

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062618\
 Data File : VX002911.D
 Acq On : 26 Jun 2018 23:17
 Operator : JC/MD
 Sample : J3707-05 50X
 Misc : 5.49g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WP021SB488-29-31-180622

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	93	rBV	486142	689540	6.93%	2.717%
2	4.599	645	658	677	rBV	445928	1231635	12.38%	4.853%
3	5.507	791	807	817	rBV2	168601	485998	4.88%	1.915%
4	5.666	823	833	858	rVB2	255405	747517	7.51%	2.946%
5	6.074	888	900	910	rBV	178493	469044	4.71%	1.848%
6	6.867	1019	1030	1048	rBV	360852	847126	8.51%	3.338%
7	7.220	1076	1088	1116	rBV	4679975	9951446	100.00%	39.213%
8	8.720	1316	1334	1340	rBV	899848	1406006	14.13%	5.540%
9	8.787	1340	1345	1352	rVB	224044	330294	3.32%	1.302%
10	10.116	1558	1563	1573	rVB	776583	1016868	10.22%	4.007%
11	10.360	1591	1603	1609	rBV	88192	146152	1.47%	0.576%
12	10.415	1609	1612	1624	rVB	98447	133875	1.35%	0.528%
13	11.140	1725	1731	1741	rVV	892077	1223144	12.29%	4.820%
