

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012524\
 Data File : VY017103.D
 Acq On : 25 Jan 2024 13:55
 Operator : SY/MD
 Sample : VY0125SBL01
 Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VY0125SBL01

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_Y\methods\82Y012424S.M

Title : SW846 8260

Signal : TIC: VY017103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.716	468	475	491	rVB4	6951	23689	2.11%	0.235%
2	6.728	760	805	806	rBV4	24423	166068	14.76%	1.647%
3	7.722	958	968	974	rBV	91090	219434	19.51%	2.176%
4	7.795	974	980	988	rBV	155371	370297	32.91%	3.672%
5	8.149	1027	1038	1050	rVB	90954	196513	17.47%	1.948%
6	8.697	1119	1128	1139	rBV	255517	490825	43.63%	4.867%
7	9.350	1221	1235	1242	rBV	77638	267016	23.73%	2.648%
8	9.441	1243	1250	1270	rVB2	62742	207465	18.44%	2.057%
9	9.813	1295	1311	1329	rVB2	16962	56794	5.05%	0.563%
10	10.185	1364	1372	1379	rBV	380902	671100	59.65%	6.654%
11	10.252	1379	1383	1391	rVV	33188	81252	7.22%	0.806%
12	10.349	1391	1399	1416	rVB	135255	332138	29.52%	3.293%
13	10.581	1427	1437	1443	rBV4	32055	80446	7.15%	0.798%
14	10.660	1443	1450	1466	rVB	152526	367696	32.68%	3.646%
15	10.837	1469	1479	1492	rBV	73294	177712	15.80%	1.762%
16	11.093	1509	1521	1527	rBV2	66275	173064	15.38%	1.716%
17	11.172	1528	1534	1540	rVV	152415	329633	29.30%	3.268%
18	11.246	1540	1546	1556	rVB	112979	255858	22.74%	2.537%
19	11.355	1556	1564	1573	rVB2	7692	16265	1.45%	0.161%
20	11.502	1575	1588	1600	rBV3	435768	1125013	100.00%	11.155%
21	11.983	1657	1667	1675	rBV2	198587	454016	40.36%	4.502%
22	12.069	1675	1681	1690	rVB	154728	285468	25.37%	2.830%
23	12.300	1709	1719	1729	rBV	167348	309483	27.51%	3.069%
24	12.404	1729	1736	1744	rVV	116548	220168	19.57%	2.183%
25	12.489	1744	1750	1753	rVV	256390	452302	40.20%	4.485%
26	12.526	1753	1756	1768	rVB3	439456	954712	84.86%	9.466%
27	12.995	1825	1833	1836	rBV	105036	185525	16.49%	1.840%
28	13.038	1836	1840	1852	rVB	178970	299669	26.64%	2.971%
29	13.312	1873	1885	1893	rBV	101046	182051	16.18%	1.805%
30	13.434	1899	1905	1914	rBV	304467	463836	41.23%	4.599%
31	13.635	1929	1938	1946	rBV2	6094	11471	1.02%	0.114%
32	13.910	1976	1983	1990	rBV3	12277	25841	2.30%	0.256%
33	14.349	2047	2055	2067	rVB	108146	176982	15.73%	1.755%
34	14.727	2111	2117	2125	rVB	82786	128286	11.40%	1.272%
35	14.867	2134	2140	2147	rBV2	84862	142251	12.64%	1.410%
36	14.977	2151	2158	2164	rBV	48641	81321	7.23%	0.806%

