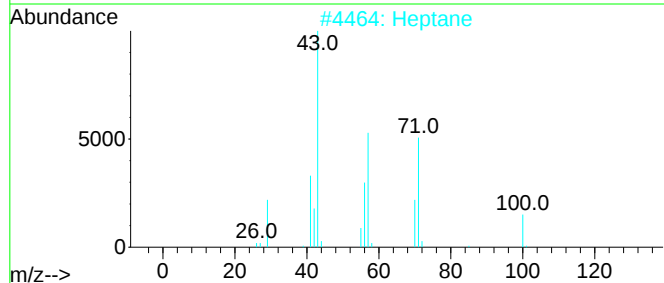
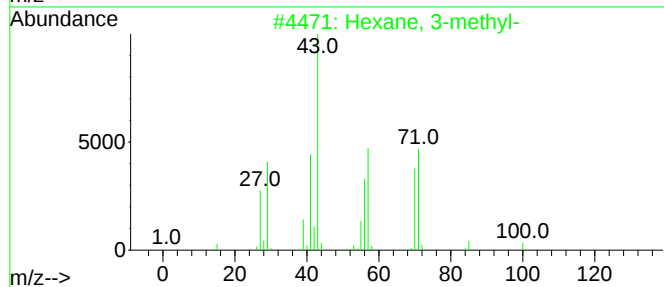
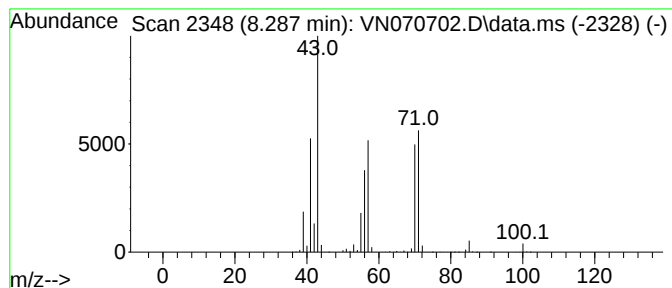
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexane, 3-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	39.54 ug/l	26837200	Pentafluorobenzene	8.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2		Heptane	100	C7H16	000142-82-5	64
3		Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	64



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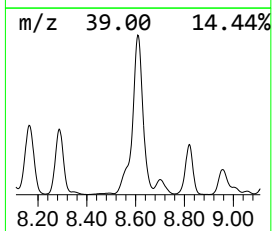
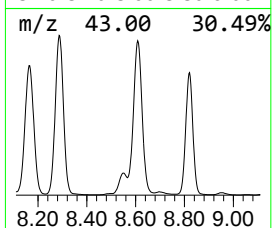
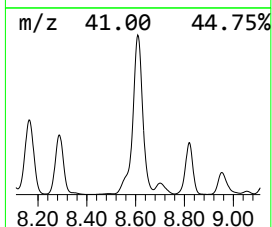
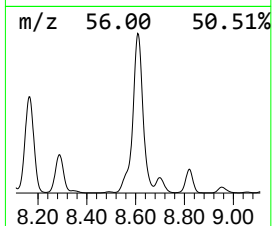
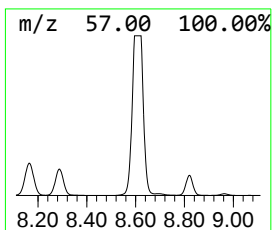
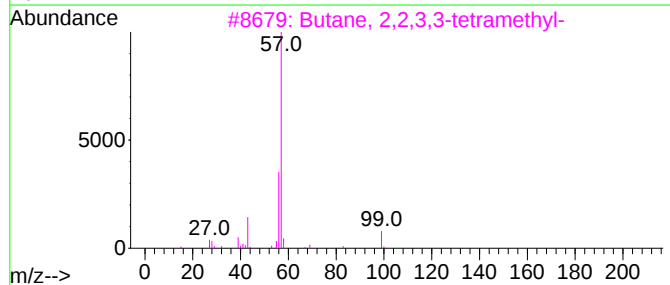
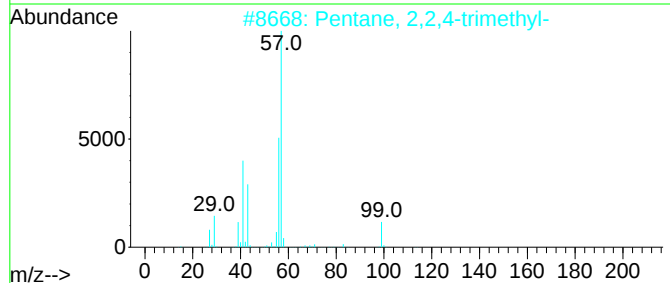
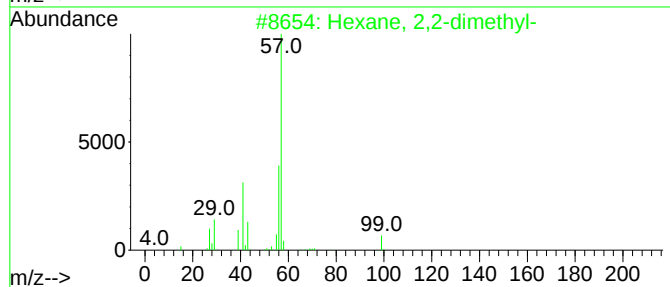
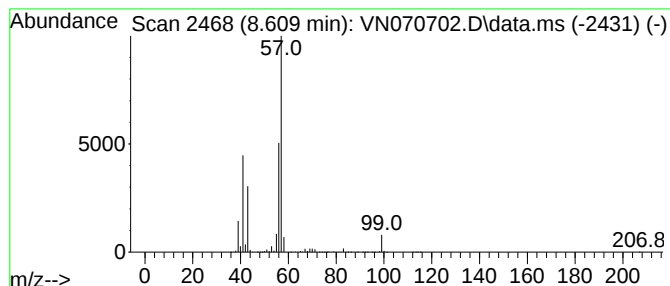
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Quant Title : SW846 8260

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

Peak Number 3 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.609	299.08 ug/l	81996700	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64
5			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

