

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
 Data File : VN070629.D
 Acq On : 14 Jan 2022 17:46
 Operator : JC/MD
 Sample : N1148-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-29R

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	408	426	454	rVB	466047	1115714	5.43%	0.924%
2	4.248	816	842	880	rBV6	77442	324991	1.58%	0.269%
3	5.074	1120	1150	1173	rBV2	332831	1346112	6.55%	1.115%
4	5.382	1235	1265	1317	rBV	611455	2202822	10.72%	1.824%
5	5.618	1319	1353	1411	rVV2	3228917	11431461	55.65%	9.466%
6	6.498	1654	1681	1707	rVB4	171596	581973	2.83%	0.482%
7	7.144	1903	1922	1944	rVV3	175906	506724	2.47%	0.420%
8	8.021	2225	2249	2260	rBV	642041	1576283	7.67%	1.305%
9	8.086	2261	2273	2292	rVV	1267012	3010434	14.66%	2.493%
10	8.174	2292	2306	2329	rVB3	334525	850996	4.14%	0.705%
11	8.450	2388	2409	2425	rBV3	1277764	3750180	18.26%	3.106%
12	8.539	2425	2442	2465	rVV	9069600	20540474	100.00%	17.010%
13	8.968	2584	2602	2628	rBV	1879928	3990093	19.43%	3.304%
14	9.880	2933	2942	2955	rVB4	165968	288999	1.41%	0.239%
15	10.017	2985	2993	3007	rVB	258458	487209	2.37%	0.403%
16	10.204	3046	3063	3065	rBV2	2558195	3748267	18.25%	3.104%
17	10.237	3067	3075	3114	rVB	5564038	10792728	52.54%	8.938%
18	10.440	3137	3151	3166	rBV	2870554	5469144	26.63%	4.529%
19	10.553	3179	3193	3209	rVB	5014974	9036340	43.99%	7.483%