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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	15.190	2188	2193	2200	rVB	60520	103792	9.23%	1.029%
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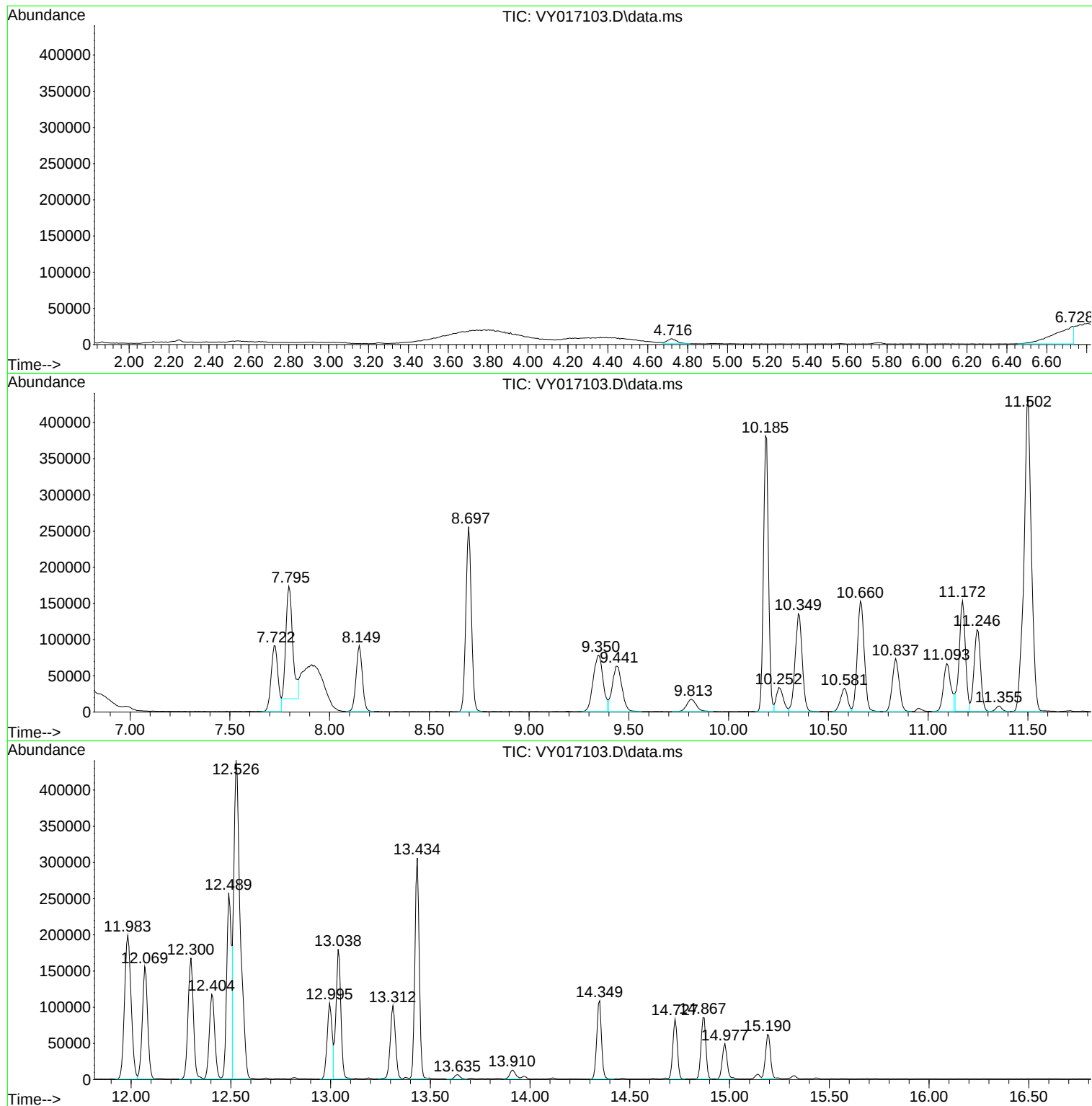
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Quant Title : SW846 8260

