

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091619\
 Data File : VX012415.D
 Acq On : 16 Sep 2019 19:05
 Operator : JC/SP
 Sample : K4830-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 S13-0277

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	42	rBV	580555	695154	10.54%	1.497%
2	2.838	312	320	323	rBV	51669	112319	1.70%	0.242%
3	2.881	323	327	341	rVB	83602	200256	3.04%	0.431%
4	3.161	362	373	385	rBV	189577	436464	6.62%	0.940%
5	4.392	565	575	592	rVB	346486	1010467	15.32%	2.176%
6	5.490	743	755	760	rBV	108055	306488	4.65%	0.660%
7	5.575	760	769	777	rVV	395012	1275159	19.33%	2.745%
8	5.654	777	782	788	rVV	138550	388180	5.89%	0.836%
9	5.721	788	793	807	rVB2	94779	266503	4.04%	0.574%
10	5.935	814	828	839	rBV5	109021	382680	5.80%	0.824%
11	6.057	839	848	861	rVB	126561	333243	5.05%	0.717%
12	6.252	866	880	890	rVV3	169358	555494	8.42%	1.196%
13	6.349	890	896	904	rVV2	171173	473843	7.18%	1.020%
14	6.447	904	912	929	rVB	290880	801010	12.14%	1.725%
15	6.849	969	978	989	rBV	200771	480450	7.28%	1.034%
16	7.459	1063	1078	1091	rBV	2899250	6595569	100.00%	14.200%
17	7.630	1101	1106	1115	rVV2	30339	67358	1.02%	0.145%
18	7.727	1115	1122	1133	rVB	299457	577940	8.76%	1.244%
19	7.843	1133	1141	1148	rBV2	108393	221579	3.36%	0.477%
20	8.026	1163	1171	1183	rVB2	121155	267087	4.05%	0.575%
21	8.386	1224	1230	1236	rVB	105639	188195	2.85%	0.405%
22	8.581	1257	1262	1268	rVB	38594	73153	1.11%	0.157%
23	8.660	1268	1275	1279	rBV2	604693	1133249	17.18%	2.440%
24	8.709	1279	1283	1297	rVV2	671865	1230162	18.65%	2.649%
25	8.837	1297	1304	1308	rVV	324505	551515	8.36%	1.187%
26	8.879	1308	1311	1312	rVV	71764	95890	1.45%	0.206%
27	8.904	1312	1315	1322	rVB	174824	278094	4.22%	0.599%
28	9.038	1331	1337	1344	rVB	558862	916816	13.90%	1.974%
29	9.160	1349	1357	1363	rBV	313126	495825	7.52%	1.068%
30	9.434	1397	1402	1407	rBV2	55785	89101	1.35%	0.192%
31	9.568	1417	1424	1428	rBV3	188866	312212	4.73%	0.672%
32	9.617	1428	1432	1437	rVV	668625	972136	14.74%	2.093%
33	9.672	1437	1441	1446	rVV	394346	597693	9.06%	1.287%
34	9.885	1469	1476	1489	rVB2	60050	131081	1.99%	0.282%

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35	10.001	1489	1495	1500	rBV2	47810	75055	1.14%	0.162%
36	10.111	1508	1513	1518	rBV	399915	555189	8.42%	1.195%
37	10.184	1518	1525	1529	rVV	379390	552647	8.38%	1.190%
38	10.233	1529	1533	1540	rVB2	40963	75057	1.14%	0.162%
39	10.330	1544	1549	1559	rBV3	199950	453129	6.87%	0.976%
40	10.507	1573	1578	1584	rVB	63497	92577	1.40%	0.199%
41	10.641	1590	1600	1608	rBV4	75346	221293	3.36%	0.476%
42	10.830	1618	1631	1639	rBV2	132855	242361	3.67%	0.522%
43	10.910	1639	1644	1651	rBV3	72226	126127	1.91%	0.272%
44	11.013	1656	1661	1674	rVB	970760	1240648	18.81%	2.671%
45	11.135	1674	1681	1685	rBV	492457	621934	9.43%	1.339%
46	11.355	1712	1717	1727	rVB	1096009	1332886	20.21%	2.870%
47	11.666	1763	1768	1777	rBV6	52513	109442	1.66%	0.236%
48	11.763	1777	1784	1787	rVV4	47941	80194	1.22%	0.173%
49	11.916	1800	1809	1810	rBV2	96484	135991	2.06%	0.293%
50	11.940	1810	1813	1821	rVB	243754	328442	4.98%	0.707%
51	12.074	1830	1835	1840	rBV	572507	685799	10.40%	1.477%
52	12.141	1840	1846	1851	rVV	2158856	2698665	40.92%	5.810%
53	12.226	1856	1860	1865	rBV	113439	146428	2.22%	0.315%
54	12.293	1865	1871	1876	rBV	963432	1224132	18.56%	2.636%
55	12.367	1876	1883	1884	rBV2	147093	201121	3.05%	0.433%
56	12.458	1892	1898	1902	rBV	186162	242268	3.67%	0.522%
57	12.513	1902	1907	1914	rBV	466268	591809	8.97%	1.274%
58	12.665	1923	1932	1935	rBV	704304	893018	13.54%	1.923%
59	12.696	1935	1937	1942	rVV	256969	306222	4.64%	0.659%
60	12.751	1942	1946	1953	rVV2	471275	819717	12.43%	1.765%
61	12.897	1960	1970	1975	rVB2	353597	507207	7.69%	1.092%
62	12.970	1975	1982	1987	rBV	532220	711802	10.79%	1.533%
63	13.080	1995	2000	2005	rBV3	73557	117562	1.78%	0.253%
64	13.147	2006	2011	2015	rBV2	70511	109514	1.66%	0.236%
65	13.190	2015	2018	2020	rBV2	105079	115314	1.75%	0.248%
66	13.220	2020	2023	2026	rVB	162731	175416	2.66%	0.378%
67	13.342	2038	2043	2048	rBV2	1412625	1861378	28.22%	4.008%
68	13.476	2060	2065	2071	rVB	492658	604622	9.17%	1.302%
69	13.562	2074	2079	2081	rBV2	59382	79544	1.21%	0.171%
70	13.598	2081	2085	2087	rVV	76482	101134	1.53%	0.218%
71	13.635	2087	2091	2095	rVV3	198120	302371	4.58%	0.651%

