

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
 Data File : VX033749.D
 Acq On : 16 Jan 2023 15:34
 Operator : JC/MD
 Sample : 01161-01 10X
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 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: VX033749.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.440	378	386	399	rBV	16547	36360	1.71%	0.205%
2	5.379	692	704	714	rBV	88247	249375	11.75%	1.404%
3	5.544	714	731	752	rVB	154166	486796	22.94%	2.740%
4	5.818	765	776	788	rBV3	11529	35099	1.65%	0.198%
5	5.946	788	797	803	rBV	88102	229353	10.81%	1.291%
6	6.031	803	811	826	rVB	299263	788138	37.13%	4.436%
7	6.604	895	905	913	rBV2	50083	119287	5.62%	0.671%
8	6.757	920	930	941	rBV	246659	587607	27.68%	3.307%
9	7.373	1022	1031	1040	rBV	40096	93447	4.40%	0.526%
10	8.269	1172	1178	1182	rBV	29126	47373	2.23%	0.267%
11	8.433	1199	1205	1209	rBV2	22367	36555	1.72%	0.206%
12	8.500	1209	1216	1226	rVB	16699	34368	1.62%	0.193%
13	8.598	1226	1232	1234	rBV	19306	31964	1.51%	0.180%
14	8.647	1234	1240	1245	rVV	512553	825375	38.89%	4.646%
15	8.714	1245	1251	1264	rVV	1223045	1878437	88.50%	10.573%
16	8.824	1264	1269	1277	rVB2	32761	58264	2.75%	0.328%
17	8.909	1277	1283	1290	rBV	99139	143694	6.77%	0.809%
18	9.561	1386	1390	1394	rVB	15229	21456	1.01%	0.121%
19	9.903	1442	1446	1450	rVB2	22010	31211	1.47%	0.176%
20	10.006	1459	1463	1466	rBV	20065	25797	1.22%	0.145%
21	10.049	1466	1470	1477	rVB	507885	682666	32.16%	3.842%
22	10.189	1488	1493	1499	rBV	1238328	1642378	77.38%	9.244%
23	10.299	1504	1511	1517	rVV	1598389	2122498	100.00%	11.946%
24	10.360	1517	1521	1531	rVB	103224	139179	6.56%	0.783%
25	10.640	1562	1567	1582	rVB	636790	836281	39.40%	4.707%
26	10.780	1582	1590	1594	rBV2	14243	22903	1.08%	0.129%
27	10.963	1612	1620	1624	rBV	61662	98945	4.66%	0.557%
28	11.079	1633	1639	1651	rVB	450836	587543	27.68%	3.307%
29	11.244	1660	1666	1671	rVB	23470	35567	1.68%	0.200%
30	11.305	1671	1676	1683	rVV	83313	105799	4.98%	0.595%
31	11.378	1683	1688	1694	rVV	310895	533424	25.13%	3.002%
32	11.451	1694	1700	1702	rVV	165423	259092	12.21%	1.458%
33	11.475	1702	1704	1714	rVB	82281	92199	4.34%	0.519%
34	11.610	1722	1726	1734	rBV	78379	118107	5.56%	0.665%
35	11.750	1744	1749	1756	rVB	414663	509770	24.02%	2.869%
36	11.969	1777	1785	1788	rBV2	31908	50170	2.36%	0.282%

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37	12.018	1788	1793	1799	rVV	534796	702323	33.09%	3.953%
38	12.085	1799	1804	1808	rVV	103936	132929	6.26%	0.748%
39	12.128	1808	1811	1816	rVB	94431	111539	5.26%	0.628%
40	12.244	1823	1830	1838	rBV2	149158	229361	10.81%	1.291%
41	12.317	1838	1842	1848	rBV4	51797	80729	3.80%	0.454%
42	12.414	1848	1858	1864	rVV	640004	862237	40.62%	4.853%
43	12.530	1873	1877	1879	rBV	19672	25942	1.22%	0.146%
44	12.609	1884	1890	1894	rBV2	45315	67192	3.17%	0.378%
45	12.701	1900	1905	1917	rVB4	10599	22285	1.05%	0.125%
46	12.963	1944	1948	1955	rVB	34387	51814	2.44%	0.292%
47	13.170	1975	1982	1986	rBV2	17459	25532	1.20%	0.144%
48	13.268	1995	1998	1999	rBV	22713	23813	1.12%	0.134%
49	13.286	1999	2001	2007	rVV3	30680	56284	2.65%	0.317%
50	13.341	2007	2010	2015	rVV	93514	106958	5.04%	0.602%
51	13.426	2019	2024	2032	rVB	85631	117630	5.54%	0.662%
52	13.499	2032	2036	2041	rBV2	16794	22807	1.07%	0.128%
53	13.774	2076	2081	2091	rBV	1019573	1218249	57.40%	6.857%
54	14.640	2217	2223	2232	rVB	143421	189032	8.91%	1.064%
55	14.780	2240	2246	2259	rVB	77148	99565	4.69%	0.560%
56	15.414	2346	2350	2356	rVB	16961	24368	1.15%	0.137%