20	11.089	3382	3393	3403	rBV	800903	1388355	6.76%	1.150%
21	11.615	3576	3589	3619	rVB2	1784408	4158708	20.25%	3.444%
22	11.744	3622	3637	3662	rVV	6106100	11453977	55.76%	9.485%
23	11.846	3664	3675	3693	rVB	1237711	2296811	11.18%	1.902%
24	11.958	3706	3717	3743	rVB4	967234	2189170	10.66%	1.813%
25	12.355	3856	3865	3876	rBV2	587589	991706	4.83%	0.821%
26	12.731	3992	4005	4030	rVB4	3220369	6217463	30.27%	5.149%
27	12.841	4036	4046	4058	rBV2	1069682	1882940	9.17%	1.559%
28	13.675	4346	4357	4390	rVB2	2161585	4371784	21.28%	3.620%
29	13.876	4425	4432	4443	rVB	1744030	2466521	12.01%	2.043%
30	14.329	4593	4601	4615	rVB	1466604	2288836	11.14%	1.895%

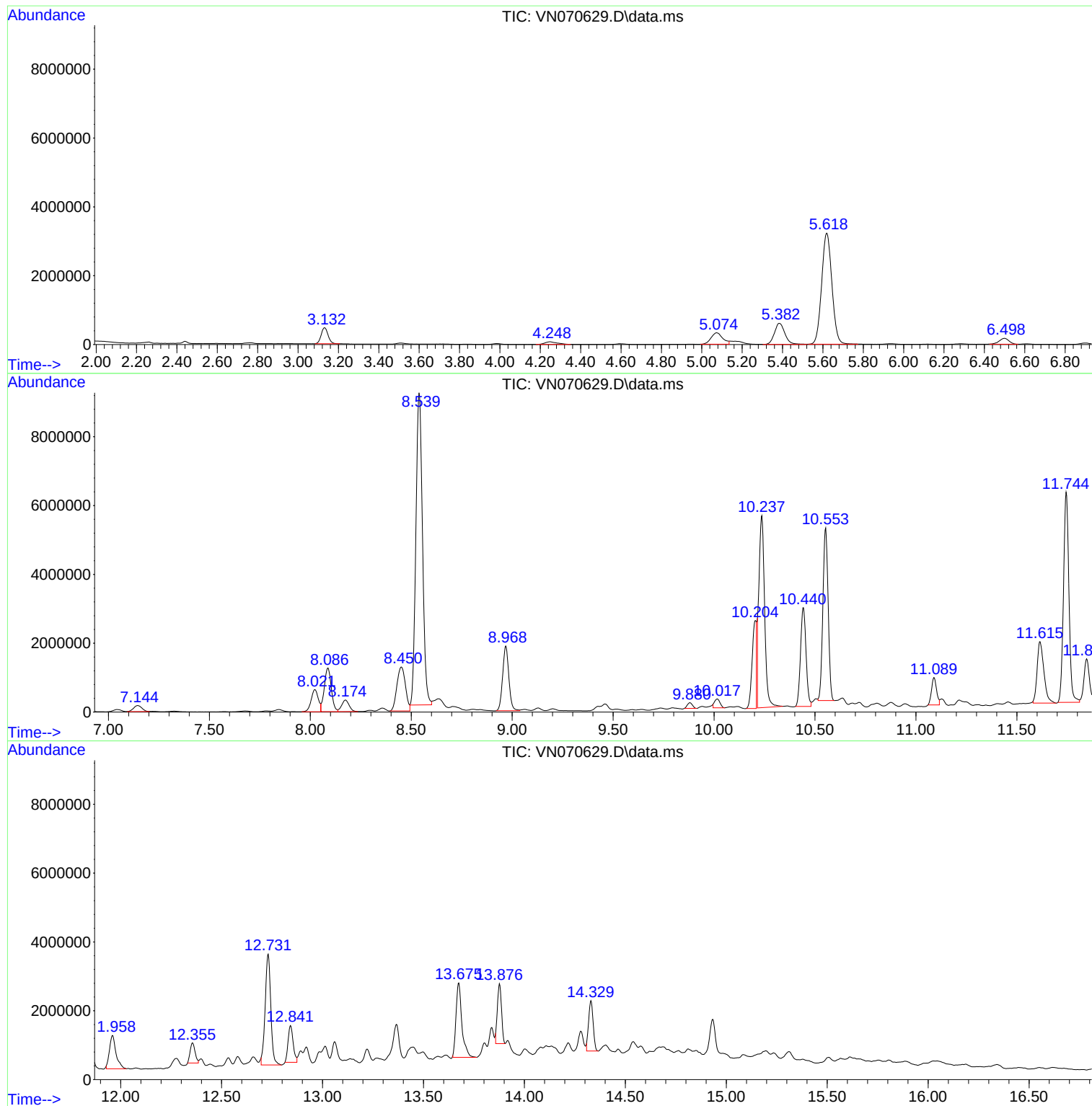
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Instrument :
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ClientSampleId :
MW-29R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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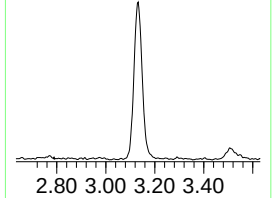
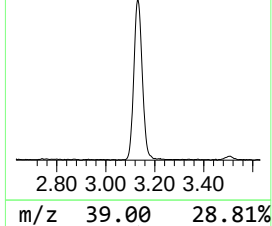
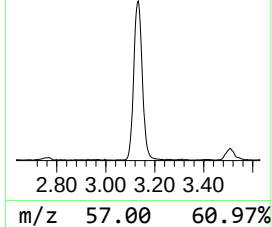
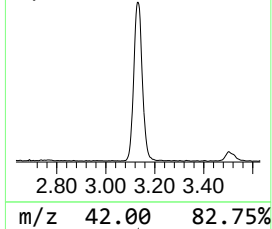
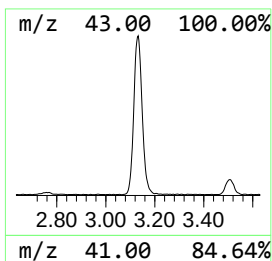
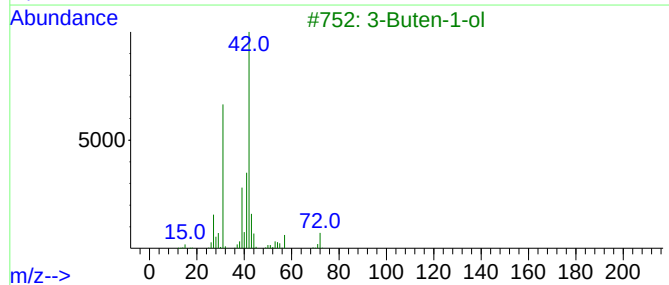
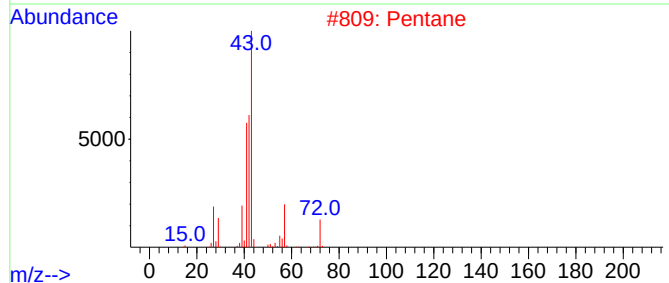
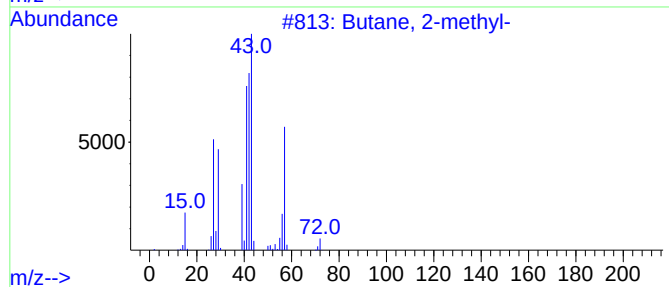
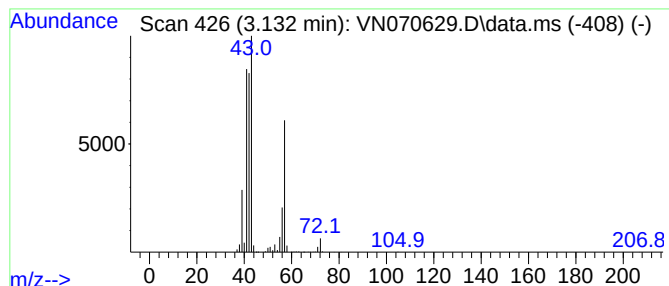
