

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
 Data File : VX038733.D
 Acq On : 10 Nov 2023 16:57
 Operator : JC/MD
 Sample : 05331-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X110723W.M
 Title : SW846 8260

Signal : TIC: VX038733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.965	139	144	152	rVB3	10871	22406	1.08%	0.098%
2	2.069	152	161	169	rBV3	11206	23127	1.11%	0.101%
3	2.215	181	185	194	rVB	17530	26572	1.28%	0.116%
4	2.380	203	212	222	rBV	58436	99191	4.77%	0.433%
5	2.867	287	292	299	rVV2	16471	35849	1.72%	0.157%
6	3.111	322	332	346	rBV3	19836	49166	2.36%	0.215%
7	4.306	518	528	539	rVB4	11982	35545	1.71%	0.155%
8	4.562	559	570	585	rBV2	21849	73433	3.53%	0.321%
9	5.032	637	647	661	rBV3	10081	32227	1.55%	0.141%
10	5.196	665	674	684	rBV2	7335	22588	1.09%	0.099%
11	5.385	694	705	715	rBV	155570	457255	21.99%	1.996%
12	5.550	723	732	750	rVB	241517	690844	33.22%	3.016%
13	5.958	789	799	805	rBV	147417	388976	18.71%	1.698%
14	6.037	805	812	830	rVV	362701	999781	48.08%	4.365%
15	6.202	832	839	855	rVB4	13321	50494	2.43%	0.220%
16	6.763	921	931	944	rBV	374980	916970	44.10%	4.003%
17	8.500	1209	1216	1225	rVB4	13973	31416	1.51%	0.137%
18	8.647	1233	1240	1247	rBV	776153	1252950	60.26%	5.470%
19	8.720	1247	1252	1262	rVB	437345	704032	33.86%	3.074%
20	8.958	1282	1291	1298	rBV	125206	200107	9.62%	0.874%
