

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034798.D
 Acq On : 28 Mar 2023 17:13
 Operator : JC/MD
 Sample : 02065-02
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1161

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.416	209	218	249	rBV	775803	2570575	40.11%	5.015%
2	5.385	693	705	714	rBV	176904	512569	8.00%	1.000%
3	5.495	714	723	724	rBV	117988	234213	3.65%	0.457%
4	5.544	725	731	739	rVB	281674	759686	11.85%	1.482%
5	5.812	763	775	789	rBV	179509	519376	8.10%	1.013%
6	5.952	789	798	815	rVB	220840	590550	9.21%	1.152%
7	6.172	823	834	841	rBV5	20102	74169	1.16%	0.145%
8	6.604	890	905	917	rBV	70899	174492	2.72%	0.340%
9	6.757	920	930	951	rVB	526738	1267038	19.77%	2.472%
10	8.647	1234	1240	1246	rBV	1098293	1686916	26.32%	3.291%
11	8.714	1246	1251	1265	rVB	4052011	6408587	100.00%	12.503%
12	9.903	1442	1446	1451	rVB	84123	122462	1.91%	0.239%
13	10.006	1457	1463	1466	rBV	77213	106220	1.66%	0.207%
14	10.055	1466	1471	1487	rVV	1005134	1504313	23.47%	2.935%
15	10.195	1487	1494	1499	rVV	326564	493639	7.70%	0.963%
16	10.299	1502	1511	1517	rVV	1548175	2314312	36.11%	4.515%
17	10.360	1517	1521	1532	rVB	277678	392722	6.13%	0.766%
