

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
 Data File : VN070381.D
 Acq On : 30 Dec 2021 6:43
 Operator : JC/MD
 Sample : M5007-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-03RE

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: VN070381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.443	160	169	190	rVB	341319	575529	5.62%	0.924%
2	3.140	417	429	451	rVB2	124869	287450	2.81%	0.462%
3	5.079	1126	1152	1174	rBV4	111960	428210	4.18%	0.688%
4	5.621	1326	1354	1384	rBV3	213969	748997	7.32%	1.203%
5	7.045	1858	1885	1913	rBV2	696881	2134575	20.85%	3.428%
6	7.327	1969	1990	2016	rVB4	59131	175477	1.71%	0.282%
7	7.844	2168	2183	2202	rVB4	57911	155035	1.51%	0.249%
8	8.024	2229	2250	2260	rBV2	636137	1517070	14.82%	2.437%
9	8.086	2261	2273	2289	rVV2	1168132	2675119	26.13%	4.296%
10	8.174	2289	2306	2334	rVB2	1590850	4000420	39.07%	6.425%
11	8.440	2386	2405	2431	rVB	789477	1822303	17.80%	2.927%
12	8.617	2438	2471	2494	rBV	4214650	10238789	100.00%	16.444%
13	8.968	2582	2602	2628	rBV	1813539	3789110	37.01%	6.086%
14	9.459	2756	2785	2796	rBV5	299792	889655	8.69%	1.429%
15	9.512	2797	2805	2819	rVV2	153398	292800	2.86%	0.470%
16	9.593	2819	2835	2861	rVV	335484	712929	6.96%	1.145%
17	9.732	2864	2887	2903	rVV6	99980	274686	2.68%	0.441%
18	9.883	2925	2943	2968	rBV	2767711	5467384	53.40%	8.781%
19	10.014	2970	2992	3021	rBV	3971458	8165719	79.75%	13.115%
20	10.199	3043	3061	3076	rBV3	116385	255179	2.49%	0.410%
21	10.371	3101	3125	3137	rBV2	463902	897041	8.76%	1.441%
22	10.440	3137	3151	3182	rVB	2752676	5201996	50.81%	8.355%
23	10.636	3205	3224	3240	rVB	82572	252330	2.46%	0.405%
24	10.867	3296	3310	3313	rBV3	128367	226084	2.21%	0.363%
25	11.130	3396	3408	3435	rVB	89022	218272	2.13%	0.351%
26	11.258	3441	3456	3470	rBV5	54982	109696	1.07%	0.176%
27	11.744	3620	3637	3656	rBV	2395268	4352851	42.51%	6.991%
28	11.993	3713	3730	3754	rVB6	65888	165601	1.62%	0.266%
29	12.731	3987	4005	4028	rBV2	1746067	3198237	31.24%	5.137%
30	13.675	4341	4357	4378	rBV	1647699	2879844	28.13%	4.625%
31	14.150	4519	4534	4547	rBV2	86176	155699	1.52%	0.250%

