

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
 Data File : VX033747.D
 Acq On : 16 Jan 2023 14:12
 Operator : JC/MD
 Sample : 01161-01 50X
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20230113-H4-STOCKPILE

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\82X011123W.M
 Title : SW846 8260

Signal : TIC: VX033747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	693	705	717	rBV	78913	230940	31.13%	3.864%
2	5.550	720	732	749	rVB2	147431	426247	57.46%	7.132%
3	5.952	788	798	806	rBV	88128	235961	31.81%	3.948%
4	6.038	806	812	826	rVB	64452	168032	22.65%	2.811%
5	6.611	898	906	915	rVB3	5575	13997	1.89%	0.234%
6	6.757	921	930	945	rBV	214003	516481	69.62%	8.641%
7	7.379	1023	1032	1039	rBV4	6645	14381	1.94%	0.241%
8	8.647	1234	1240	1246	rBV	489232	741813	100.00%	12.411%
9	8.720	1246	1252	1264	rVB	214365	348874	47.03%	5.837%
10	8.909	1278	1283	1290	rBV2	10322	15921	2.15%	0.266%
11	10.055	1465	1471	1483	rVB	448602	617312	83.22%	10.328%
12	10.195	1488	1494	1504	rBV	214518	287140	38.71%	4.804%
13	10.299	1504	1511	1517	rVV	270800	363055	48.94%	6.074%
14	10.360	1517	1521	1530	rVB	10941	15252	2.06%	0.255%
15	10.640	1562	1567	1579	rVB	108479	144551	19.49%	2.419%
16	10.963	1611	1620	1624	rBV	10567	15543	2.10%	0.260%
17	11.079	1634	1639	1654	rVB	390825	489008	65.92%	8.182%
18	11.305	1671	1676	1681	rBV	13925	16906	2.28%	0.283%
19	11.378	1683	1688	1695	rVV	46687	85000	11.46%	1.422%
20	11.451	1695	1700	1710	rVB2	26659	46529	6.27%	0.778%
21	11.610	1721	1726	1734	rBV	12459	18397	2.48%	0.308%
22	11.750	1745	1749	1756	rVB	64824	80138	10.80%	1.341%
23	12.018	1788	1793	1800	rVV	439658	576625	77.73%	9.648%
24	12.085	1800	1804	1808	rVV	16905	22087	2.98%	0.370%
25	12.128	1808	1811	1817	rVB	13474	16476	2.22%	0.276%
26	12.244	1824	1830	1838	rBV2	24302	35412	4.77%	0.592%
27	12.317	1838	1842	1849	rBV3	7019	12917	1.74%	0.216%
28	12.414	1849	1858	1864	rBV	98599	132087	17.81%	2.210%
29	12.610	1885	1890	1894	rBV2	6478	8824	1.19%	0.148%
30	13.292	1994	2002	2007	rBV6	5086	11202	1.51%	0.187%
31	13.341	2007	2010	2017	rVV	12859	15070	2.03%	0.252%
32	13.426	2019	2024	2030	rVB2	11310	14412	1.94%	0.241%
33	13.774	2076	2081	2092	rBV	162936	205583	27.71%	3.440%
34	14.640	2219	2223	2232	rBV	18158	22368	3.02%	0.374%
35	14.780	2241	2246	2251	rBV	9998	12341	1.66%	0.206%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M

