

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
 Data File : VN072968.D
 Acq On : 20 Jun 2022 17:54
 Operator : JC\MD
 Sample : N3370-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-09

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN072968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	196	204	215	rVB	42720	95779	3.77%	0.512%
2	5.004	517	530	539	rBV3	24347	92386	3.63%	0.494%
3	5.299	567	580	595	rBV2	38576	136508	5.37%	0.730%
4	5.546	609	622	635	rBV4	47476	169731	6.68%	0.907%
5	6.963	848	863	876	rBV3	137571	424330	16.69%	2.269%
6	7.769	986	1000	1010	rBV4	16043	53087	2.09%	0.284%
7	7.951	1021	1031	1036	rBV	226891	532670	20.95%	2.848%
8	8.016	1036	1042	1049	rVV	442578	991182	38.99%	5.299%
9	8.104	1049	1057	1071	rVB	576837	1430758	56.28%	7.650%
10	8.369	1093	1102	1115	rBV	229916	529029	20.81%	2.829%
11	8.545	1115	1132	1145	rVV	1034927	2541996	100.00%	13.591%
12	8.898	1184	1192	1206	rBV	586792	1222261	48.08%	6.535%
13	9.392	1264	1276	1280	rBV4	46280	139803	5.50%	0.747%
14	9.445	1280	1285	1291	rVB4	23452	48099	1.89%	0.257%
15	9.522	1291	1298	1305	rBV2	85985	172820	6.80%	0.924%