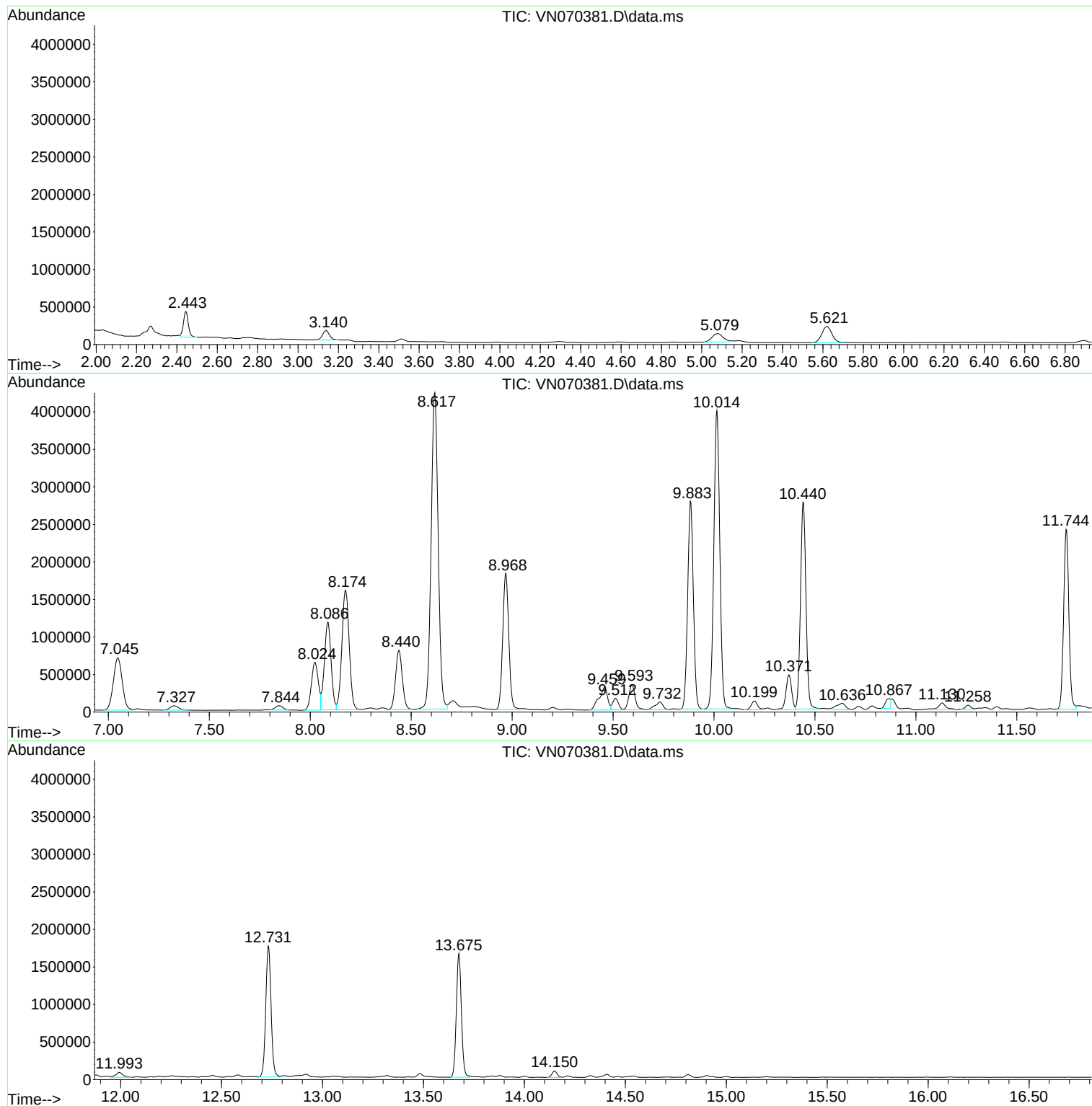
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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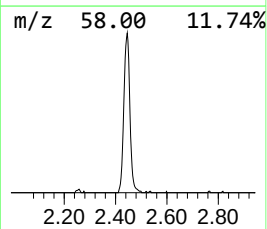
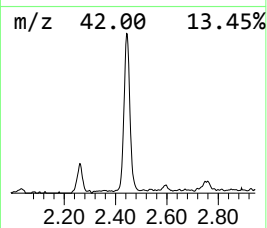
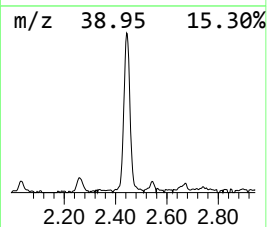
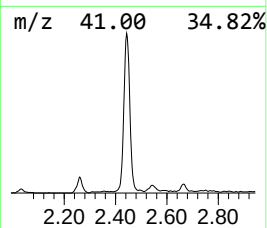
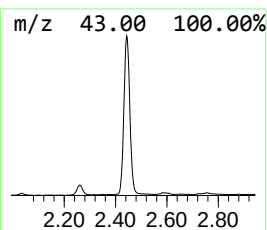
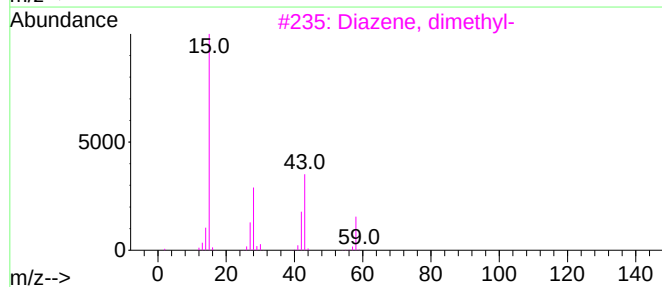
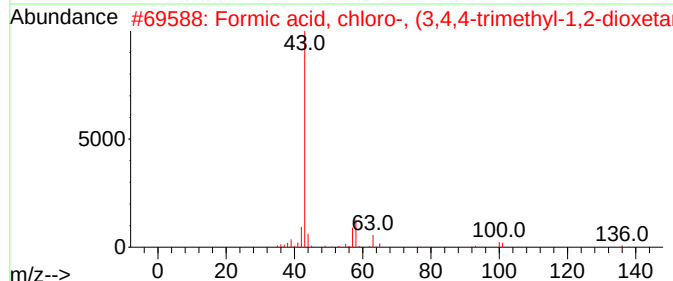
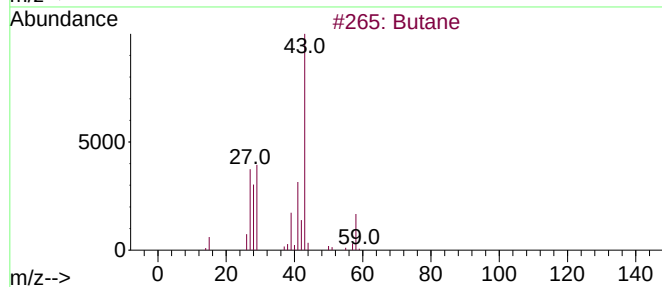
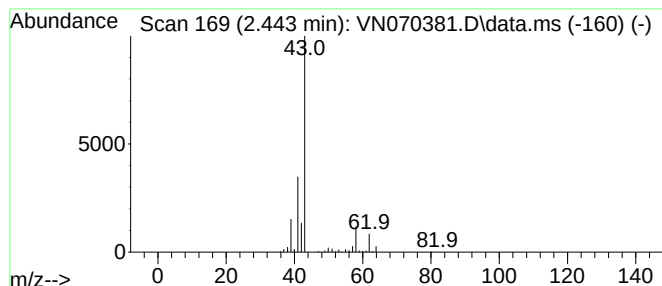
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Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.443	10.76 ug/l	575529	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	50
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	38
3			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4
4			Allyl acetate	100	C5H8O2	000591-87-7	4
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4



