

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
 Data File : VN070223.D
 Acq On : 18 Dec 2021 19:26
 Operator : JC/MD
 Sample : M5044-14 10X
 Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-14-4.5

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.119	406	421	447	rVB3	182463	424512	1.83%	0.150%
2	3.499	547	563	588	rBV4	145752	356774	1.53%	0.126%
3	5.138	1119	1174	1209	rBV3	836805	3863933	16.62%	1.363%
4	5.613	1321	1351	1393	rBV2	587950	2044164	8.79%	0.721%
5	6.114	1503	1538	1569	rBV3	588609	1830747	7.87%	0.646%
6	6.463	1651	1668	1691	rVB5	111370	339502	1.46%	0.120%
7	6.895	1805	1829	1858	rBV5	137547	439387	1.89%	0.155%
8	7.042	1858	1884	1903	rBV2	656212	1994691	8.58%	0.703%
9	7.141	1904	1921	1944	rVB	642443	1836504	7.90%	0.648%
10	7.841	2168	2182	2201	rVB3	190429	468110	2.01%	0.165%
11	8.021	2227	2249	2254	rBV	895475	1851268	7.96%	0.653%
12	8.075	2257	2269	2289	rVV3	2750790	7854963	33.78%	2.770%
13	8.171	2290	2305	2330	rVB3	1754619	4435688	19.07%	1.564%
14	8.295	2331	2351	2371	rBV	1869738	4362430	18.76%	1.538%
15	8.437	2386	2404	2433	rBV	1042268	2432208	10.46%	0.858%
16	8.614	2434	2470	2494	rVV	4613688	13283973	57.12%	4.685%
17	8.705	2495	2504	2526	rVB2	350821	870977	3.75%	0.307%
18	8.826	2527	2549	2577	rVB2	1221566	2682735	11.54%	0.946%
19	8.965	2580	2601	2629	rBV2	3160112	7266114	31.25%	2.562%
20	9.123	2648	2660	2675	rVB3	170375	335671	1.44%	0.118%
21	9.244	2697	2705	2742	rVB4	164896	493546	2.12%	0.174%
22	9.456	2750	2784	2796	rBV2	2300666	5921494	25.46%	2.088%
23	9.510	2796	2804	2821	rVV	1268332	2424014	10.42%	0.855%
24	9.590	2821	2834	2843	rVV	267823	561116	2.41%	0.198%
25	9.638	2844	2852	2865	rVV	405544	756240	3.25%	0.267%
26	9.730	2865	2886	2902	rVB5	330945	872163	3.75%	0.308%
27	9.882	2926	2943	2964	rVB	2846304	5854950	25.18%	2.065%
28	10.014	2965	2992	3005	rBV3	3738392	8478211	36.46%	2.990%
29	10.078	3006	3016	3026	rBV	1591555	2839794	12.21%	1.001%
30	10.215	3047	3067	3093	rBV	2092815	4905785	21.10%	1.730%
31	10.320	3094	3106	3112	rBV4	180477	345783	1.49%	0.122%
32	10.368	3112	3124	3137	rVV3	1405202	2568950	11.05%	0.906%
33	10.440	3137	3151	3175	rVV	5082429	9871883	42.45%	3.481%
34	10.623	3204	3219	3233	rVB2	1911760	3803786	16.36%	1.341%
35	10.682	3234	3241	3252	rVB3	201955	301381	1.30%	0.106%
36	10.784	3268	3279	3296	rBV6	274781	672526	2.89%	0.237%

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37	10.877	3296	3314	3335	rBV8	708369	2119115	9.11%	0.747%
38	10.963	3336	3346	3359	rVB2	470789	844891	3.63%	0.298%
39	11.052	3359	3379	3391	rBV2	514785	1045083	4.49%	0.369%
40	11.154	3407	3417	3434	rVB2	676004	1381933	5.94%	0.487%
41	11.221	3435	3442	3448	rBV5	173050	253423	1.09%	0.089%
42	11.344	3480	3488	3500	rBV3	252009	417559	1.80%	0.147%
43	11.454	3520	3529	3537	rBV3	419195	659835	2.84%	0.233%
44	11.526	3539	3556	3581	rVB3	2188224	5079536	21.84%	1.791%
45	11.626	3581	3593	3616	rBV	1641635	2944836	12.66%	1.039%
46	11.744	3619	3637	3653	rBV	5138017	9621360	41.37%	3.393%
47	11.843	3656	3674	3694	rVB	6291998	11264834	48.44%	3.973%
48	11.958	3702	3717	3739	rVB	6211039	11637709	50.05%	4.104%
49	12.181	3791	3800	3812	rVB6	308656	540967	2.33%	0.191%
50	12.253	3816	3827	3854	rVB6	566075	1481040	6.37%	0.522%
51	12.366	3860	3869	3880	rVB2	536306	892477	3.84%	0.315%
52	12.578	3938	3948	3958	rBV	975752	1718126	7.39%	0.606%
53	12.728	3993	4004	4015	rVB2	3534255	5819402	25.03%	2.052%
54	12.878	4050	4060	4063	rBV4	236088	362388	1.56%	0.128%
55	12.918	4064	4075	4093	rVB	3593266	5975575	25.70%	2.107%
56	13.015	4098	4111	4119	rBV	5025033	8404029	36.14%	2.964%
57	13.055	4120	4126	4143	rVB2	3213698	5396395	23.21%	1.903%
58	13.219	4171	4187	4204	rBV	2763621	5337086	22.95%	1.882%
59	13.366	4229	4242	4257	rBV	14451989	23254338	100.00%	8.201%
60	13.492	4274	4289	4298	rBV4	542225	1437612	6.18%	0.507%
61	13.608	4324	4332	4339	rBV2	502554	799582	3.44%	0.282%
62	13.675	4346	4357	4363	rBV	4862618	8231816	35.40%	2.903%
63	13.836	4406	4417	4423	rBV	1641428	2559265	11.01%	0.903%
64	13.876	4424	4432	4439	rVV	2427893	3505481	15.07%	1.236%
65	13.994	4467	4476	4489	rVB3	1085837	1634854	7.03%	0.577%
66	14.069	4494	4504	4514	rVB	1183838	1817195	7.81%	0.641%
67	14.131	4515	4527	4532	rBV	2521763	4033224	17.34%	1.422%
68	14.217	4548	4559	4572	rVB	4041029	6278125	27.00%	2.214%
69	14.326	4589	4600	4613	rVB3	1867019	3196714	13.75%	1.127%
70	14.461	4640	4650	4661	rBV	844976	1361043	5.85%	0.480%
71	14.538	4670	4679	4686	rBV	1795037	2701672	11.62%	0.953%
72	14.579	4687	4694	4703	rVV	2694086	3730140	16.04%	1.315%
73	14.621	4703	4710	4719	rVB2	862492	1126959	4.85%	0.397%
74	14.764	4756	4763	4769	rBV2	231387	272145	1.17%	0.096%
75	14.809	4769	4780	4788	rBV	1857822	3138167	13.49%	1.107%
76	14.927	4807	4824	4837	rBV4	2765710	6724545	28.92%	2.371%

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77	14.981	4838	4844	4860	rVB3	643372	1126931	4.85%	0.397%
78	15.083	4875	4882	4899	rVB2	394956	711424	3.06%	0.251%
79	15.195	4903	4924	4951	rVV5	1173891	3646450	15.68%	1.286%
80	15.311	4955	4967	4984	rVB5	805413	1846828	7.94%	0.651%
81	15.504	5016	5039	5054	rVB	1740601	3509539	15.09%	1.238%
82	15.611	5069	5079	5090	rBV4	348048	620040	2.67%	0.219%
83	15.804	5136	5151	5168	rBV	537890	1164528	5.01%	0.411%
84	16.107	5257	5264	5277	rVB2	157659	258569	1.11%	0.091%
85	16.617	5439	5454	5489	rVB	862484	2035412	8.75%	0.718%