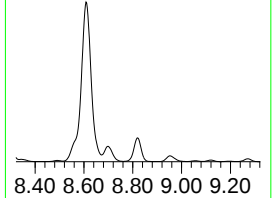
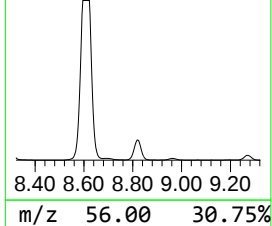
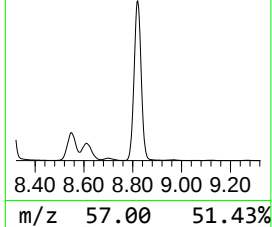
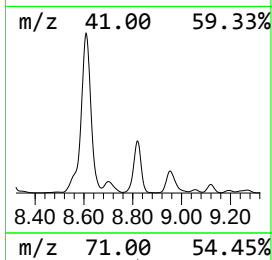
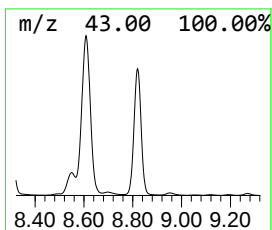
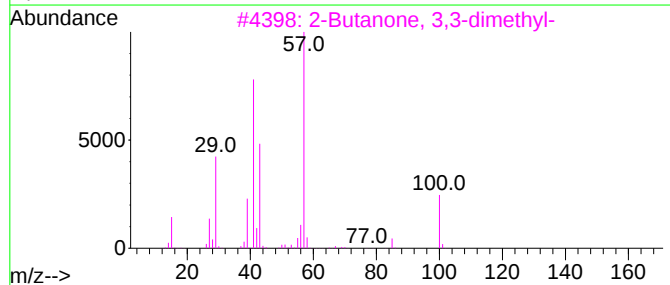
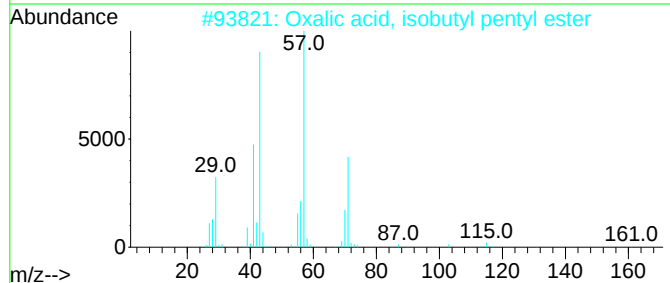
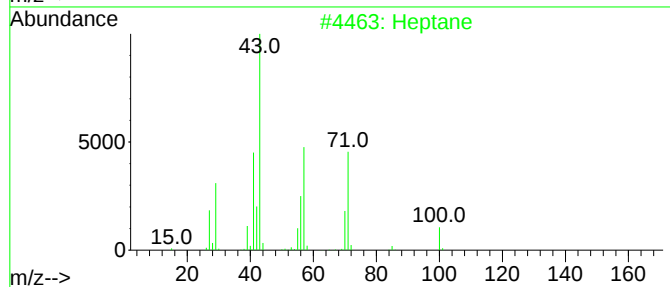
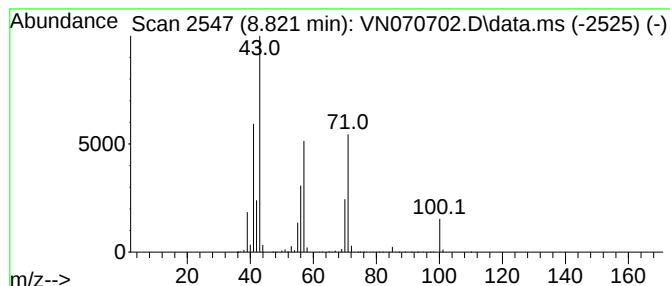
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Quant Title : SW846 8260

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

Peak Number 4 Heptane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.821	67.23 ug/l	18431300	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	95
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	43
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

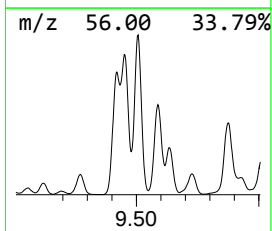
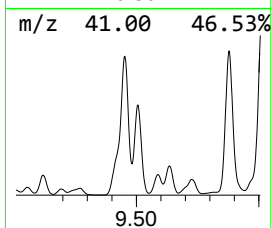
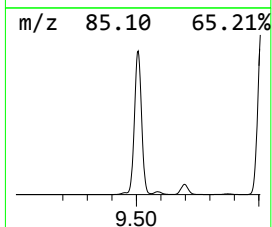
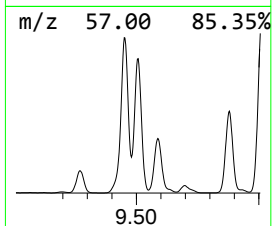
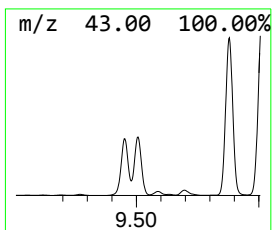
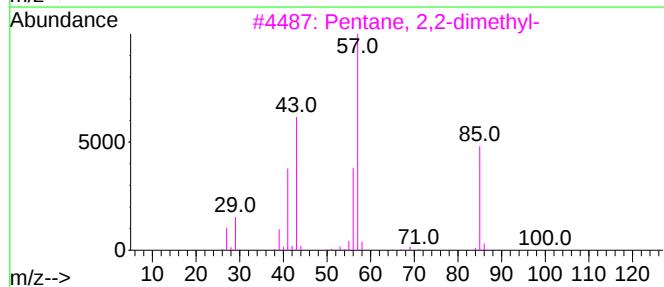
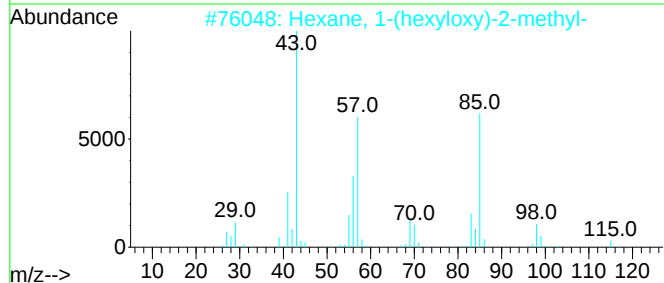
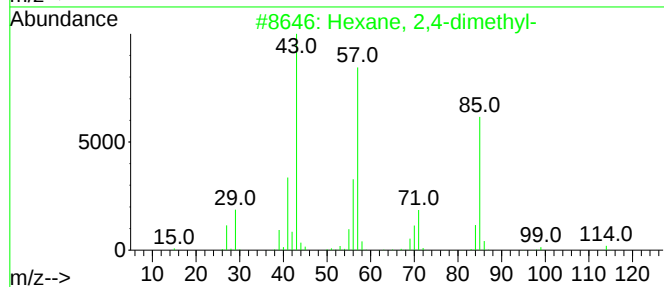
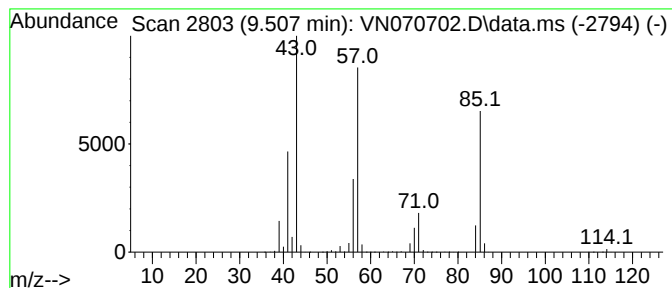
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,4-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.507	55.89 ug/l	15324100	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	91
2			Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	78
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
4			Hexane, 2-methyl-	100	C7H16	000591-76-4	59
5			2-Pentoxo-tetrahydropyran	172	C10H20O2	032767-70-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