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



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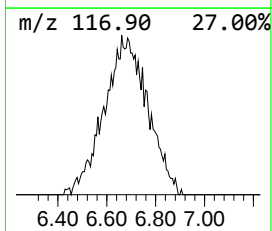
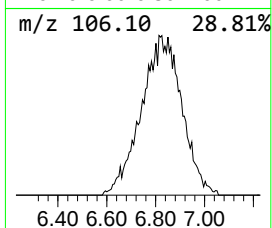
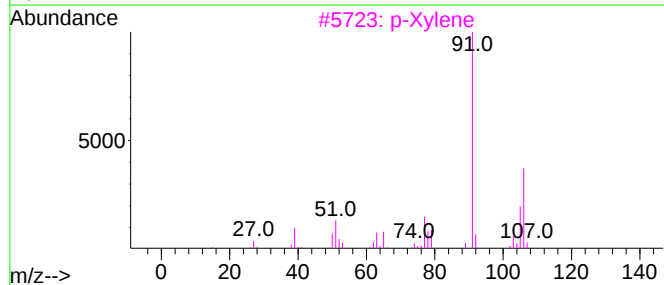
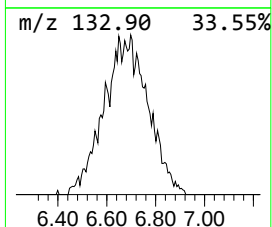
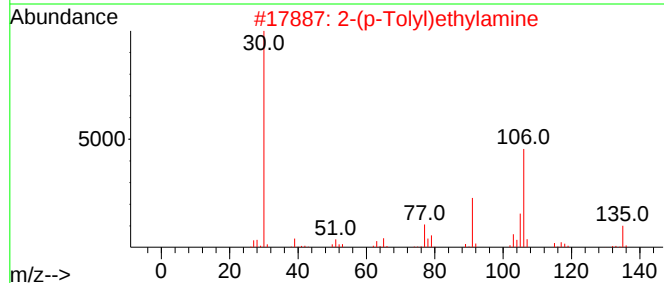
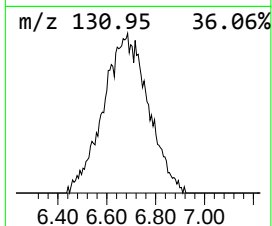
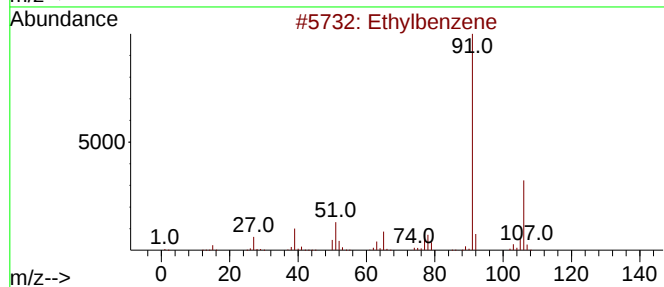
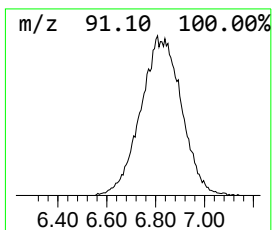
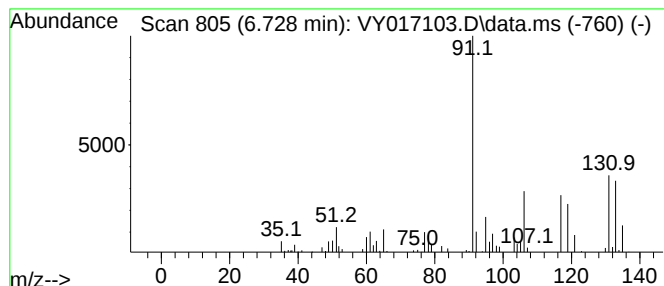
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012424S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown6.728 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	22.42 ug/l	166068	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylbenzene	106	C8H10	000100-41-4	25
2			2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	11
3			p-Xylene	106	C8H10	000106-42-3	10
4			Benzenepropanenitrile	131	C9H9N	000645-59-0	10
5			Bicyclo[3.2.1]oct-2-ene, 3-methy...	134	C10H14	049826-53-1	10



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Instrument :
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ClientSampleId :
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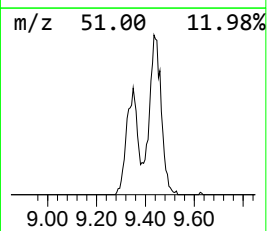
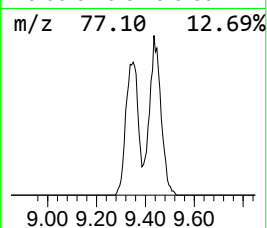
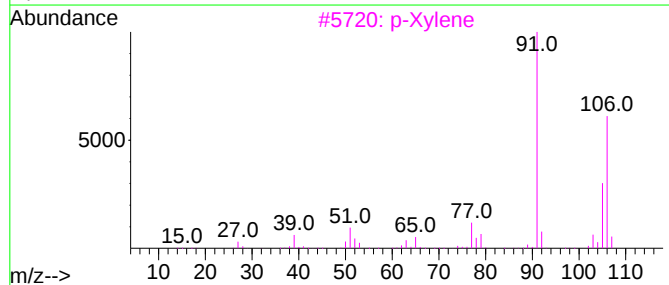
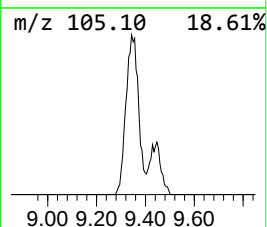
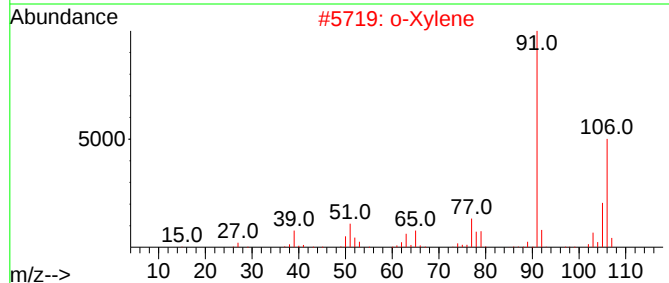
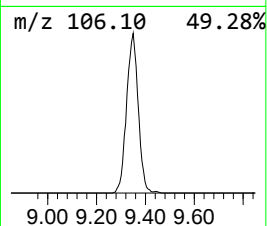
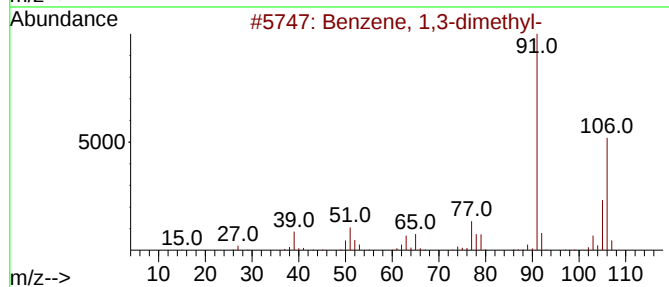
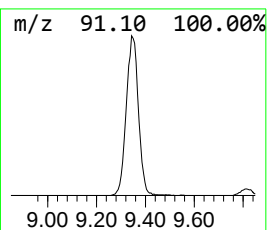
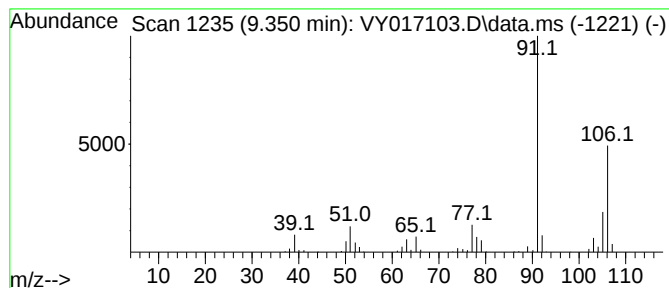
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.350	27.20 ug/l	267016	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2			o-Xylene	106	C8H10	000095-47-6	97
3			p-Xylene	106	C8H10	000106-42-3	95
4			Ethylbenzene	106	C8H10	000100-41-4	91
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	90



