

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
 Data File : VX021382.D
 Acq On : 23 Mar 2021 14:02
 Operator : JC/MD
 Sample : M1723-03
 Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RO124027

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\82X031621W.M
 Title : SW846 8260

Signal : TIC: VX021382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.764	278	285	292	rBV	41926	75738	2.32%	0.542%
2	5.464	733	744	756	rBV	47825	141803	4.35%	1.015%
3	5.623	759	771	792	rVB	86060	244923	7.52%	1.753%
4	6.029	830	840	850	rBV	59137	156222	4.79%	1.118%
5	6.829	966	976	984	rBV	131598	328153	10.07%	2.348%
6	7.482	1072	1087	1104	rVB2	62875	153184	4.70%	1.096%
7	8.629	1275	1282	1288	rBV	96473	180638	5.54%	1.293%
8	8.694	1288	1293	1299	rVV	264552	423548	13.00%	3.031%
9	8.765	1299	1305	1319	rVB	946613	1436824	44.10%	10.282%
10	9.000	1340	1345	1355	rVB	40168	67608	2.08%	0.484%
11	9.165	1365	1373	1378	rBV	92880	149019	4.57%	1.066%
12	9.624	1443	1451	1461	rVB	331864	453176	13.91%	3.243%
13	10.094	1525	1531	1541	rVB	236200	345038	10.59%	2.469%
14	10.194	1542	1548	1551	rBV	1084971	1407872	43.21%	10.075%
15	10.235	1551	1555	1560	rVV	889047	1170336	35.92%	8.375%
16	10.277	1560	1562	1566	rVV	45407	52944	1.63%	0.379%
