

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
 Data File : VN075719.D
 Acq On : 12 Dec 2022 17:41
 Operator : JC\MD
 Sample : N5978-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-03

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: VN075719.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	35	43	45	rBV2	18624	42827	2.14%	0.338%
2	2.336	45	48	58	rVB3	30432	59186	2.96%	0.467%
3	2.524	74	80	87	rBV	51069	85364	4.26%	0.673%
4	3.259	198	205	213	rVB3	24043	58896	2.94%	0.464%
5	5.289	536	550	561	rBV4	14312	52410	2.62%	0.413%
6	5.818	628	640	655	rVB3	27065	96657	4.83%	0.762%
7	7.236	868	881	895	rBV2	124192	366121	18.29%	2.887%
8	7.494	918	925	936	rBV4	9847	27801	1.39%	0.219%
9	8.012	1005	1013	1023	rVB2	9420	23830	1.19%	0.188%
10	8.171	1029	1040	1045	rBV	147734	361683	18.07%	2.852%
11	8.230	1045	1050	1059	rVV	292714	648076	32.37%	5.111%
12	8.335	1059	1068	1078	rVB	276927	664006	33.17%	5.237%
13	8.582	1102	1110	1124	rVB	146406	332705	16.62%	2.624%
14	8.765	1127	1141	1152	rBV	850867	2002104	100.00%	15.790%
15	8.859	1152	1157	1164	rVB5	12553	26893	1.34%	0.212%
16	9.106	1190	1199	1212	rBV	398072	811214	40.52%	6.398%
17	9.594	1270	1282	1287	rBV4	75666	185522	9.27%	1.463%
18	9.647	1287	1291	1298	rVV3	30323	59063	2.95%	0.466%
19	9.729	1298	1305	1318	rVB2	59435	128191	6.40%	1.011%
20	9.871	1324	1329	1337	rVB3	19091	42518	2.12%	0.335%
21	10.018	1344	1354	1364	rVB	554754	1080289	53.96%	8.520%
22	10.153	1364	1377	1390	rBV	703916	1444756	72.16%	11.394%
23	10.329	1399	1407	1414	rBV2	20968	43677	2.18%	0.344%
24	10.500	1424	1436	1441	rBV	138434	245498	12.26%	1.936%
25	10.571	1441	1448	1461	rVB	598001	1112883	55.59%	8.777%
26	10.759	1468	1480	1488	rVB6	16763	45336	2.26%	0.358%
27	10.918	1501	1507	1513	rBV6	10013	24639	1.23%	0.194%
28	10.988	1513	1519	1520	rVV2	28673	45800	2.29%	0.361%
29	11.012	1521	1523	1529	rVB2	34429	47430	2.37%	0.374%
30	11.253	1556	1564	1570	rBV3	15985	35422	1.77%	0.279%
31	11.871	1658	1669	1676	rBV	523183	943750	47.14%	7.443%
32	12.112	1703	1710	1715	rBV4	11454	22066	1.10%	0.174%
33	12.853	1827	1836	1845	rBV	396851	683516	34.14%	5.391%
34	13.794	1989	1996	2005	rBV	491820	804954	40.21%	6.348%
35	14.276	2072	2078	2083	rBV2	15956	24845	1.24%	0.196%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