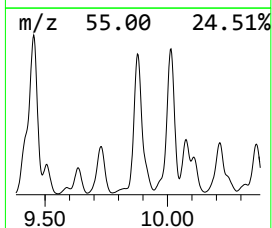
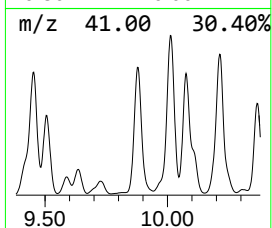
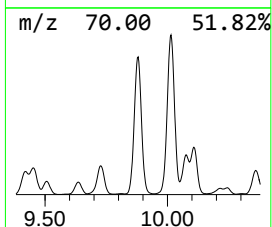
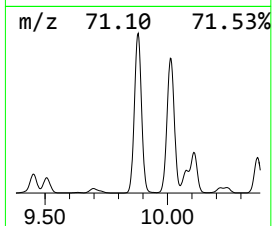
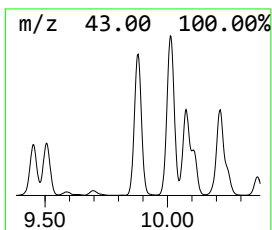
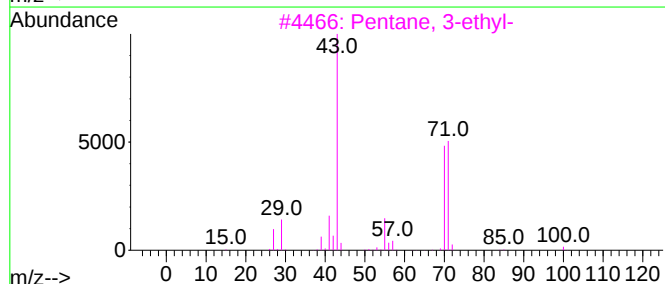
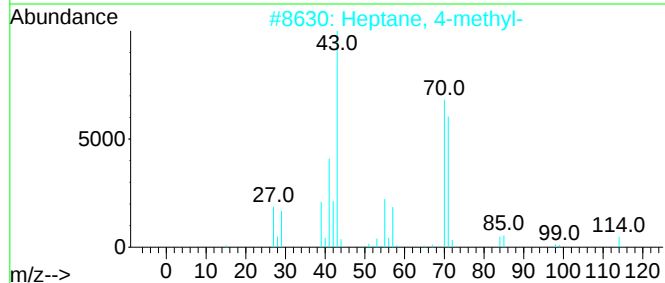
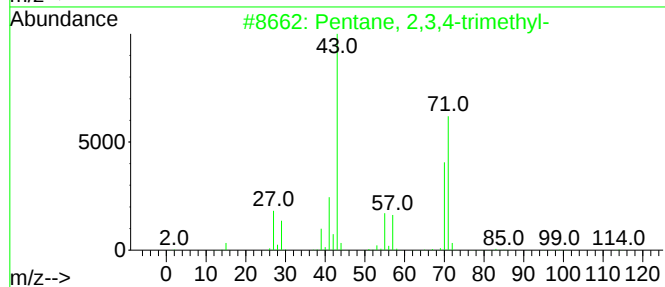
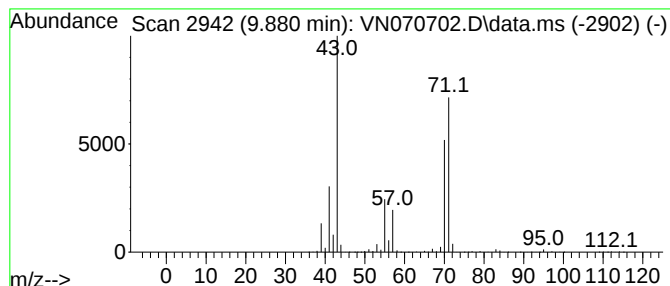
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	132.85 ug/l	36421200	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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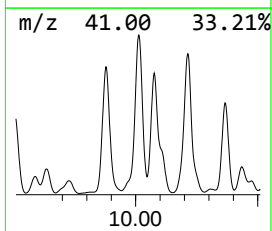
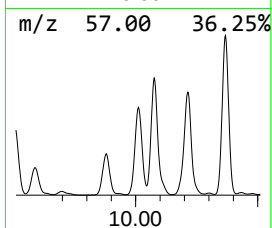
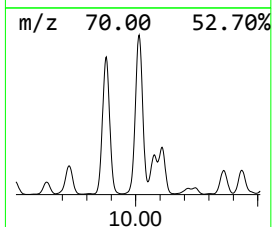
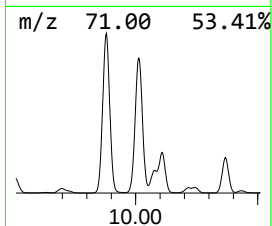
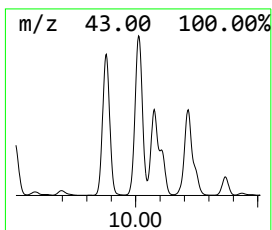
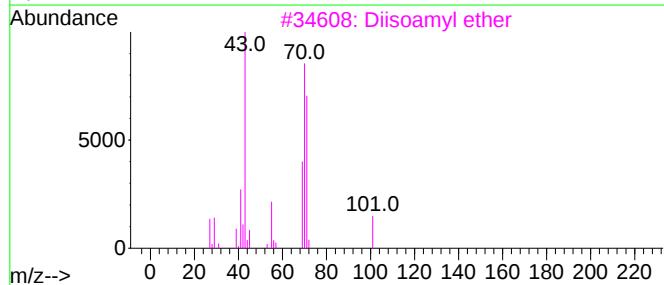
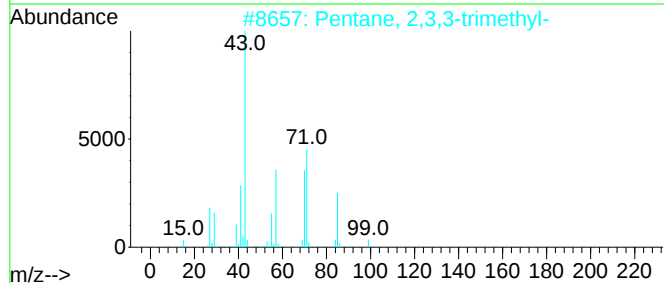
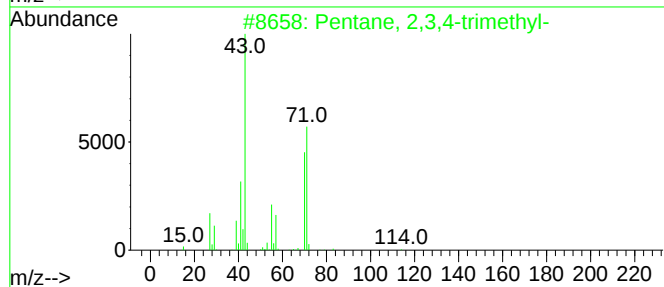
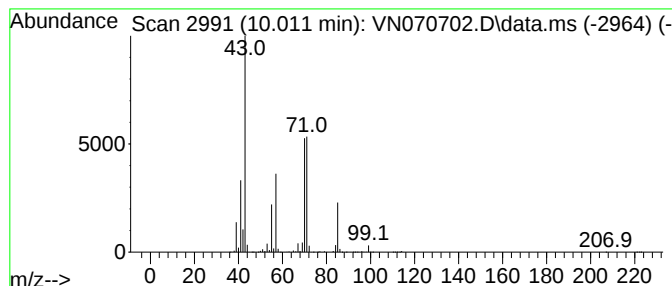
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.011	169.46 ug/l	46460500	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	81
2			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
3			Diisoamyl ether	158	C10H22O	000544-01-4	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	56
5			Pyrrolidine	71	C4H9N	000123-75-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

