

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
 Data File : VN075725.D
 Acq On : 12 Dec 2022 20:05
 Operator : JC\MD
 Sample : N5978-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 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\82N120922W.M
 Title : SW846 8260

Signal : TIC: VN075725.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	35	42	45	rBV	21422	49066	4.24%	0.472%
2	2.330	45	47	53	rVB	17624	27895	2.41%	0.269%
3	2.836	126	133	141	rVB4	12451	34892	3.02%	0.336%
4	3.259	195	205	218	rVB	55720	135884	11.75%	1.308%
5	5.289	539	550	560	rBV2	16630	54905	4.75%	0.529%
6	5.536	581	592	603	rBV2	15141	50599	4.37%	0.487%
7	5.818	627	640	653	rVB3	28019	97458	8.42%	0.938%
8	6.683	778	787	796	rVB4	5649	17055	1.47%	0.164%
9	7.230	870	880	893	rBV2	61180	178356	15.42%	1.717%
10	8.171	1031	1040	1045	rBV	153038	379692	32.82%	3.656%
11	8.230	1045	1050	1059	rVV	300791	681865	58.94%	6.566%
12	8.335	1059	1068	1081	rVB	265904	642335	55.52%	6.185%
13	8.588	1102	1111	1121	rBV	154472	350331	30.28%	3.373%
14	8.765	1124	1141	1153	rVV	433596	1051518	90.90%	10.125%
15	8.853	1153	1156	1168	rVB4	5117	11857	1.02%	0.114%
16	9.106	1188	1199	1209	rBV	408724	830268	71.77%	7.995%
17	9.594	1270	1282	1287	rBV7	21883	68159	5.89%	0.656%
18	9.653	1287	1292	1298	rVV2	11439	22875	1.98%	0.220%
19	9.729	1298	1305	1316	rVV	35077	75907	6.56%	0.731%
20	9.871	1317	1329	1335	rVB6	9504	28518	2.47%	0.275%
21	10.018	1345	1354	1364	rBV	317162	621590	53.73%	5.986%
22	10.147	1364	1376	1390	rBV	479666	997625	86.24%	9.607%
23	10.324	1400	1406	1413	rBV3	19609	45907	3.97%	0.442%
24	10.500	1425	1436	1441	rBV	43124	79530	6.87%	0.766%
25	10.571	1441	1448	1463	rVB	605064	1156842	100.00%	11.140%
