

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
 Data File : VX043317.D
 Acq On : 08 Oct 2024 11:40
 Operator : JC/MD
 Sample : P4342-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PORT-ELIZABETH-1201

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\82X100124W.M
 Title : SW846 8260

Signal : TIC: VX043317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.617	71	87	90	rBV	5764	24354	4.35%	0.315%
2	2.392	207	214	224	rBV	13290	24416	4.36%	0.316%
3	5.385	693	705	720	rBV2	54864	160626	28.70%	2.076%
4	5.550	720	732	752	rVV	86009	248376	44.37%	3.211%
5	5.952	790	798	816	rBV	64373	172969	30.90%	2.236%
6	6.757	921	930	945	rBV	143462	348675	62.29%	4.507%
7	7.811	1097	1103	1115	rBV	4438	10205	1.82%	0.132%
8	8.647	1234	1240	1258	rBV	293751	471586	84.25%	6.096%
9	10.055	1465	1471	1486	rBV	281312	399363	71.35%	5.162%
10	10.195	1489	1494	1501	rBV	42344	59989	10.72%	0.775%
11	10.299	1505	1511	1526	rVV	230208	315746	56.41%	4.082%
12	10.640	1562	1567	1577	rBV	154752	201418	35.98%	2.604%
13	11.024	1625	1630	1635	rBV	110181	160460	28.67%	2.074%
14	11.079	1635	1639	1651	rVB	234863	304826	54.46%	3.940%
15	11.305	1671	1676	1683	rBV	18898	23861	4.26%	0.308%
16	11.378	1683	1688	1696	rVV	120083	199630	35.66%	2.581%
17	11.451	1696	1700	1707	rVB	84050	103463	18.48%	1.337%
18	11.610	1722	1726	1731	rBV	75538	95378	17.04%	1.233%
19	11.658	1731	1734	1740	rVB2	5699	8655	1.55%	0.112%
20	11.750	1744	1749	1757	rBV	411632	504200	90.08%	6.518%
21	11.890	1770	1772	1779	rVB2	5048	5619	1.00%	0.073%
22	11.969	1779	1785	1788	rBV	21892	26750	4.78%	0.346%
23	12.018	1788	1793	1799	rVV	269320	356685	63.72%	4.611%
24	12.085	1799	1804	1811	rVB	256866	318624	56.92%	4.119%
25	12.244	1823	1830	1833	rBV	136757	194929	34.82%	2.520%
26	12.268	1833	1834	1838	rVV	57517	43430	7.76%	0.561%
27	12.317	1838	1842	1852	rVB2	114858	158387	28.30%	2.047%
28	12.408	1852	1857	1862	rBV3	13493	20157	3.60%	0.261%
29	12.463	1862	1866	1872	rVB	31820	38327	6.85%	0.495%
30	12.530	1872	1877	1879	rBV	103303	133975	23.94%	1.732%
31	12.554	1879	1881	1886	rVV	89538	96251	17.20%	1.244%
32	12.609	1886	1890	1895	rVB	183158	215114	38.43%	2.781%
33	12.713	1900	1907	1913	rVB2	25603	50707	9.06%	0.655%
34	12.817	1914	1924	1926	rBV4	15999	23377	4.18%	0.302%
35	12.847	1926	1929	1934	rVB	72224	85885	15.34%	1.110%
36	12.920	1934	1941	1944	rBV	174974	205850	36.78%	2.661%

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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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37	12.963	1944	1948	1954	rVB	347669	410076	73.26%	5.301%
38	13.024	1954	1958	1959	rBV	5883	6659	1.19%	0.086%
39	13.067	1963	1965	1968	rVB2	5864	6083	1.09%	0.079%
40	13.170	1975	1982	1986	rBV	99129	128163	22.90%	1.657%
41	13.286	1996	2001	2007	rVB2	411123	559744	100.00%	7.236%
42	13.371	2012	2015	2019	rVB	11329	13451	2.40%	0.174%
43	13.420	2019	2023	2029	rVB2	15014	21420	3.83%	0.277%
44	13.481	2029	2033	2035	rBV	14283	19782	3.53%	0.256%
45	13.591	2045	2051	2057	rVV3	43348	86899	15.52%	1.123%
46	13.676	2060	2065	2070	rVB2	13129	19862	3.55%	0.257%
47	13.774	2076	2081	2092	rVB	408944	500369	89.39%	6.468%
48	13.926	2099	2106	2109	rBV3	4949	7069	1.26%	0.091%
49	14.073	2126	2130	2136	rVB	7076	9234	1.65%	0.119%
50	14.213	2150	2153	2156	rBV2	4810	6374	1.14%	0.082%
51	14.249	2156	2159	2167	rVB	10344	14779	2.64%	0.191%
52	14.639	2217	2223	2229	rBV	6828	9475	1.69%	0.122%
53	15.121	2297	2302	2311	rBV	14969	26868	4.80%	0.347%
54	15.219	2312	2318	2336	rVB	35402	65047	11.62%	0.841%
55	15.499	2358	2364	2370	rVB3	7195	12338	2.20%	0.159%