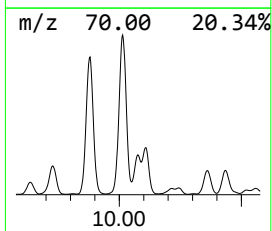
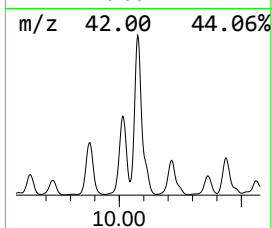
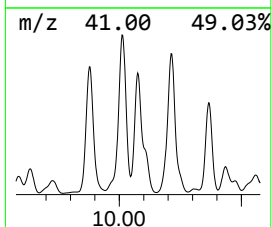
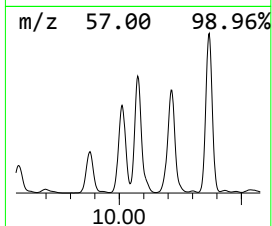
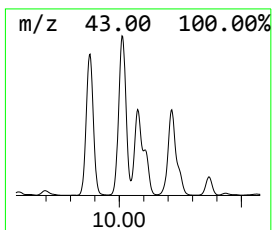
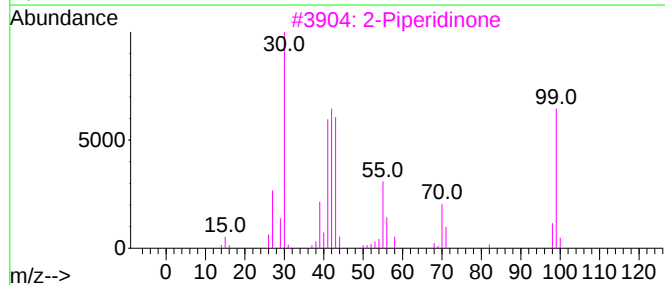
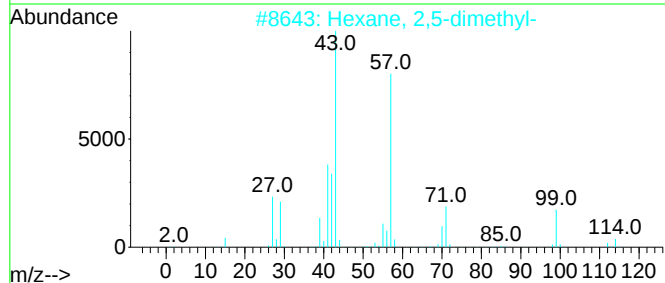
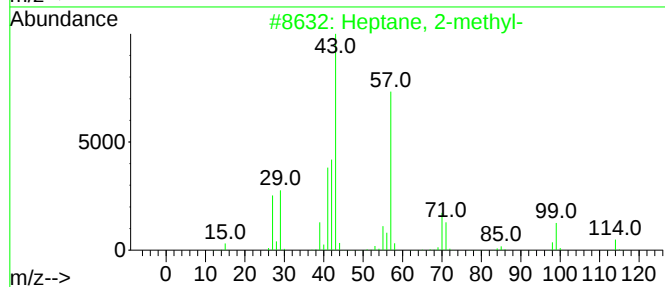
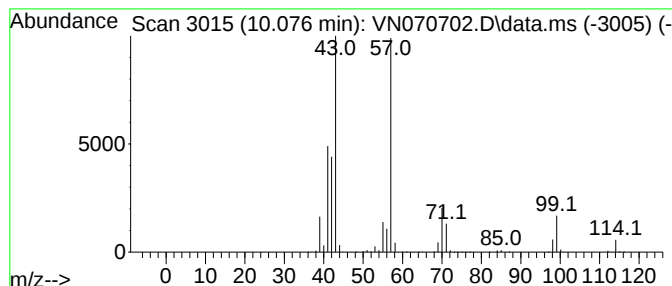
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Quant Title : SW846 8260

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

Peak Number 8 Heptane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.076	65.32 ug/l	17909500	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	80
3			2-Piperidinone	99	C5H9NO	000675-20-7	40
4			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	38
5			Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A3-8-5.5

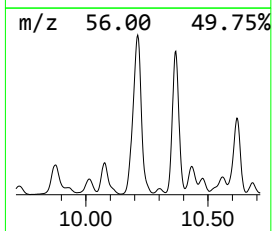
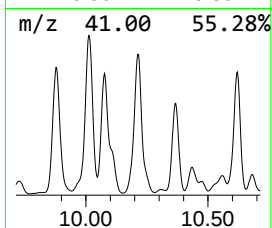
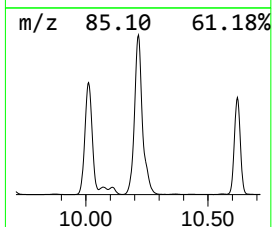
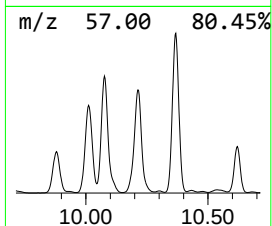
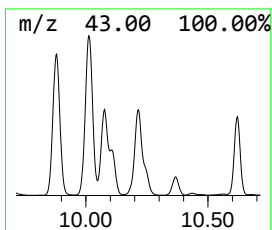
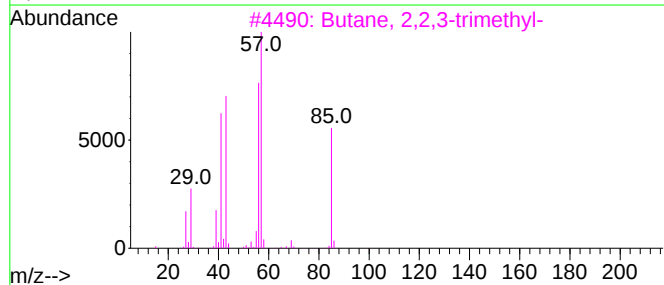
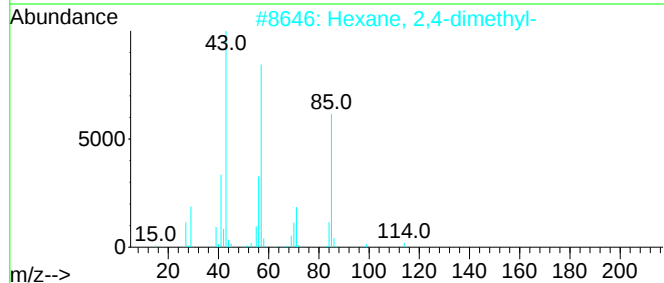
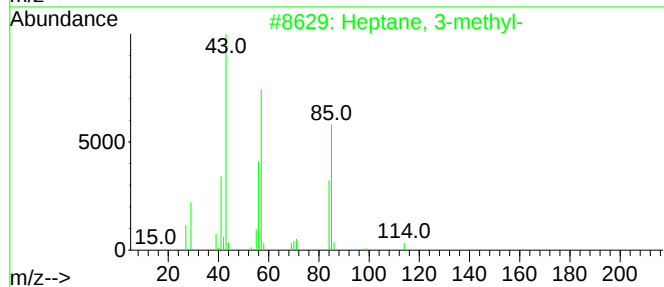
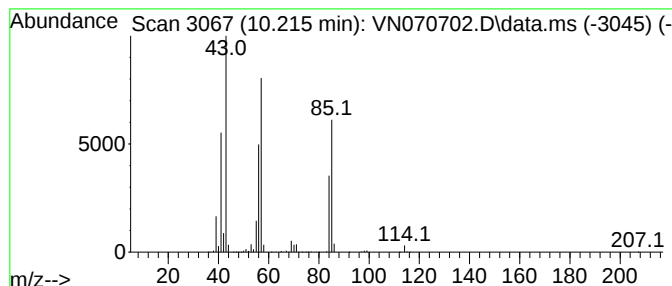
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Quant Title : SW846 8260