17	10.341	1566	1573	1580	rVV	2456626	3258088	100.00%	23.315%
18	10.394	1580	1582	1587	rVB	29315	34037	1.04%	0.244%
19	10.624	1614	1621	1625	rBV2	29089	53923	1.66%	0.386%
20	10.683	1625	1631	1645	rVB2	742618	1103277	33.86%	7.895%
21	10.806	1645	1652	1658	rBV	139213	211992	6.51%	1.517%
22	10.894	1663	1667	1678	rVB5	37316	71165	2.18%	0.509%
23	11.000	1678	1685	1689	rBV	60477	88530	2.72%	0.634%
24	11.124	1700	1706	1711	rBV	222904	298261	9.15%	2.134%
25	11.347	1737	1744	1751	rBV2	277956	393242	12.07%	2.814%
26	11.418	1751	1756	1763	rBV	300340	515745	15.83%	3.691%
27	11.489	1764	1768	1771	rBV	75930	88227	2.71%	0.631%
28	11.653	1791	1796	1804	rVB	88523	121930	3.74%	0.873%
29	11.789	1815	1819	1825	rBV	183571	223531	6.86%	1.600%
30	11.924	1835	1842	1848	rVB3	25454	47494	1.46%	0.340%
31	12.012	1853	1857	1860	rVV	53759	69356	2.13%	0.496%
32	12.059	1860	1865	1871	rVB2	278456	364306	11.18%	2.607%
33	12.130	1871	1877	1889	rBV2	41387	93095	2.86%	0.666%
34	12.283	1896	1903	1906	rBV2	45853	78629	2.41%	0.563%
35	12.353	1911	1915	1923	rVB3	44498	72089	2.21%	0.516%

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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\82X031621W.M
Title : SW846 8260

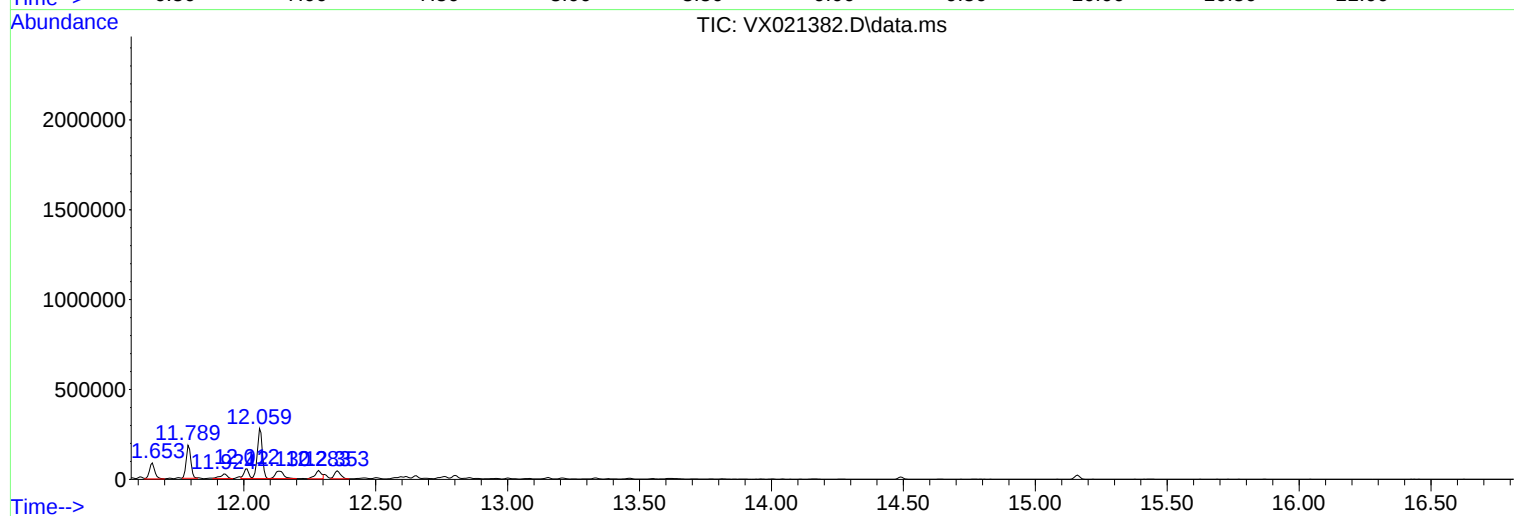
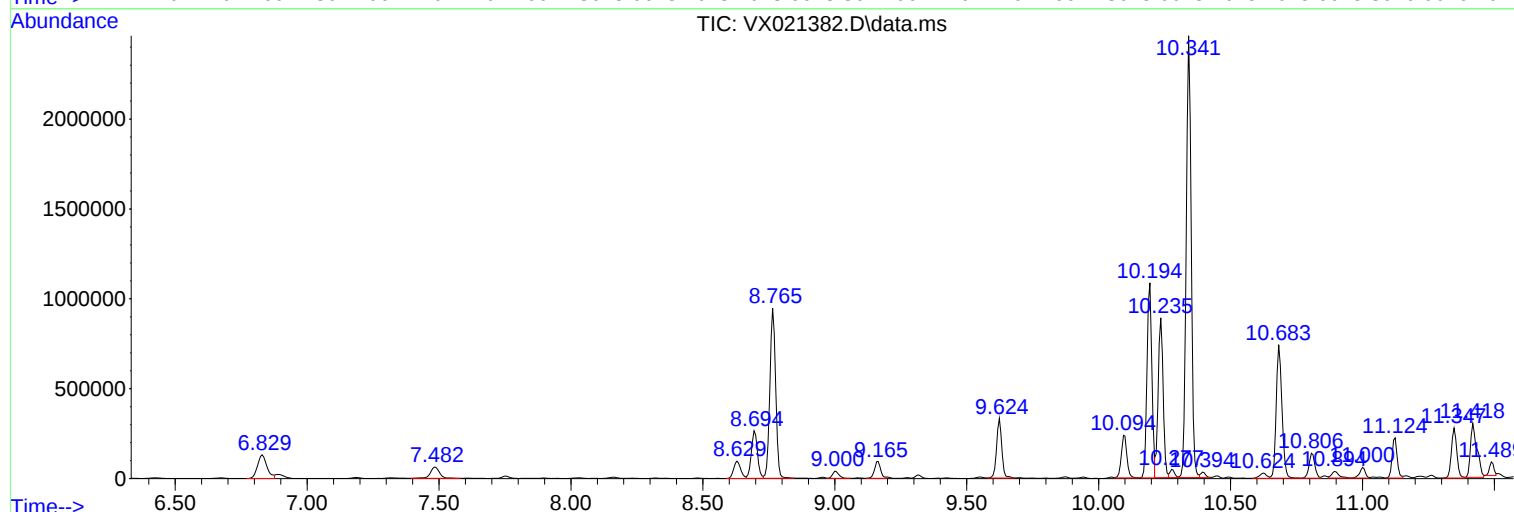