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

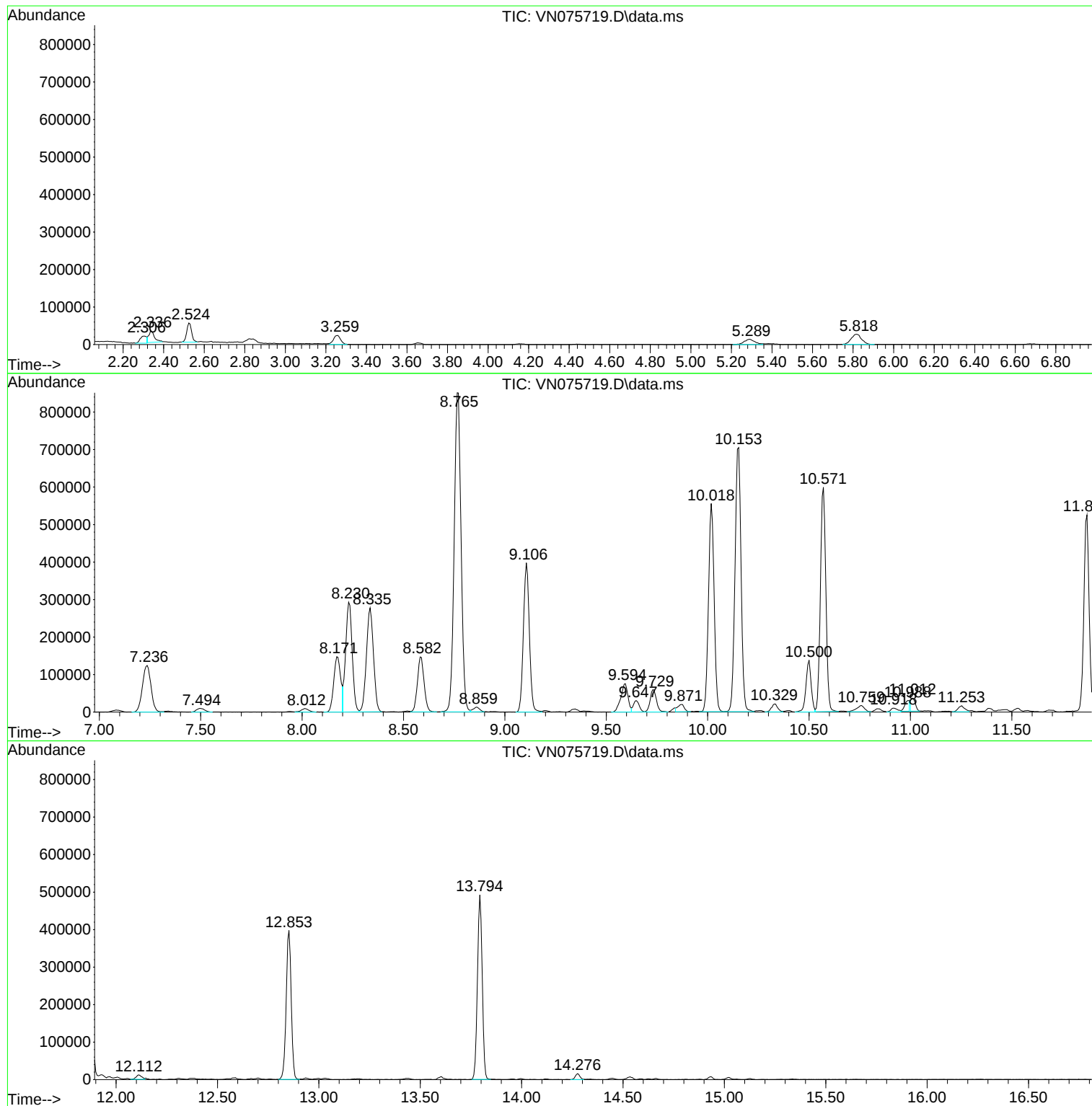
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



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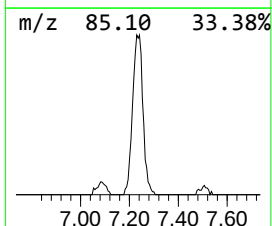
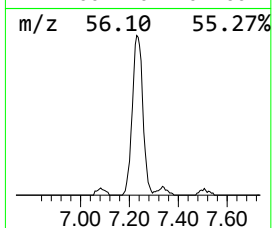
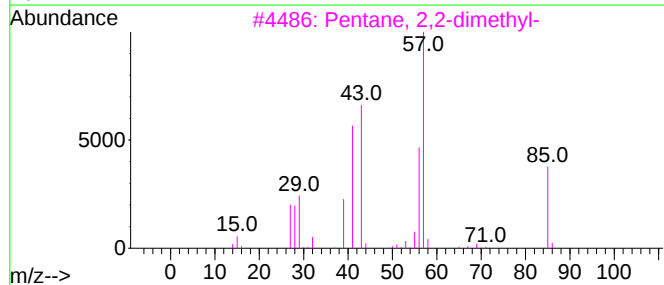
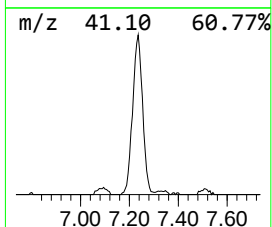
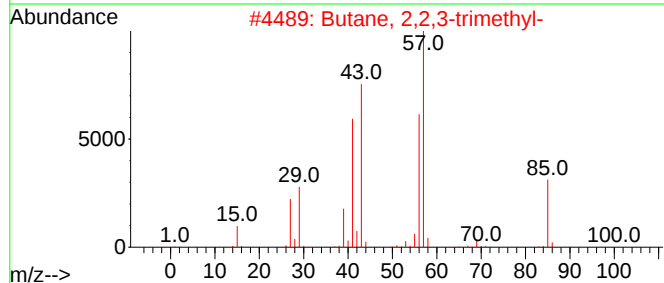
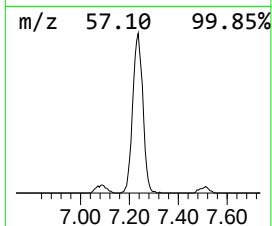
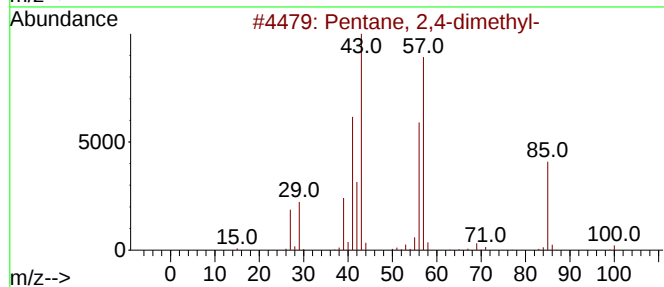
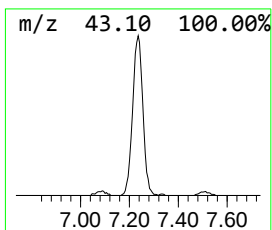
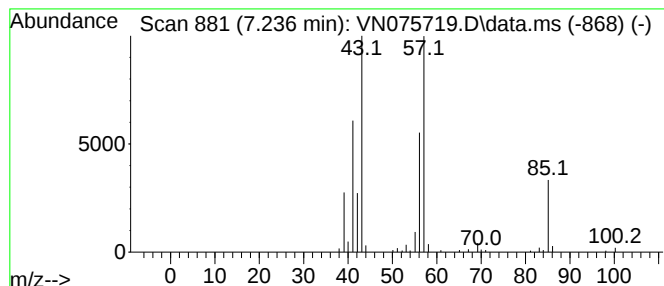
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.236	28.25 ug/l	366121	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
5			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	50