14	11.244	1741	1748	1752	rVV	75753	119157	1.20%	0.470%
15	11.439	1776	1780	1786	rBV	89615	153700	1.54%	0.606%
16	11.537	1786	1796	1801	rVB2	628167	932273	9.37%	3.674%
17	11.671	1813	1818	1825	rBV4	51191	117728	1.18%	0.464%
18	11.774	1831	1835	1838	rBV	124085	134041	1.35%	0.528%
19	11.811	1838	1841	1851	rVB	245762	369183	3.71%	1.455%
20	12.079	1880	1885	1891	rVV	960307	1335938	13.42%	5.264%
21	12.152	1891	1897	1902	rVV3	161029	322567	3.24%	1.271%
22	12.323	1919	1925	1929	rVB2	124123	208570	2.10%	0.822%
23	12.378	1929	1934	1941	rVB4	231675	457430	4.60%	1.802%
24	12.481	1945	1951	1955	rBV	506424	588822	5.92%	2.320%
25	12.524	1955	1958	1964	rVB	99054	137270	1.38%	0.541%
26	12.591	1964	1969	1971	rBV	135043	191782	1.93%	0.756%
27	12.616	1971	1973	1978	rVV	128888	141156	1.42%	0.556%
28	12.670	1978	1982	1986	rVB	206714	229718	2.31%	0.905%
29	12.774	1991	1999	2005	rVB5	82897	189535	1.90%	0.747%
30	12.981	2024	2033	2036	rBV	150924	236197	2.37%	0.931%
31	13.024	2036	2040	2046	rVB	216395	282582	2.84%	1.113%
