

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060921\
 Data File : VX022628.D
 Acq On : 09 Jun 2021 20:49
 Operator : JC/MD
 Sample : M2610-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 W-8

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\82X060721W.M
 Title : SW846 8260

Signal : TIC: VX022628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.557	74	77	82	rVB5	2985	4207	1.13%	0.152%
2	1.752	105	109	114	rVB4	2444	3921	1.05%	0.142%
3	2.550	230	240	247	rBV3	2669	6167	1.66%	0.223%
4	2.788	273	279	281	rBV4	2264	4720	1.27%	0.171%
5	2.825	281	285	292	rVB3	4563	8436	2.26%	0.305%
6	3.105	324	331	340	rVB2	4957	11408	3.06%	0.413%
7	4.312	520	529	540	rVB2	7997	22738	6.10%	0.823%
8	4.501	551	560	567	rVB4	1993	5311	1.43%	0.192%
9	5.397	695	707	717	rBV	38825	112922	30.32%	4.089%
10	5.562	724	734	745	rBV	63129	173079	46.47%	6.267%
11	5.830	770	778	788	rBV5	3372	9668	2.60%	0.350%
12	5.964	791	800	811	rBV2	50046	134649	36.15%	4.875%
13	6.178	825	835	838	rBV7	2805	7753	2.08%	0.281%
