

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031420.D
 Acq On : 16 Sep 2022 19:09
 Operator : JC/MD
 Sample : N4645-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 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_X\Method\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	37	rBV3	19993	43893	5.24%	0.743%
2	1.368	43	46	52	rVB	44795	43892	5.24%	0.743%
3	1.605	74	85	96	rVB6	11402	43920	5.25%	0.744%
4	1.746	104	108	116	rVB2	21145	29852	3.57%	0.505%
5	1.953	137	142	148	rVB2	7393	11596	1.39%	0.196%
6	2.215	180	185	191	rVB2	5564	9687	1.16%	0.164%
7	2.782	271	278	285	rBV	11713	26238	3.13%	0.444%
8	3.111	323	332	342	rBV3	18592	48284	5.77%	0.817%
9	4.215	501	513	524	rBV2	52707	155822	18.62%	2.638%
10	4.489	544	558	567	rVB7	3306	13221	1.58%	0.224%
11	5.391	691	706	719	rBV	88718	253819	30.32%	4.297%
12	5.556	723	733	738	rVV	87815	248746	29.72%	4.211%
13	5.623	738	744	758	rVB2	82496	252954	30.22%	4.283%
14	5.958	789	799	817	rBV2	96967	258421	30.87%	4.375%
15	6.251	835	847	859	rBV	244895	718771	85.87%	12.169%
16	6.763	921	931	943	rBV2	137814	325056	38.83%	5.503%
17	7.360	1022	1029	1038	rVB4	8589	21887	2.61%	0.371%
18	7.501	1044	1052	1057	rBV	25024	51375	6.14%	0.870%
19	7.562	1057	1062	1065	rVV2	12447	24896	2.97%	0.422%
20	7.604	1065	1069	1077	rVB2	20871	43761	5.23%	0.741%
21	7.775	1089	1097	1106	rVB3	9686	21476	2.57%	0.364%
22	7.988	1122	1132	1143	rVB	206376	405038	48.39%	6.857%
23	8.110	1143	1152	1161	rBV	274906	537053	64.16%	9.093%
24	8.391	1192	1198	1202	rBV	5311	9649	1.15%	0.163%
25	8.513	1208	1218	1225	rVB5	4497	11080	1.32%	0.188%
26	8.653	1228	1241	1250	rBV	478980	837022	100.00%	14.171%
27	8.976	1287	1294	1299	rVB4	6012	13358	1.60%	0.226%
28	9.104	1308	1315	1320	rVB4	6052	13031	1.56%	0.221%
29	9.159	1320	1324	1328	rBV	12101	19354	2.31%	0.328%
30	9.201	1328	1331	1335	rVB2	9302	13537	1.62%	0.229%
31	9.458	1365	1373	1377	rBV	18558	29489	3.52%	0.499%
32	9.506	1377	1381	1388	rVB4	5015	9215	1.10%	0.156%
33	10.055	1465	1471	1476	rBV	309445	395163	47.21%	6.690%
34	10.098	1476	1478	1486	rVV4	4942	11371	1.36%	0.193%
35	10.963	1616	1620	1625	rBV2	7635	10126	1.21%	0.171%
36	11.079	1634	1639	1644	rBV	387804	509062	60.82%	8.619%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : SW846 8260

37	11.122	1644	1646	1651	rVB4	6883	8909	1.06%	0.151%
38	12.024	1789	1794	1802	rVB	306117	374053	44.69%	6.333%
39	12.244	1826	1830	1836	rVB2	9322	11632	1.39%	0.197%
40	12.475	1863	1868	1873	rVB	9872	11765	1.41%	0.199%
41	12.719	1901	1908	1912	rVB7	4879	10769	1.29%	0.182%
42	12.920	1933	1941	1947	rVB	6113	9667	1.15%	0.164%
43	13.298	1998	2003	2008	rBV3	6542	8592	1.03%	0.145%