16	9.663	1310	1322	1330	rVV3	24065	68354	2.69%	0.365%
17	9.816	1339	1348	1359	rBV	734910	1453757	57.19%	7.773%
18	9.945	1359	1370	1386	rVB	1109078	2281214	89.74%	12.197%
19	10.133	1395	1402	1407	rBV2	46656	89952	3.54%	0.481%
20	10.181	1407	1410	1421	rVB4	11259	26148	1.03%	0.140%
21	10.304	1421	1431	1436	rBV3	82195	156356	6.15%	0.836%
22	10.375	1436	1443	1457	rVB	806854	1507383	59.30%	8.059%
23	10.545	1466	1472	1483	rVB7	18891	57642	2.27%	0.308%
24	10.716	1496	1501	1505	rBV3	15751	29155	1.15%	0.156%
25	10.804	1505	1516	1524	rVB9	51762	144778	5.70%	0.774%
26	11.192	1574	1582	1587	rBV7	16815	36964	1.45%	0.198%
27	11.680	1657	1665	1676	rBV	821042	1436573	56.51%	7.681%
28	11.922	1702	1706	1719	rVB7	11788	33329	1.31%	0.178%
29	12.669	1825	1833	1841	rBV	643529	1111592	43.73%	5.943%
30	13.416	1956	1960	1967	rVB4	14309	25983	1.02%	0.139%
31	13.610	1985	1993	2008	rBV	794918	1351986	53.19%	7.229%
32	14.080	2066	2073	2078	rBV	37228	63214	2.49%	0.338%
33	14.263	2098	2104	2109	rBV3	19387	32267	1.27%	0.173%
34	14.339	2109	2117	2122	rVB7	20320	40901	1.61%	0.219%
35	14.468	2131	2139	2148	rVB5	23471	53707	2.11%	0.287%
