

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071385.D
 Acq On : 18 Mar 2022 20:20
 Operator : JC\MD
 Sample : N2015-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-07

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\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	44	rBV2	111876	213331	5.09%	0.805%
2	2.263	45	47	59	rVB2	128079	335798	8.01%	1.267%
3	5.087	512	527	540	rBV5	18222	72949	1.74%	0.275%
4	5.622	603	618	634	rVB2	59800	215601	5.14%	0.814%
5	7.045	850	860	865	rBV5	20086	58065	1.39%	0.219%
6	7.322	898	907	915	rBV6	16856	47677	1.14%	0.180%
7	8.022	1015	1026	1031	rBV	498429	1230337	29.36%	4.644%
8	8.087	1031	1037	1045	rVV	947742	2182309	52.07%	8.237%
9	8.175	1045	1052	1064	rVB	151588	392864	9.37%	1.483%
10	8.434	1086	1096	1109	rBV	567257	1326772	31.66%	5.008%
11	8.616	1113	1127	1138	rBV	703041	1772263	42.29%	6.689%
12	8.963	1176	1186	1198	rBV	1444352	2989580	71.33%	11.283%
13	9.428	1257	1265	1276	rBV9	15266	45269	1.08%	0.171%
14	9.592	1285	1293	1301	rBV2	54243	109669	2.62%	0.414%
15	9.880	1334	1342	1354	rVB	445682	863944	20.61%	3.261%
16	10.010	1354	1364	1381	rBV	599961	1217803	29.06%	4.596%
17	10.198	1390	1396	1402	rBV3	23916	48660	1.16%	0.184%
18	10.369	1418	1425	1430	rBV	54753	101346	2.42%	0.383%
19	10.439	1430	1437	1456	rVB	2290879	4191040	100.00%	15.818%
20	10.857	1503	1508	1518	rVB5	29089	78427	1.87%	0.296%
21	11.745	1648	1659	1673	rBV	2024905	3681908	87.85%	13.896%
22	12.727	1817	1826	1836	rBV	1620147	2732489	65.20%	10.313%
23	13.674	1978	1987	1999	rBV	1460116	2532904	60.44%	9.560%