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.132	18.53 ug/l	1115710	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	56
3			3-Buten-1-ol	72	C4H8O	000627-27-0	47
4			2-Butene, (Z)-	56	C4H8	000590-18-1	9
5			1-Butene	56	C4H8	000106-98-9	9



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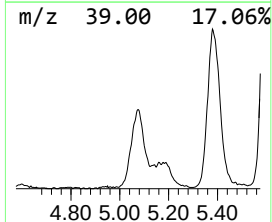
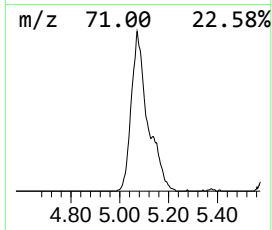
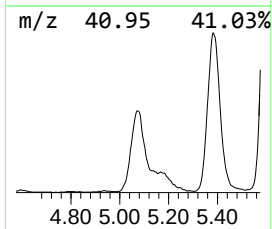
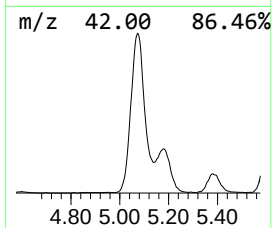
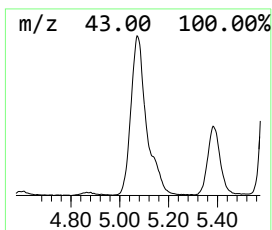
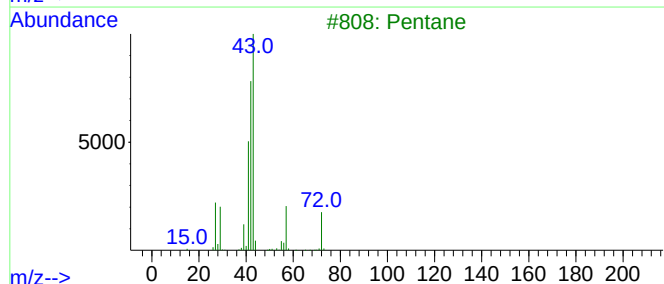
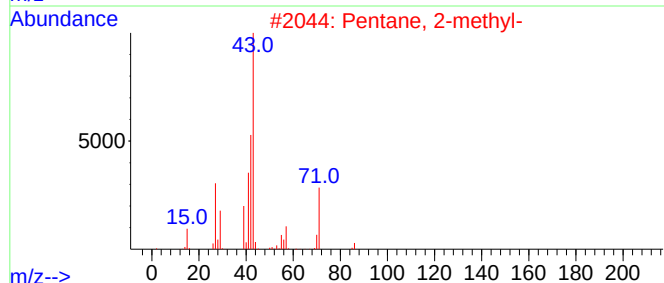
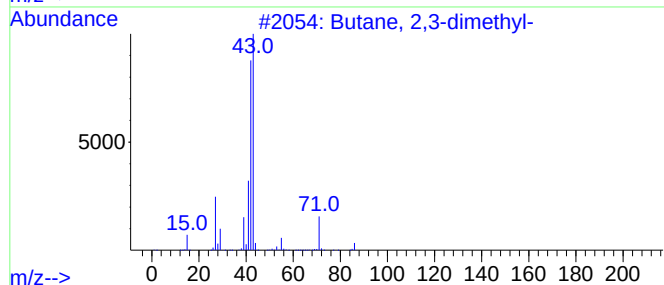
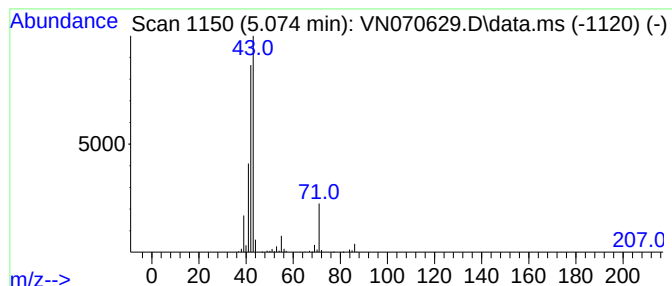
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.074	22.36 ug/l	1346110	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			Pentane	72	C5H12	000109-66-0	38
4			Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	12
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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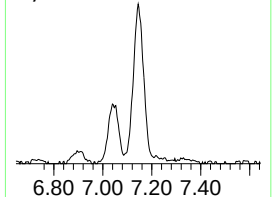
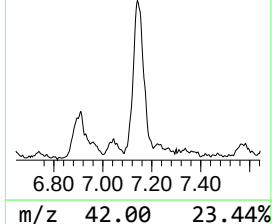
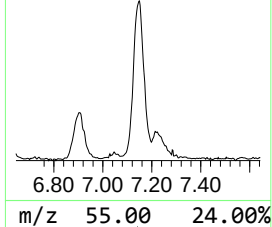
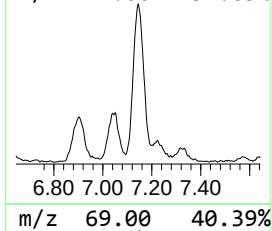
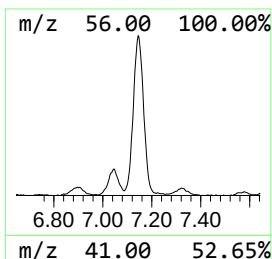
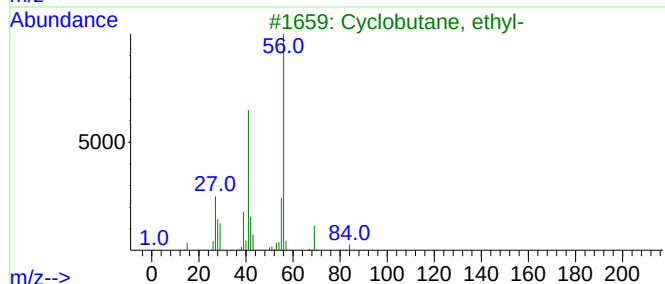
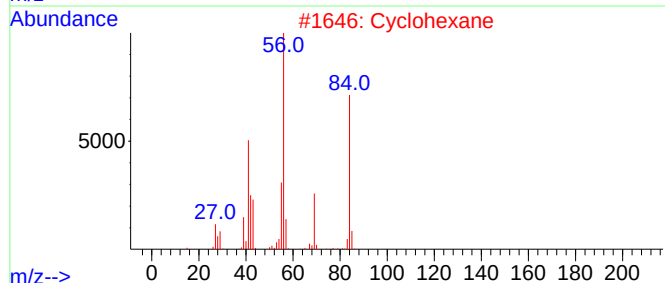
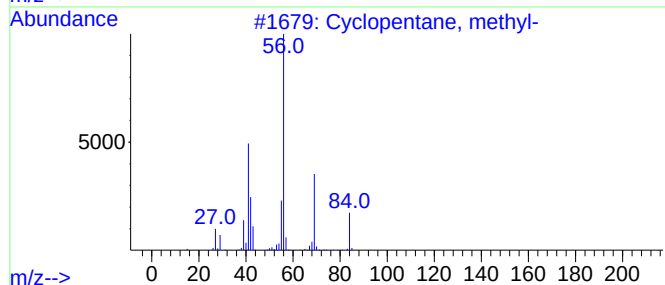
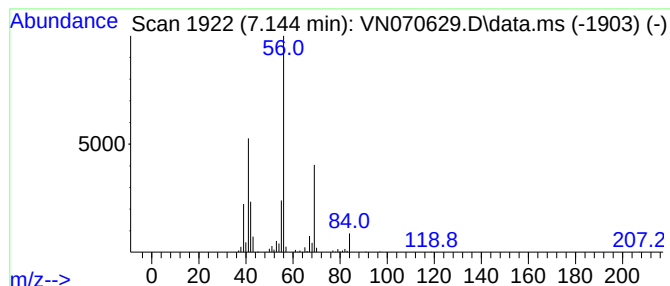