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72	13.696	2095	2101	2102	rVV2	113637	188088	2.85%	0.405%
73	13.714	2102	2104	2112	rVB2	171911	280752	4.26%	0.604%
74	13.830	2113	2123	2131	rVB	845212	1202233	18.23%	2.588%
75	13.909	2131	2136	2140	rVB	68426	87405	1.33%	0.188%
76	13.982	2140	2148	2152	rBV2	151858	238009	3.61%	0.512%
77	14.025	2152	2155	2159	rBV2	55770	66970	1.02%	0.144%
78	14.129	2167	2172	2174	rBV2	55353	73659	1.12%	0.159%
79	14.159	2174	2177	2184	rVB3	47045	66006	1.00%	0.142%
80	14.281	2189	2197	2204	rVB3	148944	321538	4.88%	0.692%
81	14.372	2209	2212	2216	rVV	66297	83220	1.26%	0.179%
82	14.427	2216	2221	2225	rVB2	68569	90383	1.37%	0.195%
83	14.537	2234	2239	2248	rVB2	171765	244271	3.70%	0.526%
84	14.689	2257	2264	2268	rBV	744765	920363	13.95%	1.982%
85	14.836	2283	2288	2296	rBV	588973	793432	12.03%	1.708%
86	15.439	2379	2387	2390	rBV	40434	68312	1.04%	0.147%
87	15.543	2398	2404	2409	rBV	89679	139652	2.12%	0.301%
88	15.683	2417	2427	2430	rBV	120342	210426	3.19%	0.453%
89	15.720	2430	2433	2439	rVB2	81163	121515	1.84%	0.262%

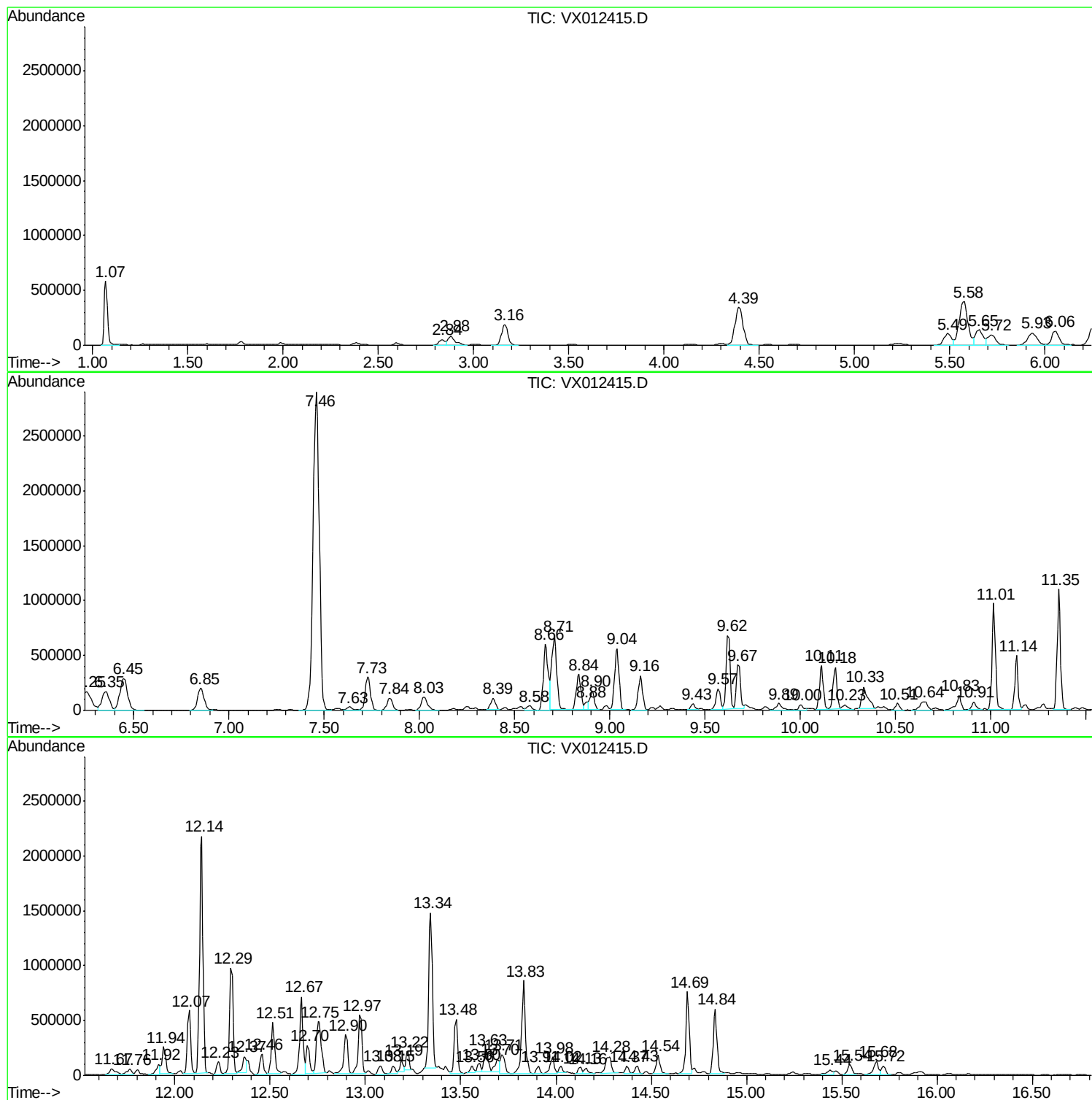
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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