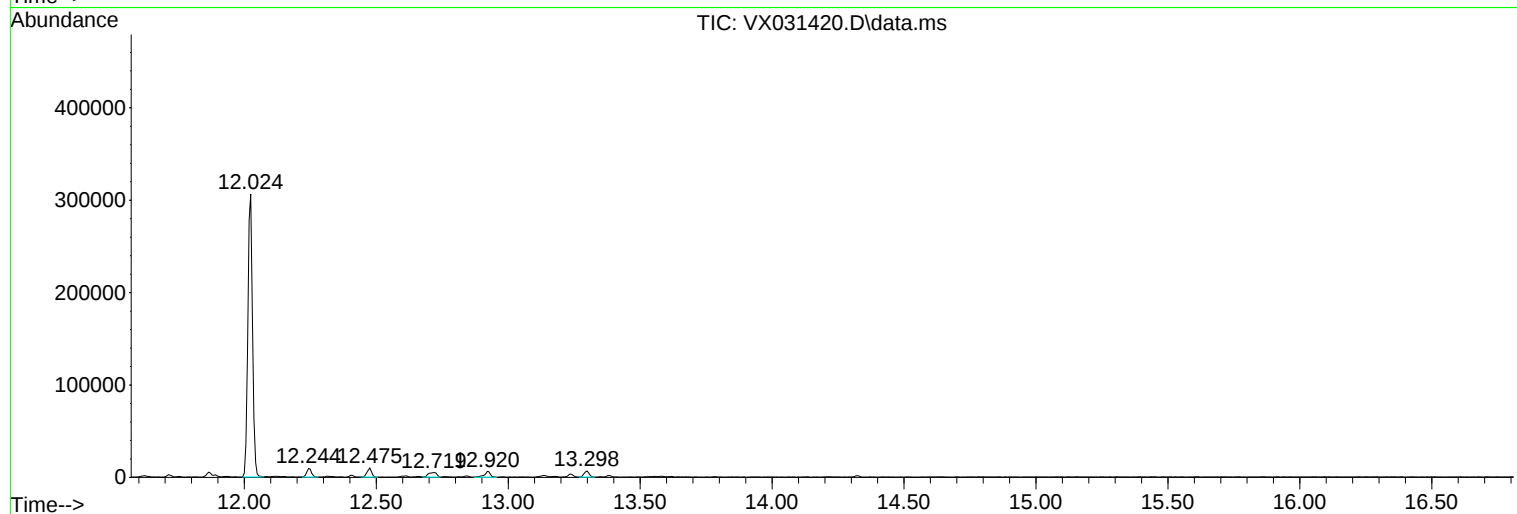
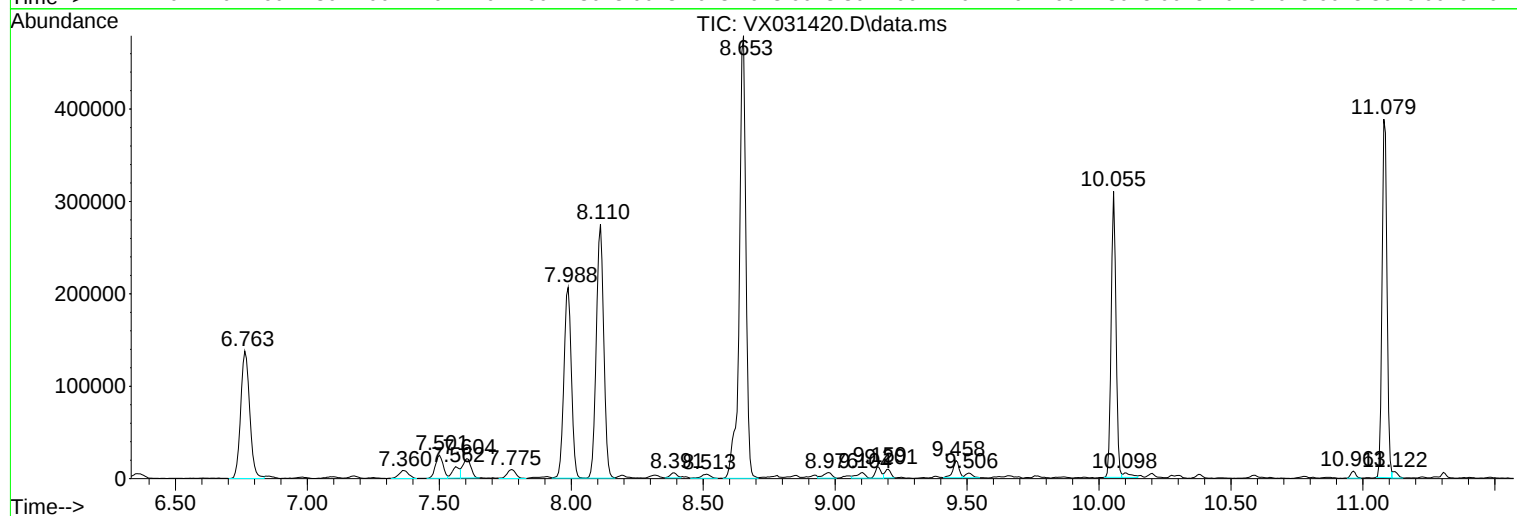
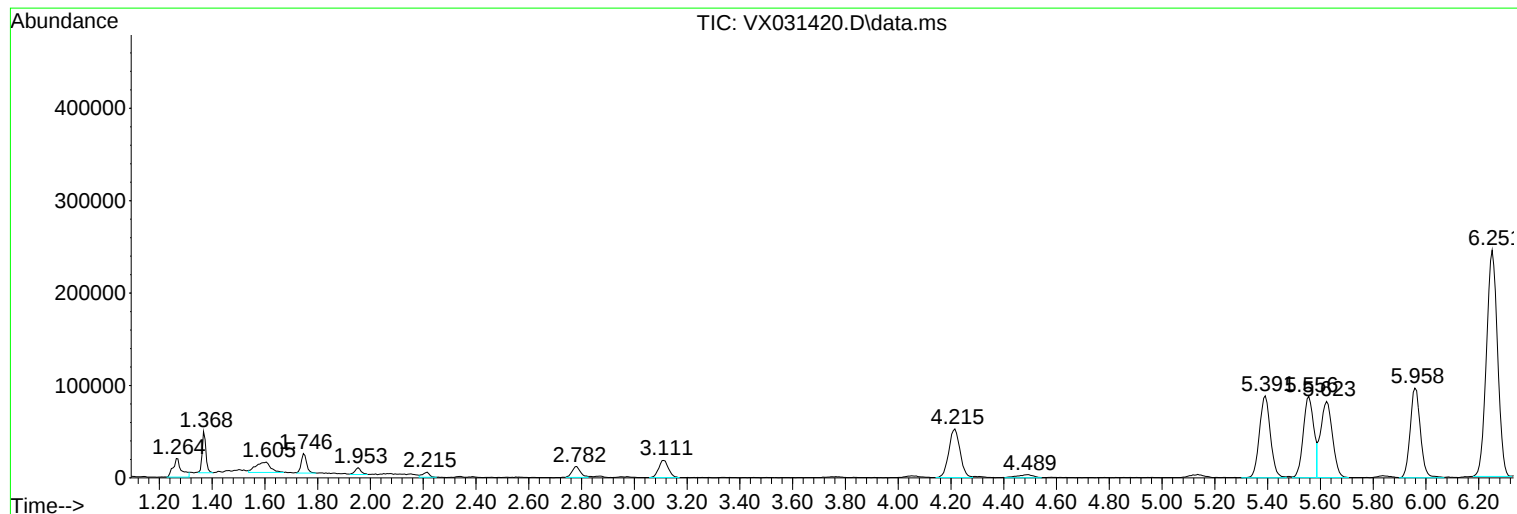
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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