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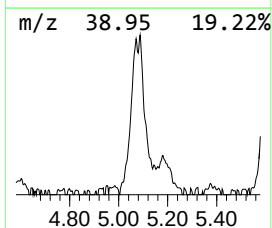
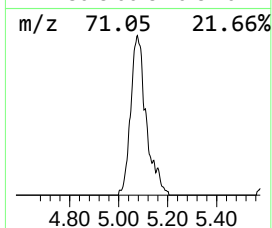
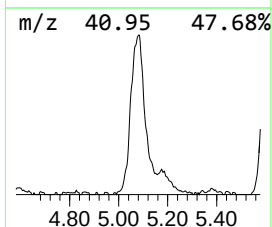
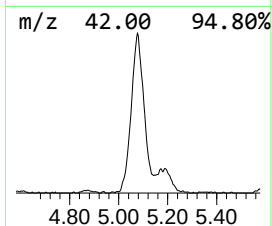
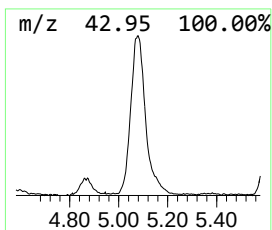
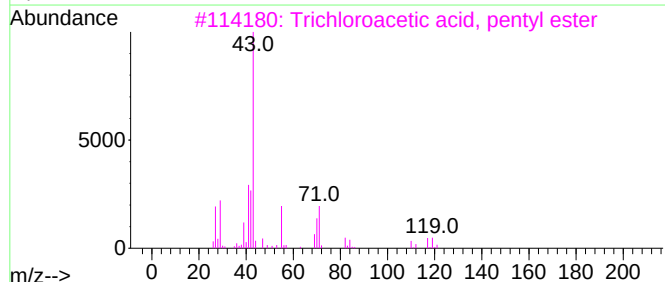
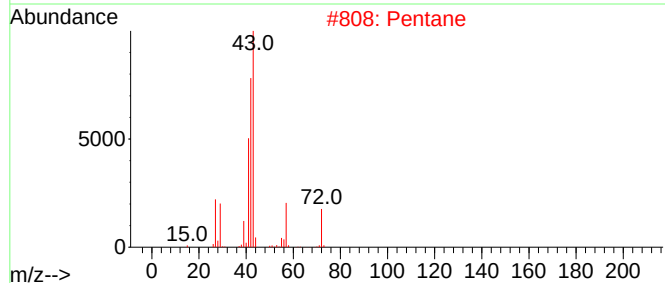
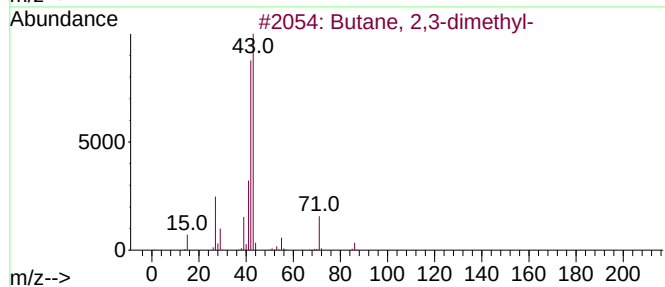
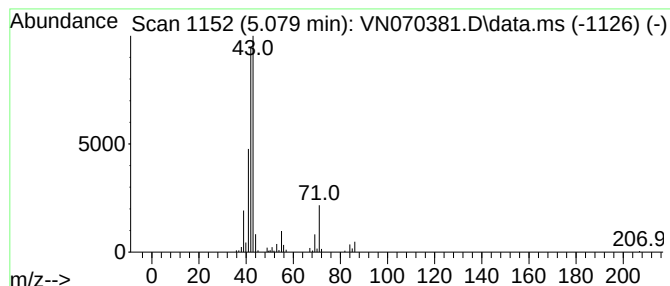
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	8.00 ug/l	428210	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane	72	C5H12	000109-66-0	40
3			Trichloroacetic acid, pentyl ester	232	C7H11Cl3O2	033972-81-5	23
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	17
5			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

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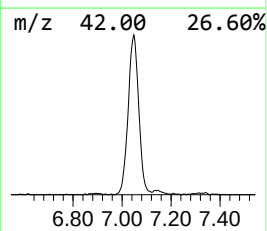
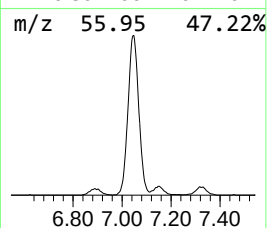
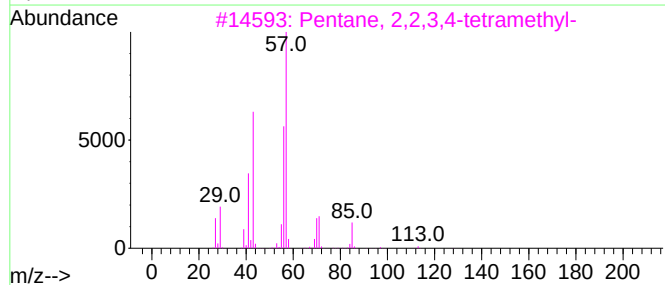
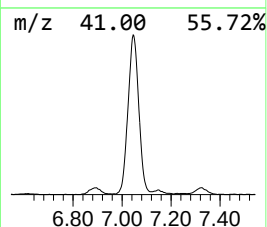
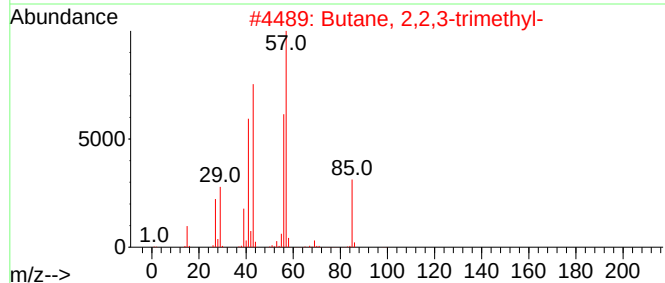
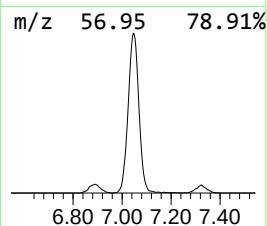
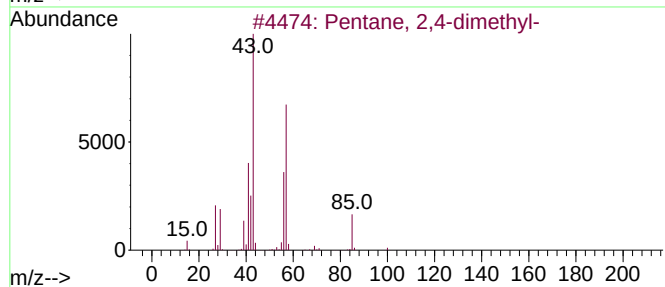
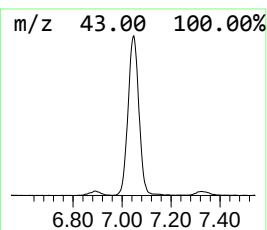
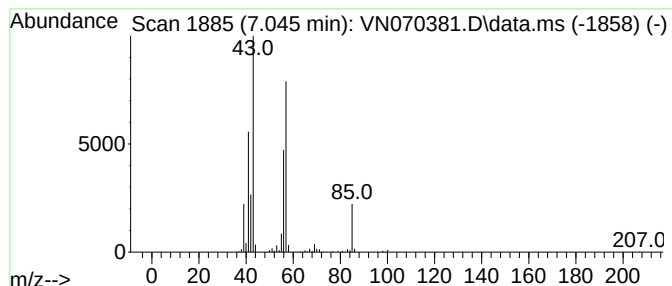
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	39.90 ug/l	2134580	Pentafluorobenzene	8.088