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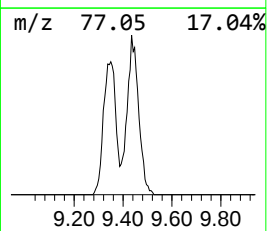
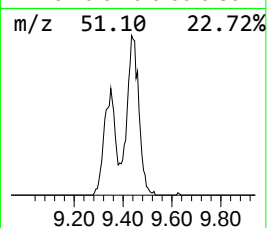
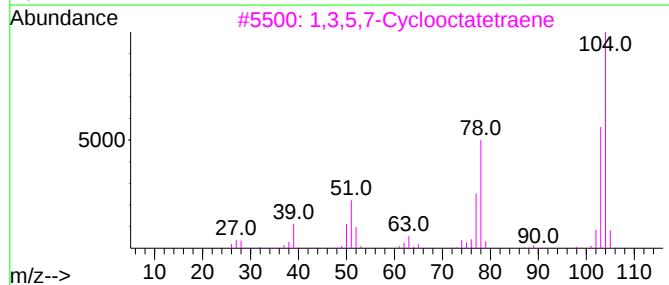
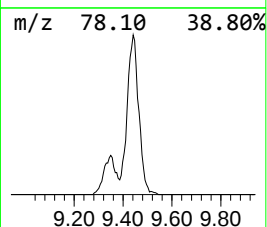
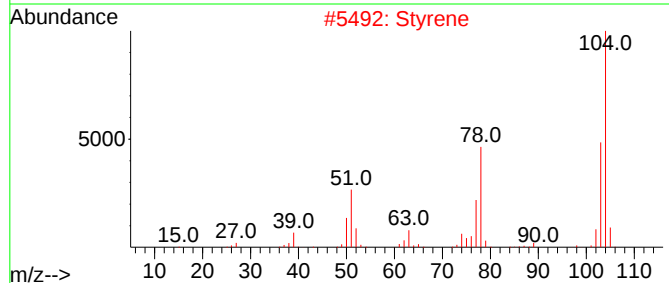
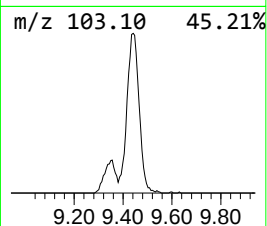
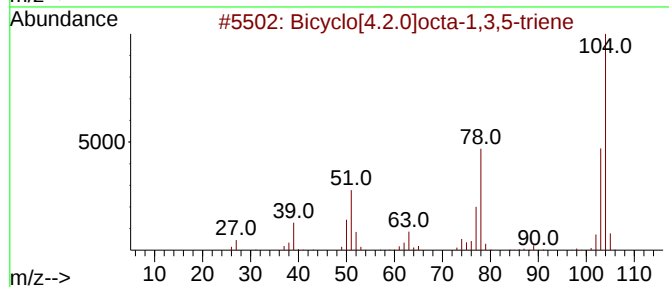
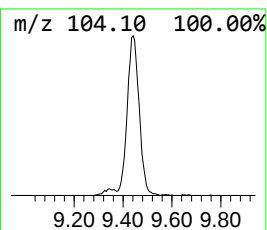
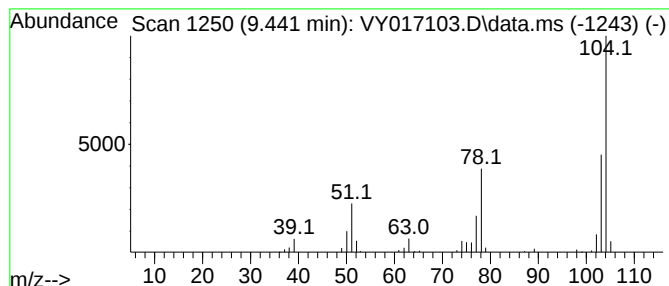
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012424S.M
Quant Title : SW846 8260