18	10.585	1551	1558	1562	rBV3	103507	178987	2.79%	0.349%
19	10.640	1562	1567	1576	rVV	610579	918249	14.33%	1.791%
20	10.781	1587	1590	1593	rVV	129493	157609	2.46%	0.307%
21	10.817	1593	1596	1599	rVV3	42647	66738	1.04%	0.130%
22	10.854	1599	1602	1606	rVV3	125250	200290	3.13%	0.391%
23	10.945	1613	1617	1623	rBV2	82069	169287	2.64%	0.330%
24	11.085	1634	1640	1653	rBV2	910017	1654201	25.81%	3.227%
25	11.189	1653	1657	1660	rBV2	163618	250945	3.92%	0.490%
26	11.305	1669	1676	1680	rBV	187336	280328	4.37%	0.547%
27	11.378	1684	1688	1694	rBV	790523	1458058	22.75%	2.845%
28	11.451	1698	1700	1701	rVV	445110	440654	6.88%	0.860%
29	11.476	1701	1704	1709	rVB	1181876	1475189	23.02%	2.878%
30	11.530	1709	1713	1717	rVB2	75617	97971	1.53%	0.191%
31	11.616	1722	1727	1734	rVB3	383100	713777	11.14%	1.393%
32	11.683	1734	1738	1740	rBV3	166503	205974	3.21%	0.402%
33	11.713	1740	1743	1746	rBV2	538589	616573	9.62%	1.203%
34	11.756	1746	1750	1759	rVB	1614380	2569155	40.09%	5.012%
35	11.841	1759	1764	1766	rBV	209449	343609	5.36%	0.670%
36	11.890	1768	1772	1776	rVB	432225	580815	9.06%	1.133%

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Title : SW846 8260