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.144	8.42 ug/l	506724	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	78
2			Cyclohexane	84	C6H12	000110-82-7	74
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5			Cyclobutane, butyl-	112	C8H16	013152-44-8	45



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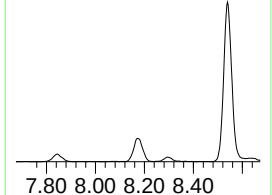
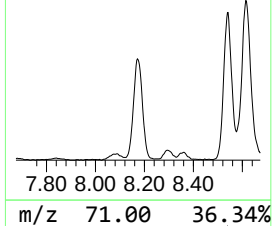
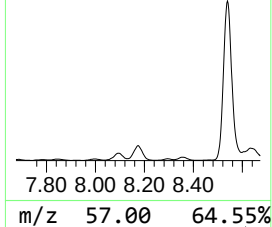
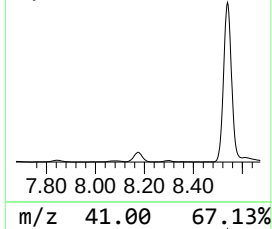
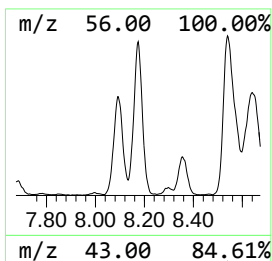
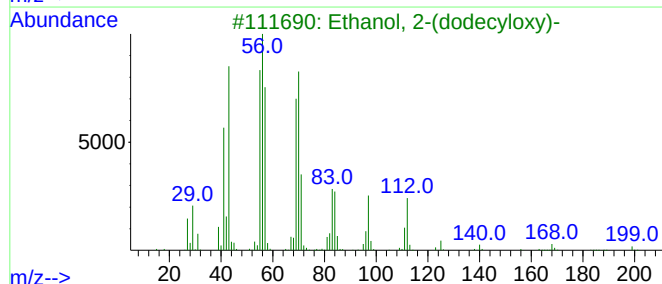
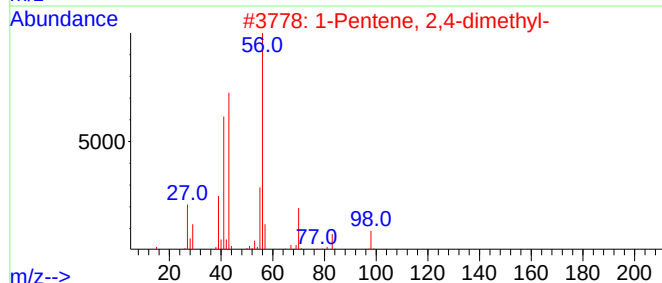
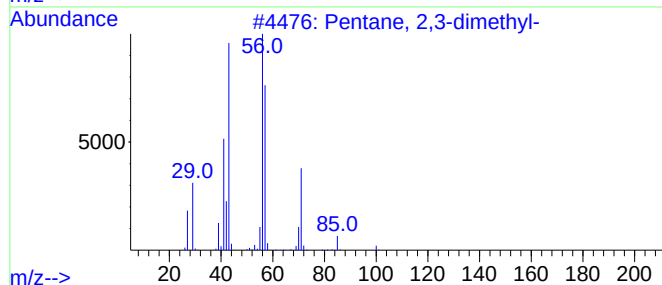
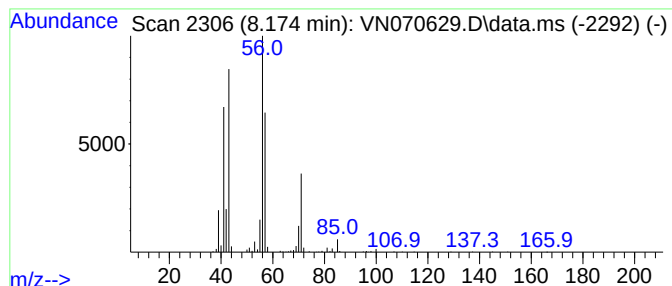
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	14.13 ug/l	850996	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	59
3			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	56
4			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	50
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	49



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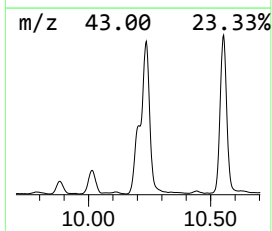
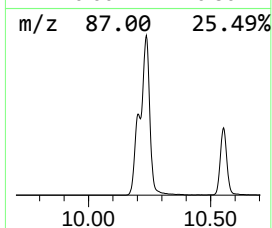
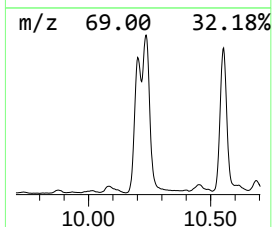
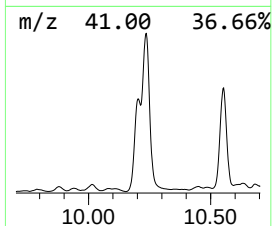
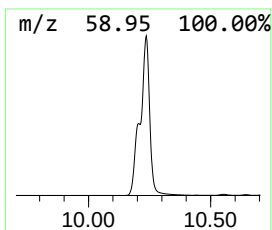
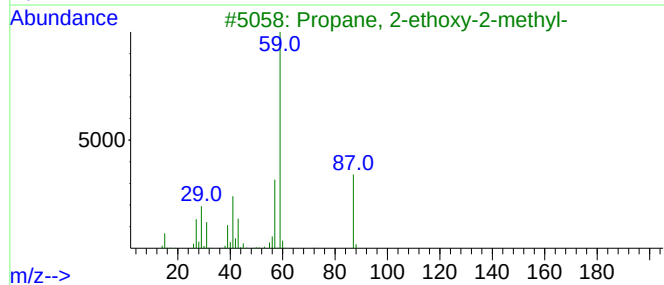
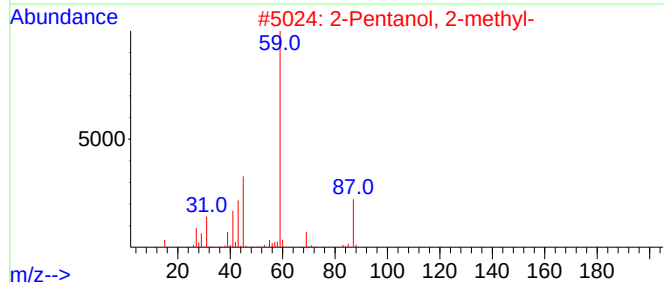