14	6.257	841	848	858	rVB4	8944	25186	6.76%	0.912%
15	6.367	858	866	873	rBV6	2566	6295	1.69%	0.228%
16	6.769	923	932	942	rBV	112720	270456	72.61%	9.793%
17	6.848	942	945	955	rVB5	3094	7741	2.08%	0.280%
18	7.379	1023	1032	1039	rVB5	6471	18834	5.06%	0.682%
19	7.659	1074	1078	1085	rVB4	2336	4163	1.12%	0.151%
20	7.988	1124	1132	1138	rVB3	4739	9747	2.62%	0.353%
21	8.110	1146	1152	1157	rBV3	5875	12946	3.48%	0.469%
22	8.507	1213	1217	1225	rVB5	2788	5516	1.48%	0.200%
23	8.653	1234	1241	1249	rVB	240344	372478	100.00%	13.487%
24	9.165	1319	1325	1330	rVB4	3433	5414	1.45%	0.196%
25	9.506	1376	1381	1387	rVB5	1995	3947	1.06%	0.143%
26	10.055	1466	1471	1481	rBV	230298	316284	84.91%	11.452%
27	10.195	1491	1494	1499	rBV	2932	4250	1.14%	0.154%
28	10.305	1508	1512	1518	rVB	4321	5084	1.36%	0.184%
29	10.963	1616	1620	1626	rVB	20663	26376	7.08%	0.955%
30	11.085	1635	1640	1649	rVB	173982	217738	58.46%	7.884%
31	11.305	1672	1676	1681	rVB	23659	27555	7.40%	0.998%
32	11.616	1724	1727	1731	rVB2	4307	4691	1.26%	0.170%