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, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59
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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ALS Vial : 47 Sample Multiplier: 1

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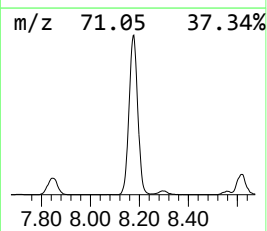
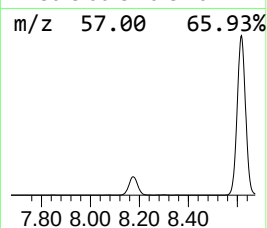
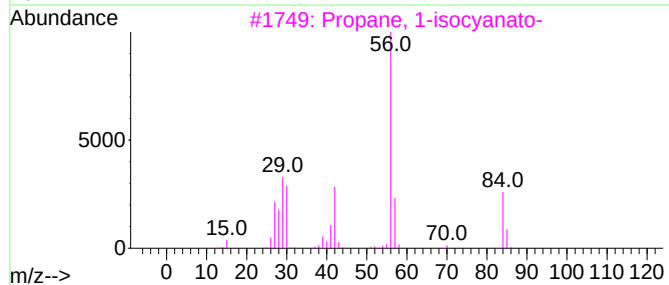
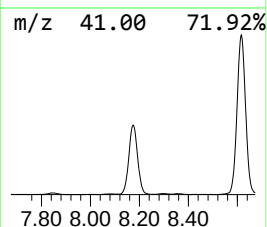
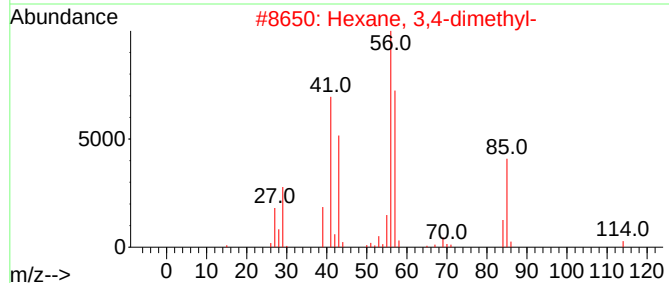
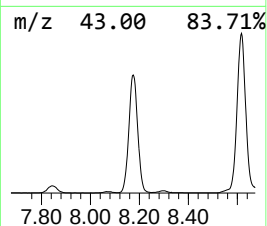
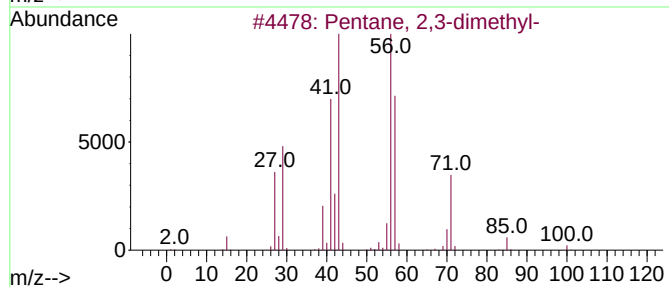
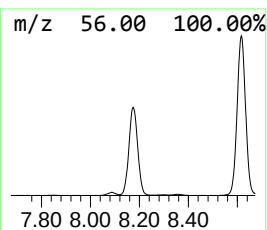
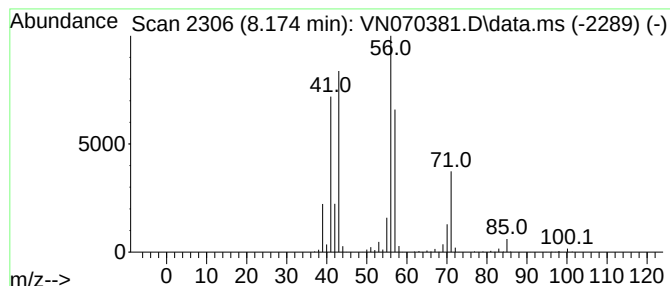
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	74.77 ug/l	4000420	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40
3			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38
5			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37