21	9.043	1298	1305	1320	rVB	139111	231731	11.14%	1.012%
22	10.055	1461	1471	1483	rBV	863555	1250786	60.15%	5.461%
23	10.195	1488	1494	1505	rVV	1252691	1671561	80.39%	7.298%
24	10.305	1506	1512	1520	rVB	805272	1066771	51.30%	4.657%
25	10.640	1562	1567	1583	rVB	1611881	2079311	100.00%	9.078%
26	10.963	1613	1620	1624	rBV	49841	70877	3.41%	0.309%
27	11.079	1634	1639	1649	rVV	839361	1066779	51.30%	4.658%
28	11.171	1649	1654	1660	rVB5	12042	23887	1.15%	0.104%
29	11.305	1672	1676	1684	rVB	64486	85916	4.13%	0.375%
30	11.402	1684	1692	1696	rBV	153198	234127	11.26%	1.022%
31	11.451	1696	1700	1705	rVB	155020	187656	9.02%	0.819%
32	11.610	1721	1726	1737	rBV	695174	897129	43.15%	3.917%
33	11.750	1744	1749	1755	rVB	772976	930124	44.73%	4.061%
34	12.018	1788	1793	1799	rVV	1100241	1445172	69.50%	6.310%
35	12.085	1799	1804	1810	rVB	1106347	1299120	62.48%	5.672%
36	12.244	1821	1830	1838	rBV	1288689	1748560	84.09%	7.634%

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37	12.317	1838	1842	1850	rVB2	52612	81495	3.92%	0.356%
38	12.414	1852	1858	1862	rBV	101058	138767	6.67%	0.606%
39	12.463	1862	1866	1872	rVB	29769	38320	1.84%	0.167%
40	12.530	1872	1877	1880	rBV	61513	84240	4.05%	0.368%
41	12.609	1886	1890	1894	rBV	125405	159775	7.68%	0.698%
42	12.646	1894	1896	1899	rVV	32366	32499	1.56%	0.142%
43	12.701	1899	1905	1912	rVV2	144751	200103	9.62%	0.874%