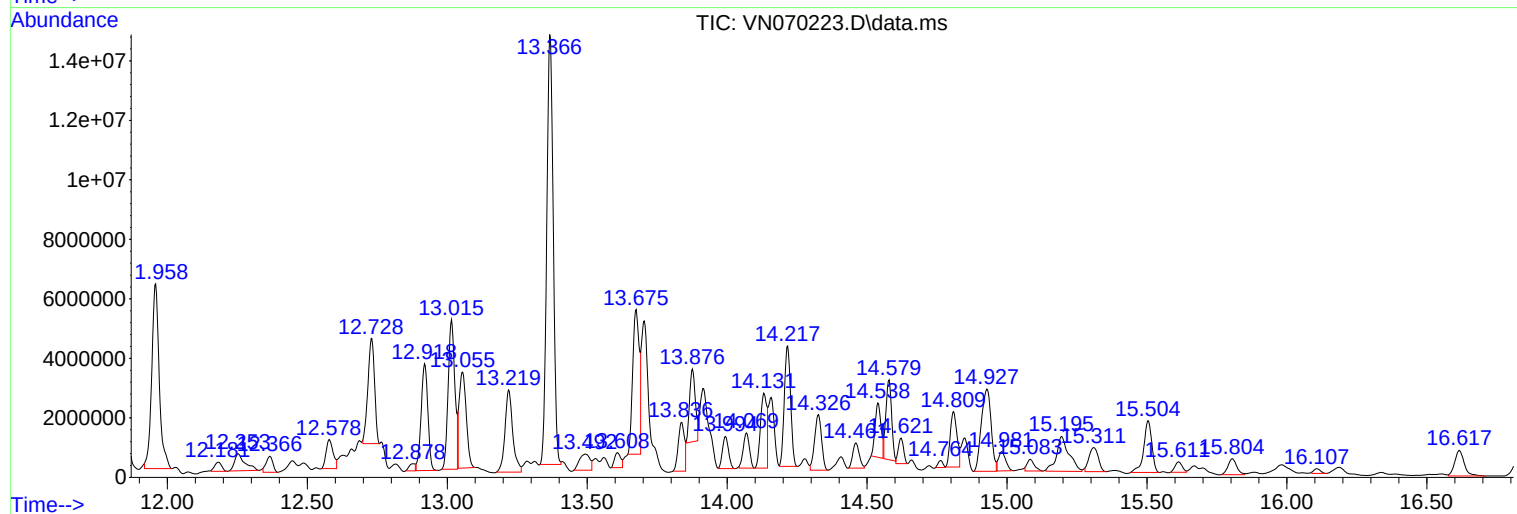
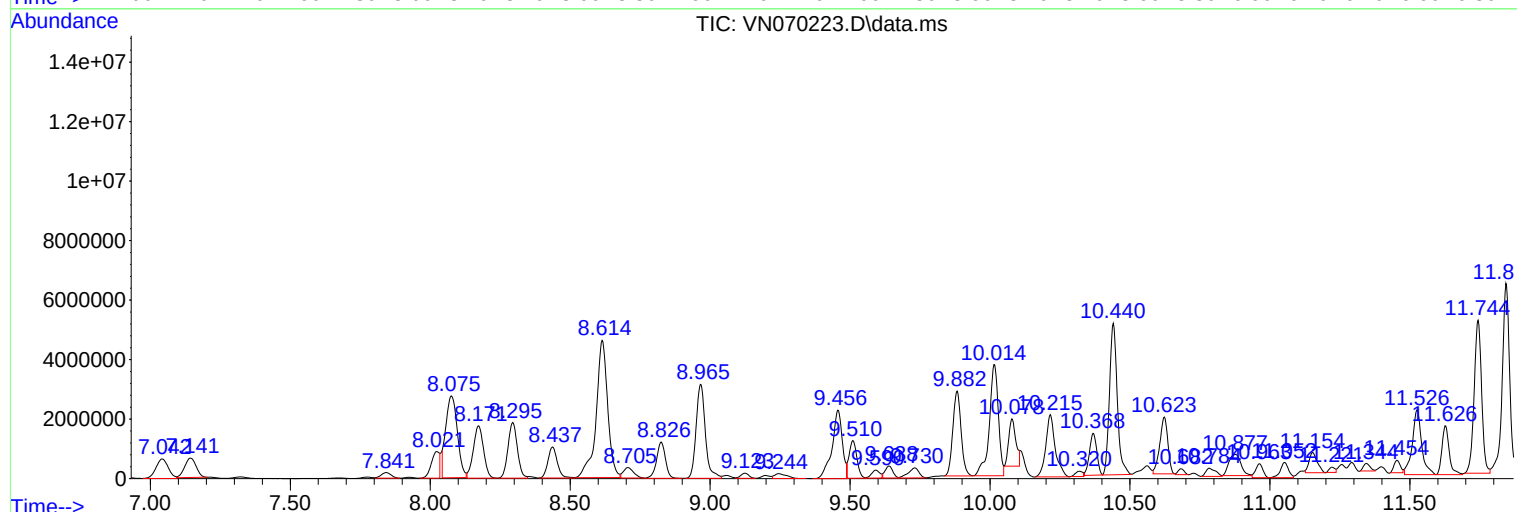
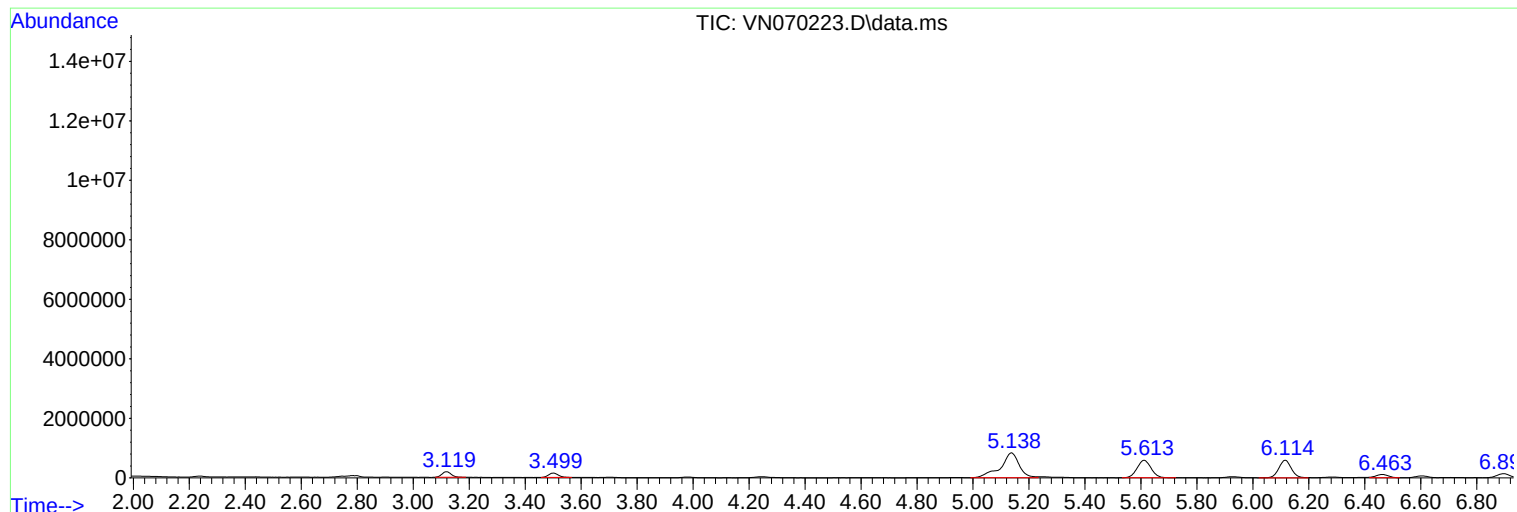
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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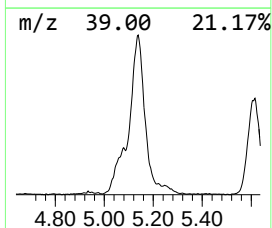
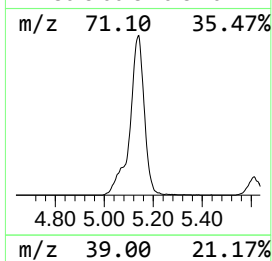
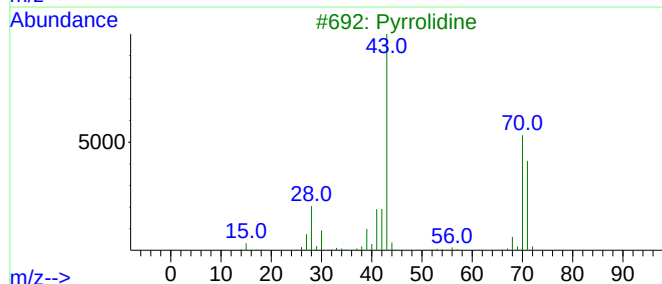
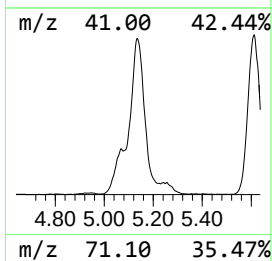
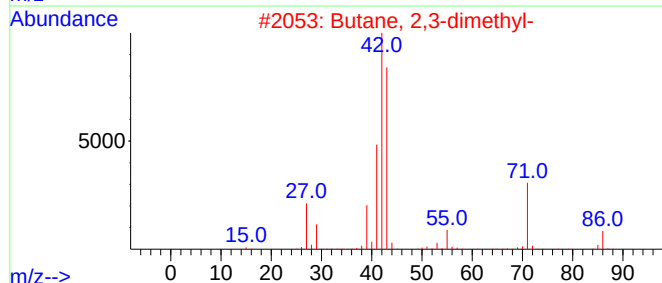
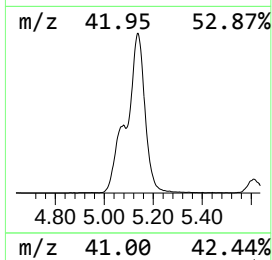
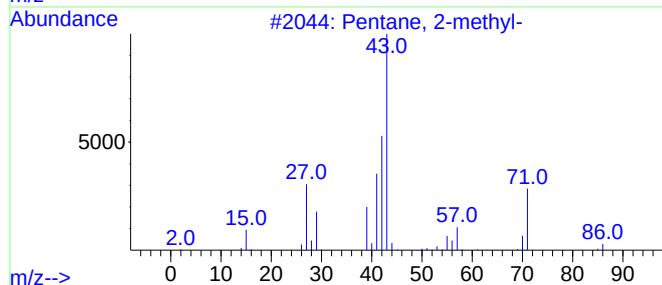
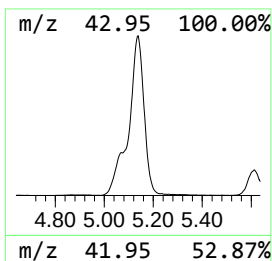
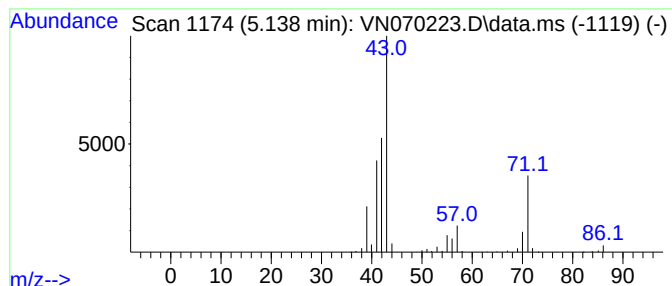
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.138	24.60 ug/l	3863930	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53
3			Pyrrolidine	71	C4H9N	000123-75-1	37
4			Pentane	72	C5H12	000109-66-0	33
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	33