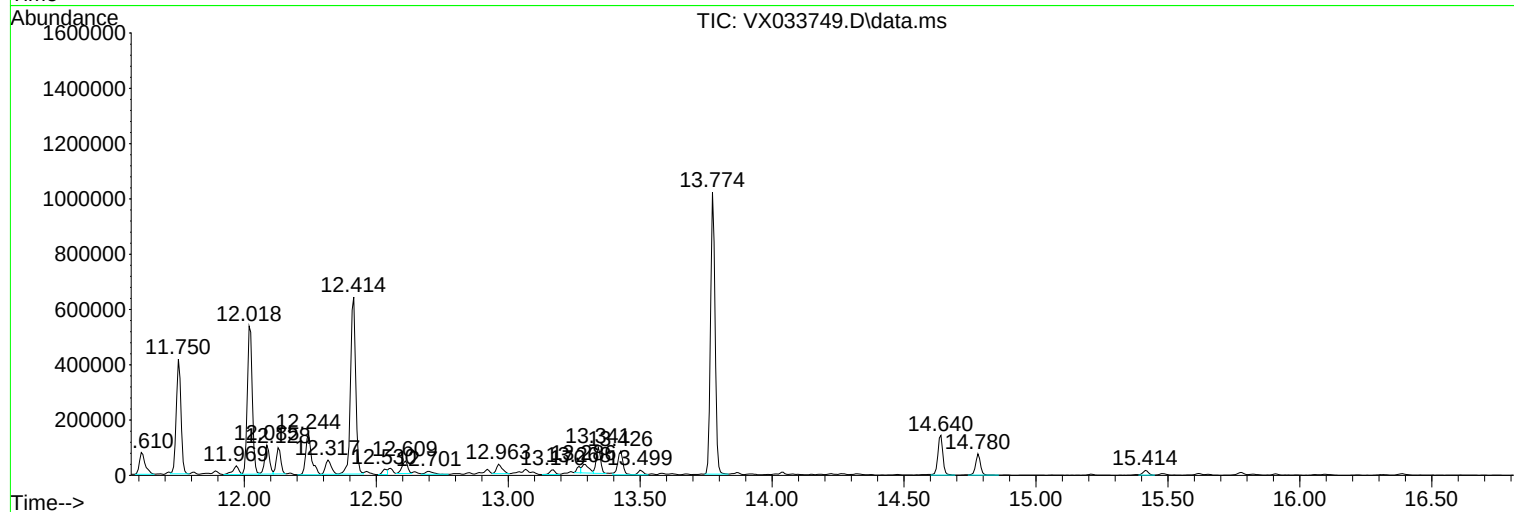
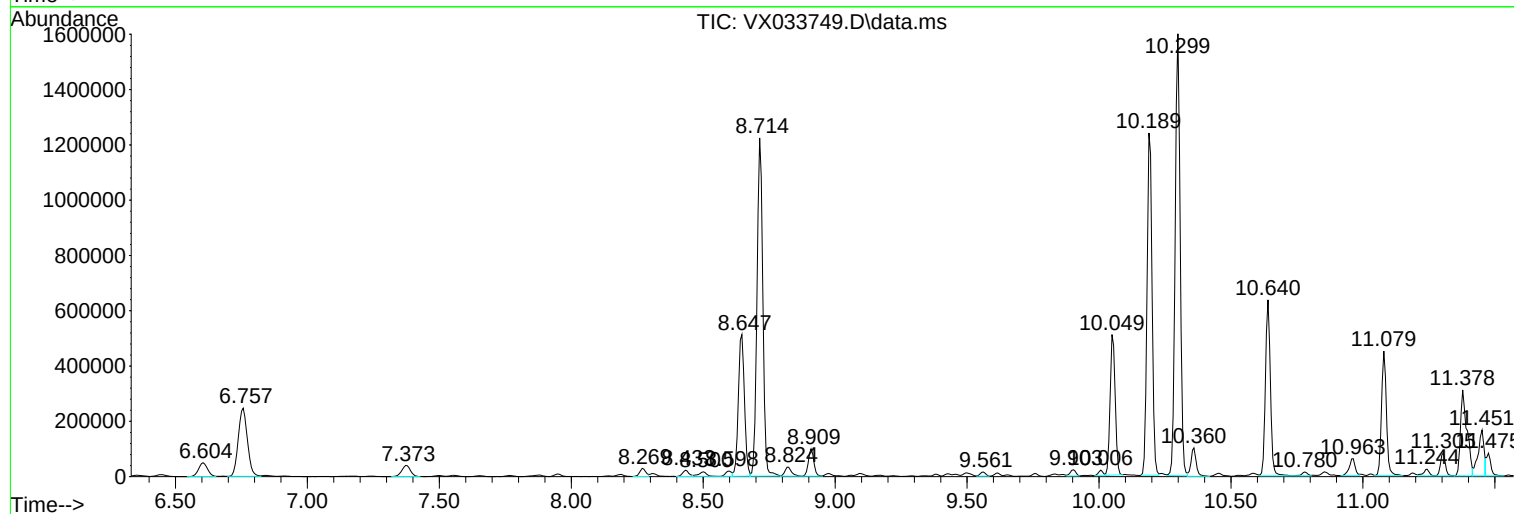
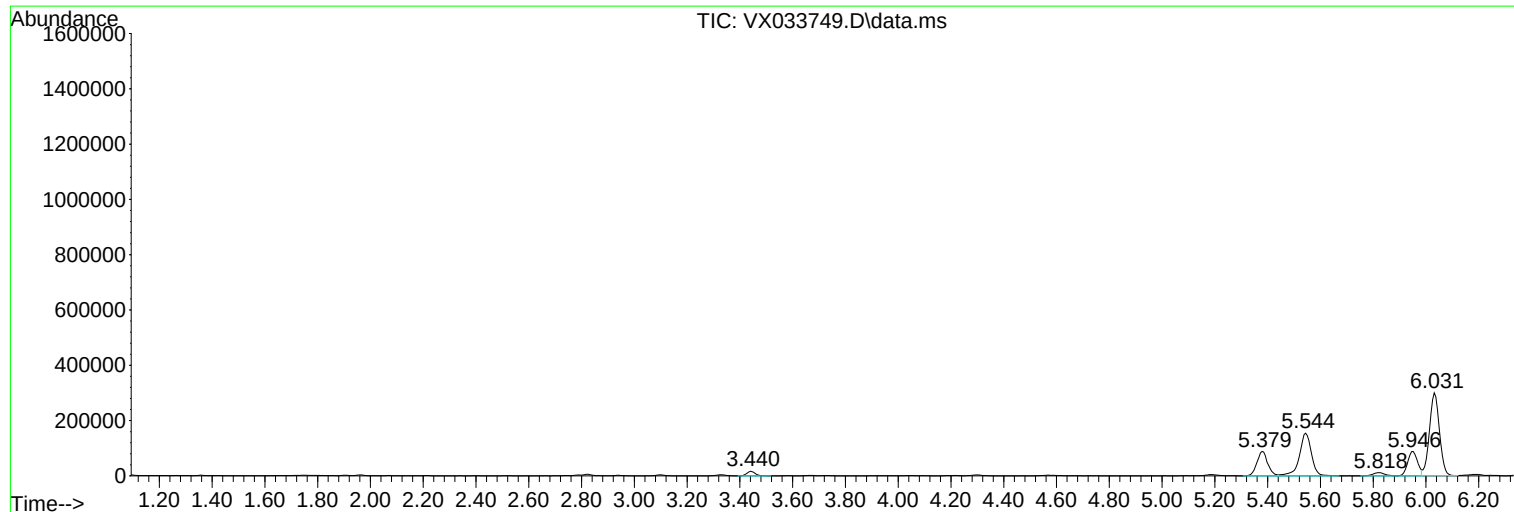
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Quant Title : SW846 8260

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



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MSVOA_X
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20230113-H4-STOCKPILE