44	12.847	1924	1929	1935	rVB	55786	76993	3.70%	0.336%
45	12.920	1935	1941	1944	rBV	83150	103454	4.98%	0.452%
46	12.963	1944	1948	1953	rVB	77728	96352	4.63%	0.421%
47	13.170	1977	1982	1987	rVB	82954	101266	4.87%	0.442%
48	13.292	1996	2002	2007	rVB2	300981	396870	19.09%	1.733%
49	13.347	2007	2011	2018	rVB3	22940	36511	1.76%	0.159%
50	13.420	2019	2023	2029	rVB	58667	78052	3.75%	0.341%
51	13.585	2046	2050	2056	rBV4	16014	32637	1.57%	0.142%
52	13.664	2060	2063	2069	rVB2	15777	22925	1.10%	0.100%
53	13.774	2074	2081	2091	rBV	378329	475739	22.88%	2.077%
54	13.865	2091	2096	2102	rVB	140083	181418	8.72%	0.792%
55	14.182	2143	2148	2151	rBV	48186	62682	3.01%	0.274%
56	14.414	2183	2186	2194	rVB	15724	24134	1.16%	0.105%
57	14.780	2240	2246	2251	rBV2	56083	77838	3.74%	0.340%

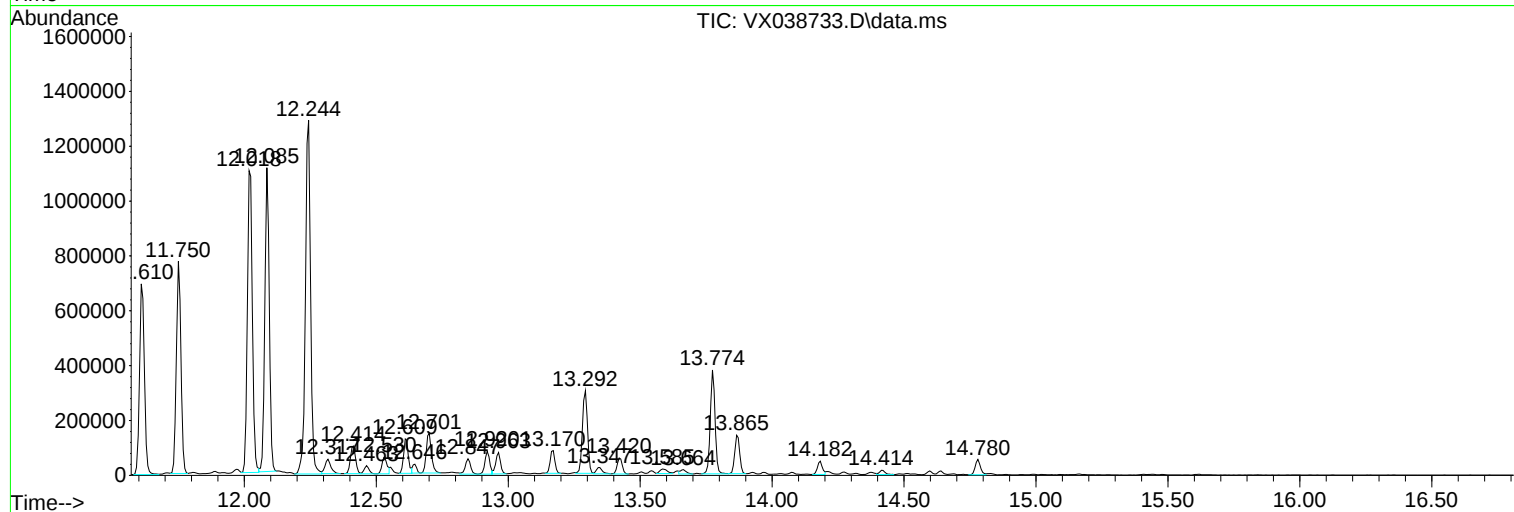
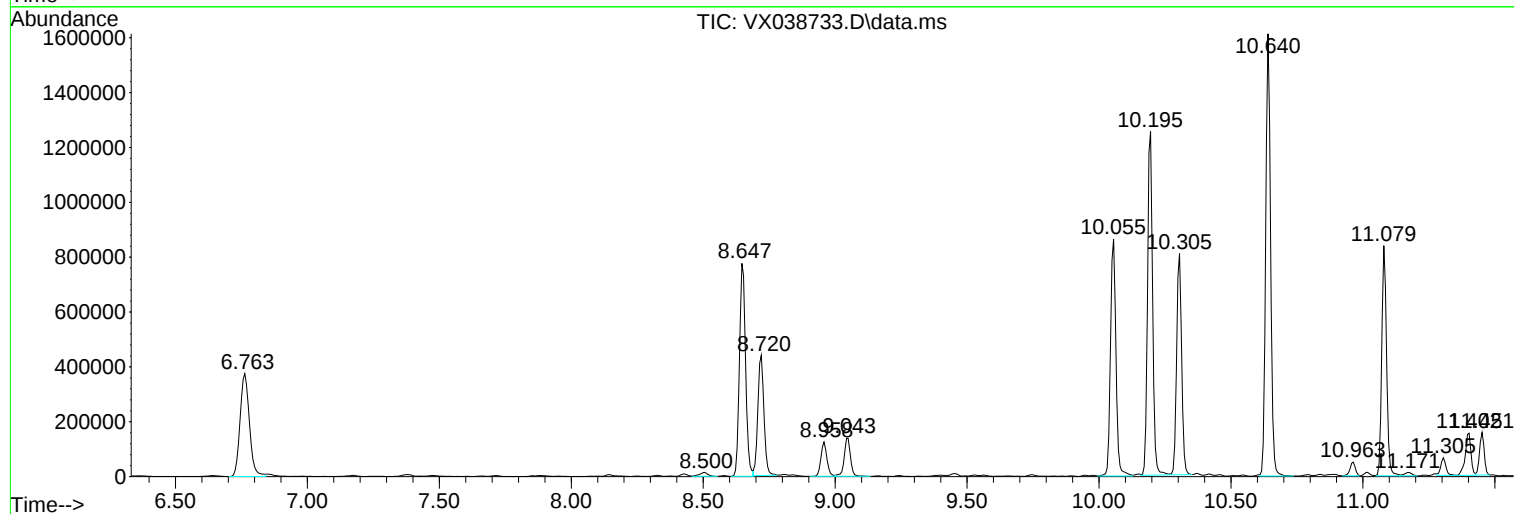
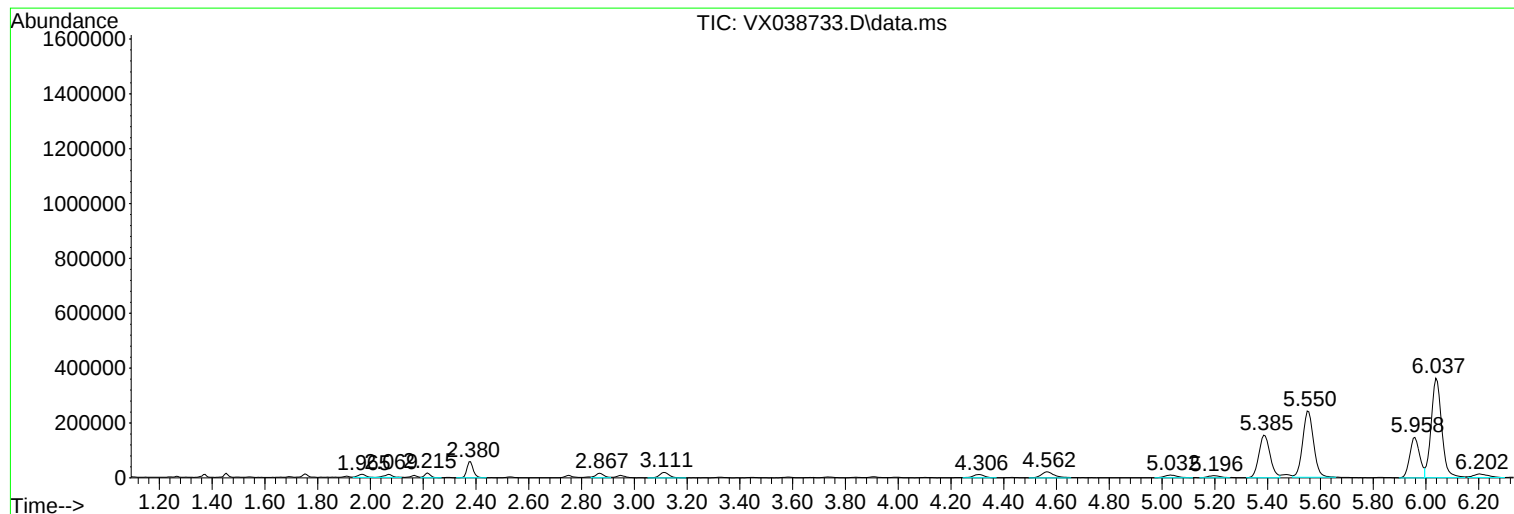
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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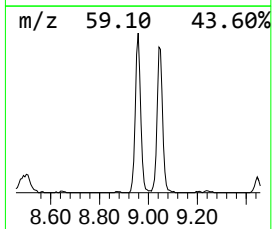
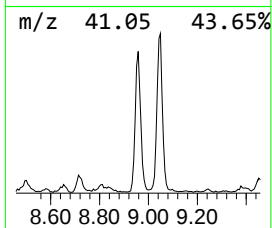
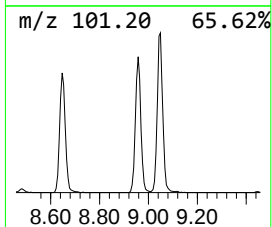
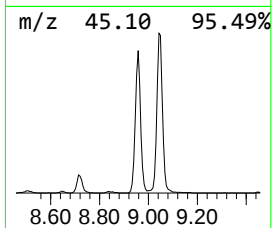
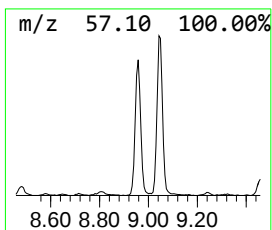
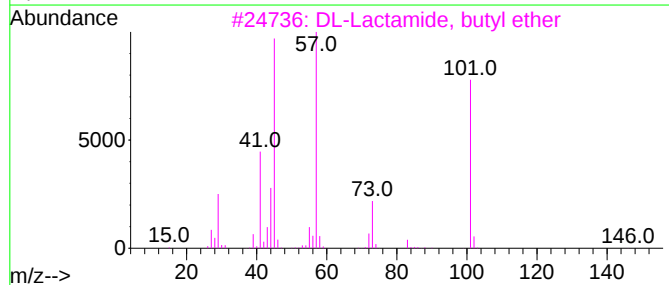
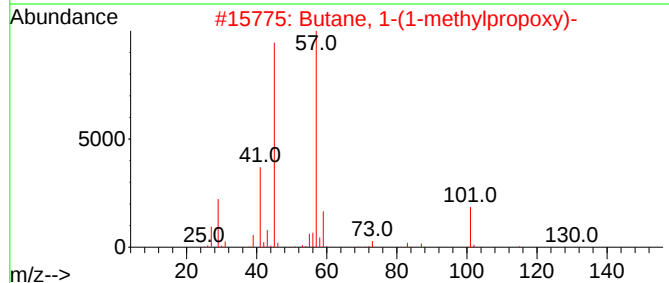
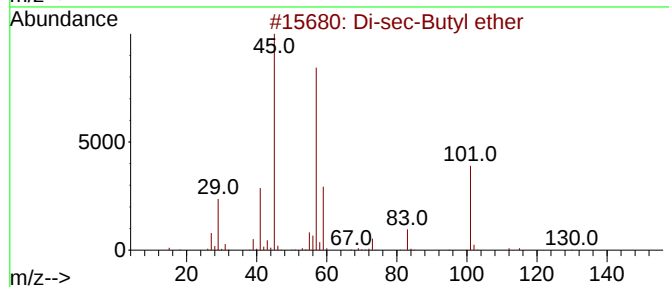
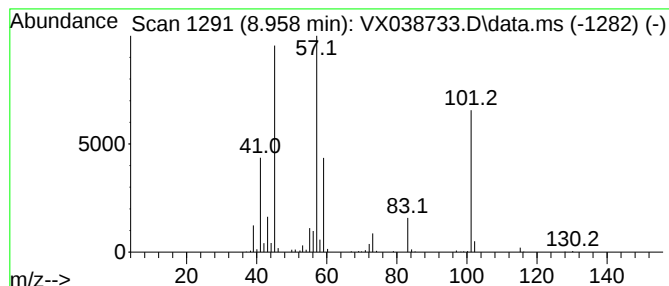