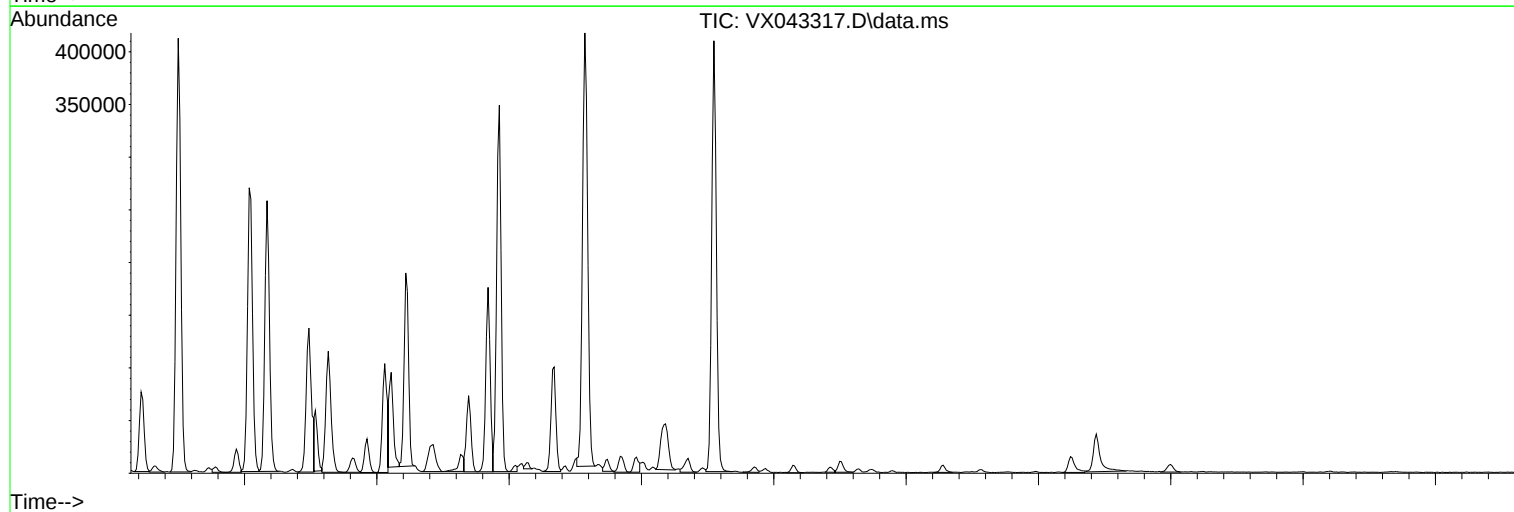
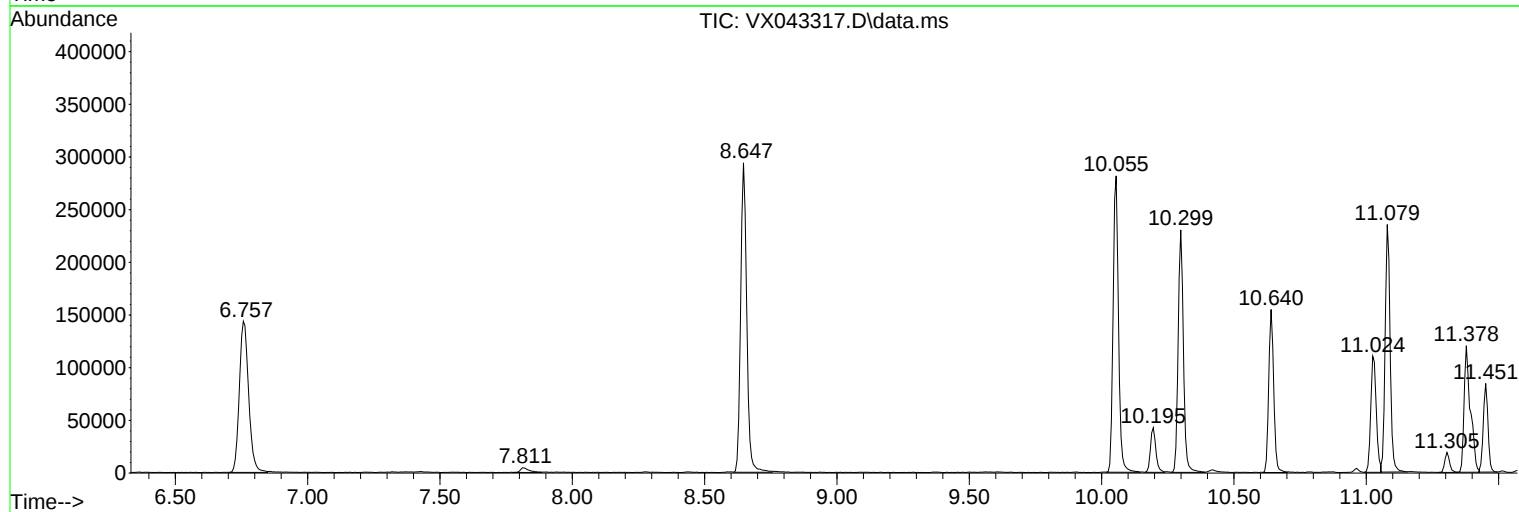
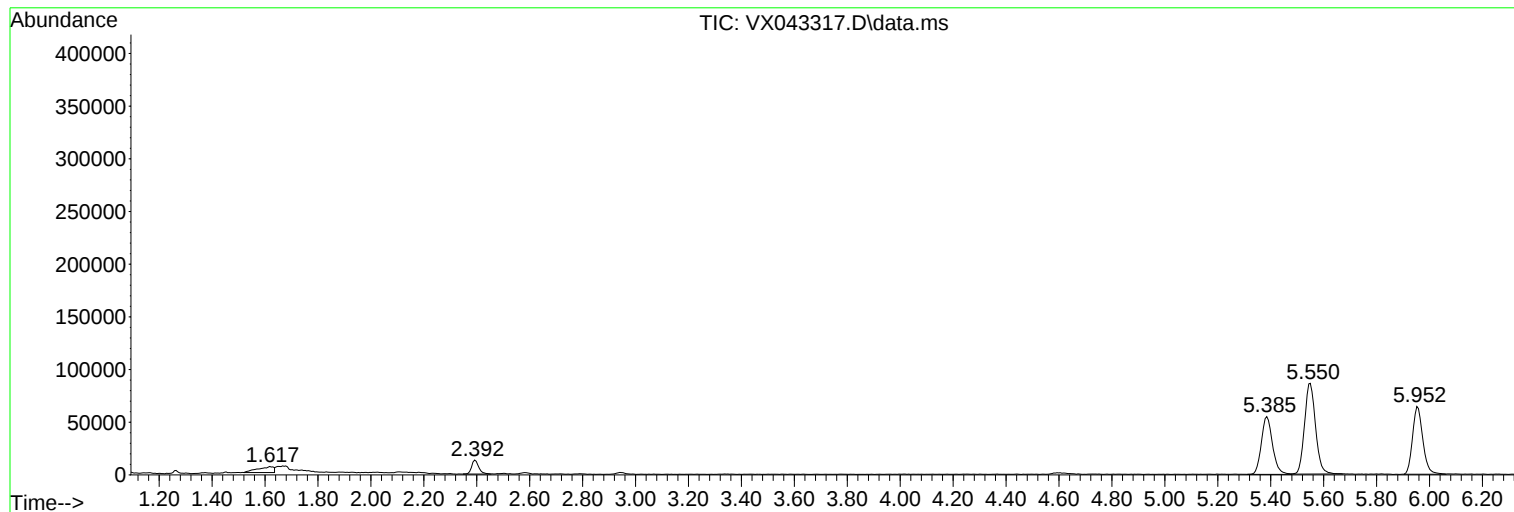
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