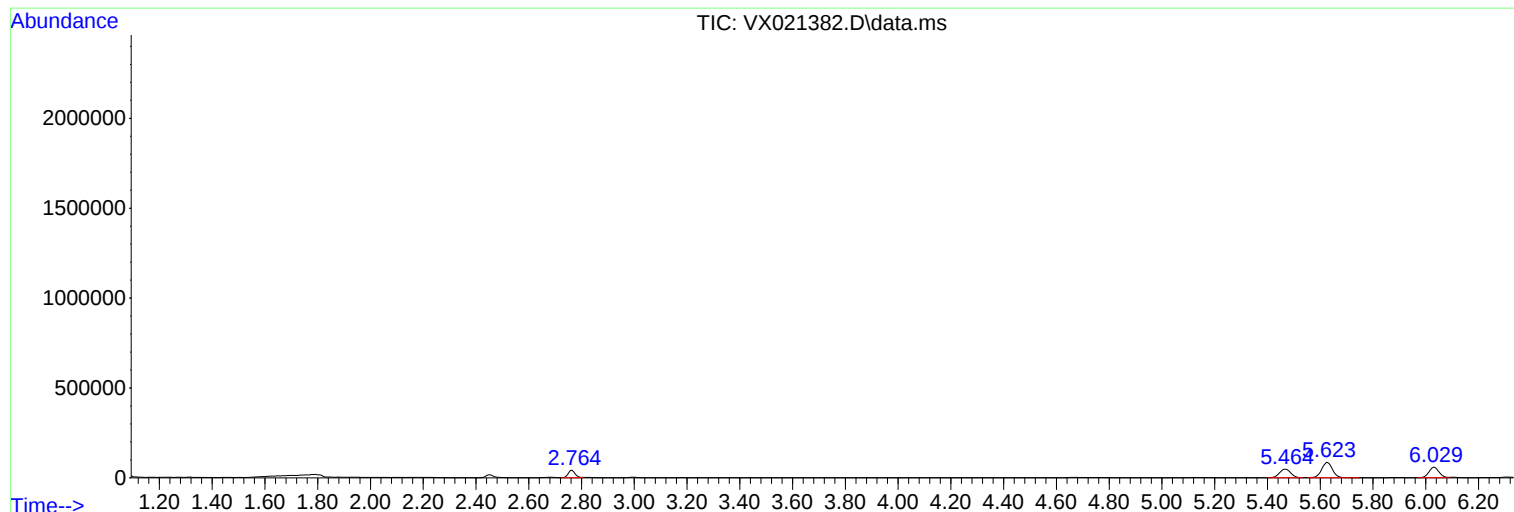
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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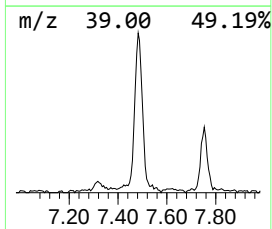
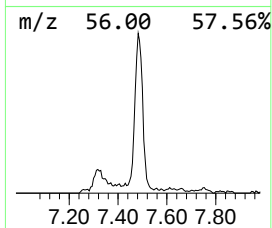
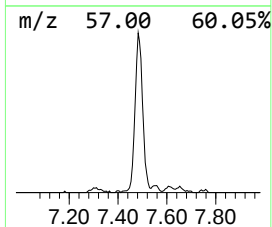
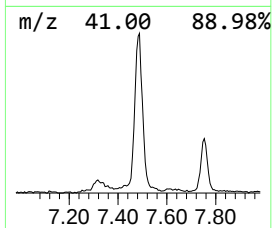
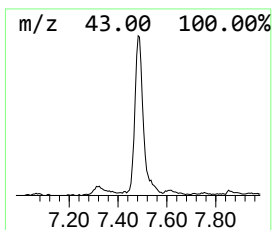
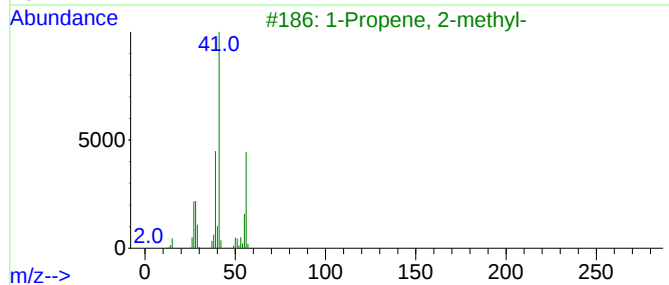
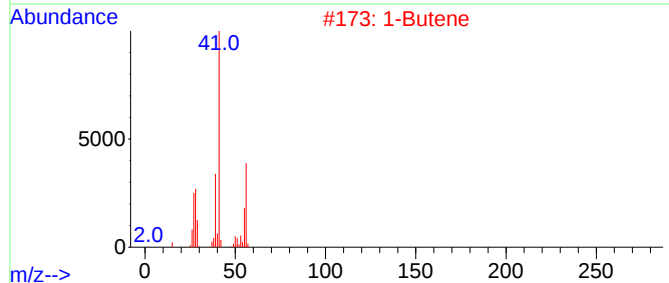
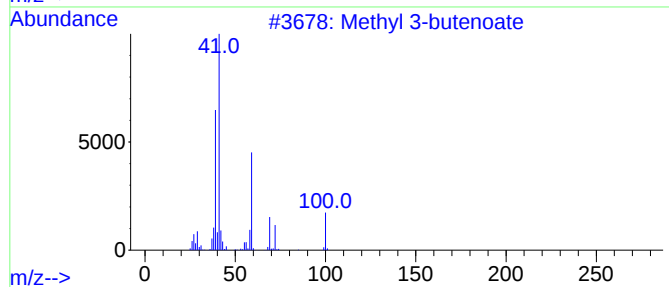
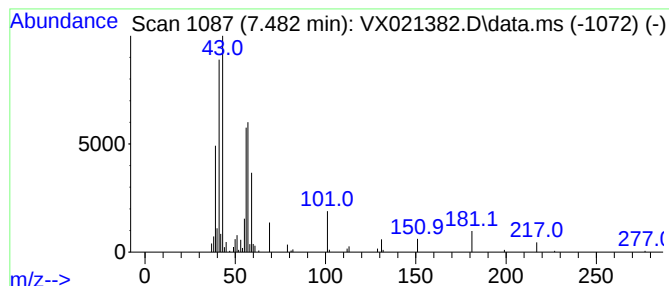
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.482 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.482	23.34 ug/l	153184	1,4-Difluorobenzene	6.829

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 3-butenolate	100	C5H8O2	003724-55-8	35
2			1-Butene	56	C4H8	000106-98-9	32
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	32
4			2-Butene, (E)-	56	C4H8	000624-64-6	23
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

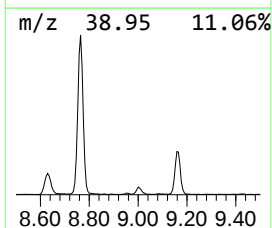
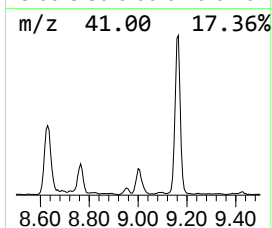
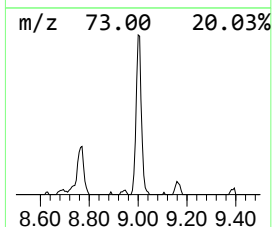
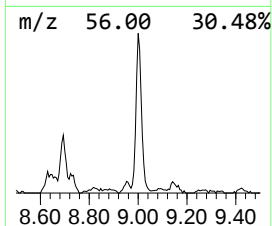
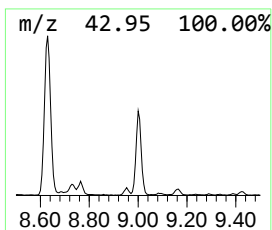
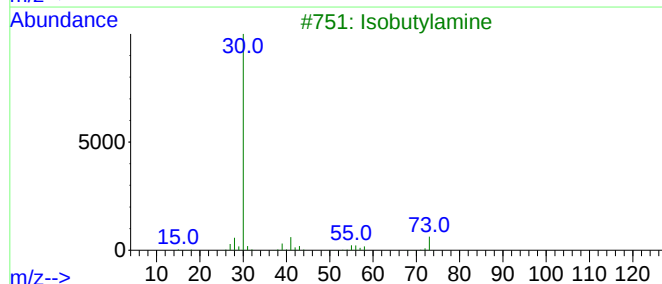
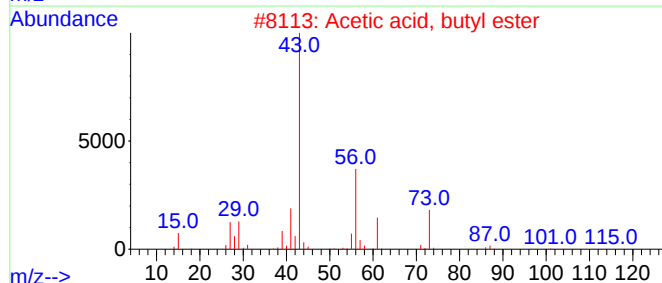