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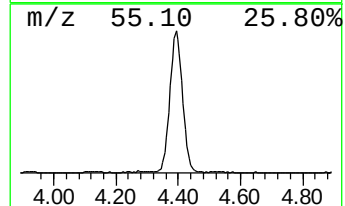
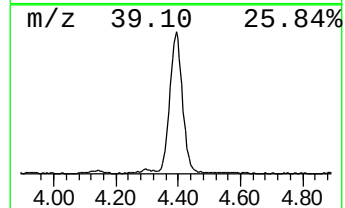
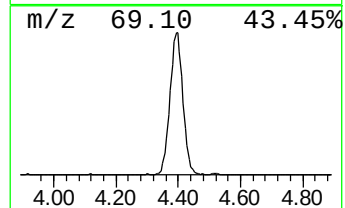
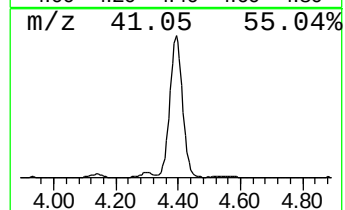
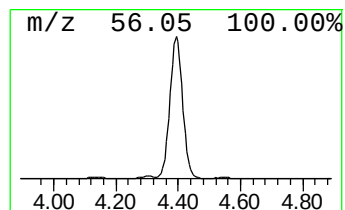
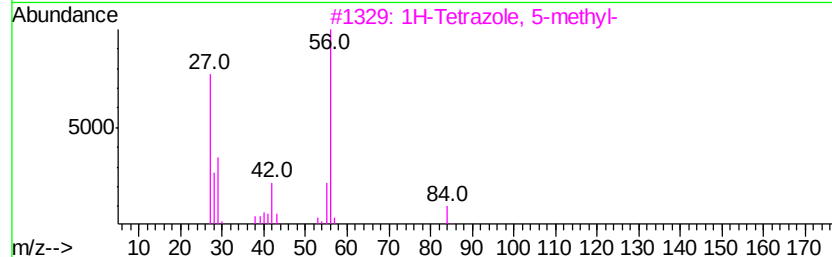
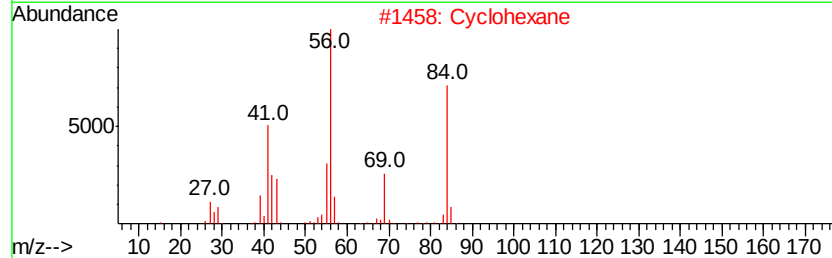
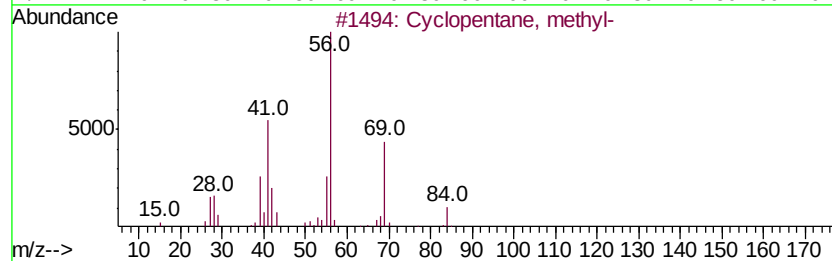
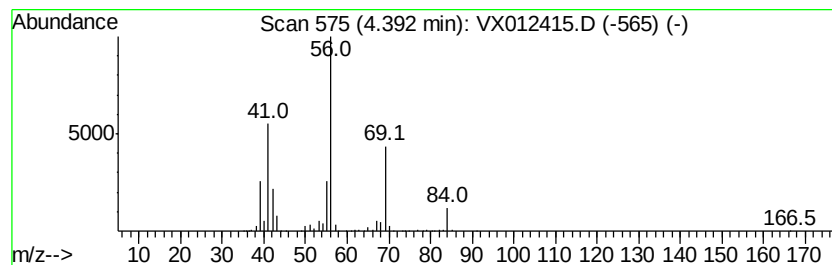
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	130.15 ug/l	1010470	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclohexane	84	C6H12	000110-82-7	83
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5		Cyclobutane	56	C4H8	000287-23-0	50



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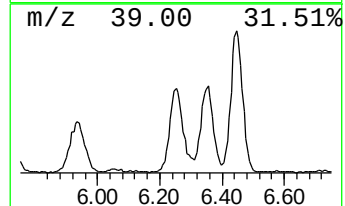
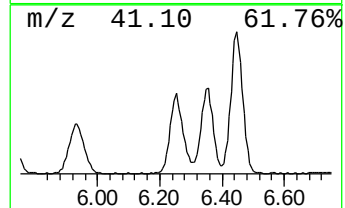
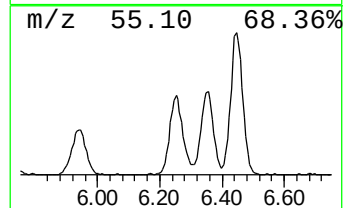
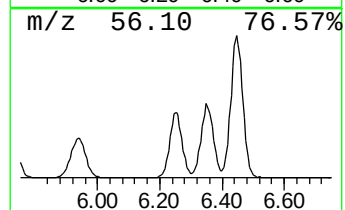
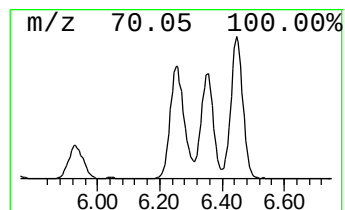
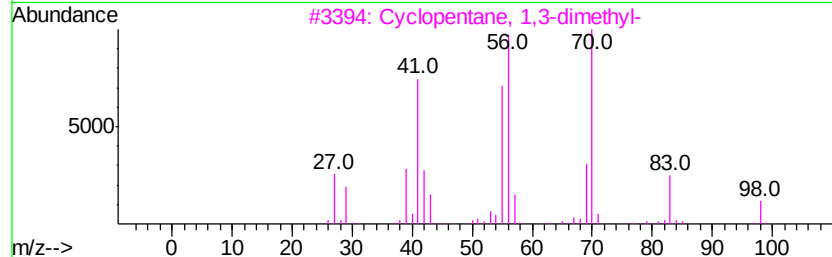
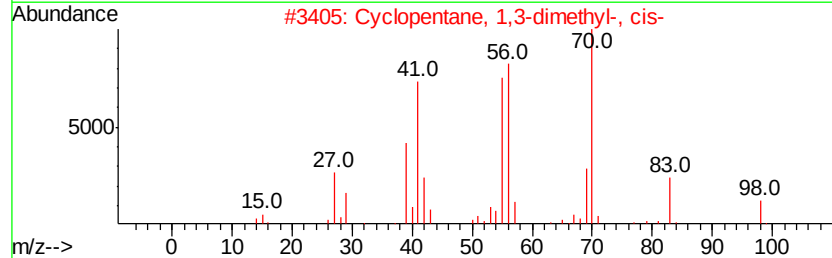
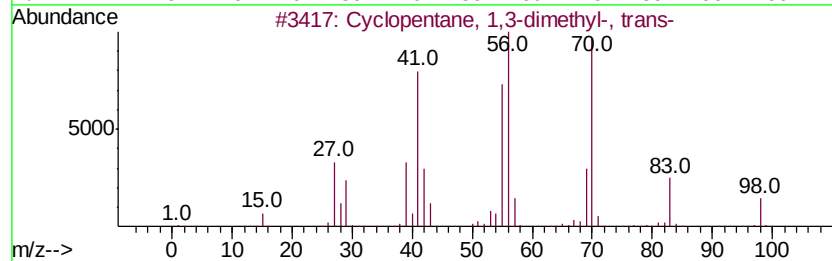
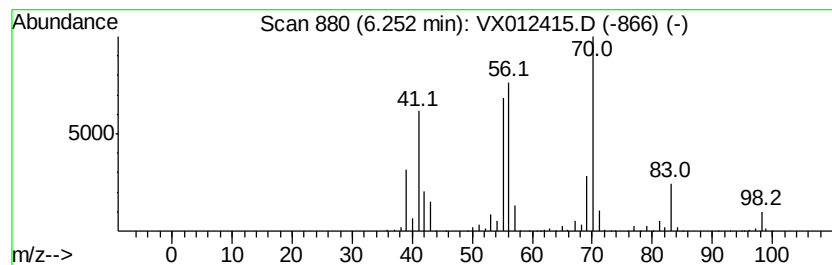
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclopentane, 1,3-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	71.55 ug/l	555494	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	97
2		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	97
3		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	95
4		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	76
5		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	58