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 1 Di-sec-Butyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	8.00 ug/l	200107	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42
4			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39
5			1,2-Hexanediol, 2-methyl-	132	C7H16O2	056255-50-6	38



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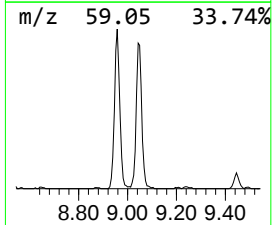
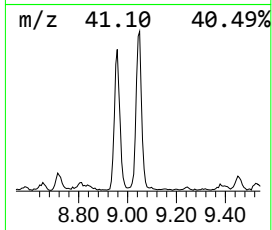
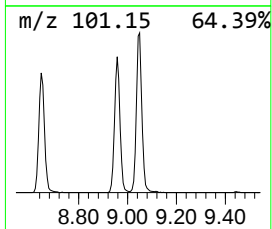
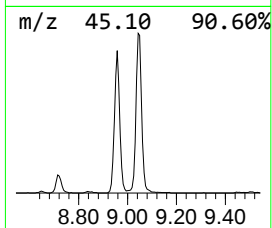
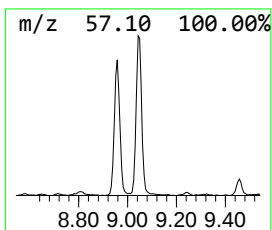
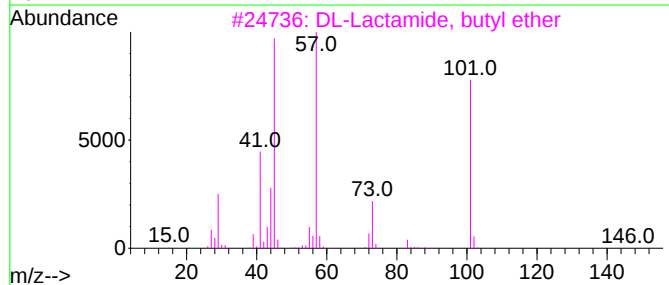
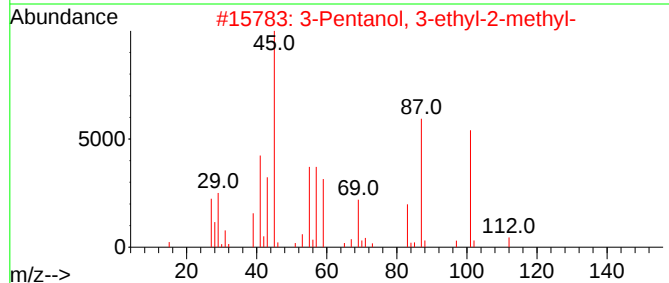
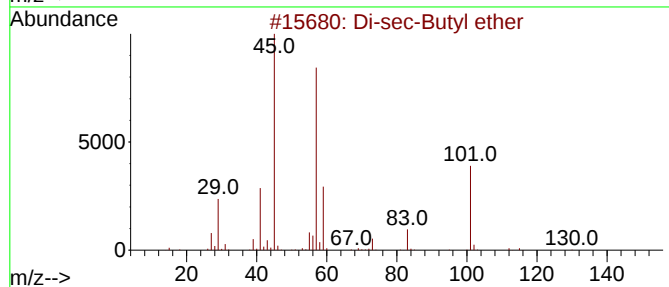
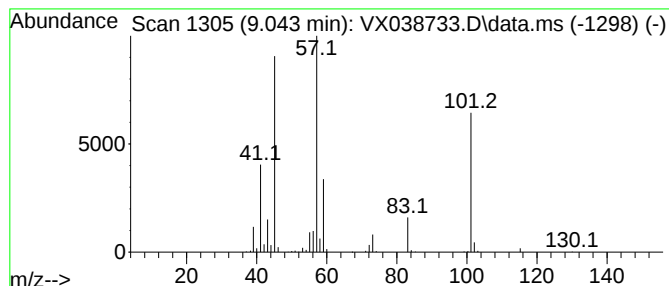
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 2 3-Pentanol, 3-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.043	9.26 ug/l	231731	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
3			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	64
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	50



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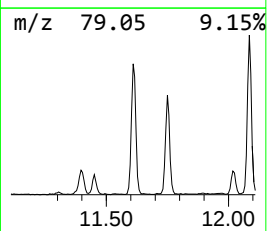
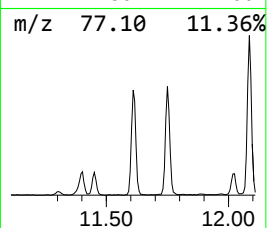
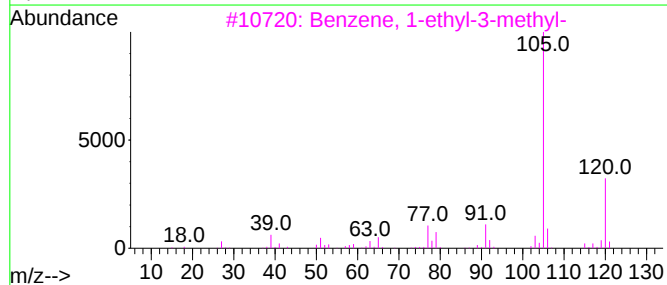
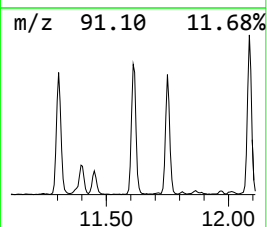
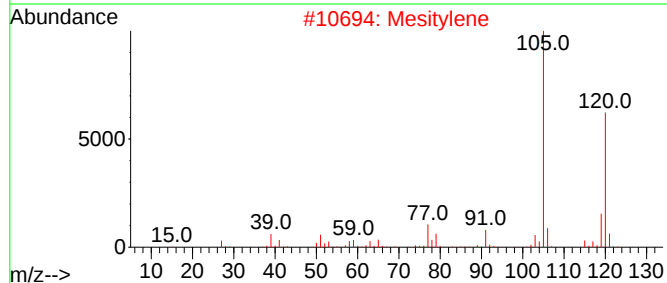
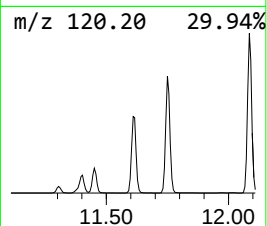
