

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070048.D
 Acq On : 13 Dec 2021 23:17
 Operator : JC/MD
 Sample : M5007-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 28 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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.446	160	170	188	rVB	354077	571615	5.22%	0.721%
2	3.140	419	429	446	rVB	128209	274520	2.51%	0.346%
3	5.077	1121	1151	1178	rBV4	112301	447266	4.09%	0.564%
4	5.618	1323	1353	1381	rBV3	208587	739161	6.75%	0.932%
5	7.048	1858	1886	1912	rBV3	757276	2343096	21.41%	2.955%
6	7.327	1967	1990	2012	rVB8	60038	170243	1.56%	0.215%
7	7.844	2168	2183	2204	rVB4	59687	163863	1.50%	0.207%
8	8.021	2225	2249	2261	rBV	845912	2087883	19.08%	2.633%
9	8.086	2261	2273	2289	rVV	1424239	3292401	30.09%	4.152%
10	8.174	2290	2306	2335	rVB	1565055	3915683	35.78%	4.938%
11	8.440	2385	2405	2433	rBV	969032	2268280	20.73%	2.861%
12	8.617	2449	2471	2495	rBV	4551581	10943419	100.00%	13.802%
13	8.705	2496	2504	2523	rVB5	81843	183445	1.68%	0.231%
14	8.968	2582	2602	2627	rBV	2436062	5136286	46.93%	6.478%
15	9.201	2676	2689	2701	rBV6	54126	119486	1.09%	0.151%
16	9.456	2747	2784	2796	rBV6	399042	1090833	9.97%	1.376%
17	9.513	2796	2805	2820	rVV2	190533	377747	3.45%	0.476%
18	9.593	2820	2835	2862	rVV2	334006	743620	6.80%	0.938%
19	9.732	2863	2887	2904	rVV6	107712	312187	2.85%	0.394%
20	9.883	2925	2943	2968	rVB	2953192	5873977	53.68%	7.408%
21	10.014	2969	2992	3022	rBV	3979795	8189081	74.83%	10.328%
22	10.199	3047	3061	3076	rBV2	115468	235588	2.15%	0.297%
23	10.371	3099	3125	3137	rBV3	580678	1148413	10.49%	1.448%
24	10.441	3137	3151	3182	rVB	4001114	7545131	68.95%	9.516%
25	10.864	3295	3309	3331	rVB7	154072	494706	4.52%	0.624%
26	11.130	3394	3408	3420	rBV5	72806	150587	1.38%	0.190%
27	11.744	3619	3637	3657	rBV	4273673	7804754	71.32%	9.843%
28	11.993	3721	3730	3747	rVB5	55603	116615	1.07%	0.147%
29	12.731	3988	4005	4030	rBV	3331272	5971981	54.57%	7.532%
30	13.675	4341	4357	4384	rBV	3694648	6433495	58.79%	8.114%
31	14.150	4522	4534	4548	rBV3	82881	145195	1.33%	0.183%

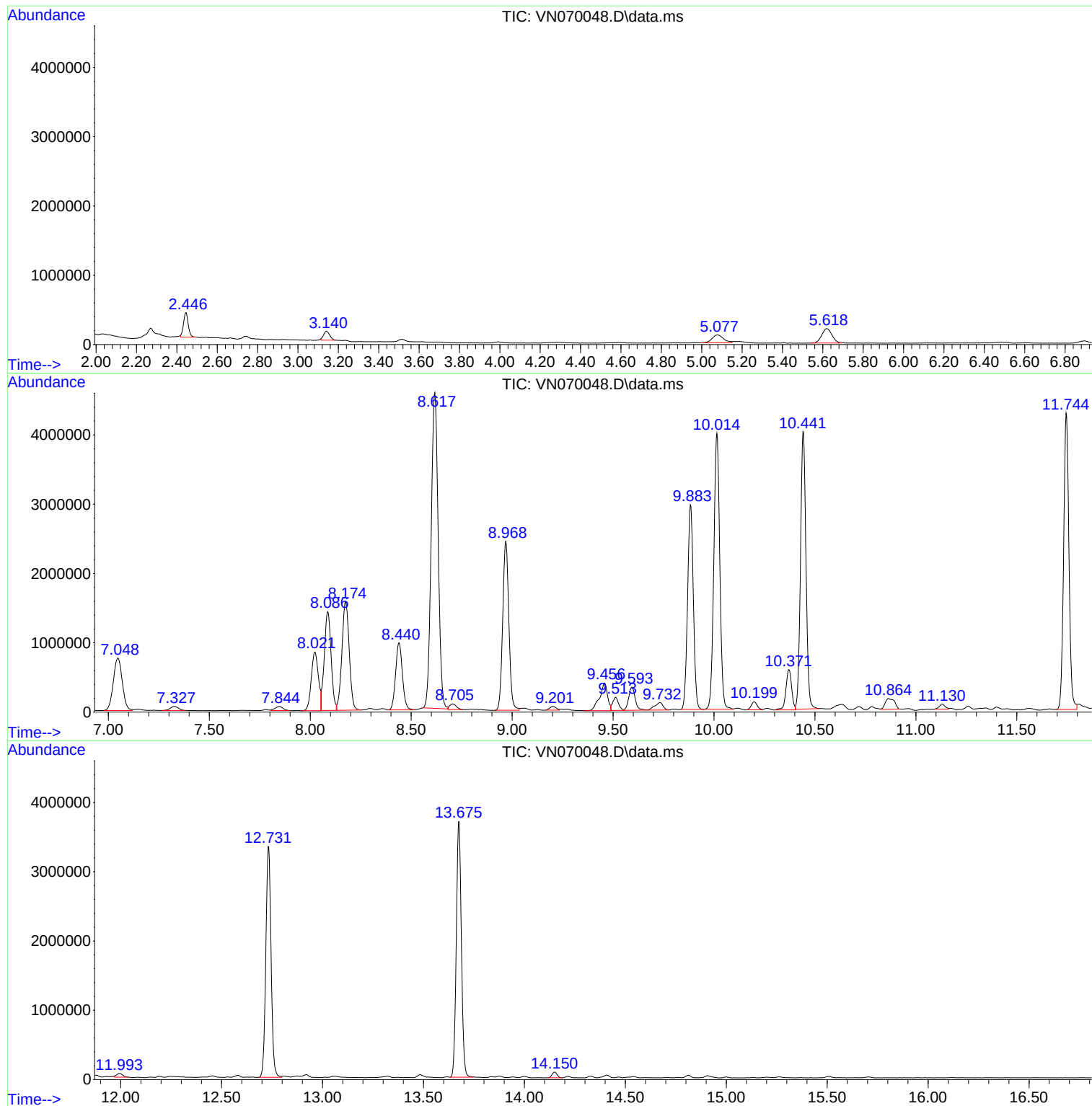
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