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MSVOA_X
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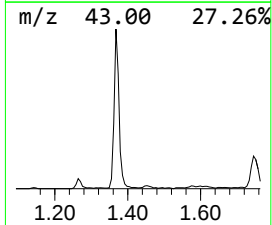
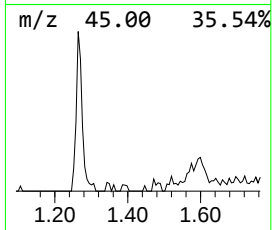
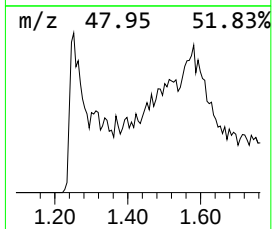
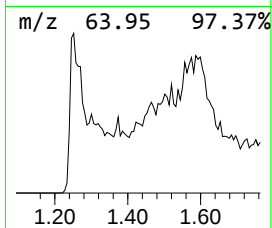
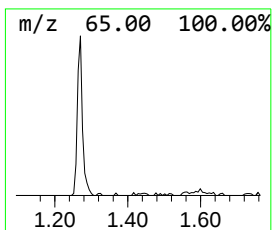
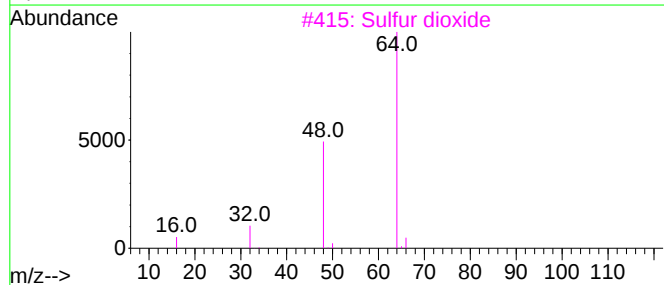
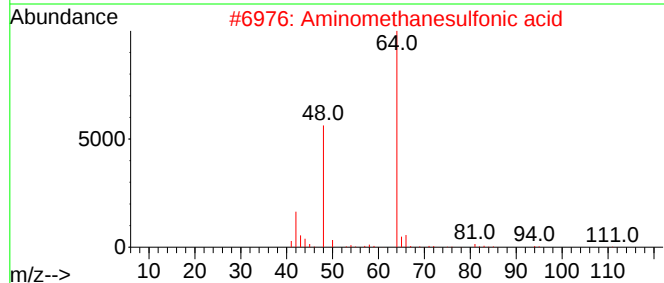
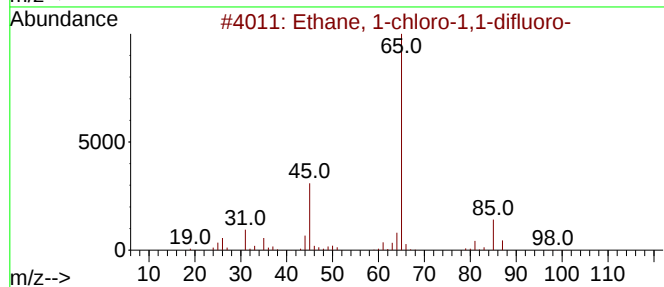
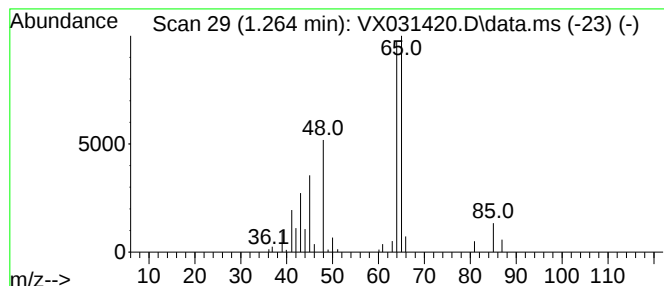
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.264 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	8.82 ug/l	43893	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	38
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	32
3			Sulfur dioxide	64	O2S	007446-09-5	32
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	9
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

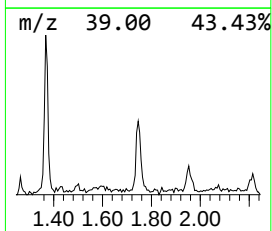
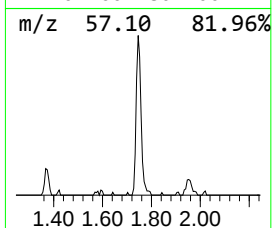
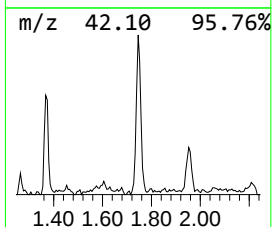
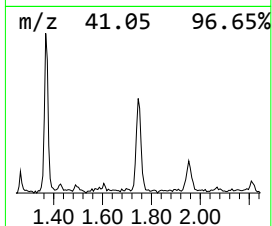
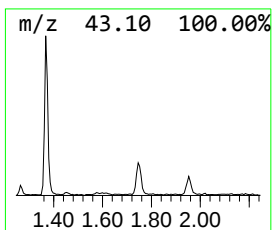
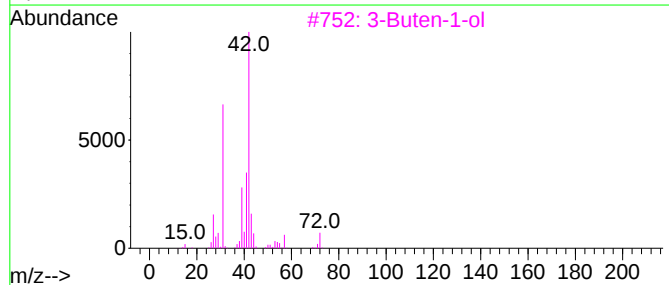
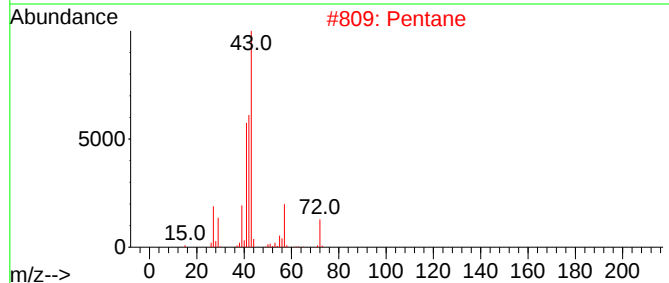
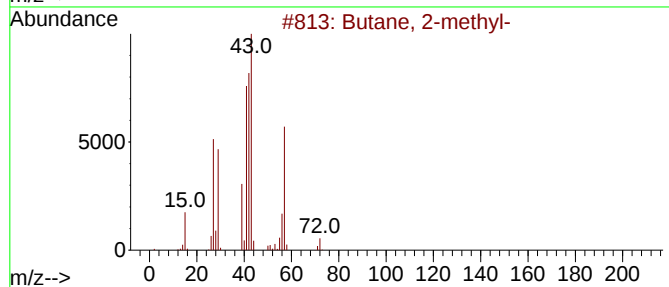
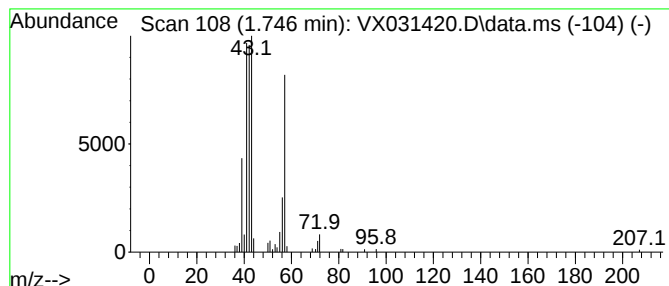
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	6.00 ug/l	29852	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	35
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	25
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	23



