

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
 Data File : VX021574.D
 Acq On : 29 Mar 2021 14:05
 Operator : JC/MD
 Sample : M1785-15 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

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\82X032421W.M
 Title : SW846 8260

Signal : TIC: VX021574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	732	744	756	rBV2	50475	140945	17.63%	3.065%
2	5.623	759	771	784	rBV2	71409	199371	24.93%	4.336%
3	6.029	829	840	853	rBV	54079	141462	17.69%	3.077%
4	6.829	966	976	987	rBV	122593	287708	35.98%	6.257%
5	8.694	1286	1293	1311	rBV	263671	405649	50.73%	8.822%
6	10.094	1525	1531	1541	rBV	285099	386685	48.35%	8.410%
7	10.235	1549	1555	1564	rBV	43214	59765	7.47%	1.300%
8	10.341	1564	1573	1580	rBV	25587	37801	4.73%	0.822%
9	11.000	1679	1685	1690	rBV	44366	55732	6.97%	1.212%
10	11.118	1700	1705	1711	rBV	247229	315553	39.46%	6.863%
11	11.341	1737	1743	1751	rBV	72259	90329	11.30%	1.965%
12	11.418	1751	1756	1757	rBV	23903	27343	3.42%	0.595%
13	11.435	1757	1759	1763	rVV	27149	32628	4.08%	0.710%
14	11.488	1763	1768	1773	rVB	17267	21354	2.67%	0.464%
15	11.653	1791	1796	1803	rBV	29935	41075	5.14%	0.893%
16	11.753	1808	1813	1815	rVV	8584	12839	1.61%	0.279%
17	11.788	1815	1819	1830	rVB	683544	799686	100.00%	17.392%
18	11.900	1830	1838	1840	rBV	11205	15690	1.96%	0.341%
19	11.930	1840	1843	1848	rVB	24039	29400	3.68%	0.639%
20	12.059	1860	1865	1871	rVV	318553	392708	49.11%	8.541%
21	12.124	1871	1876	1885	rVB	304760	371990	46.52%	8.090%
22	12.218	1885	1892	1897	rVB	13337	17695	2.21%	0.385%
23	12.283	1897	1903	1910	rBV	109418	137783	17.23%	2.997%
24	12.353	1910	1915	1923	rVB2	23116	44864	5.61%	0.976%
25	12.441	1925	1930	1936	rBV	16699	20434	2.56%	0.444%
26	12.500	1936	1940	1947	rVB	9759	11662	1.46%	0.254%
27	12.571	1947	1952	1954	rBV	31589	44252	5.53%	0.962%
28	12.594	1954	1956	1960	rVB	31430	30298	3.79%	0.659%
29	12.653	1960	1966	1969	rBV	53339	67129	8.39%	1.460%
30	12.683	1969	1971	1976	rVB	22233	23905	2.99%	0.520%
31	12.742	1976	1981	1988	rBV2	50895	85828	10.73%	1.867%
32	12.883	2000	2005	2010	rVB2	21427	30069	3.76%	0.654%
33	12.959	2010	2018	2022	rVV	26959	38685	4.84%	0.841%
34	13.000	2022	2025	2031	rVV	35921	41800	5.23%	0.909%
35	13.330	2076	2081	2087	rVB2	41040	59896	7.49%	1.303%
36	13.459	2098	2103	2108	rVB	25951	33274	4.16%	0.724%

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MW-4

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\82X032421W.M
Title : SW846 8260