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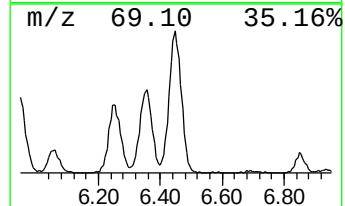
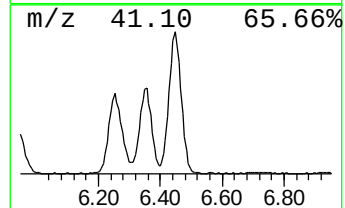
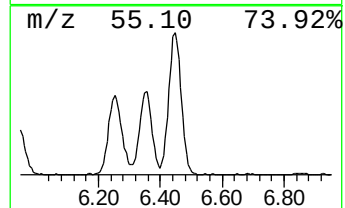
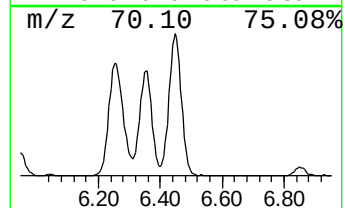
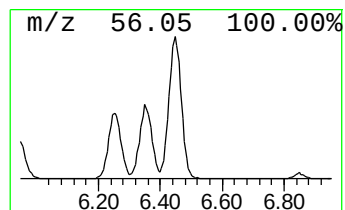
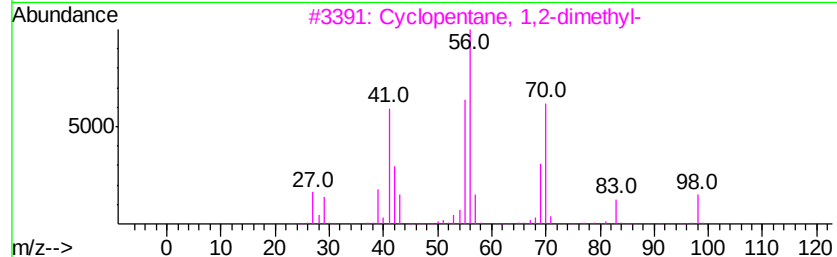
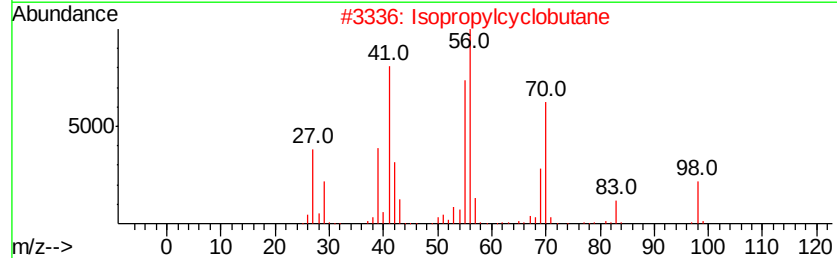
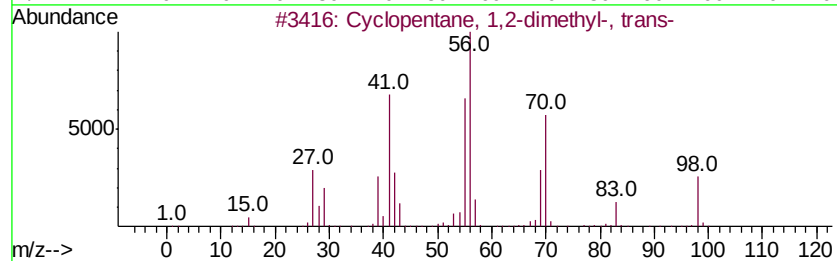
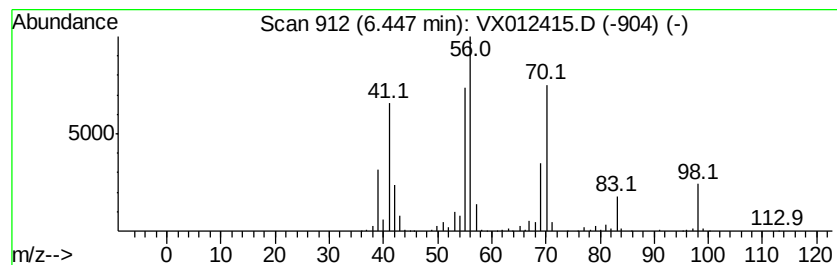
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	83.36 ug/l	801010	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	94
2		Isopropylcyclobutane	98	C7H14	000872-56-0	93
3		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
4		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	86
5		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	78