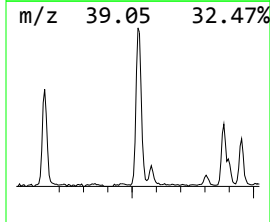
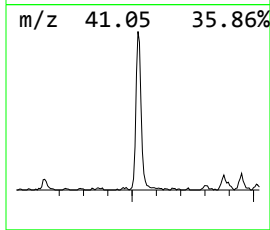
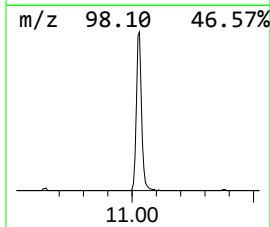
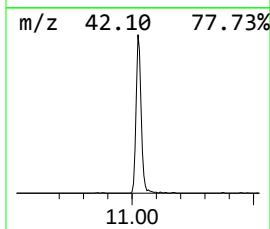
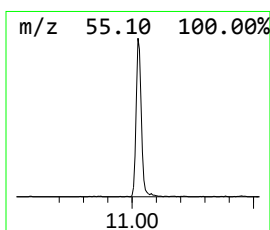
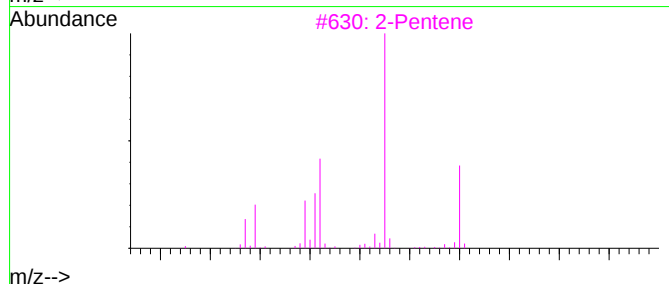
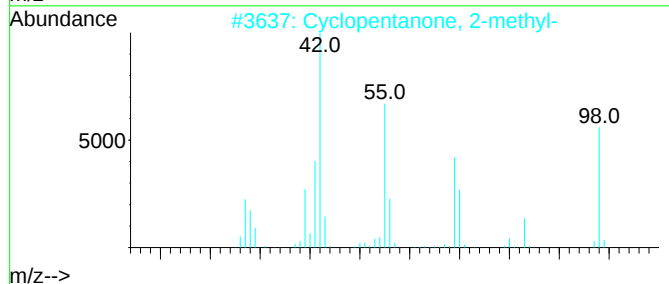
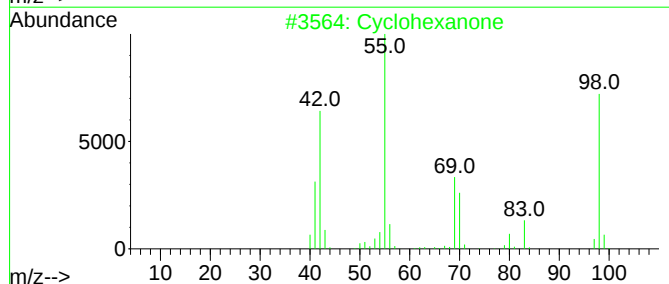
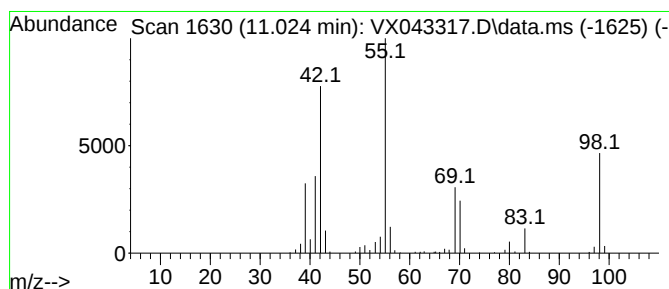
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Quant Title : SW846 8260

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

Peak Number 1 Cyclohexanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.024	20.09 ug/l	160460	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	80
3	2-Pentene	70	C5H10	000109-68-2	46
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	46
5	2-Pentene, (E)-	70	C5H10	000646-04-8	43