24	14.145	2061	2067	2074	rBV3	33244	54562	1.30%	0.206%

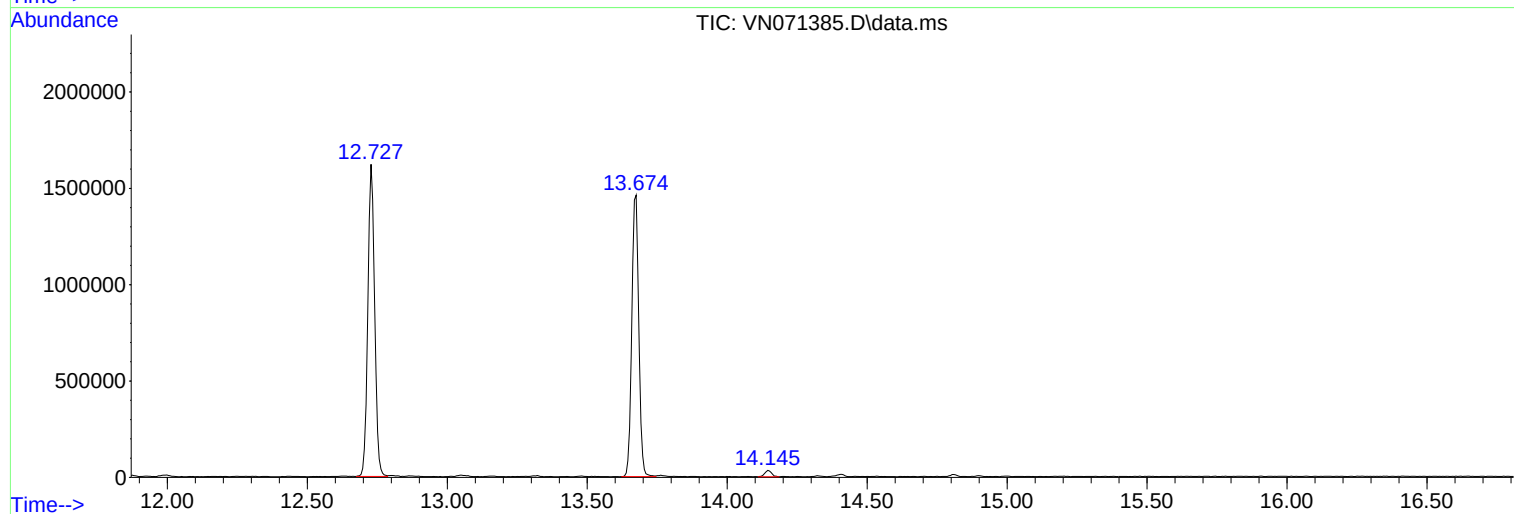
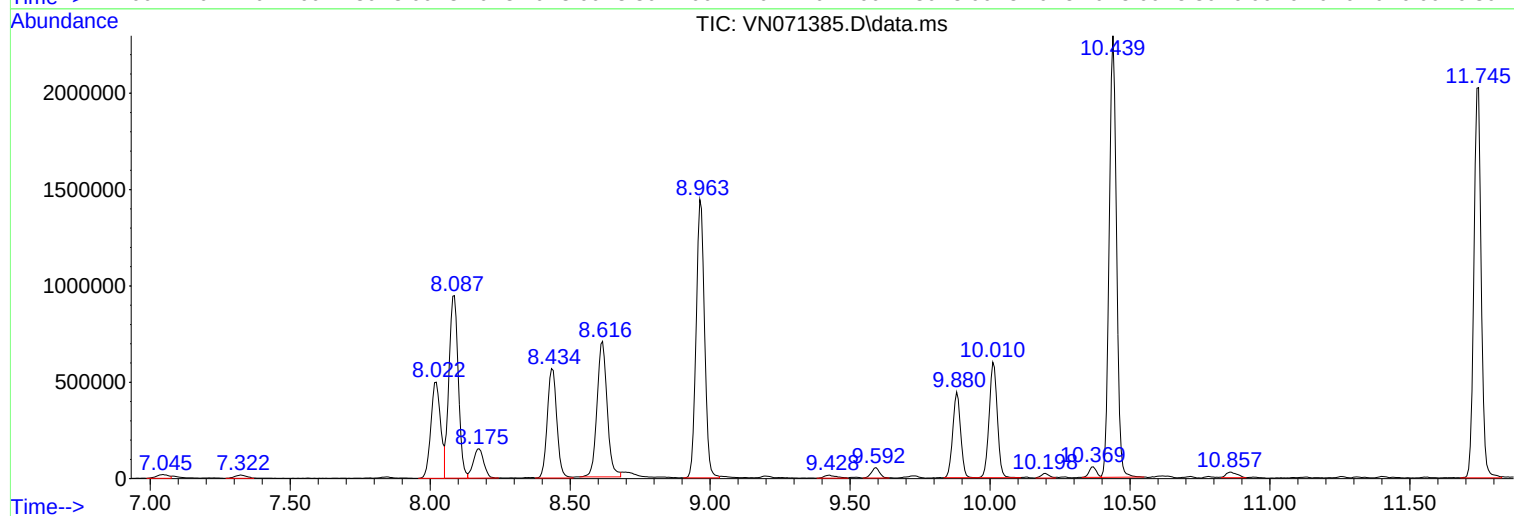
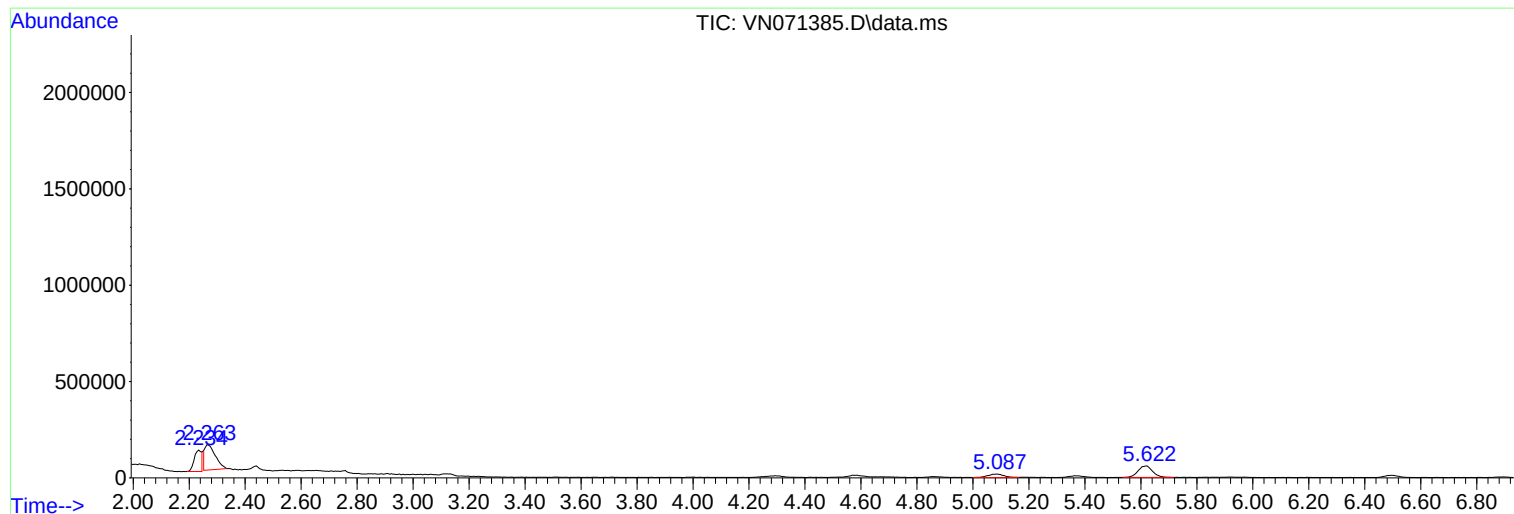
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Instrument :
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ClientSampleId :
TOLL-MW-07

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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Sample : N2015-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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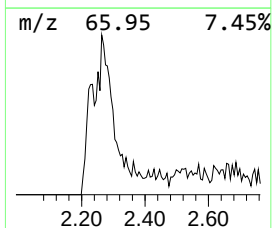
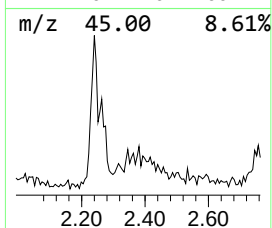
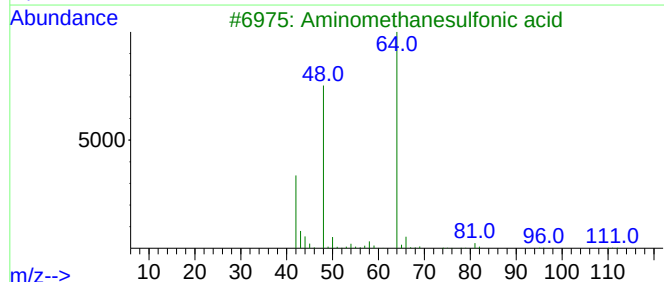
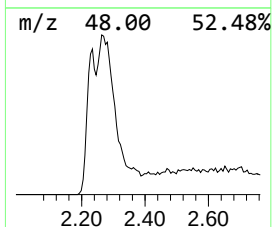
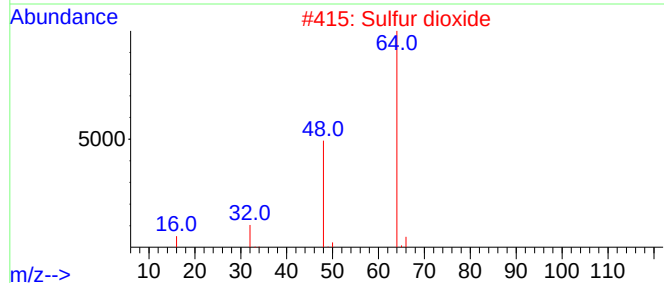