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

Peak Number 9 Heptane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	112.48 ug/l	30838800	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4			Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	53
5			Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

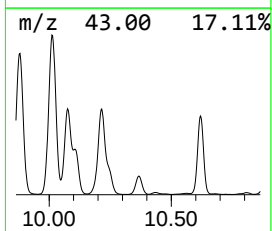
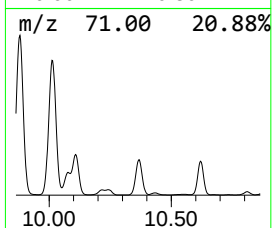
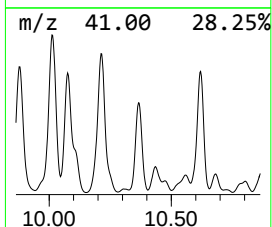
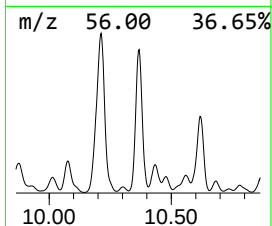
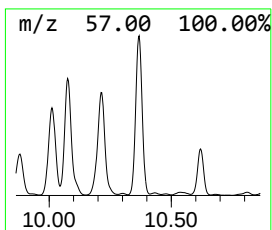
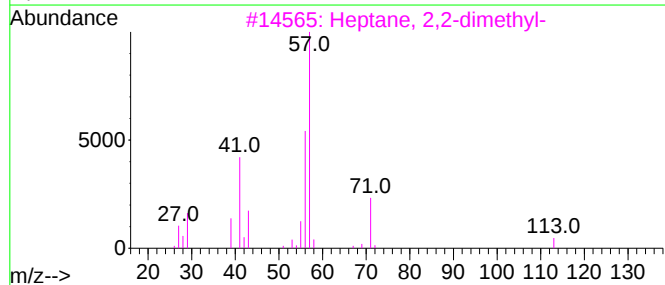
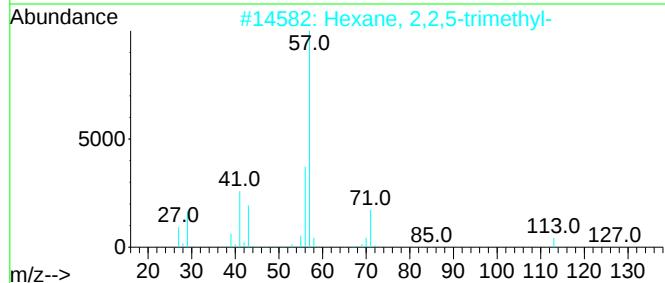
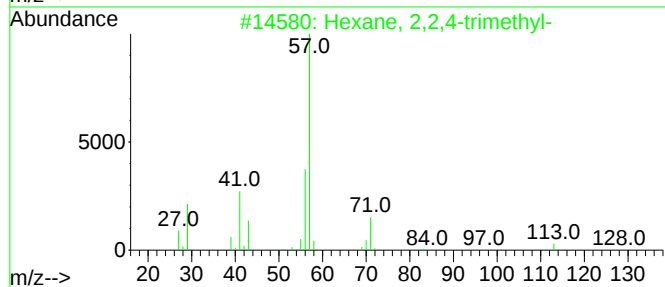
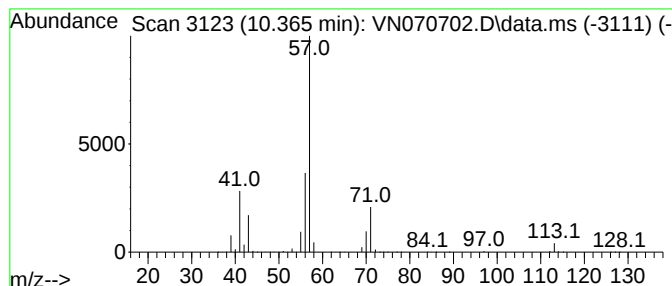
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Quant Title : SW846 8260

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

Peak Number 10 Hexane, 2,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	94.40 ug/l	16342100	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	83
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	78
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