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

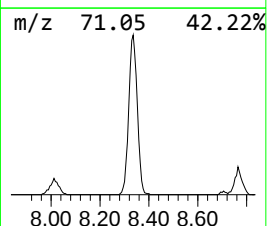
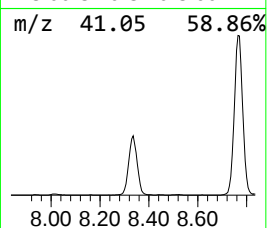
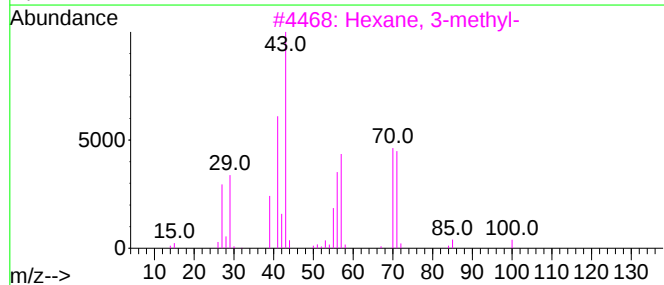
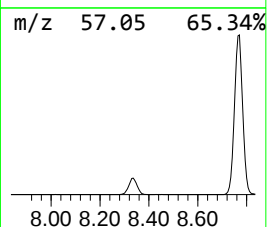
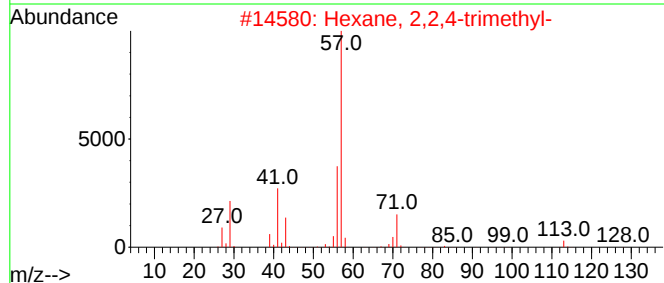
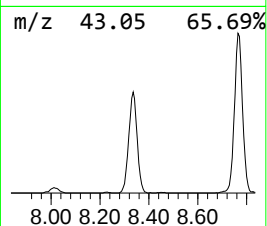
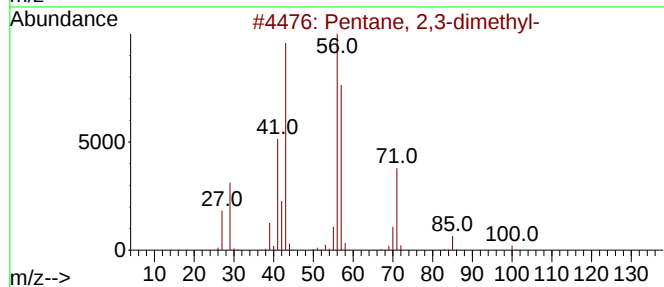
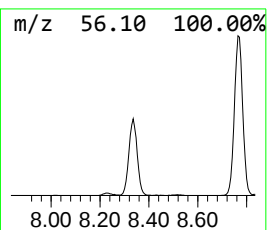
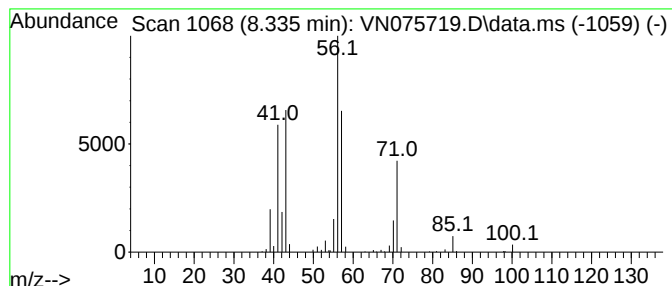
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.335	51.23 ug/l	664006	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	49
4			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	46