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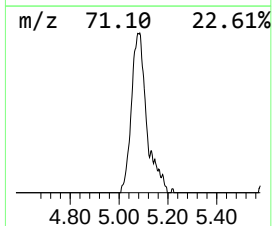
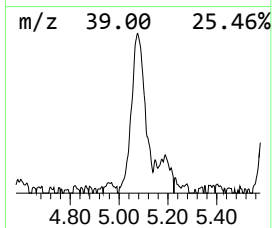
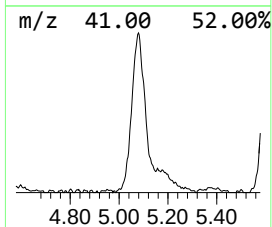
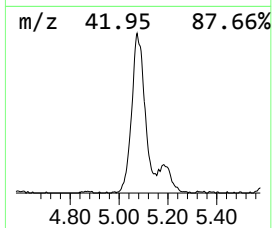
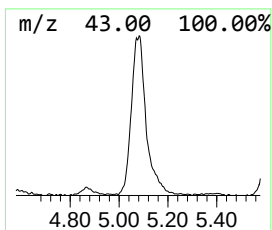
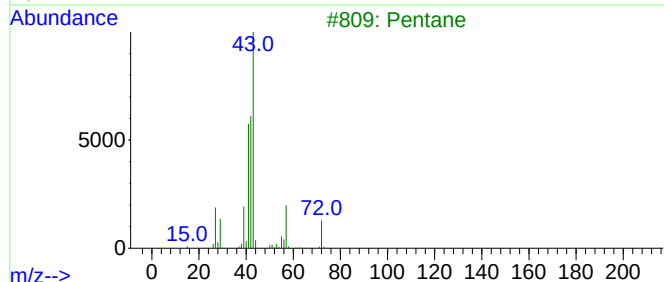
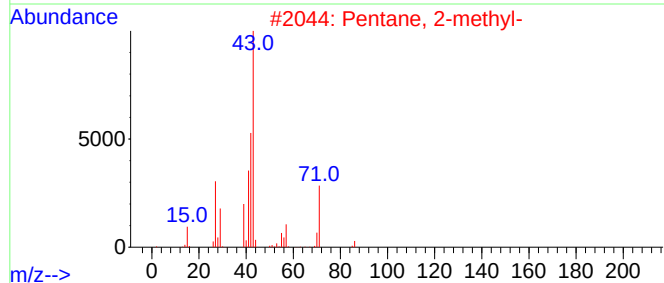
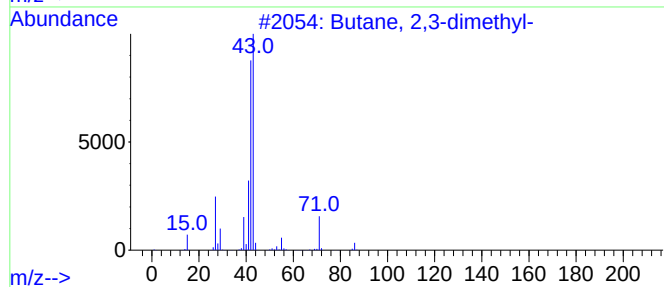
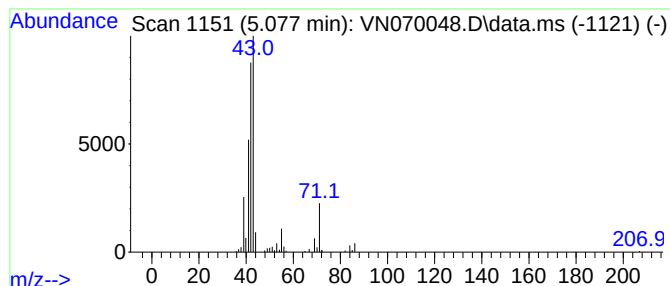
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.077	6.79 ug/l	447266	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			Pentane	72	C5H12	000109-66-0	36
4			Isobutylene carbonate	116	C5H8O3	035466-83-2	9
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	9



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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