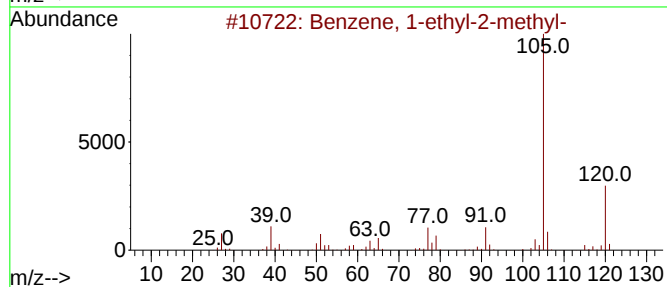
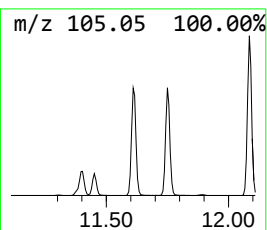
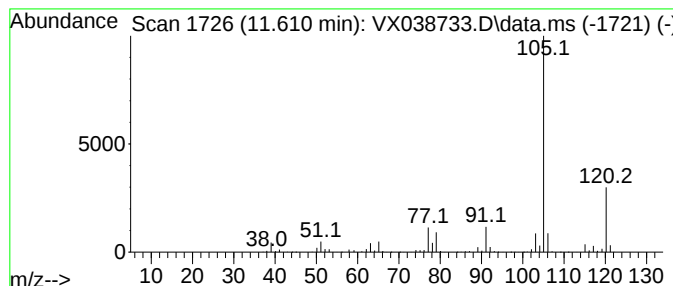
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	31.04 ug/l	897129	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	94
2			Mesitylene	120	C9H12	000108-67-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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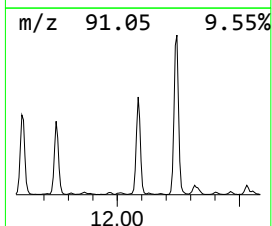
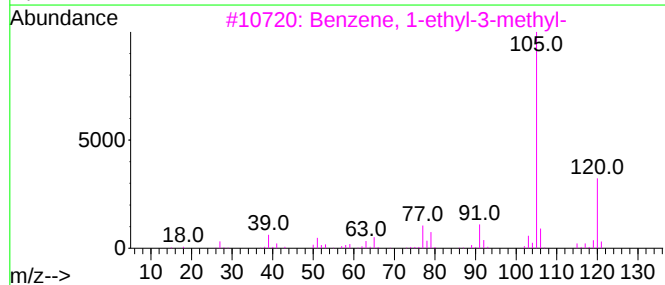
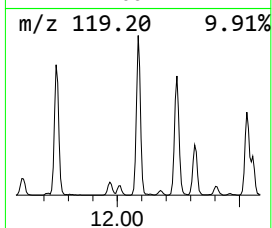
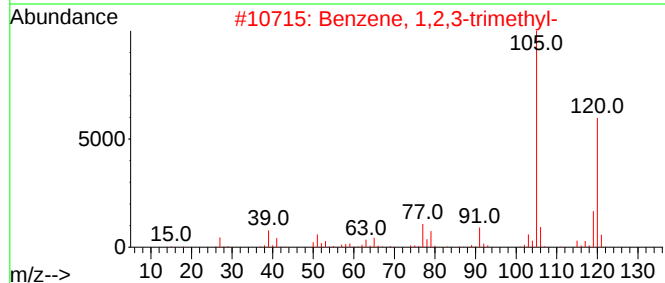
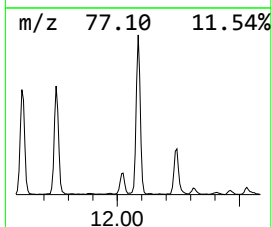
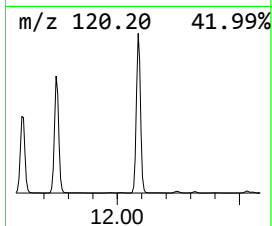
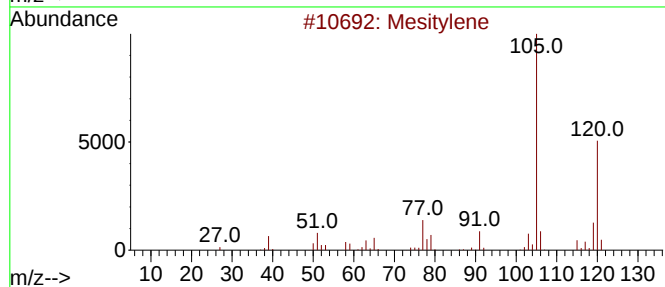
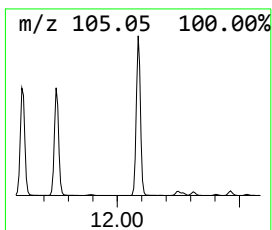
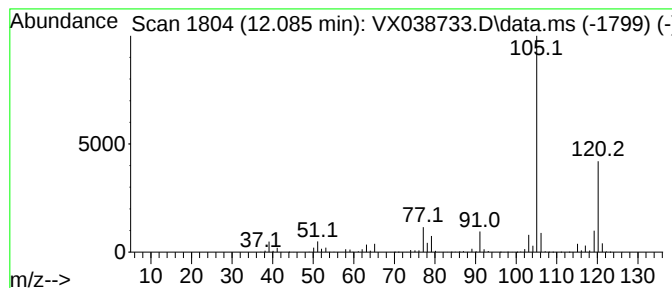
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 4 Mesitylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	44.95 ug/l	1299120	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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MW-12

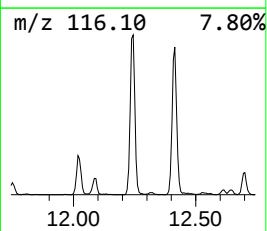
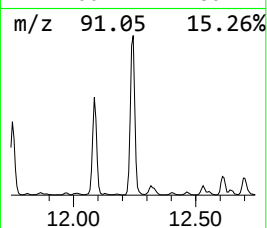
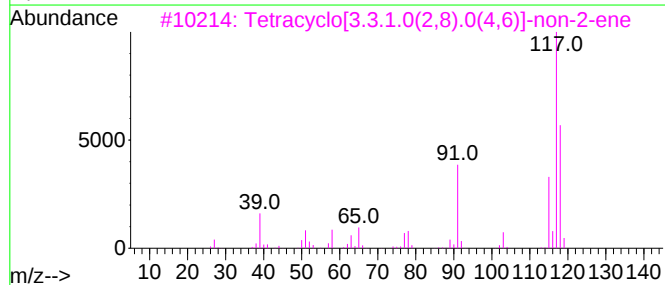
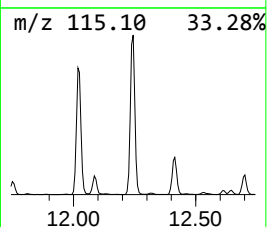
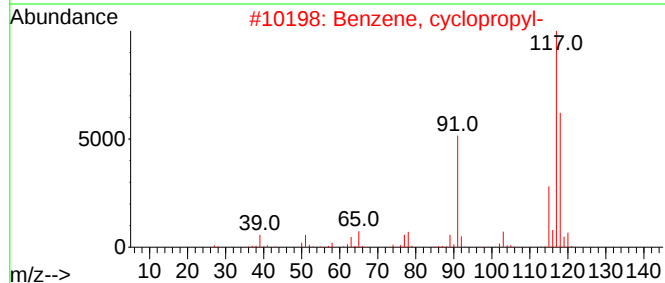
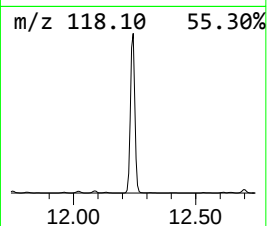
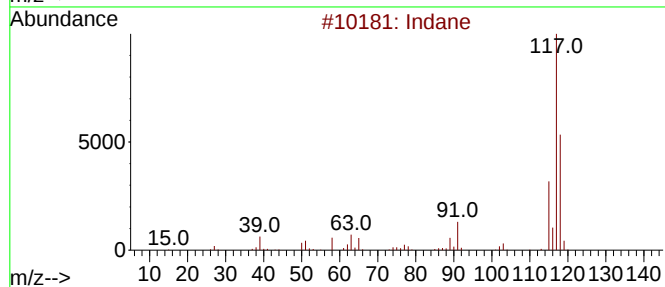
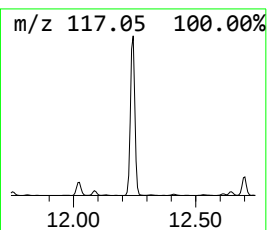