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

Peak Number 3 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.441	21.13 ug/l	207465	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	95
2			Styrene	104	C8H8	000100-42-5	94
3			1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	59
4			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	50
5			Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	50



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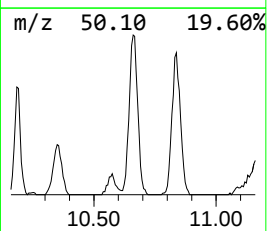
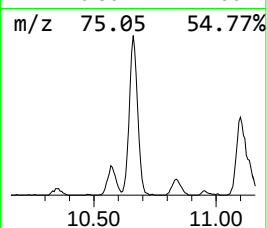
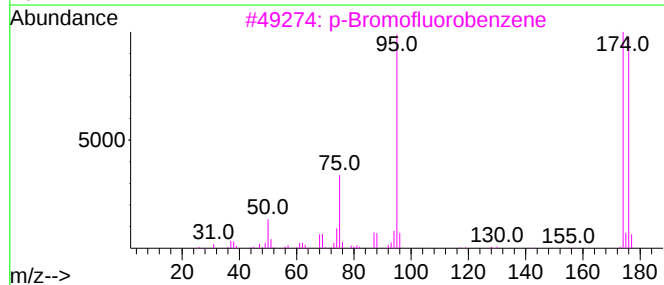
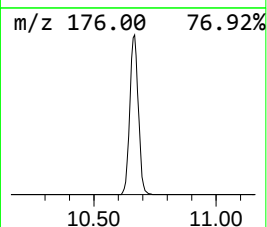
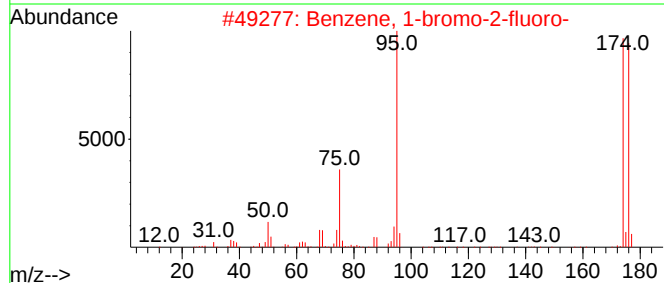
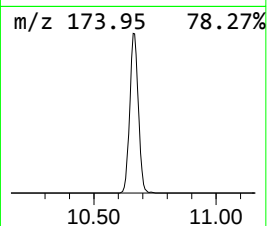
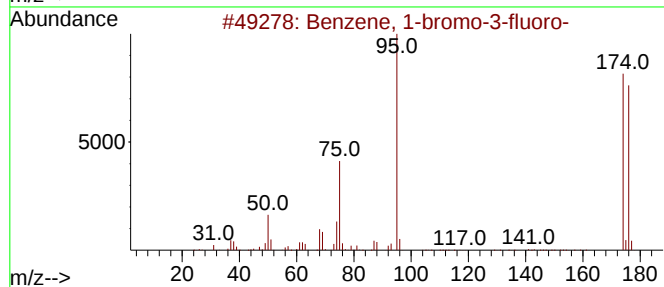
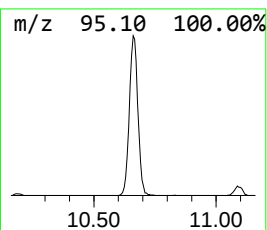
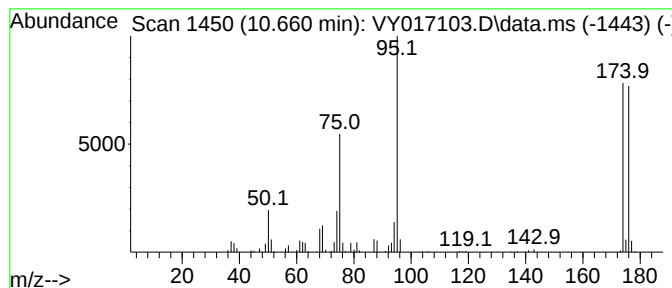
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-bromo-3-fluoro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.660	16.34 ug/l	367696	Chlorobenzene-d5	11.502