32	13.103	2046	2053	2056	rBV5	45598	106477	1.07%	0.420%
33	13.323	2084	2089	2091	rBV3	81048	128726	1.29%	0.507%
34	13.347	2091	2093	2099	rVB2	146818	197674	1.99%	0.779%

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ClientSampleId :
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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

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Title : SW846 8260

35	13.835	2169	2173	2180	rVB	82774	118712	1.19%	0.468%
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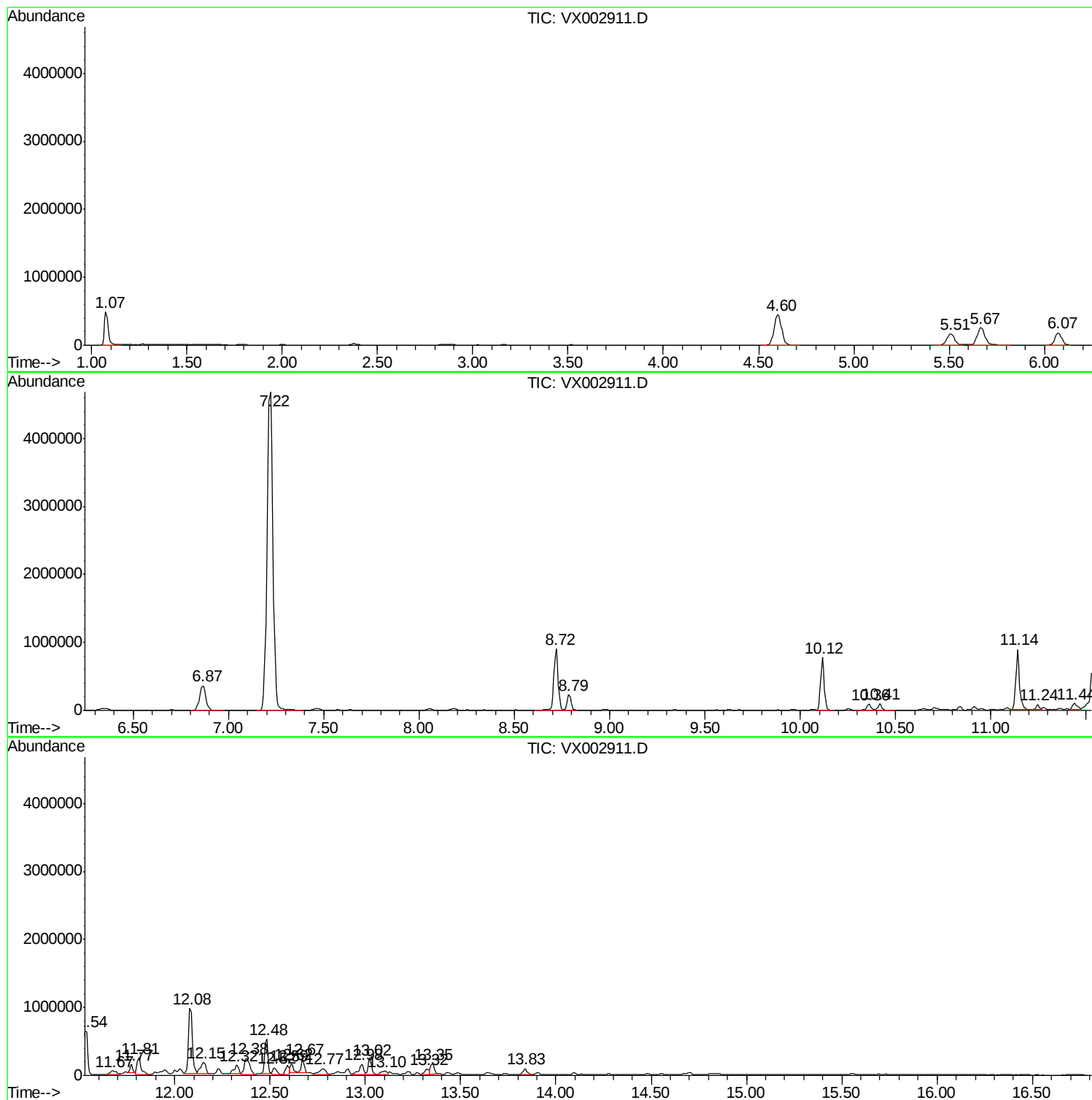
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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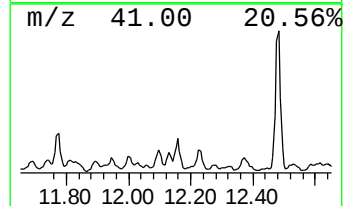
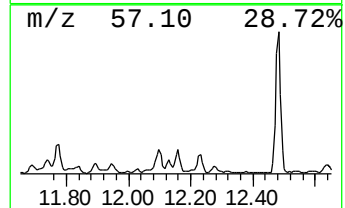
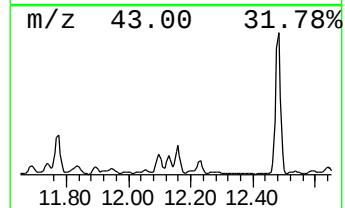
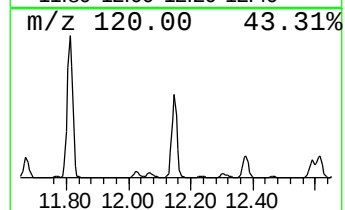
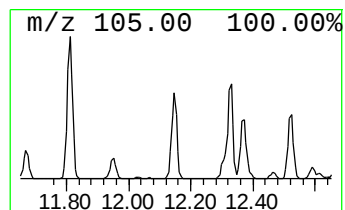
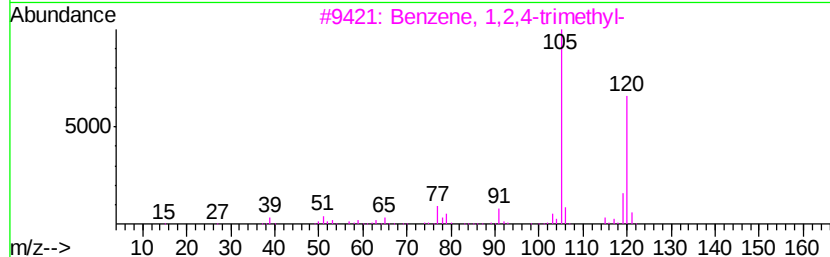
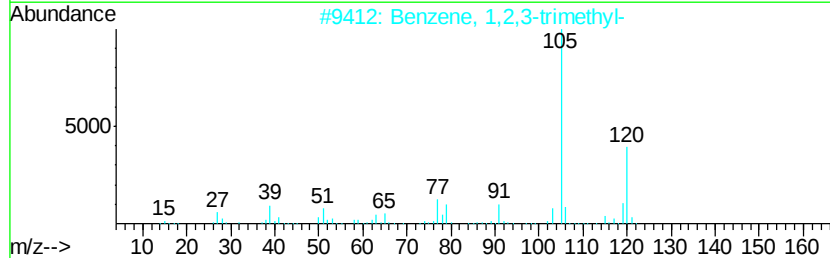