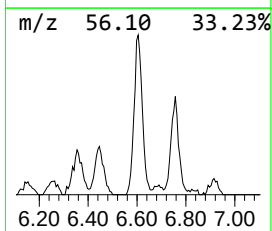
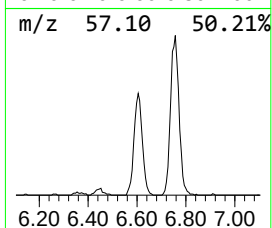
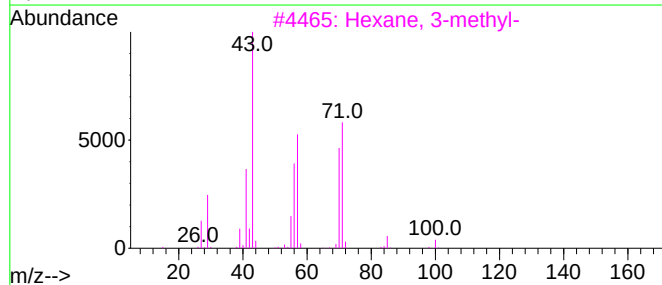
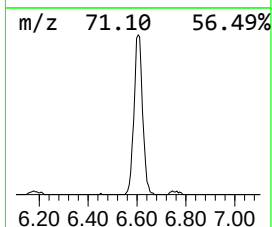
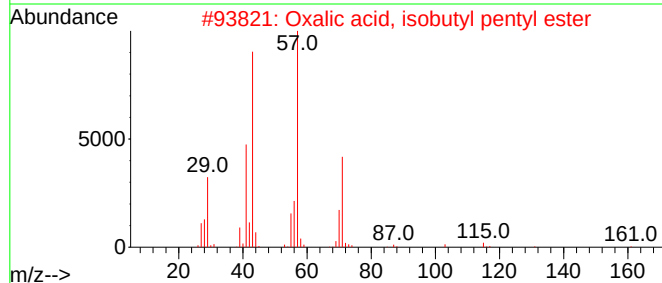
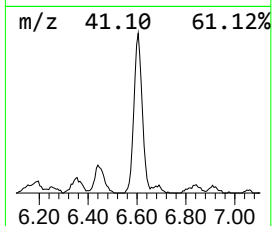
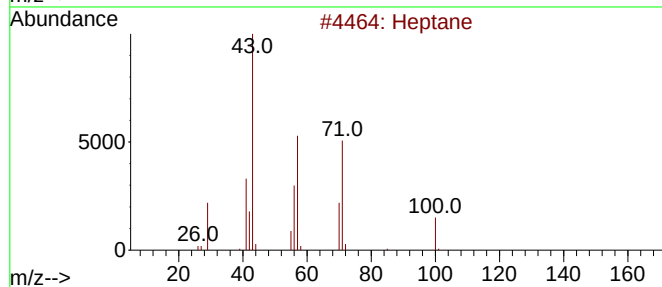
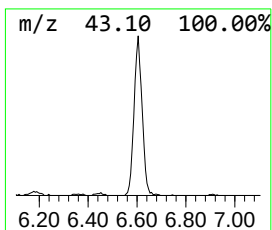
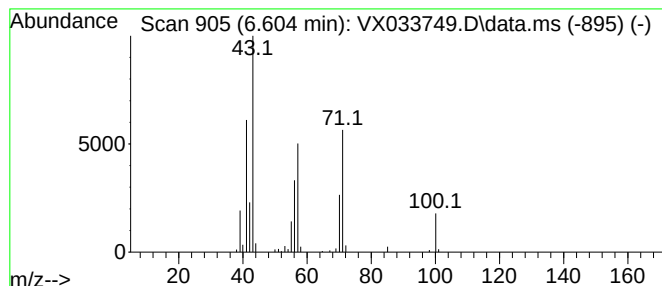
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Quant Title : SW846 8260

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

Peak Number 1 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	10.15 ug/l	119287	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38



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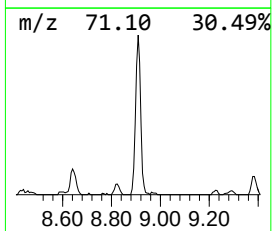
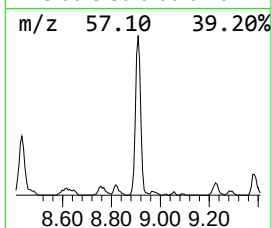
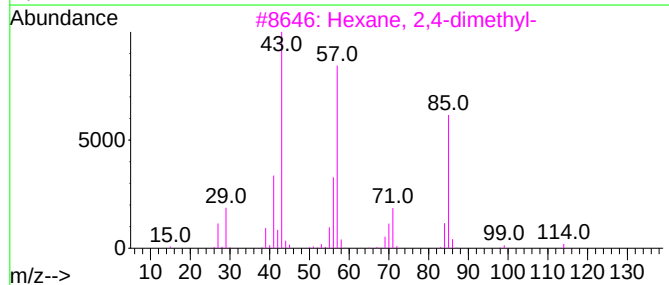
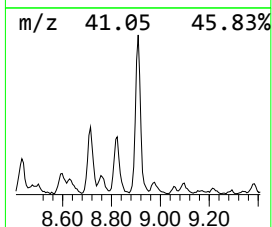
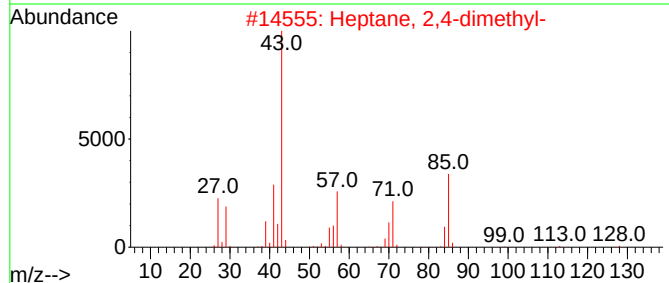
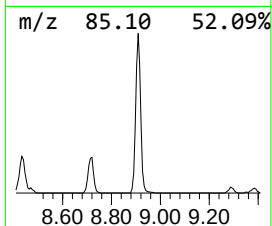
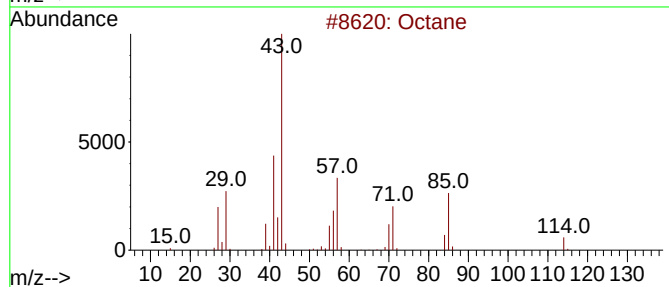
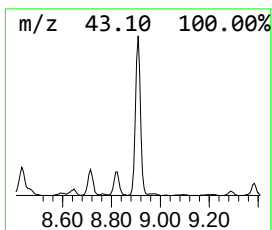
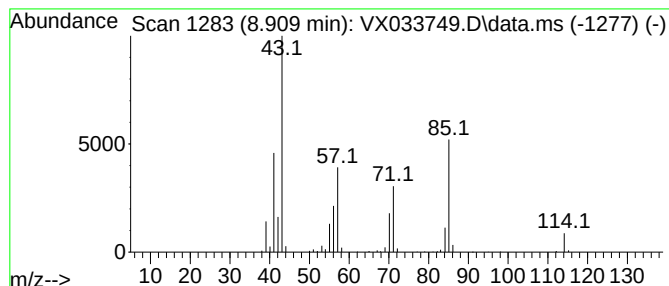
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 2 Octane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.909	10.52 ug/l	143694	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	94
2	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	86
3	Hexane, 2,4-dimethyl-			114	C8H18	000589-43-5	64
4	Undecane, 2,4-dimethyl-			184	C13H28	017312-80-0	64
5	Oxalic acid, butyl isohexyl ester			230	C12H22O4	1000309-32-7	59