37	11.939	1776	1780	1784	rBV3	627694	959073	14.97%	1.871%
38	11.975	1784	1786	1789	rVB2	263220	262951	4.10%	0.513%
39	12.024	1790	1794	1799	rBV2	1095301	1721477	26.86%	3.358%
40	12.097	1799	1806	1810	rBV3	507536	1132758	17.68%	2.210%
41	12.152	1812	1815	1817	rBV4	110880	136361	2.13%	0.266%
42	12.250	1825	1831	1832	rBV3	484866	753934	11.76%	1.471%
43	12.317	1837	1842	1848	rVB5	885115	1739149	27.14%	3.393%
44	12.384	1849	1853	1854	rBV2	124631	166260	2.59%	0.324%
45	12.421	1855	1859	1863	rVV	2066339	2449868	38.23%	4.780%
46	12.469	1863	1867	1873	rVB4	565315	994825	15.52%	1.941%
47	12.555	1874	1881	1884	rBV2	571736	1202822	18.77%	2.347%
48	12.689	1899	1903	1906	rBV3	212287	422348	6.59%	0.824%
49	12.762	1912	1915	1920	rVB3	167203	220088	3.43%	0.429%
50	12.817	1920	1924	1931	rVB3	544990	789599	12.32%	1.540%
51	12.884	1931	1935	1938	rBV2	409881	561345	8.76%	1.095%
52	12.963	1944	1948	1949	rBV	311053	333767	5.21%	0.651%
53	13.042	1955	1961	1964	rBV4	252607	379734	5.93%	0.741%
54	13.170	1975	1982	1986	rBV4	217020	449150	7.01%	0.876%
55	13.213	1986	1989	1991	rVV3	98254	133352	2.08%	0.260%
56	13.268	1995	1998	1999	rVV2	267474	323125	5.04%	0.630%