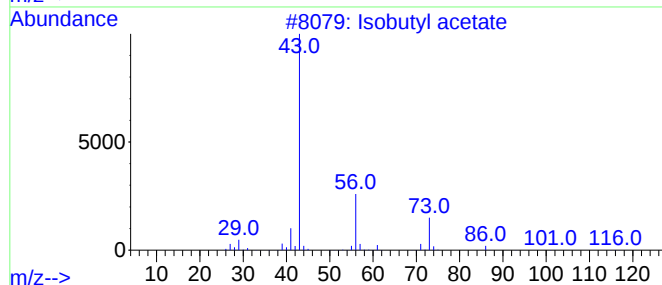
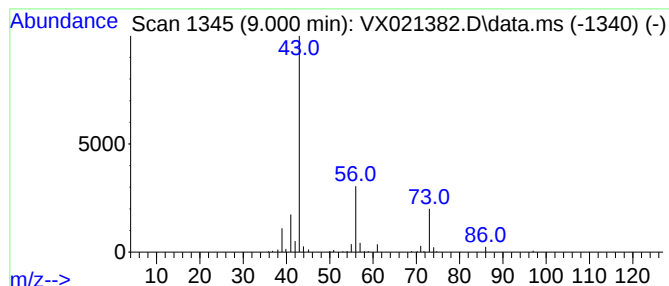
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Isobutyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	9.80 ug/l	67608	Chlorobenzene-d5	10.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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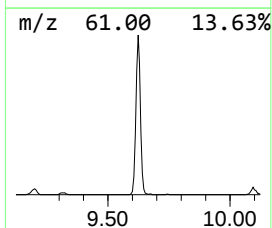
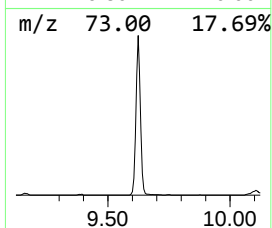
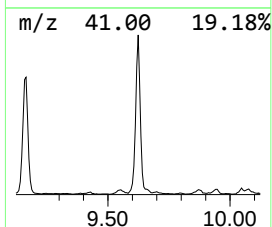
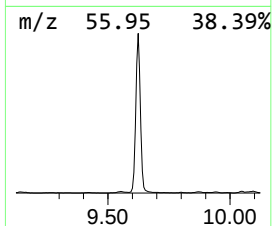
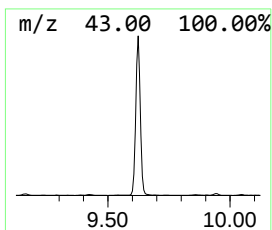
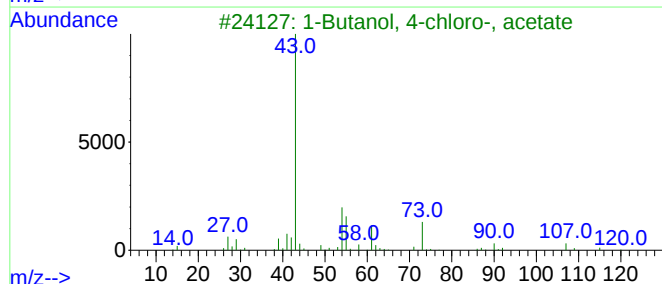
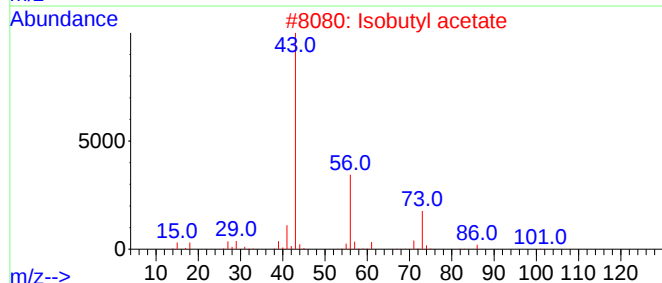
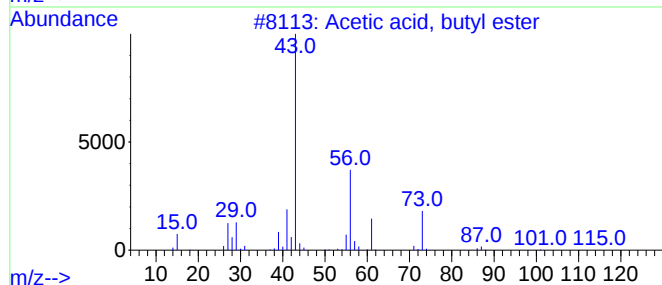
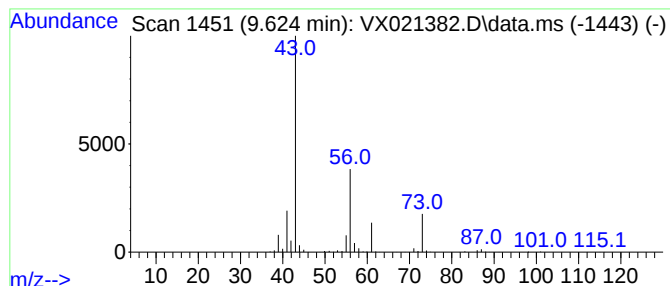
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.624	65.67 ug/l	453176	Chlorobenzene-d5	10.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
5			Isobutylamine	73	C4H11N	000078-81-9	9



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Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
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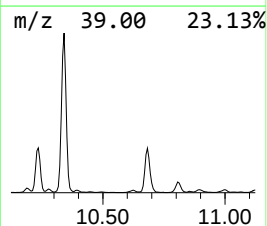
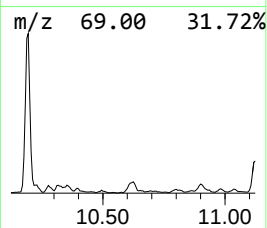
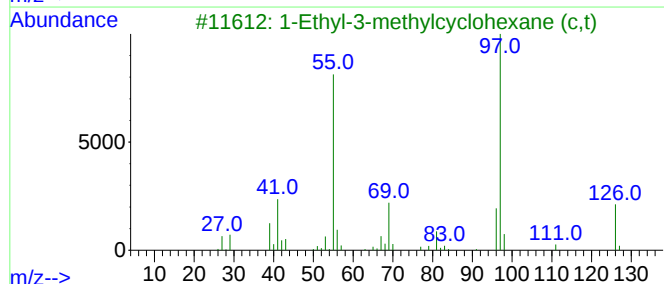
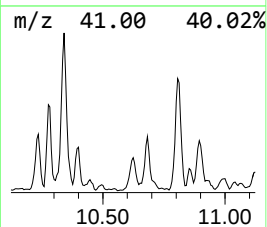
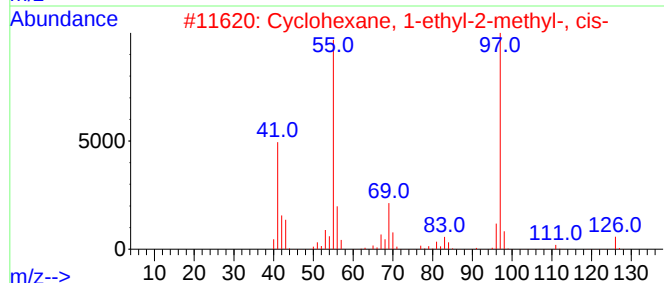