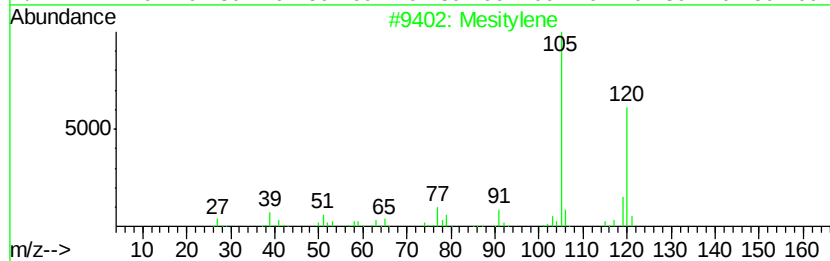
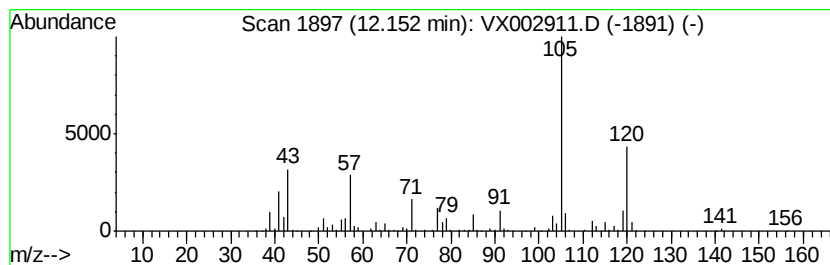
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Mesitylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	12.07 ug/l	322567	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Mesitylene	120 C9H12	000108-67-8	94
2	Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8	91
3	Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6	90
4	Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4	90
5	Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3	87



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Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-29-31-180622

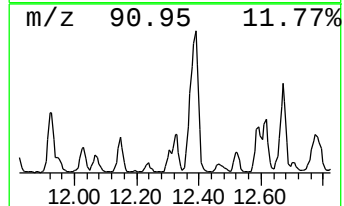
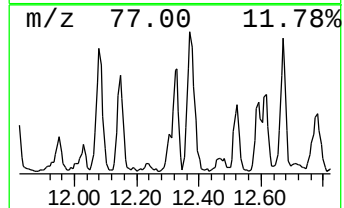
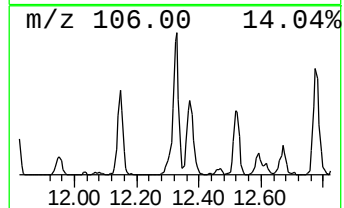
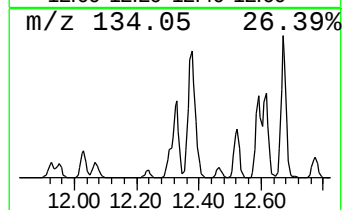
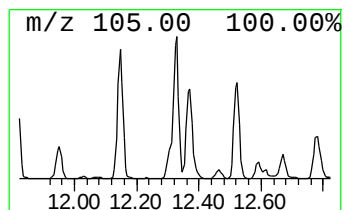
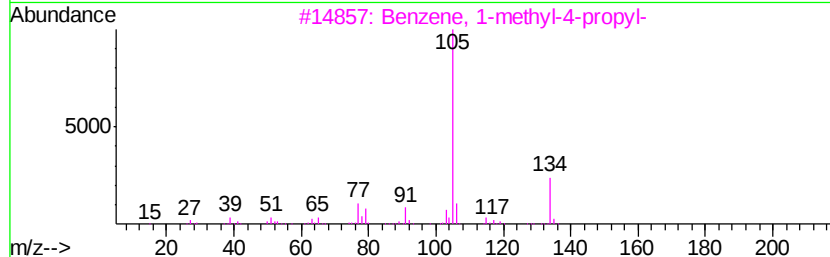
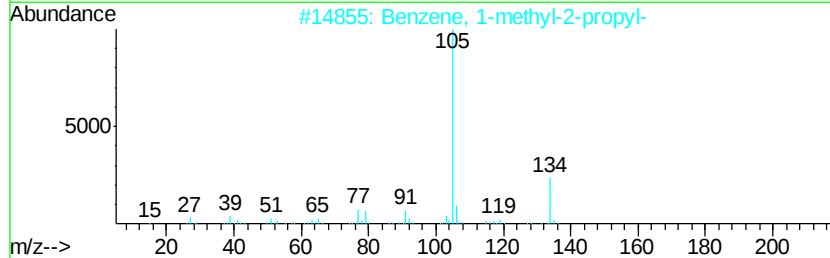
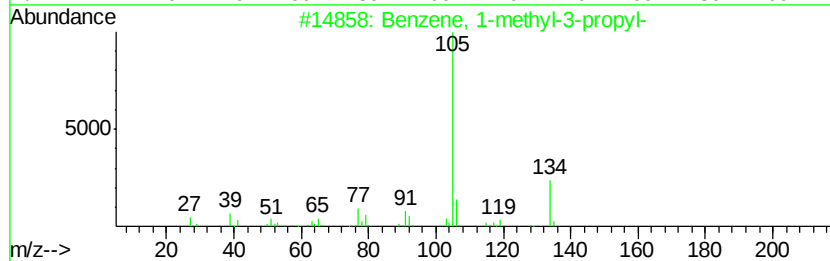