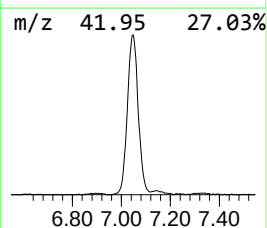
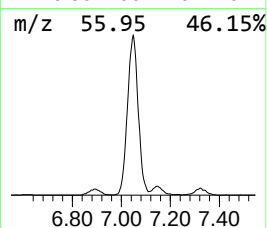
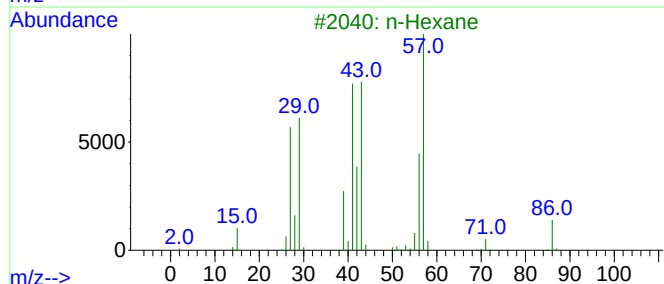
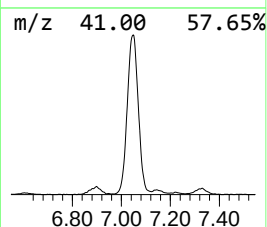
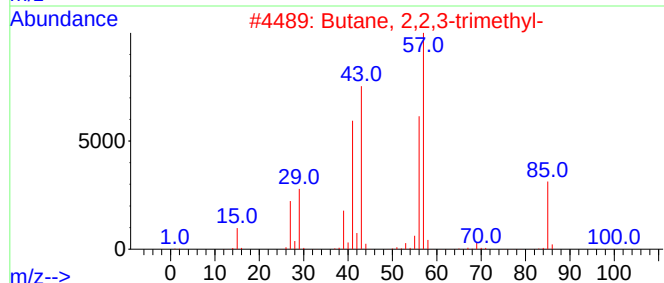
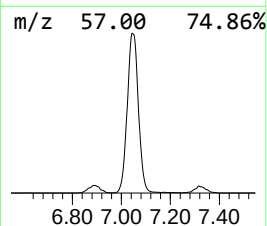
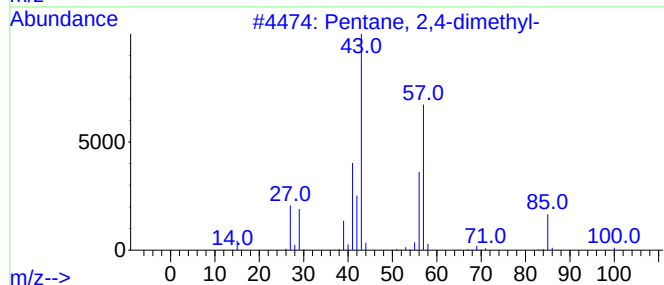
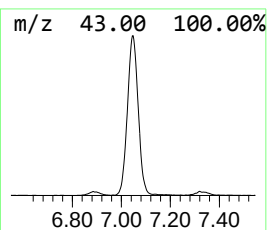
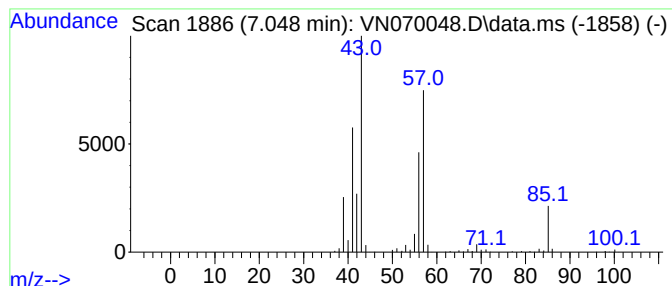
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.048	35.58 ug/l	2343100	Pentafluorobenzene	8.086

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			n-Hexane	86	C6H14	000110-54-3	53
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	50