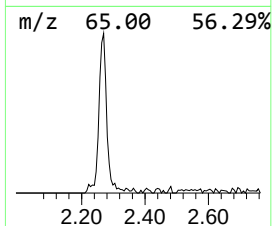
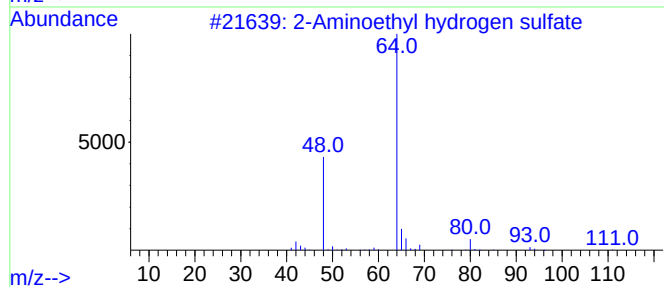
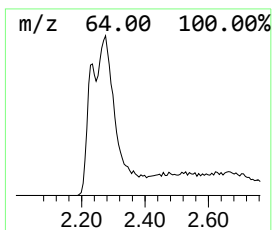
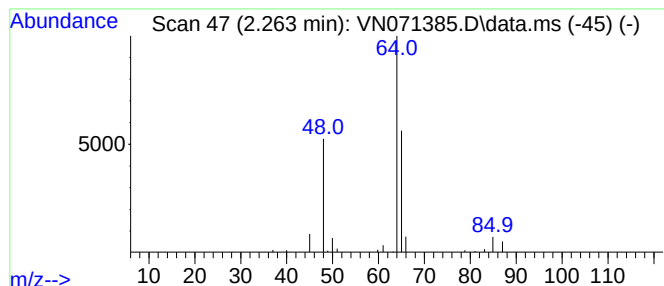
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.263 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	7.69 ug/l	335798	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	42
2			Sulfur dioxide	64	O2S	007446-09-5	40
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40
4			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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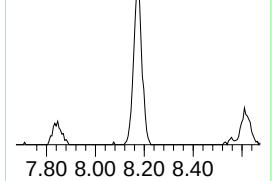
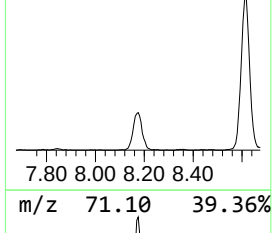
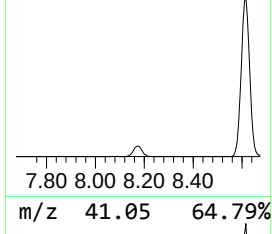
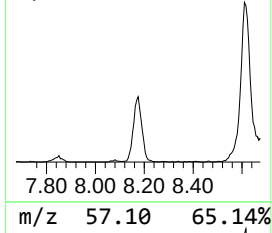
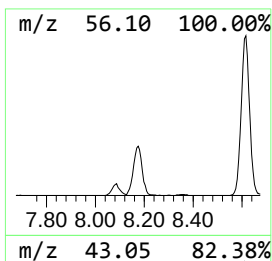