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

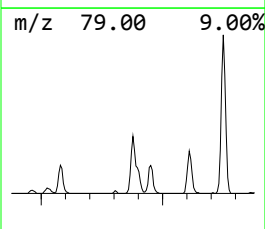
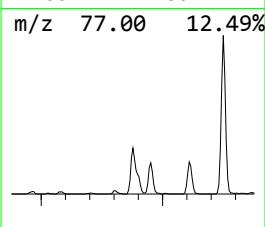
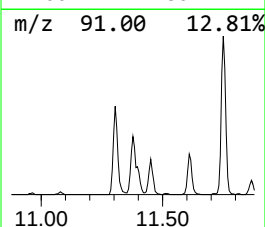
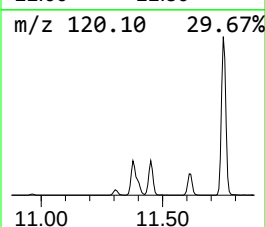
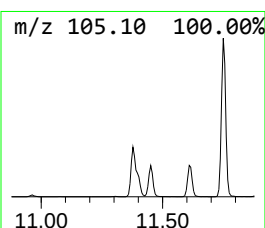
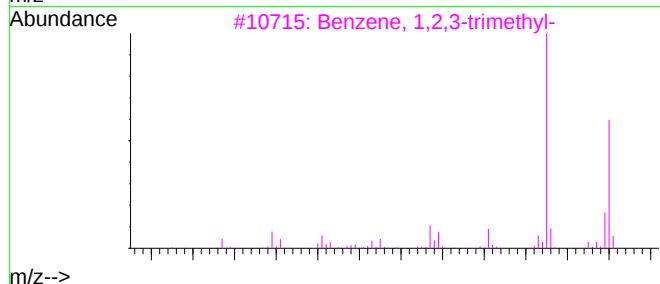
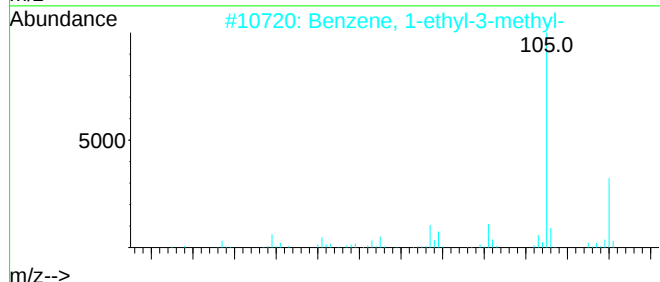
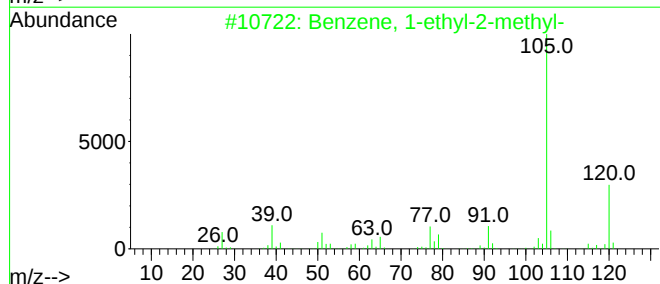
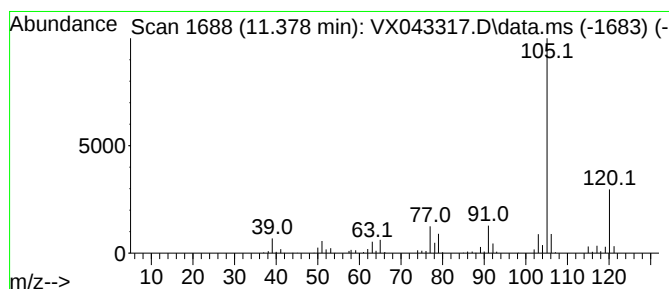
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	27.98 ug/l	199630	1,4-Dichlorobenzene-d4	12.024

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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
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Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

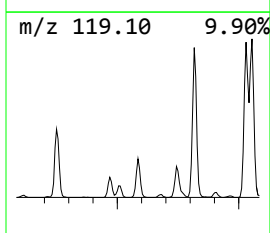
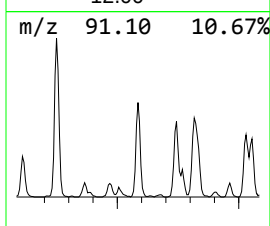
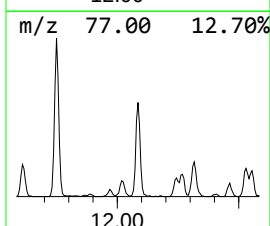
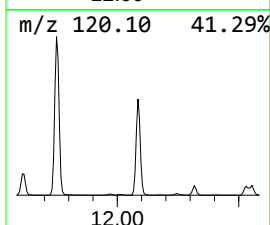
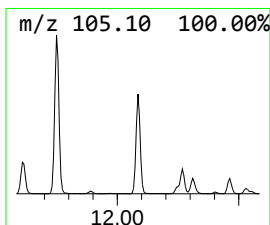
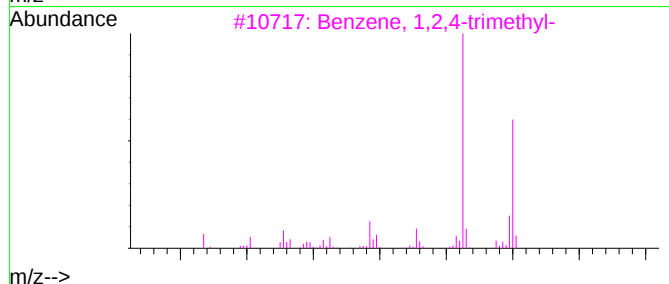
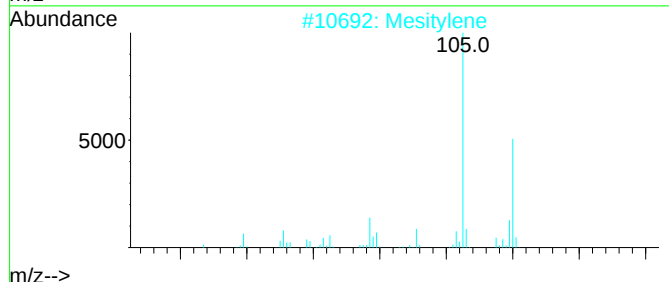
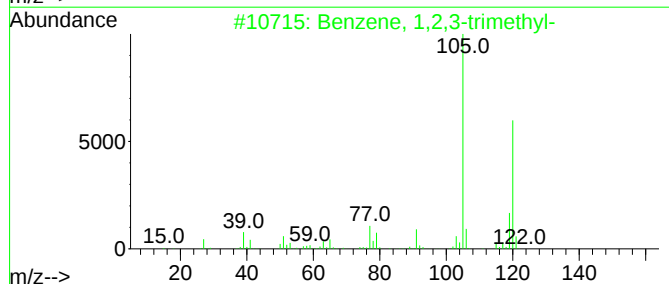
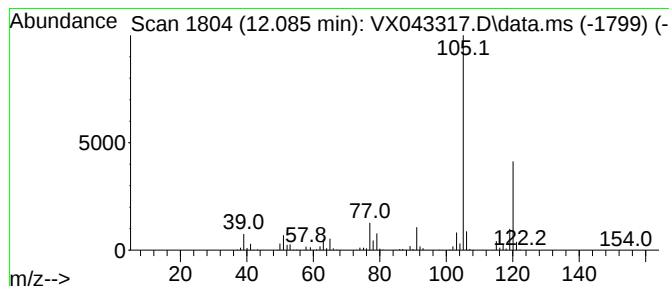
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.085	44.66 ug/l	318624	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-		120	C9H12	000526-73-8	95
2	Mesitylene		120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-		120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-		120	C9H12	000622-96-8	90
5	Benzene, 1-ethyl-3-methyl-		120	C9H12	000620-14-4	90