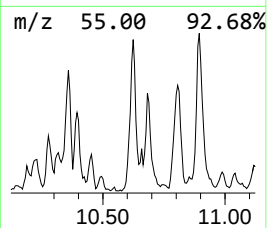
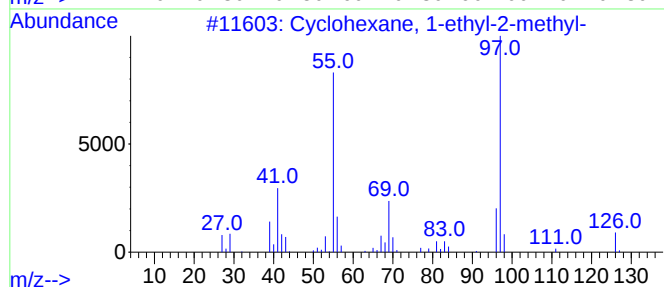
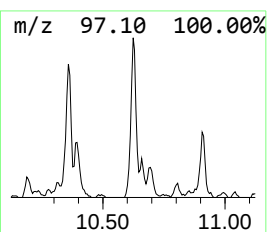
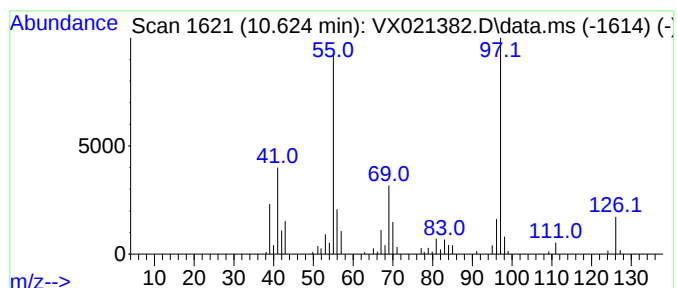
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.624	7.81 ug/l	53923	Chlorobenzene-d5	10.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	83
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	78
3			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	74
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	72
5			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	72



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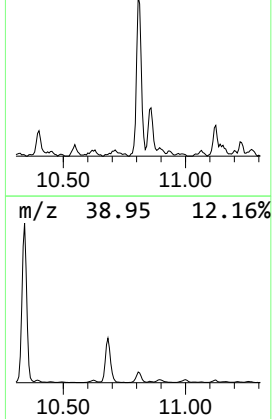
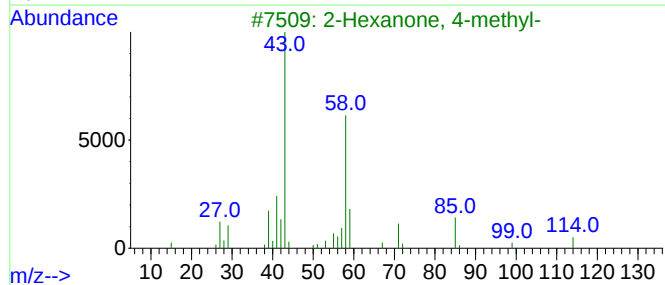
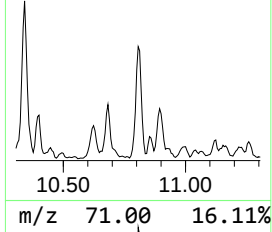
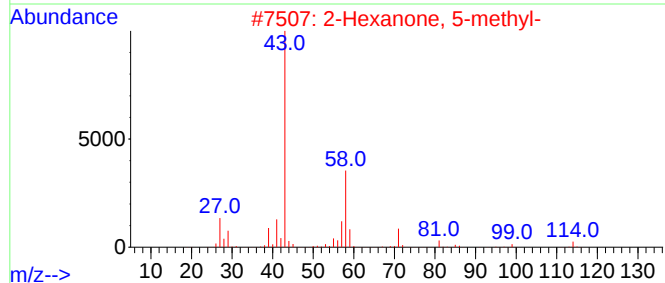
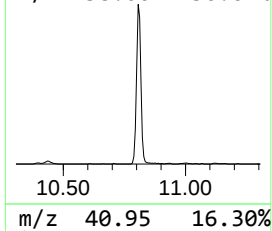
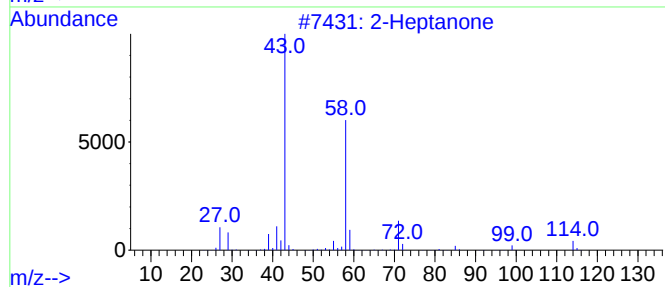
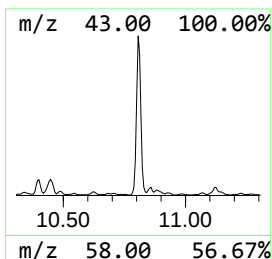
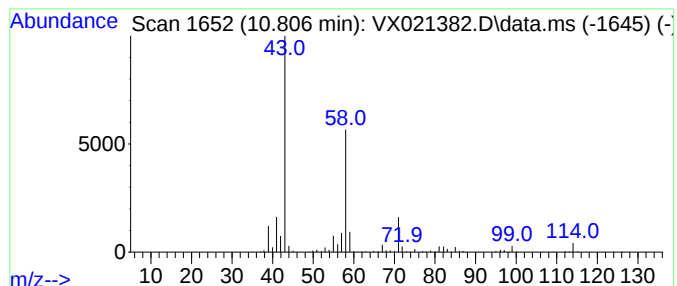
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.806	30.72 ug/l	211992	Chlorobenzene-d5	10.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	90
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	56
5			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

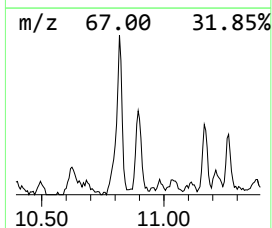