37	13.812	2157	2163	2171	rVB	33509	44679	5.59%	0.972%
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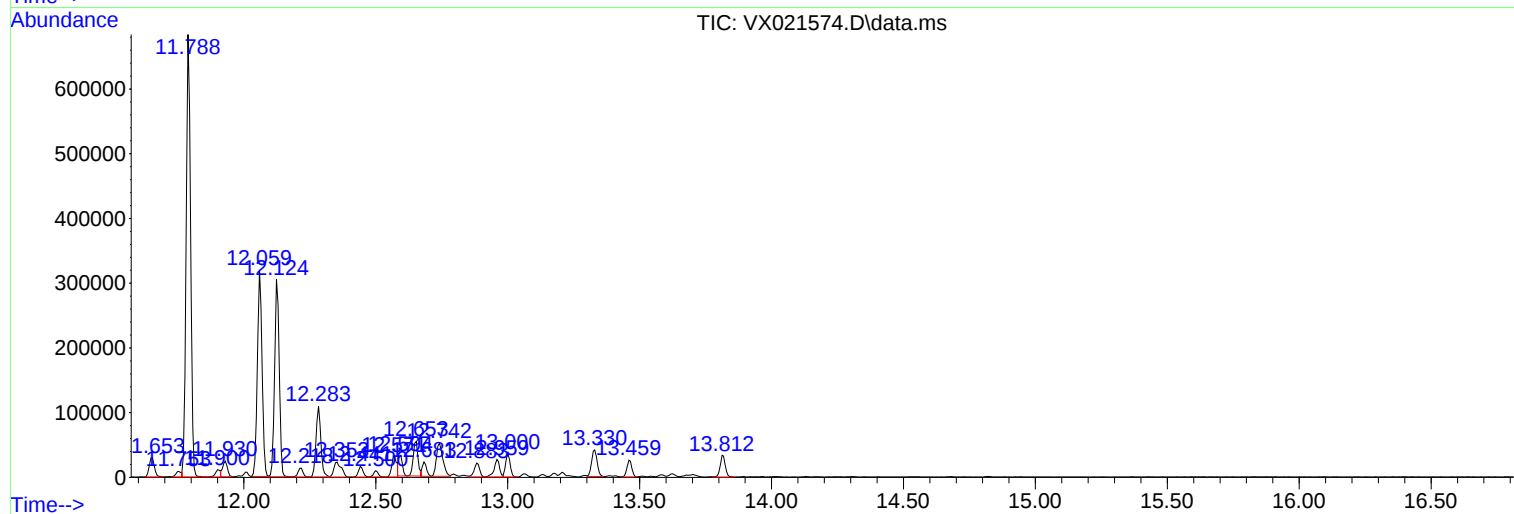
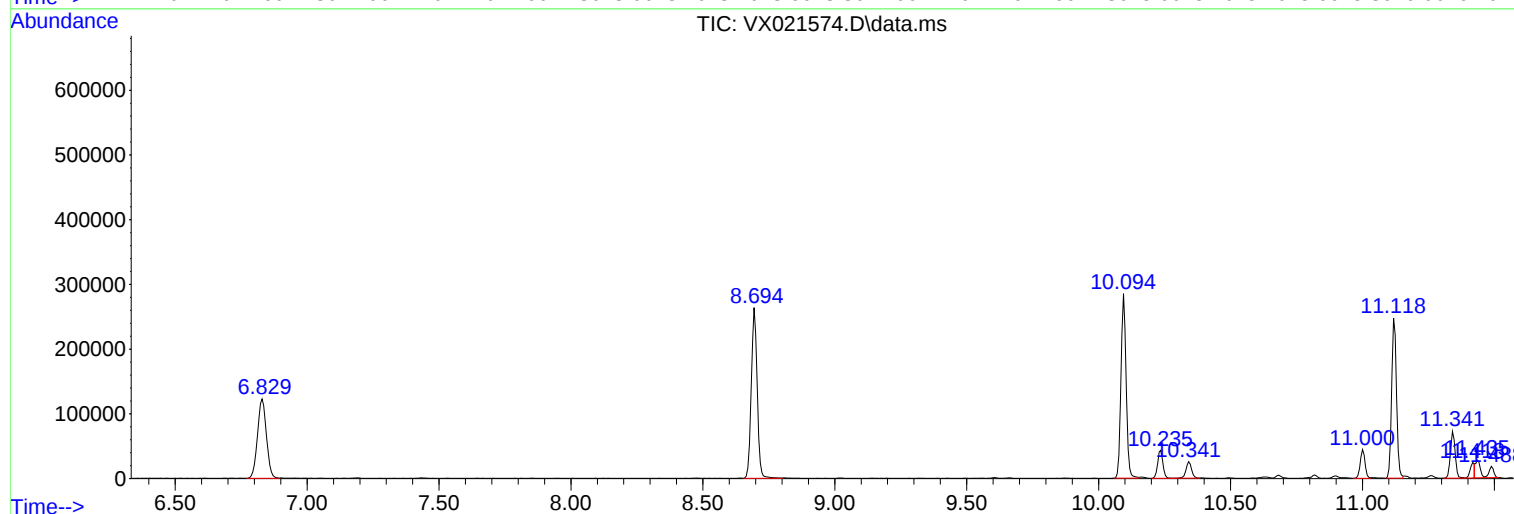
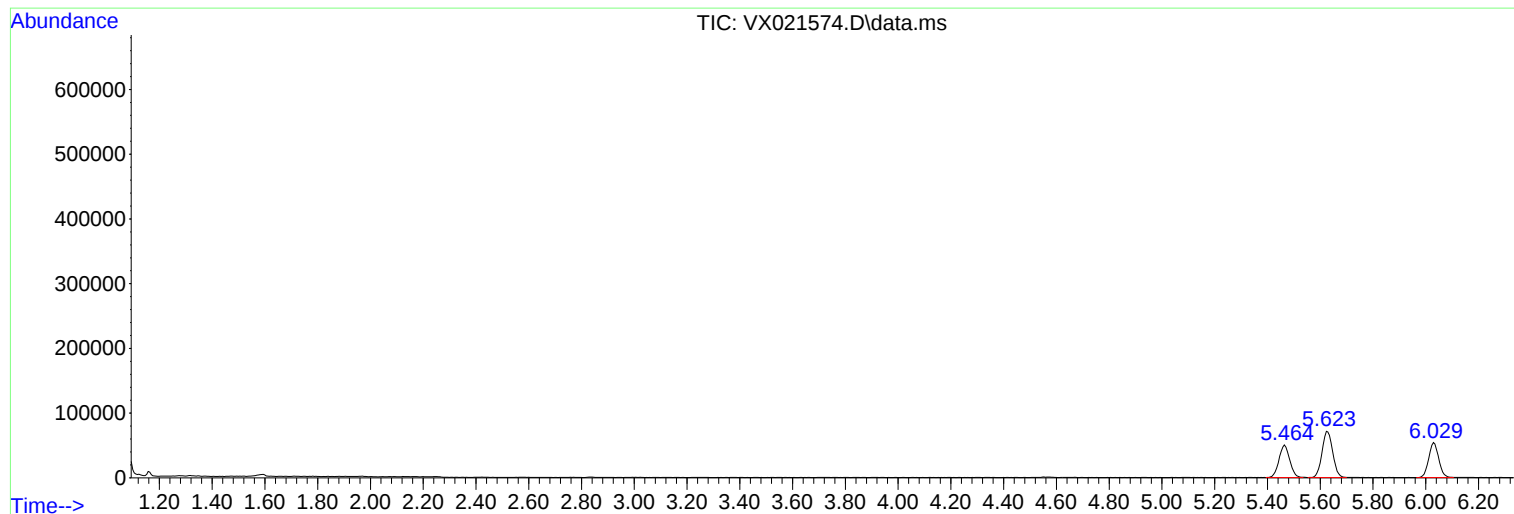
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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