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	97
2			Benzene, 1-bromo-2-fluoro-	174	C6H4BrF	001072-85-1	94
3			p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	93
4			Pyrazole, 3-(2-bromoethyl)-	174	C5H7BrN2	211738-72-6	42
5			4(1H)-Pyrimidinone, 5-bromo-	174	C4H3BrN2O	019808-30-1	32



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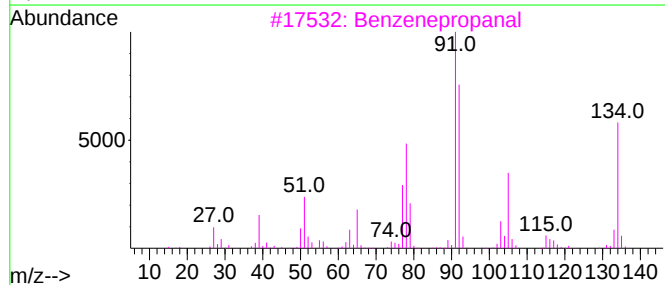
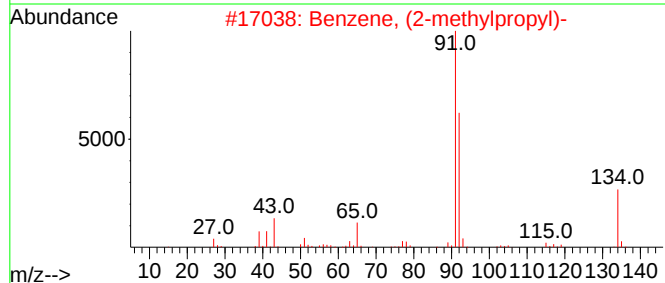
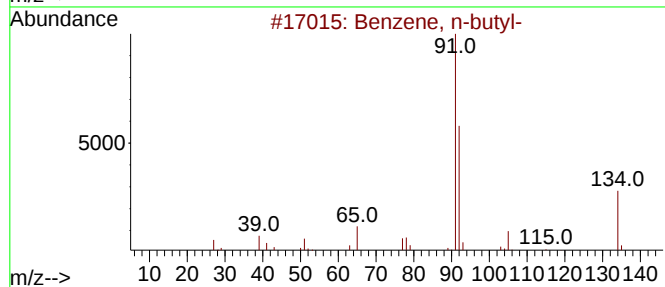
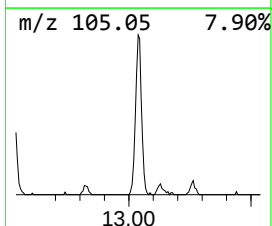
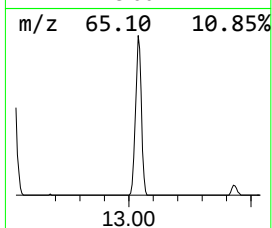
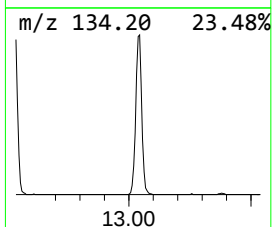
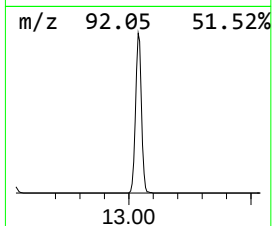
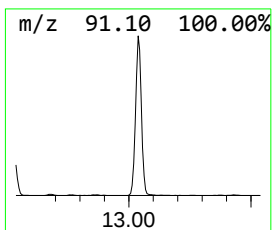
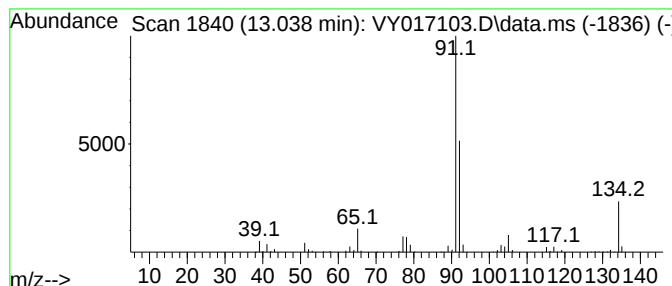
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012424S.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, (2-methylpropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.038	32.30 ug/l	299669	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, n-butyl-	134	C10H14	000104-51-8	95
2			Benzene, (2-methylpropyl)-	134	C10H14	000538-93-2	83
3			Benzenepropanal	134	C9H10O	000104-53-0	64
4			Naphthalene, 1,2,3,4,4a,8a-hexah...	134	C10H14	062690-62-4	59
5			Acetaldehyde dibenzyl acetal	242	C16H18O2	1000431-44-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012524\
Data File : VY017103.D
Acq On : 25 Jan 2024 13:55
Operator : SY/MD
Sample : VY0125SBL01
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VY0125SBL01