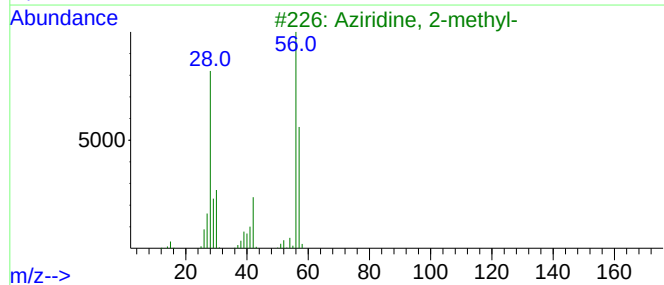
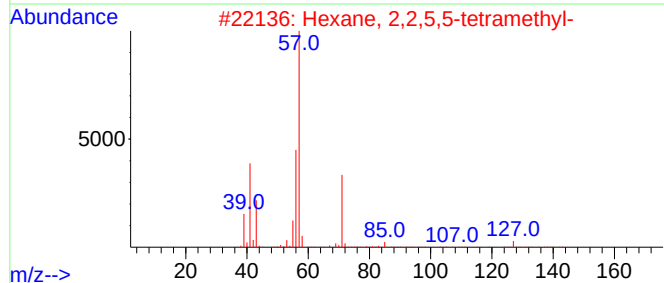
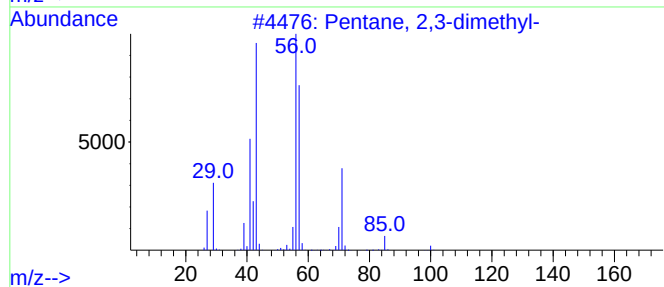
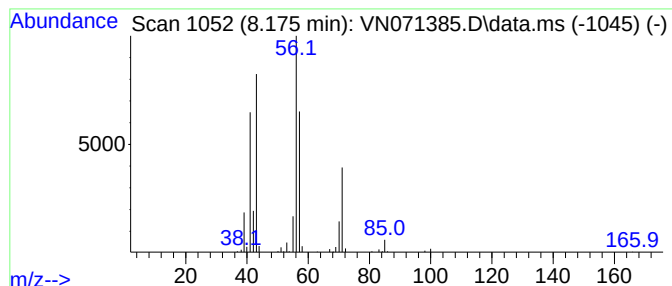
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	9.00 ug/l	392864	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5			Heptane	100	C7H16	000142-82-5	40



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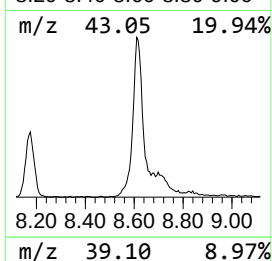
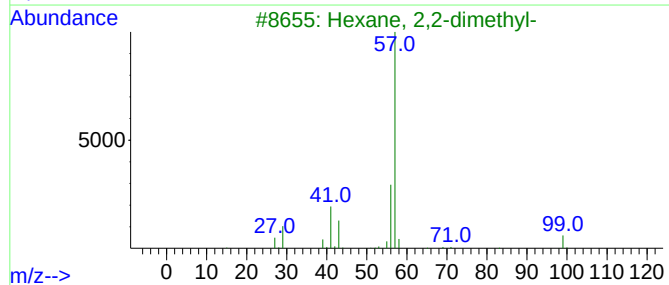
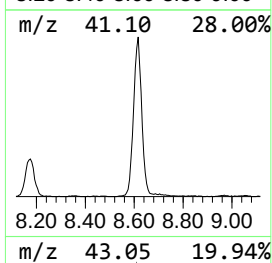
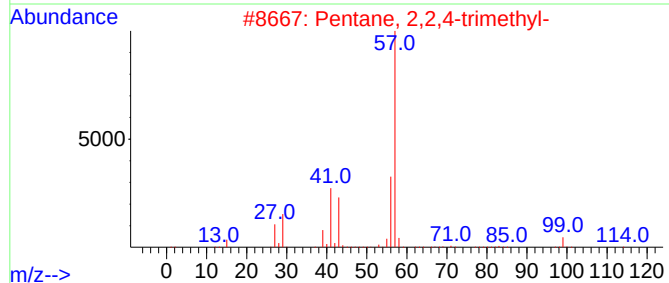
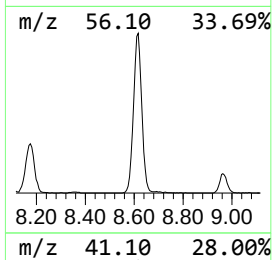
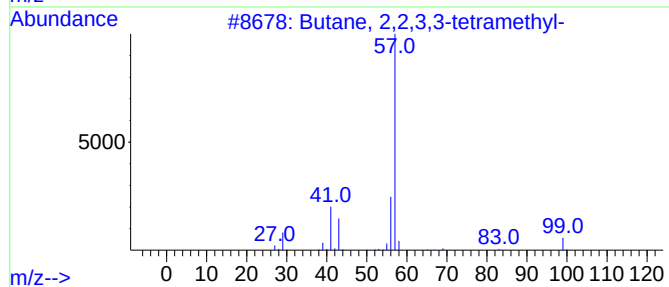
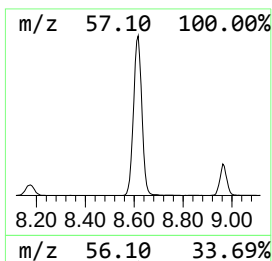
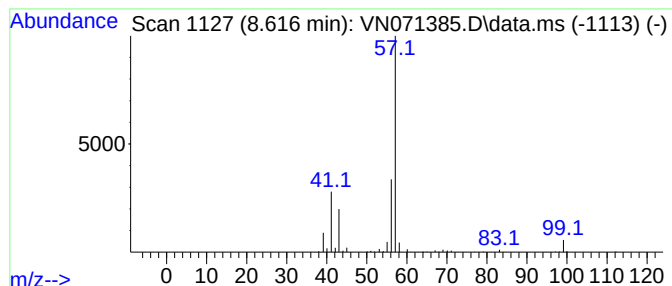
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	29.64 ug/l	1772260	1,4-Difluorobenzene	8.963