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Instrument :
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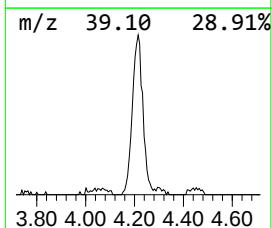
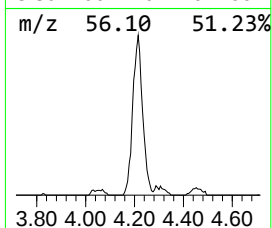
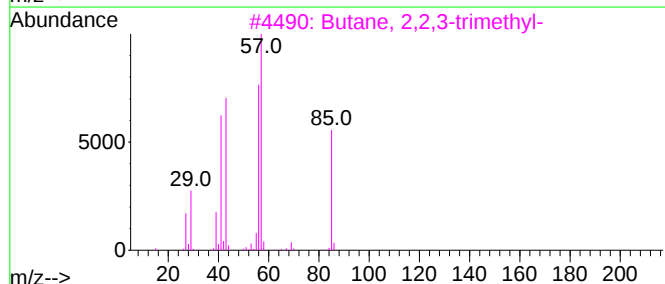
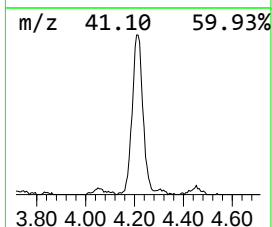
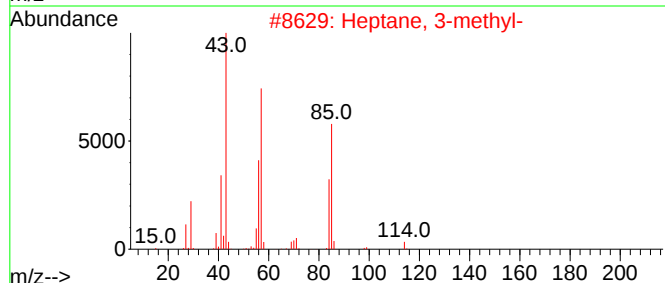
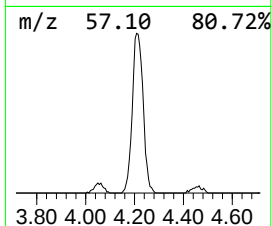
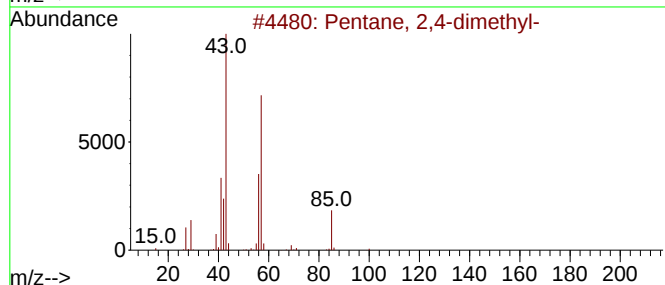
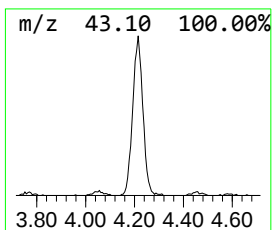
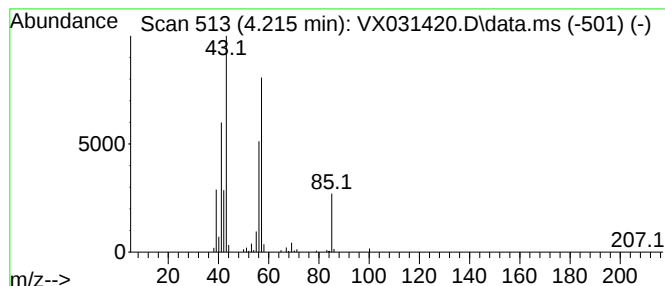
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.215	31.32 ug/l	155822	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
2			Heptane, 3-methyl-	114	C8H18	000589-81-1	72
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	47