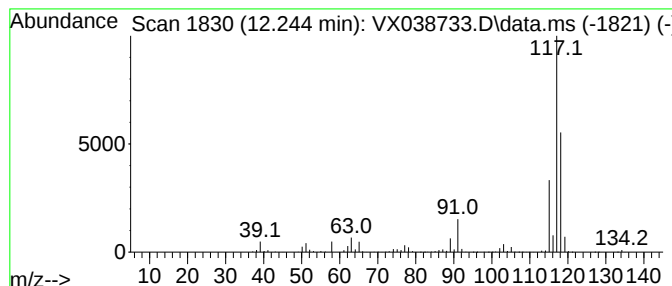
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	60.50 ug/l	1748560	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	83
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5			Deltacyclene	118	C9H10	007785-10-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038733.D
Acq On : 10 Nov 2023 16:57
Operator : JC/MD
Sample : 05331-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

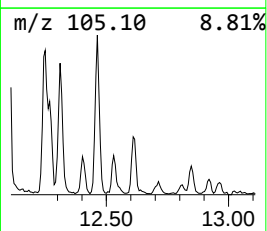
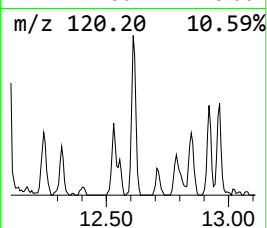
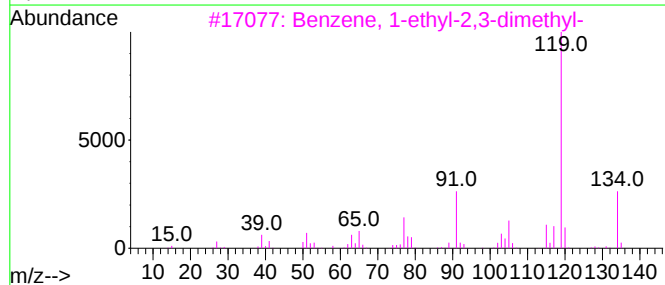
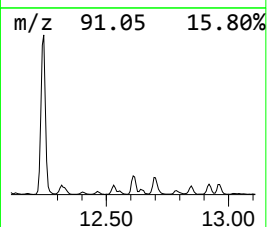
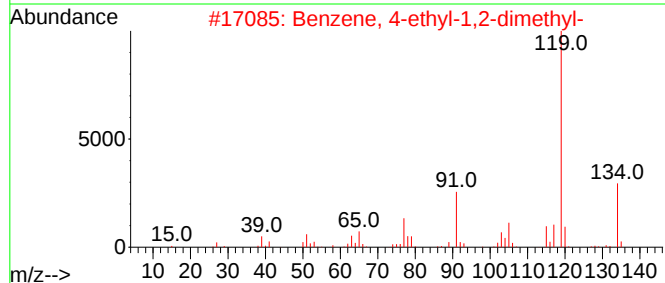
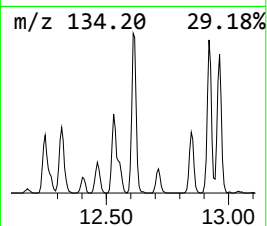
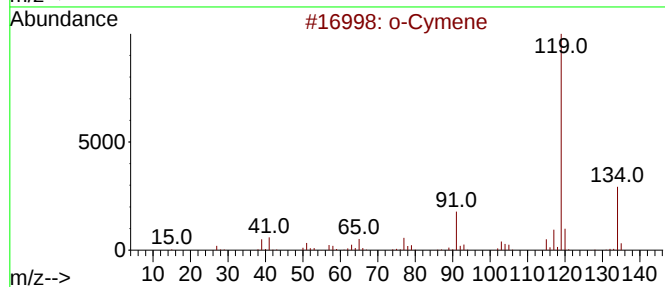
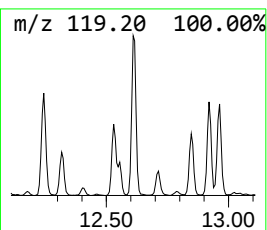
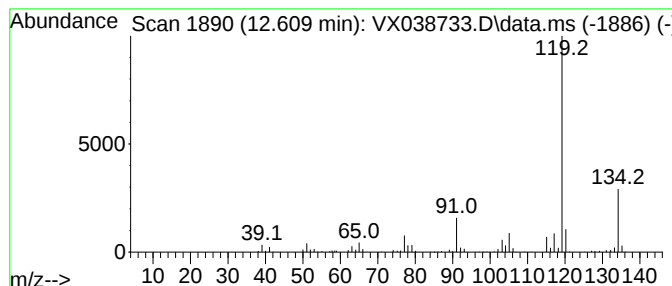
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	5.53 ug/l	159775	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, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038733.D
Acq On : 10 Nov 2023 16:57
Operator : JC/MD
Sample : 05331-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

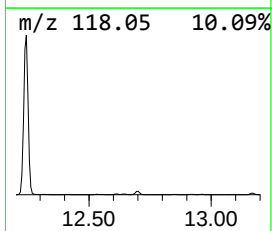
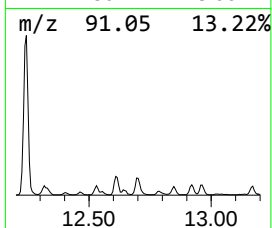
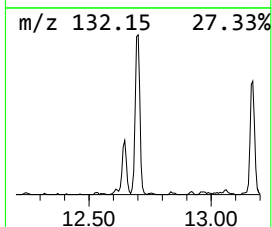
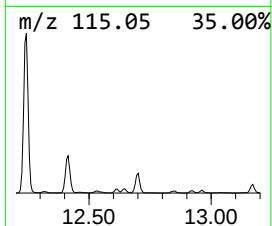
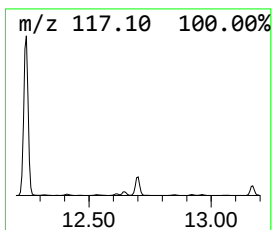
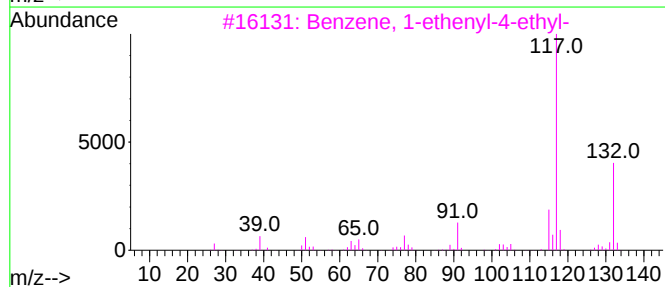