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S13-0277

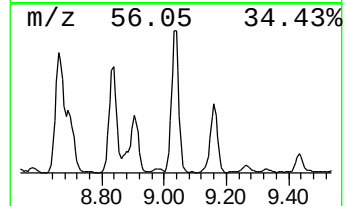
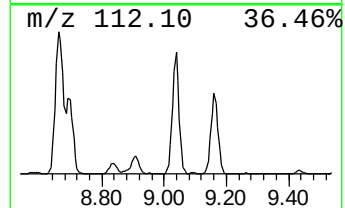
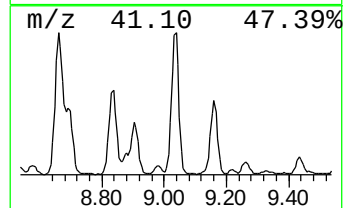
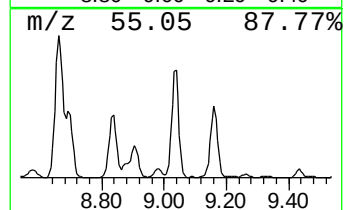
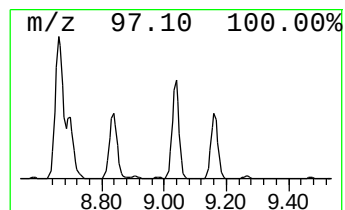
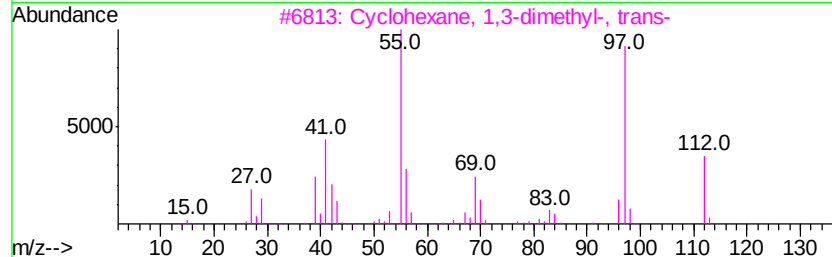
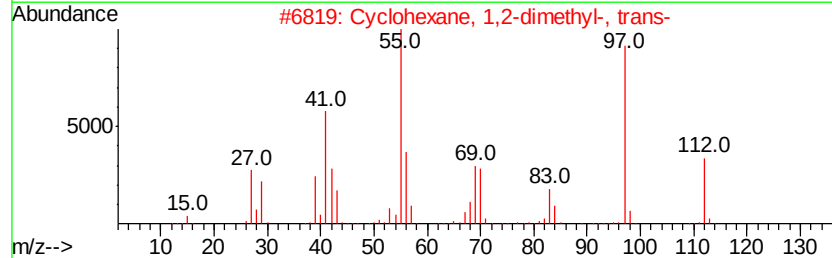
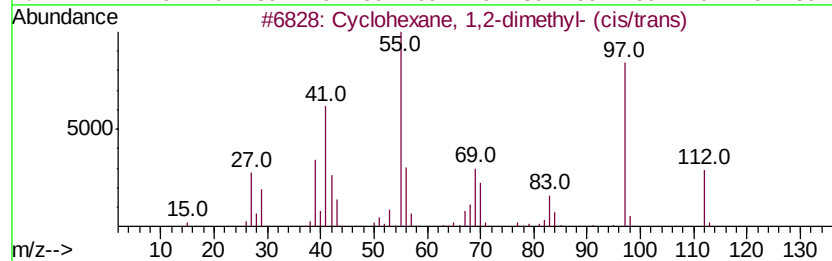
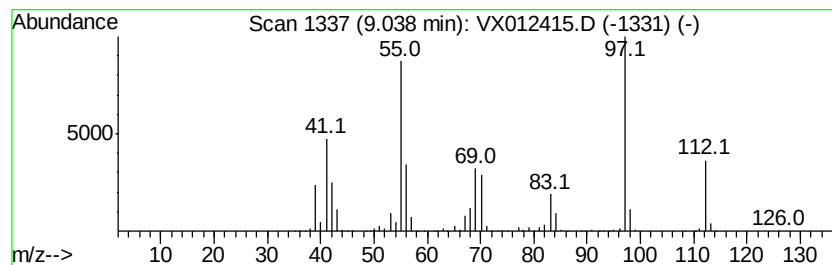
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,2-dimethyl- ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	82.57 ug/l	916816	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	97
2		Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
3		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	90
4		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	86
5		Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0277

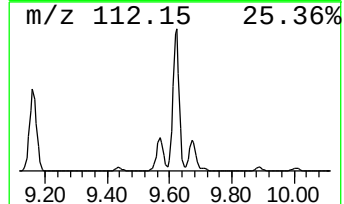
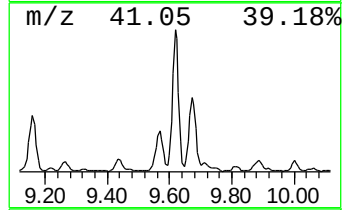
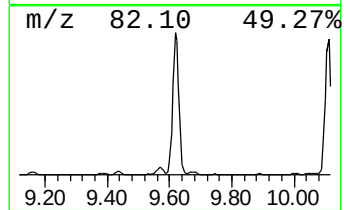
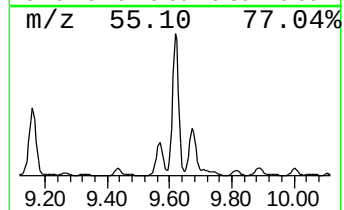
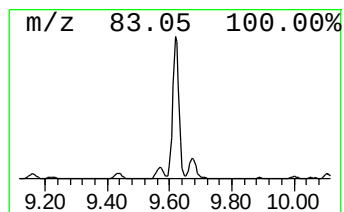
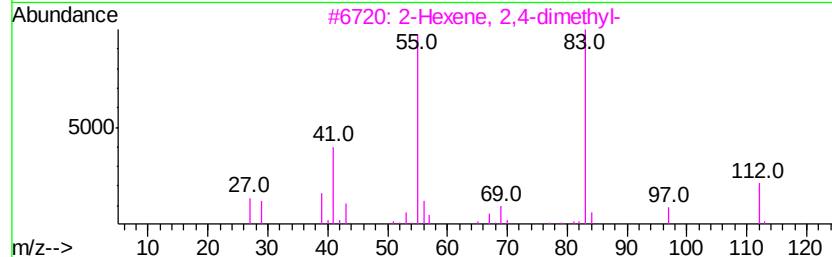
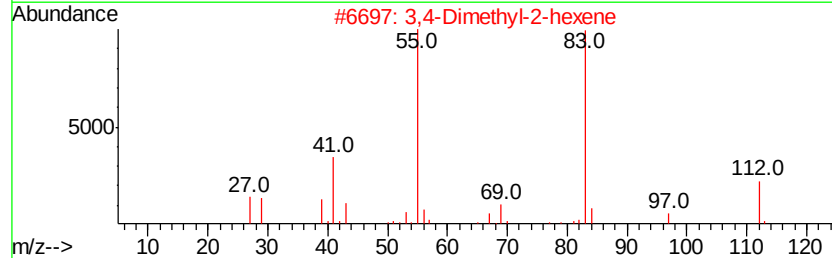
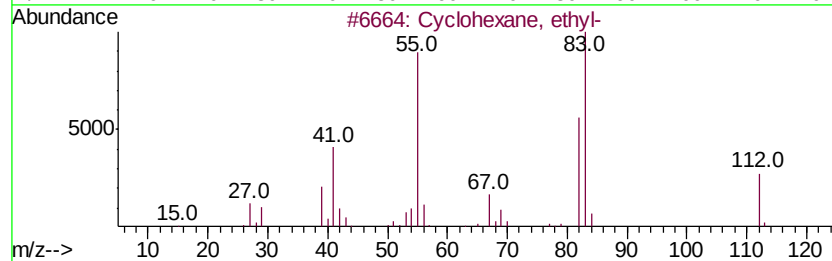
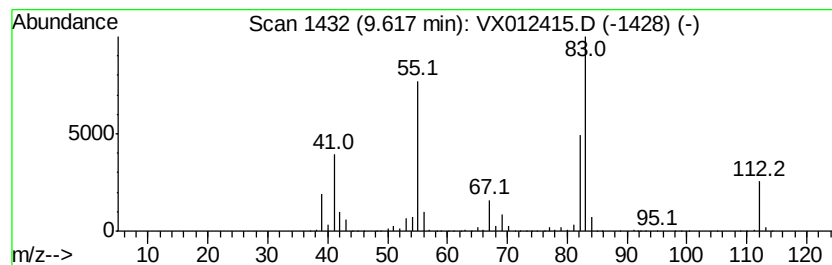
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	87.55 ug/l	972136	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	97
2		3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	68
3		2-Hexene, 2,4-dimethyl-	112	C8H16	014255-23-3	59
4		trans-3,4-Dimethyl-2-hexene	112	C8H16	019550-82-4	59
5		2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
S13-0277