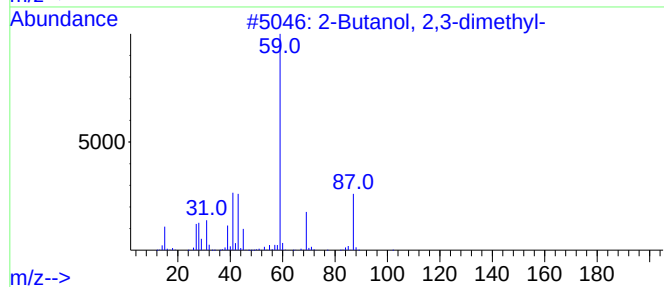
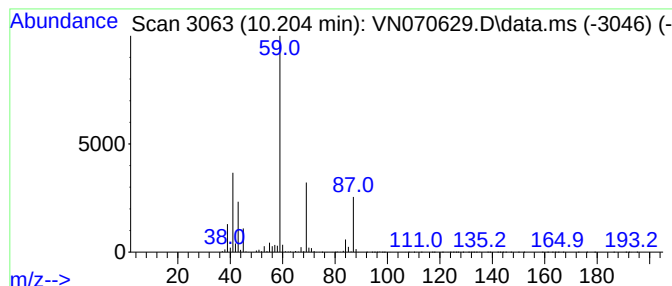
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 5 2-Butanol, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	46.97 ug/l	3748270	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4			Amylene hydrate	88	C5H12O	000075-85-4	50
5			2-Decanol, methyl ether	172	C11H24O	1000333-83-9	40



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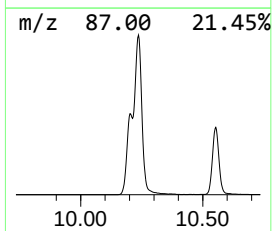
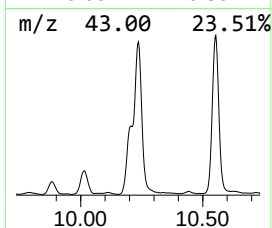
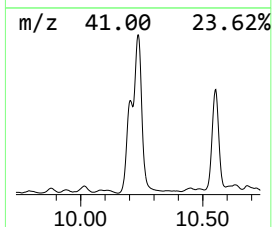
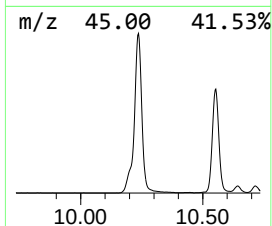
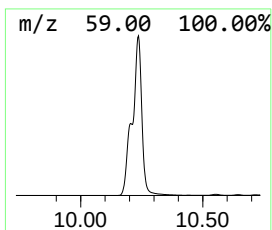
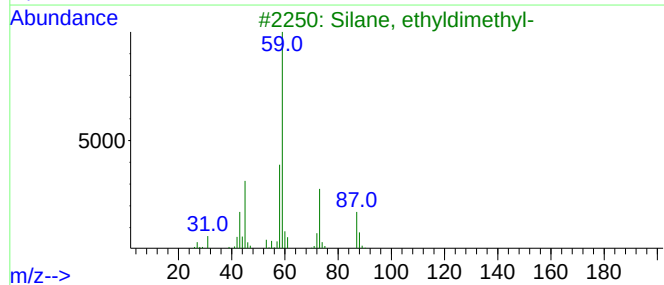
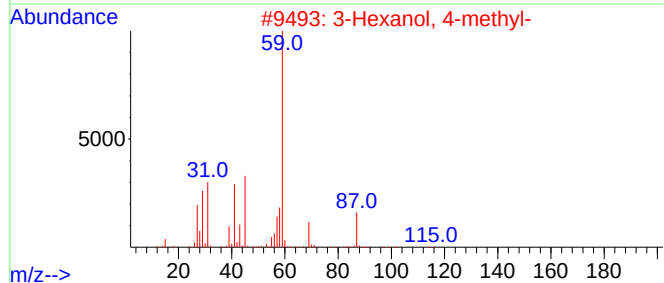
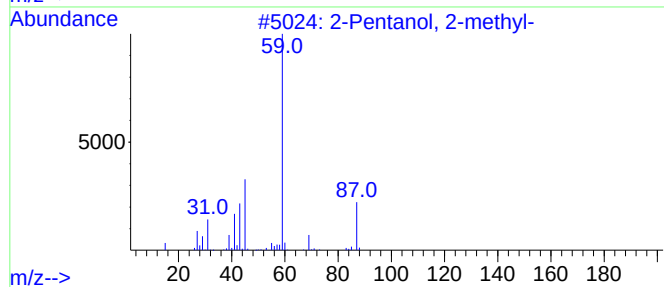
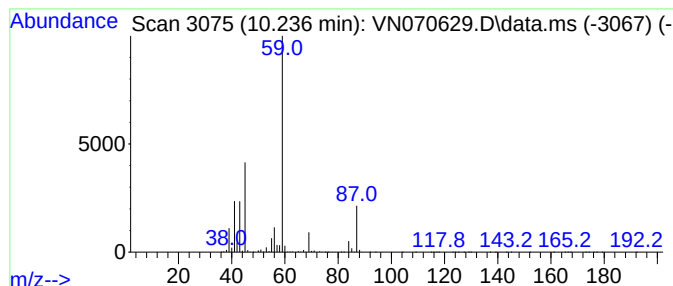
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.236	135.24 ug/l	10792700	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	56
3			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	39
4			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	38
5			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070629.D
Acq On : 14 Jan 2022 17:46
Operator : JC/MD
Sample : N1148-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

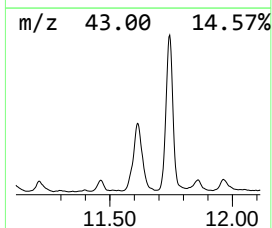
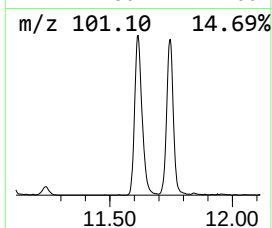