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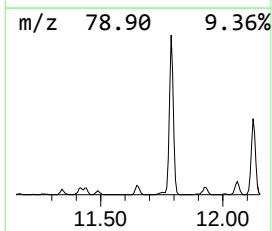
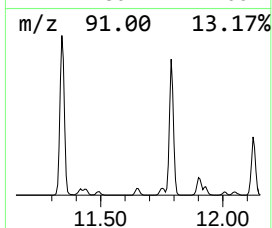
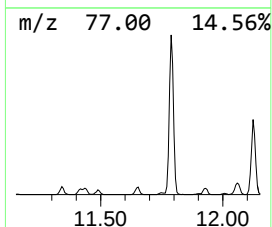
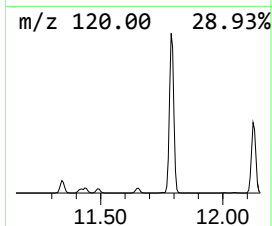
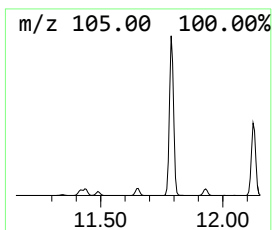
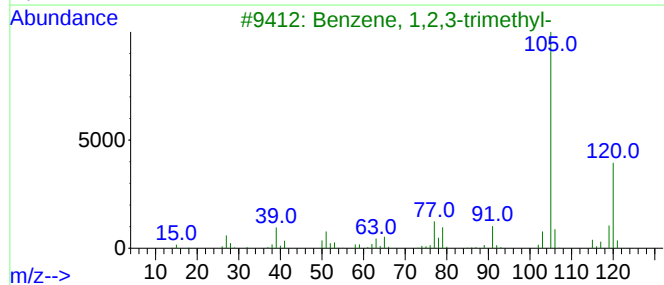
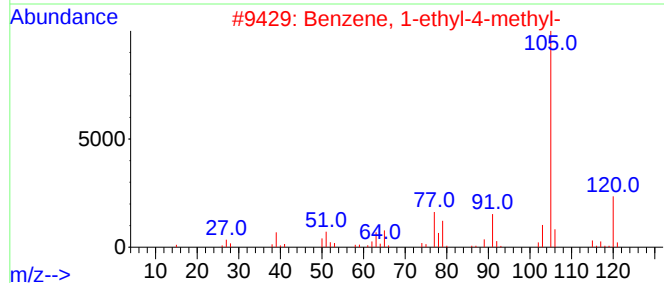
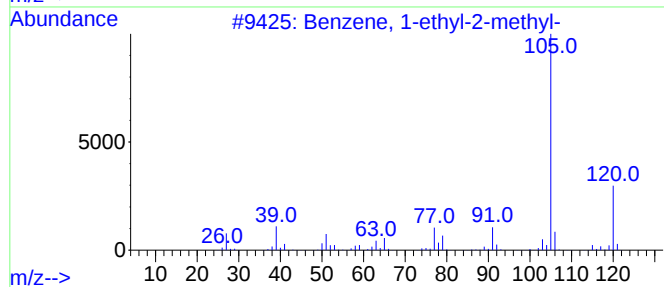
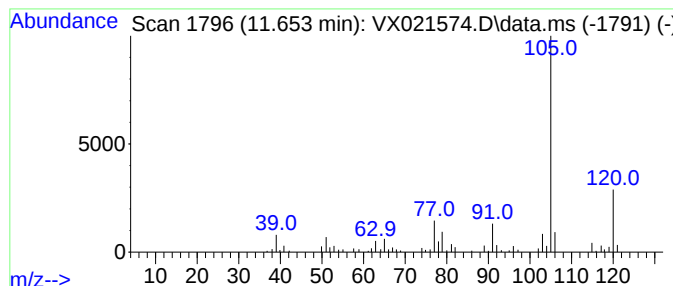
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.653	5.23 ug/l	41075	1,4-Dichlorobenzene-d4	12.059

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-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Instrument :
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ClientSampleId :
MW-4