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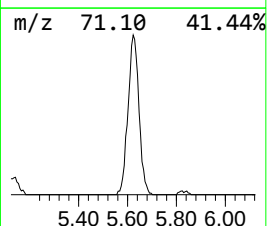
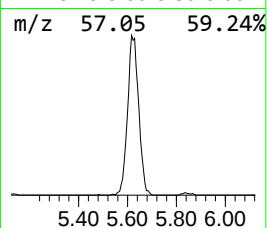
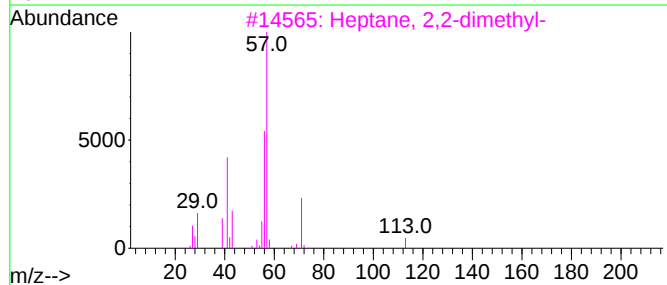
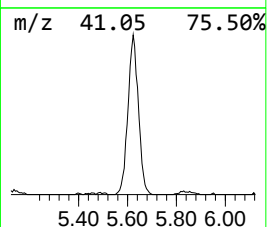
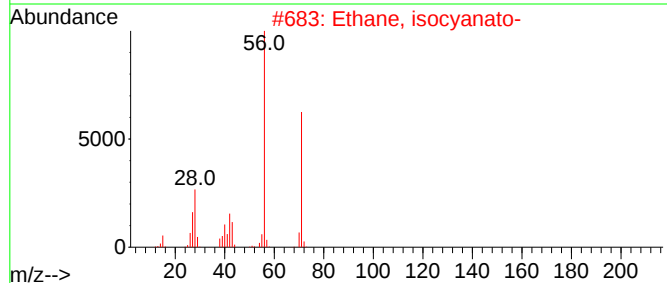
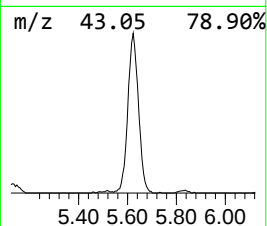
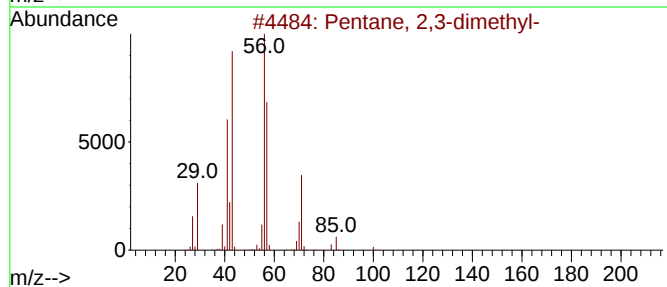
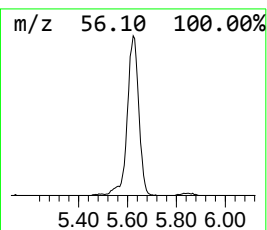
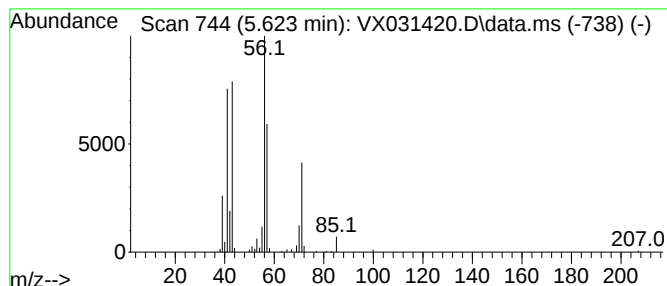
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	50.85 ug/l	252954	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
2			Ethane, isocyanato-	71	C3H5NO	000109-90-0	53
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	43
5			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	38



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TOLL-MW-03

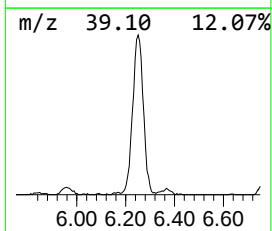
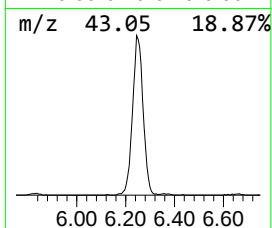
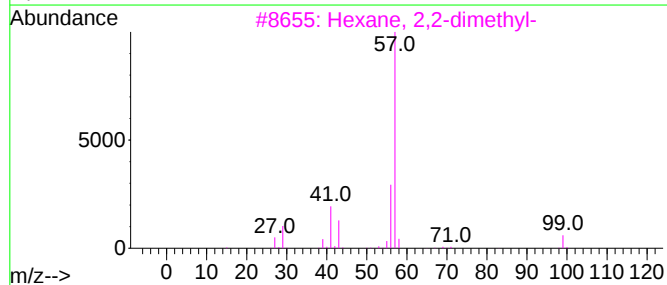
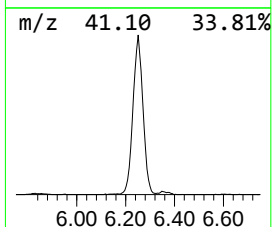
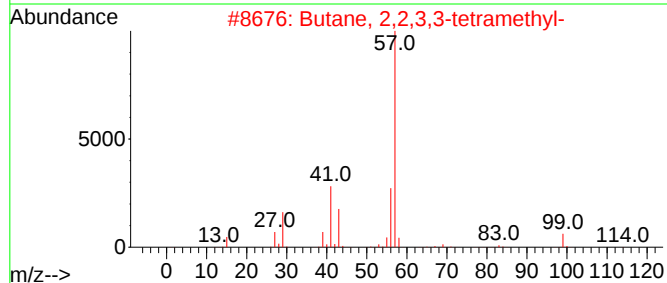
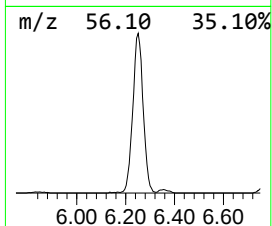
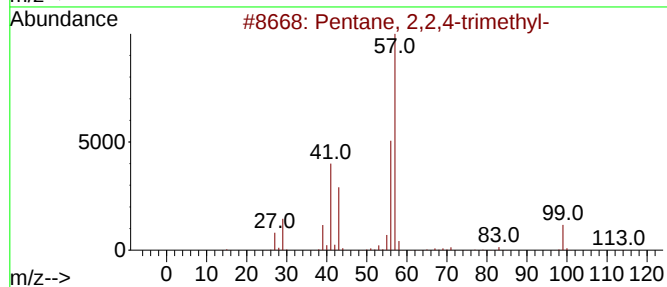
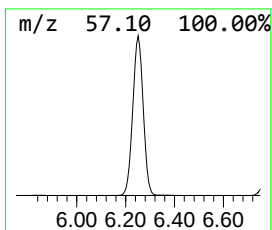
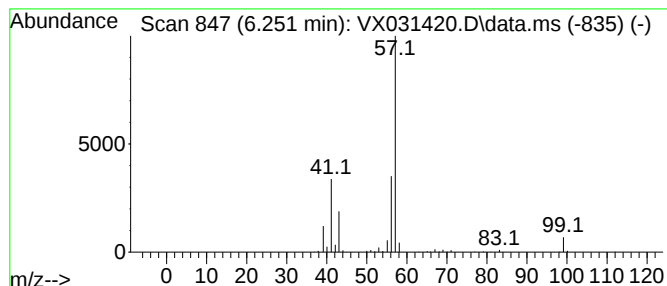
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	110.56 ug/l	718771	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031420.D
Acq On : 16 Sep 2022 19:09
Operator : JC/MD
Sample : N4645-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