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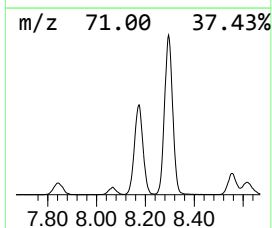
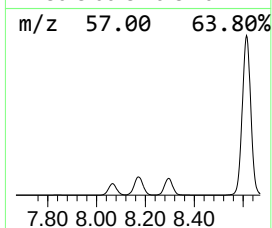
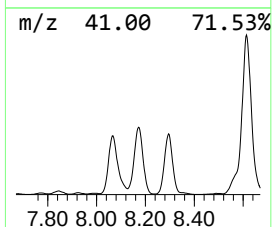
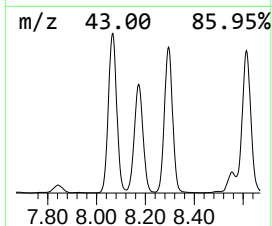
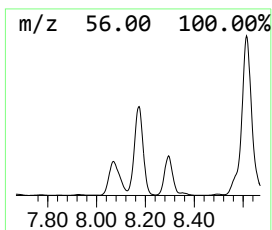
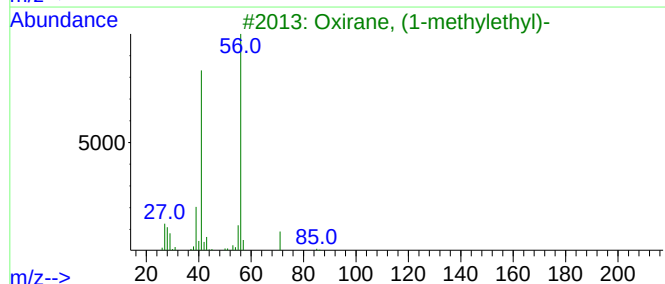
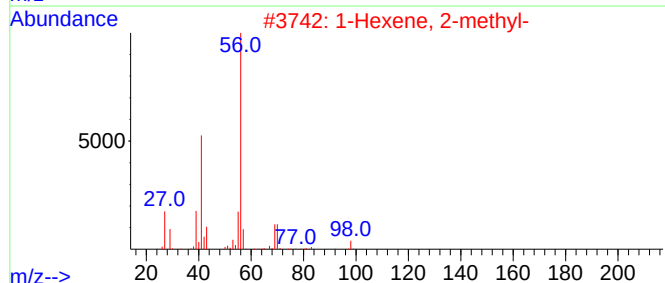
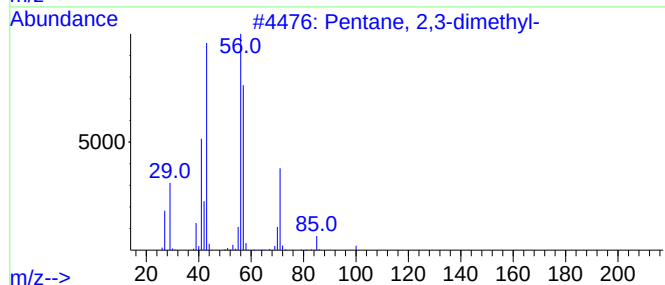
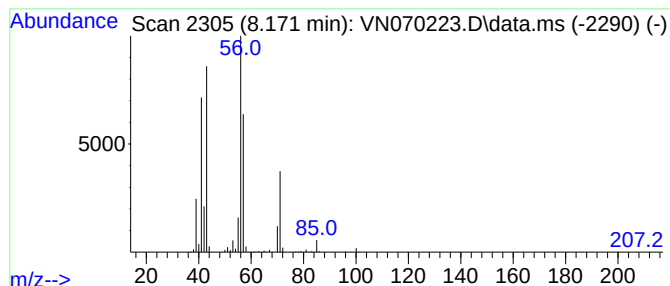
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.171	28.23 ug/l	4435690	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	37
4			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	37
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	28