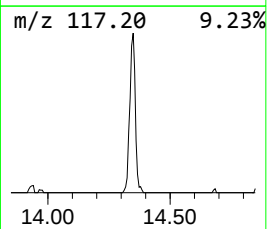
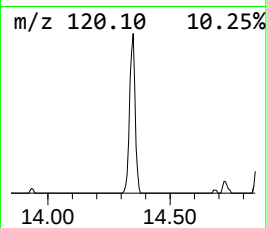
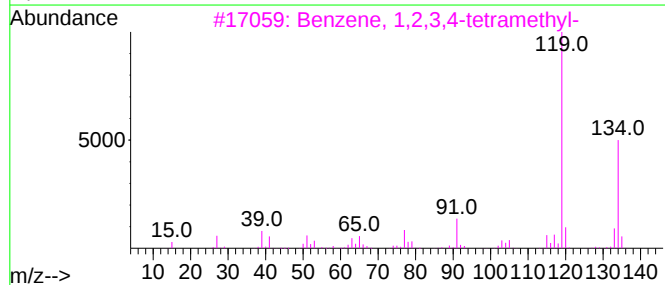
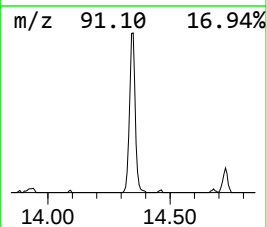
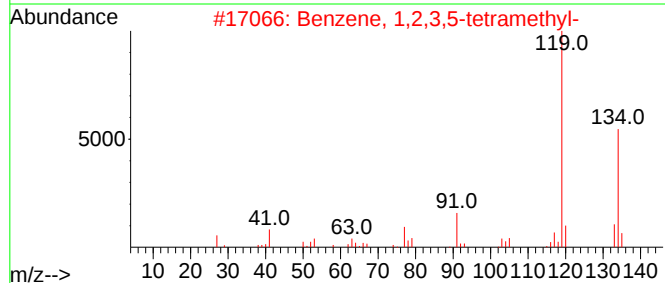
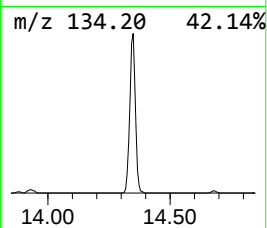
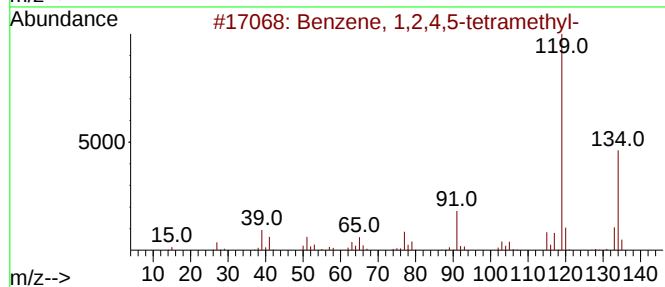
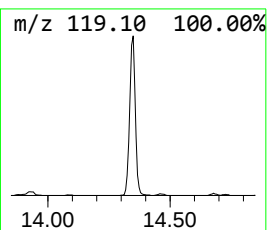
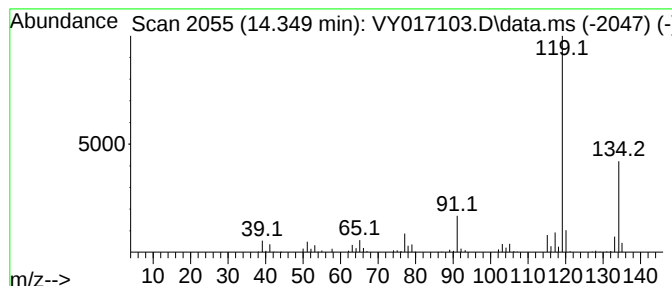
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.349	19.08 ug/l	176982	1,4-Dichlorobenzene-d4	13.434

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	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012524\
Data File : VY017103.D
Acq On : 25 Jan 2024 13:55
Operator : SY/MD
Sample : VY0125SBL01
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VY0125SBL01