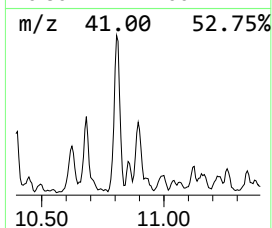
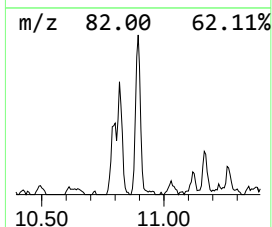
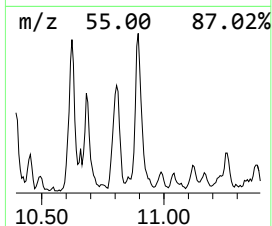
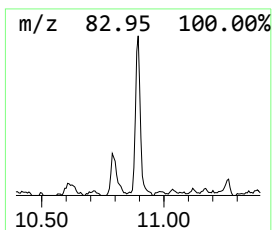
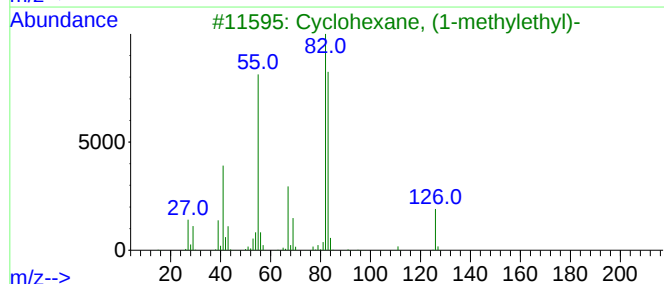
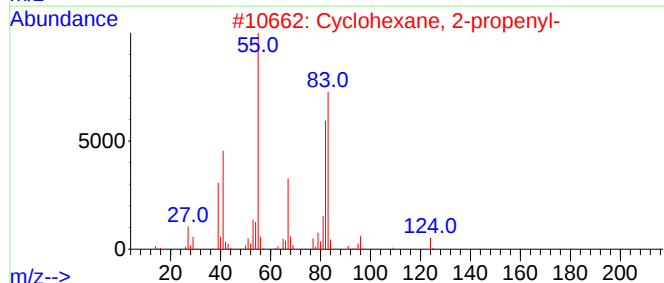
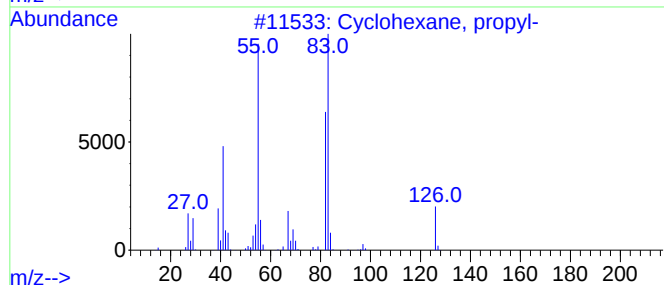
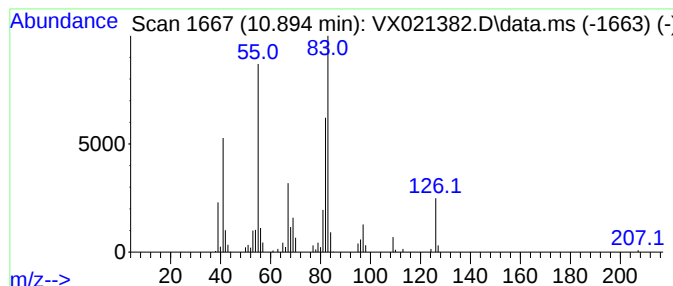
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexane, propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.894	10.31 ug/l	71165	Chlorobenzene-d5	10.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	72
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	70
4			Cyclohexane, 1,1'-(1,2-ethanedi...	194	C14H26	003321-50-4	64
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

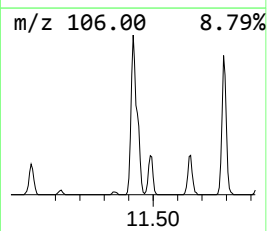
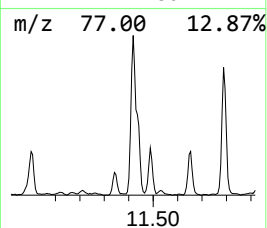
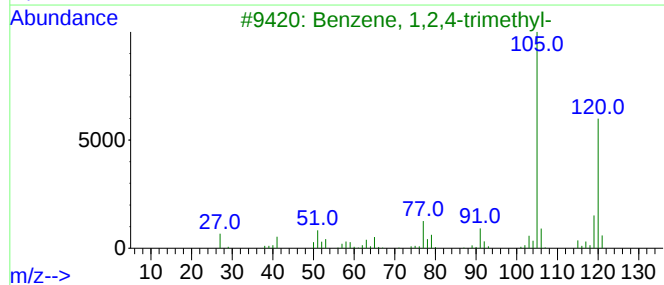
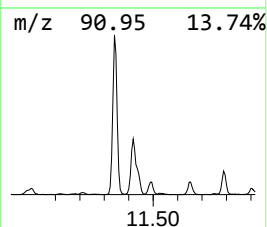
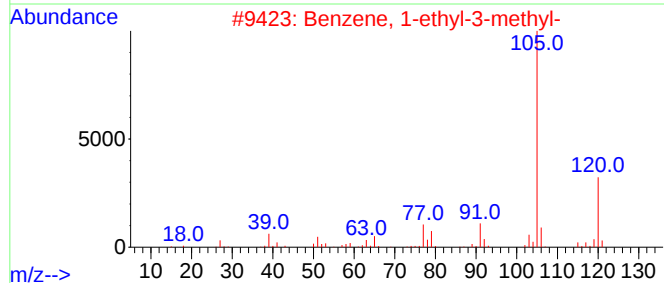
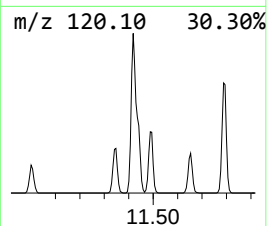
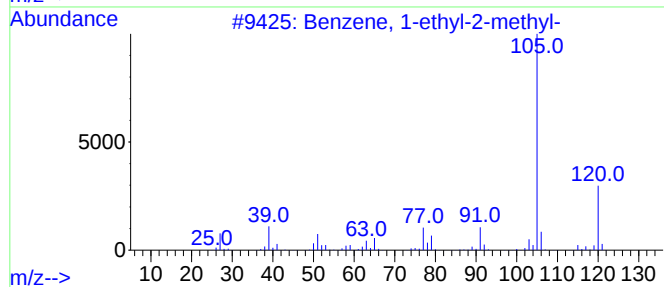
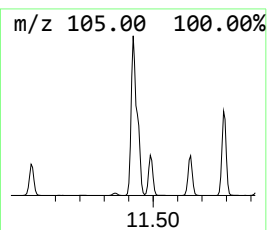
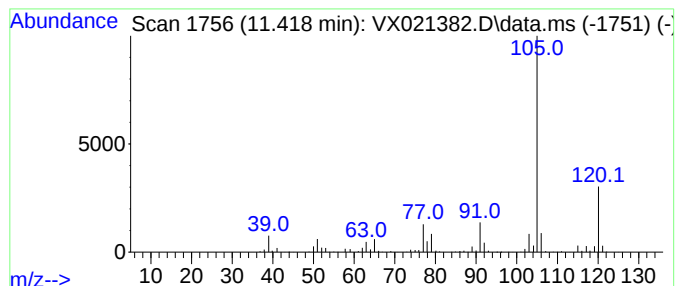
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.418	70.78 ug/l	515745	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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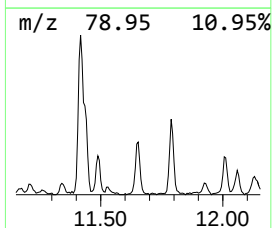