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

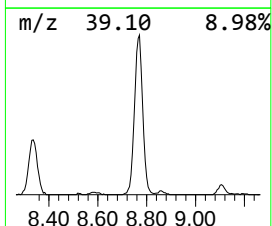
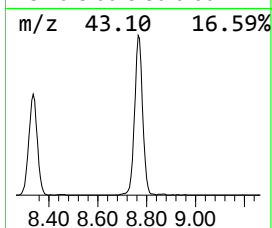
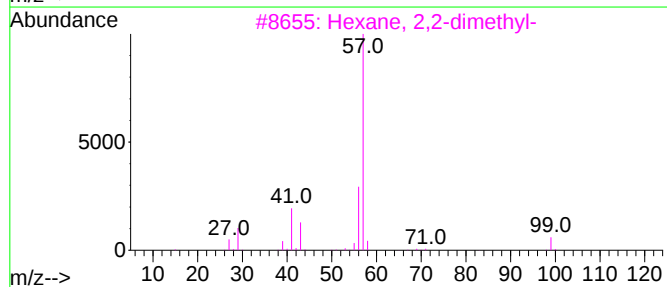
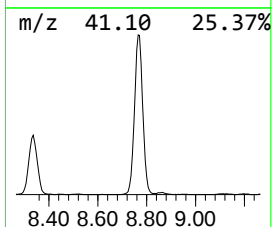
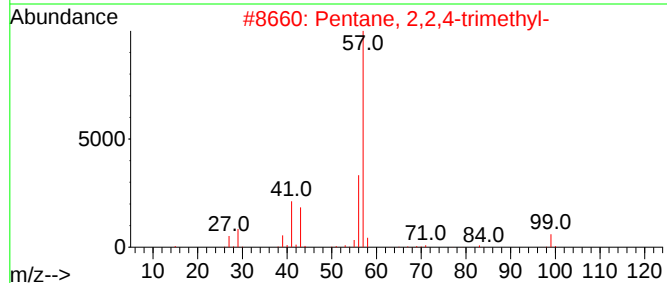
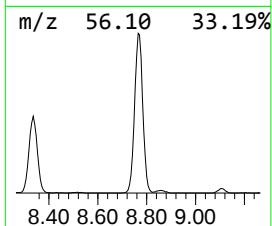
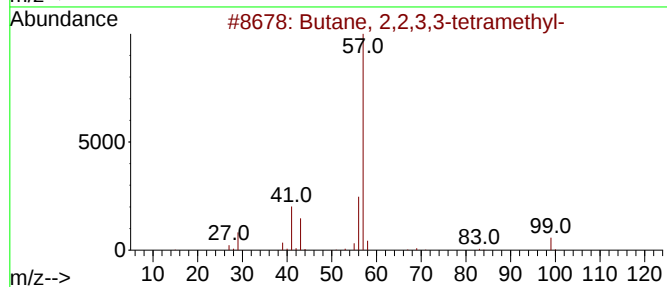
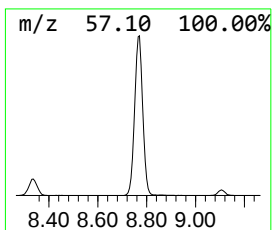
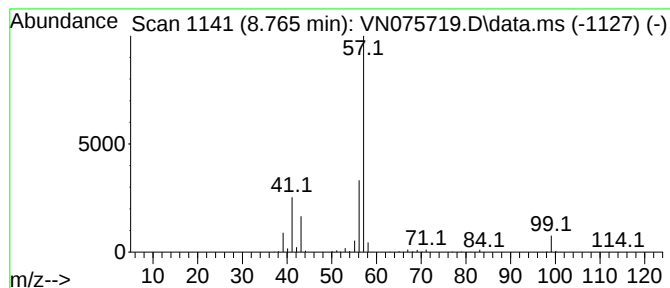
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	123.40 ug/l	2002100	1,4-Difluorobenzene	9.106

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	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	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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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