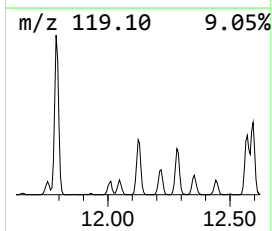
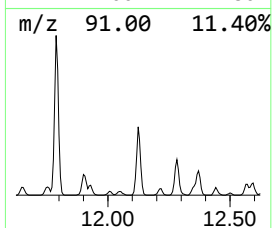
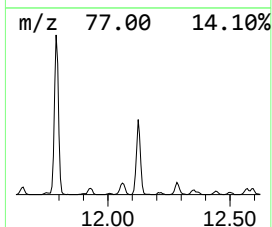
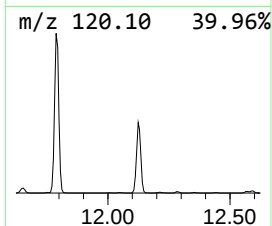
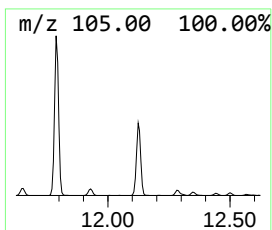
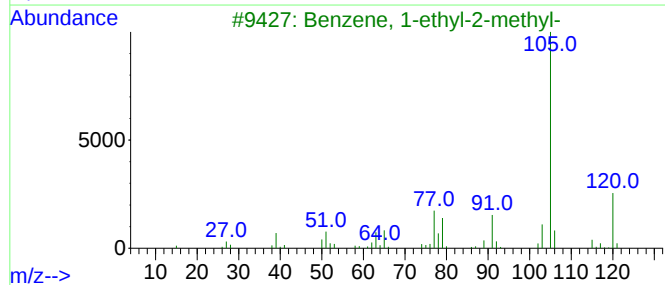
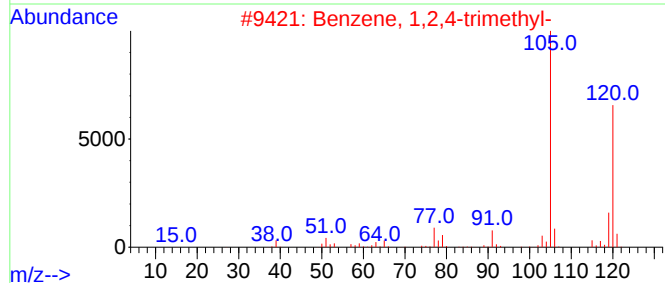
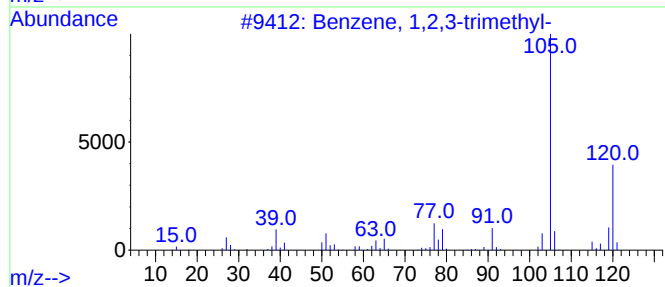
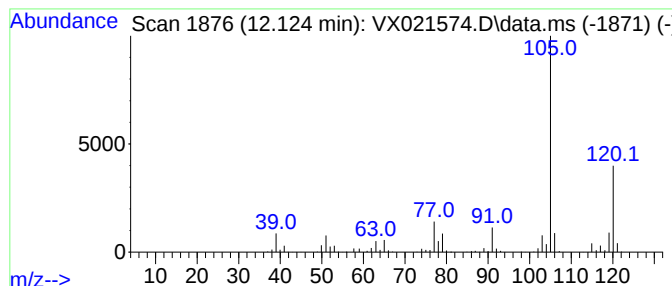
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Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.124	47.36 ug/l	371990	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

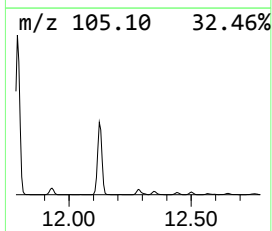
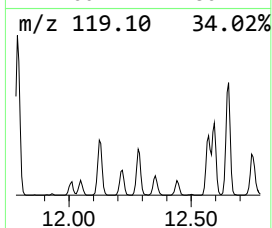
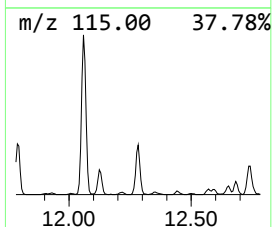
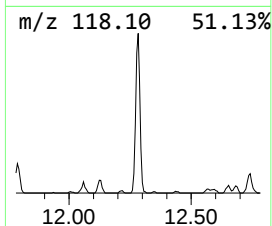
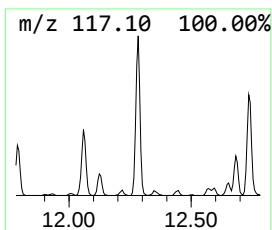
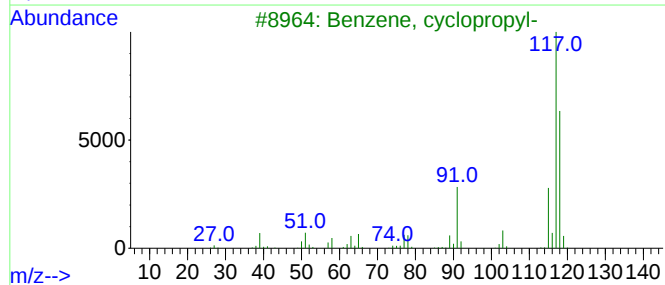
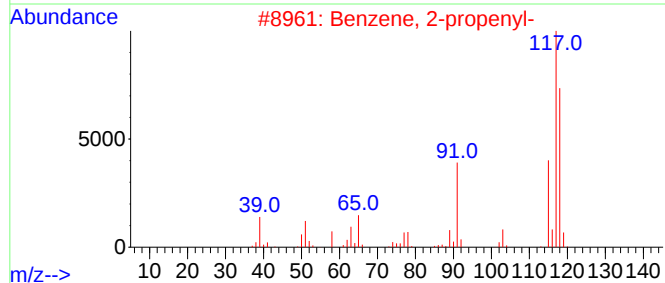
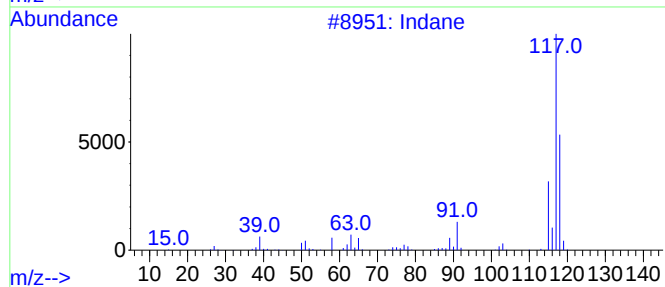
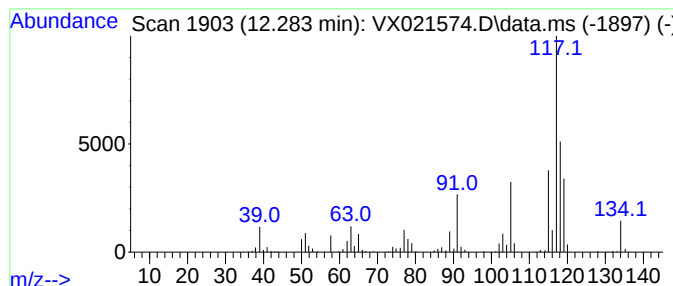
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.283	17.54 ug/l	137783	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	92
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	60