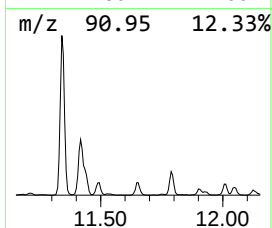
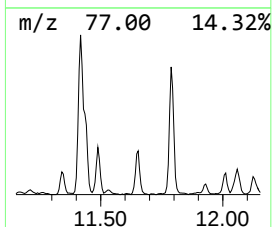
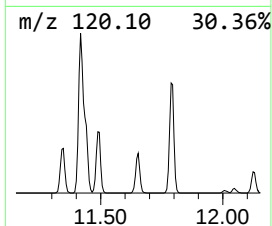
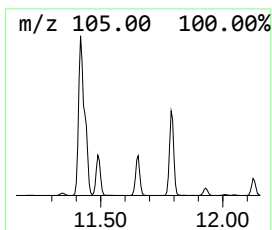
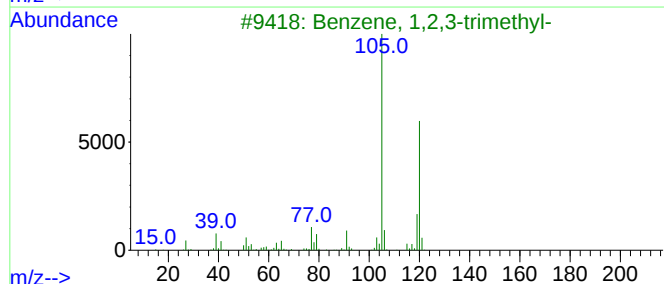
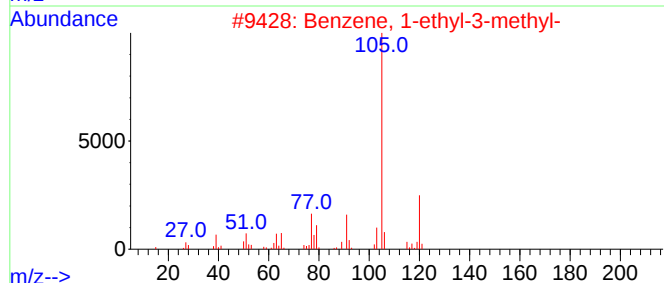
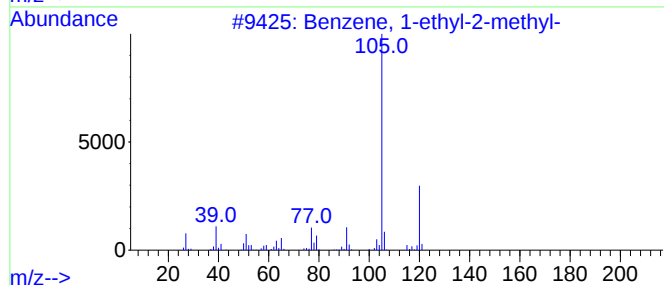
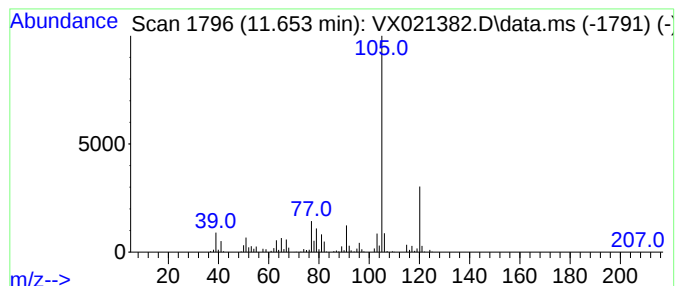
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.653	16.73 ug/l	121930	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

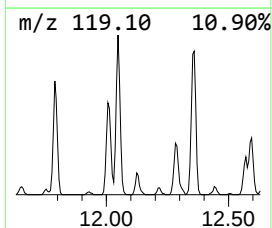
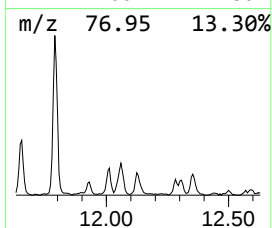
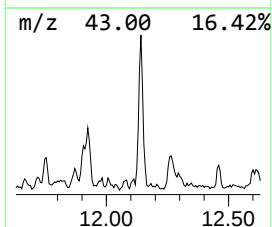
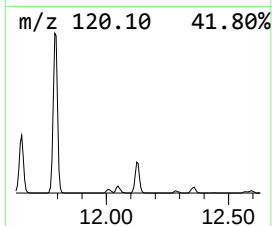
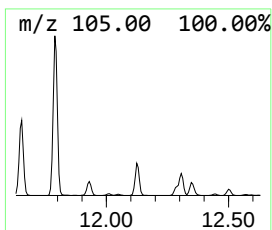
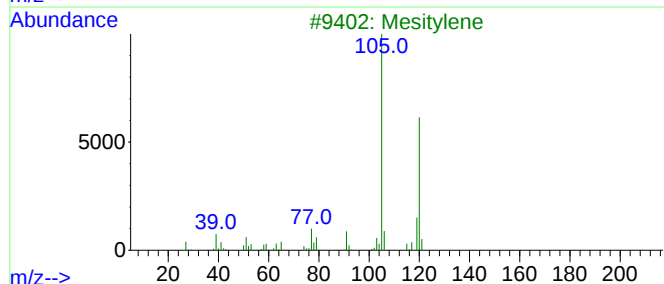
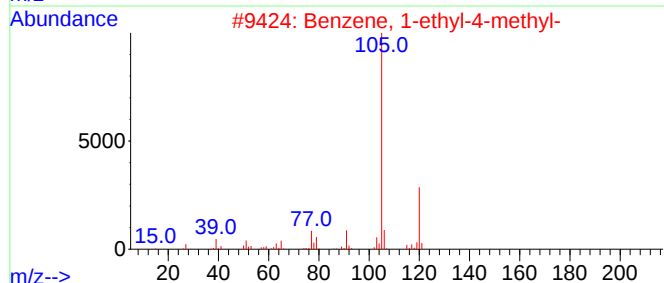
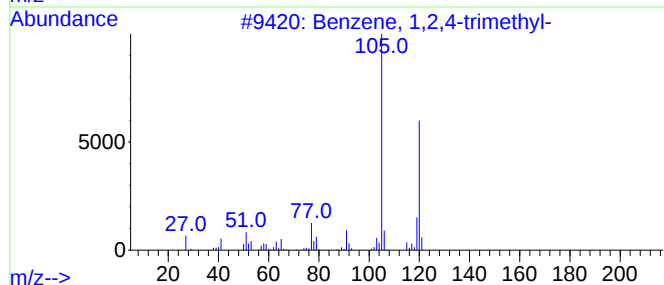
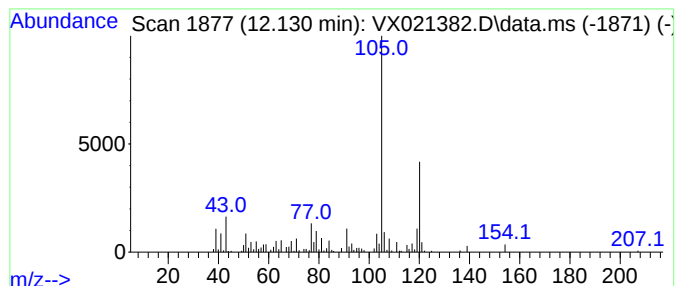
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.130	12.78 ug/l	93095	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

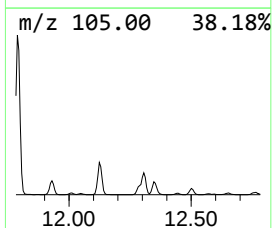
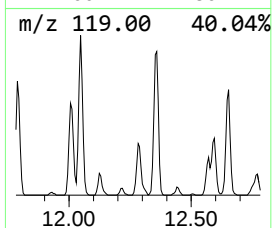
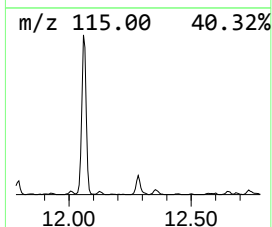
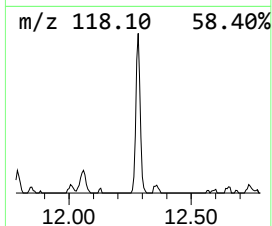
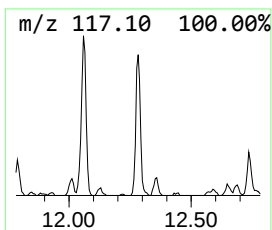
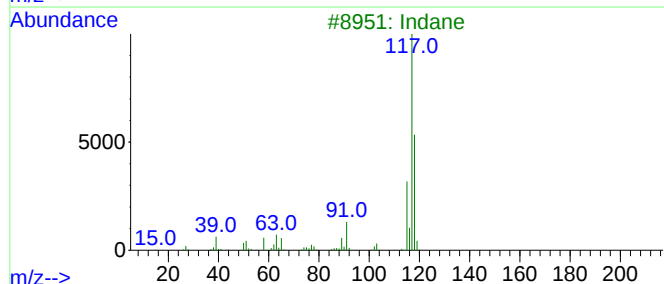