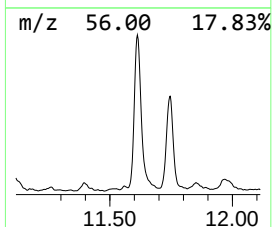
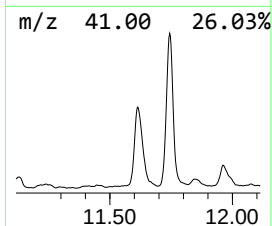
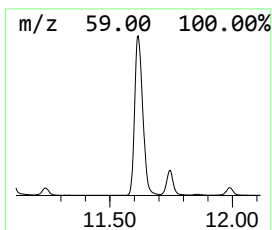
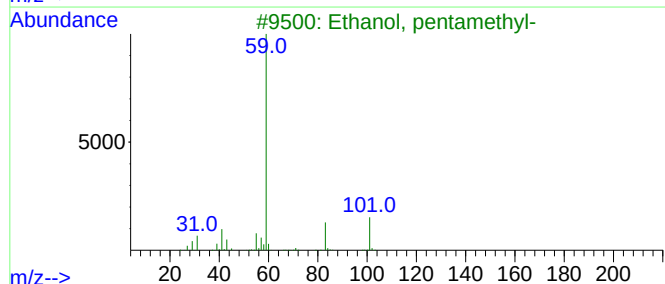
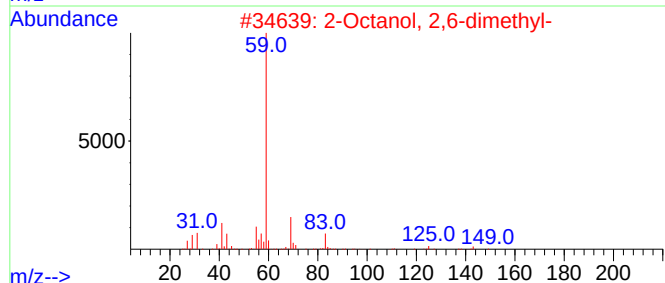
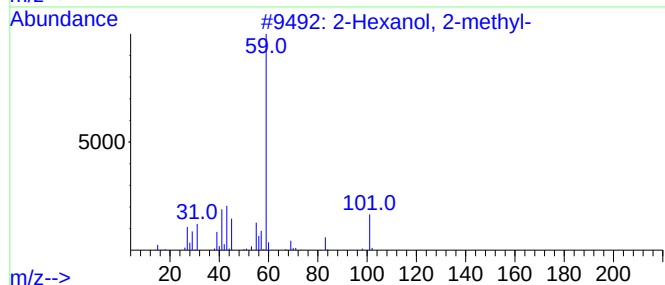
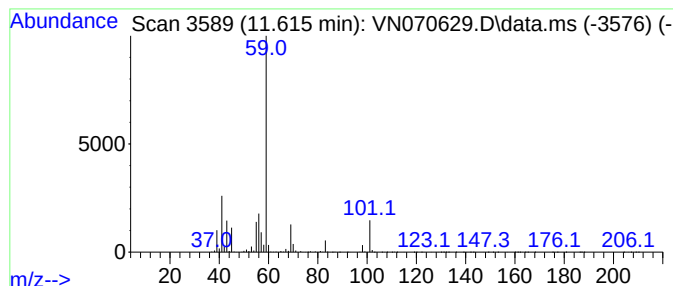
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ClientSampleId :
MW-29R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 7 2-Hexanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.615	18.15 ug/l	4158710	Chlorobenzene-d5			11.744
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	72
2	2-Octanol, 2,6-dimethyl-		158	C10H22O	018479-57-7	64
3	Ethanol, pentamethyl-		116	C7H16O	000594-83-2	53
4	2-Pentanol, 2,3-dimethyl-		116	C7H16O	004911-70-0	50
5	3-Heptanol, 4-methyl-		130	C8H18O	014979-39-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070629.D
Acq On : 14 Jan 2022 17:46
Operator : JC/MD
Sample : N1148-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-29R

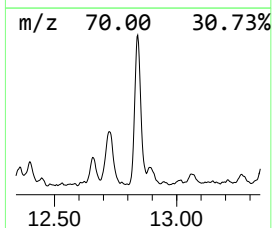
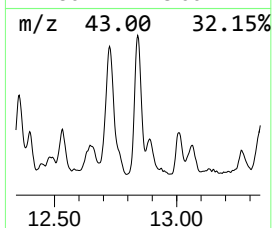
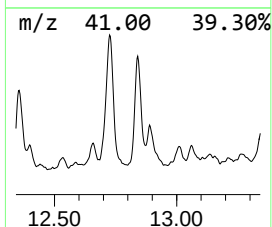
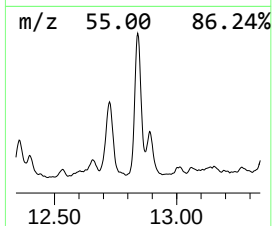
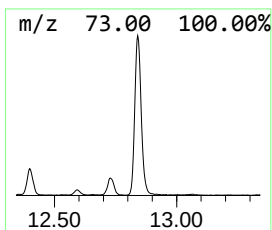
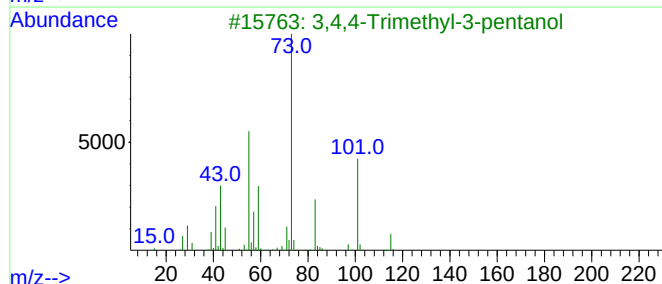
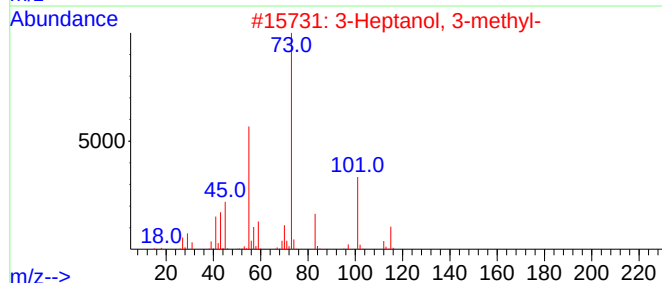
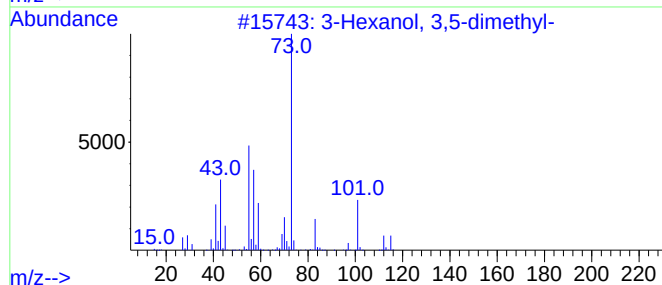
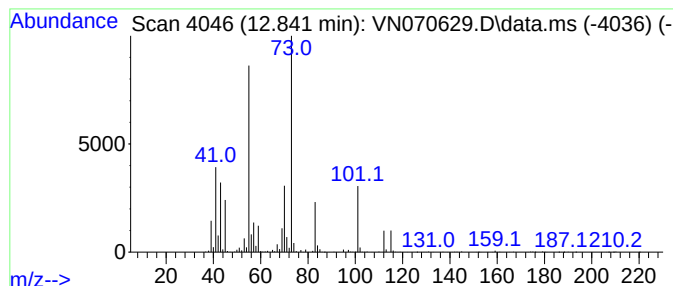