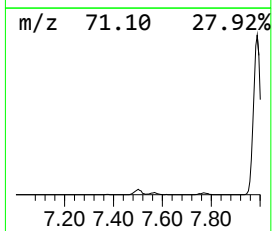
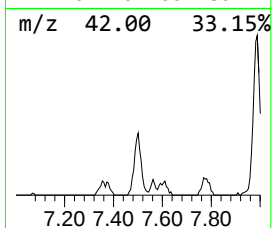
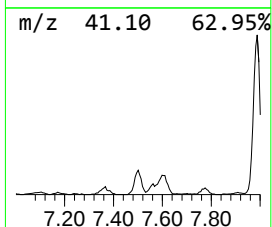
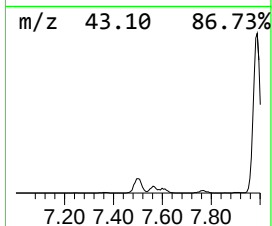
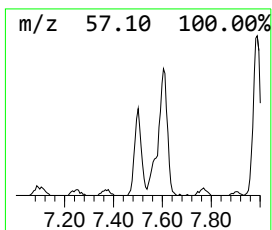
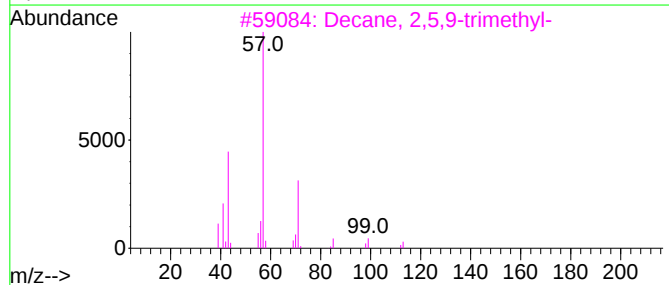
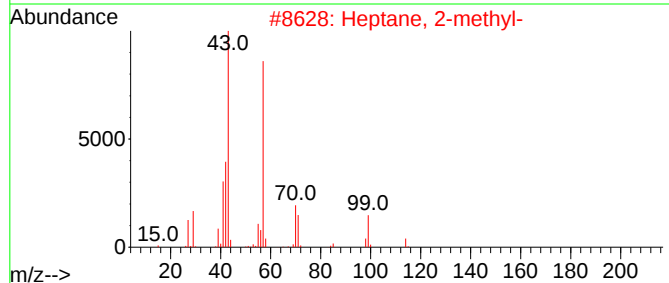
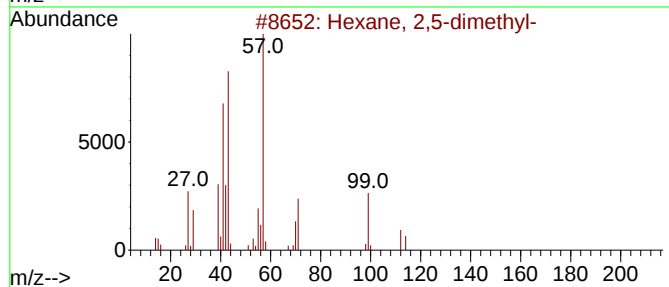
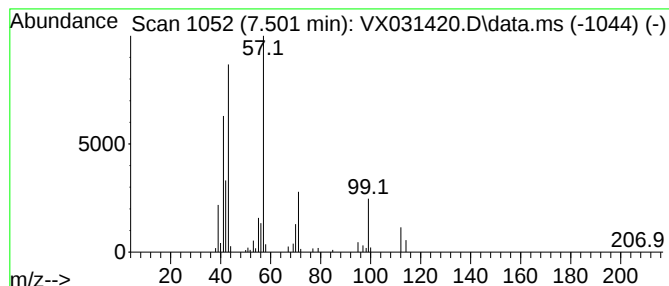
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.501	7.90 ug/l	51375	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	94
2			Heptane, 2-methyl-	114	C8H18	000592-27-8	64
3			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	53
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031420.D
Acq On : 16 Sep 2022 19:09
Operator : JC/MD
Sample : N4645-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