26	10.753	1471	1479	1486	rVB6	7127	19139	1.65%	0.184%
27	10.912	1501	1506	1513	rBV3	7727	14557	1.26%	0.140%
28	11.006	1513	1522	1528	rBV5	23372	58932	5.09%	0.567%
29	11.388	1579	1587	1592	rBV7	8117	17775	1.54%	0.171%
30	11.870	1661	1669	1677	rBV	534269	948185	81.96%	9.130%
31	12.853	1827	1836	1846	rVB	405842	695394	60.11%	6.696%
32	13.794	1988	1996	2012	rBB	508791	846651	73.19%	8.153%
33	14.276	2072	2078	2084	rBV	20255	32535	2.81%	0.313%
34	14.447	2101	2107	2112	rBV3	7586	11859	1.03%	0.114%
35	14.535	2114	2122	2126	rVV5	9318	17561	1.52%	0.169%
36	14.659	2137	2143	2150	rVB3	8026	12901	1.12%	0.124%

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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	14.935	2185	2190	2195	rVB3	11253	18469	1.60%	0.178%
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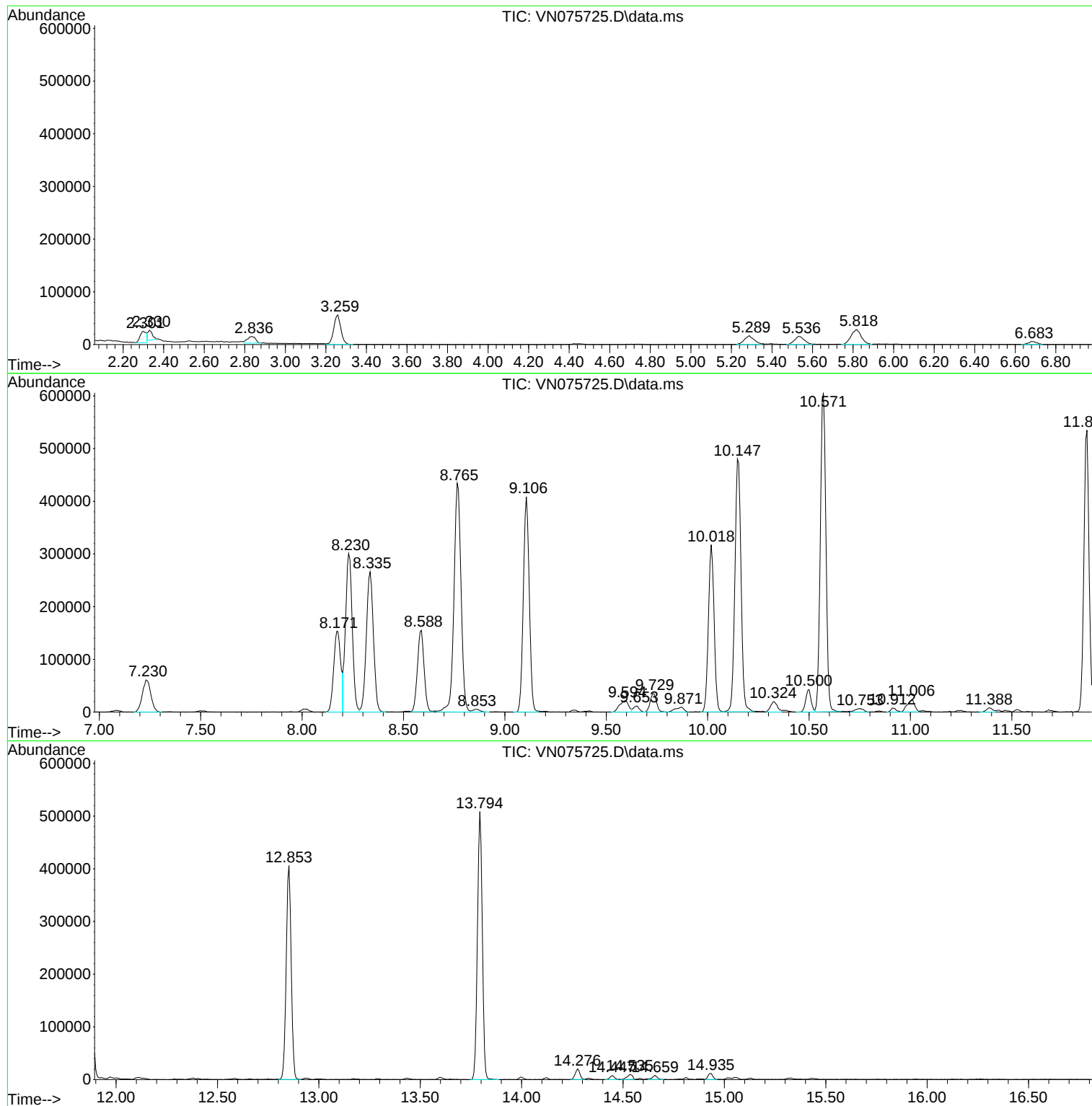