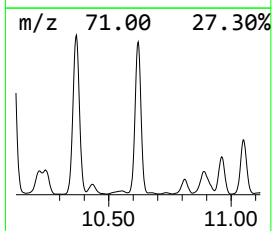
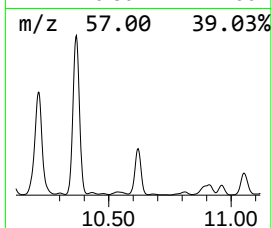
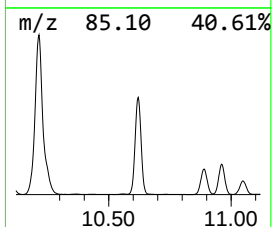
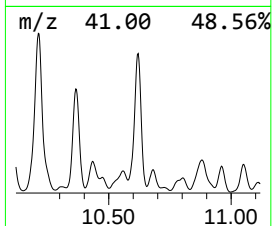
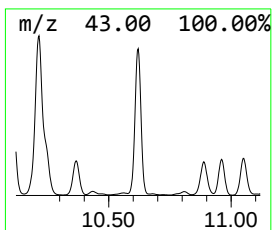
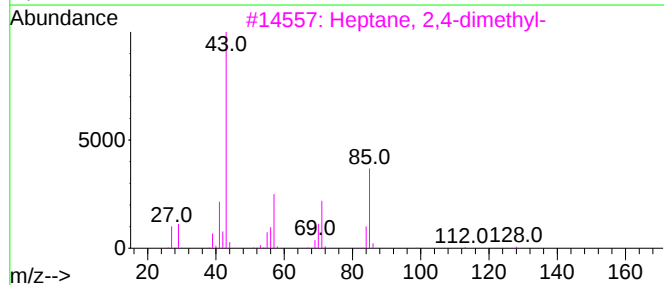
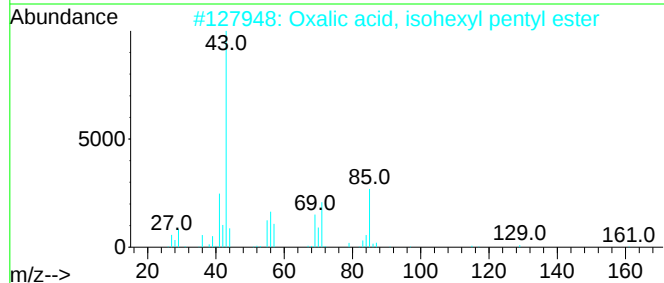
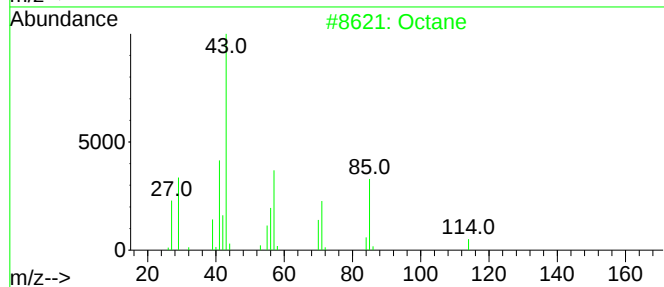
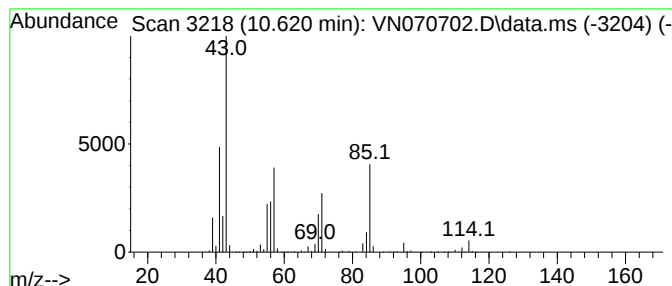
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Quant Title : SW846 8260

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

Peak Number 11 Octane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.620	127.96 ug/l	22152400	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	94
2			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	64
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	59
5			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

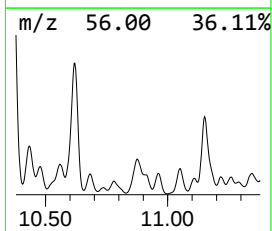
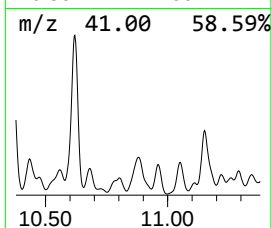
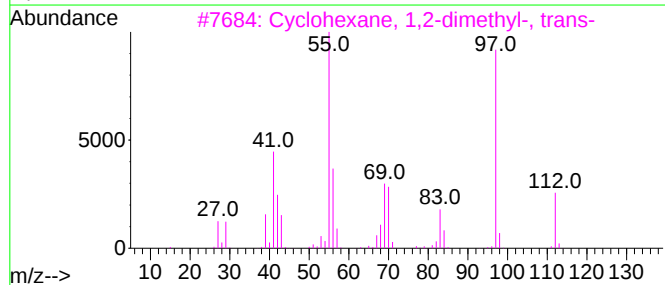
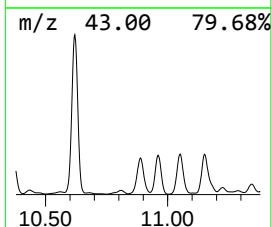
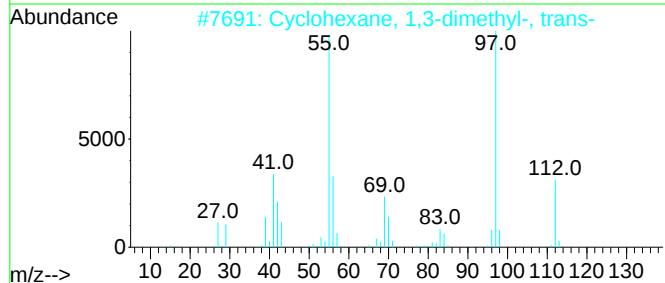
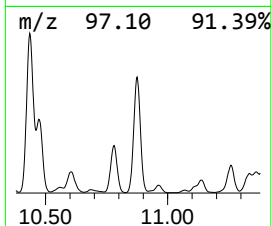
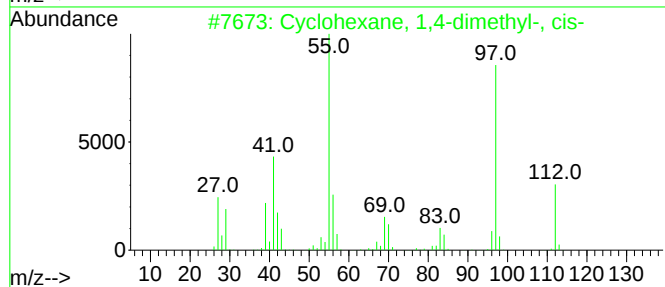
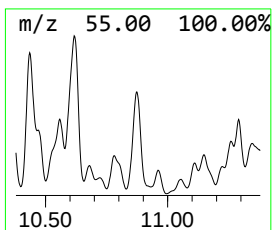
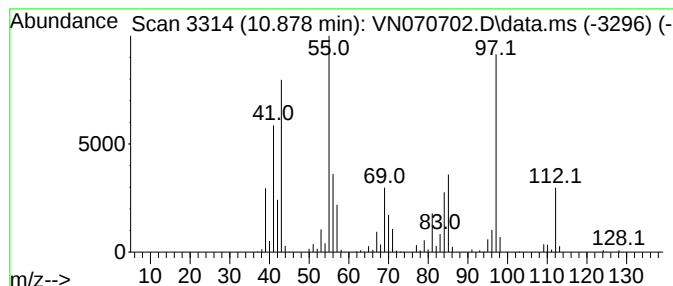
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Quant Title : SW846 8260

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

Peak Number 12 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.878	61.27 ug/l	10607100	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	81
2			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	81
3			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	76
4			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	74
5			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