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Instrument :
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ClientSampleId :
MW-4

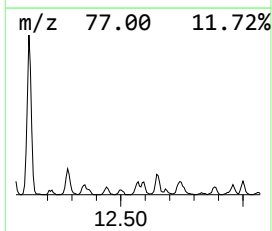
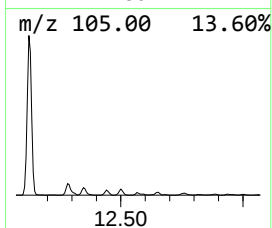
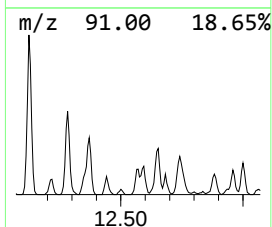
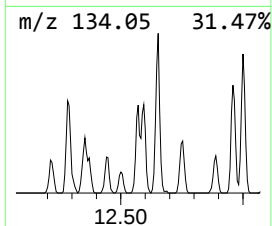
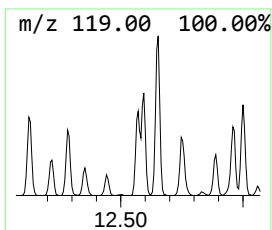
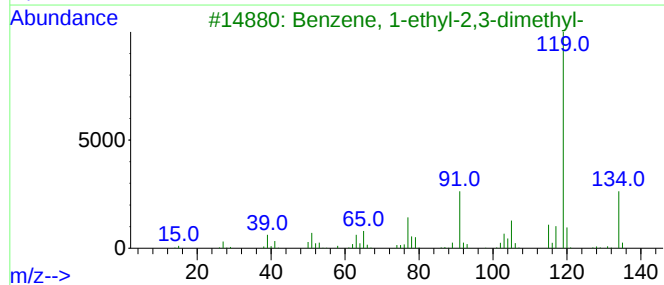
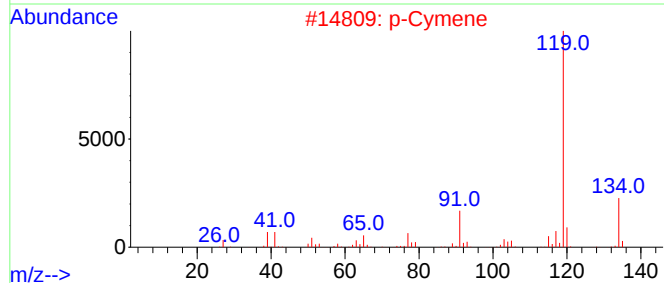
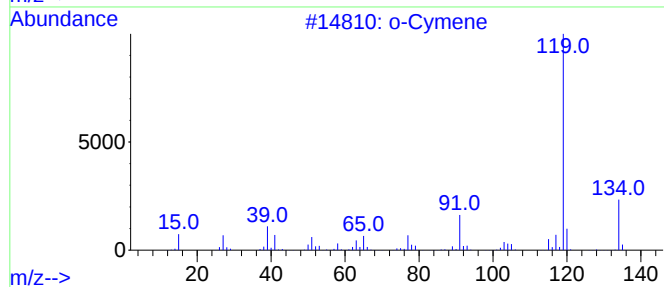
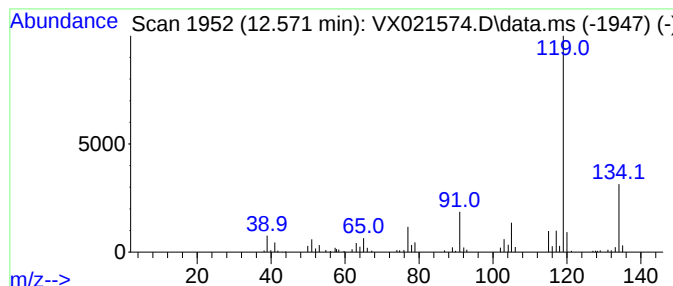
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Quant Title : SW846 8260

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

Peak Number 4 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.571	5.63 ug/l	44252	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			p-Cymene	134	C10H14	000099-87-6	97
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96