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TOLL-MW-03

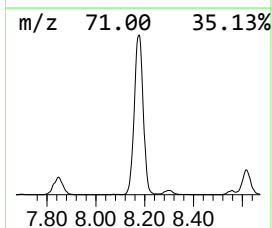
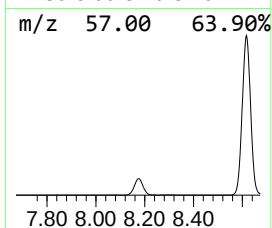
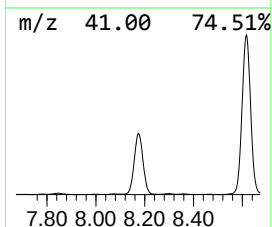
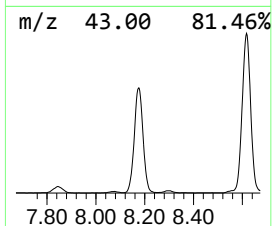
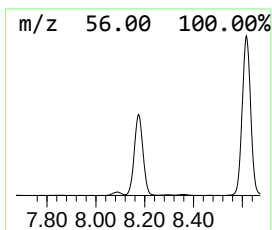
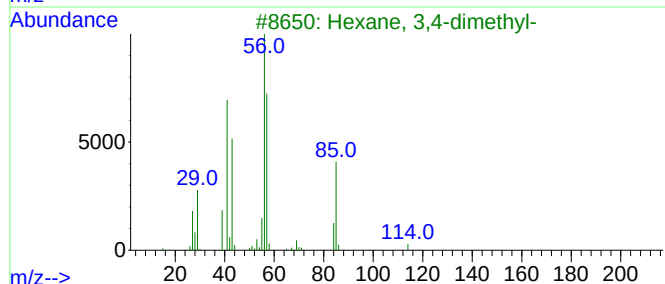
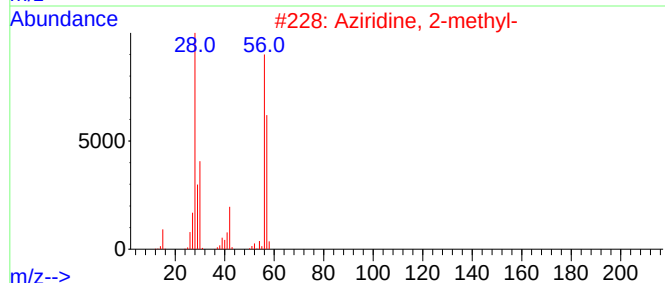
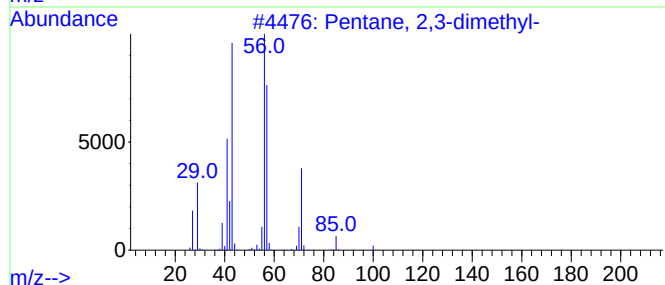
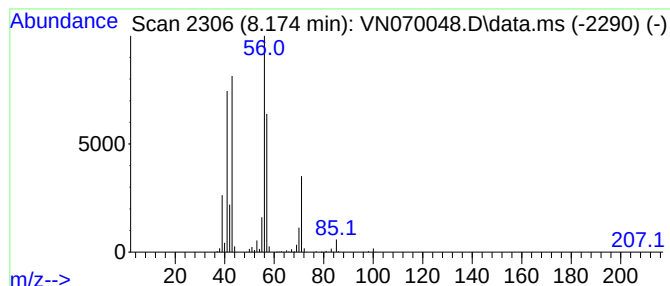
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	59.47 ug/l	3915680	Pentafluorobenzene	8.086

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			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40
4			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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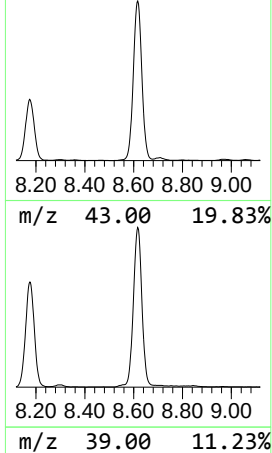
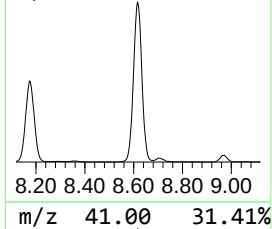
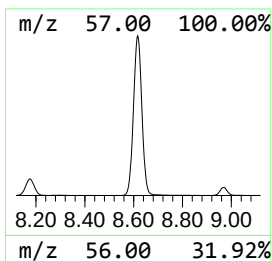
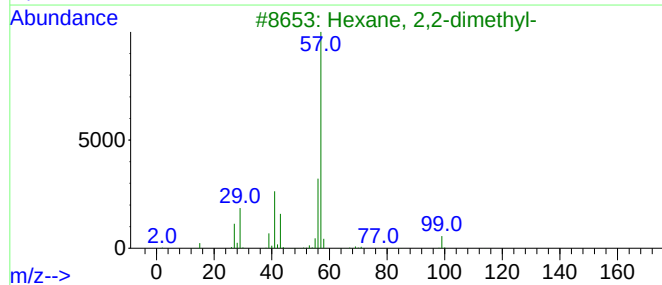
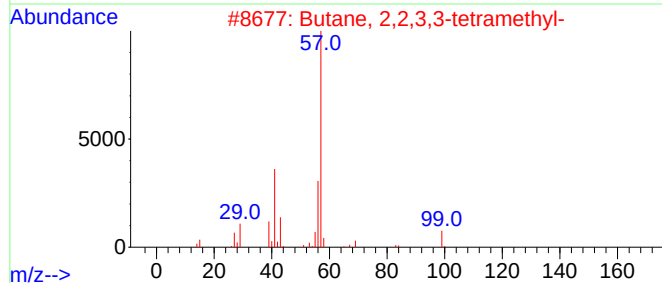
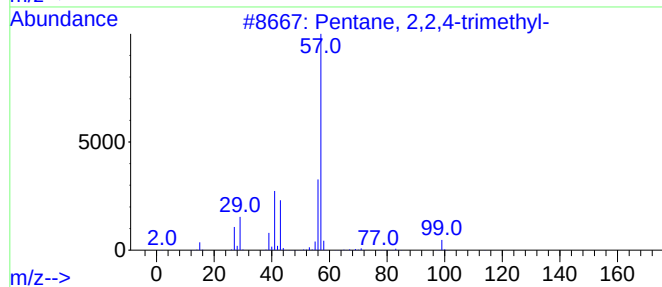
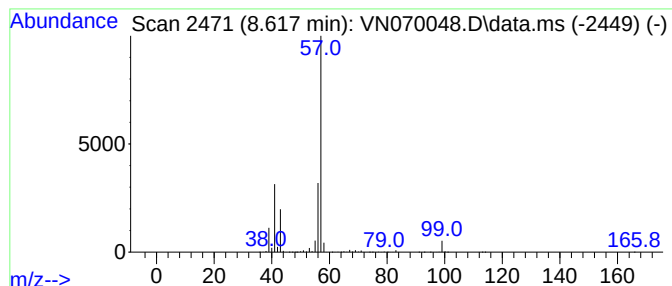
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	106.53 ug/l	10943400	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	38