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Quant Title : SW846 8260

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

Peak Number 8 3-Hexanol, 3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	21.54 ug/l	1882940	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanol, 3,5-dimethyl-	130	C8H18O	004209-91-0	59
2			3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	53
3			3,4,4-Trimethyl-3-pentanol	130	C8H18O	007294-05-5	50
4			Heptane, 3-chloro-3-methyl-	148	C8H17Cl	005272-02-6	27
5			3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070629.D
Acq On : 14 Jan 2022 17:46
Operator : JC/MD
Sample : N1148-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-29R

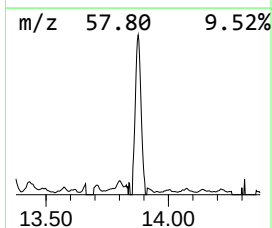
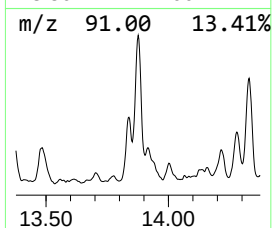
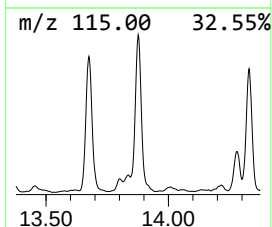
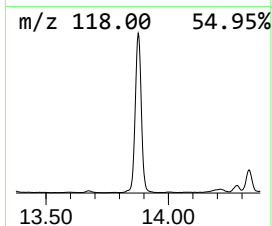
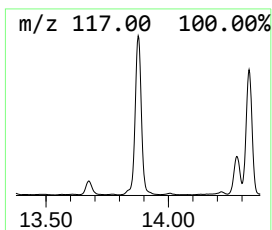
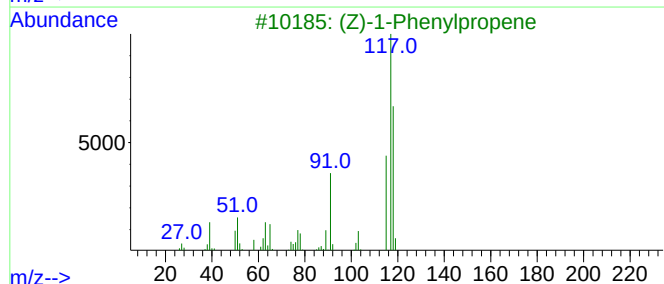
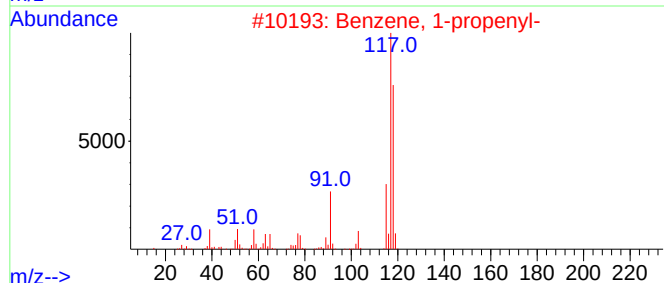
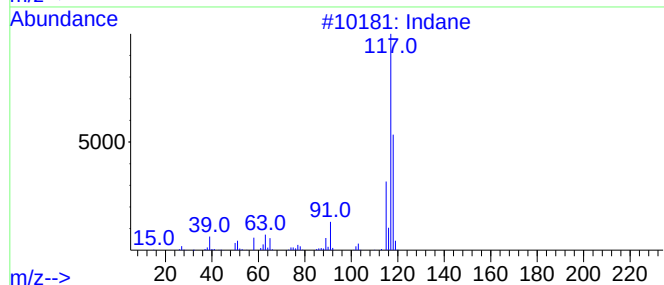
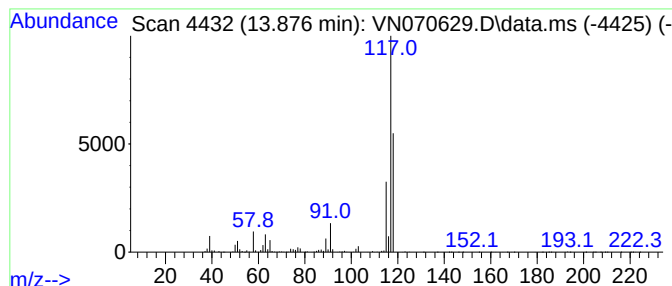
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	28.21 ug/l	2466520	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070629.D
Acq On : 14 Jan 2022 17:46
Operator : JC/MD
Sample : N1148-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-29R

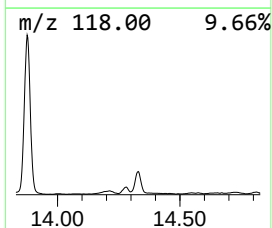