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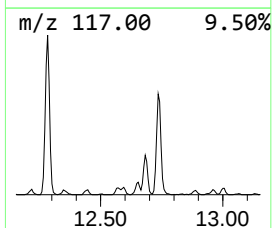
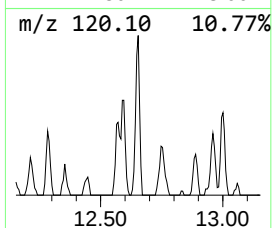
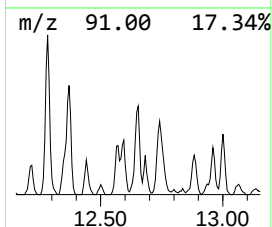
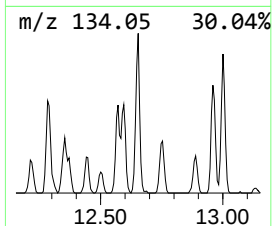
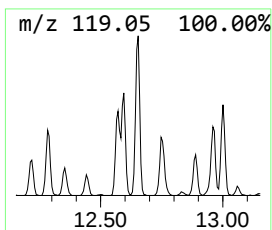
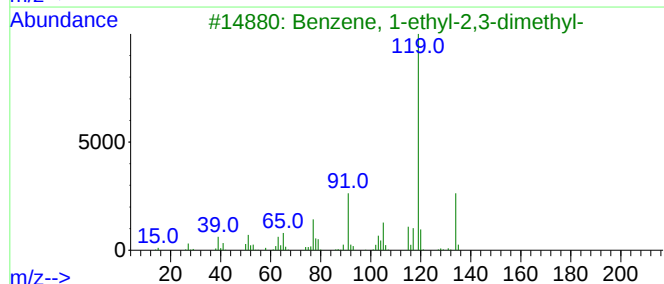
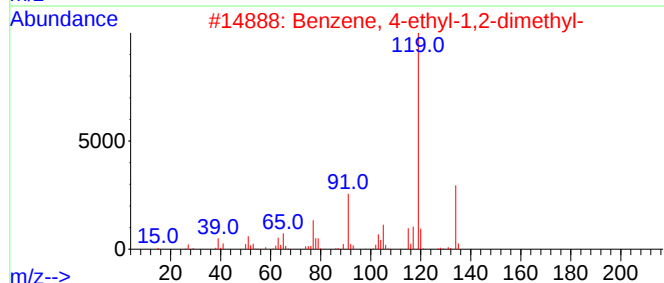
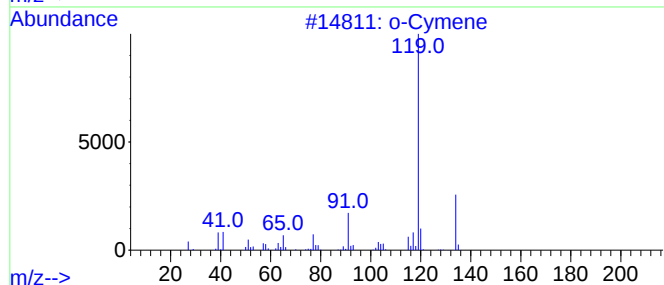
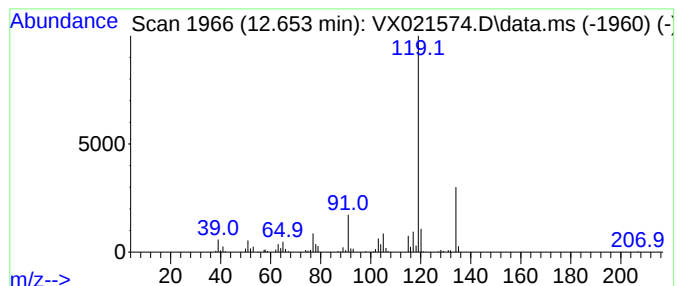
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.653	8.55 ug/l	67129	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021574.D
Acq On : 29 Mar 2021 14:05
Operator : JC/MD
Sample : M1785-15 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

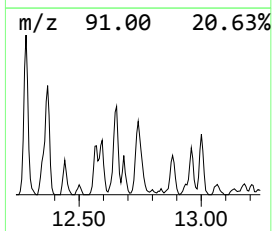
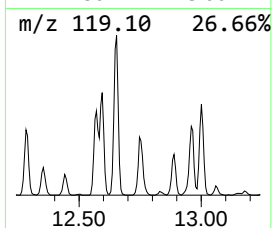
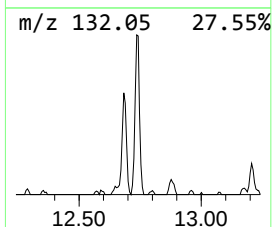
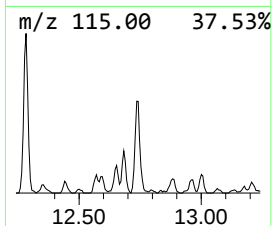
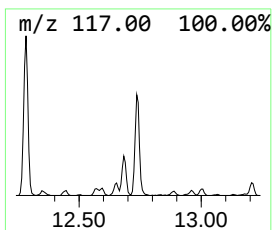
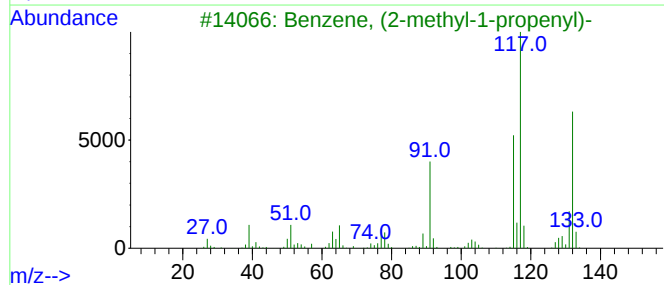
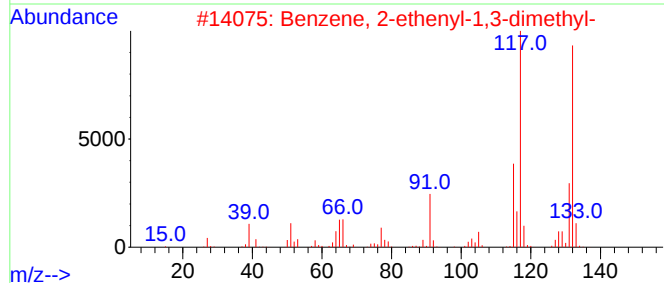
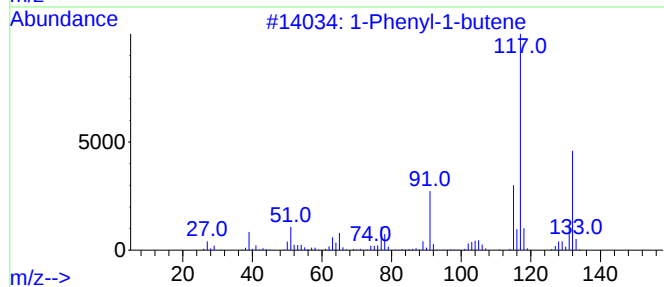
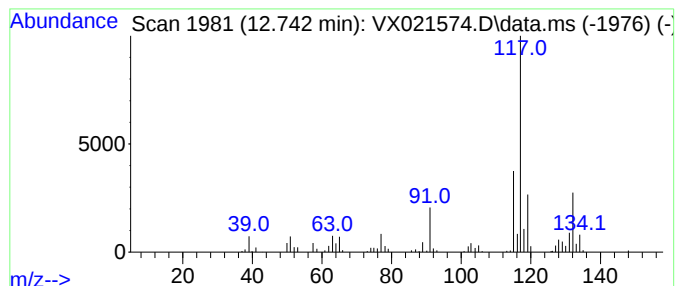
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Quant Title : SW846 8260