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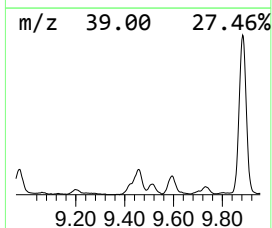
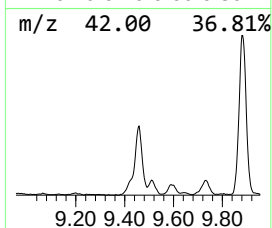
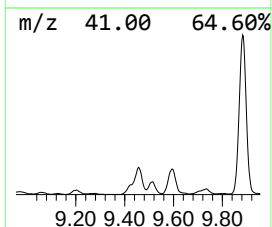
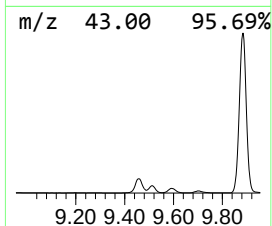
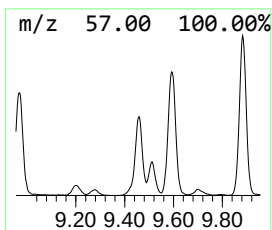
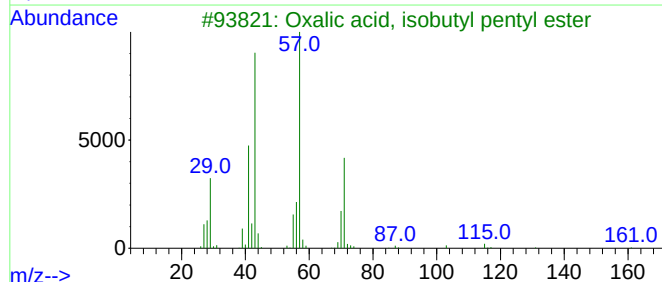
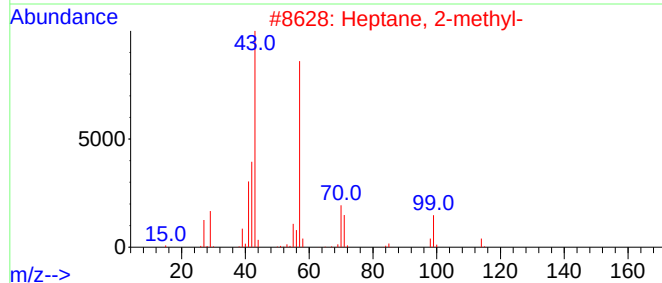
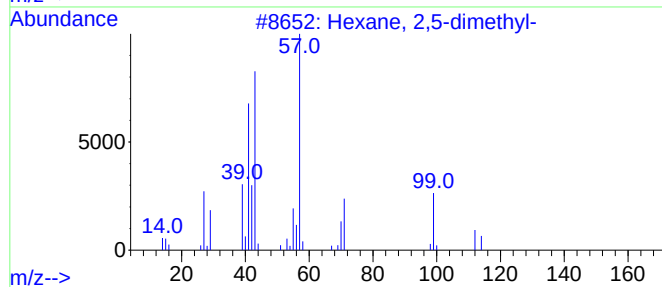
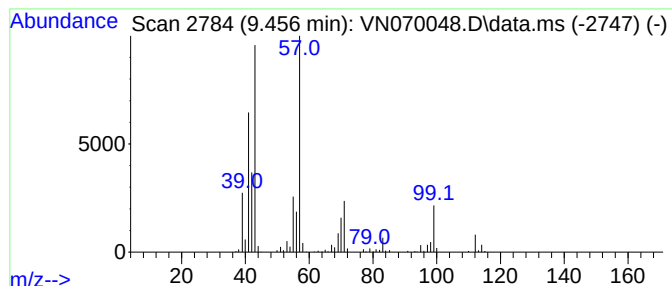
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.456	10.62 ug/l	1090830	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	91
2			Heptane, 2-methyl-	114	C8H18	000592-27-8	64
3			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	50
4			Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	47
5			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	43