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



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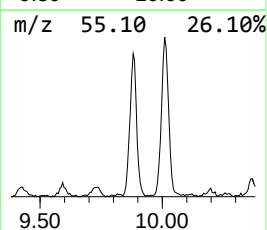
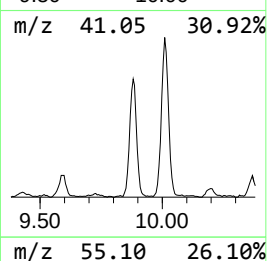
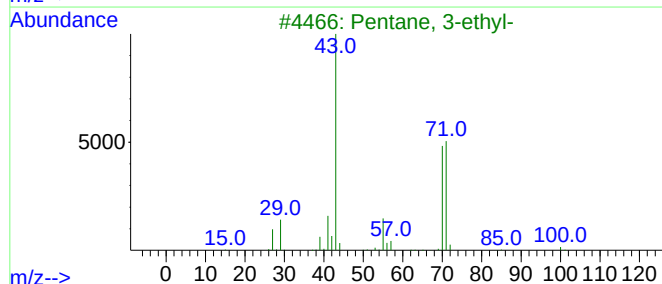
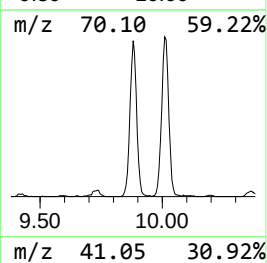
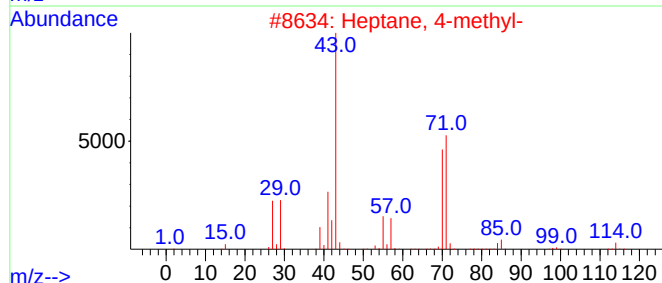
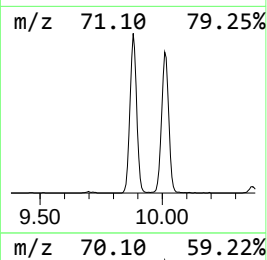
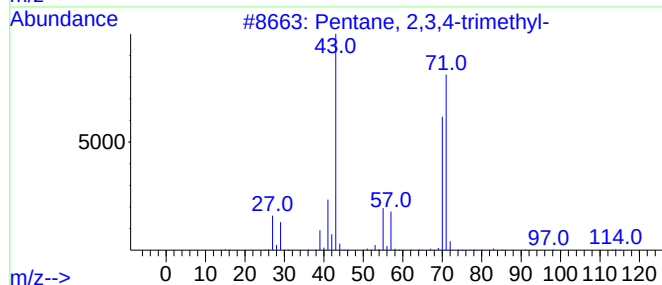
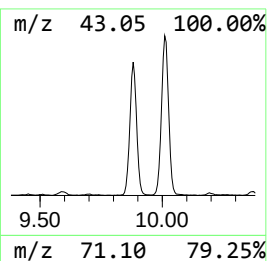
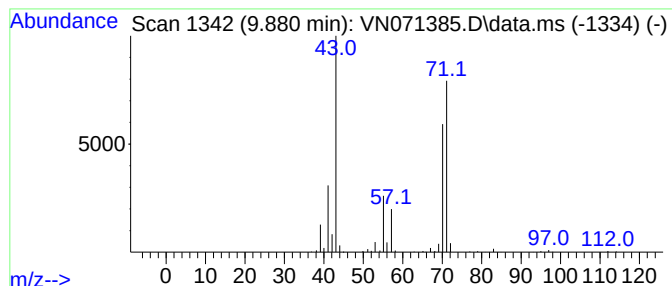
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	14.45 ug/l	863944	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	86
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



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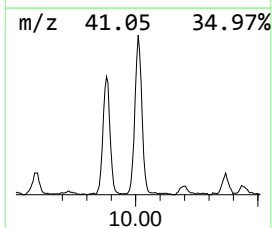