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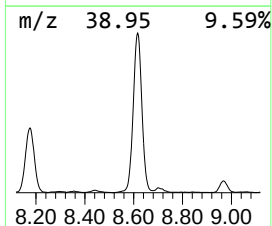
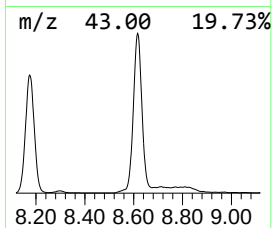
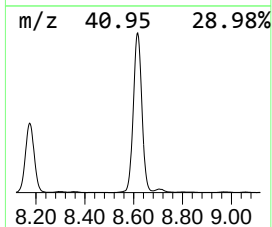
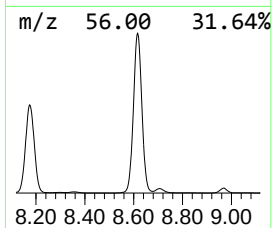
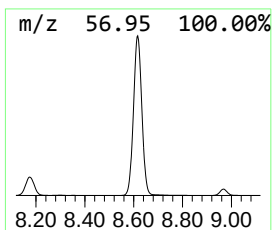
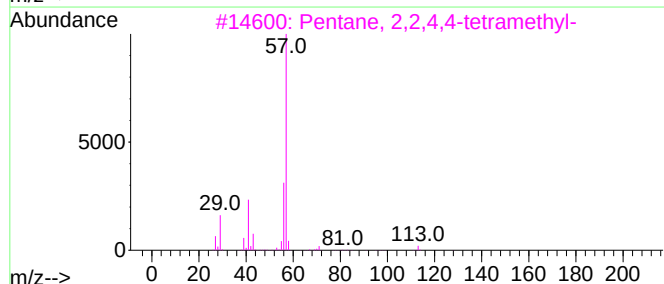
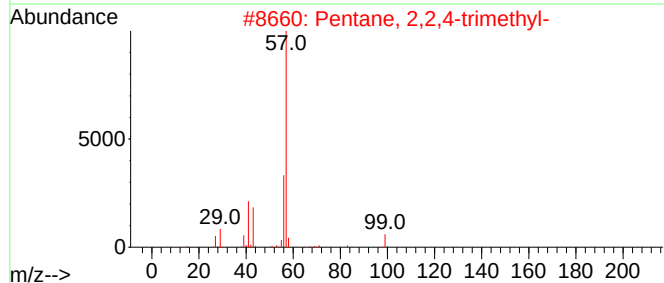
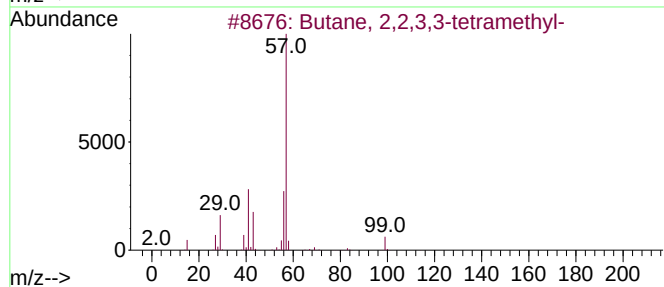
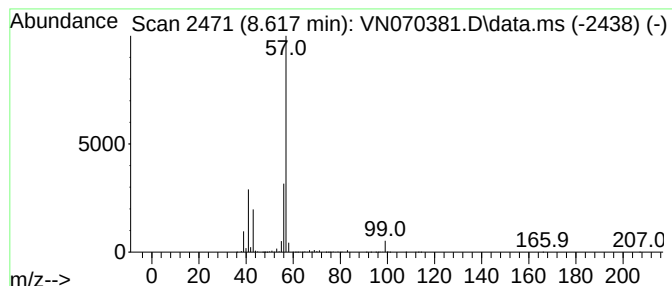
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Quant Title : SW846 8260

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

Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	135.11 ug/l	10238800	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
5			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	56



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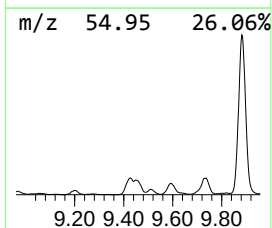
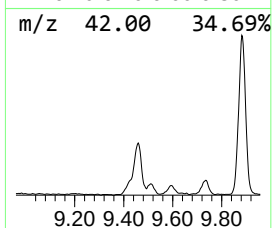
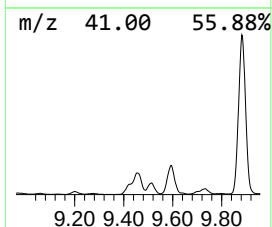
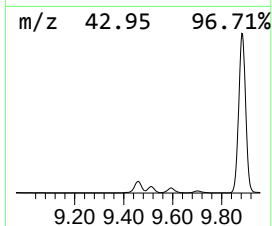
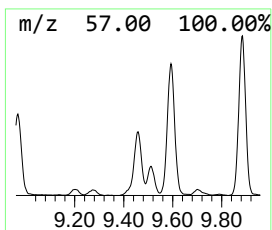
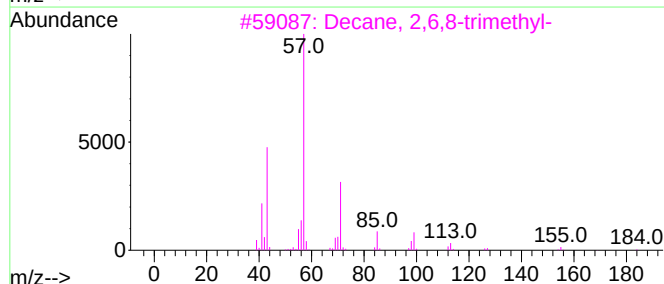
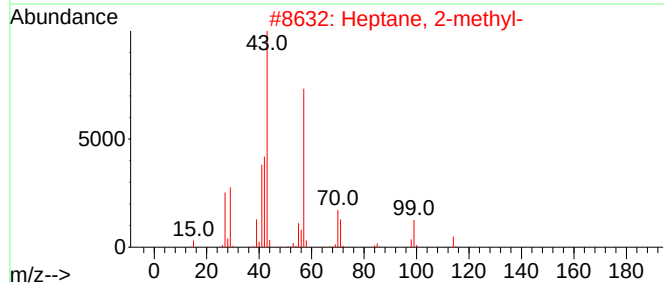
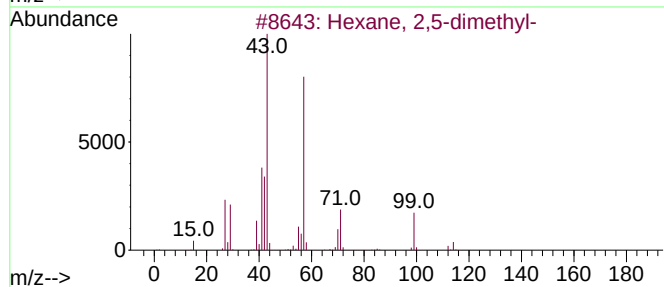
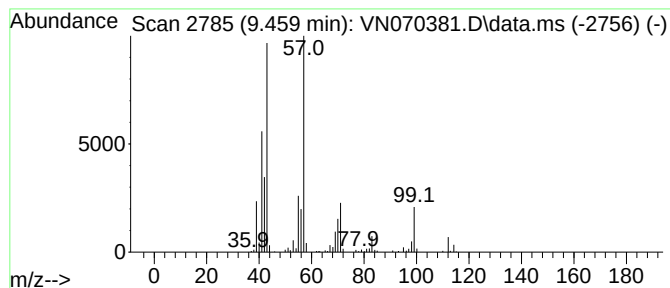
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.459	11.74 ug/l	889655	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	76
2			Heptane, 2-methyl-	114	C8H18	000592-27-8	59
3			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	47
4			4-Bromoheptane	178	C7H15Br	000998-93-6	47
5			1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070381.D
Acq On : 30 Dec 2021 6:43
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03RE