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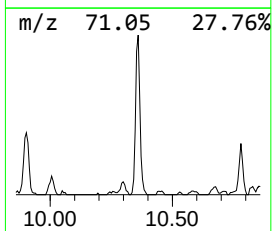
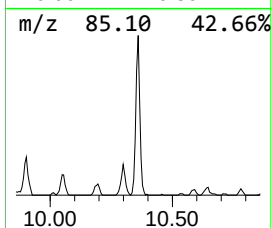
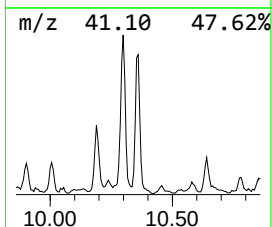
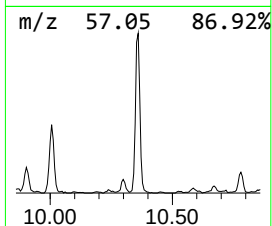
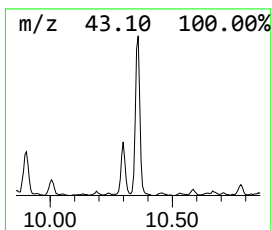
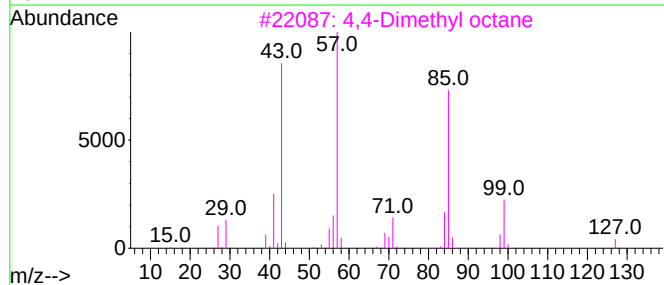
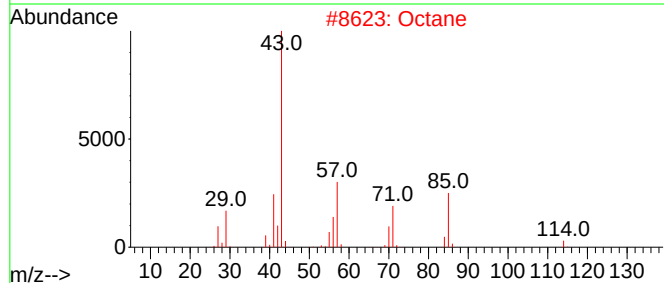
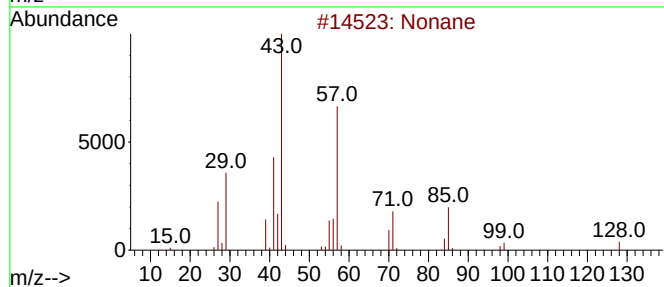
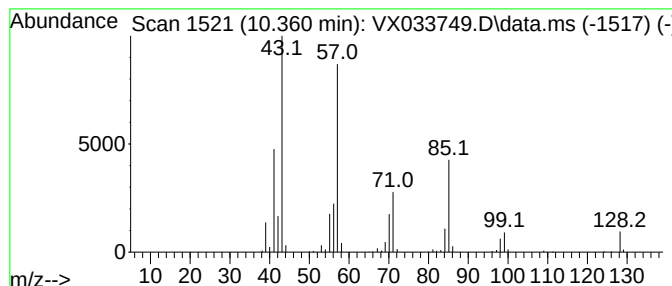
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 3 Nonane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	10.19 ug/l	139179	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	94
2			Octane	114	C8H18	000111-65-9	59
3			4,4-Dimethyl octane	142	C10H22	015869-95-1	53
4			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	50
5			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	50