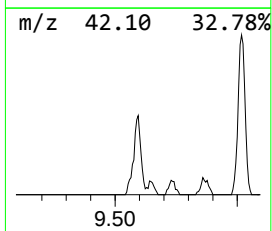
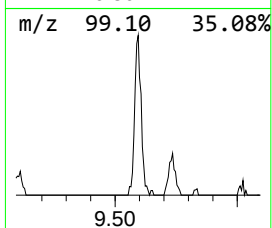
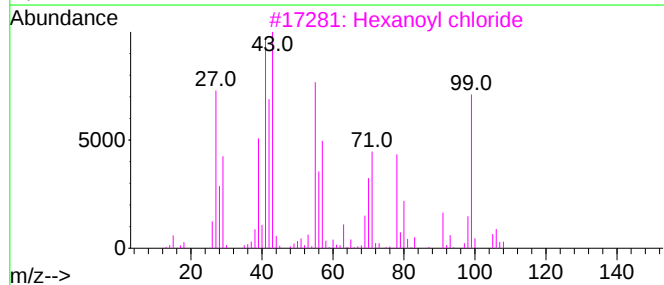
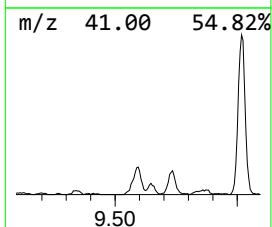
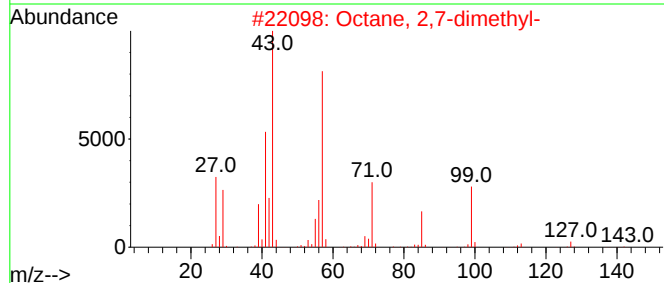
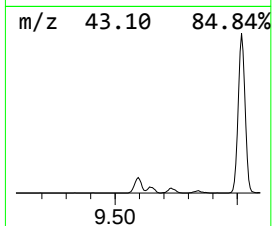
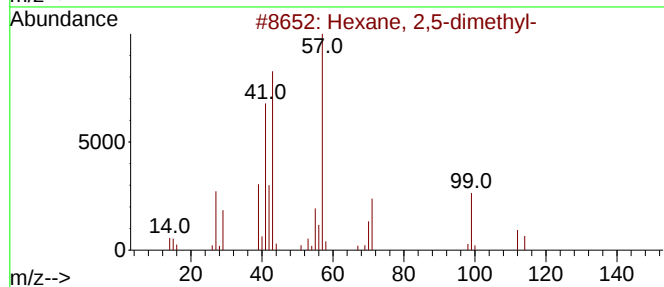
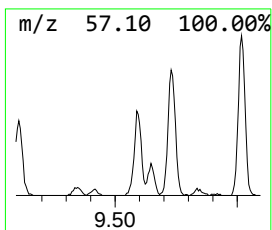
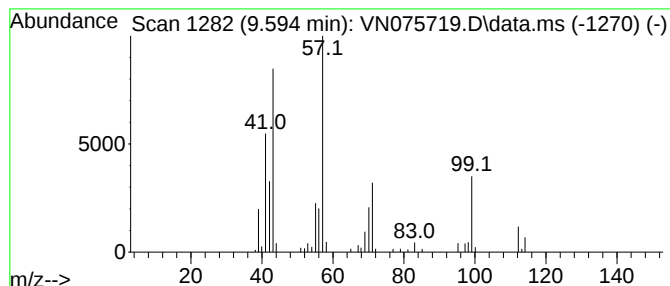
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.594	11.43 ug/l	185522	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	76
2			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	53
3			Hexanoyl chloride	134	C6H11ClO	000142-61-0	53
4			Heptane, 2-methyl-	114	C8H18	000592-27-8	52
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47



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TOLL-MW-03

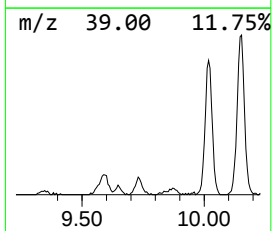
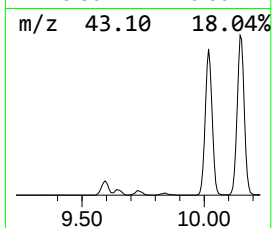
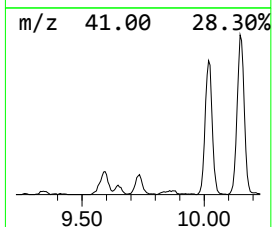
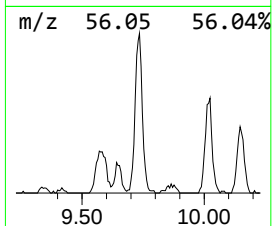
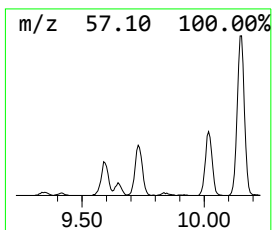
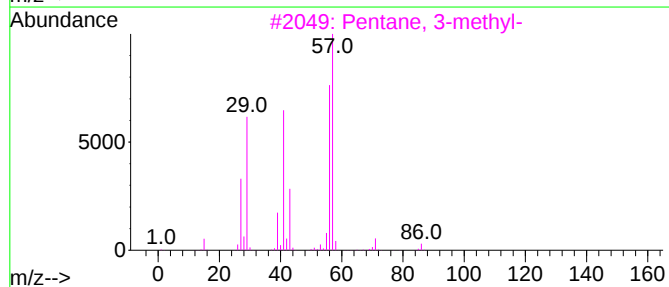
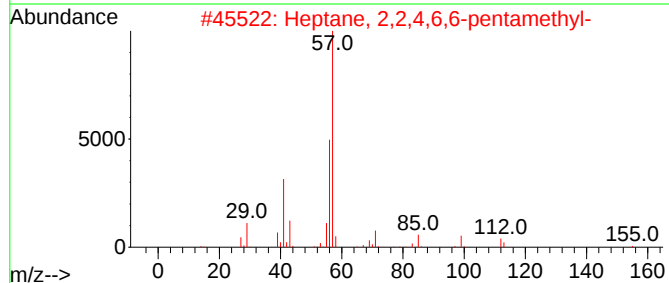
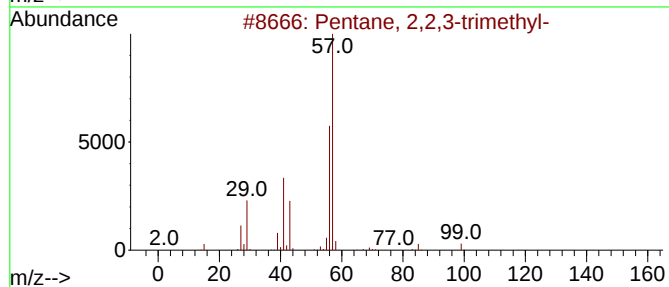
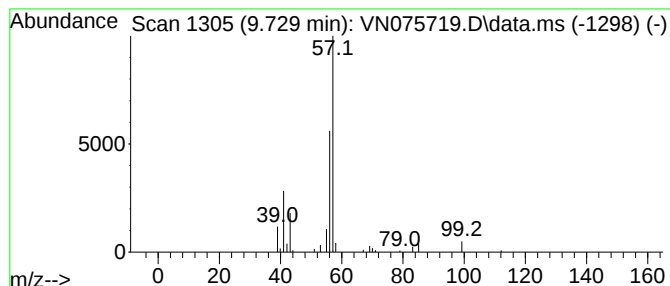
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentane, 2,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.729	7.90 ug/l	128191	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	78
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	74
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	64
4			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075719.D
Acq On : 12 Dec 2022 17:41
Operator : JC\MD
Sample : N5978-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