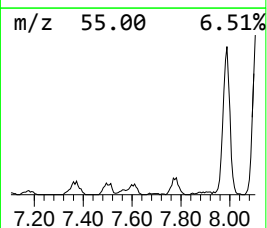
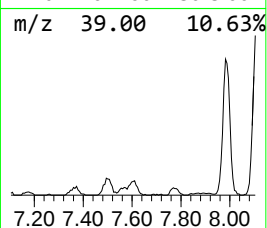
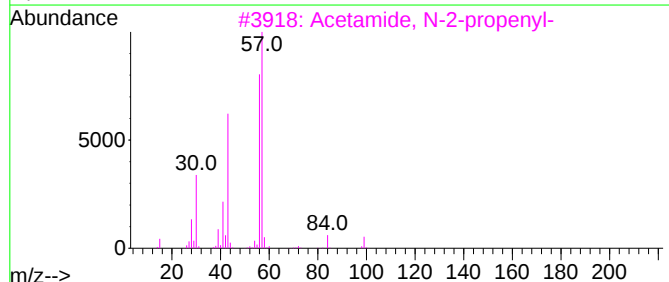
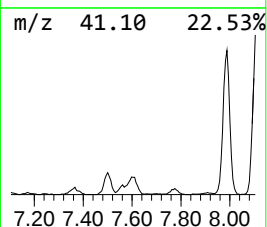
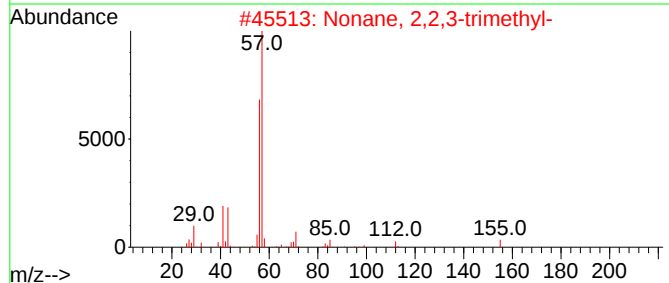
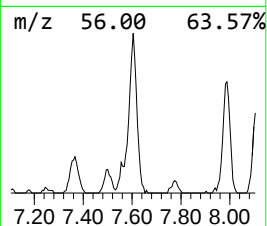
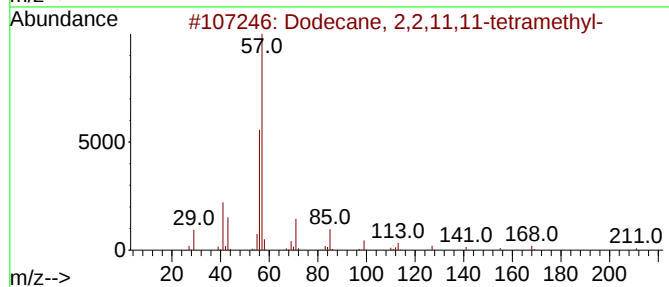
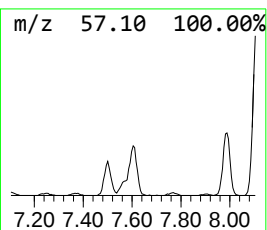
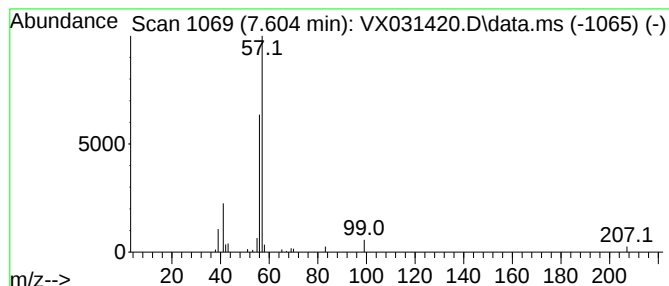
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane, 2,2,11,11-tetrame... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.604	6.73 ug/l	43761	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	56
2	Nonane, 2,2,3-trimethyl-	170	C12H26	055499-04-2	56
3	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	45
4	Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	43
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031420.D
Acq On : 16 Sep 2022 19:09
Operator : JC/MD
Sample : N4645-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

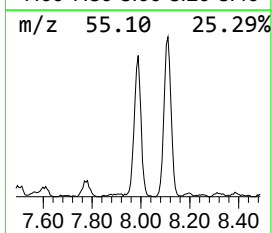
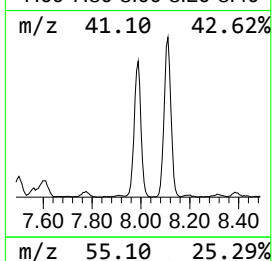
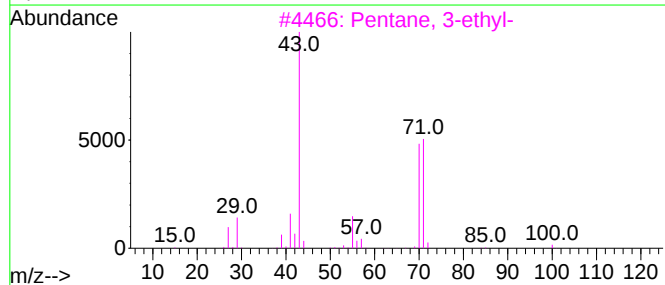
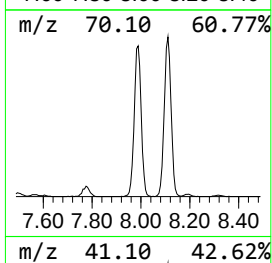
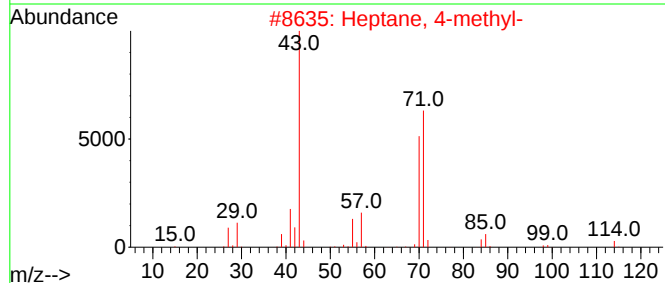
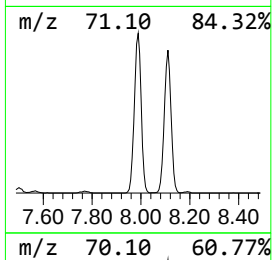
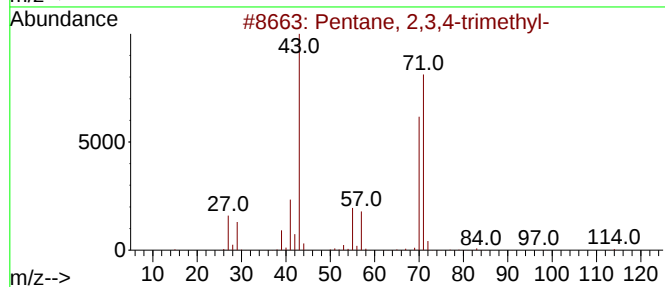
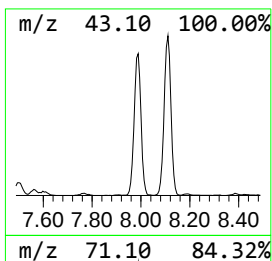
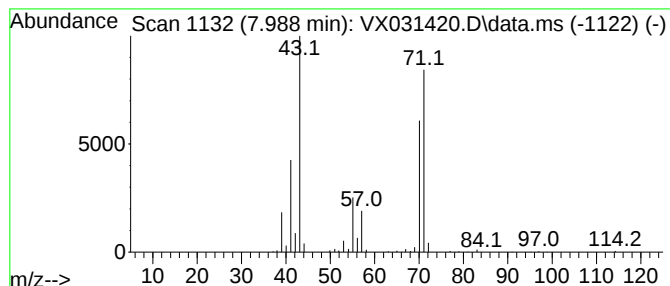
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	62.30 ug/l	405038	1,4-Difluorobenzene	6.763