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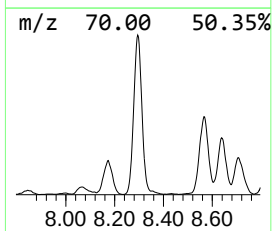
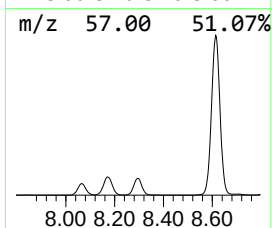
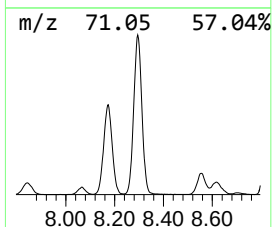
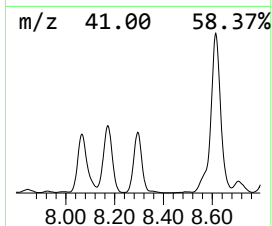
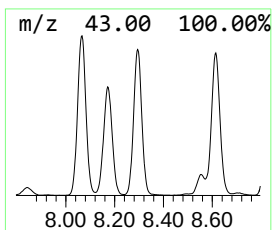
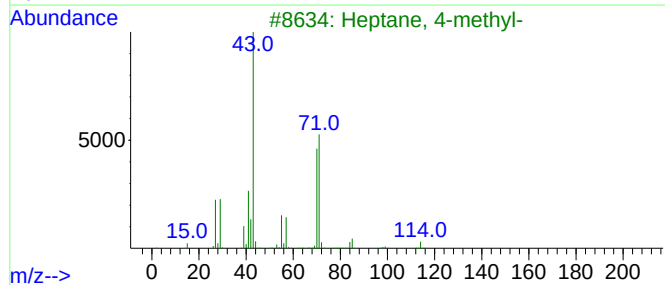
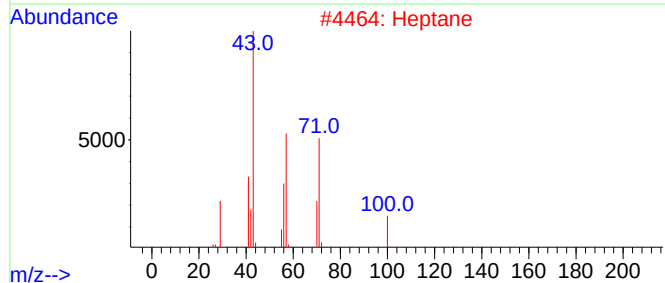
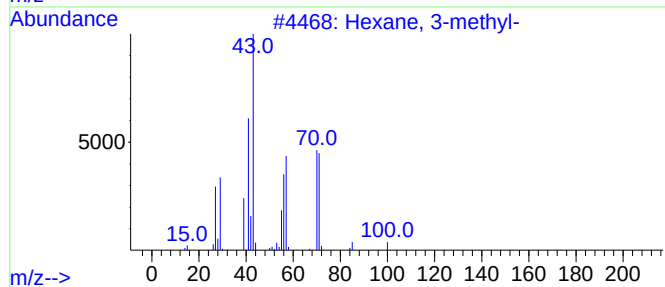
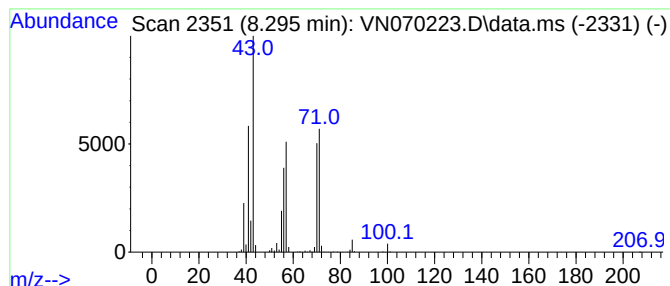
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.295	27.77 ug/l	4362430	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane	100	C7H16	000142-82-5	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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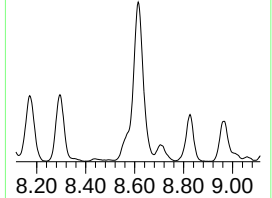
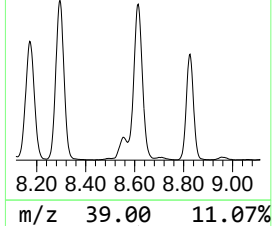
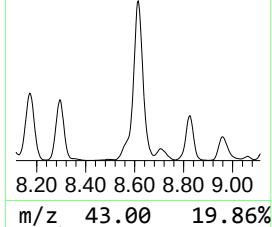
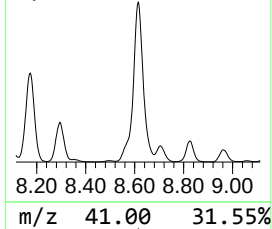
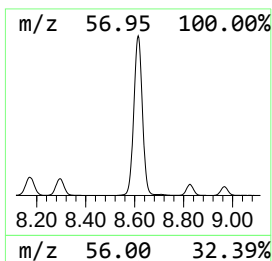
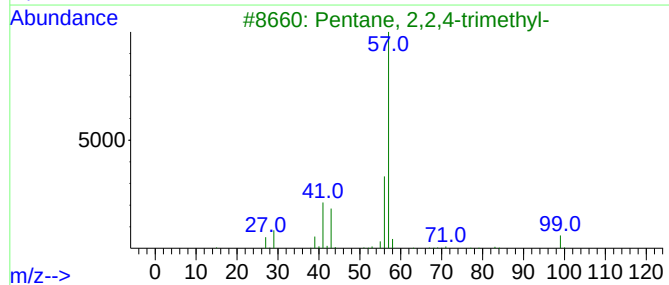
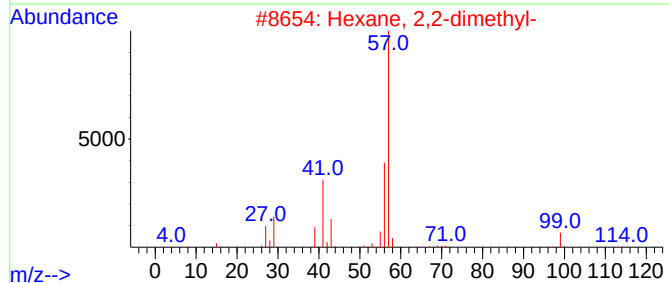
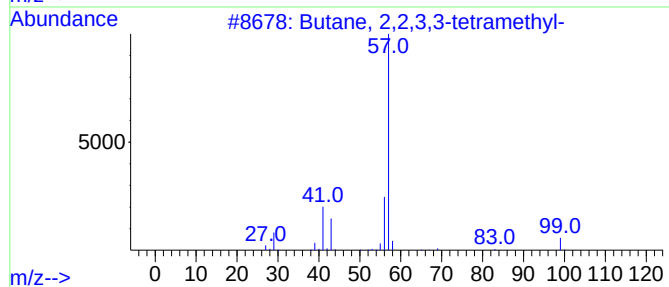
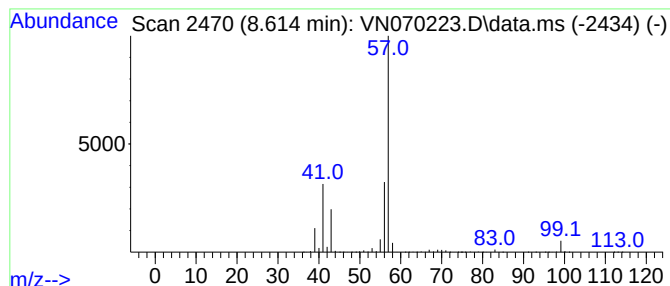
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	91.41 ug/l	13284000	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

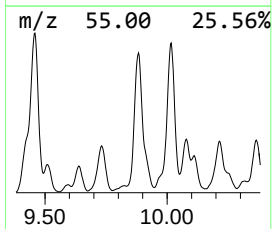
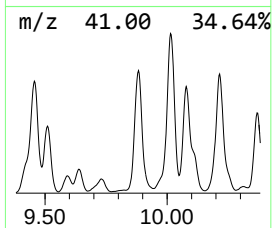
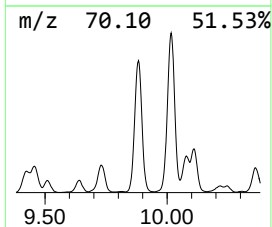
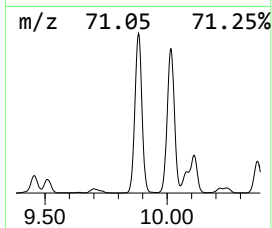
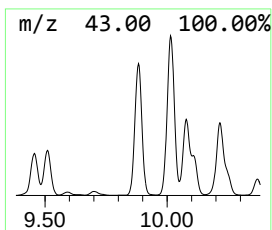
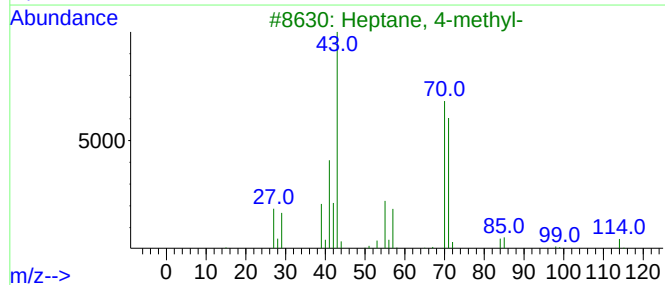
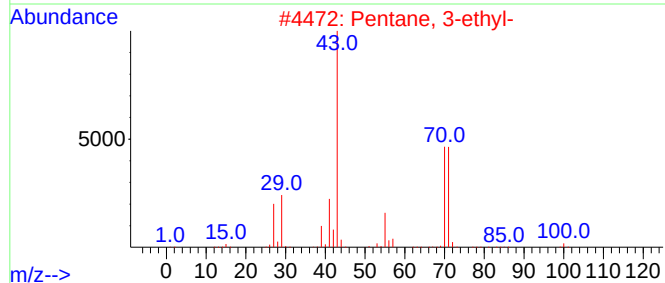
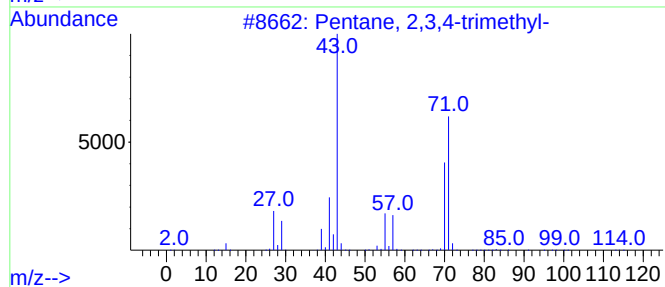
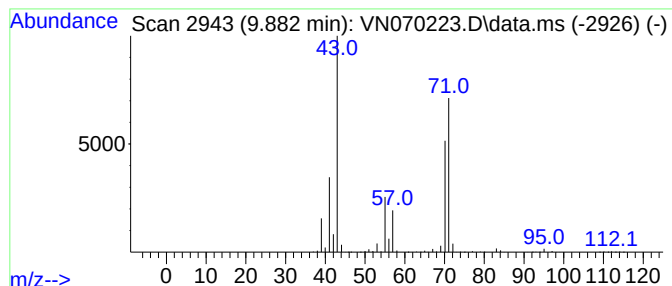
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.882	40.29 ug/l	5854950	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	74
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