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



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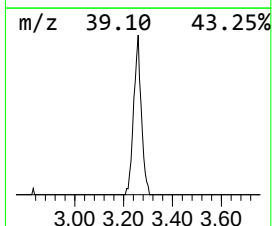
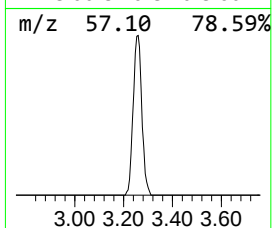
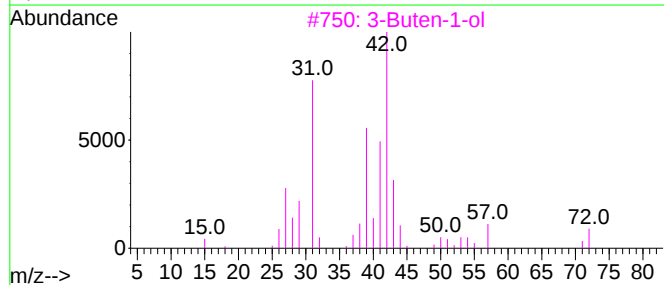
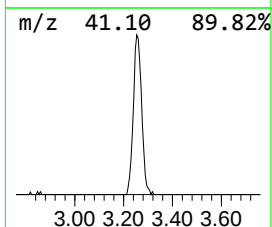
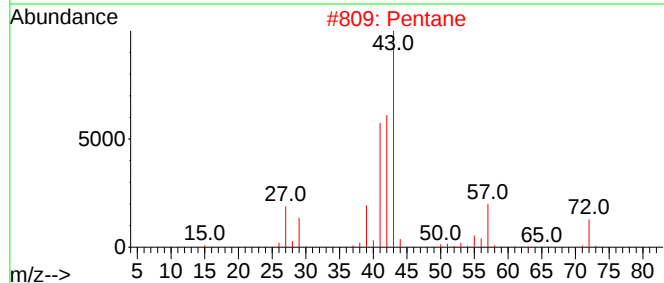
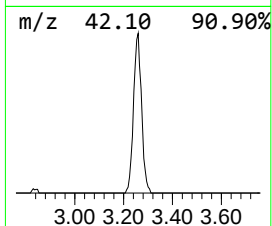
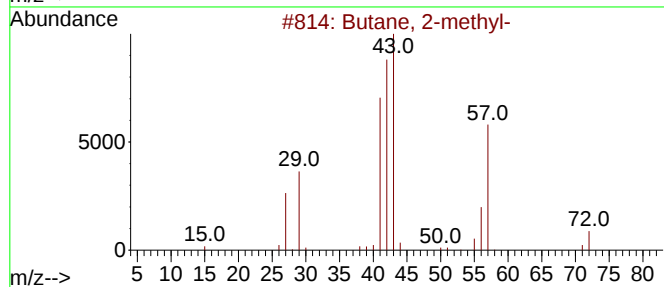
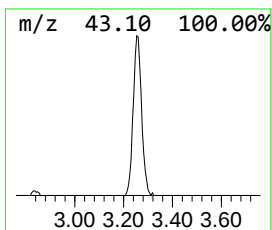
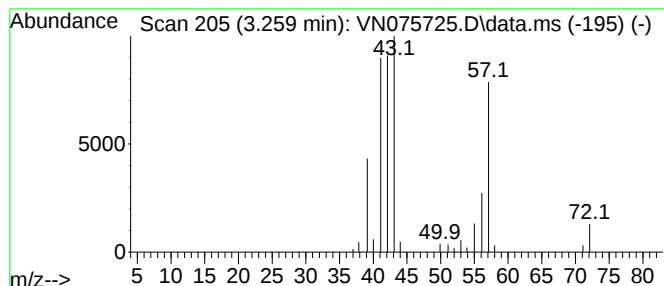
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.259	9.96 ug/l	135884	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	38
3			3-Buten-1-ol	72	C4H8O	000627-27-0	33
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
5			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25



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Instrument :