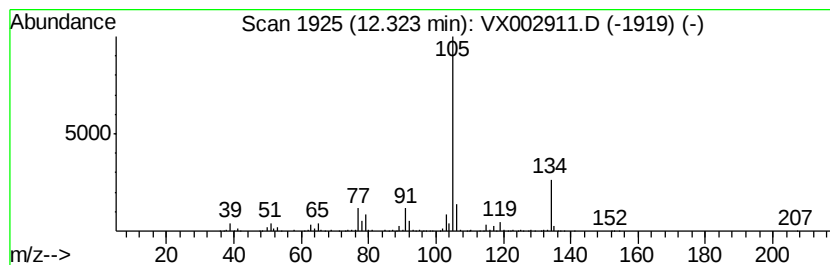
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-methyl-3-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	7.81 ug/l	208570	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	95
2		Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91
3		Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	91
4		Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	86
5		2-Tolyloxirane	134	C9H10O	002783-26-8	74



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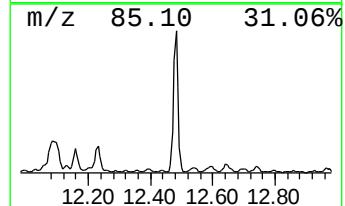
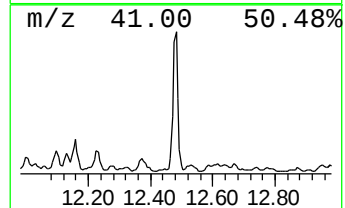
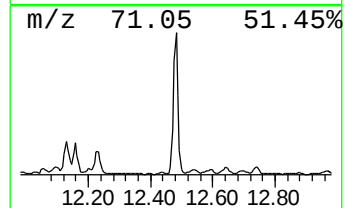
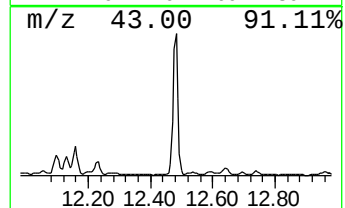
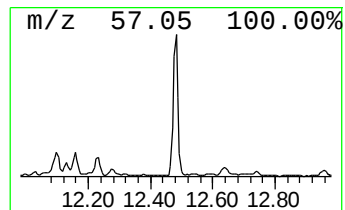
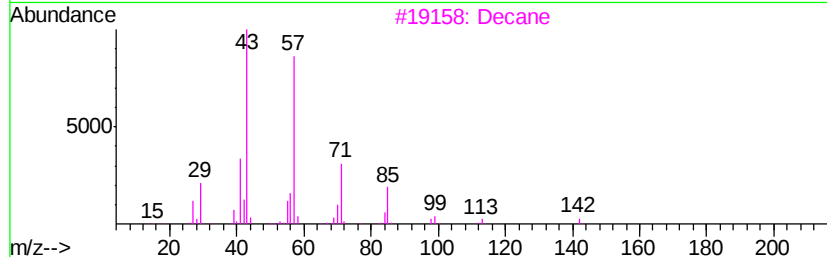
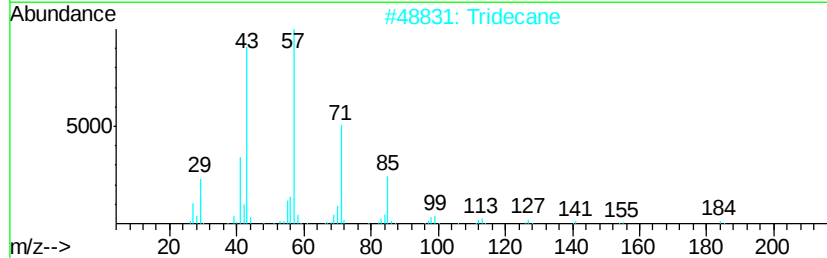
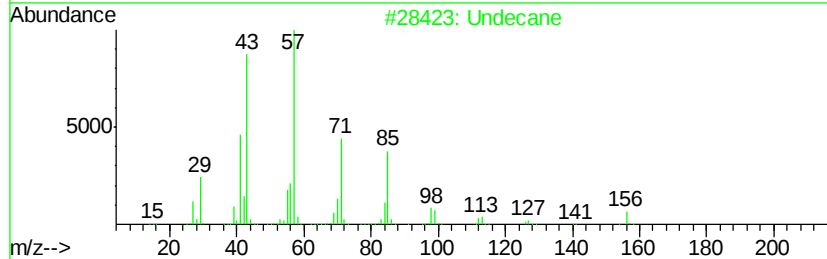
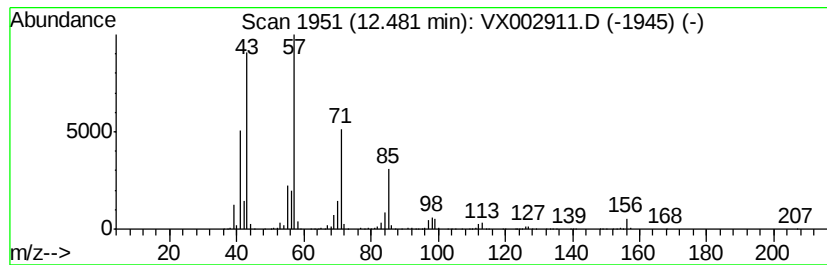
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	22.04 ug/l	588822	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	93