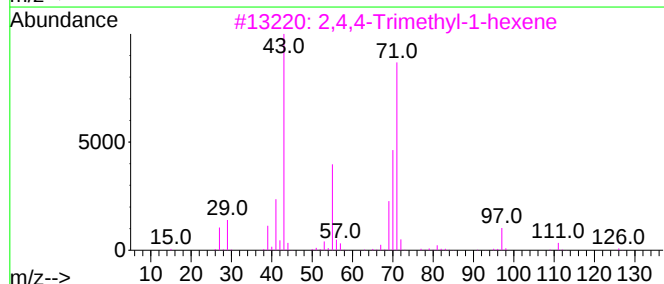
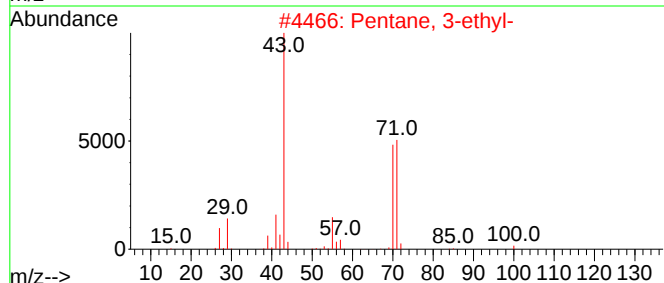
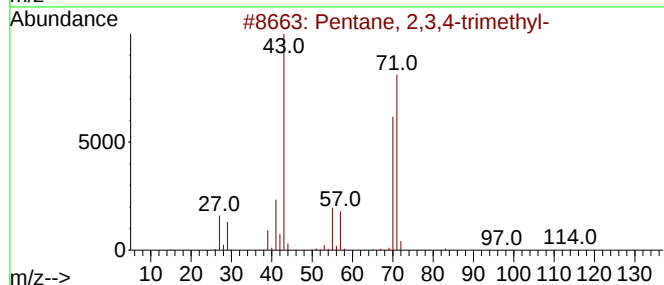
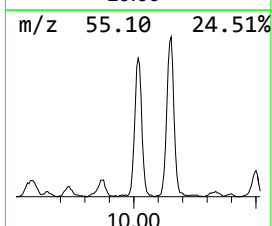
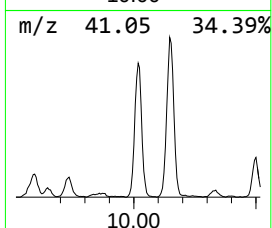
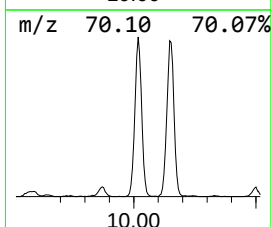
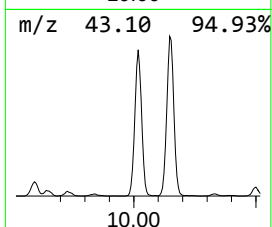
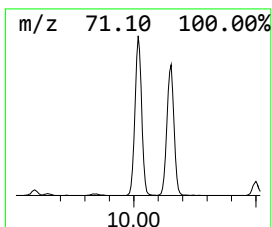
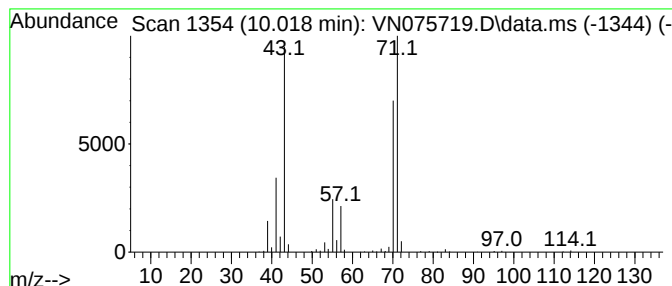
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.018	66.58 ug/l	1080290	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			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78
5			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075719.D
Acq On : 12 Dec 2022 17:41
Operator : JC\MD
Sample : N5978-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