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Instrument :
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ClientSampleId :
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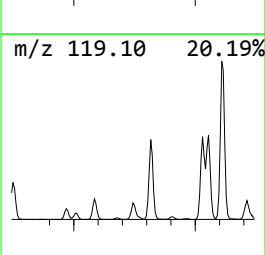
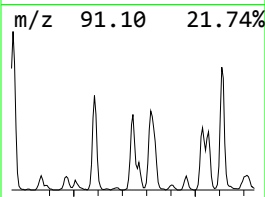
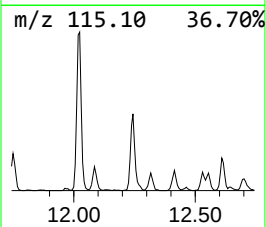
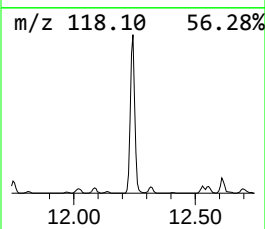
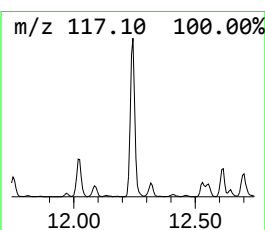
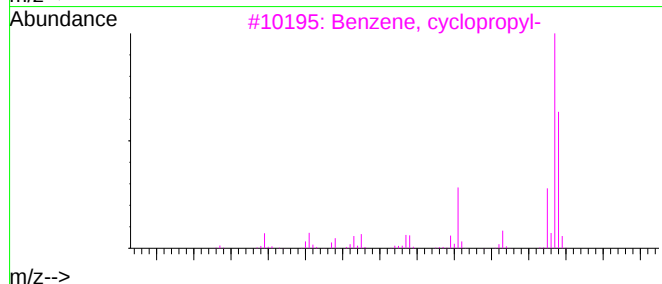
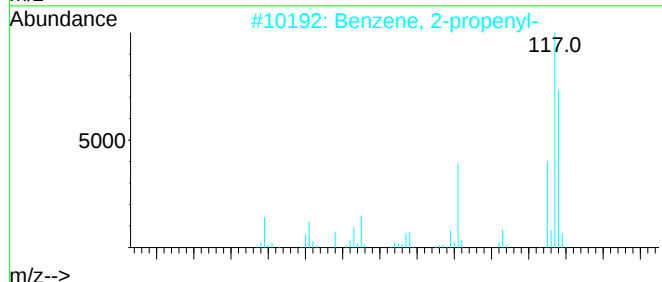
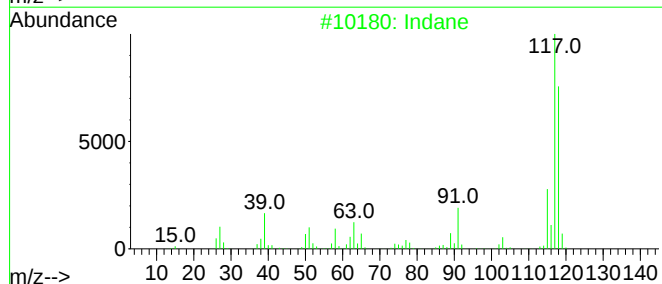
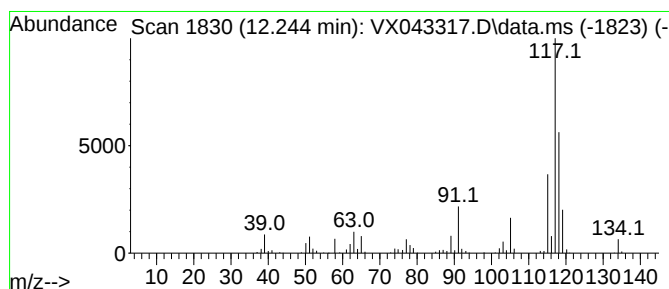
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	27.33 ug/l	194929	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	58



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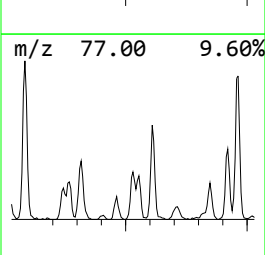
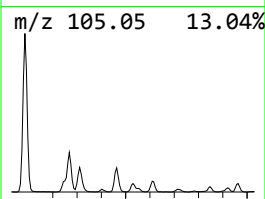
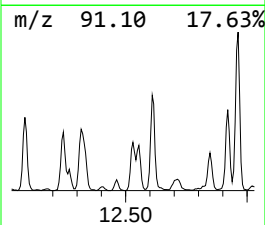
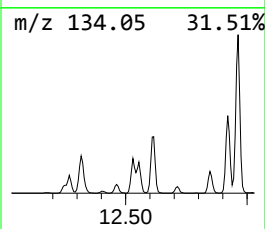
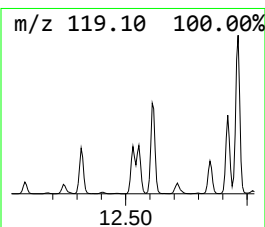
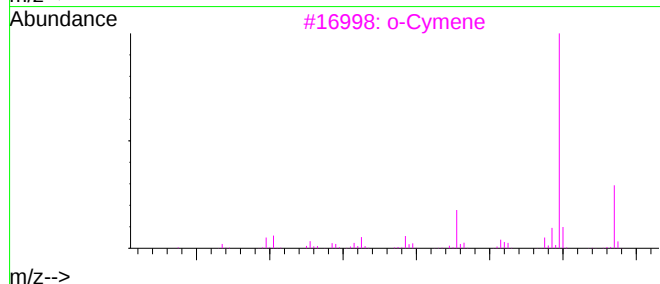
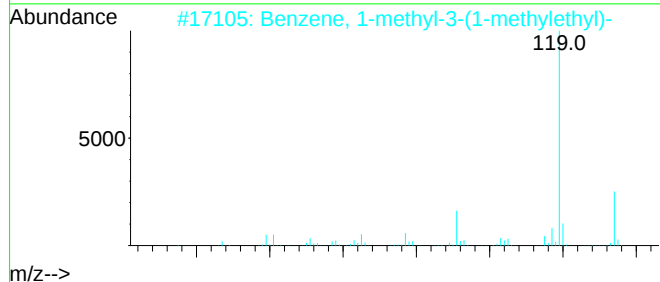
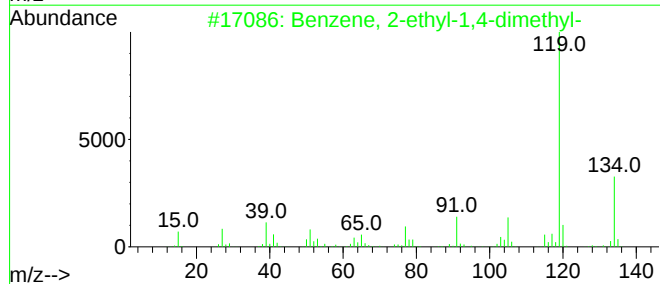
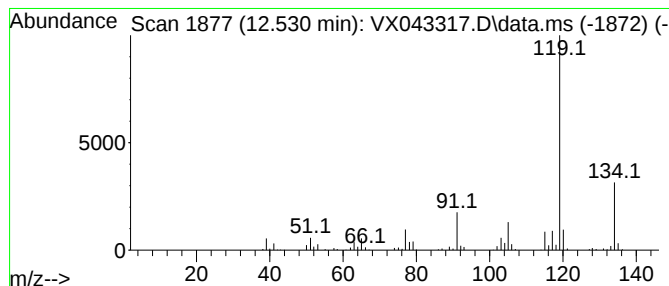
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.530	18.78 ug/l	133975	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
Acq On : 08 Oct 2024 11:40
Operator : JC/MD
Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