57	13.292	1999	2002	2007	rVB2	633839	885839	13.82%	1.728%
58	13.341	2007	2010	2013	rBV3	58813	75464	1.18%	0.147%
59	13.420	2018	2023	2031	rVB3	318764	690983	10.78%	1.348%
60	13.500	2033	2036	2040	rBV4	109971	143694	2.24%	0.280%
61	13.542	2040	2043	2046	rBV	57622	67275	1.05%	0.131%
62	13.585	2046	2050	2054	rBV4	120197	204720	3.19%	0.399%
63	13.670	2061	2064	2068	rBV3	86195	124366	1.94%	0.243%
64	13.774	2078	2081	2083	rBV	102348	120123	1.87%	0.234%
65	14.073	2126	2130	2133	rBV4	59398	85819	1.34%	0.167%
66	14.225	2150	2155	2159	rVB4	121740	214181	3.34%	0.418%
67	14.481	2194	2197	2205	rVB3	66792	142593	2.23%	0.278%
68	14.615	2216	2219	2220	rBV	64247	65075	1.02%	0.127%
69	14.634	2220	2222	2226	rVB	97157	117494	1.83%	0.229%
70	15.182	2307	2312	2320	rVB4	33555	71282	1.11%	0.139%
71	15.560	2369	2374	2379	rBV	393405	542410	8.46%	1.058%
72	15.969	2434	2441	2456	rBV	189808	463823	7.24%	0.905%

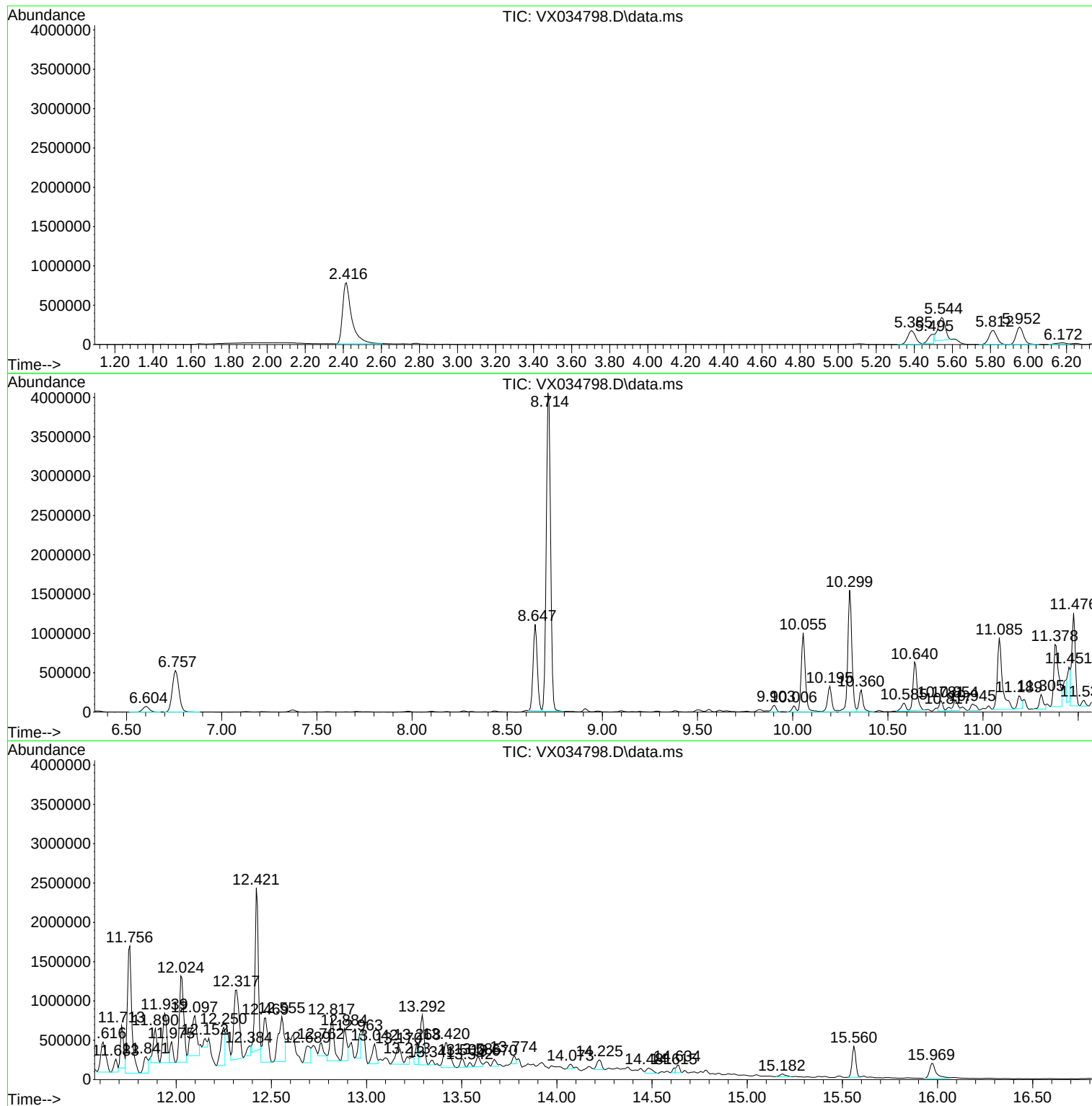
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Instrument :
MSVOA_X
ClientSampleId :
1161

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

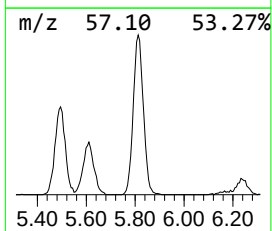