36	14.627	2162	2166	2172	rBV5	16144	25582	1.01%	0.137%

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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

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37	14.745	2181	2186	2191	rBV5	25593	41707	1.64%	0.223%
38	14.868	2203	2207	2212	rVB3	15888	27458	1.08%	0.147%
39	15.127	2245	2251	2255	rBV5	13531	26981	1.06%	0.144%

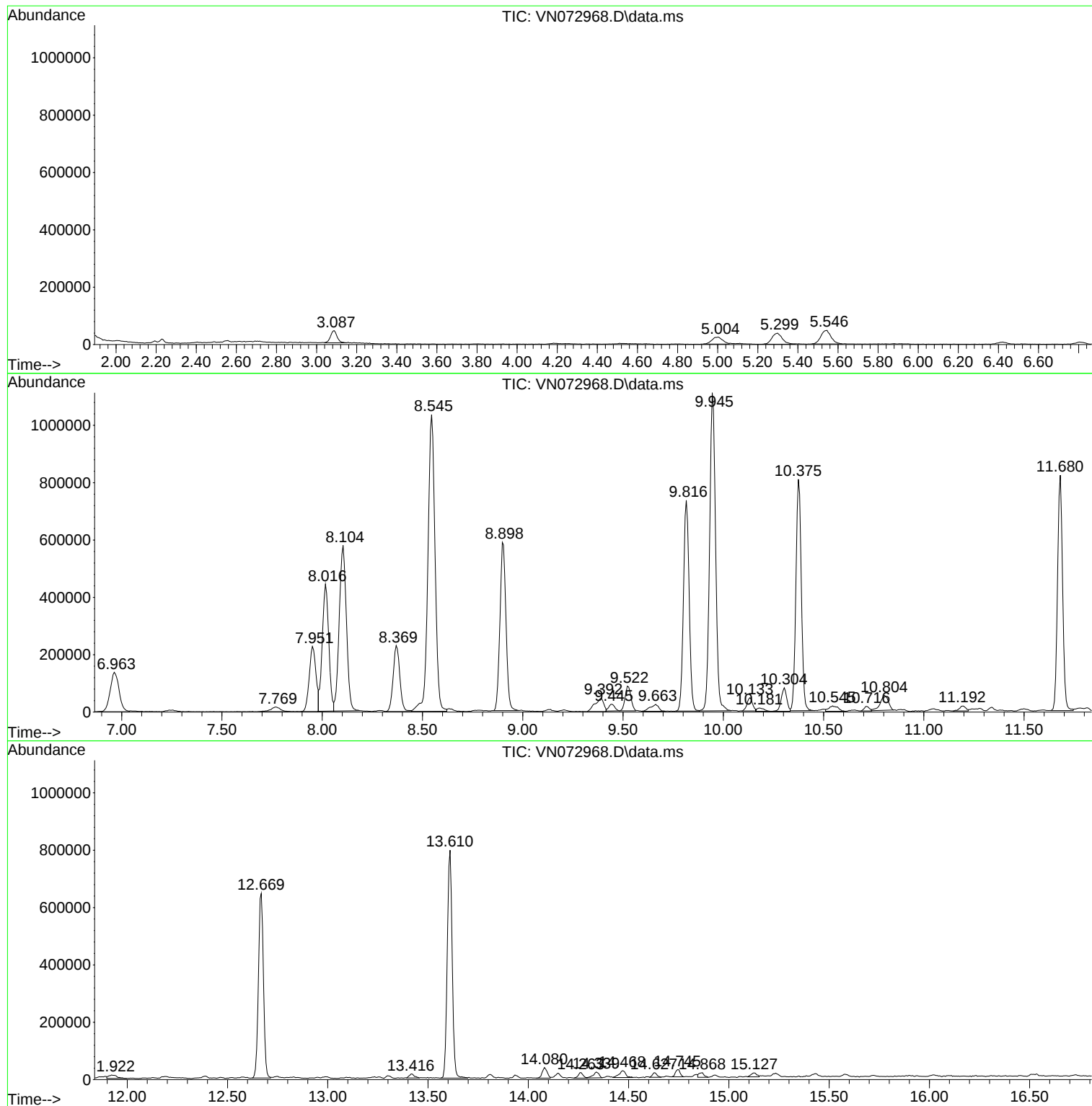
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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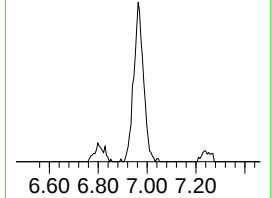
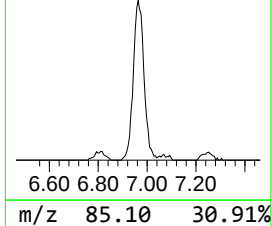
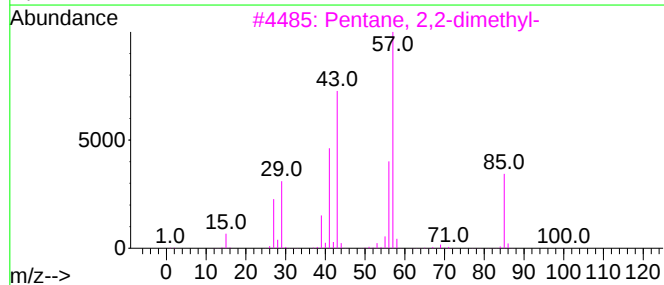
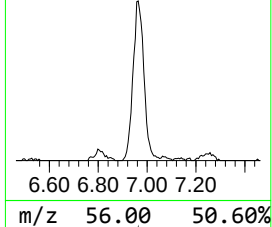
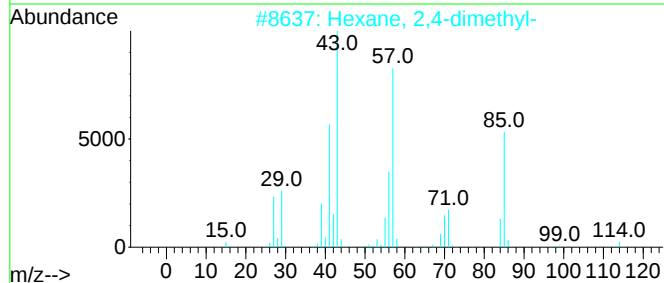
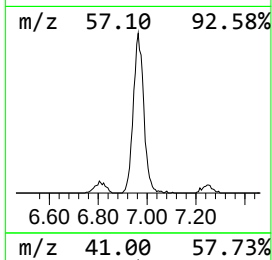
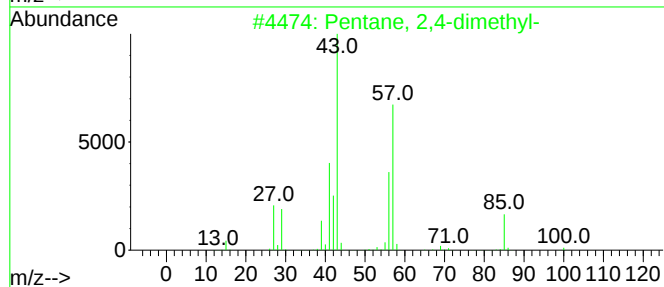
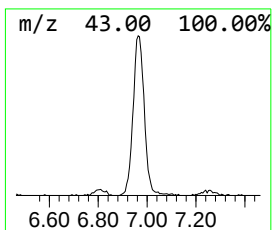
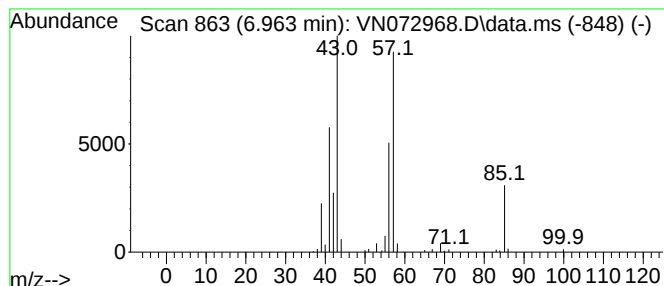
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	21.41 ug/l	424330	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	87
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