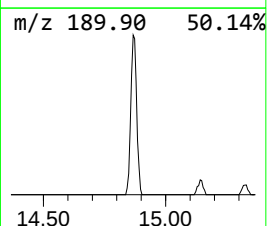
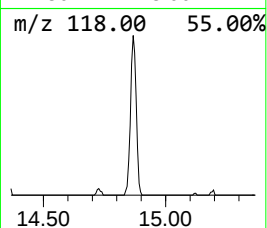
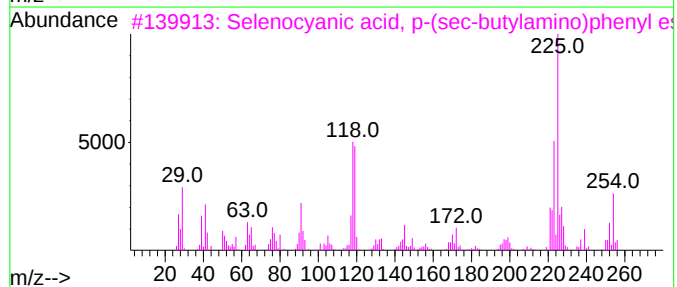
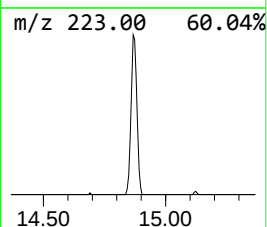
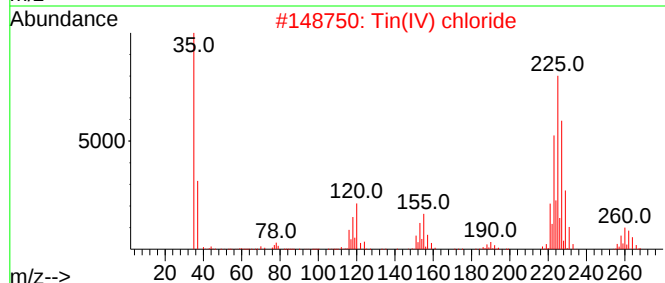
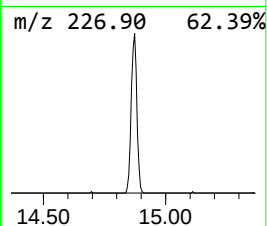
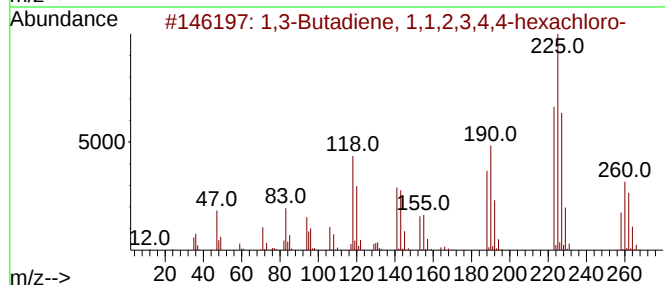
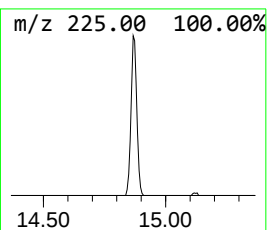
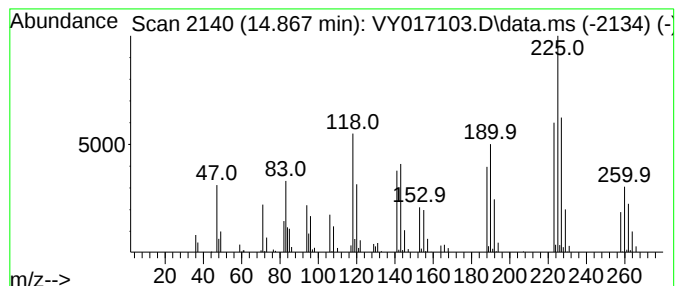
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012424S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.867	15.33 ug/l	142251	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			Tin(IV) chloride	260	Cl4Sn	007646-78-8	38
3			Selenocyanic acid, p-(sec-butyla...	254	C11H14N2Se	022037-11-2	17
4			Spiro[benzocyclobutene-1,2'-(1',...	190	C12H14O2	1000159-59-8	10
5			3-Bromo-4,5-dichloropyridine	225	C5H2BrCl2N	1001056-83-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012524\
Data File : VY017103.D
Acq On : 25 Jan 2024 13:55
Operator : SY/MD
Sample : VY0125SBL01
Misc : 5.00g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VY0125SBL01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012424S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.728	6.728	22.4	ug/l	166068	1	7.795	370297	50.0
Benzene, 1,3-di...	9.350	27.2	ug/l	267016	2	8.697	490825	50.0
Bicyclo[4.2.0]o...	9.441	21.1	ug/l	207465	2	8.697	490825	50.0
Benzene, 1-brom...	10.660	16.3	ug/l	367696	3	11.502	1125010	50.0
Benzene, (2-met...	13.038	32.3	ug/l	299669	4	13.434	463836	50.0
Benzene, 1,2,4,...	14.349	19.1	ug/l	176982	4	13.434	463836	50.0
1,3-Butadiene, ...	14.867	15.3	ug/l	142251	4	13.434	463836	50.0