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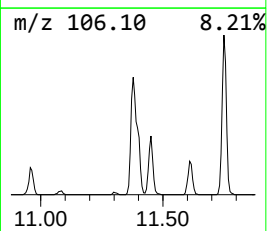
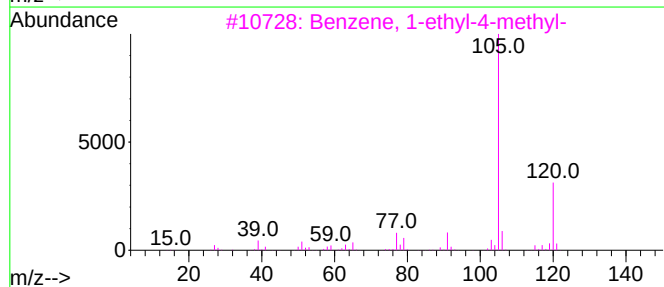
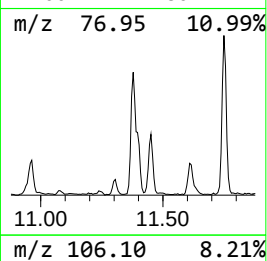
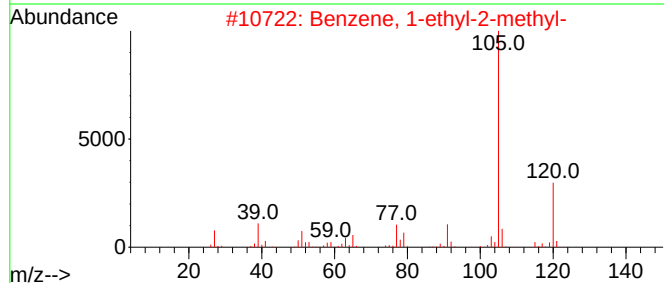
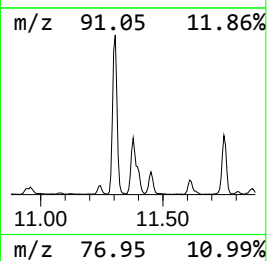
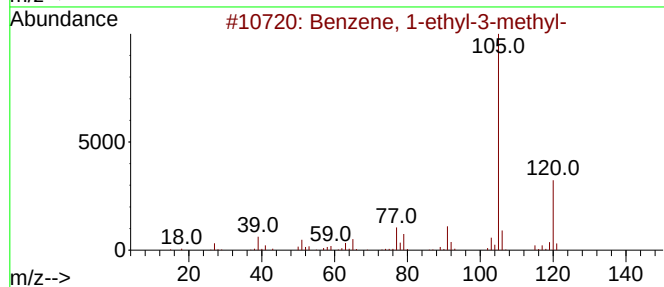
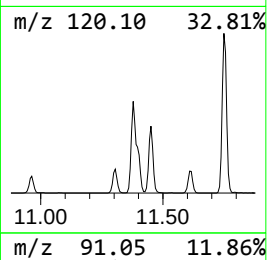
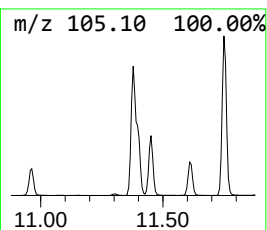
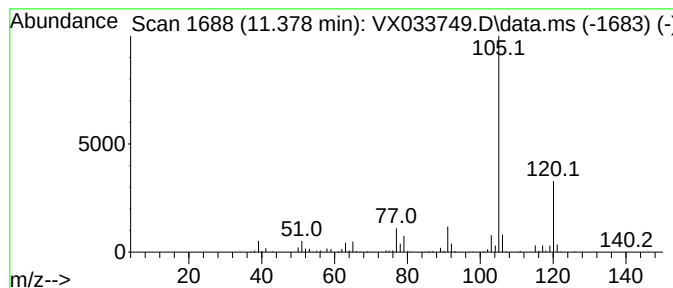
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	37.98 ug/l	533424	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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20230113-H4-STOCKPILE

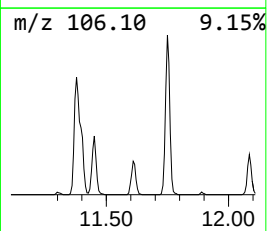
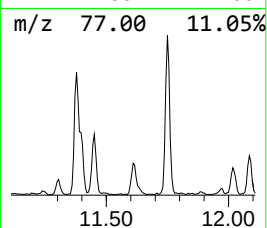
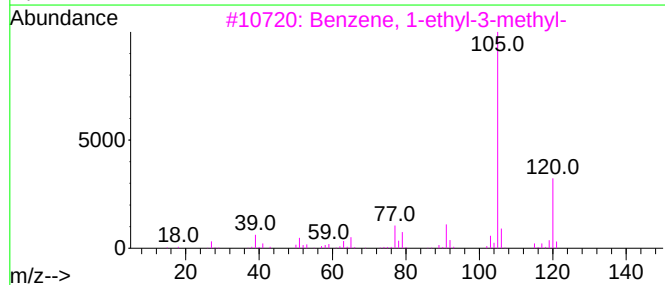
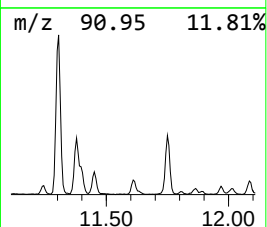
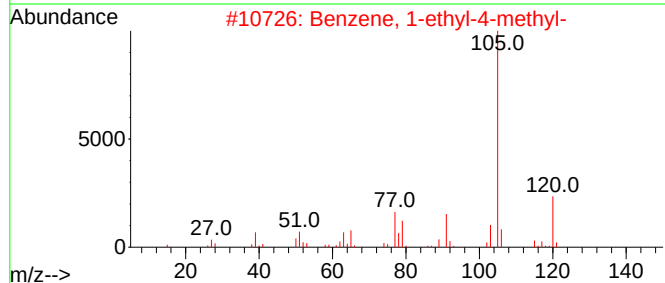
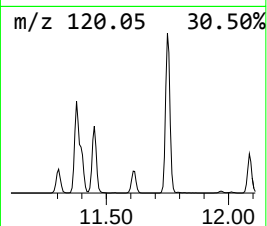
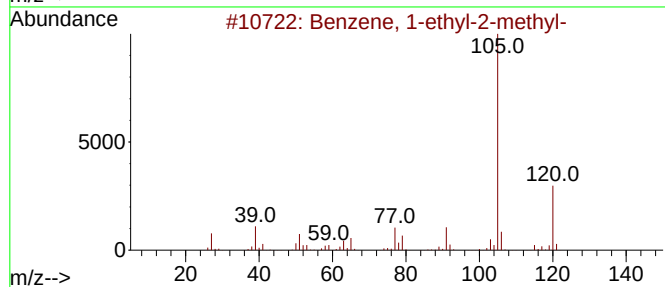
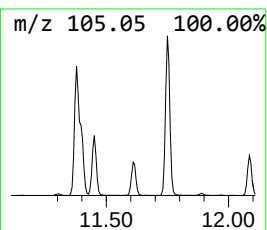
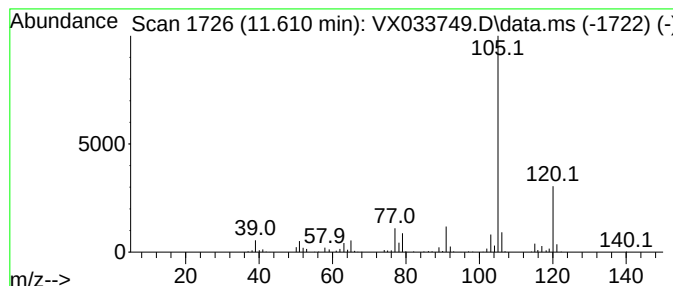
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	8.41 ug/l	118107	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	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Mesitylene	120	C9H12	000108-67-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