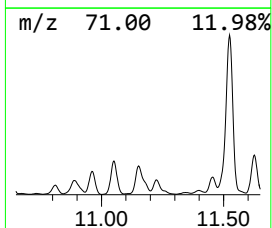
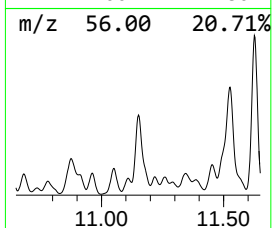
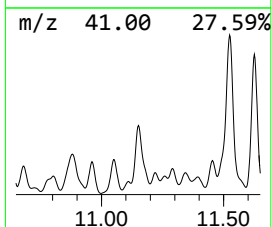
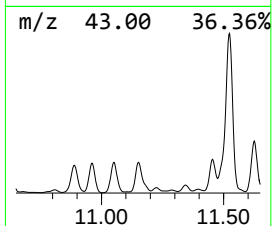
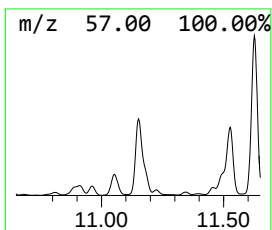
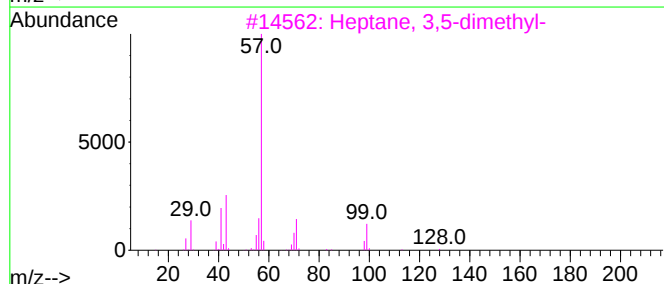
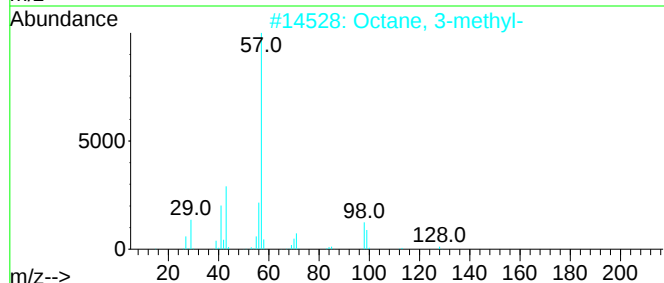
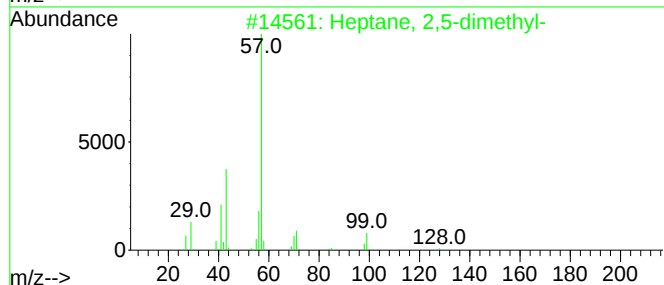
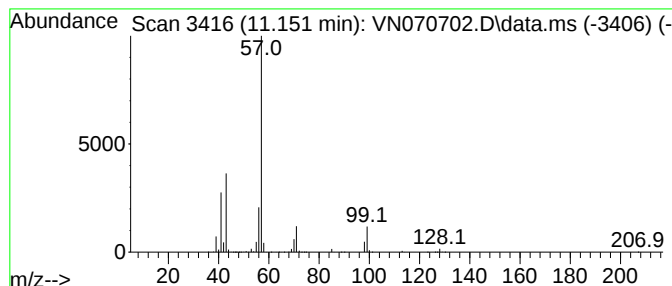
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Quant Title : SW846 8260

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

Peak Number 13 Heptane, 2,5-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.151	49.74 ug/l	8611770	Chlorobenzene-d5	11.744

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	91
2		Octane, 3-methyl-	128	C9H20	002216-33-3	83
3		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	80
4		Hexanoic acid, 1,1-dimethylethyl...	172	C10H20O2	002492-18-4	72
5		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

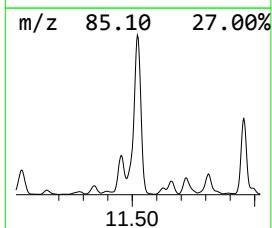
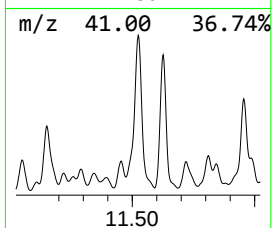
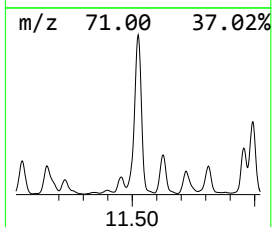
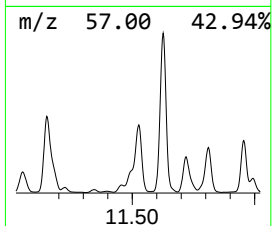
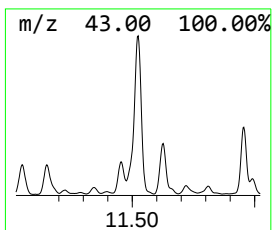
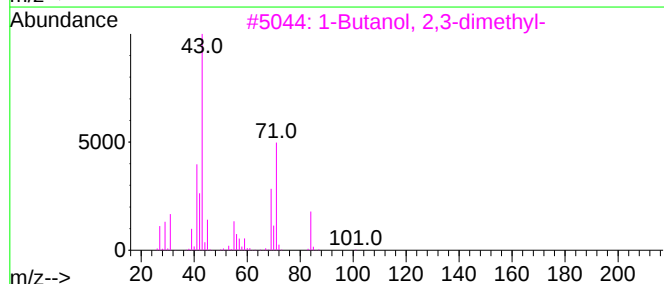
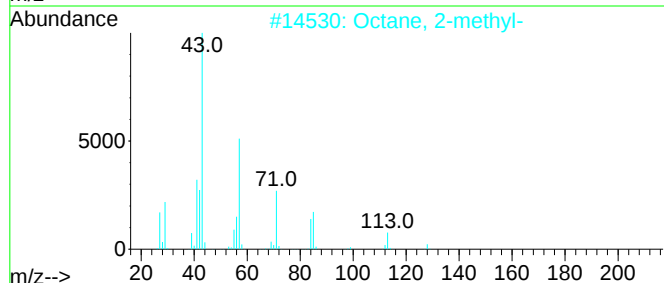
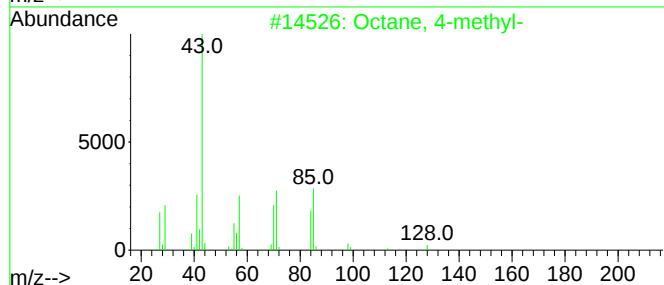
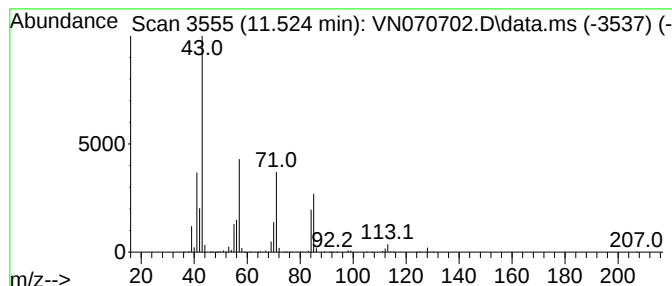
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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