5			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	50



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Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

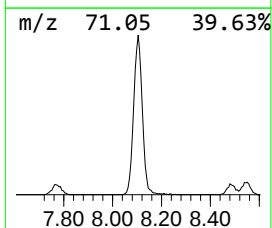
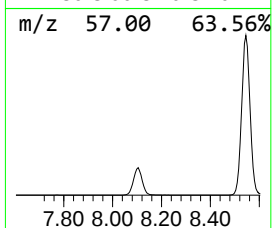
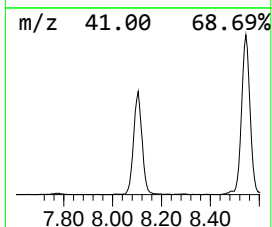
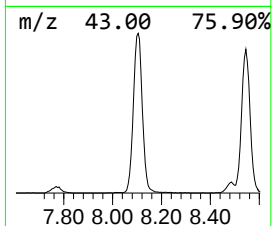
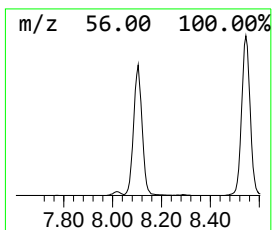
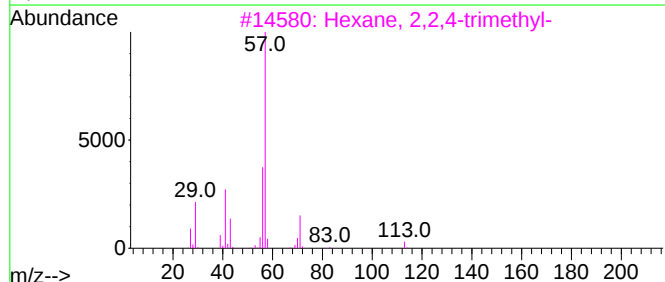
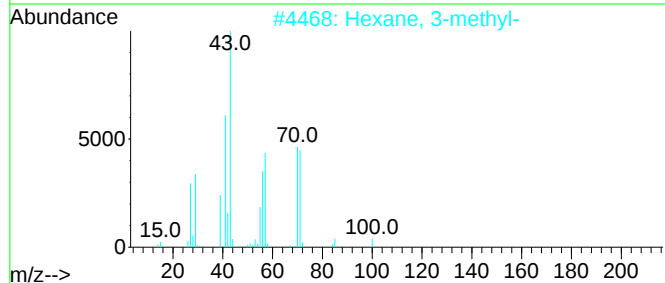
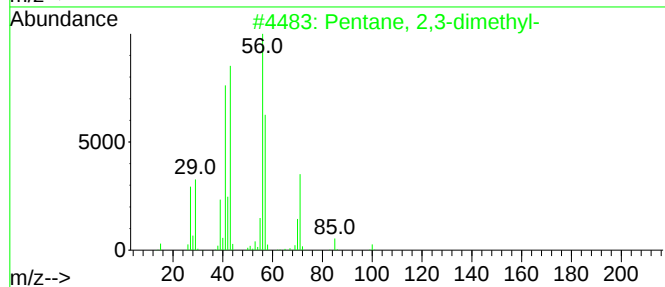
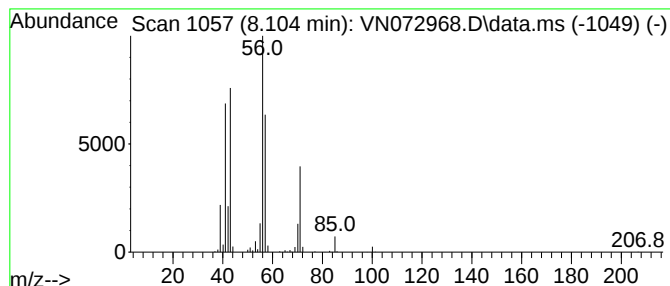
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	72.17 ug/l	1430760	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	38



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MSVOA_N
ClientSampleId :
TOLL-MW-09

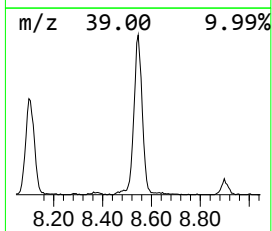
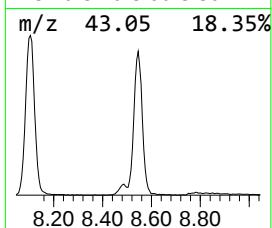
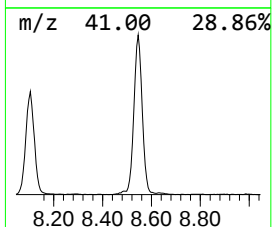
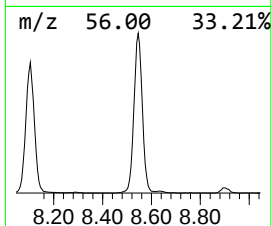
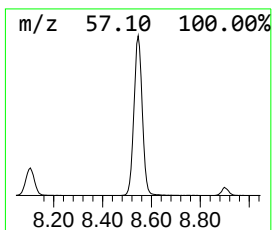
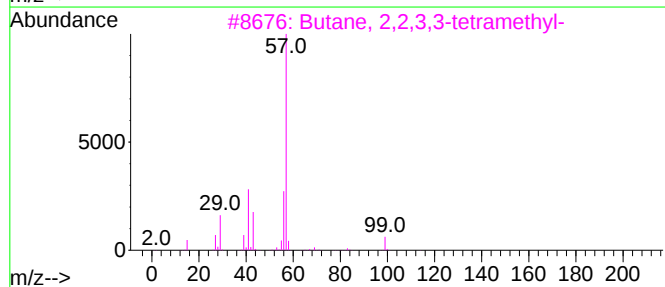
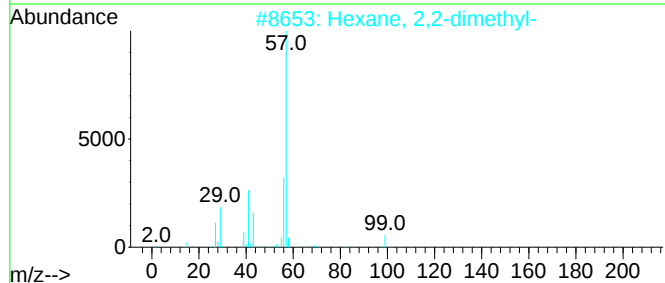
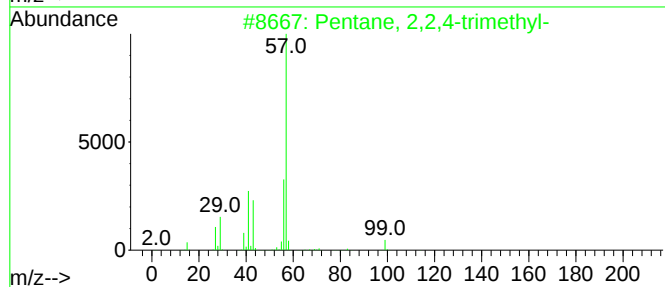