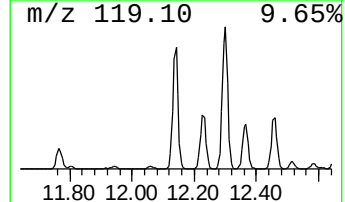
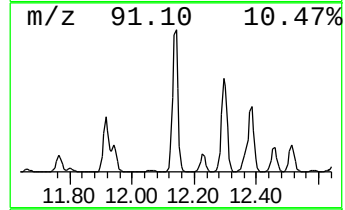
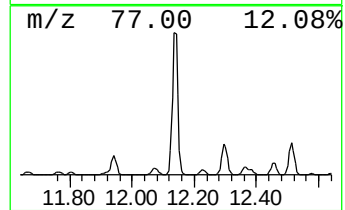
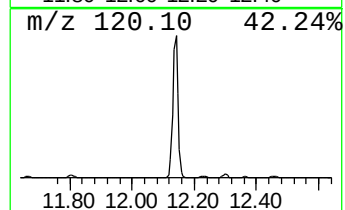
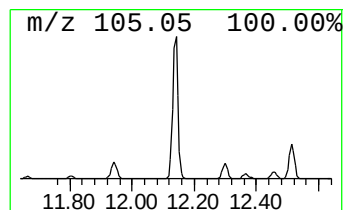
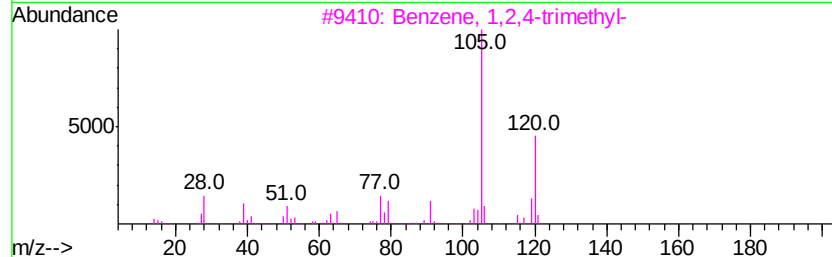
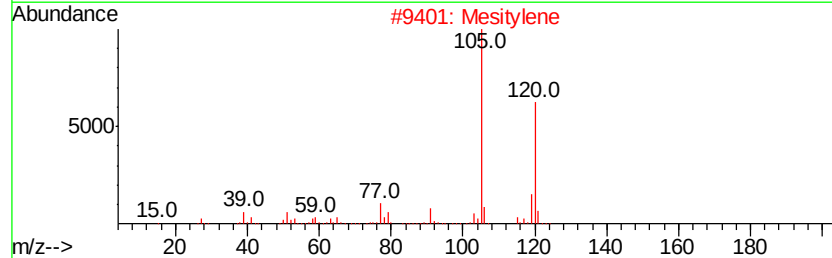
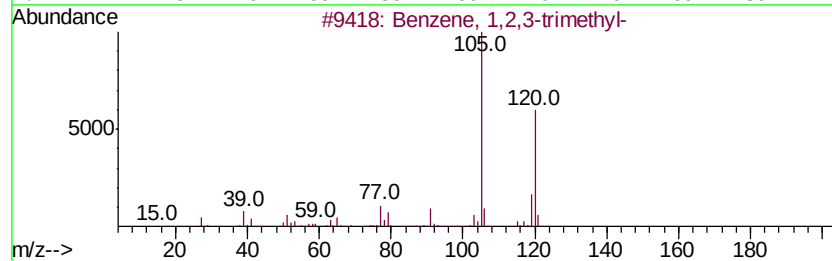
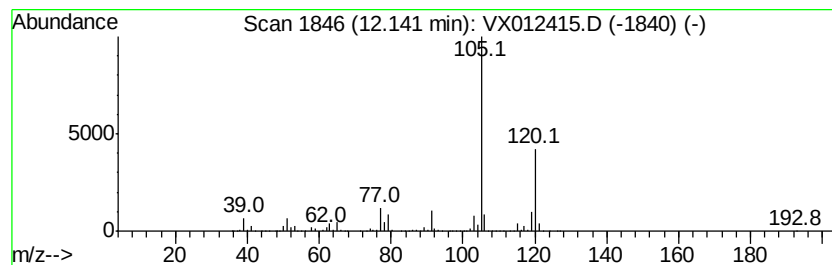
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	196.75 ug/l	2698670	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
S13-0277