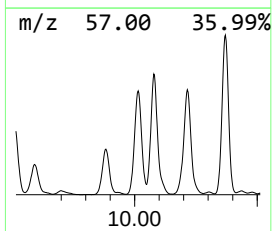
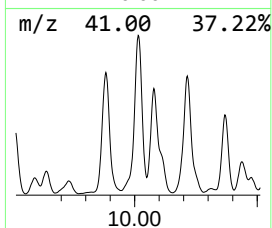
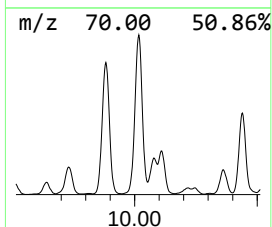
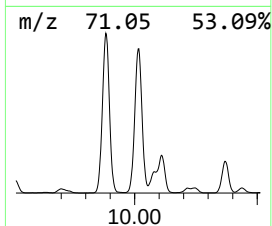
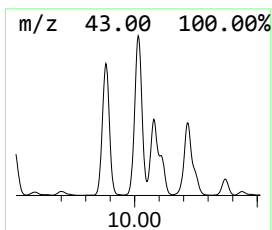
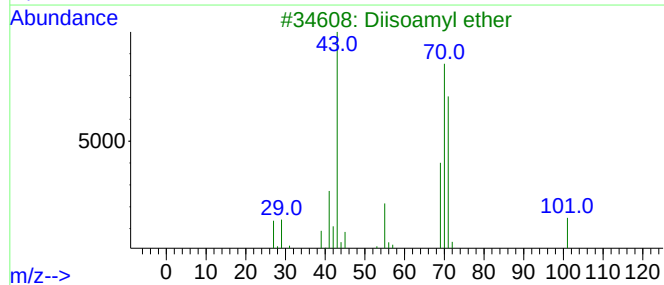
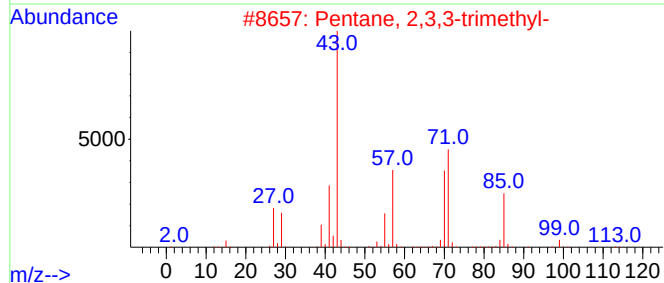
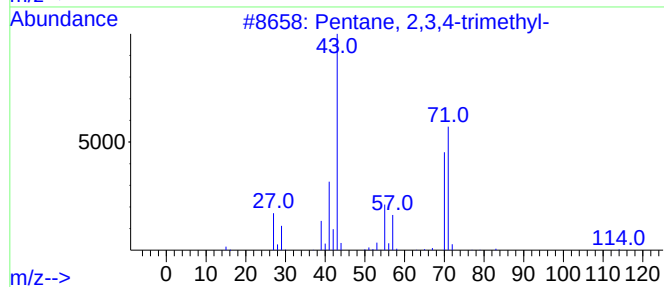
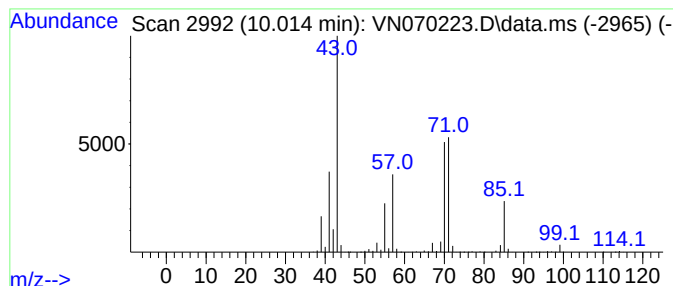
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	58.34 ug/l	8478210	1,4-Difluorobenzene	8.968

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	72
3			Diisoamyl ether	158	C10H22O	000544-01-4	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	56
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

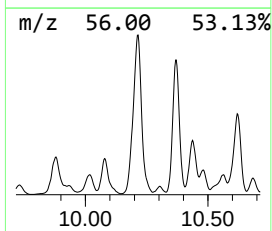
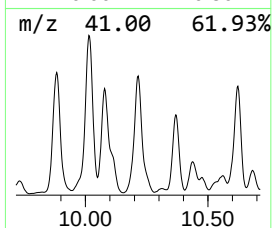
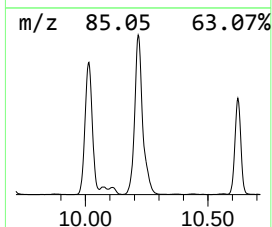
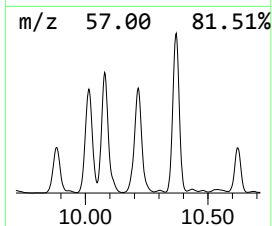
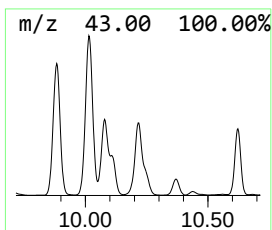
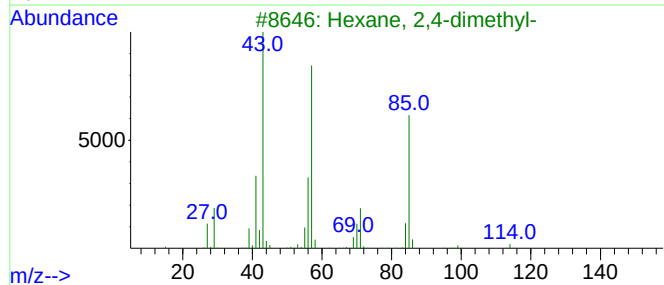
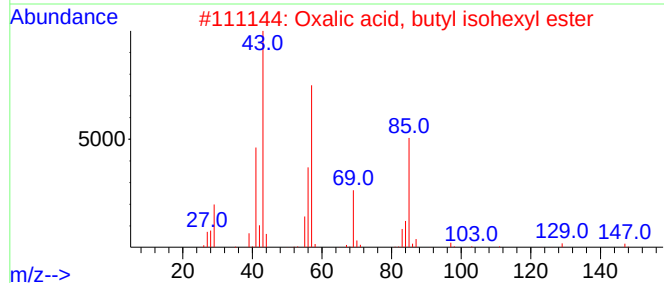
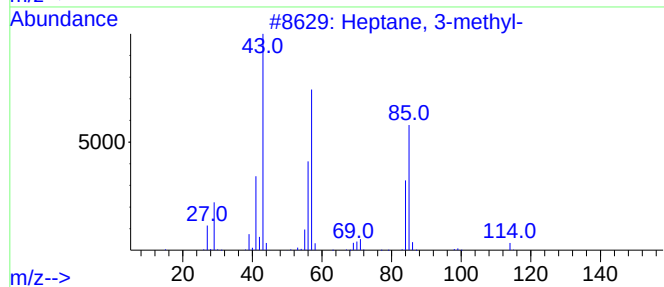
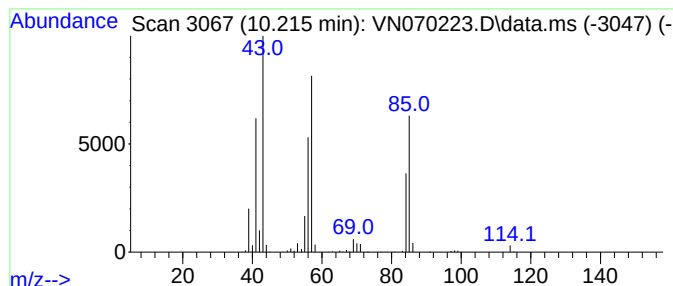
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Quant Title : SW846 8260

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

Peak Number 7 Heptane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	33.76 ug/l	4905790	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	78
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4			Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	59
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

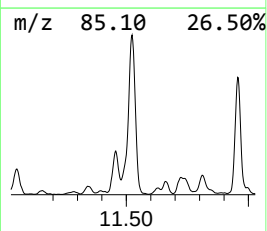
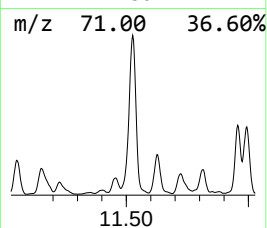
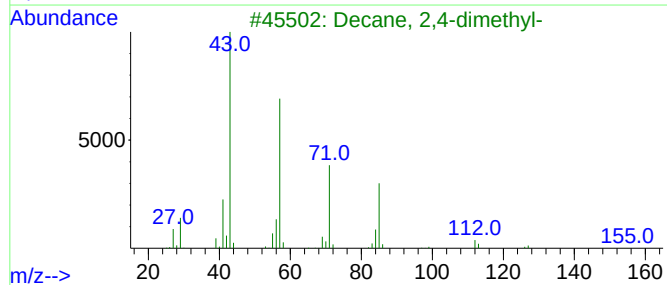
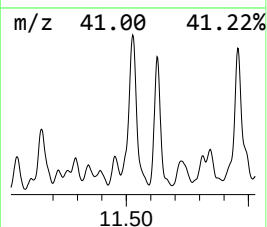
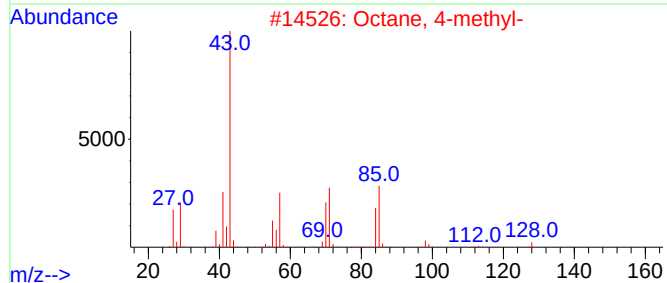
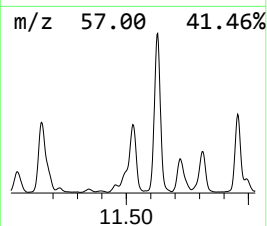
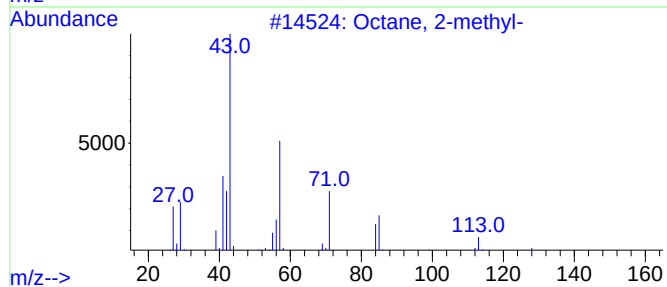
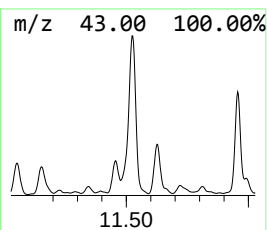
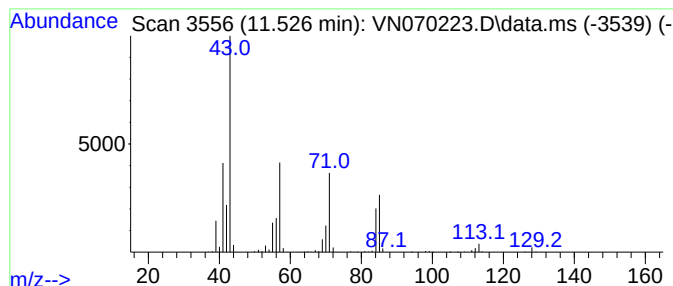
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.527	26.40 ug/l	5079540	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	72
2			Octane, 4-methyl-	128	C9H20	002216-34-4	64
3			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53
4			Octane	114	C8H18	000111-65-9	53
5			Ether, hexyl pentyl	172	C11H24O	032357-83-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DA-14-4.5