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

Peak Number 6 1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.742	10.93 ug/l	85828	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	81
2			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	81
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
4			Indan, 1-methyl-	132	C10H12	000767-58-8	81
5			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021574.D
Acq On : 29 Mar 2021 14:05
Operator : JC/MD
Sample : M1785-15 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

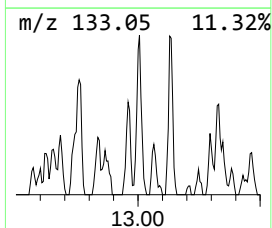
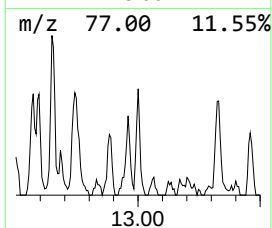
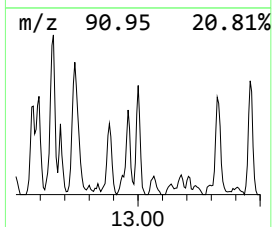
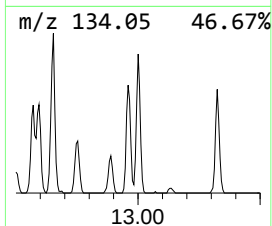
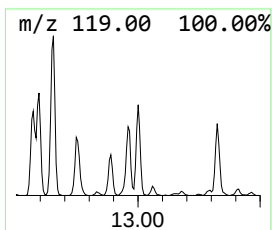
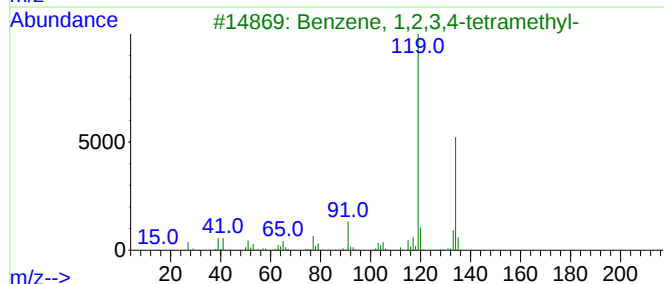
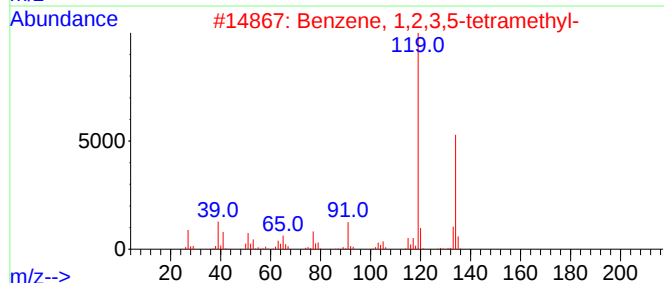
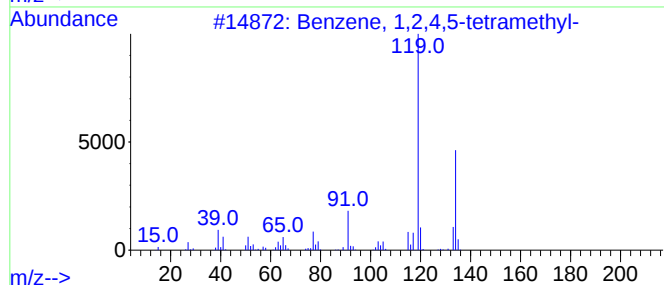
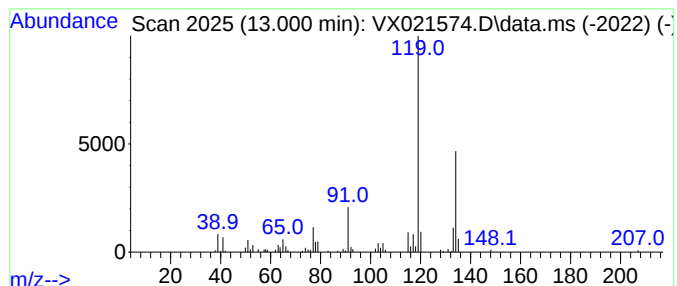
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	5.32 ug/l	41800	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
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	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021574.D
Acq On : 29 Mar 2021 14:05
Operator : JC/MD
Sample : M1785-15 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