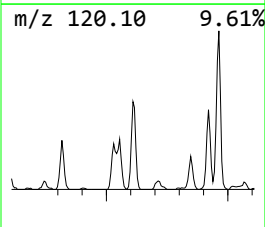
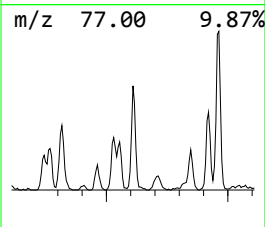
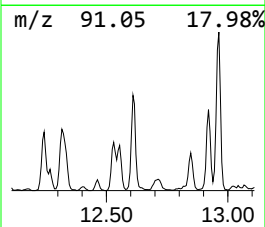
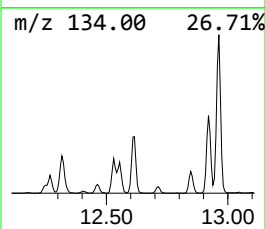
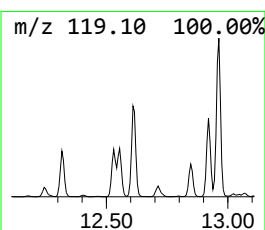
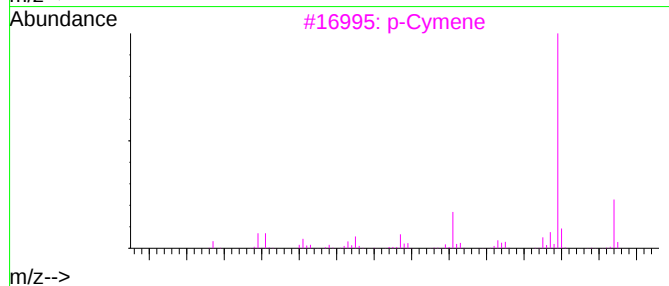
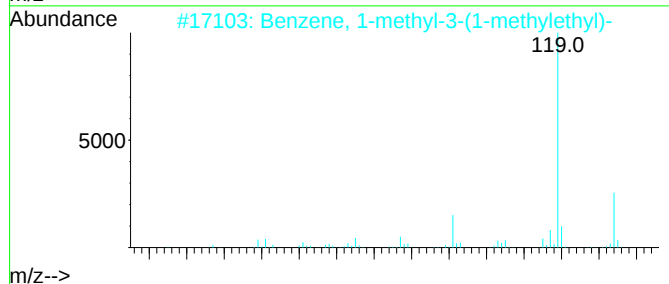
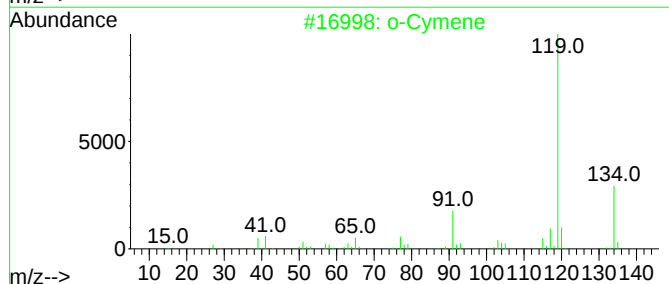
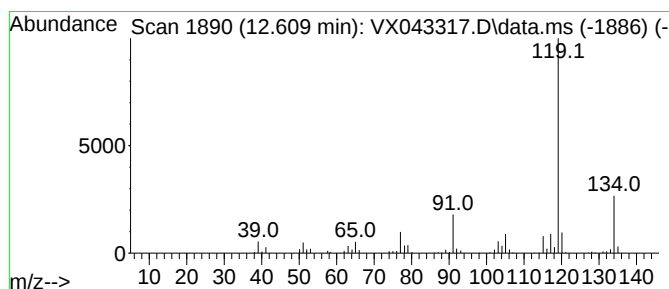
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.609	30.15 ug/l	215114	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	97
3	p-Cymene	134	C10H14	000099-87-6	97
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
Acq On : 08 Oct 2024 11:40
Operator : JC/MD
Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