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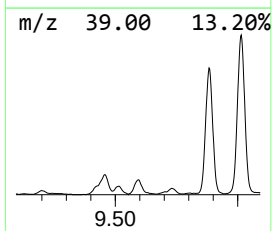
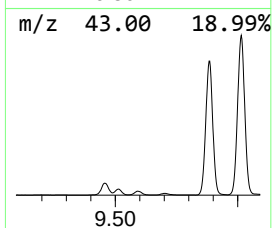
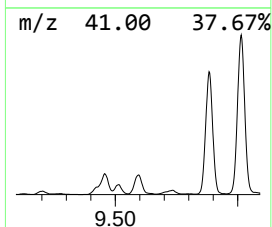
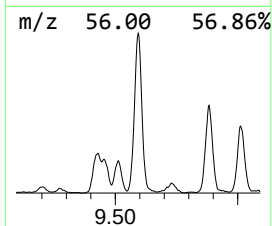
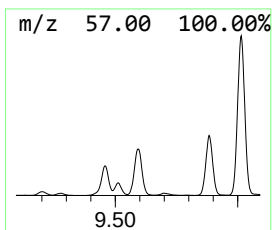
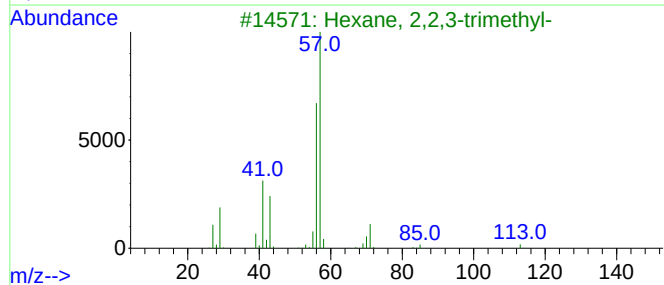
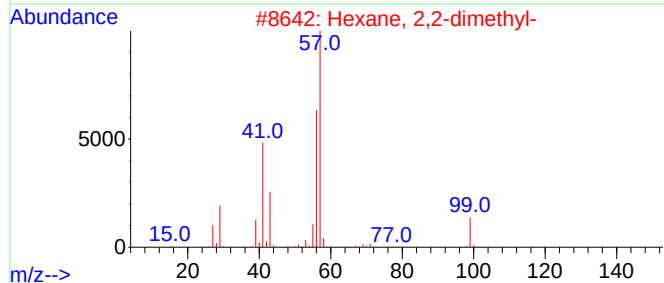
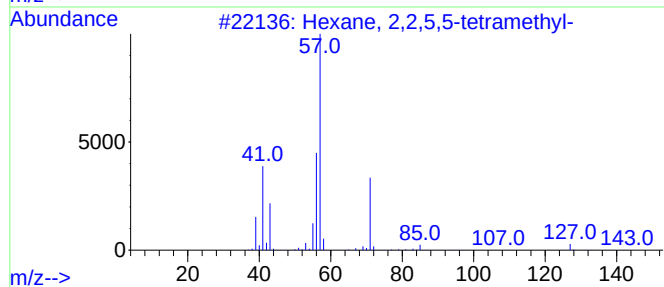
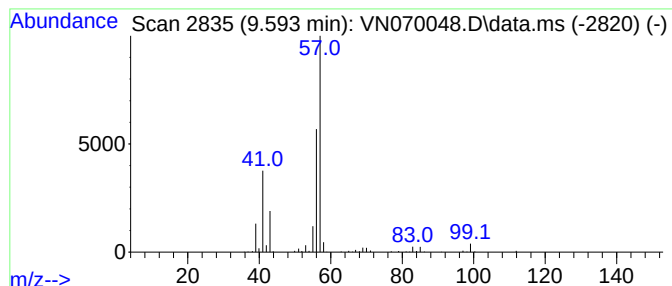
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.593	7.24 ug/l	743620	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	64
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070048.D
Acq On : 13 Dec 2021 23:17
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

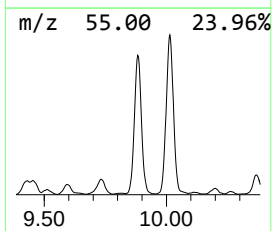
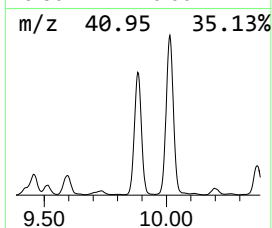
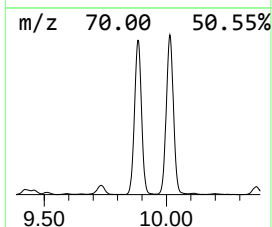
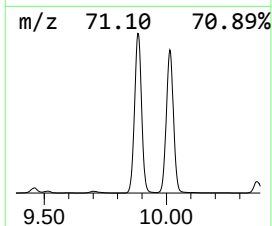
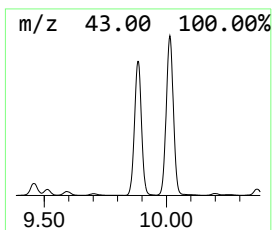
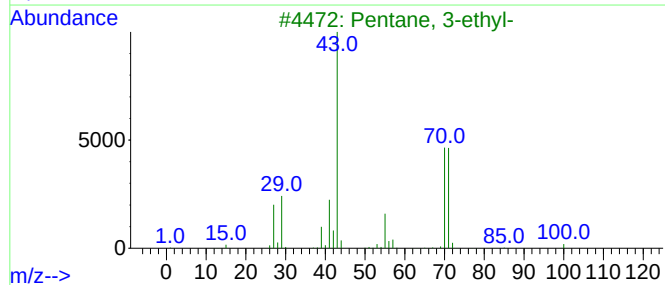
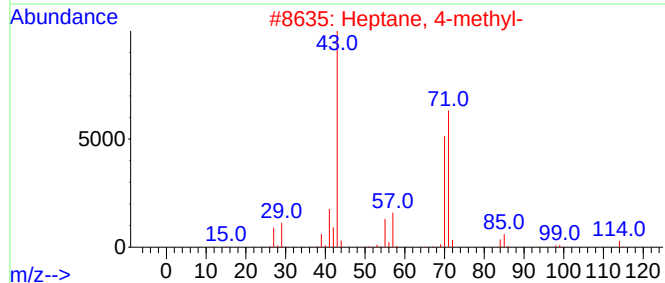
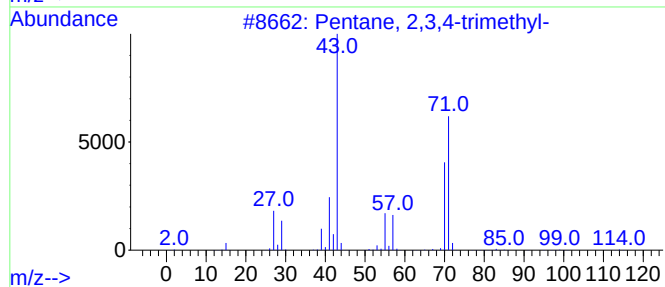
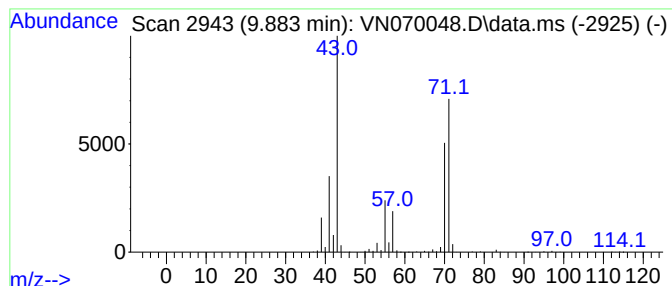
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	57.18 ug/l	5873980	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070048.D
Acq On : 13 Dec 2021 23:17
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