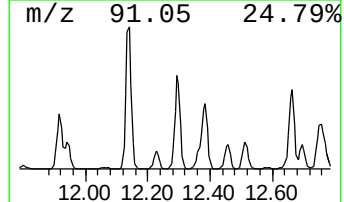
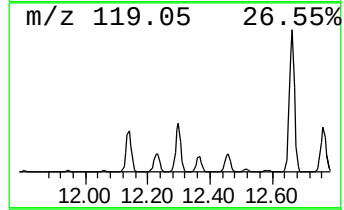
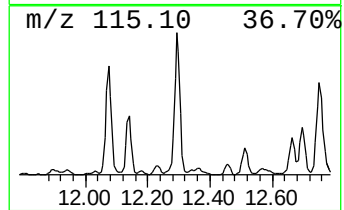
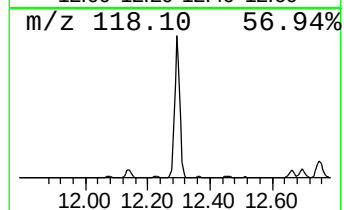
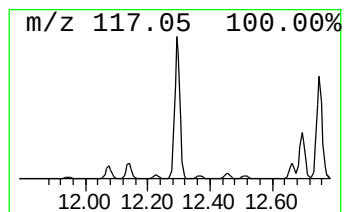
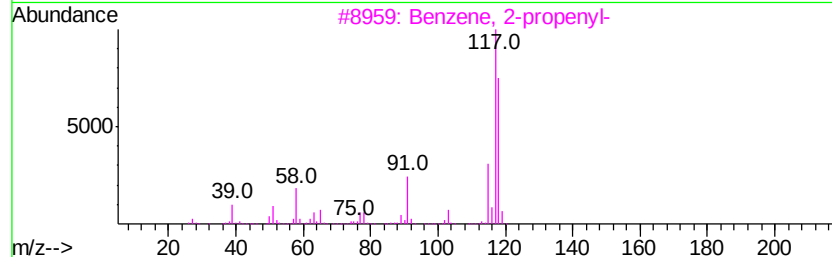
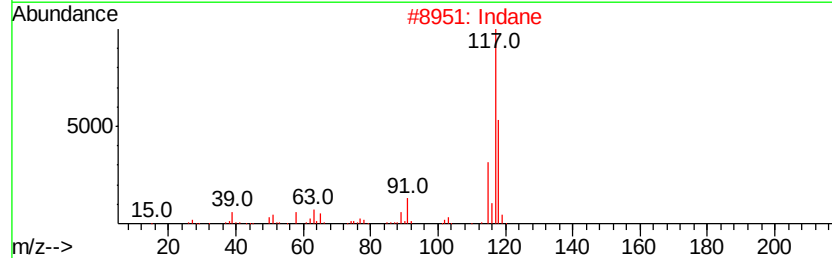
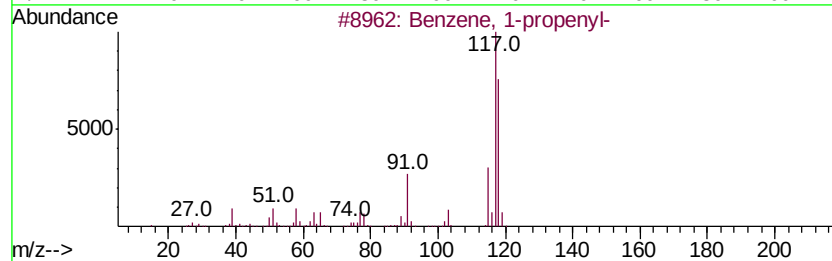
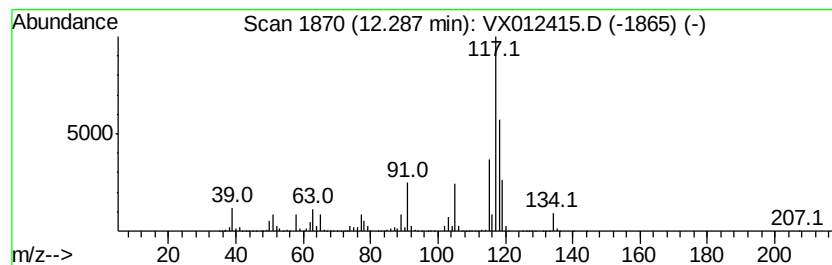
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	89.25 ug/l	1224130	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	90
2		Indane	118	C9H10	000496-11-7	87
3		Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5		Benzene, cyclopropyl-	118	C9H10	000873-49-4	60



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0277

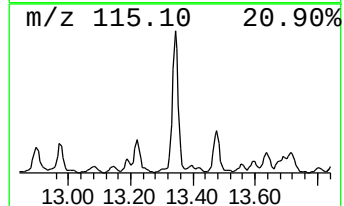
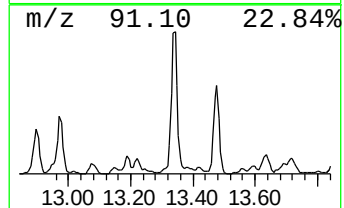
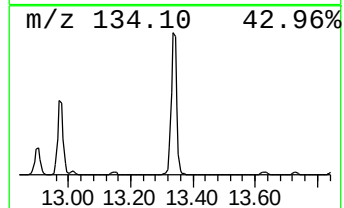
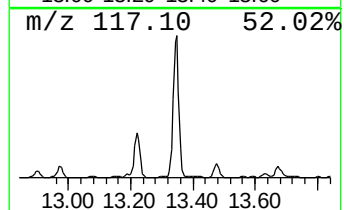
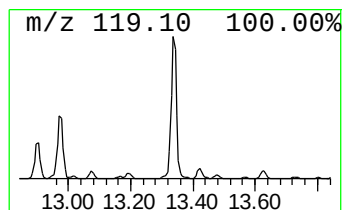
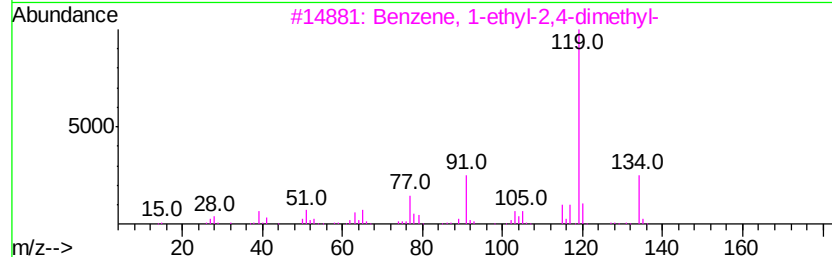
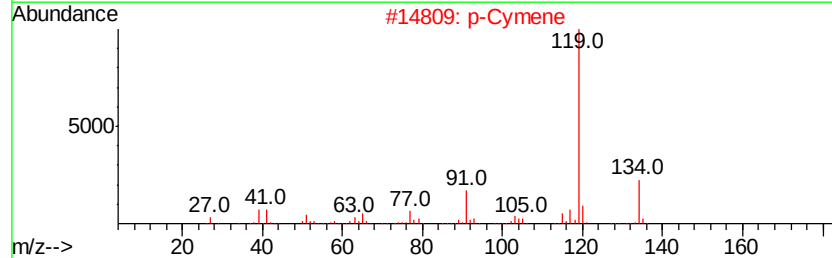
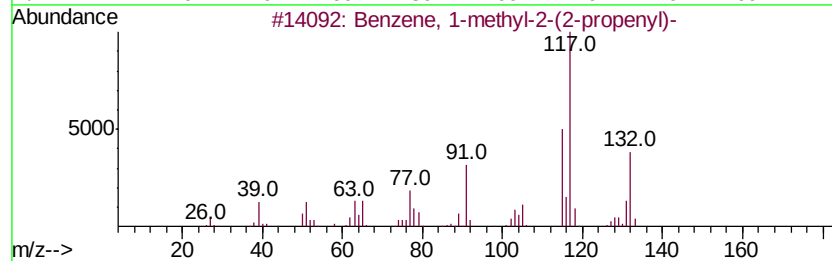
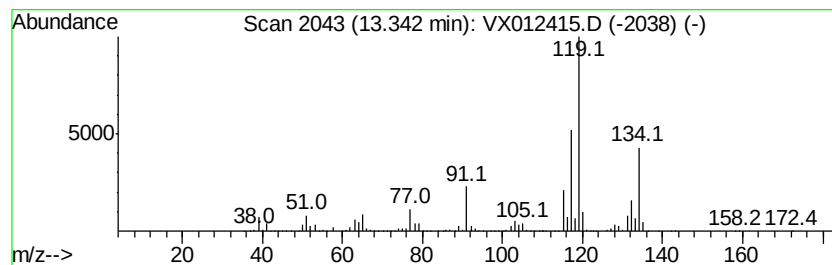
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-methyl-2-(2-prop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	135.71 ug/l	1861380	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2		p-Cymene	134	C10H14	000099-87-6	64
3		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
5		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0277