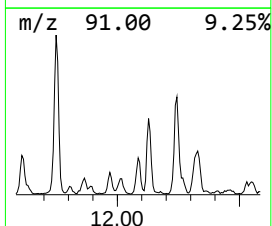
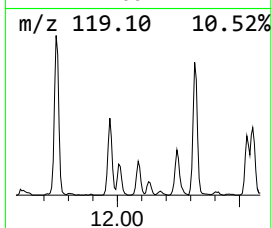
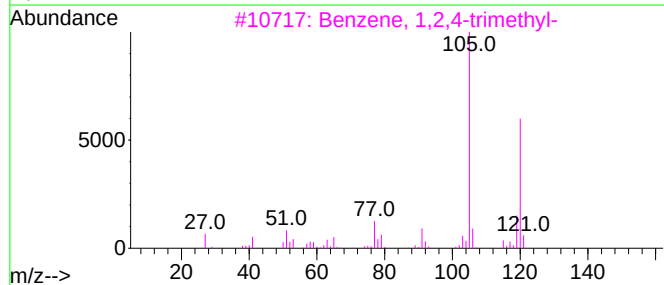
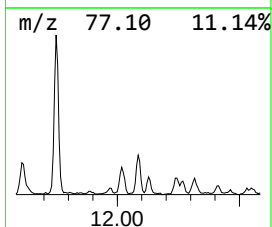
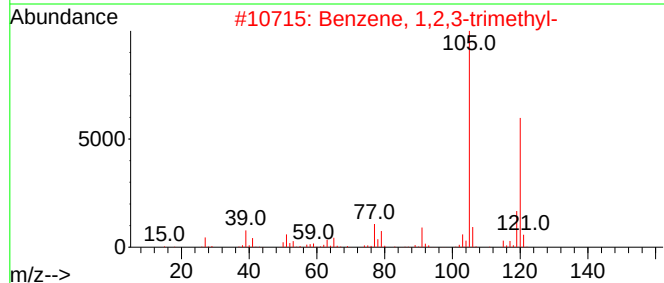
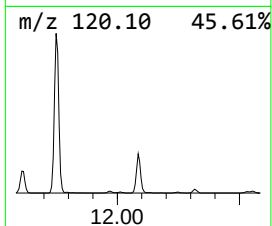
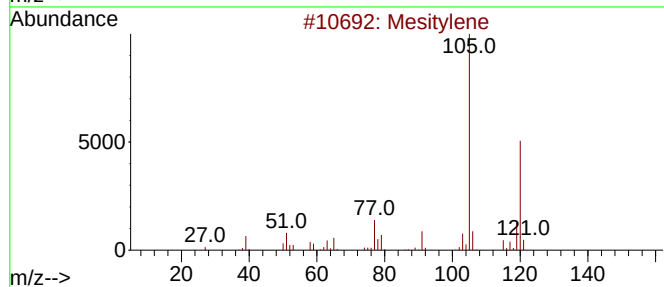
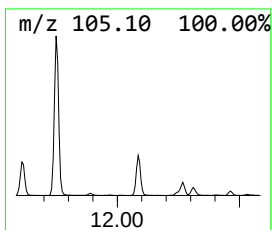
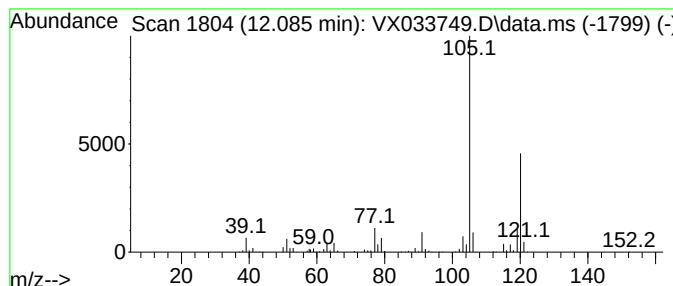
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	9.46 ug/l	132929	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	95
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

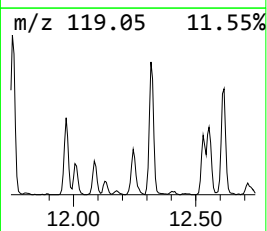
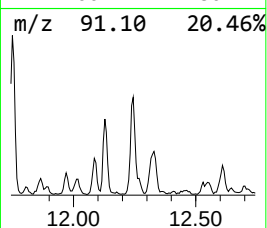
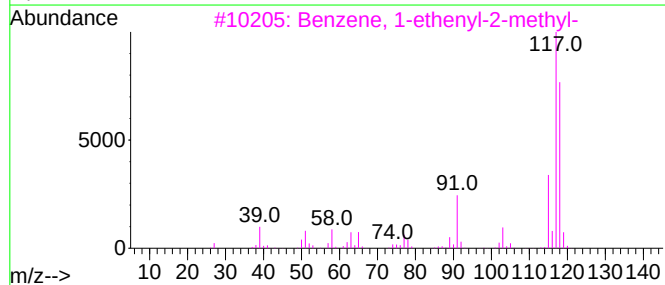
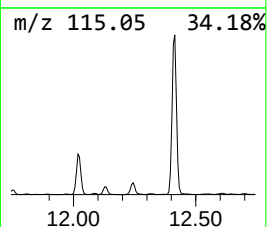
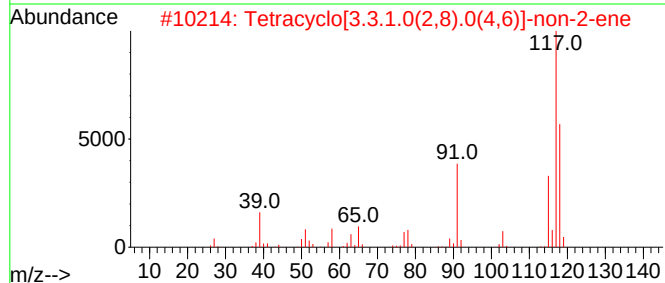
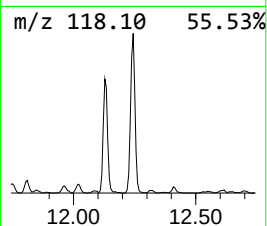
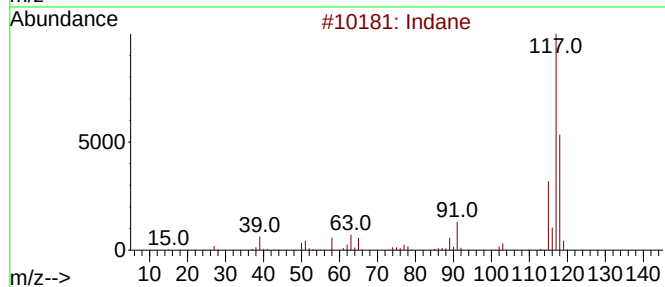
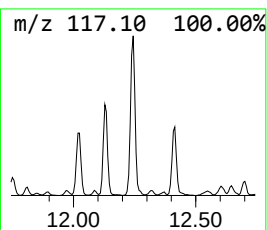
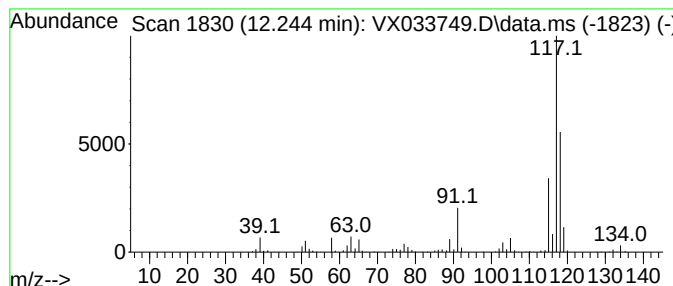
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	16.33 ug/l	229361	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	74
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			Deltacyclene	118	C9H10	007785-10-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