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			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031420.D
Acq On : 16 Sep 2022 19:09
Operator : JC/MD
Sample : N4645-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

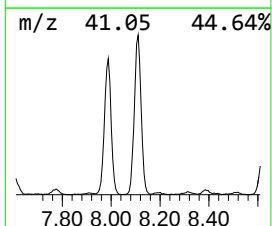
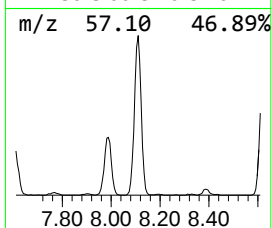
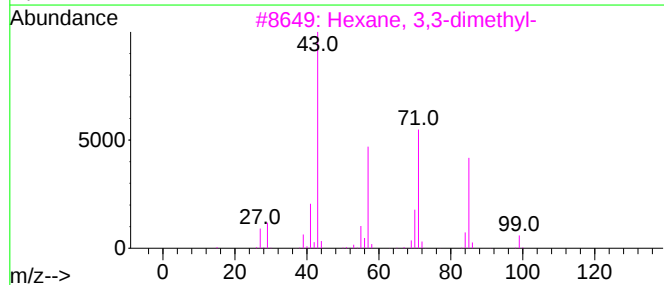
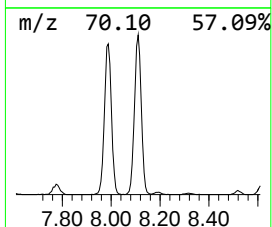
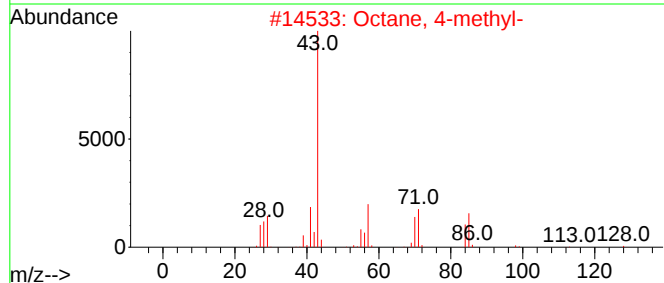
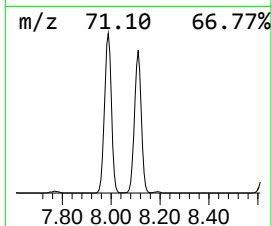
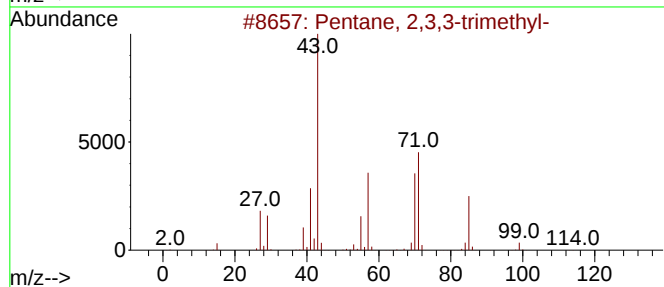
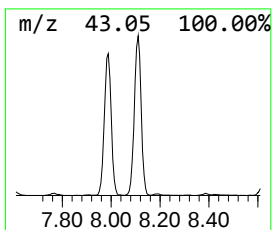
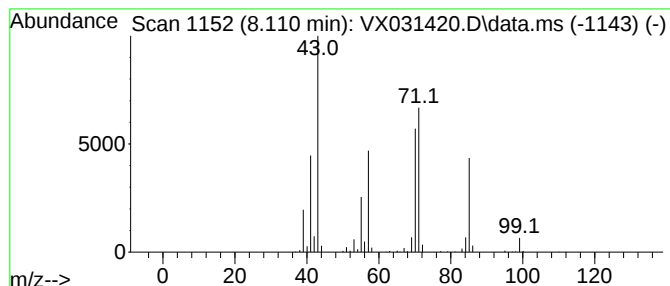
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Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	82.61 ug/l	537053	1,4-Difluorobenzene	6.763

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	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031420.D
Acq On : 16 Sep 2022 19:09
Operator : JC/MD
Sample : N4645-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.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...	4.215	31.3	ug/l	155822	1	5.556	248746	50.0
Pentane, 2,3-di...	5.623	50.9	ug/l	252954	1	5.556	248746	50.0
Pentane, 2,2,4-...	6.251	110.6	ug/l	718771	2	6.763	325056	50.0
Hexane, 2,5-dim...	7.501	7.9	ug/l	51375	2	6.763	325056	50.0
Dodecane, 2,2,1...	7.604	6.7	ug/l	43761	2	6.763	325056	50.0
Pentane, 2,3,4-...	7.988	62.3	ug/l	405038	2	6.763	325056	50.0
Pentane, 2,3,3-...	8.110	82.6	ug/l	537053	2	6.763	325056	50.0