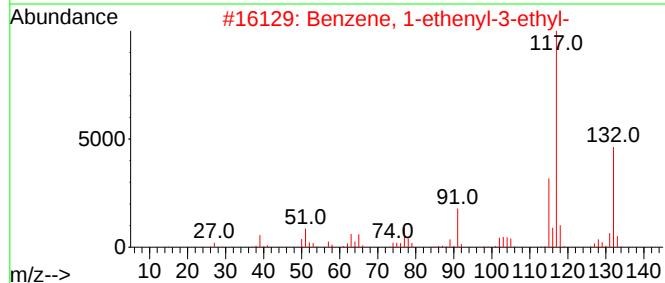
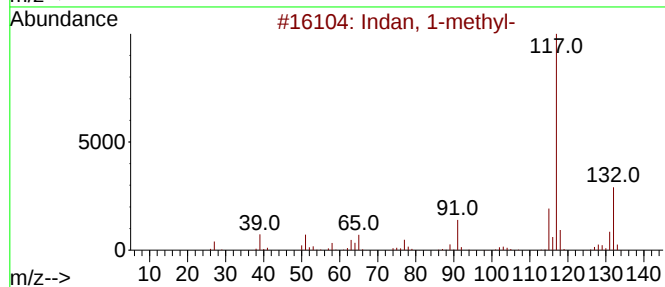
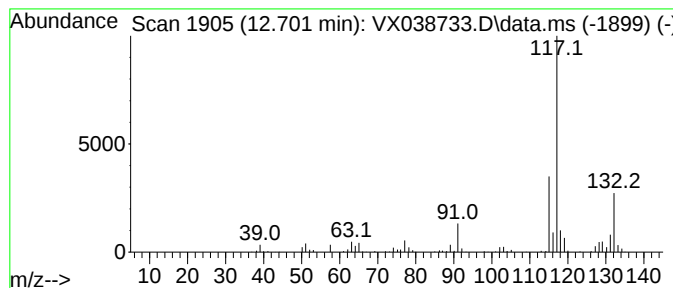
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Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	6.92 ug/l	200103	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indan, 1-methyl-	132	C10H12	000767-58-8	87
2		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83
4		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5		Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038733.D
Acq On : 10 Nov 2023 16:57
Operator : JC/MD
Sample : 05331-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

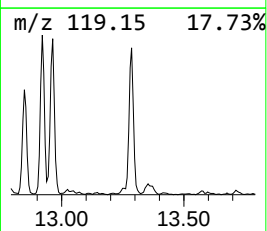
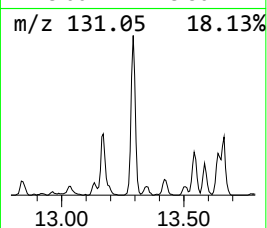
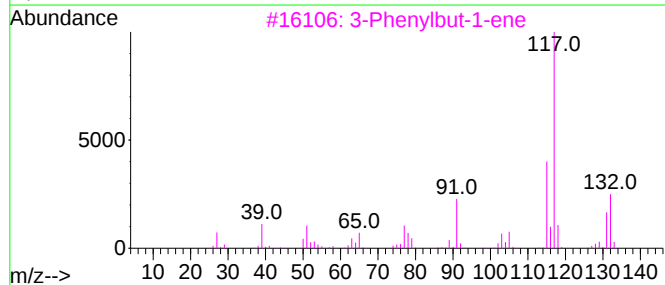
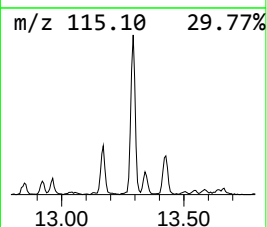
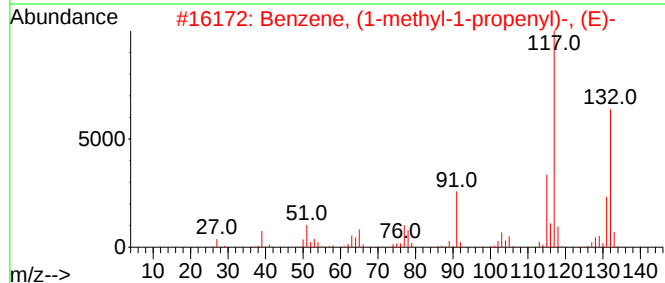
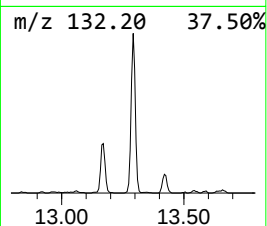
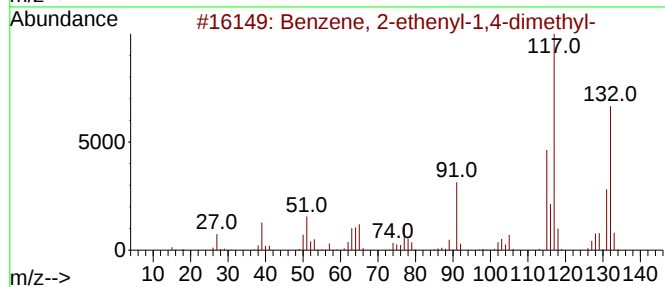
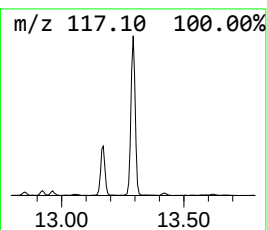
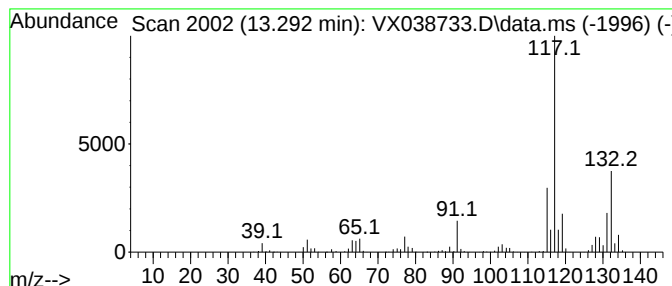
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	13.73 ug/l	396870	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038733.D
Acq On : 10 Nov 2023 16:57
Operator : JC/MD
Sample : 05331-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

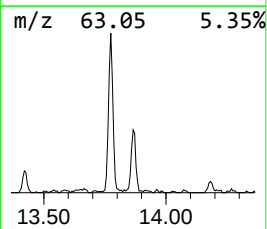
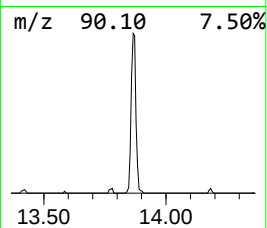