33	11.890	1770	1772	1777	rVB2	3343	4017	1.08%	0.145%
34	12.024	1789	1794	1802	rVV	209847	254767	68.40%	9.225%
35	12.244	1825	1830	1837	rVB2	134493	178583	47.94%	6.466%
36	12.317	1837	1842	1850	rBV4	9456	14311	3.84%	0.518%

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37	12.408	1853	1857	1863	rVB3	9525	12599	3.38%	0.456%
38	12.469	1863	1867	1872	rBV3	3192	4638	1.25%	0.168%
39	12.616	1887	1891	1894	rBV	16390	19550	5.25%	0.708%
40	12.646	1894	1896	1901	rVV	9351	10129	2.72%	0.367%
41	12.701	1901	1905	1913	rVB2	49453	66534	17.86%	2.409%
42	12.847	1925	1929	1935	rVB4	2558	4928	1.32%	0.178%
43	12.927	1935	1942	1947	rBV	68383	81822	21.97%	2.963%
44	13.030	1955	1959	1966	rVB5	4021	6230	1.67%	0.226%
45	13.140	1972	1977	1979	rBV2	3917	4829	1.30%	0.175%
46	13.170	1979	1982	1990	rVB	28063	35148	9.44%	1.273%
47	13.292	1990	2002	2007	rBV2	76010	103659	27.83%	3.753%
48	13.426	2021	2024	2029	rVB3	5508	6530	1.75%	0.236%
49	13.548	2040	2044	2047	rVV3	9583	14650	3.93%	0.530%
50	13.579	2047	2049	2054	rVV2	10208	13294	3.57%	0.481%