2	Tridecane	184 C13H28	000629-50-5	80
3	Decane	142 C10H22	000124-18-5	78
4	Hexadecane	226 C16H34	000544-76-3	72
5	Tetradecane	198 C14H30	000629-59-4	64



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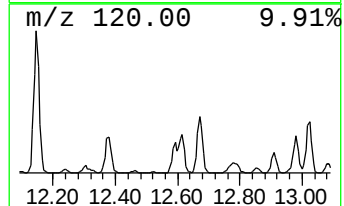
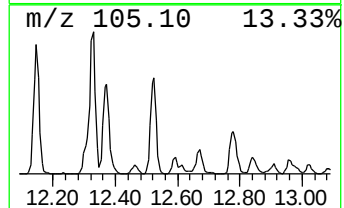
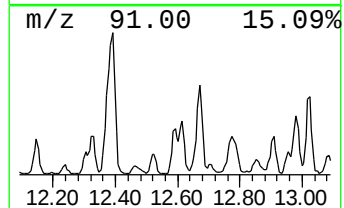
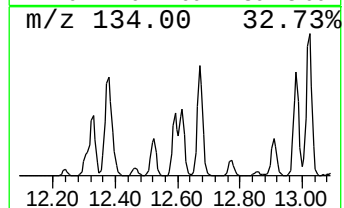
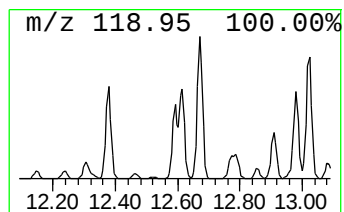
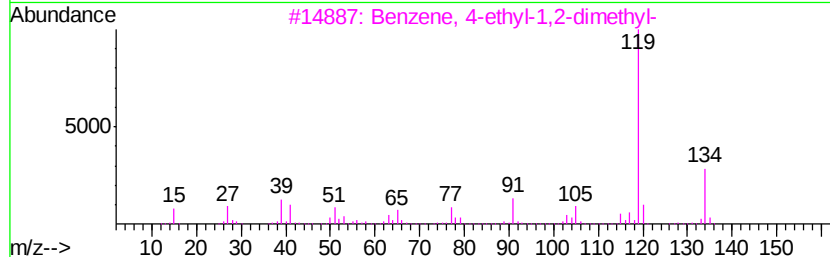
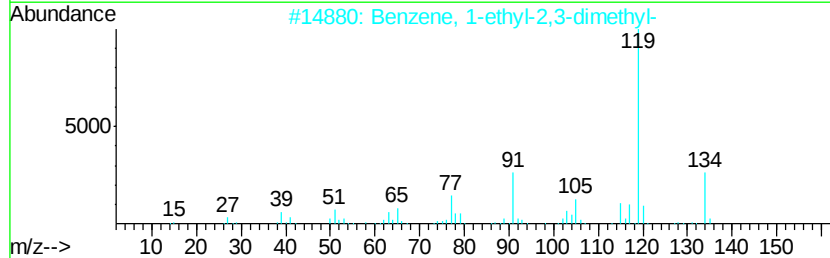
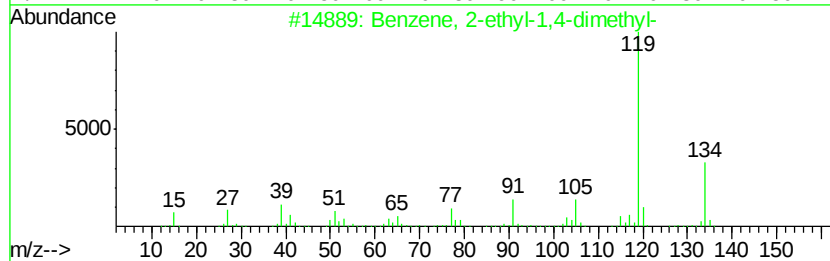
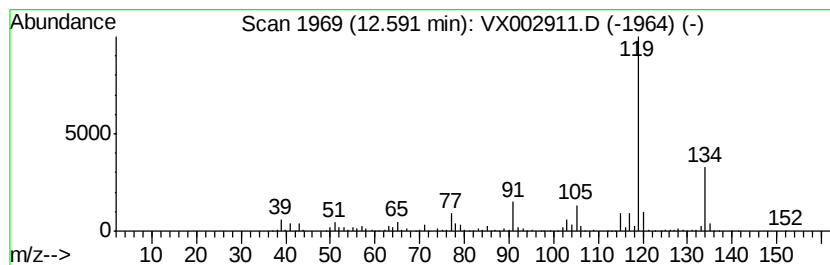
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	7.18 ug/l	191782	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4		o-Cymene	134	C10H14	000527-84-4	95
5		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93



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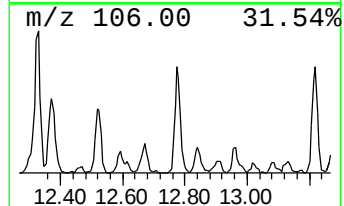
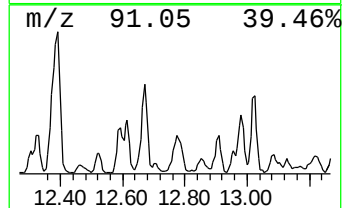
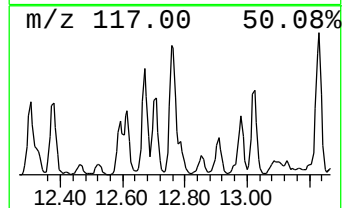