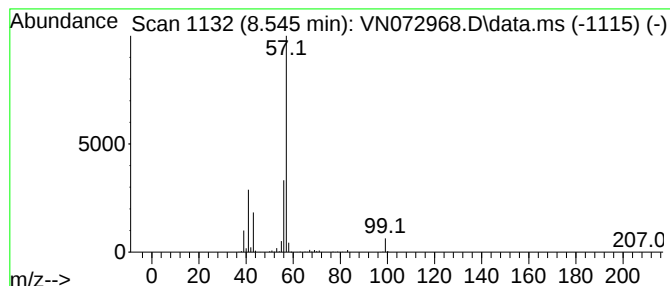
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	103.99 ug/l	2542000	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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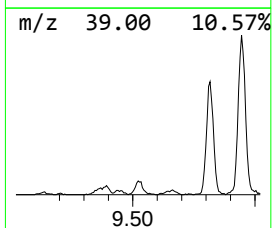
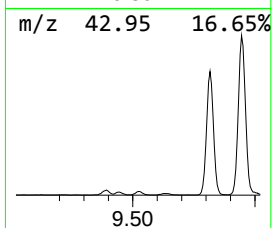
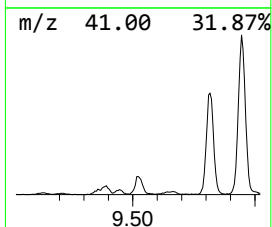
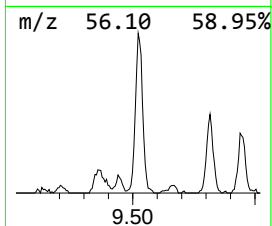
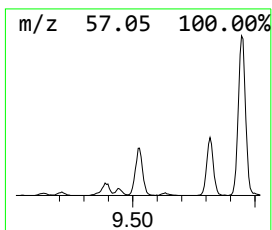
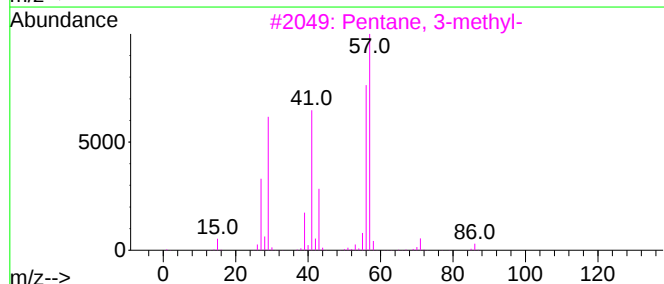
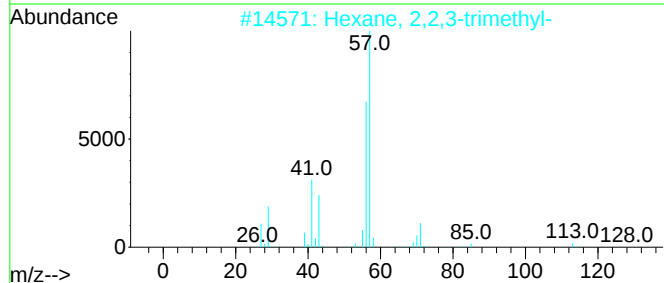
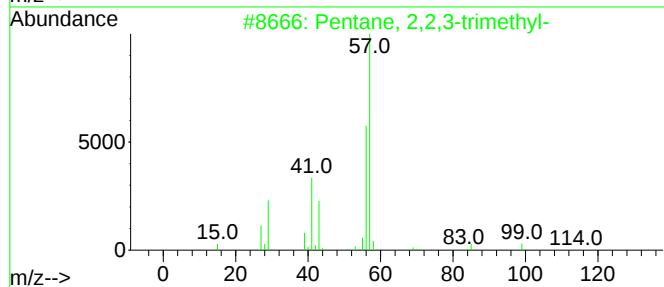
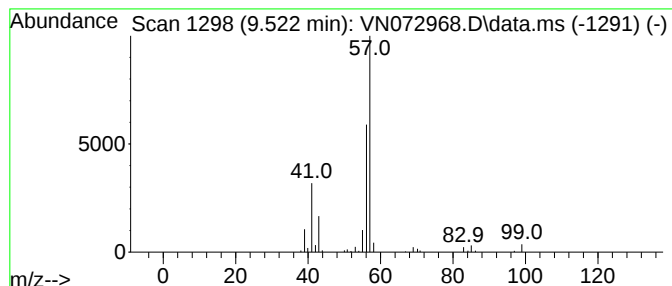
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.522	7.07 ug/l	172820	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	72
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	64
4			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	59



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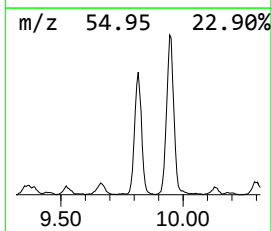
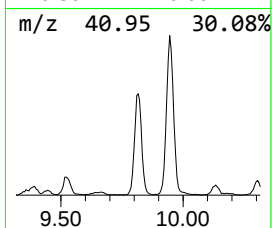
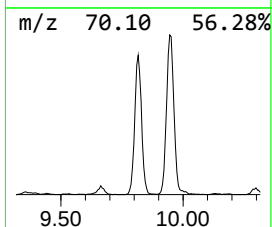
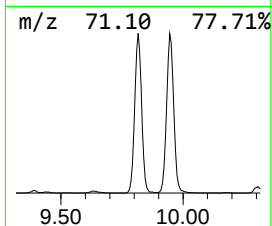
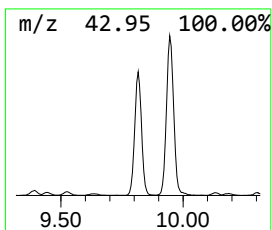