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ClientSampleId :
TOLL-MW-09

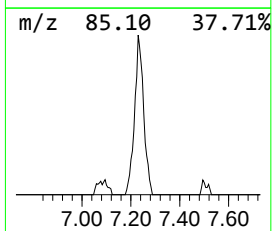
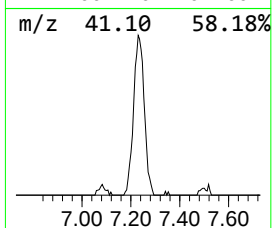
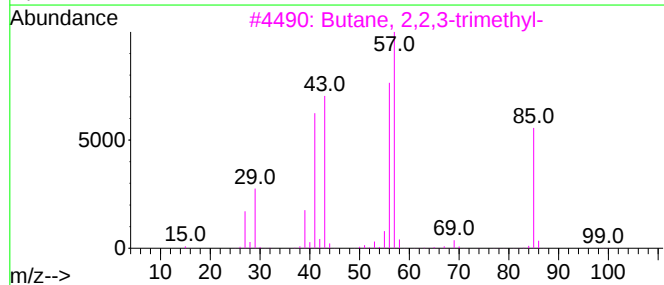
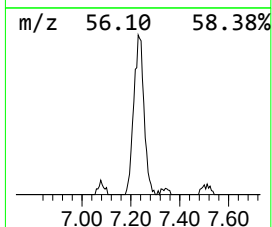
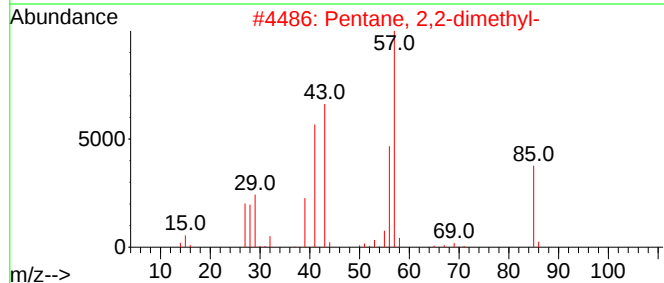
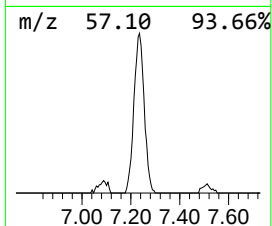
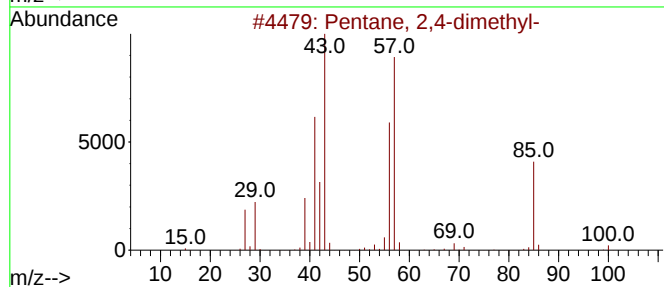
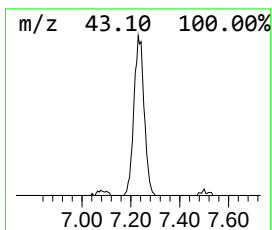
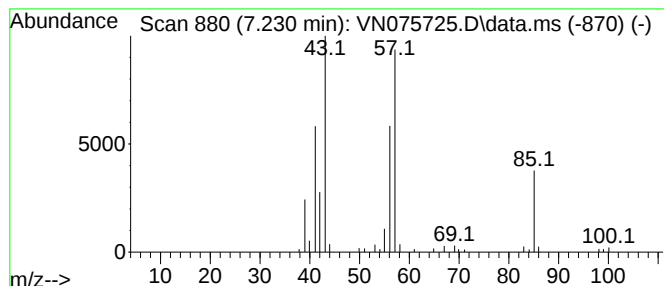
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	13.08 ug/l	178356	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	52
5			Pentane, 3-methyl-	86	C6H14	000096-14-0	43



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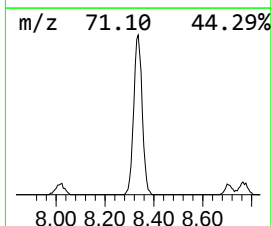
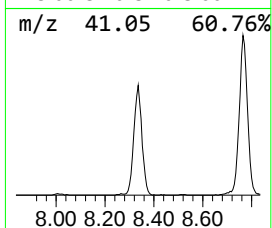
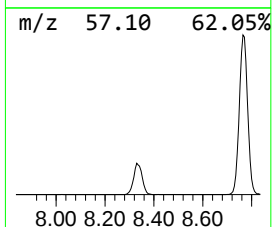
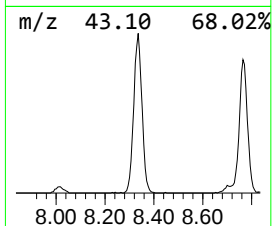