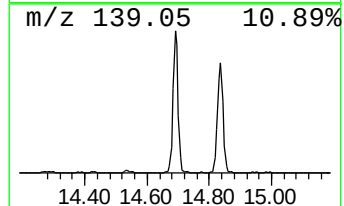
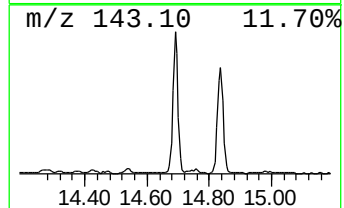
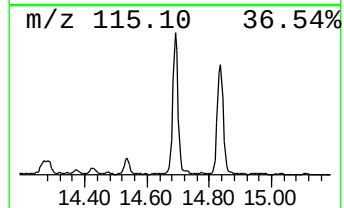
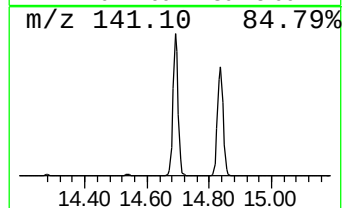
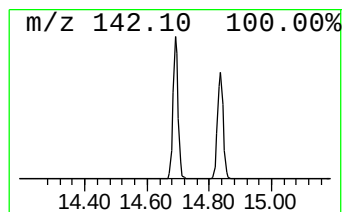
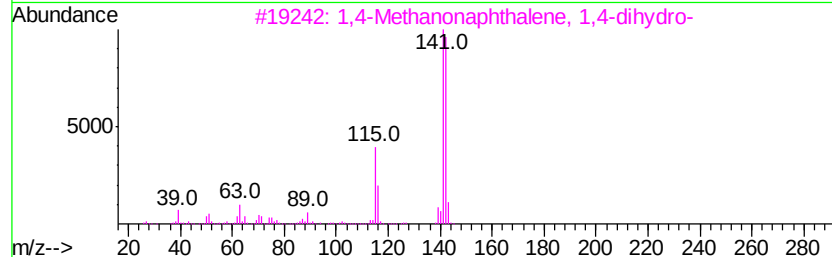
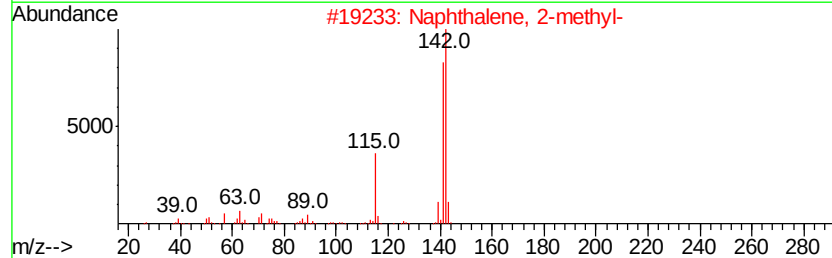
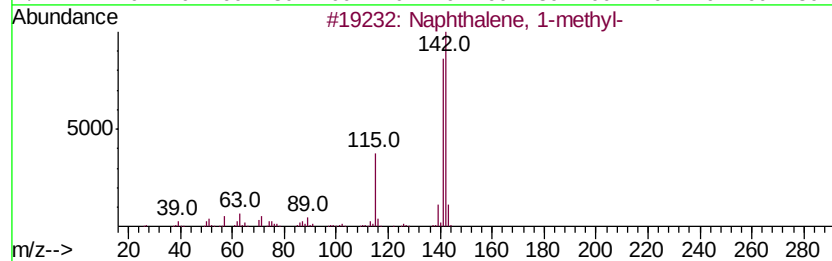
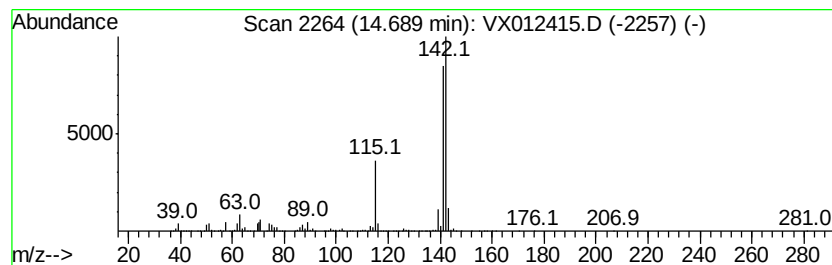
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	67.10 ug/l	920363	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	94
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091619\
Data File : VX012415.D
Acq On : 16 Sep 2019 19:05
Operator : JC/SP
Sample : K4830-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0277

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.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, met...	4.39	130.2	ug/l	1010470	1	5.65	388180	50.0
Cyclopentane, 1,3...	6.25	71.5	ug/l	555494	1	5.65	388180	50.0
Cyclopentane, 1,2...	6.45	83.4	ug/l	801010	2	6.86	480450	50.0
Cyclohexane, 1,2-...	9.04	82.6	ug/l	916816	3	10.11	555189	50.0
Cyclohexane, ethyl-	9.62	87.5	ug/l	972136	3	10.11	555189	50.0
Benzene, 1,2,3-tr...	12.14	196.8	ug/l	2698670	4	12.07	685799	50.0
Benzene, 1-propenyl-	12.29	89.3	ug/l	1224130	4	12.07	685799	50.0
Benzene, 1-methyl...	13.34	135.7	ug/l	1861380	4	12.07	685799	50.0
Naphthalene, 1-me...	14.69	67.1	ug/l	920363	4	12.07	685799	50.0