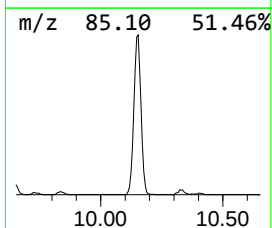
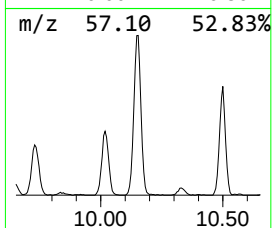
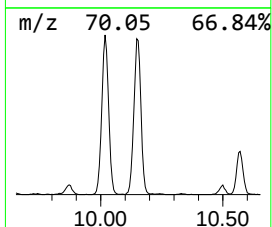
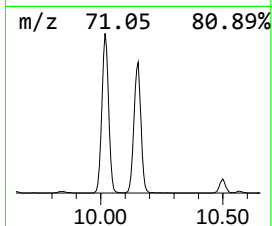
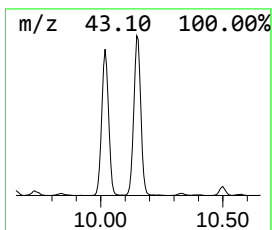
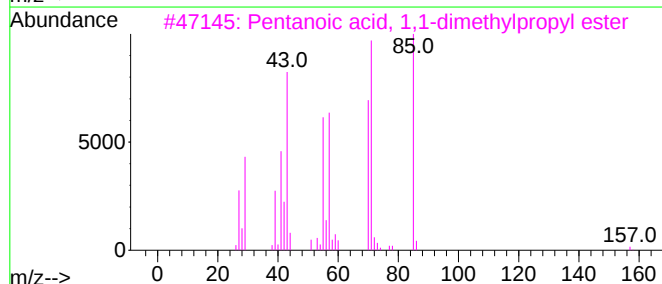
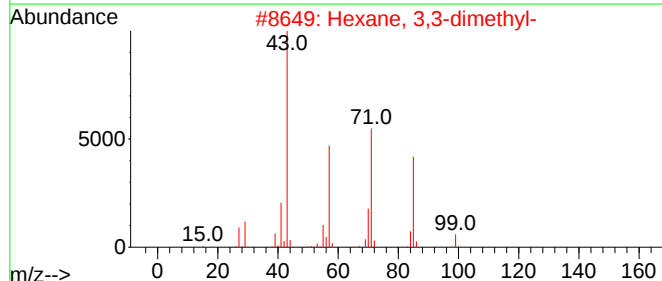
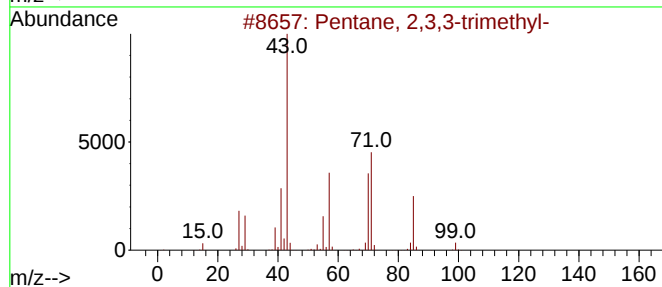
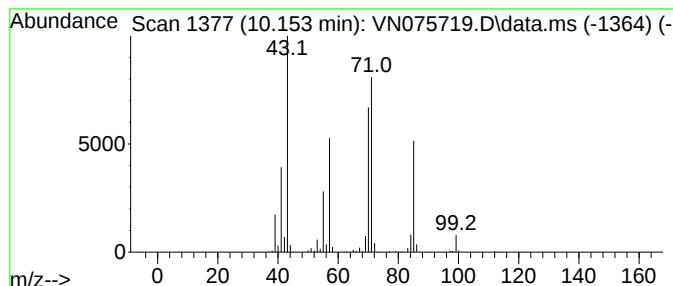
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	89.05 ug/l	1444760	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	72
3			Pentanoic acid, 1,1-dimethylprop...	172	C10H20O2	117421-32-6	72
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075719.D
Acq On : 12 Dec 2022 17:41
Operator : JC\MD
Sample : N5978-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