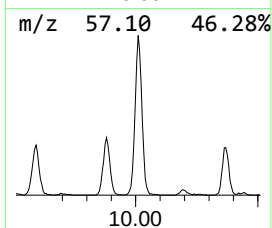
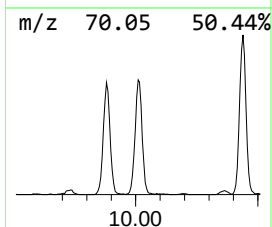
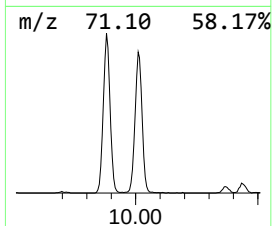
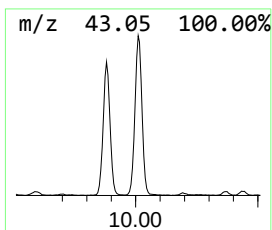
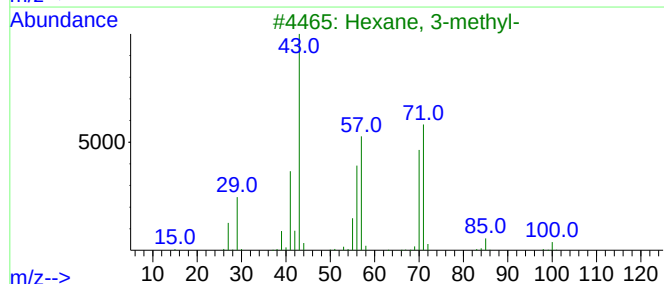
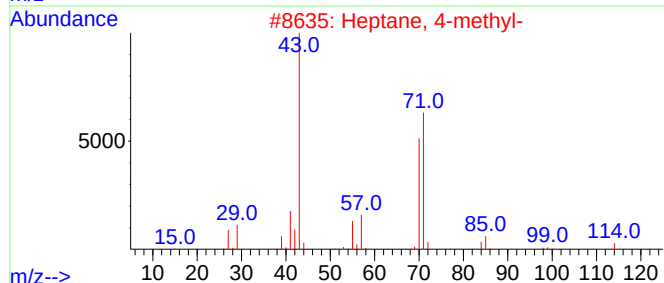
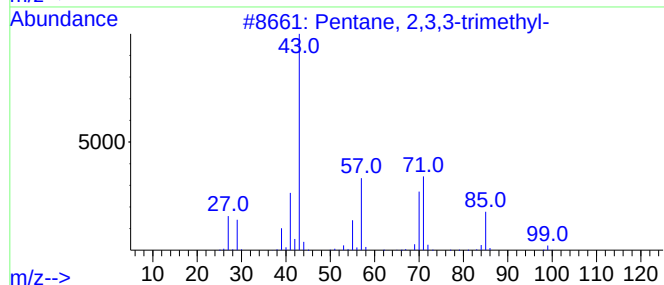
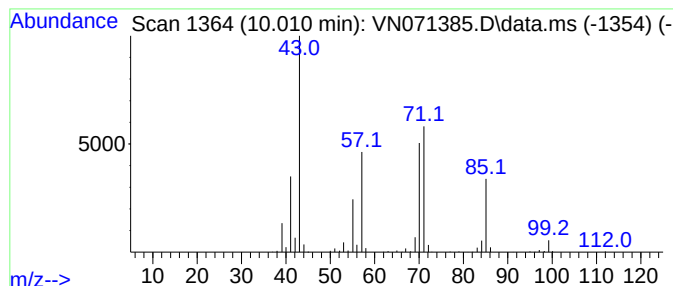
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	20.37 ug/l	1217800	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.263	2.263	7.7	ug/l	335798	1	8.086	2182310	50.0
Pentane, 2,3-di...	8.175	9.0	ug/l	392864	1	8.086	2182310	50.0
Butane, 2,2,3,3...	8.616	29.6	ug/l	1772260	2	8.963	2989580	50.0
Pentane, 2,3,4-...	9.880	14.4	ug/l	863944	2	8.963	2989580	50.0
Pentane, 2,3,3-...	10.010	20.4	ug/l	1217800	2	8.963	2989580	50.0