51	13.646	2054	2060	2061	rVV2	9061	14041	3.77%	0.508%
52	13.664	2061	2063	2069	rVB4	8897	12735	3.42%	0.461%
53	13.926	2099	2106	2110	rBV4	3454	4959	1.33%	0.180%
54	13.975	2110	2114	2118	rVB	3734	4455	1.20%	0.161%
55	14.219	2150	2154	2162	rVB	7140	9577	2.57%	0.347%
56	14.323	2167	2171	2175	rBV	4881	6115	1.64%	0.221%
57	14.371	2175	2179	2184	rVB3	5460	6775	1.82%	0.245%
58	14.780	2242	2246	2252	rBV	13813	17200	4.62%	0.623%

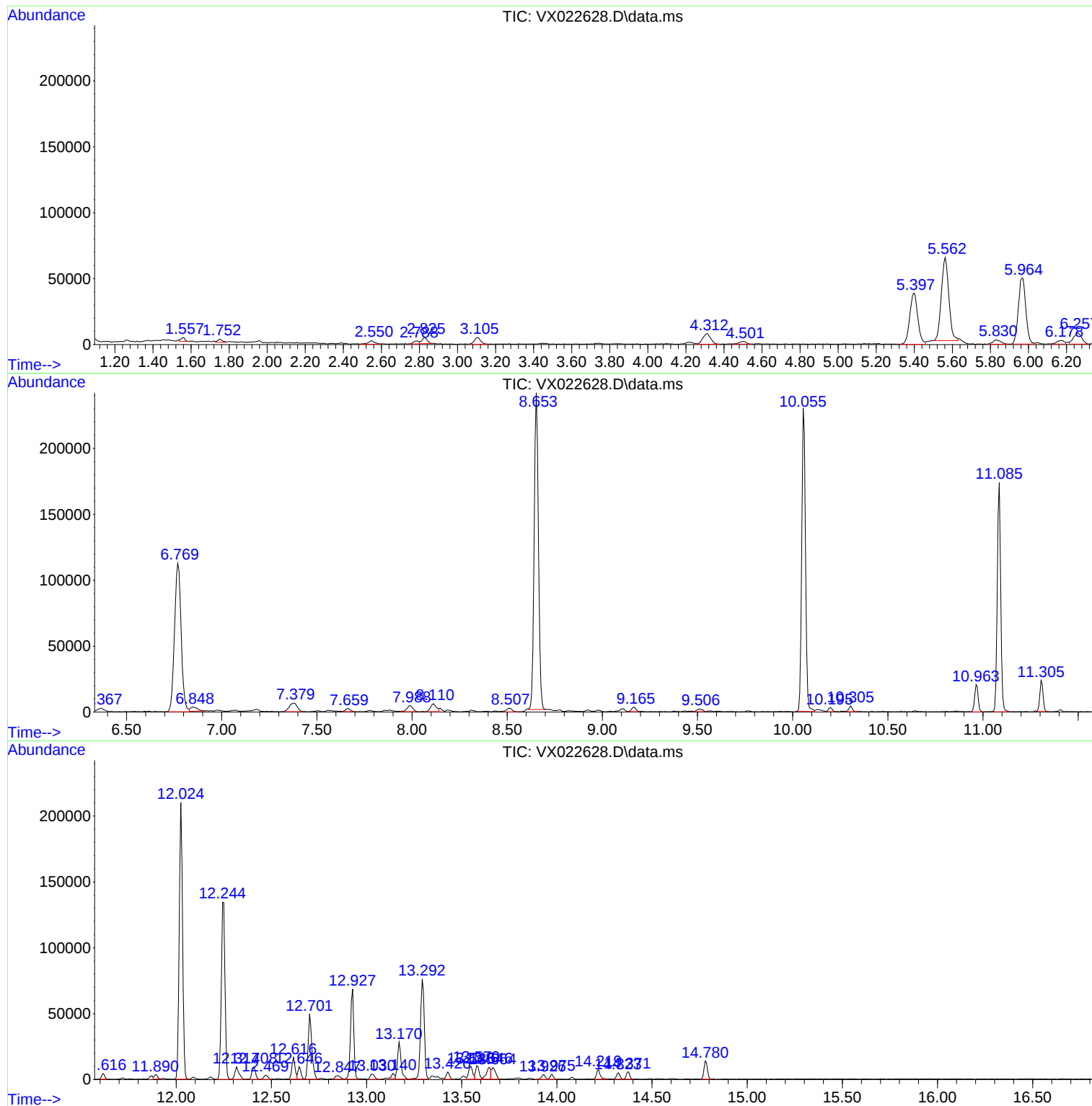
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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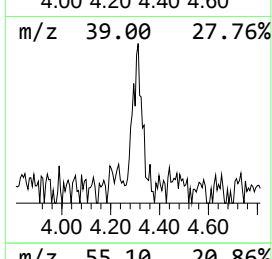
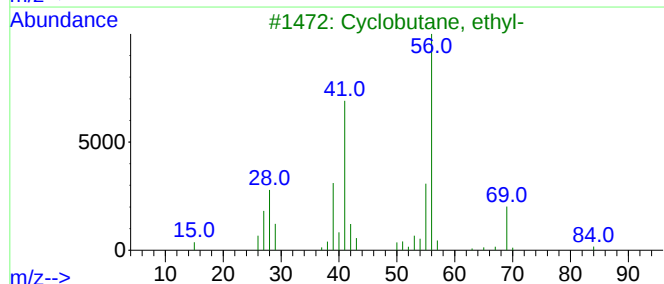
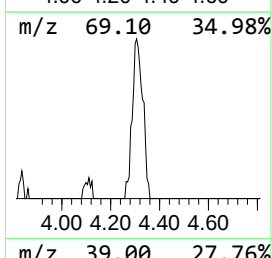
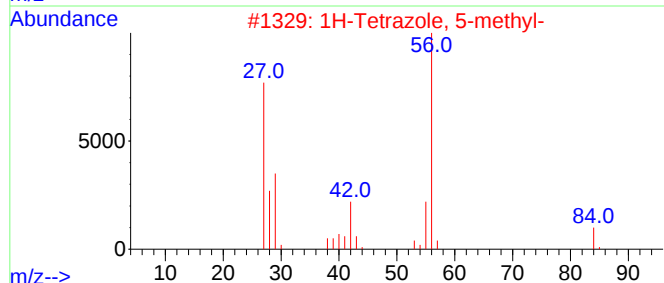
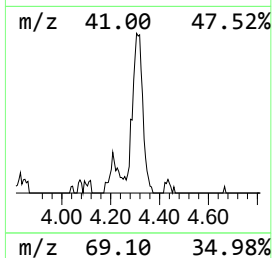
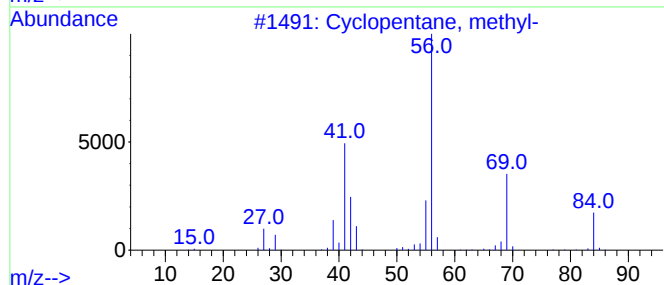
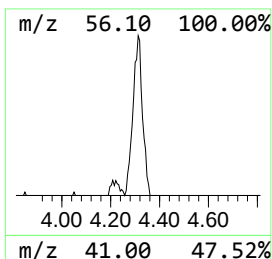
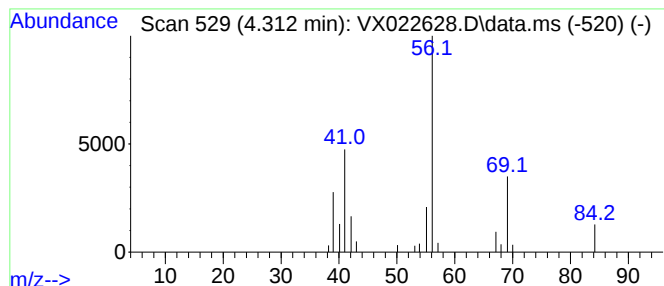
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	6.57 ug/l	22738	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45