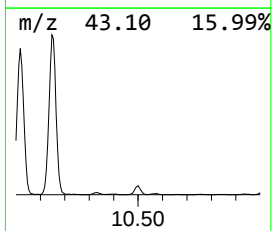
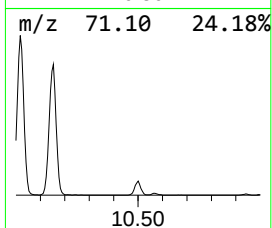
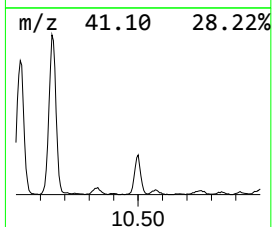
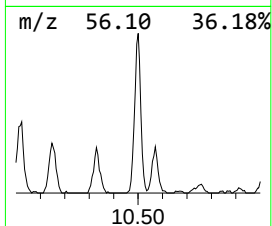
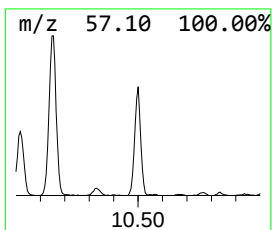
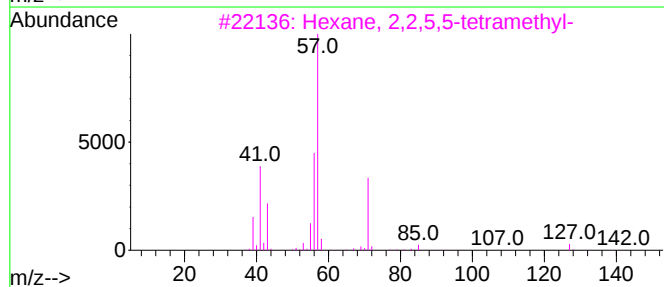
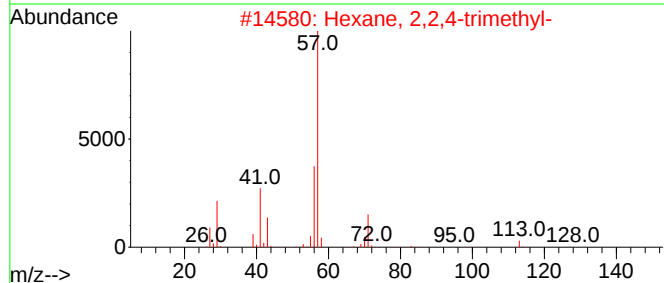
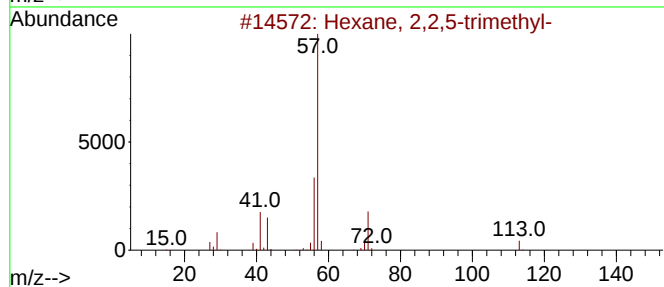
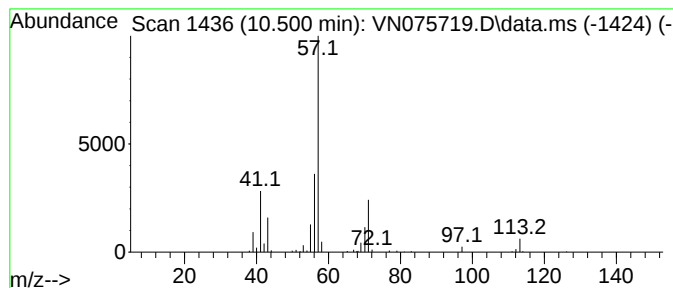
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

Peak Number 8 Hexane, 2,2,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.500	13.01 ug/l	245498	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
5			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075719.D
Acq On : 12 Dec 2022 17:41
Operator : JC\MD
Sample : N5978-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.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...	7.236	28.3	ug/l	366121	1	8.230	648076	50.0
Pentane, 2,3-di...	8.335	51.2	ug/l	664006	1	8.230	648076	50.0
Butane, 2,2,3,3...	8.765	123.4	ug/l	2002100	2	9.106	811214	50.0
Hexane, 2,5-dim...	9.594	11.4	ug/l	185522	2	9.106	811214	50.0
Pentane, 2,2,3-...	9.729	7.9	ug/l	128191	2	9.106	811214	50.0
Pentane, 2,3,4-...	10.018	66.6	ug/l	1080290	2	9.106	811214	50.0
Pentane, 2,3,3-...	10.153	89.0	ug/l	1444760	2	9.106	811214	50.0
Hexane, 2,2,5-t...	10.500	13.0	ug/l	245498	3	11.871	943750	50.0