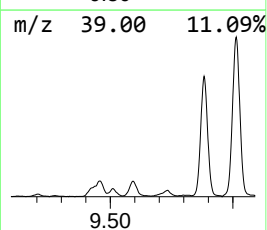
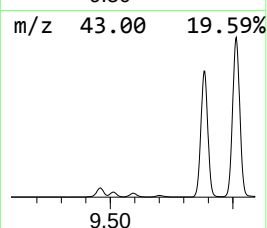
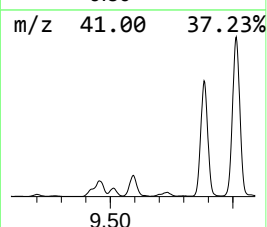
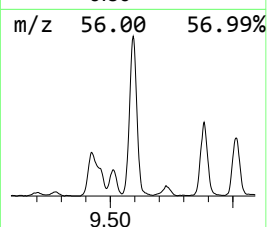
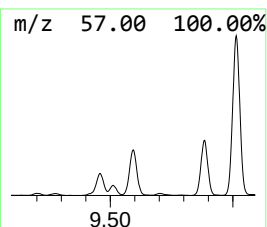
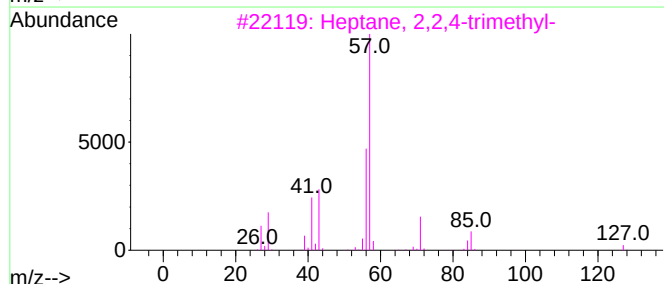
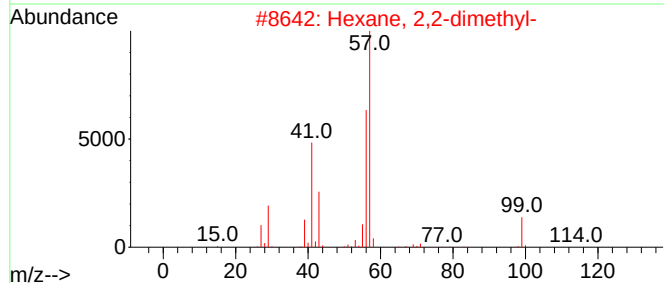
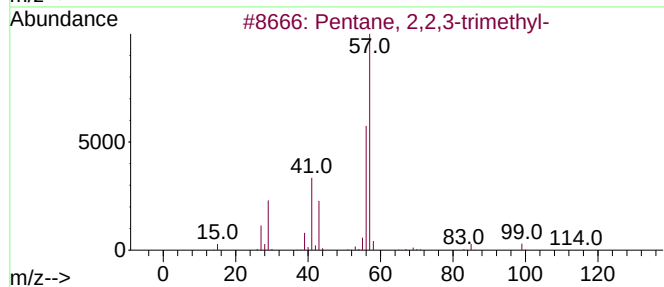
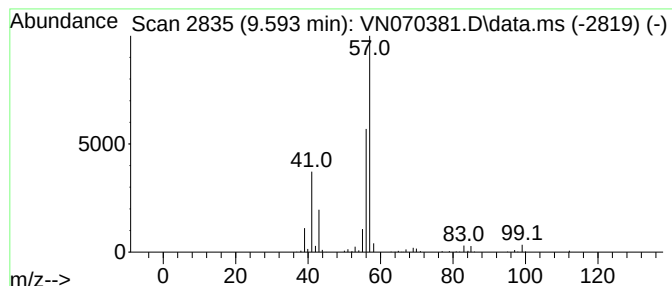
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.593	9.41 ug/l	712929	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	72
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	59
5			Pentane, 3-methyl-	86	C6H14	000096-14-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070381.D
Acq On : 30 Dec 2021 6:43
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03RE