5			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	36



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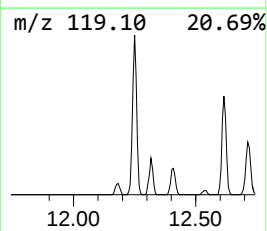
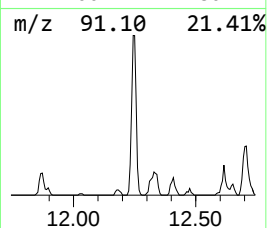
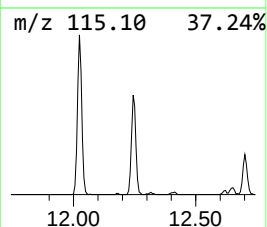
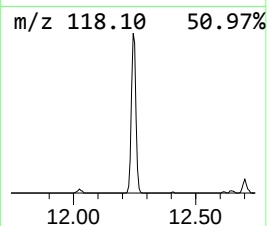
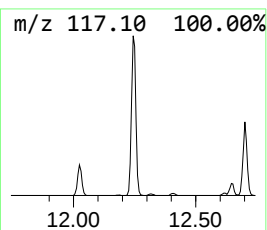
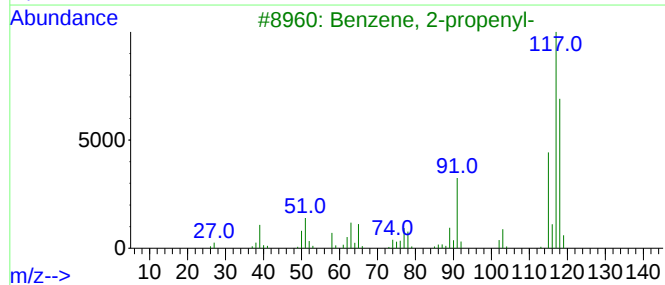
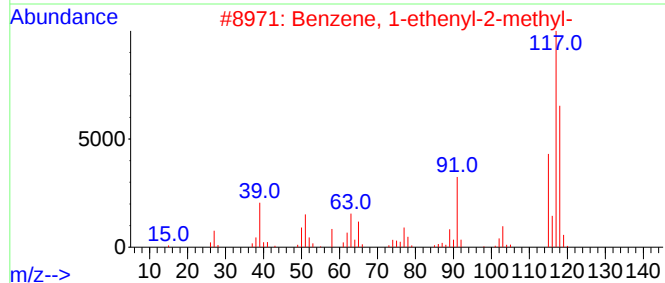
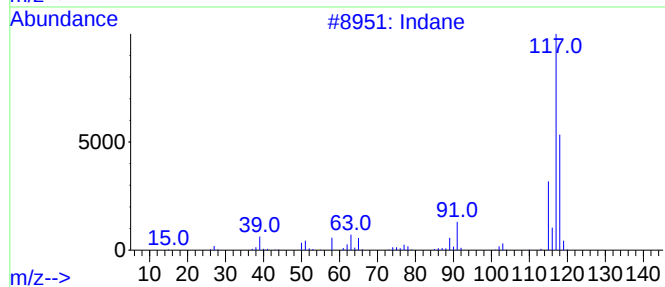
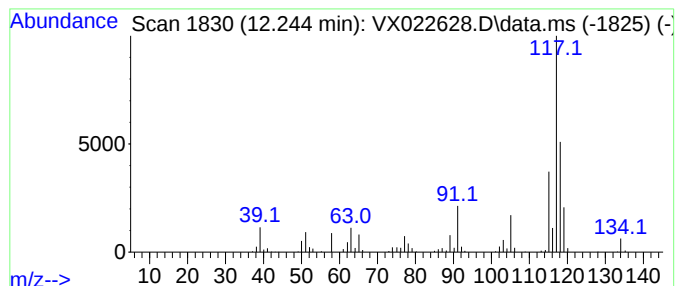
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	35.05 ug/l	178583	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, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	86
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
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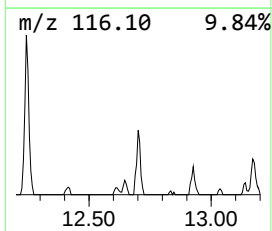
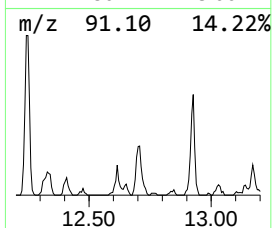
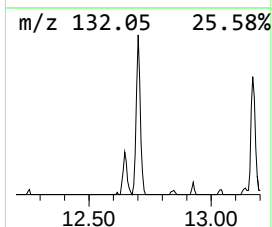
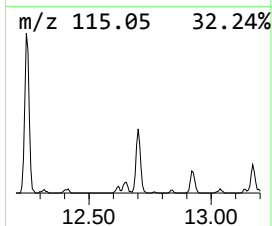
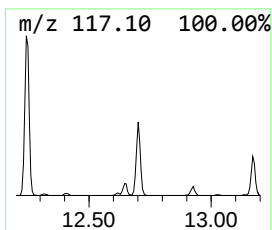
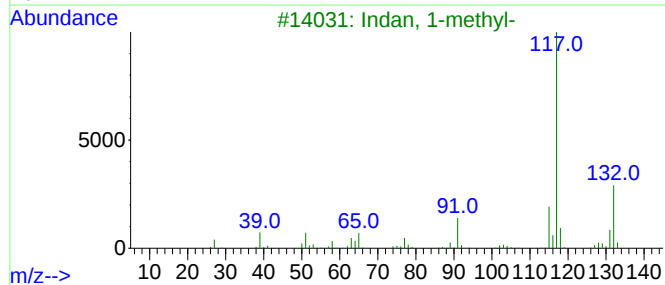