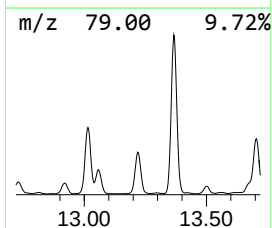
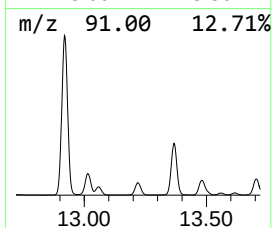
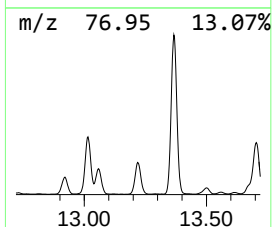
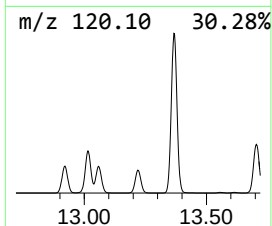
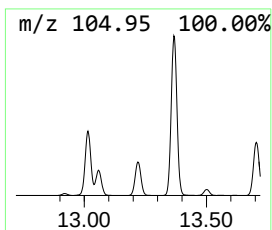
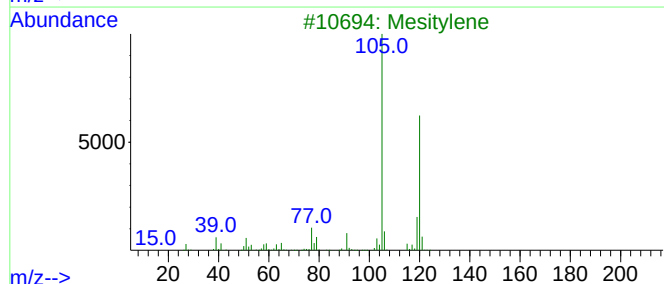
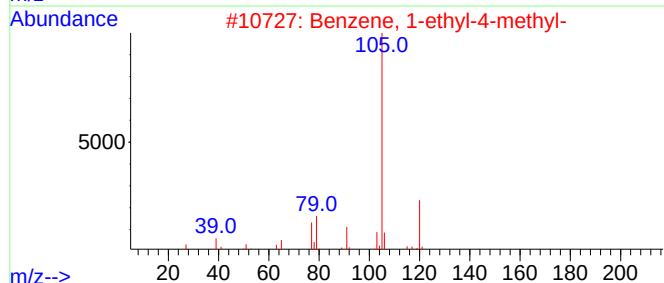
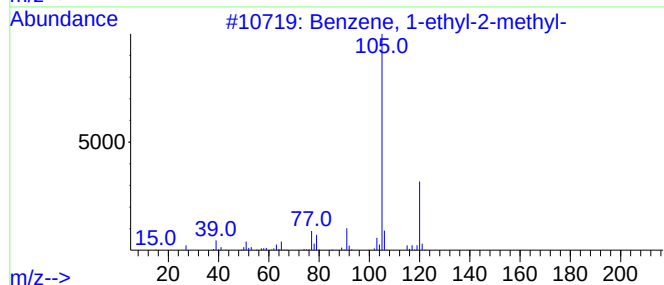
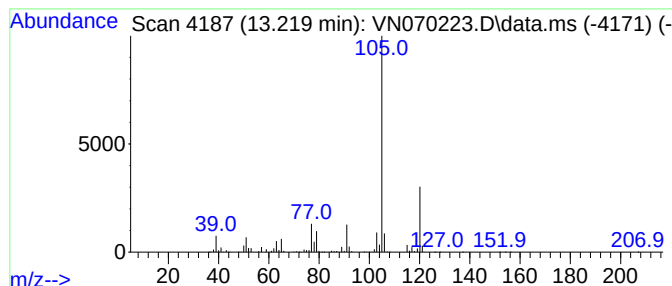
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	32.42 ug/l	5337090	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-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

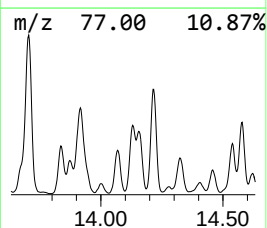
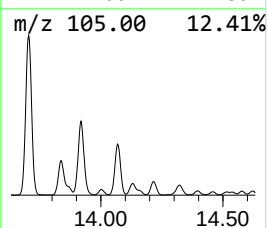
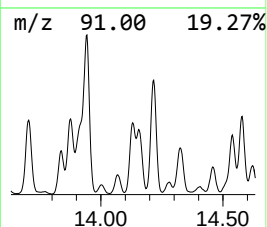
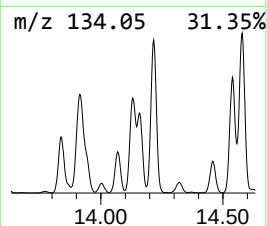
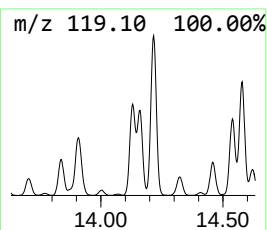
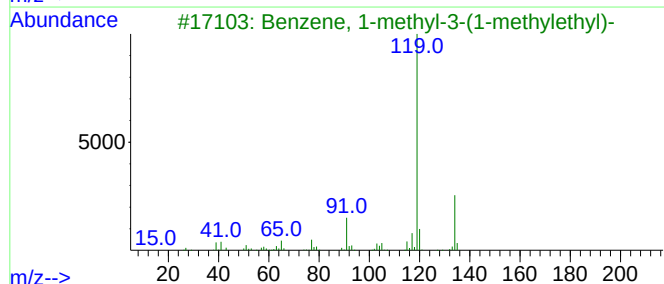
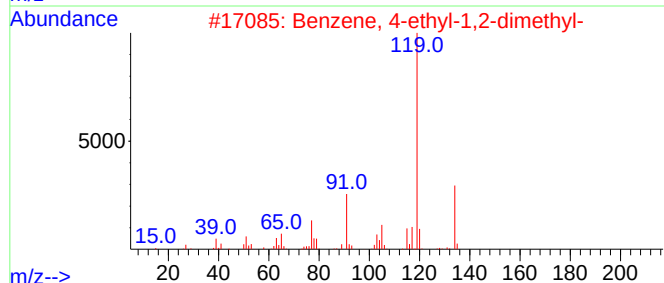
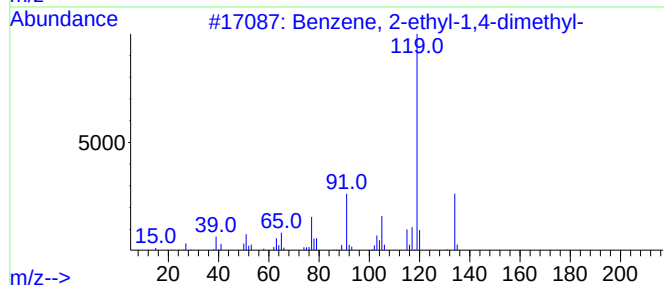
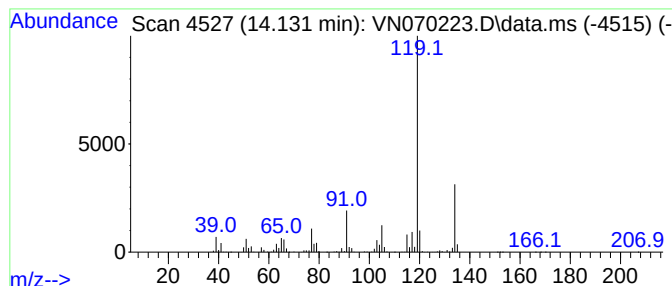
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 11 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.131	24.50 ug/l	4033220	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