Peak Number 14 Octane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.524	167.98 ug/l	29080800	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	64
2			Octane, 2-methyl-	128	C9H20	003221-61-2	64
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	59
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	58
5			Dodecane, 5-methyl-	184	C13H28	017453-93-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

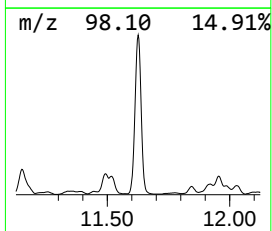
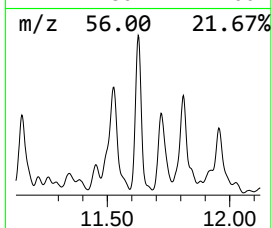
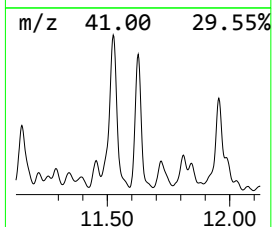
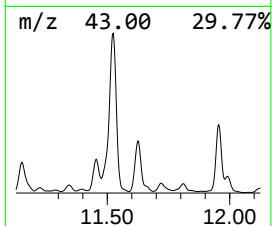
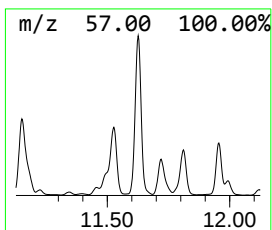
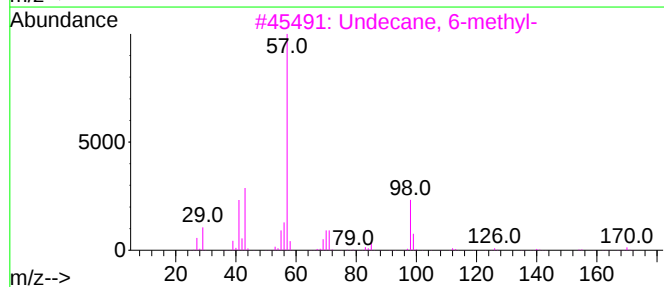
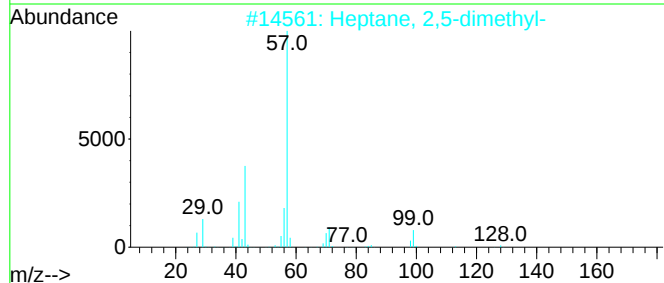
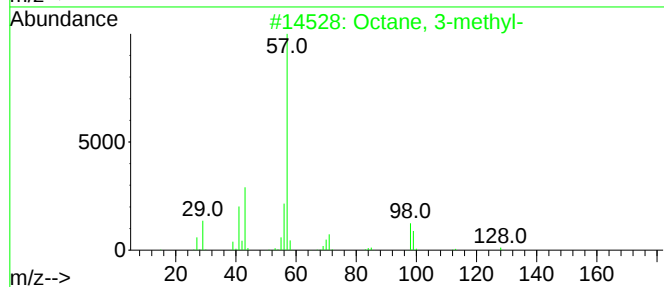
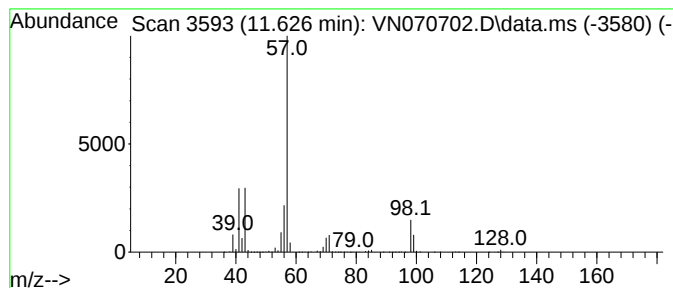
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Quant Title : SW846 8260

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

Peak Number 15 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.626	98.09 ug/l	16981100	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	91
2			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3			Undecane, 6-methyl-	170	C12H26	017302-33-9	64
4			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50
5			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011922\
Data File : VN070702.D
Acq On : 19 Jan 2022 16:12
Operator : JC/MD
Sample : N1145-08
Misc : 5.98g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A3-8-5.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.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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Hexane, 3-methyl-	8.287	39.5	ug/l	26837200	1	8.080	33934800	50.0
Hexane, 2,2-dim...	8.609	299.1	ug/l	81996700	2	8.965	13708100	50.0
Heptane	8.821	67.2	ug/l	18431300	2	8.965	13708100	50.0
Hexane, 2,4-dim...	9.507	55.9	ug/l	15324100	2	8.965	13708100	50.0
Pentane, 2,3,4-...	9.880	132.8	ug/l	36421200	2	8.965	13708100	50.0
Pentane, 2,3,3-...	10.011	169.5	ug/l	46460500	2	8.965	13708100	50.0
Heptane, 2-methyl-	10.076	65.3	ug/l	17909500	2	8.965	13708100	50.0
Heptane, 3-methyl-	10.215	112.5	ug/l	30838800	2	8.965	13708100	50.0
Hexane, 2,2,4-t...	10.365	94.4	ug/l	16342100	3	11.744	8656020	50.0
Octane	10.620	128.0	ug/l	22152400	3	11.744	8656020	50.0
Cyclohexane, 1,...	10.878	61.3	ug/l	10607100	3	11.744	8656020	50.0
Heptane, 2,5-di...	11.151	49.7	ug/l	8611770	3	11.744	8656020	50.0
Octane, 4-methyl-	11.524	168.0	ug/l	29080800	3	11.744	8656020	50.0
Octane, 3-methyl-	11.626	98.1	ug/l	16981100	3	11.744	8656020	50.0