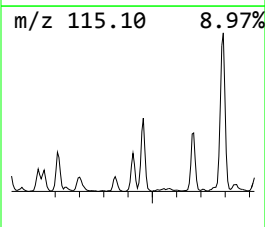
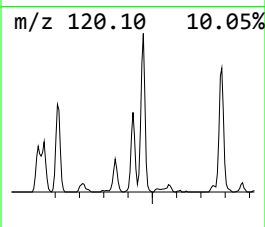
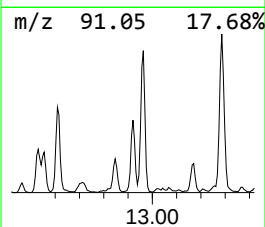
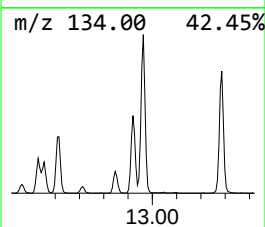
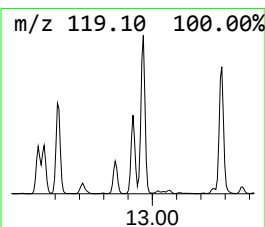
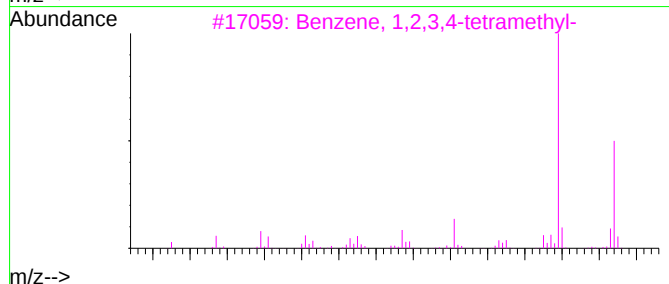
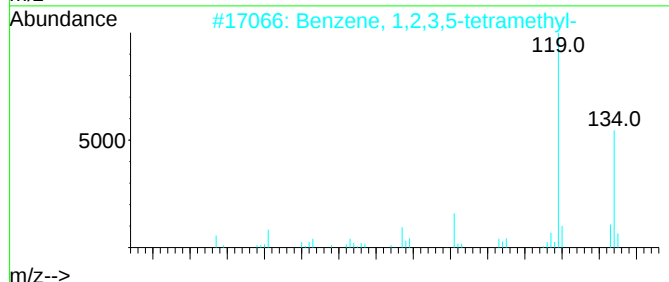
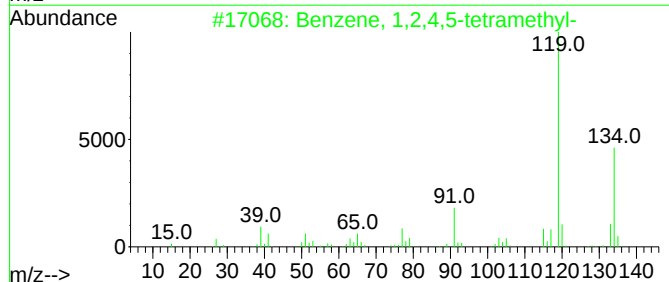
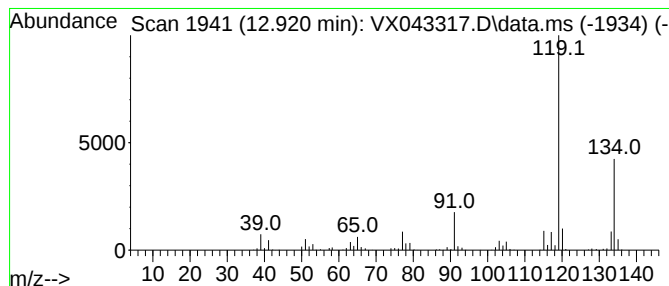
Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.920	28.86 ug/l	205850	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID		MW MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-		134 C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-		134 C10H14	000527-53-7	96
3	Benzene, 1,2,3,4-tetramethyl-		134 C10H14	000488-23-3	95
4	o-Cymene		134 C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-		134 C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
Acq On : 08 Oct 2024 11:40
Operator : JC/MD
Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

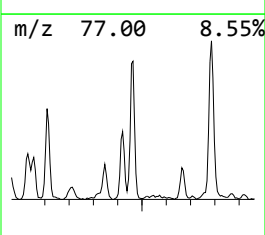
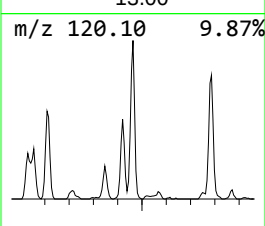
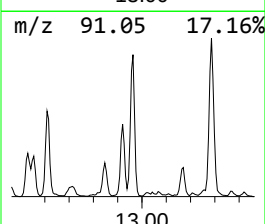
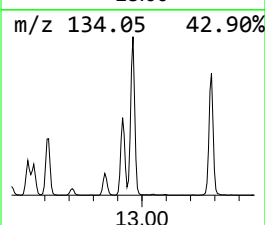
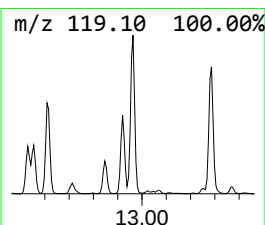
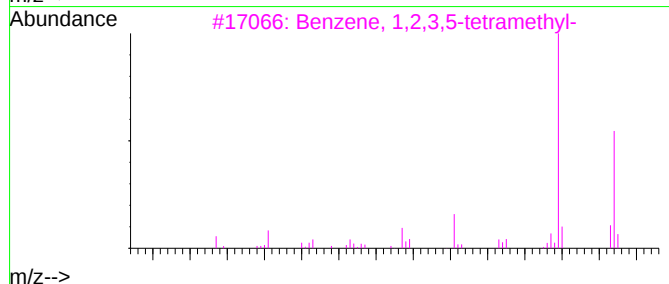
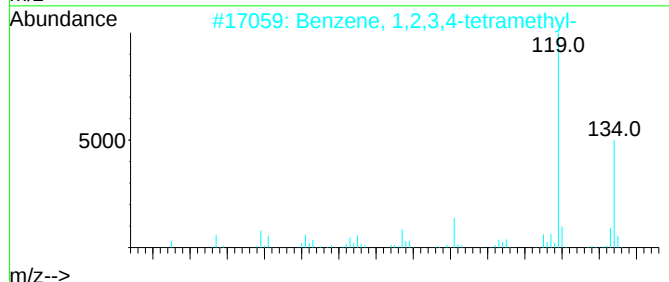
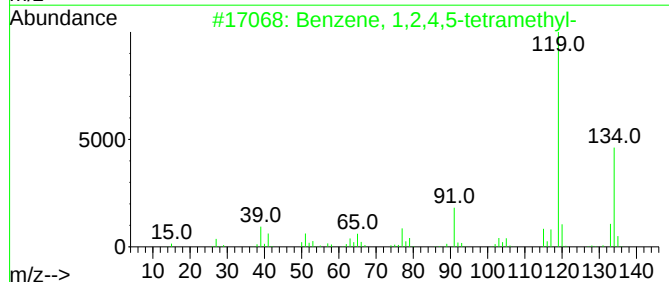
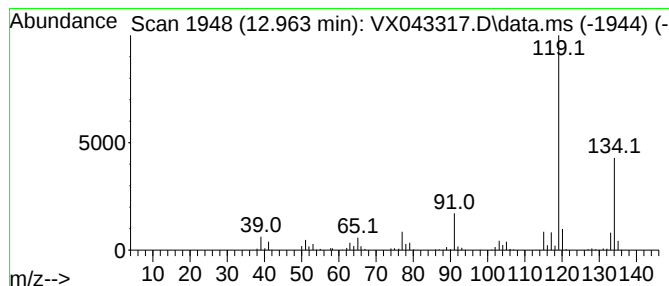
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	57.48 ug/l	410076	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
Acq On : 08 Oct 2024 11:40
Operator : JC/MD
Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