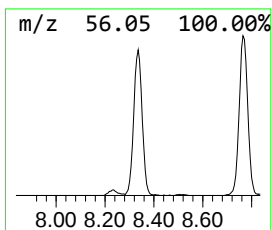
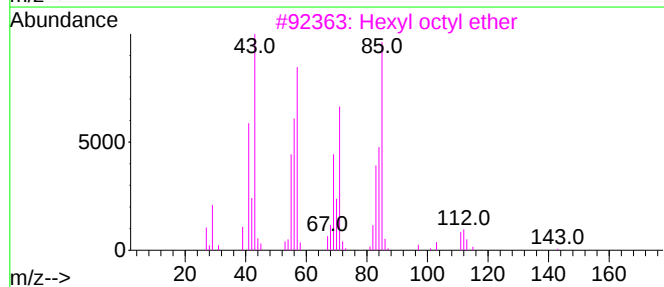
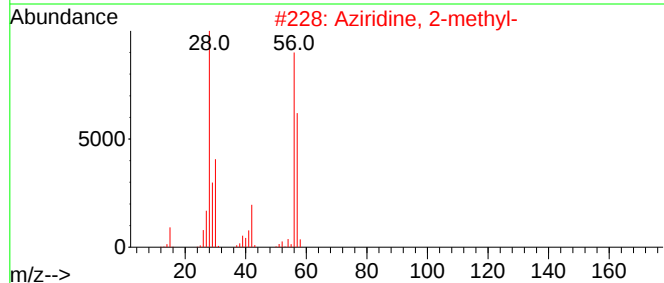
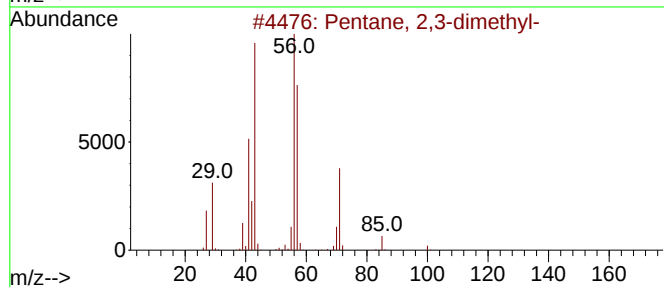
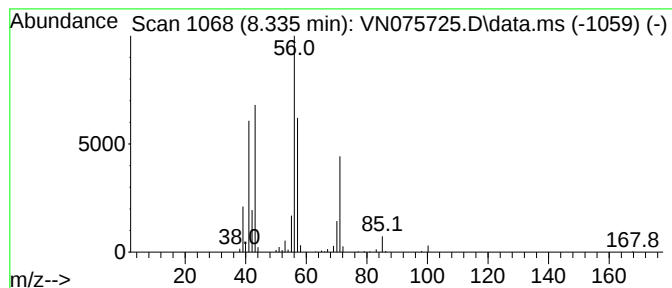
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.335	47.10 ug/l	642335	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3			Hexyl octyl ether	214	C14H30O	017071-54-4	47
4			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	47
5			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	43



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ALS Vial : 22 Sample Multiplier: 1

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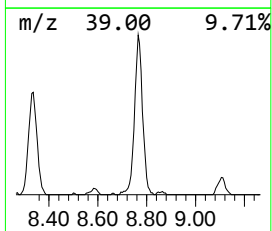
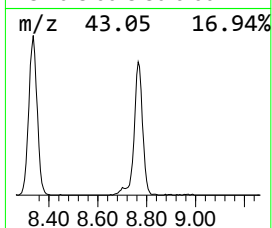
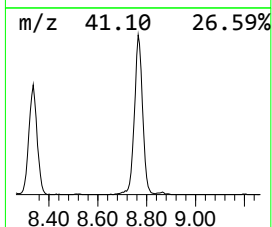
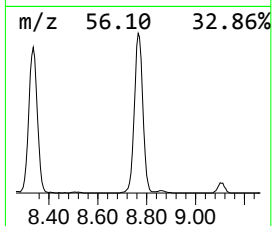
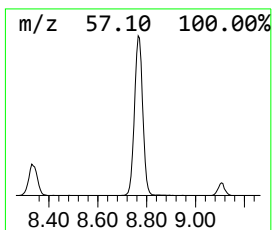