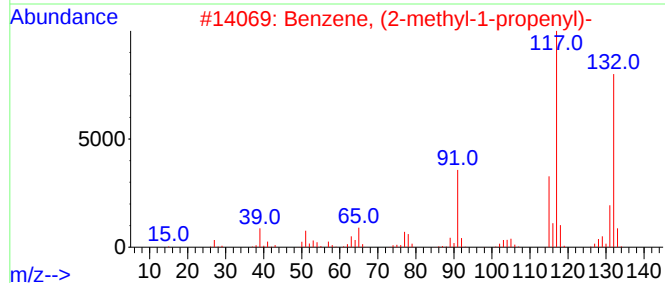
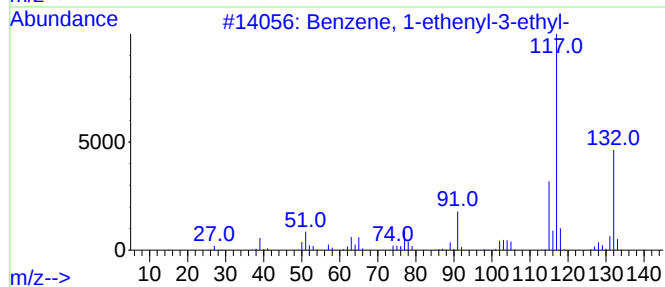
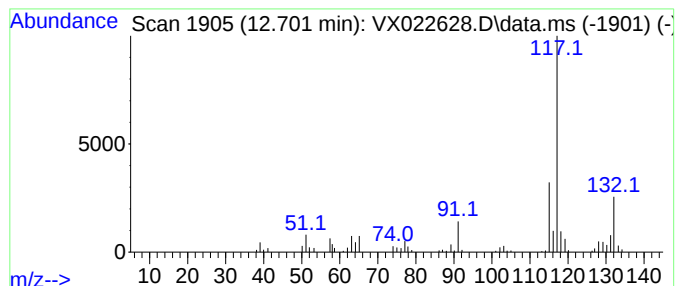
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	13.06 ug/l	66534	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
3			Indan, 1-methyl-	132	C10H12	000767-58-8	86
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	83



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ClientSampled :
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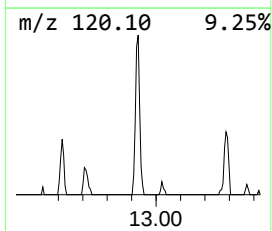
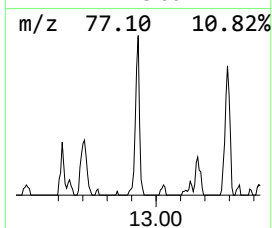
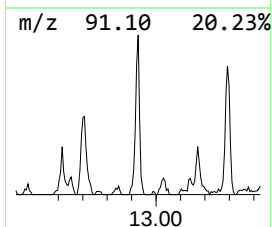
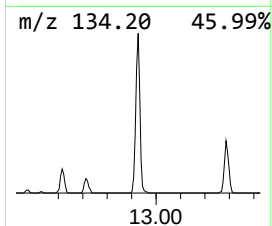
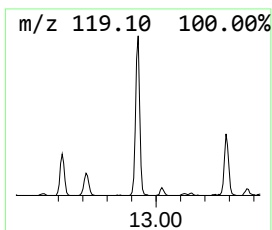
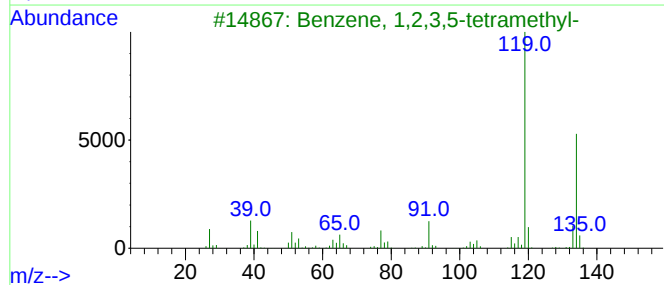
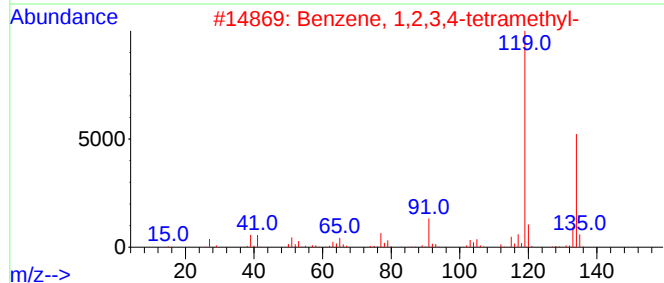
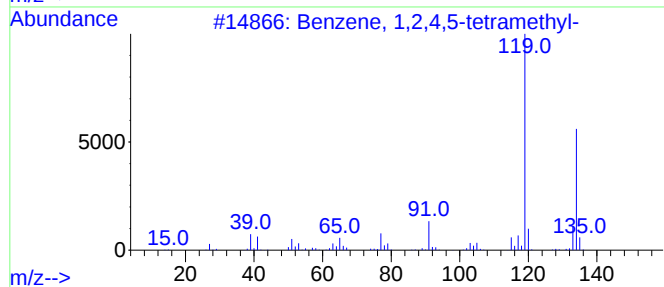
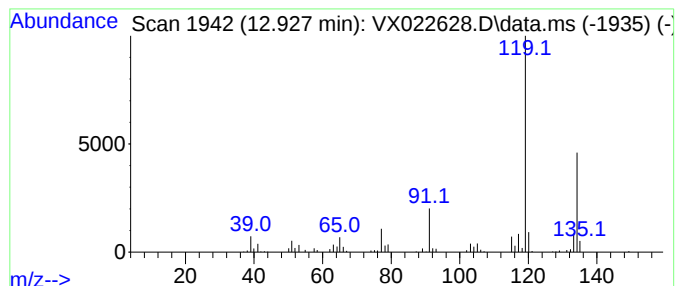
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	16.06 ug/l	81822	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	95