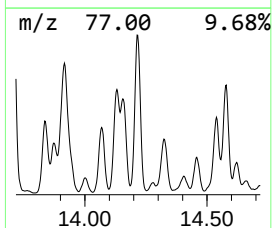
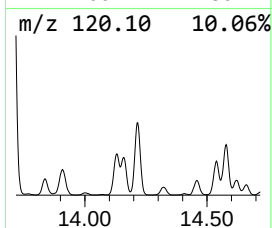
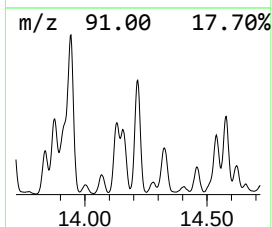
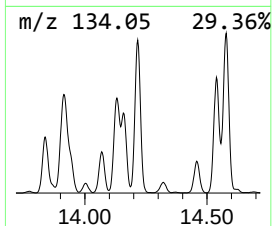
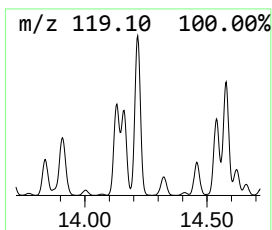
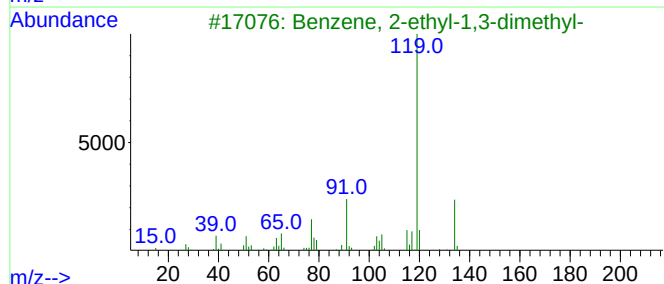
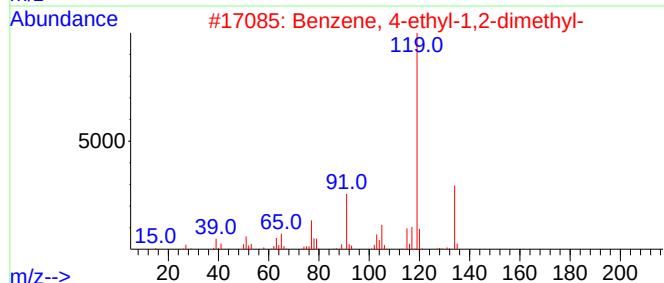
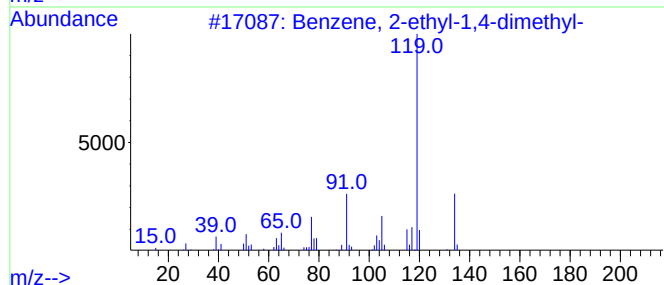
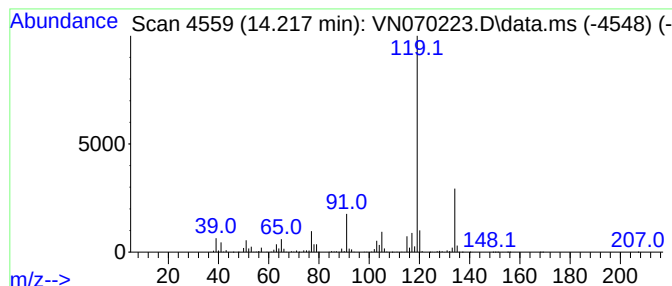
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Quant Title : SW846 8260

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

Peak Number 12 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	38.13 ug/l	6278130	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

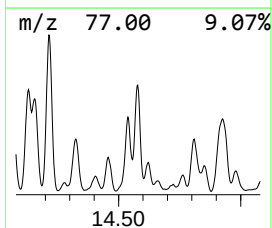
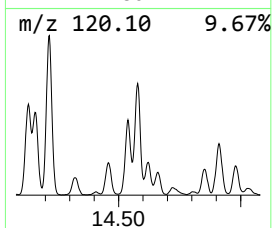
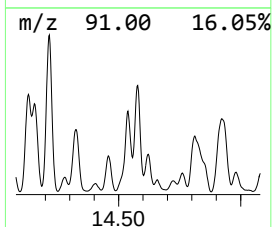
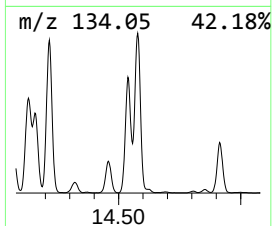
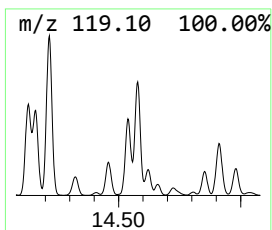
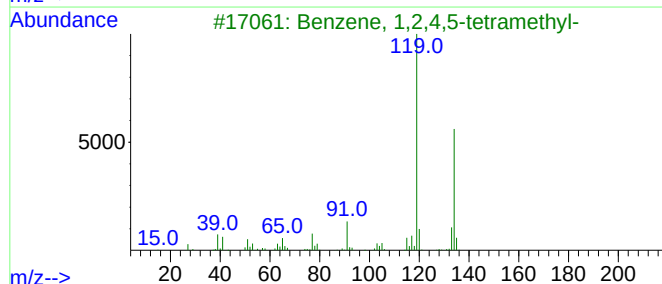
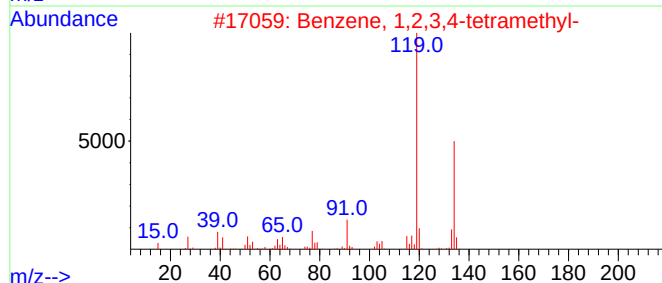
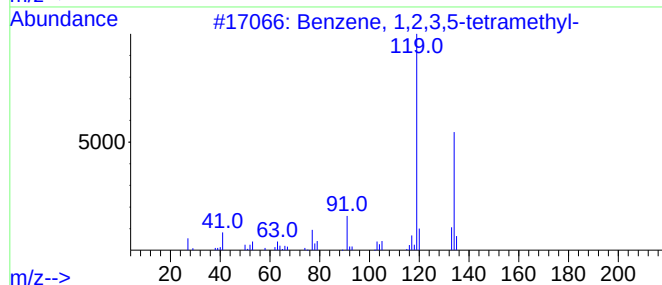
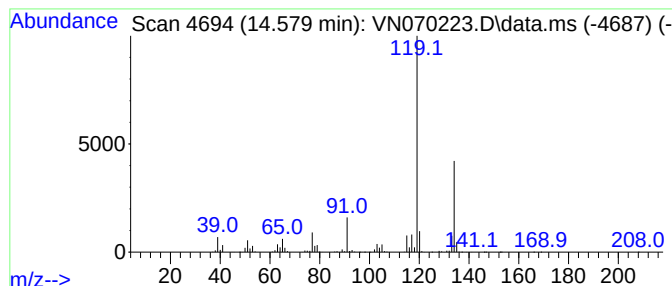
Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

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 13 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.579	22.66 ug/l	3730140	1,4-Dichlorobenzene-d4			13.675
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	97
2	Benzene, 1,2,3,4-tetramethyl-		134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-		134	C10H14	000095-93-2	94
4	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	94
5	o-Cymene		134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