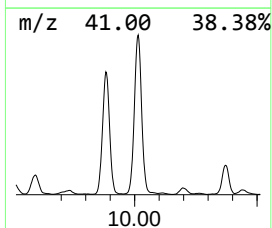
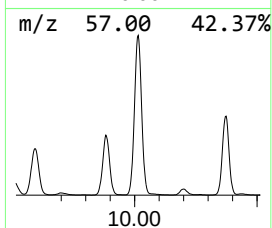
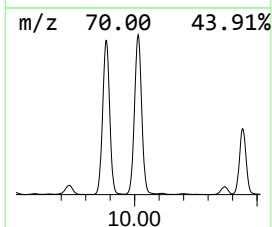
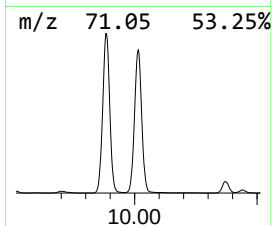
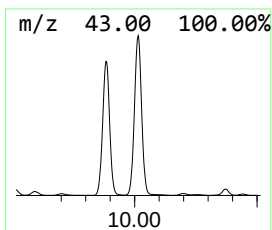
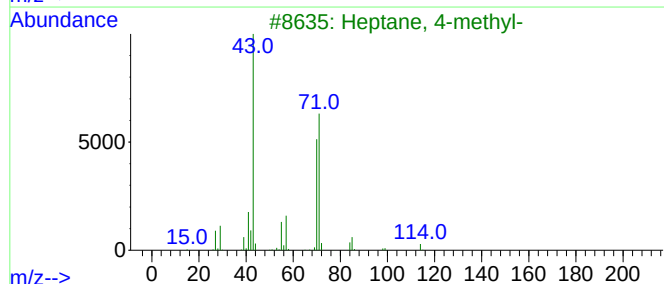
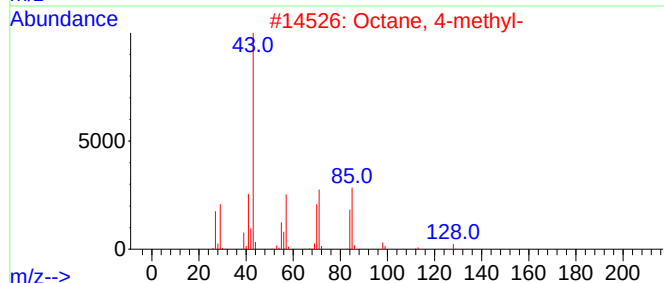
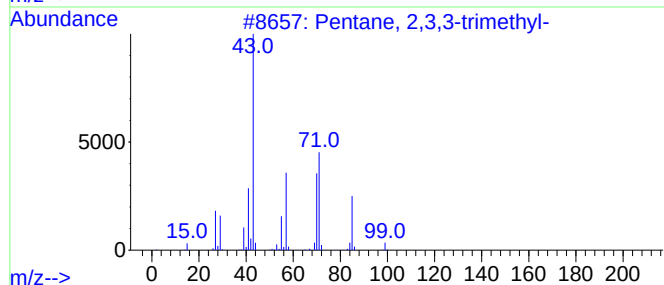
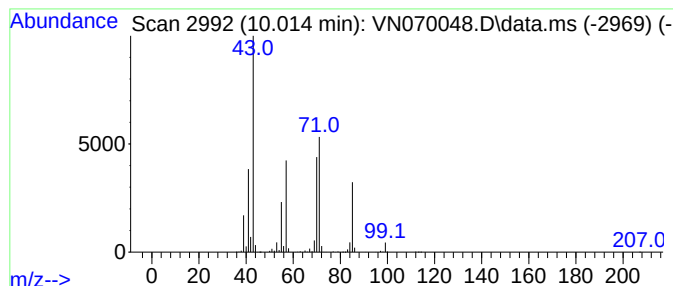
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	79.72 ug/l	8189080	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Octane, 4-methyl-	128	C9H20	002216-34-4	78
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070048.D
Acq On : 13 Dec 2021 23:17
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