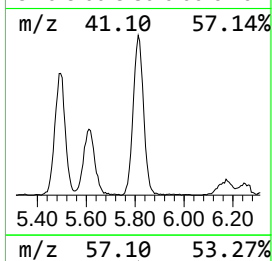
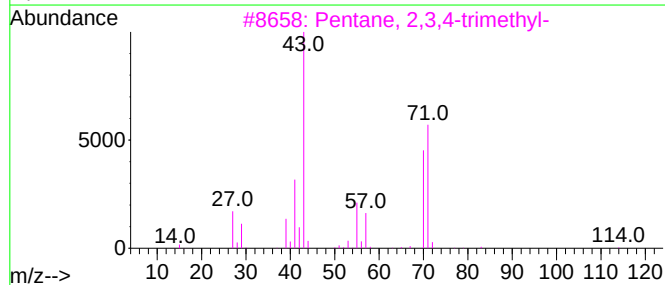
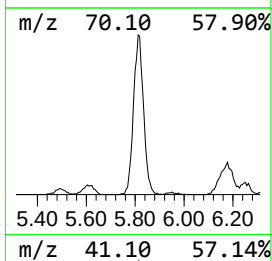
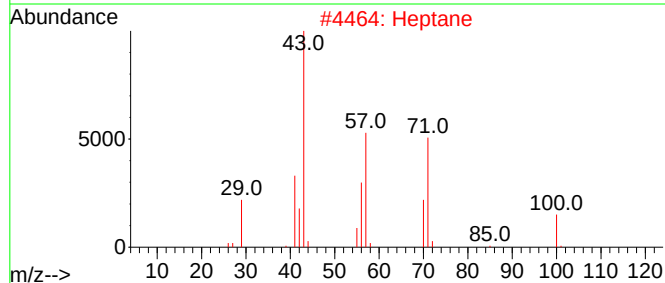
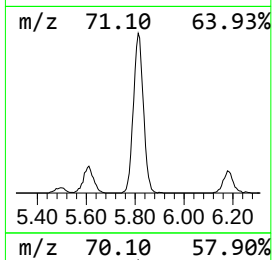
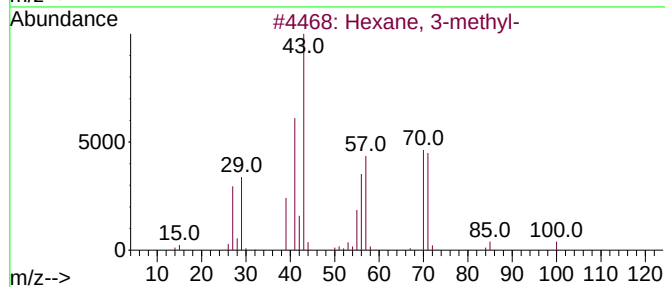
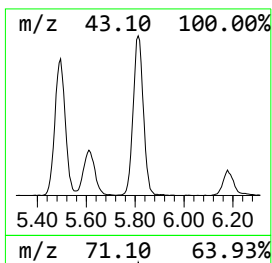
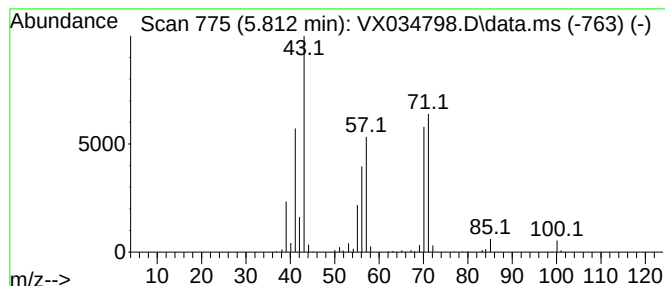
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	34.18 ug/l	519376	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Pyrrolidine	71	C4H9N	000123-75-1	50
5			Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	47



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Instrument :
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ClientSampleId :
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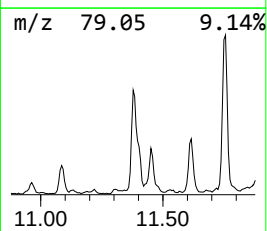
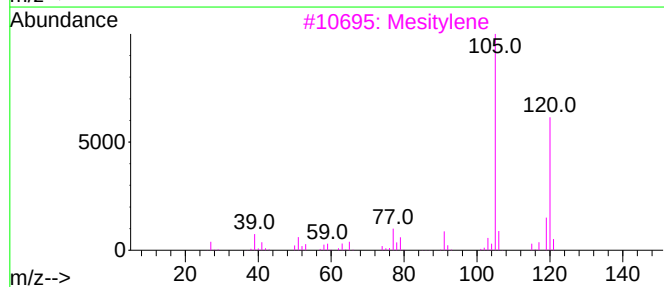
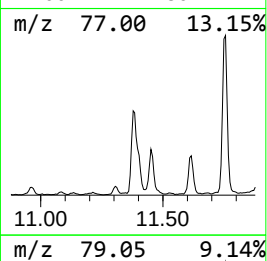
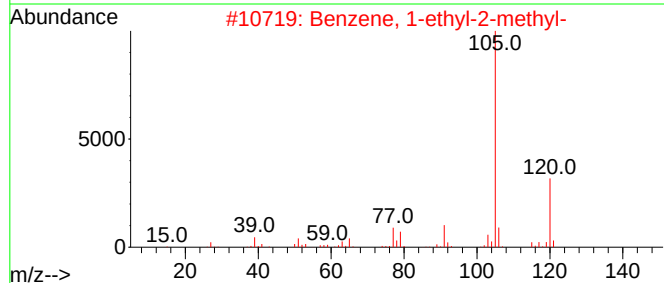
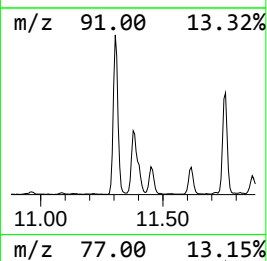
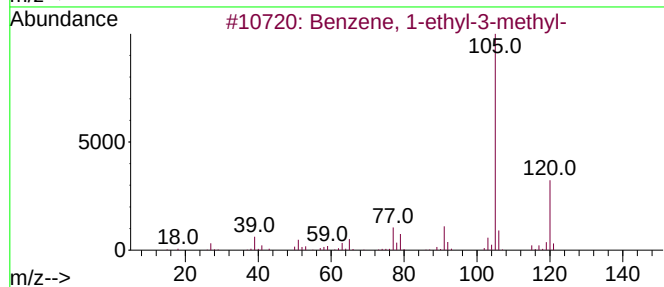
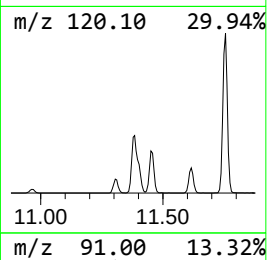
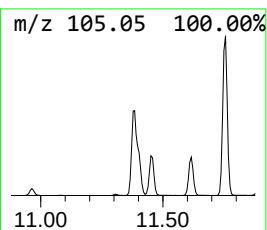
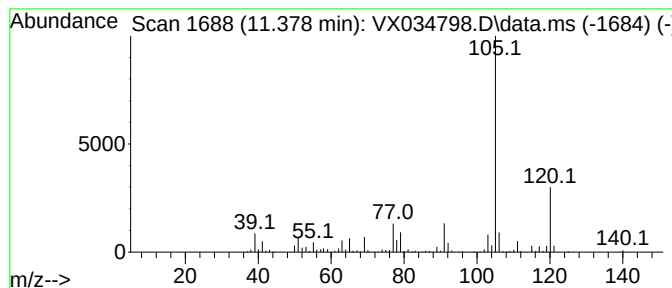