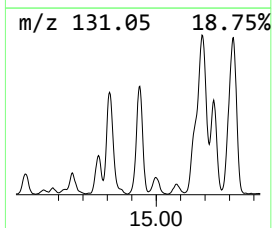
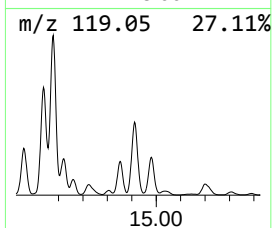
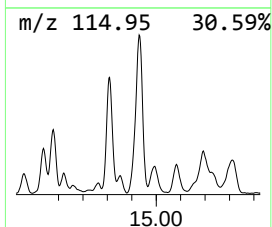
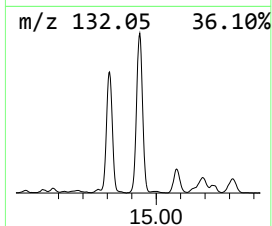
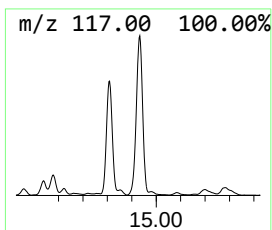
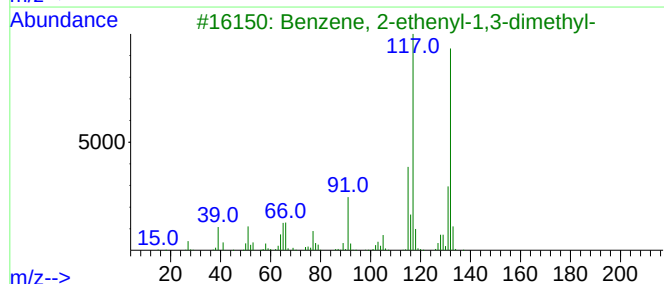
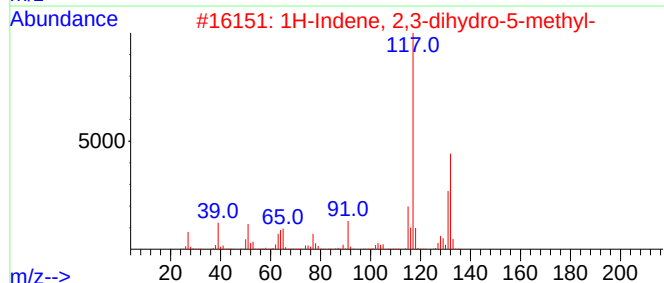
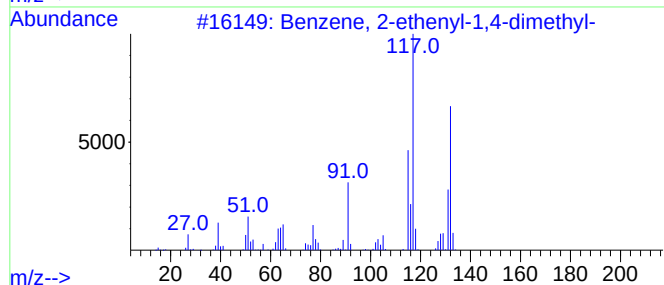
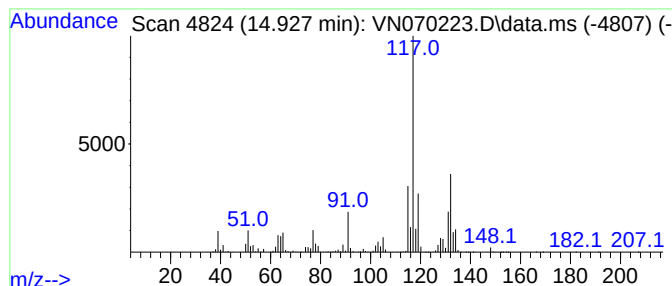
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Quant Title : SW846 8260

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

Peak Number 14 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	40.84 ug/l	6724550	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	81
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	81
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

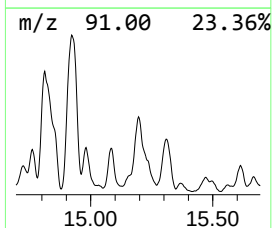
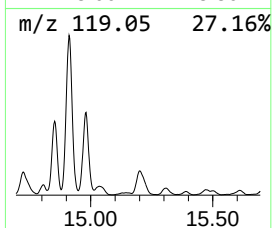
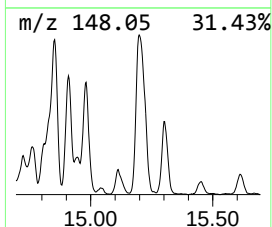
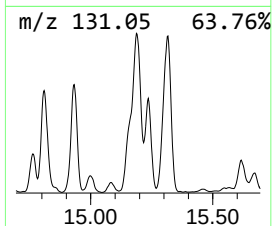
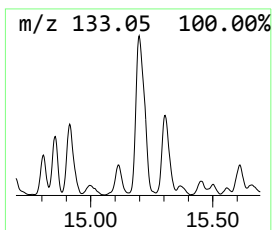
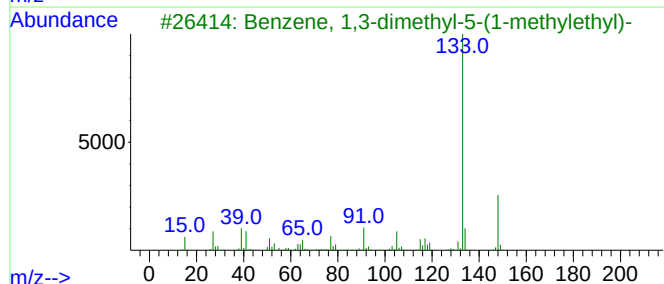
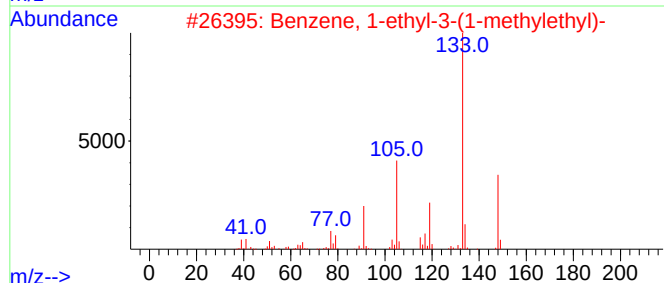
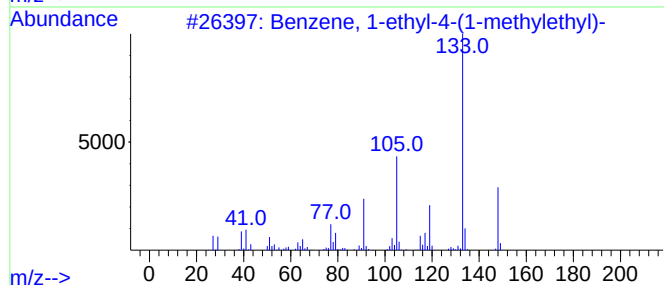
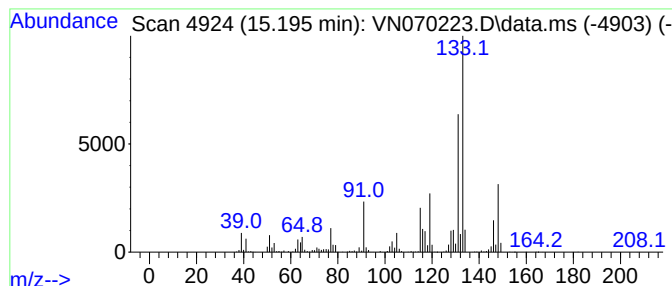
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 15 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.195	22.15 ug/l	3646450	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	64
2			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	58
3			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	49
4			Benzene, pentamethyl-	148	C11H16	000700-12-9	49
5			Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121821\
Data File : VN070223.D
Acq On : 18 Dec 2021 19:26
Operator : JC/MD
Sample : M5044-14 10X
Misc : 6.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-14-4.5

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
Pentane, 2-methyl-	5.138	24.6	ug/l	3863930	1	8.086	7854960	50.0
Pentane, 2,3-di...	8.171	28.2	ug/l	4435690	1	8.086	7854960	50.0
Hexane, 3-methyl-	8.295	27.8	ug/l	4362430	1	8.086	7854960	50.0
Butane, 2,2,3,3...	8.614	91.4	ug/l	13284000	2	8.968	7266110	50.0
Pentane, 2,3,4-...	9.882	40.3	ug/l	5854950	2	8.968	7266110	50.0
Pentane, 2,3,3-...	10.014	58.3	ug/l	8478210	2	8.968	7266110	50.0
Heptane, 3-methyl-	10.215	33.8	ug/l	4905790	2	8.968	7266110	50.0
Octane, 2-methyl-	11.527	26.4	ug/l	5079540	3	11.744	9621360	50.0
Benzene, 1-ethy...	13.219	32.4	ug/l	5337090	4	13.675	8231820	50.0
Benzene, 2-ethy...	14.131	24.5	ug/l	4033220	4	13.675	8231820	50.0
Benzene, 4-ethy...	14.217	38.1	ug/l	6278130	4	13.675	8231820	50.0
Benzene, 1,2,3,...	14.579	22.7	ug/l	3730140	4	13.675	8231820	50.0
Benzene, 2-ethe...	14.927	40.8	ug/l	6724550	4	13.675	8231820	50.0
Benzene, 1-ethy...	15.195	22.1	ug/l	3646450	4	13.675	8231820	50.0