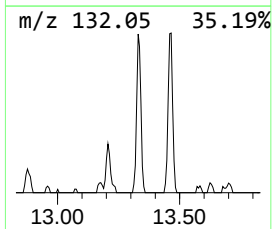
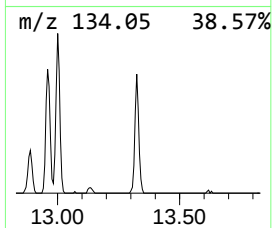
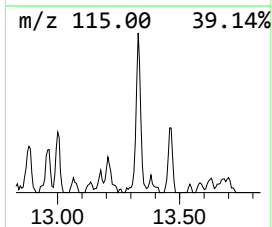
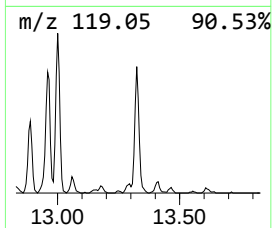
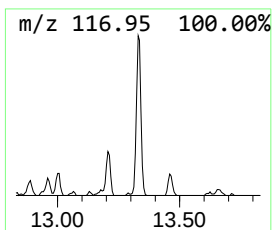
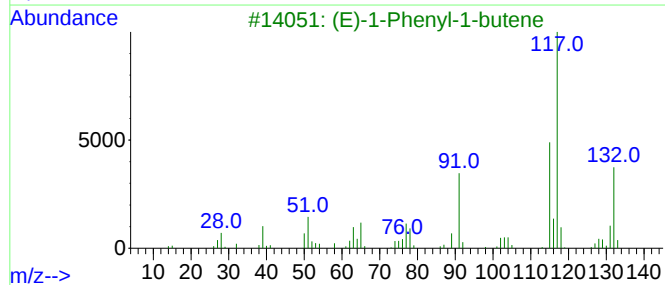
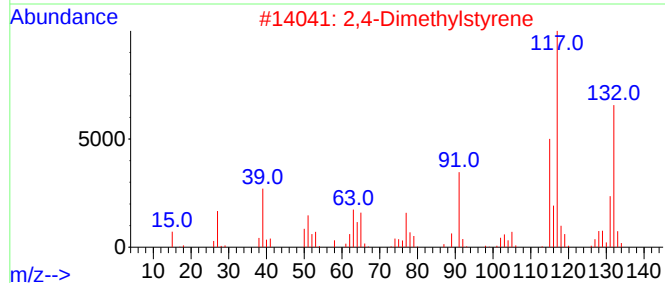
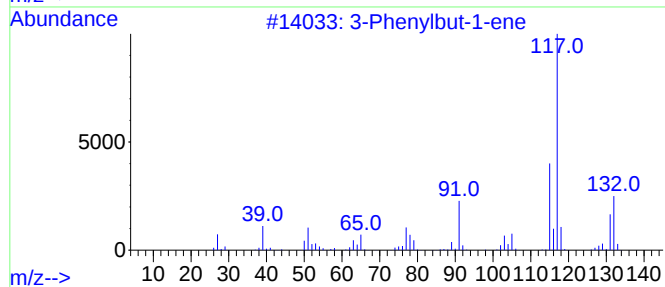
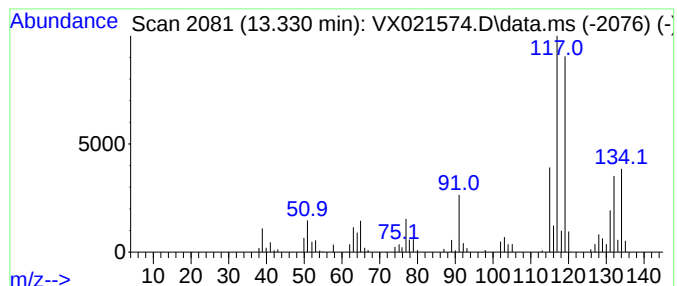
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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

Peak Number 8 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	7.63 ug/l	59896	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	80
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	70
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	64
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032921\
Data File : VX021574.D
Acq On : 29 Mar 2021 14:05
Operator : JC/MD
Sample : M1785-15 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.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
Benzene, 1-ethy...	11.653	5.2	ug/l	41075	4	12.059	392708	50.0
Benzene, 1,2,3-...	12.124	47.4	ug/l	371990	4	12.059	392708	50.0
Indane	12.283	17.5	ug/l	137783	4	12.059	392708	50.0
o-Cymene	12.571	5.6	ug/l	44252	4	12.059	392708	50.0
Benzene, 4-ethy...	12.653	8.6	ug/l	67129	4	12.059	392708	50.0
1-Phenyl-1-butene	12.742	10.9	ug/l	85828	4	12.059	392708	50.0
Benzene, 1,2,4,...	13.000	5.3	ug/l	41800	4	12.059	392708	50.0
3-Phenylbut-1-ene	13.330	7.6	ug/l	59896	4	12.059	392708	50.0