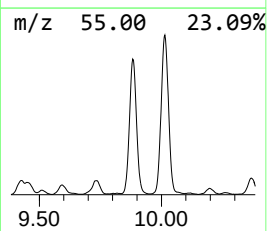
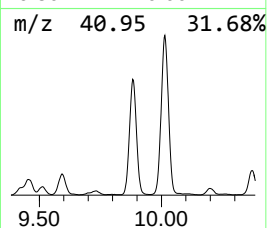
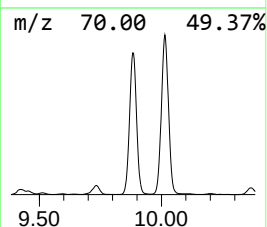
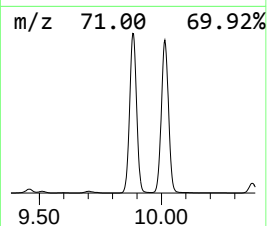
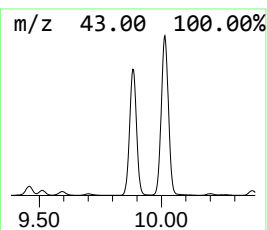
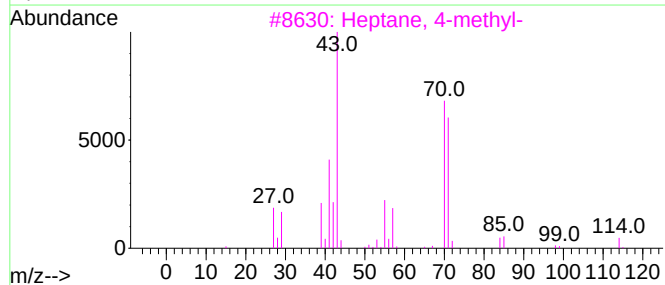
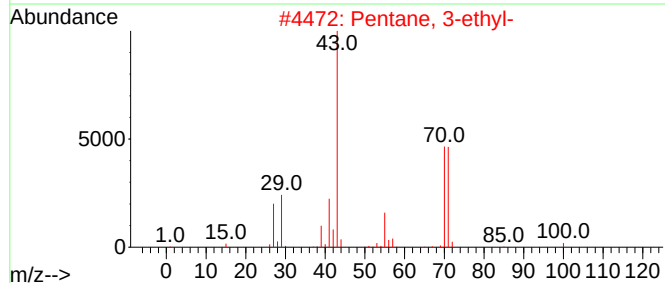
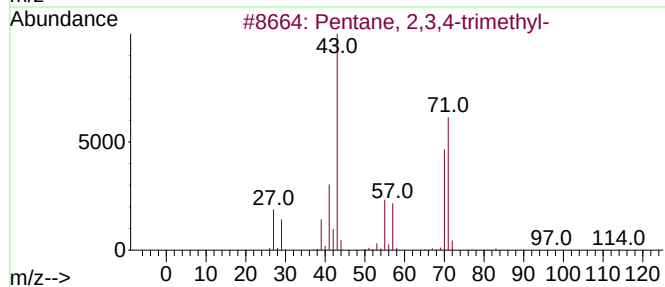
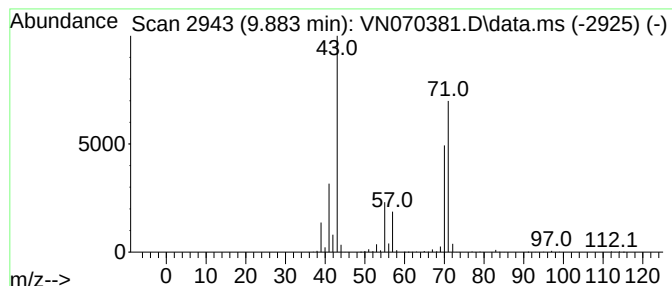
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	72.15 ug/l	5467380	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			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070381.D
Acq On : 30 Dec 2021 6:43
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03RE

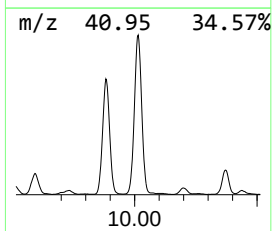
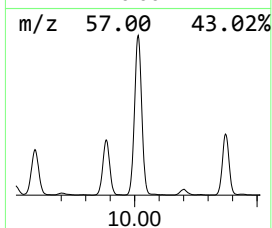
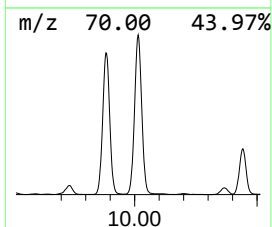
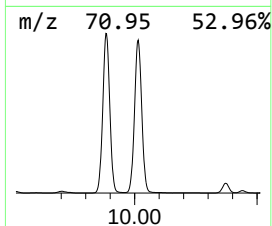
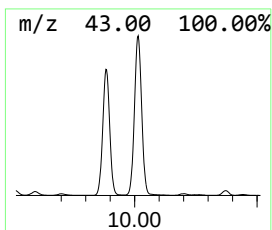
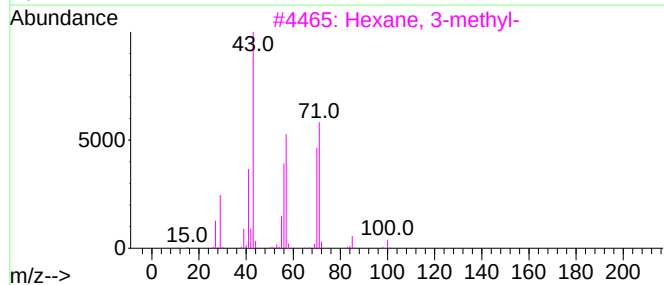
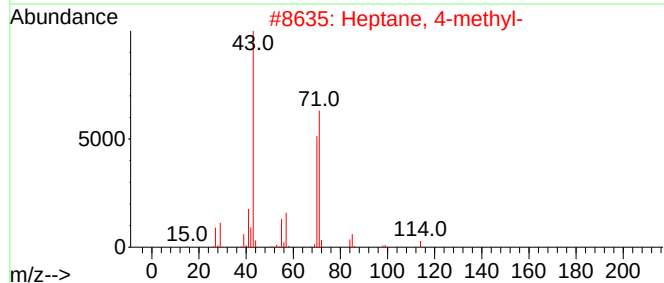
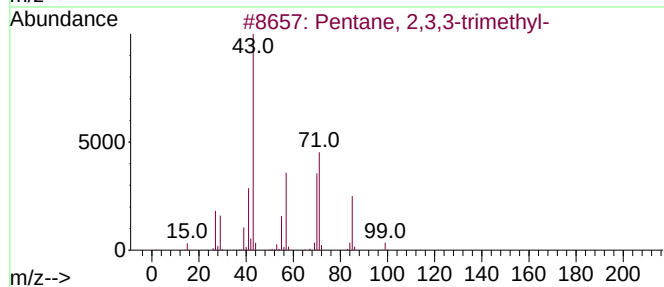
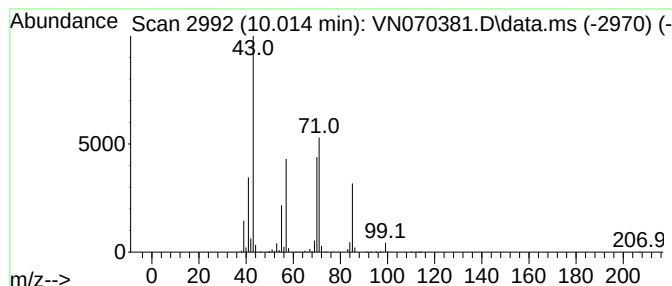
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Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	107.75 ug/l	8165720	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070381.D
Acq On : 30 Dec 2021 6:43
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03RE