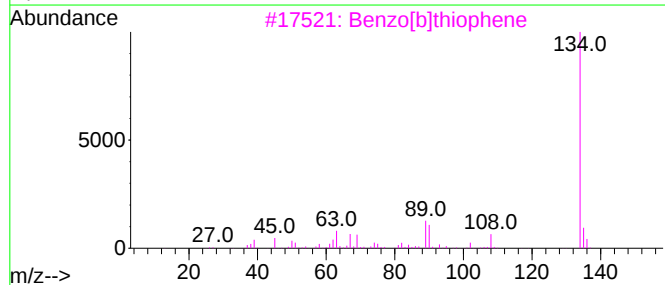
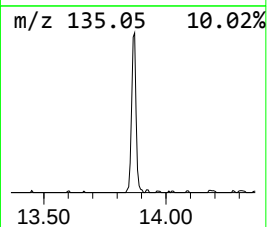
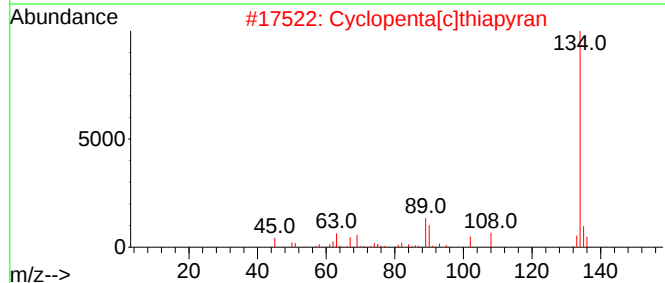
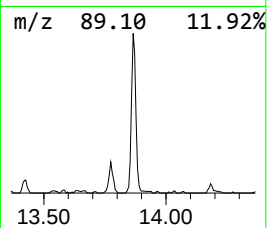
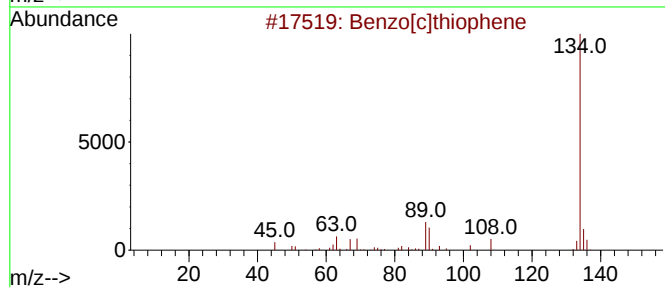
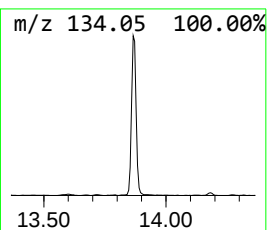
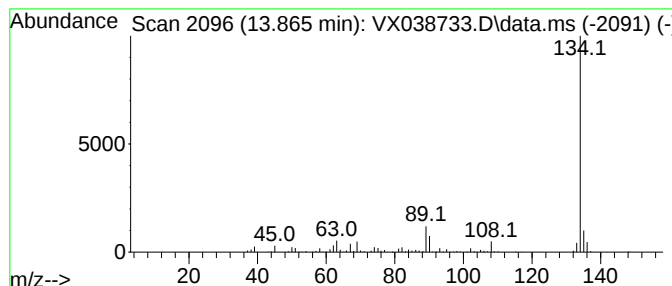
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[c]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.865	6.28 ug/l	181418	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
3			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
4			3-Deazaadenine	134	C6H6N4	006811-77-4	59
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038733.D
Acq On : 10 Nov 2023 16:57
Operator : JC/MD
Sample : 05331-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.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
Di-sec-Butyl ether	8.958	8.0	ug/l	200107	3	10.055	1250790	50.0
3-Pentanol, 3-e...	9.043	9.3	ug/l	231731	3	10.055	1250790	50.0
Benzene, 1-ethy...	11.610	31.0	ug/l	897129	4	12.024	1445170	50.0
Mesitylene	12.085	45.0	ug/l	1299120	4	12.024	1445170	50.0
Indane	12.244	60.5	ug/l	1748560	4	12.024	1445170	50.0
o-Cymene	12.610	5.5	ug/l	159775	4	12.024	1445170	50.0
Indan, 1-methyl-	12.701	6.9	ug/l	200103	4	12.024	1445170	50.0
Benzene, 2-ethe...	13.292	13.7	ug/l	396870	4	12.024	1445170	50.0
Benzo[c]thiophene	13.865	6.3	ug/l	181418	4	12.024	1445170	50.0