Title : SW846 8260

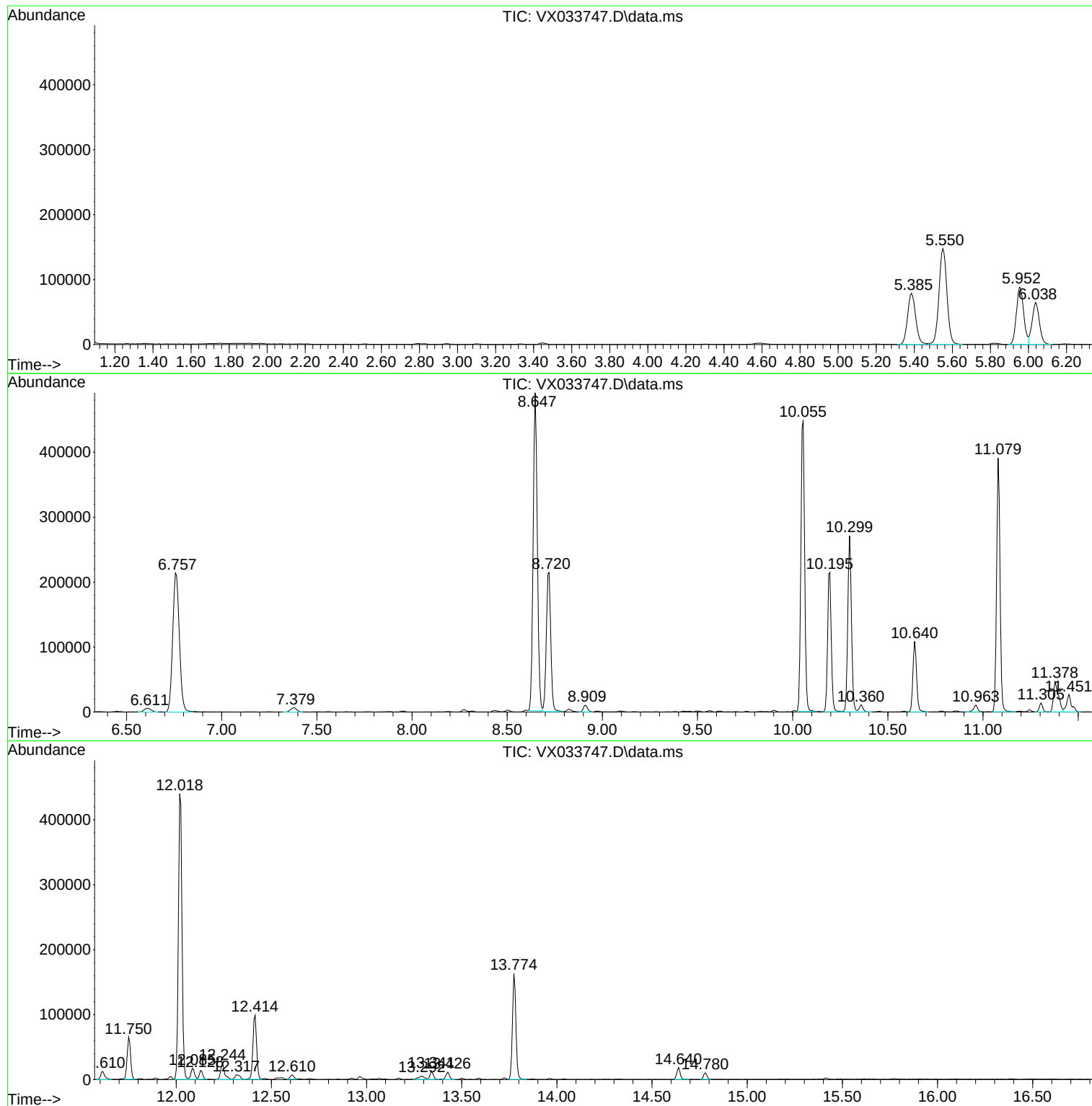
Sum of corrected areas: 5976882

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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



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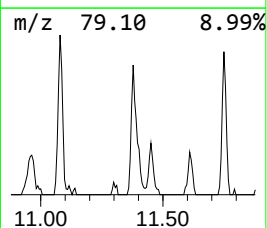
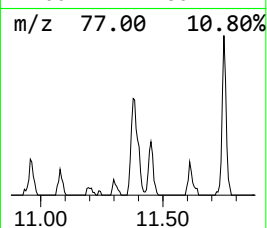
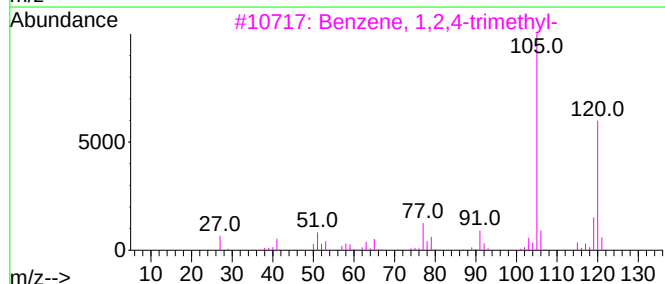
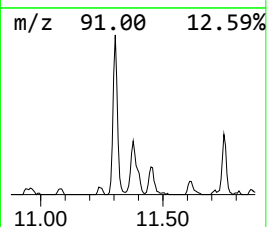
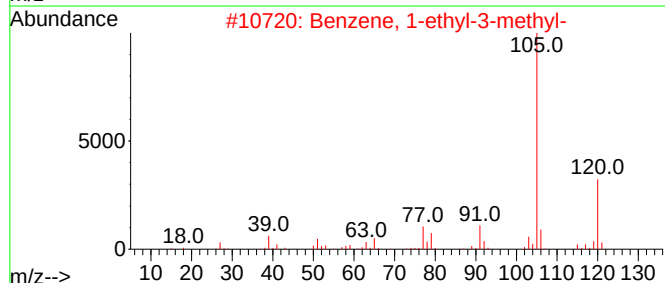
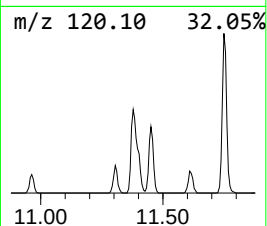
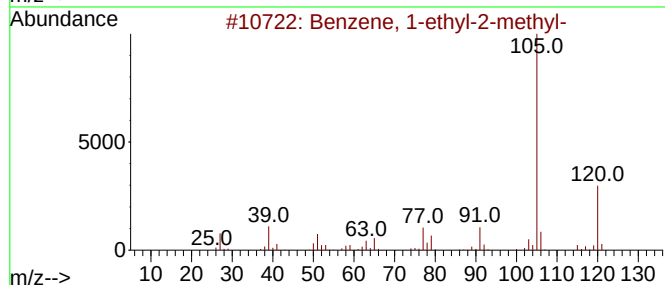
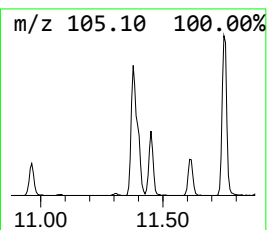
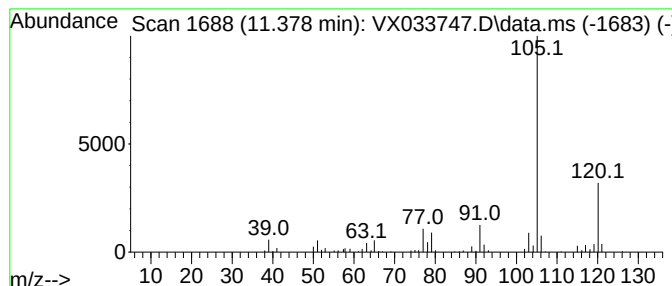
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	7.37 ug/l	85000	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	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	90