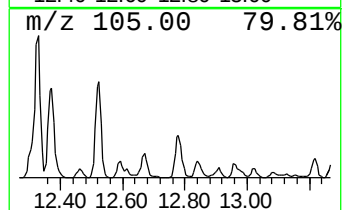
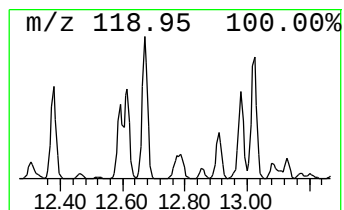
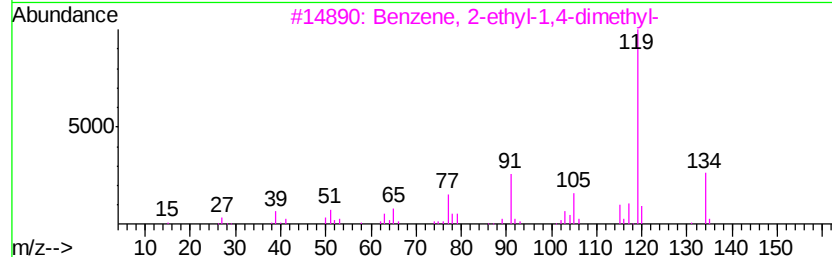
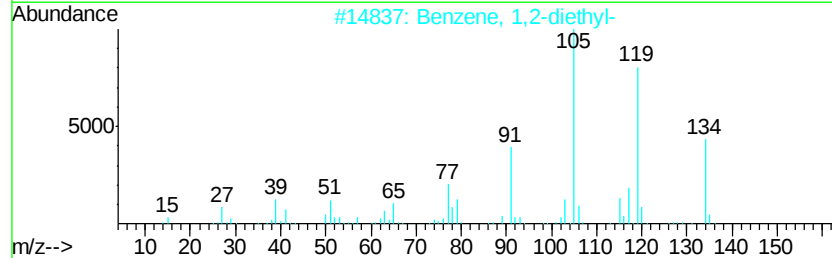
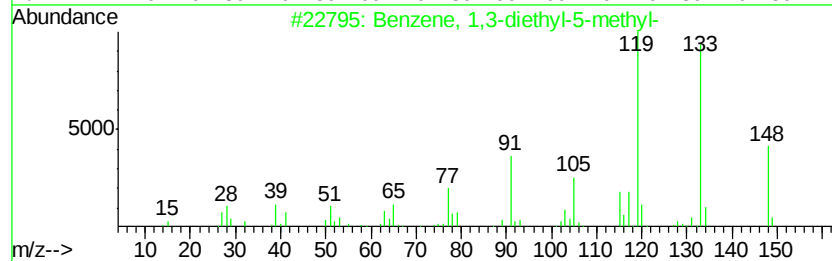
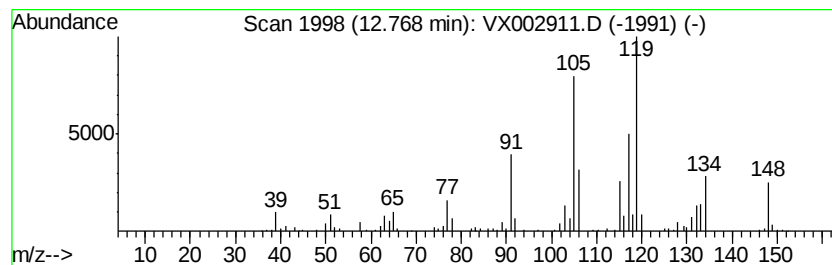
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,3-diethyl-5-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	7.09 ug/l	189535	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	76
2		Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	62
3		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	53
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	49
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
Data File : VX002911.D
Acq On : 26 Jun 2018 23:17
Operator : JC/MD
Sample : J3707-05 50X
Misc : 5.49g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
WP021SB488-29-31-180622

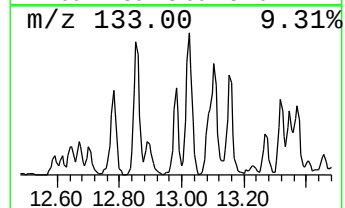
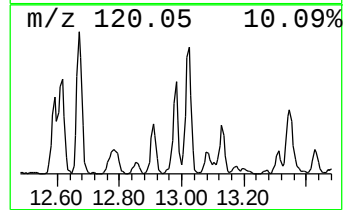
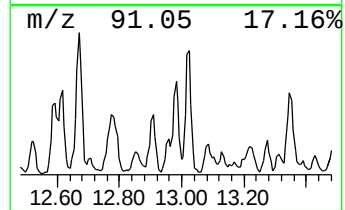