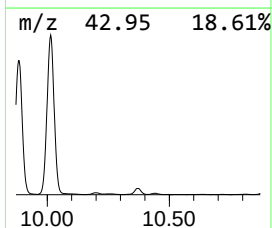
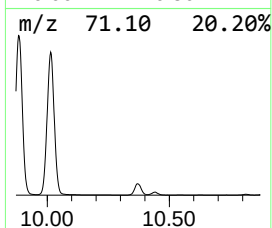
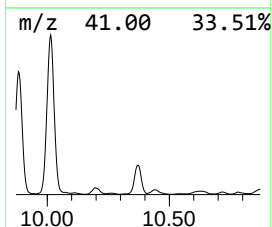
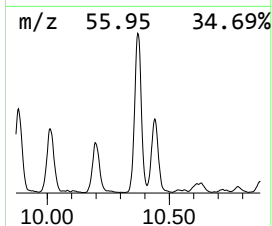
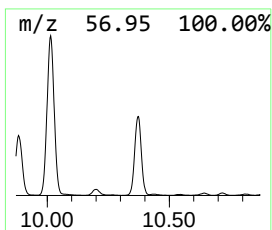
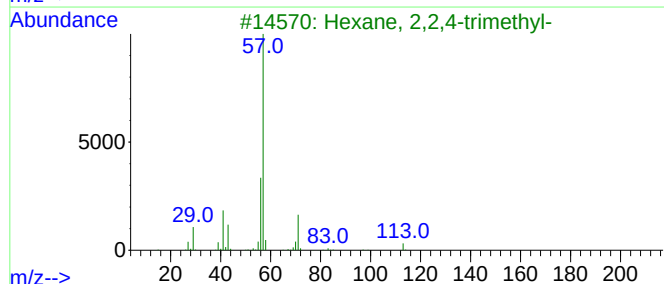
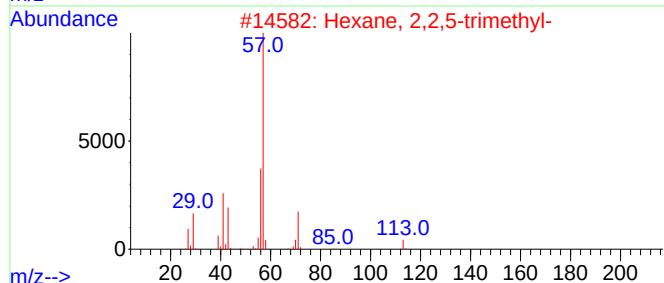
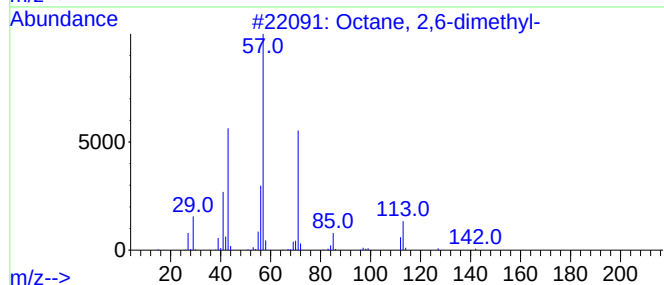
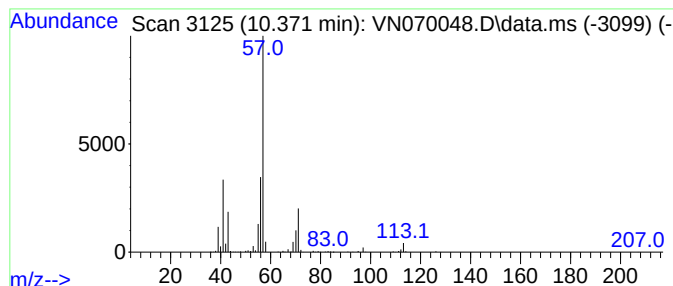
Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

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 9 Octane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.371	7.36 ug/l	1148410	Chlorobenzene-d5		11.744	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	72
2	Hexane, 2,2,5-trimethyl-		128	C9H20	003522-94-9	72
3	Hexane, 2,2,4-trimethyl-		128	C9H20	016747-26-5	56
4	Heptane, 2,2-dimethyl-		128	C9H20	001071-26-7	50
5	Pentane, 2,2,4,4-tetramethyl-		128	C9H20	001070-87-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070048.D
Acq On : 13 Dec 2021 23:17
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

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
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Pentane, 2,4-di...	7.048	35.6	ug/l	2343100	1	8.086	3292400	50.0
Pentane, 2,3-di...	8.174	59.5	ug/l	3915680	1	8.086	3292400	50.0
Pentane, 2,2,4-...	8.617	106.5	ug/l	10943400	2	8.968	5136290	50.0
Hexane, 2,5-dim...	9.456	10.6	ug/l	1090830	2	8.968	5136290	50.0
Hexane, 2,2,5,5...	9.593	7.2	ug/l	743620	2	8.968	5136290	50.0
Pentane, 2,3,4-...	9.883	57.2	ug/l	5873980	2	8.968	5136290	50.0
Pentane, 2,3,3-...	10.014	79.7	ug/l	8189080	2	8.968	5136290	50.0
Octane, 2,6-dim...	10.371	7.4	ug/l	1148410	3	11.744	7804750	50.0