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			p-Cymene	134	C10H14	000099-87-6	94



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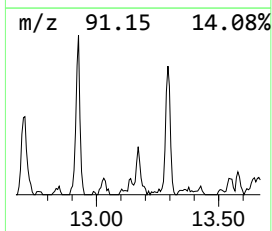
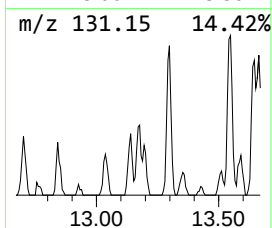
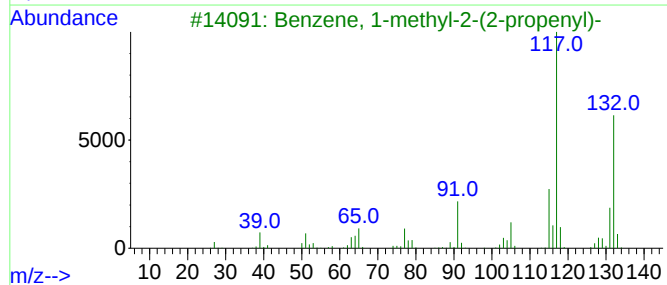
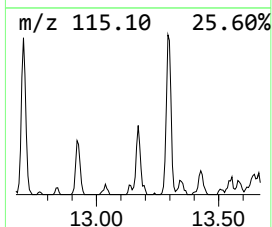
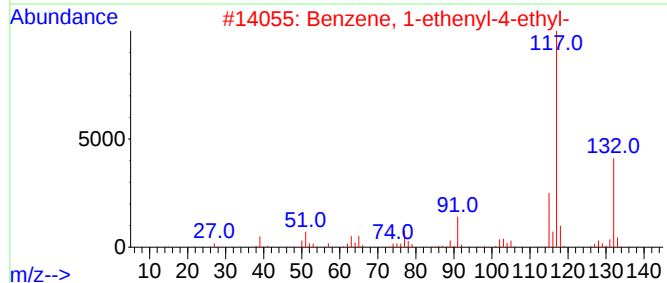
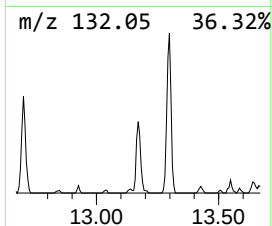
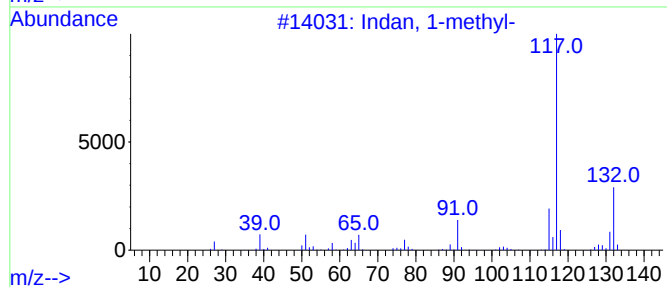
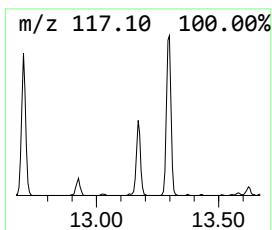
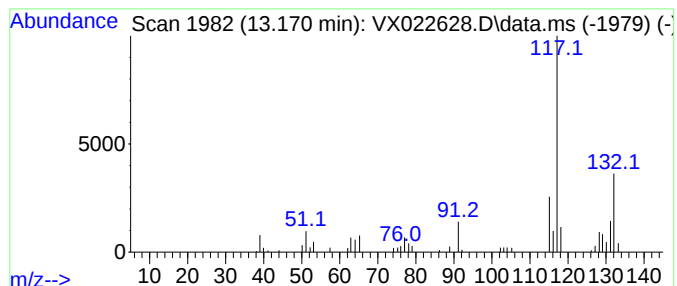
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	6.90 ug/l	35148	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	90
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060921\
Data File : VX022628.D
Acq On : 09 Jun 2021 20:49
Operator : JC/MD
Sample : M2610-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

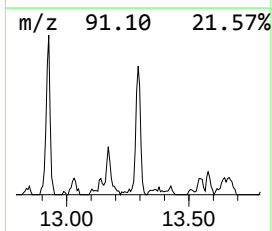
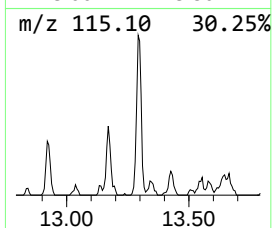
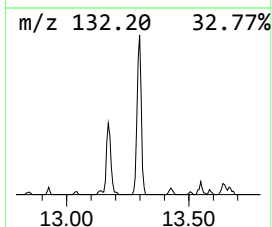
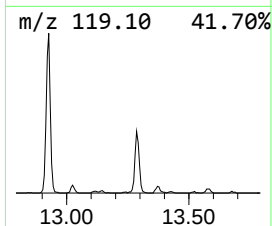
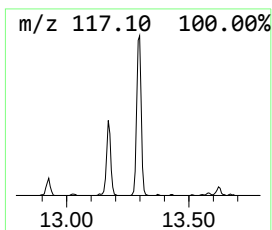