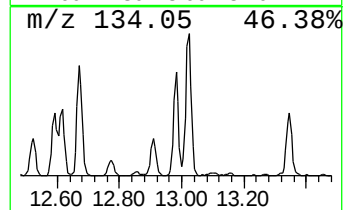
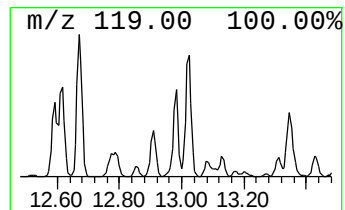
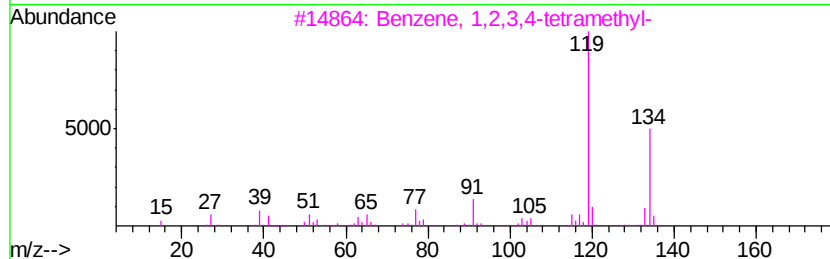
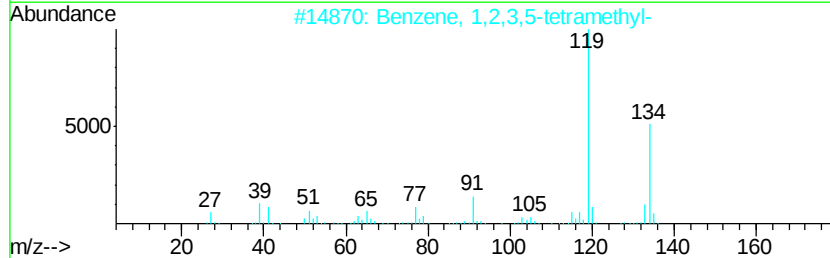
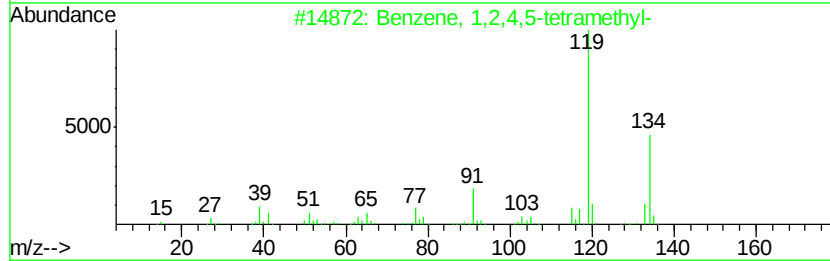
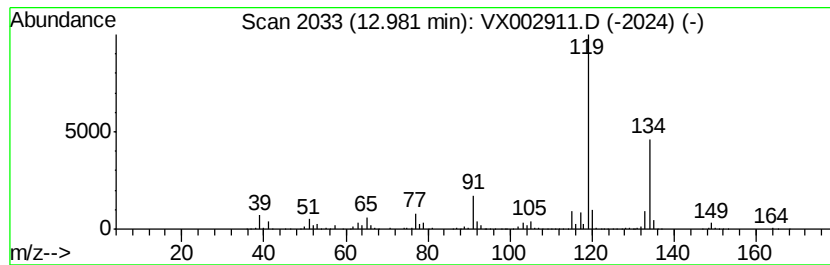
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	8.84 ug/l	236197	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062618\
Data File : VX002911.D
Acq On : 26 Jun 2018 23:17
Operator : JC/MD
Sample : J3707-05 50X
Misc : 5.49g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-29-31-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.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
Mesitylene	12.15	12.1	ug/l	322567	4	12.09	1335940	50.0
Benzene, 1-methyl...	12.32	7.8	ug/l	208570	4	12.09	1335940	50.0
Undecane	12.48	22.0	ug/l	588822	4	12.09	1335940	50.0
Benzene, 2-ethyl...	12.59	7.2	ug/l	191782	4	12.09	1335940	50.0
Benzene, 1,3-diet...	12.77	7.1	ug/l	189535	4	12.09	1335940	50.0
Benzene, 1,2,4,5...	12.98	8.8	ug/l	236197	4	12.09	1335940	50.0