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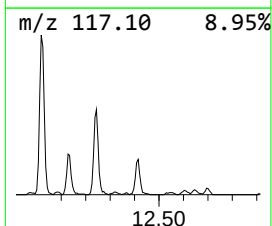
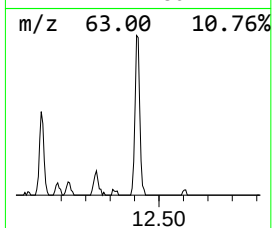
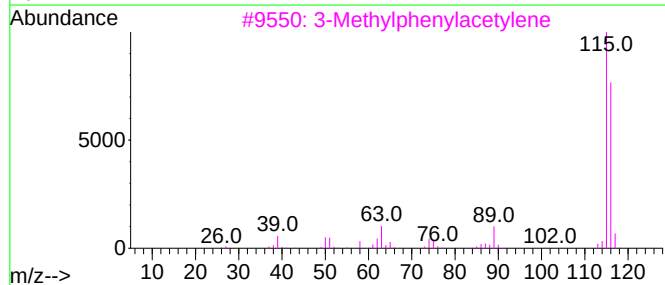
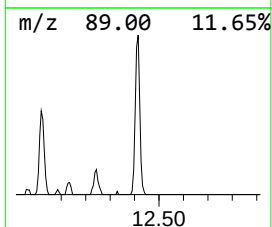
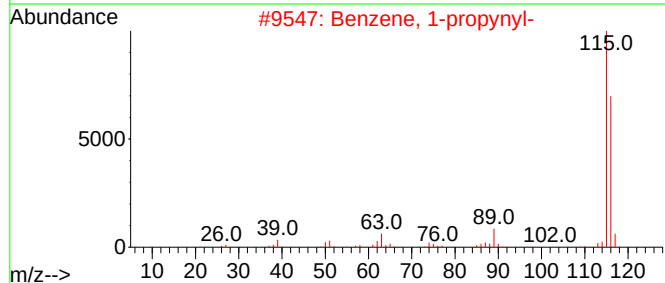
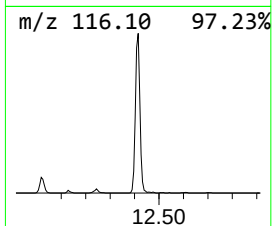
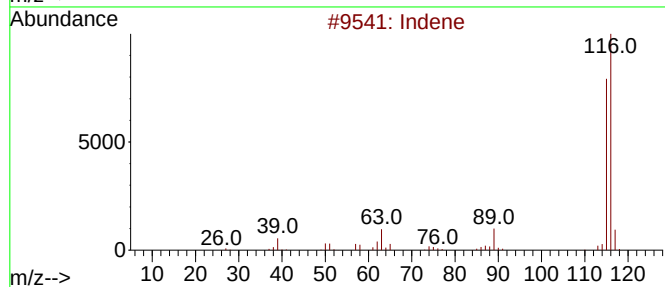
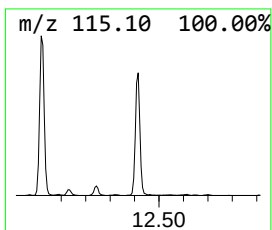
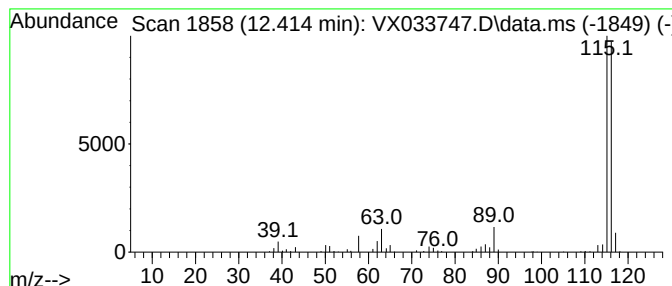
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 2 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	11.45 ug/l	132087	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethy...	11.378	7.4	ug/l	85000	4	12.024	576625	50.0
Indene	12.414	11.4	ug/l	132087	4	12.024	576625	50.0