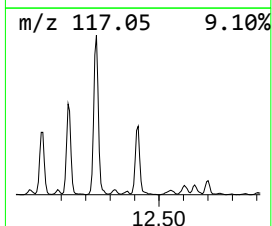
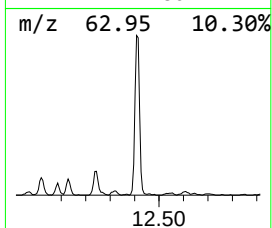
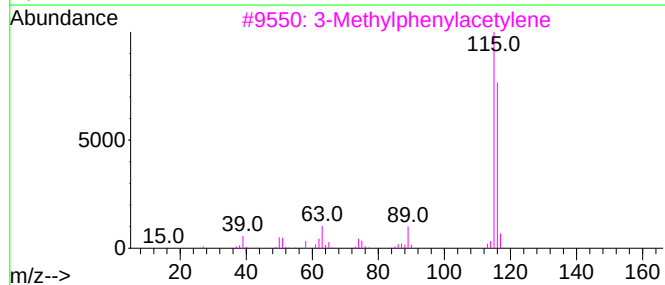
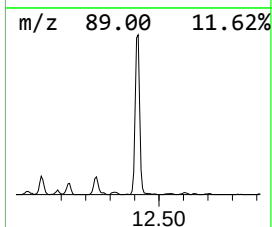
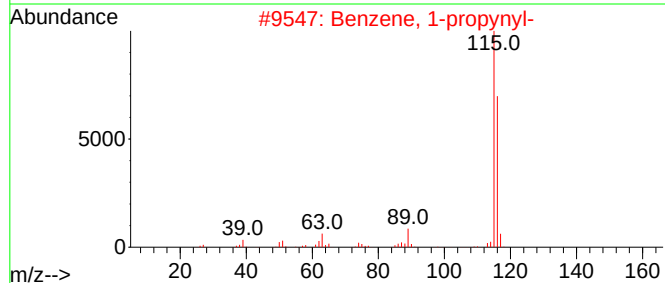
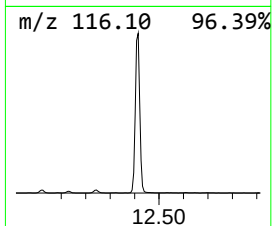
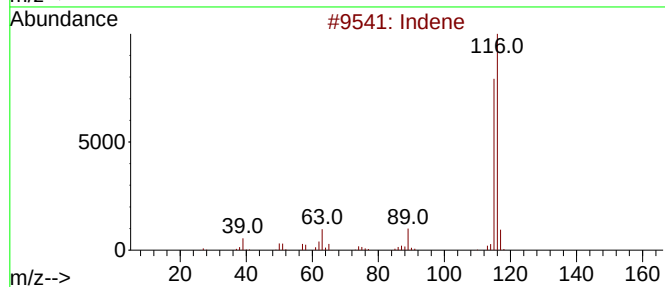
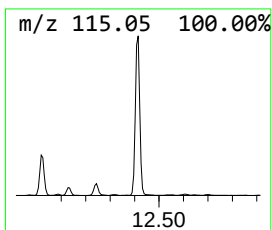
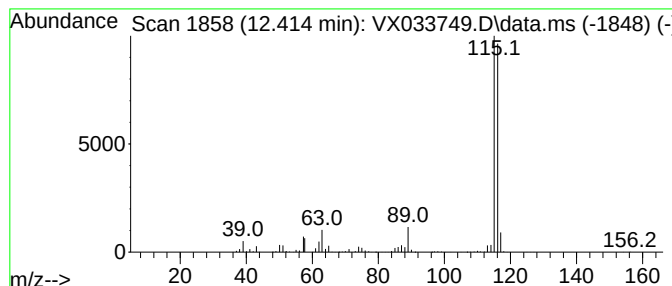
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	61.38 ug/l	862237	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	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

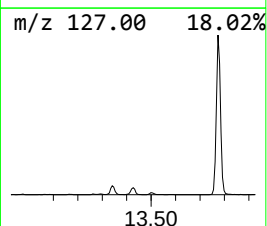
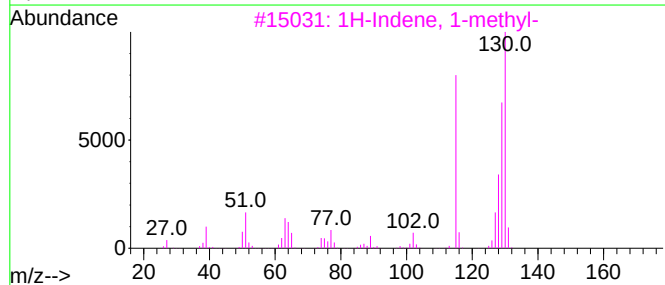
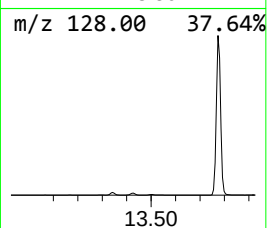
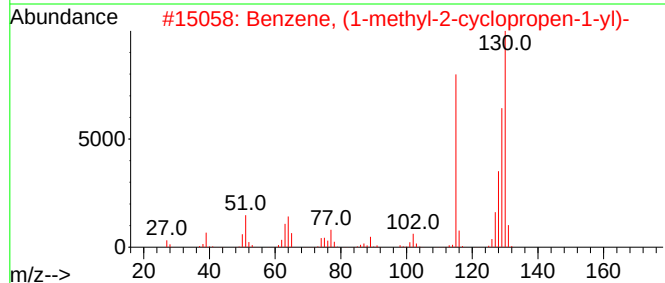
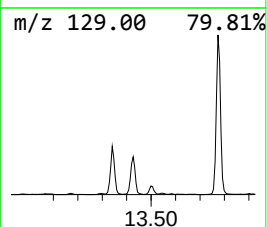
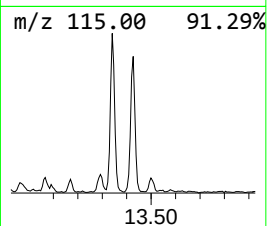
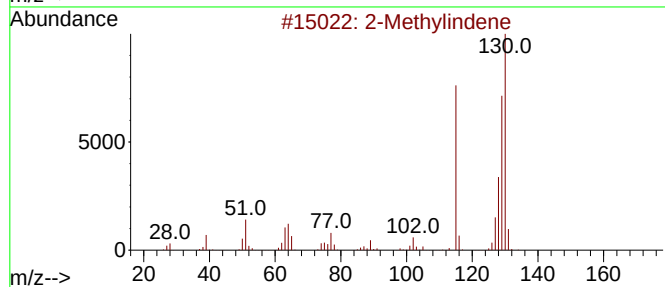
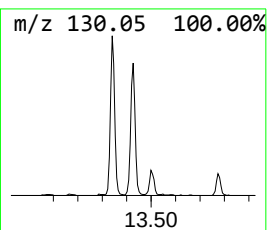
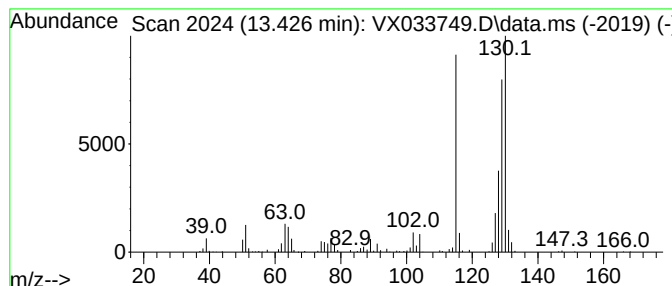
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Quant Title : SW846 8260