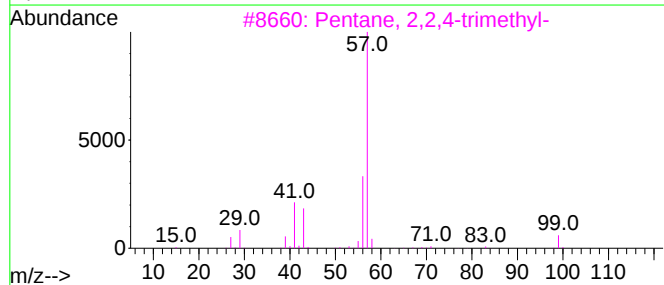
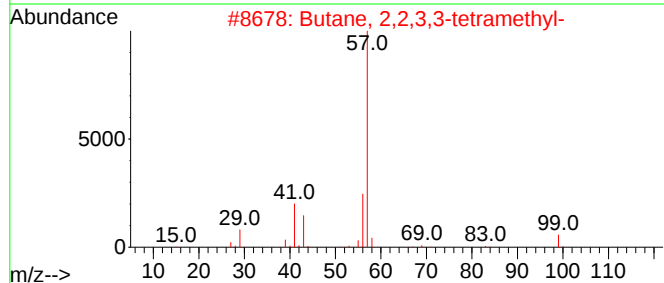
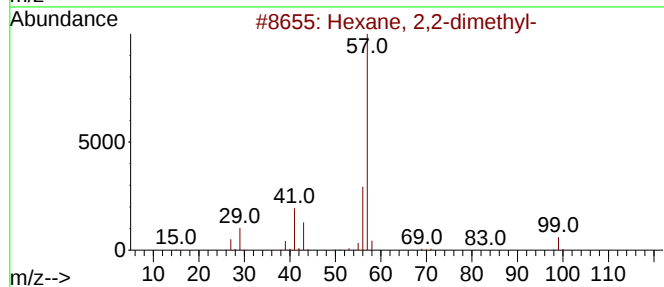
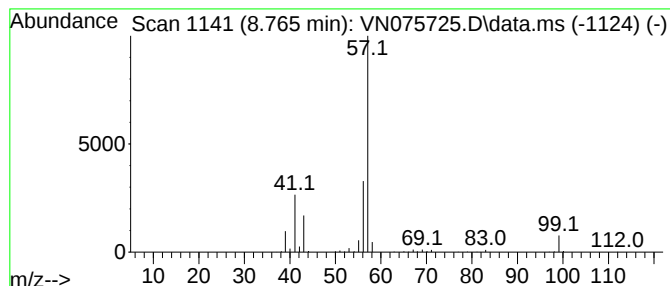
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	63.32 ug/l	1051520	1,4-Difluorobenzene	9.106

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



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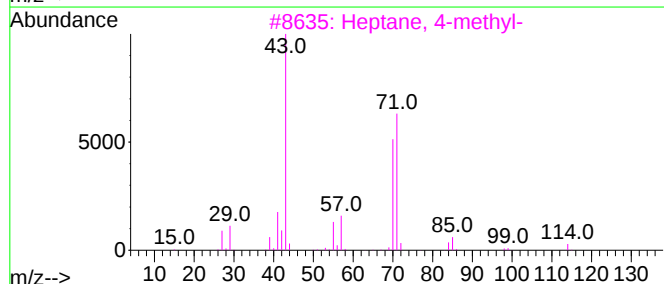
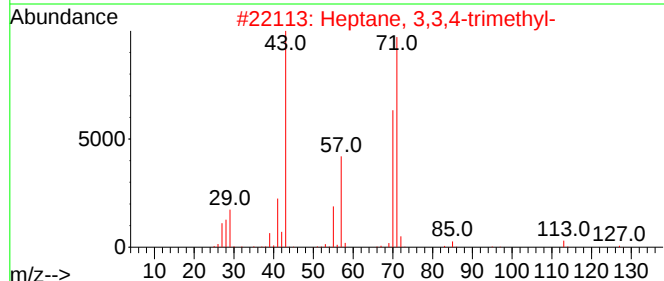
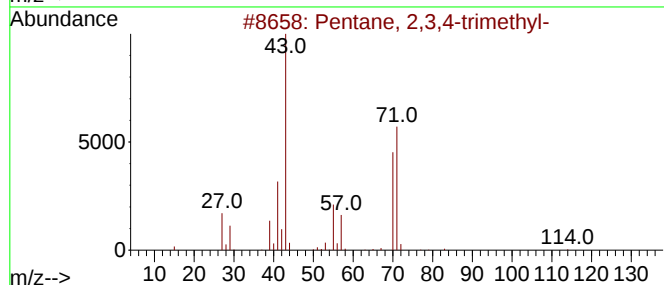
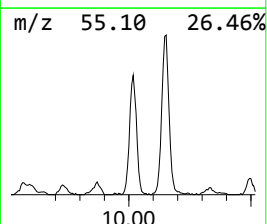
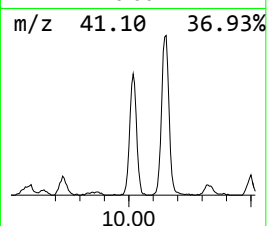
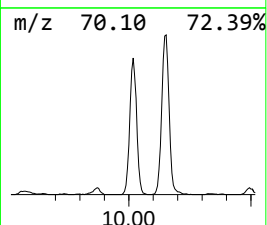
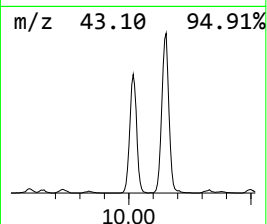
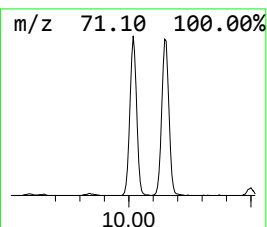
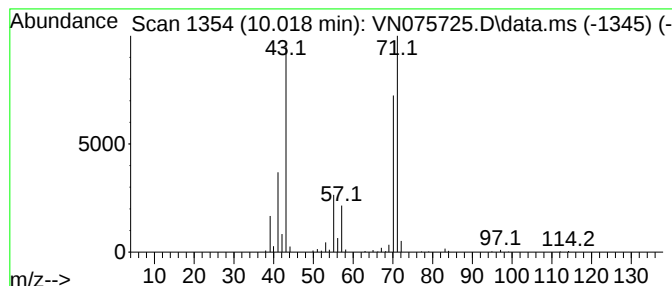
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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.