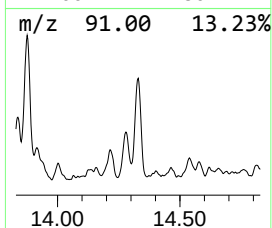
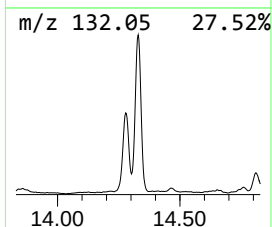
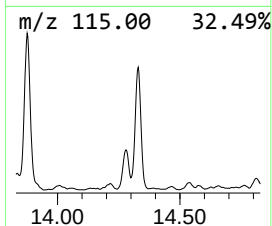
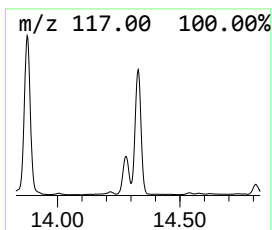
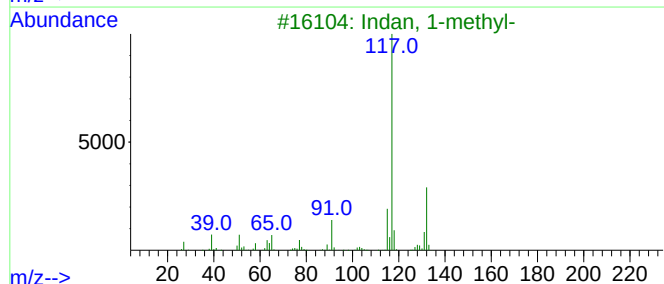
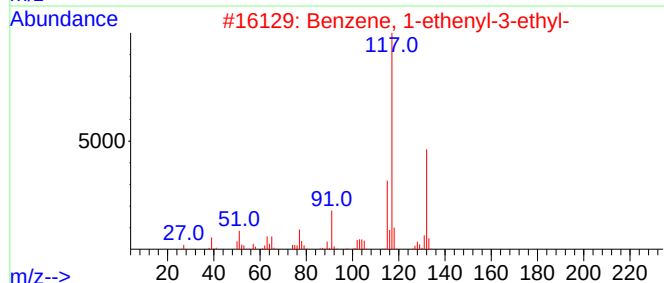
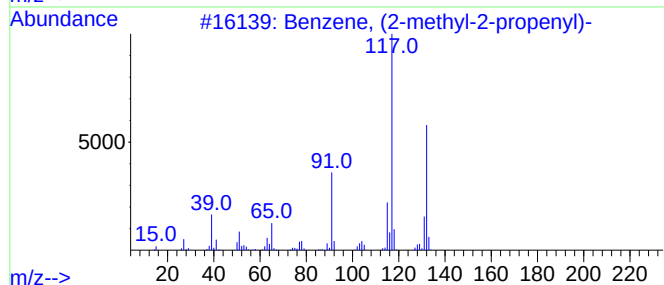
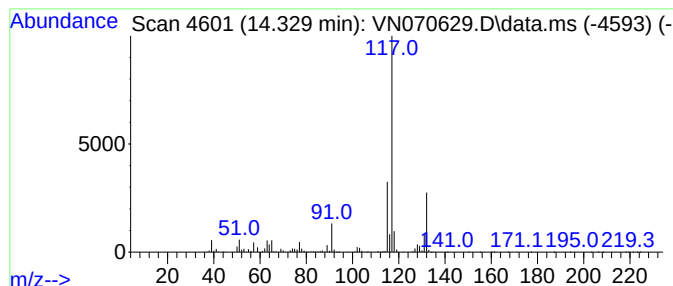
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, (2-methyl-2-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	26.18 ug/l	2288840	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070629.D
Acq On : 14 Jan 2022 17:46
Operator : JC/MD
Sample : N1148-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-29R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Butane, 2-methyl-	3.132	18.5	ug/l	1115710	1	8.086	3010430	50.0
Butane, 2,3-dim...	5.074	22.4	ug/l	1346110	1	8.086	3010430	50.0
Cyclopentane, m...	7.144	8.4	ug/l	506724	1	8.086	3010430	50.0
Pentane, 2,3-di...	8.174	14.1	ug/l	850996	1	8.086	3010430	50.0
2-Butanol, 2,3-...	10.204	47.0	ug/l	3748270	2	8.968	3990090	50.0
2-Pentanol, 2-m...	10.236	135.2	ug/l	10792700	2	8.968	3990090	50.0
2-Hexanol, 2-me...	11.615	18.1	ug/l	4158710	3	11.744	11454000	50.0
3-Hexanol, 3,5-...	12.841	21.5	ug/l	1882940	4	13.675	4371780	50.0
Indane	13.876	28.2	ug/l	2466520	4	13.675	4371780	50.0
Benzene, (2-met...	14.329	26.2	ug/l	2288840	4	13.675	4371780	50.0