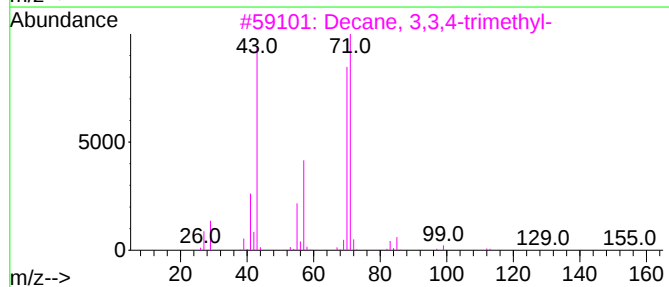
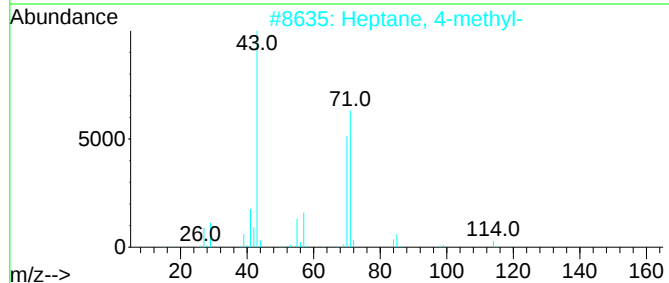
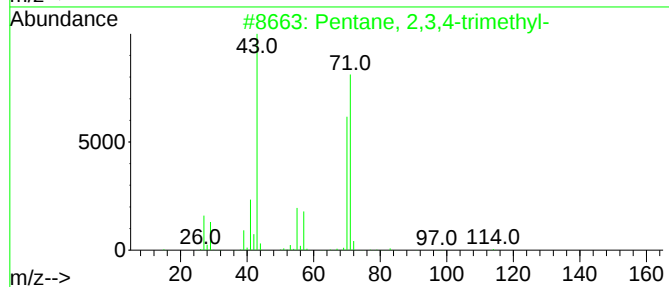
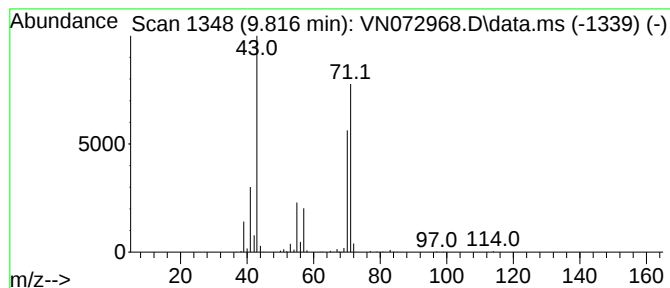
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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.
9.816	59.47 ug/l	1453760	1,4-Difluorobenzene	8.904

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			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072968.D
Acq On : 20 Jun 2022 17:54
Operator : JC\MD
Sample : N3370-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

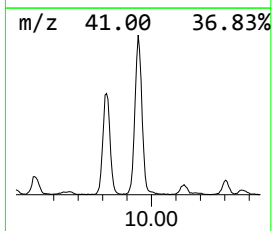
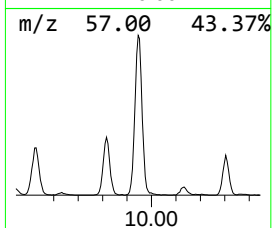
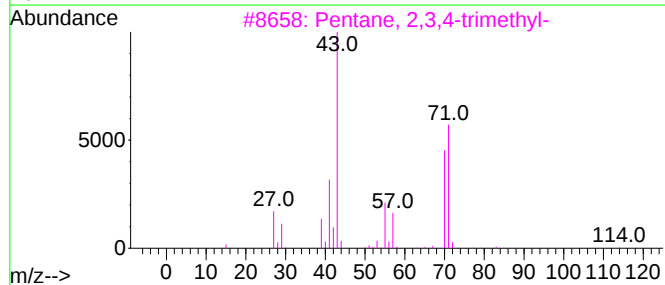
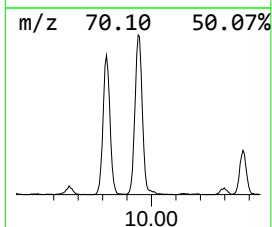
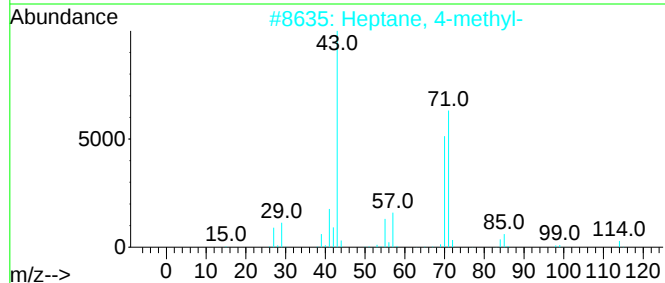
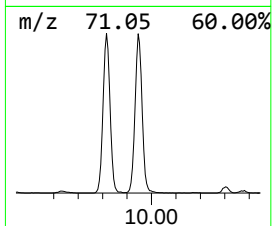
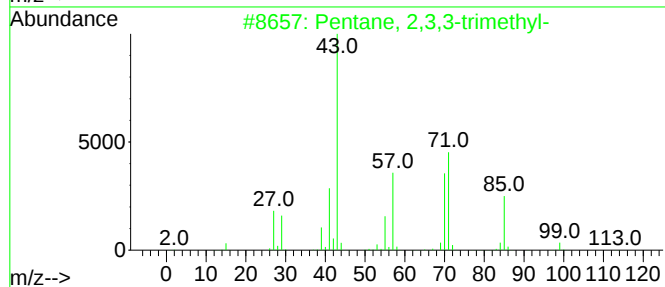
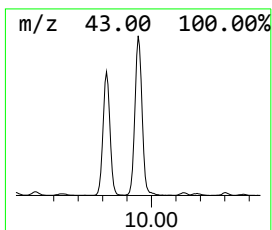
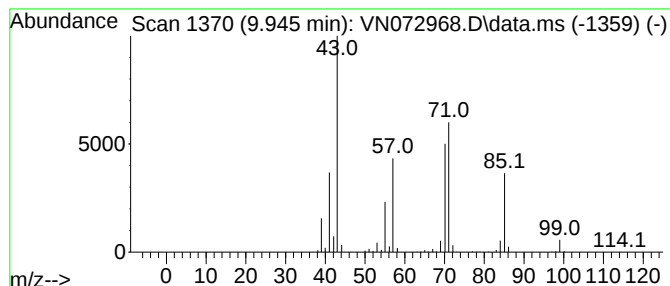
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	93.32 ug/l	2281210	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072968.D
Acq On : 20 Jun 2022 17:54
Operator : JC\MD