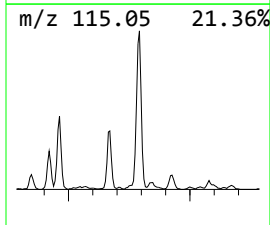
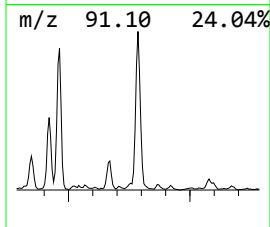
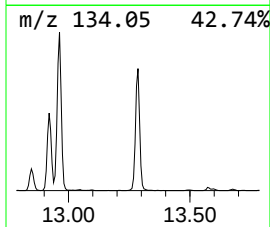
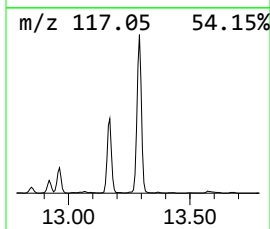
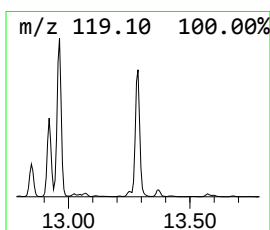
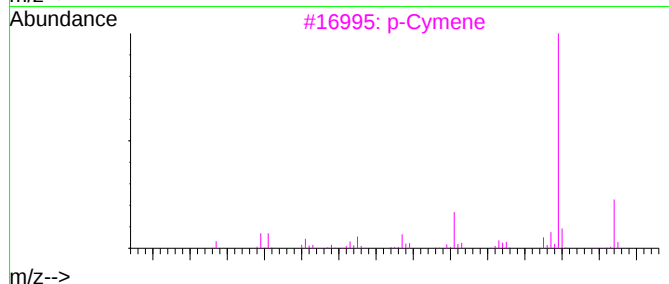
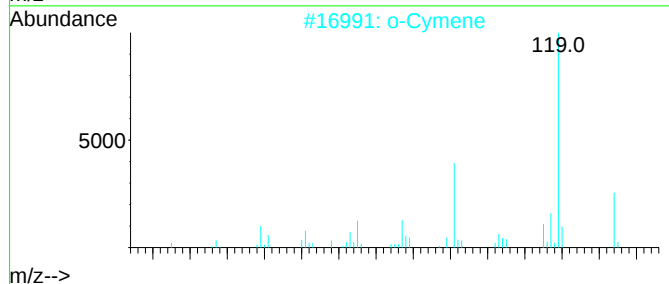
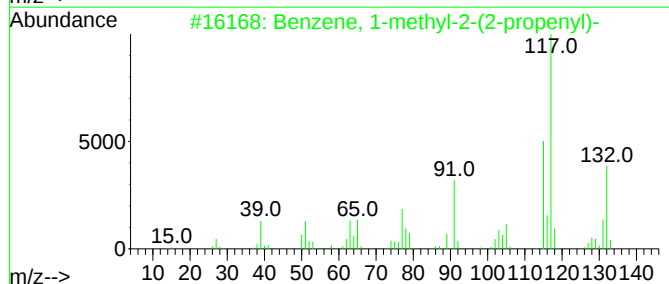
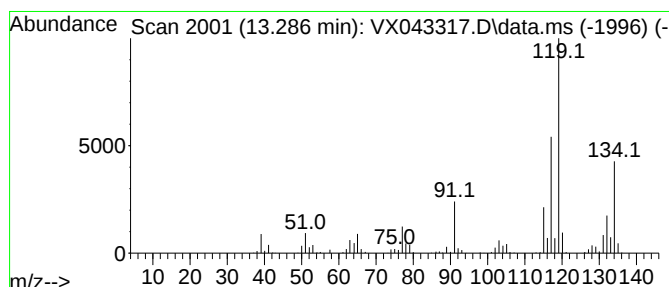
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-methyl-2-(2-propenyl) Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	78.46 ug/l	559744	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2	o-Cymene	134	C10H14	000527-84-4	70
3	p-Cymene	134	C10H14	000099-87-6	64
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100824\
Data File : VX043317.D
Acq On : 08 Oct 2024 11:40
Operator : JC/MD
Sample : P4342-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PORT-ELIZABETH-1201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone	11.024	20.1	ug/l	160460	3	10.055	399363	50.0
Benzene, 1-ethy...	11.378	28.0	ug/l	199630	4	12.024	356685	50.0
Benzene, 1,2,3-...	12.085	44.7	ug/l	318624	4	12.024	356685	50.0
Indane	12.244	27.3	ug/l	194929	4	12.024	356685	50.0
Benzene, 2-ethy...	12.530	18.8	ug/l	133975	4	12.024	356685	50.0
o-Cymene	12.609	30.1	ug/l	215114	4	12.024	356685	50.0
Benzene, 1,2,4,...	12.920	28.9	ug/l	205850	4	12.024	356685	50.0
Benzene, 1,2,3,...	12.963	57.5	ug/l	410076	4	12.024	356685	50.0
Benzene, 1-meth...	13.286	78.5	ug/l	559744	4	12.024	356685	50.0