10.018	37.43 ug/l	621590	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Hexanoic acid, 1,1-dimethylpropy...	186	C11H22O2	116423-69-9	83
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075725.D
Acq On : 12 Dec 2022 20:05
Operator : JC\MD
Sample : N5978-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

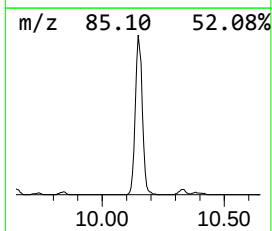
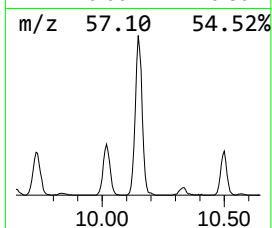
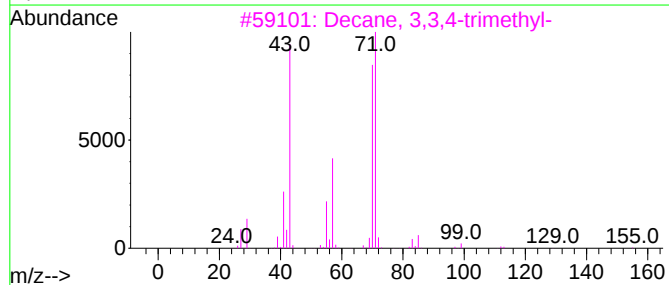
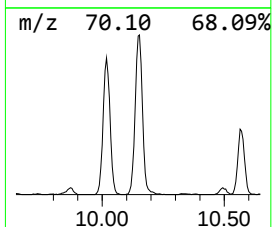
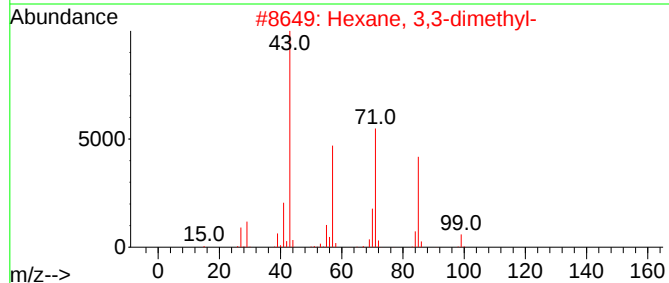
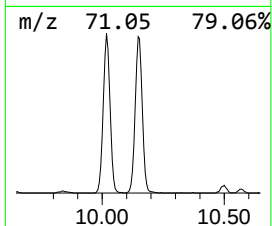
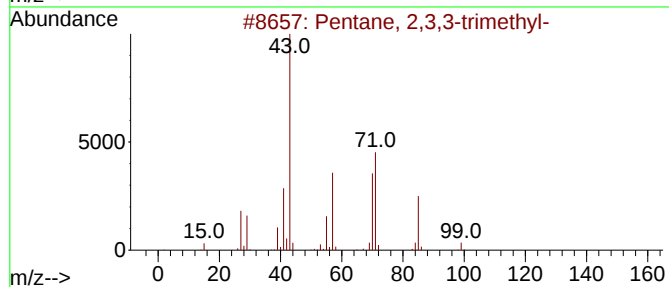
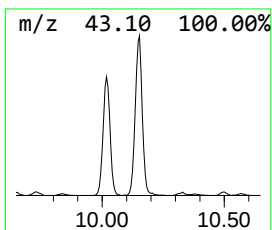
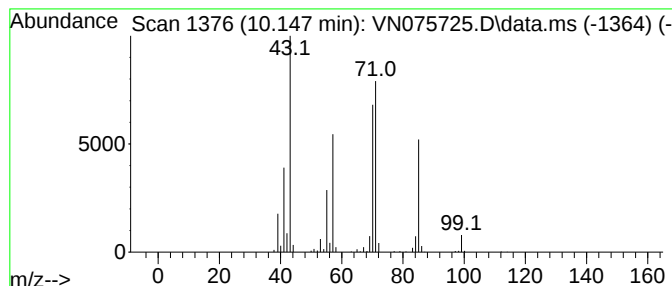
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Quant Title : SW846 8260

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.
10.147	60.08 ug/l	997625	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075725.D
Acq On : 12 Dec 2022 20:05
Operator : JC\MD
Sample : N5978-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.259	10.0	ug/l	135884	1	8.230	681865	50.0
Pentane, 2,4-di...	7.230	13.1	ug/l	178356	1	8.230	681865	50.0
Pentane, 2,3-di...	8.335	47.1	ug/l	642335	1	8.230	681865	50.0
Hexane, 2,2-dim...	8.765	63.3	ug/l	1051520	2	9.106	830268	50.0
Pentane, 2,3,4-...	10.018	37.4	ug/l	621590	2	9.106	830268	50.0
Pentane, 2,3,3-...	10.147	60.1	ug/l	997625	2	9.106	830268	50.0