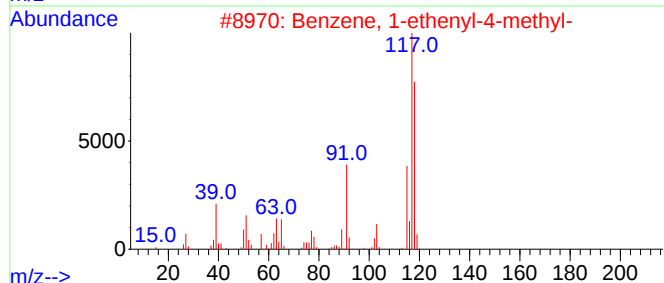
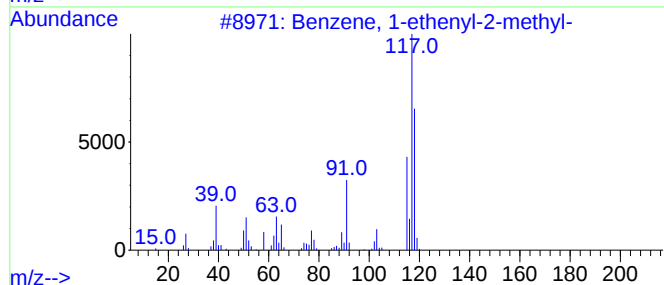
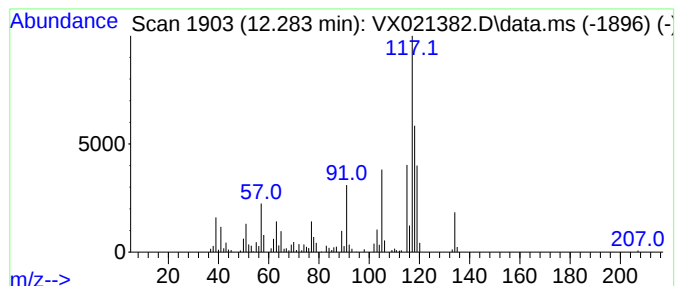
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	10.79 ug/l	78629	1,4-Dichlorobenzene-d4	12.065

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	95
2		Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	91
3		Indane	118	C9H10	000496-11-7	90
4		Benzene, 1-propenyl-	118	C9H10	000637-50-3	78
5		Benzene, 2-propenyl-	118	C9H10	000300-57-2	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032321\
Data File : VX021382.D
Acq On : 23 Mar 2021 14:02
Operator : JC/MD
Sample : M1723-03
Misc : 11.36g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO124027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Acetic acid, bu...	9.624	65.7	ug/l	453176	3	10.100	345038	50.0
Cyclohexane, 1-...	10.624	7.8	ug/l	53923	3	10.100	345038	50.0
2-Heptanone	10.806	30.7	ug/l	211992	3	10.100	345038	50.0
Cyclohexane, pr...	10.894	10.3	ug/l	71165	3	10.100	345038	50.0
Benzene, 1-ethy...	11.418	70.8	ug/l	515745	4	12.065	364306	50.0
Benzene, 1-ethy...	11.653	16.7	ug/l	121930	4	12.065	364306	50.0
Benzene, 1,2,4-...	12.130	12.8	ug/l	93095	4	12.065	364306	50.0
Benzene, 1-ethe...	12.283	10.8	ug/l	78629	4	12.065	364306	50.0