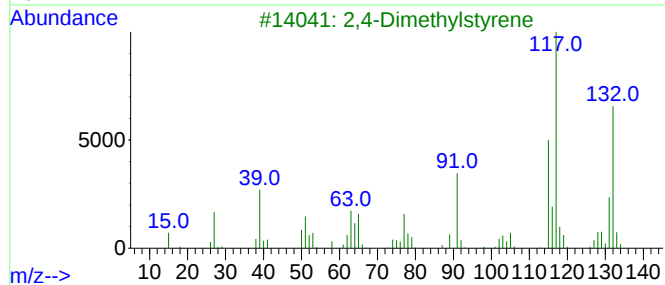
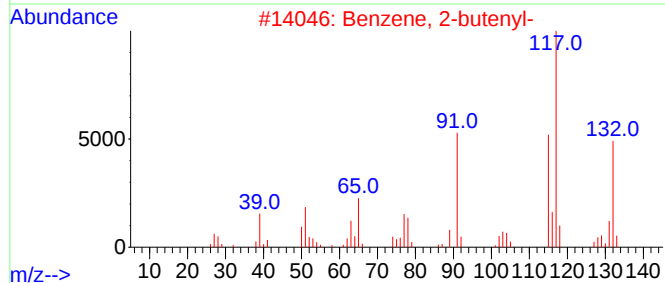
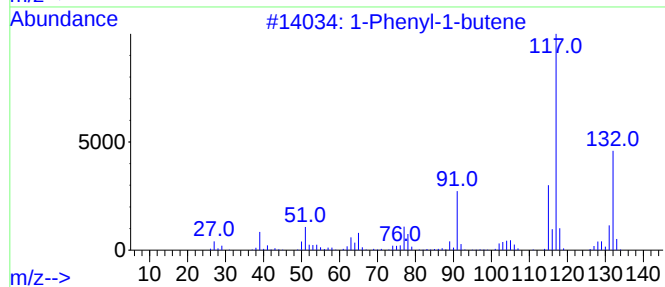
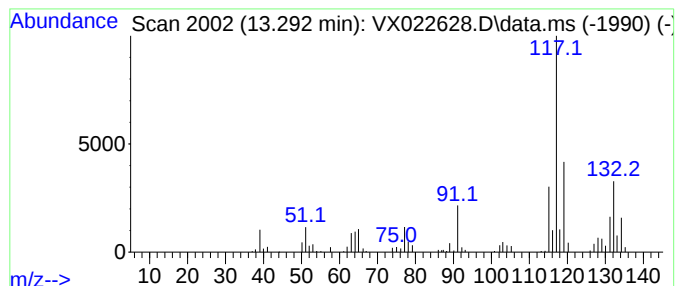
Instrument :
MSVOA_X
ClientSampleId :
W-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Phenyl-1-butene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.292	20.34 ug/l	103659	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
3	2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060921\
Data File : VX022628.D
Acq On : 09 Jun 2021 20:49
Operator : JC/MD
Sample : M2610-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
W-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, m...	4.312	6.6	ug/l	22738	1	5.562	173079	50.0
Indane	12.244	35.0	ug/l	178583	4	12.024	254767	50.0
Benzene, 1-ethe...	12.701	13.1	ug/l	66534	4	12.024	254767	50.0
Benzene, 1,2,4,...	12.927	16.1	ug/l	81822	4	12.024	254767	50.0
Indan, 1-methyl-	13.170	6.9	ug/l	35148	4	12.024	254767	50.0
1-Phenyl-1-butene	13.292	20.3	ug/l	103659	4	12.024	254767	50.0