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

Peak Number 9 2-Methylindene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	8.37 ug/l	117630	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	97
2			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	94
5			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

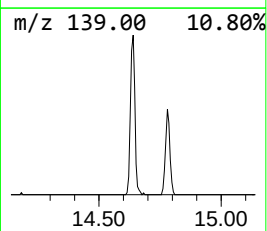
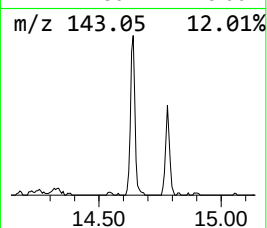
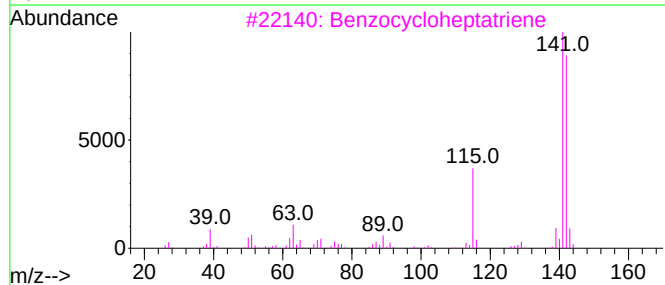
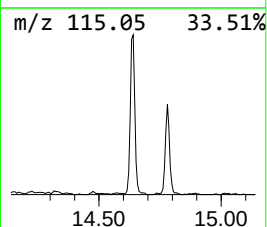
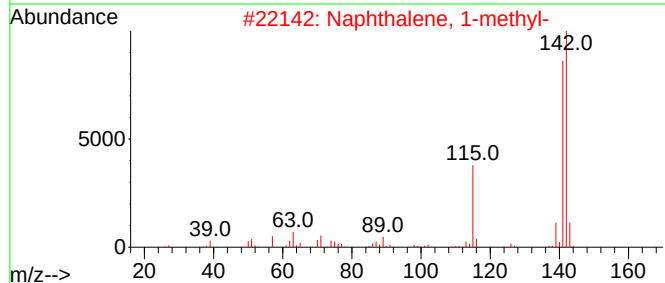
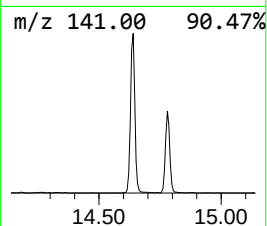
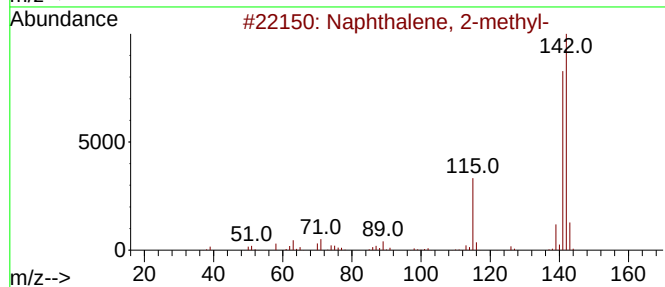
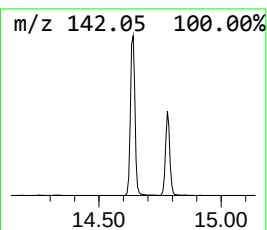
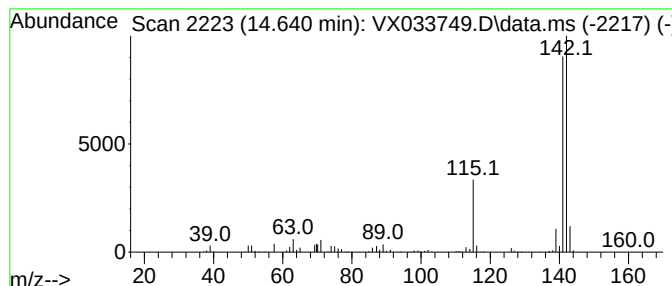
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	13.46 ug/l	189032	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011623\
Data File : VX033749.D
Acq On : 16 Jan 2023 15:34
Operator : JC/MD
Sample : 01161-01 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20230113-H4-STOCKPILE

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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
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Octane	8.909	10.5	ug/l	143694	3	10.049	682666	50.0
Nonane	10.360	10.2	ug/l	139179	3	10.049	682666	50.0
Benzene, 1-ethy...	11.378	38.0	ug/l	533424	4	12.024	702323	50.0
Benzene, 1-ethy...	11.610	8.4	ug/l	118107	4	12.024	702323	50.0
Benzene, 1,2,3-...	12.085	9.5	ug/l	132929	4	12.024	702323	50.0
Indane	12.244	16.3	ug/l	229361	4	12.024	702323	50.0
Indene	12.414	61.4	ug/l	862237	4	12.024	702323	50.0
2-Methylindene	13.426	8.4	ug/l	117630	4	12.024	702323	50.0
Benzocyclohepta...	14.640	13.5	ug/l	189032	4	12.024	702323	50.0