Sample : N3370-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

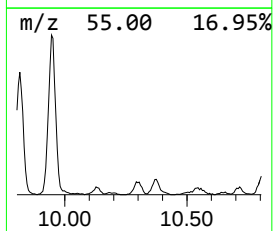
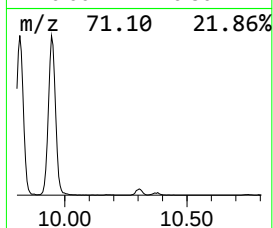
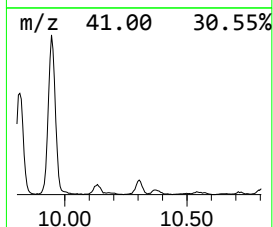
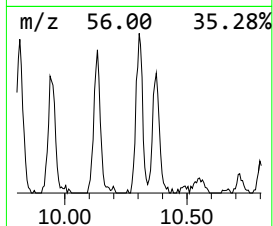
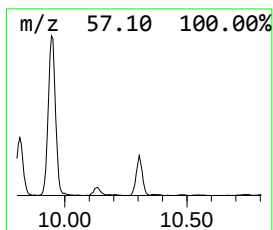
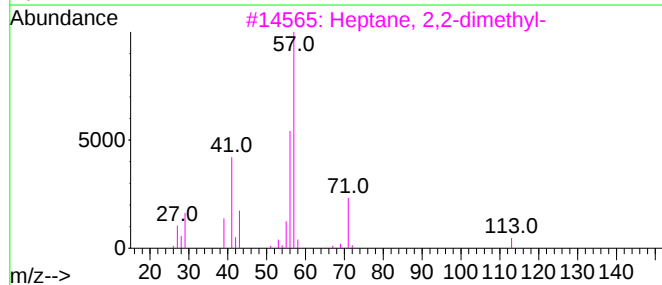
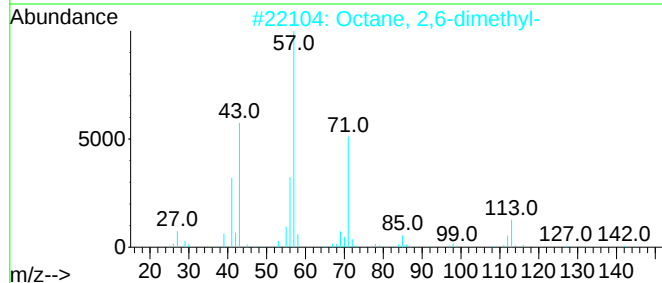
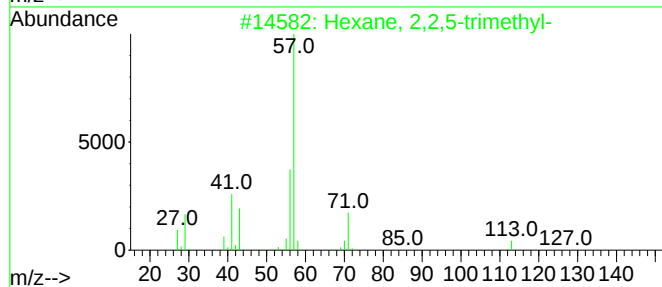
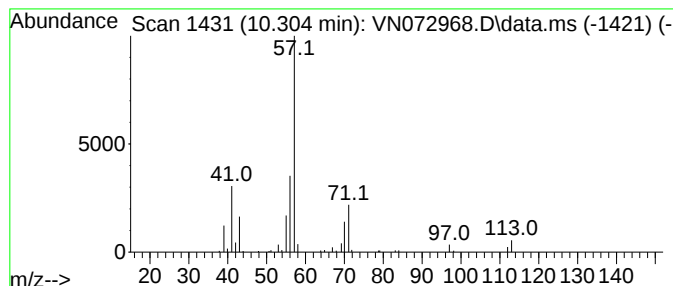
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,2,5-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.304	5.44 ug/l	156356	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
5			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072968.D
Acq On : 20 Jun 2022 17:54
Operator : JC\MD
Sample : N3370-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

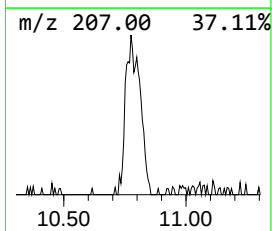
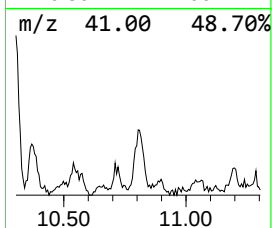
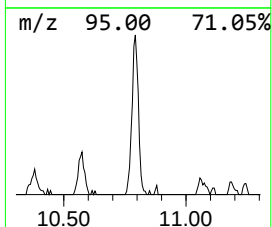
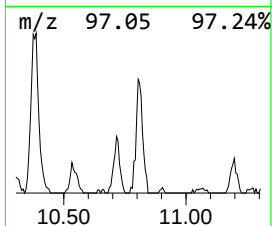
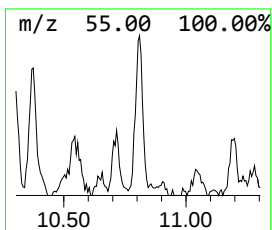
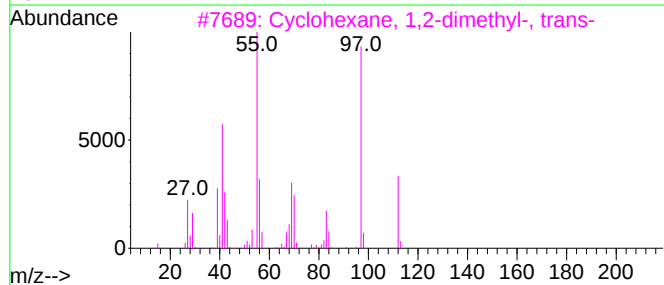
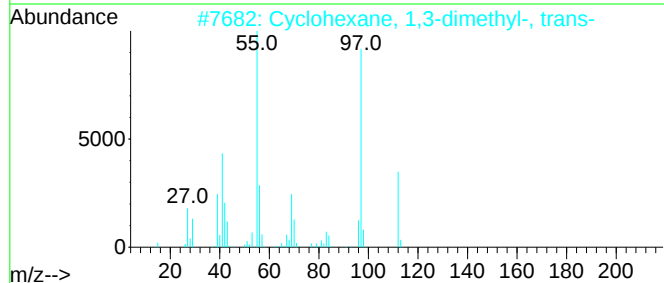