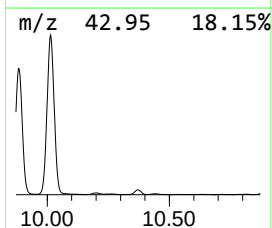
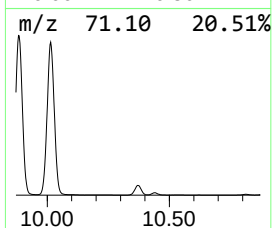
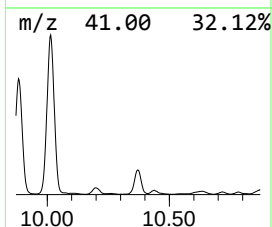
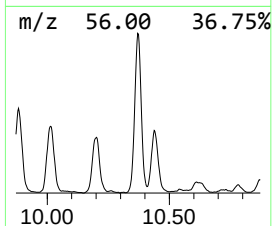
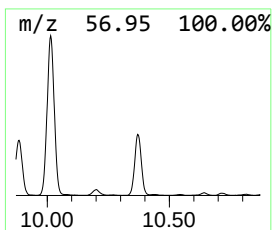
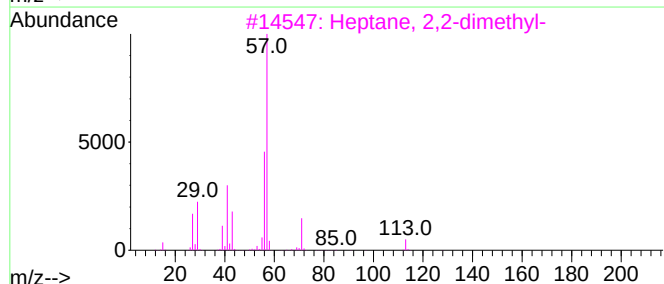
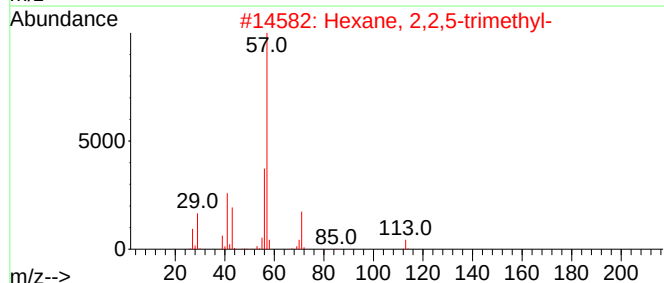
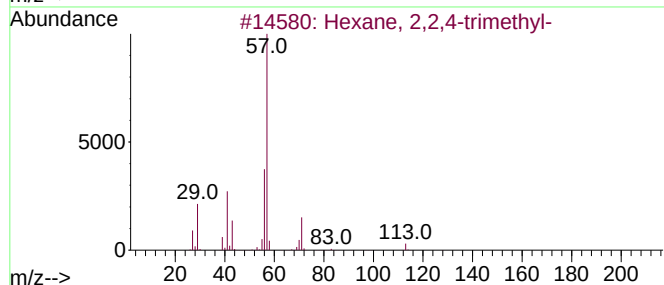
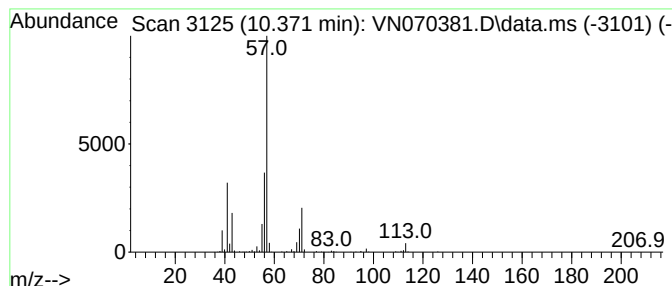
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Quant Title : SW846 8260

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

Peak Number 10 Hexane, 2,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.371	10.30 ug/l	897041	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	72
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	56
5			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070381.D
Acq On : 30 Dec 2021 6:43
Operator : JC/MD
Sample : M5007-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03RE

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
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Butane, 2,3-dim...	5.079	8.0	ug/l	428210	1	8.088	2675120	50.0
Pentane, 2,4-di...	7.045	39.9	ug/l	2134580	1	8.088	2675120	50.0
Pentane, 2,3-di...	8.174	74.8	ug/l	4000420	1	8.088	2675120	50.0
Butane, 2,2,3,3...	8.617	135.1	ug/l	10238800	2	8.968	3789110	50.0
Hexane, 2,5-dim...	9.459	11.7	ug/l	889655	2	8.968	3789110	50.0
Pentane, 2,2,3-...	9.593	9.4	ug/l	712929	2	8.968	3789110	50.0
Pentane, 2,3,4-...	9.883	72.2	ug/l	5467380	2	8.968	3789110	50.0
Pentane, 2,3,3-...	10.014	107.8	ug/l	8165720	2	8.968	3789110	50.0
Hexane, 2,2,4-t...	10.371	10.3	ug/l	897041	3	11.746	4352850	50.0