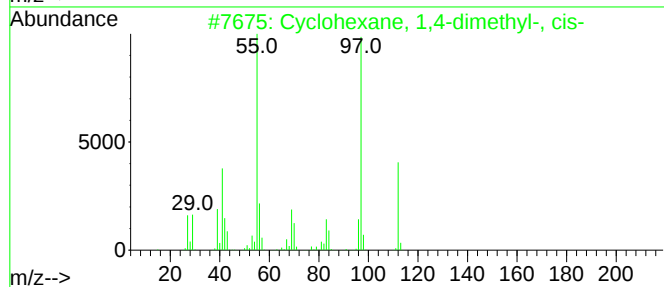
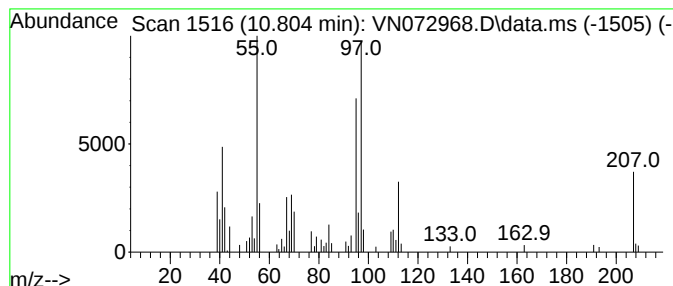
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	5.04 ug/l	144778	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	60
2			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	53
3			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50
4			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	49
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072968.D
Acq On : 20 Jun 2022 17:54
Operator : JC\MD
Sample : N3370-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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, 2,4-di...	6.963	21.4	ug/l	424330	1	8.016	991182	50.0
Pentane, 2,3-di...	8.104	72.2	ug/l	1430760	1	8.016	991182	50.0
Pentane, 2,2,4-...	8.545	104.0	ug/l	2542000	2	8.904	1222260	50.0
Pentane, 2,2,3-...	9.522	7.1	ug/l	172820	2	8.904	1222260	50.0
Pentane, 2,3,4-...	9.816	59.5	ug/l	1453760	2	8.904	1222260	50.0
Pentane, 2,3,3-...	9.945	93.3	ug/l	2281210	2	8.904	1222260	50.0
Hexane, 2,2,5-t...	10.304	5.4	ug/l	156356	3	11.680	1436570	50.0
Cyclohexane, 1,...	10.804	5.0	ug/l	144778	3	11.680	1436570	50.0