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	42.35 ug/l	1458060	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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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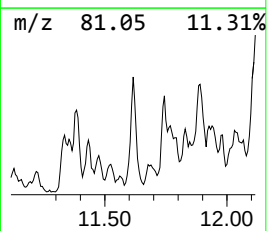
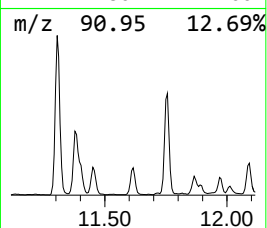
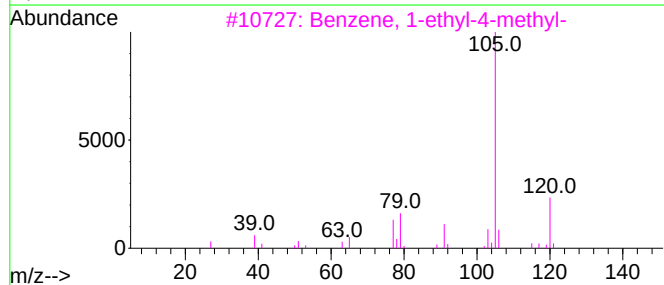
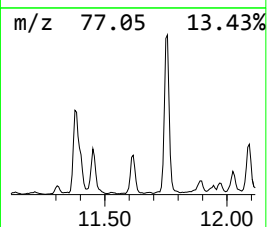
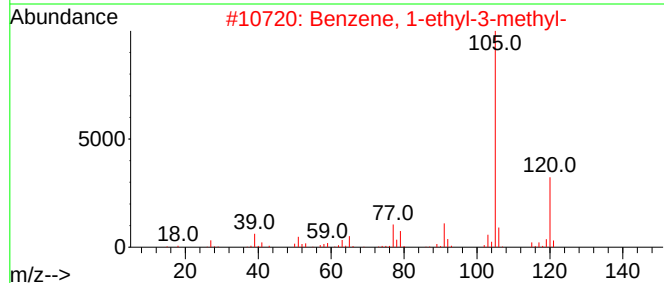
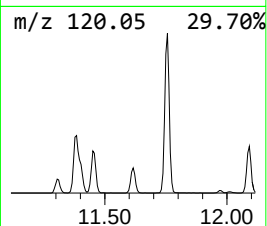
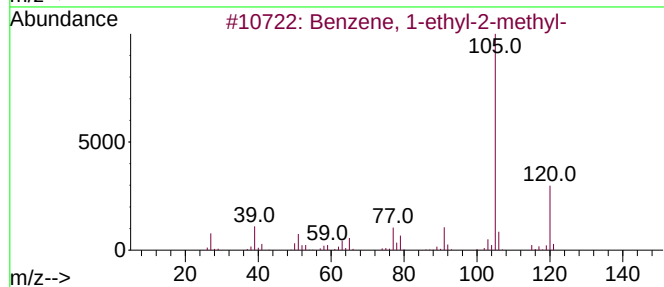
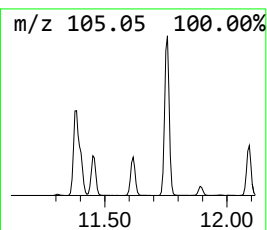
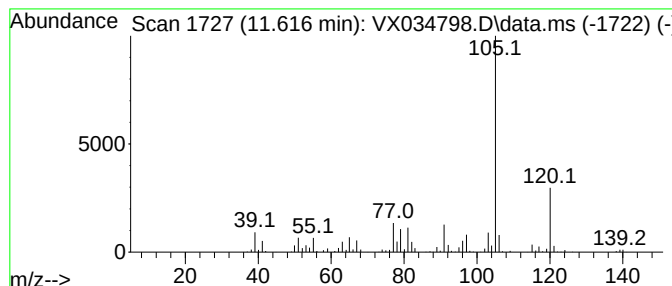
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	20.73 ug/l	713777	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-3-methyl-	120	C9H12	000620-14-4	90
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	86
4			Mesitylene	120	C9H12	000108-67-8	81
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	81



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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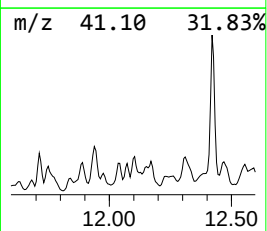
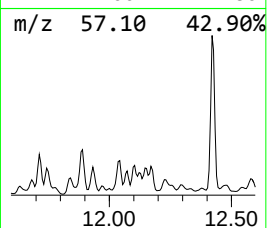
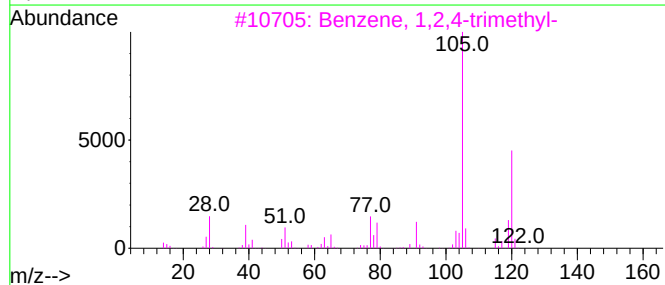
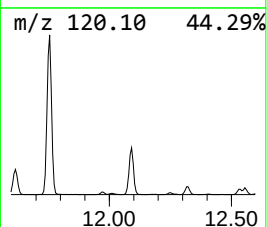
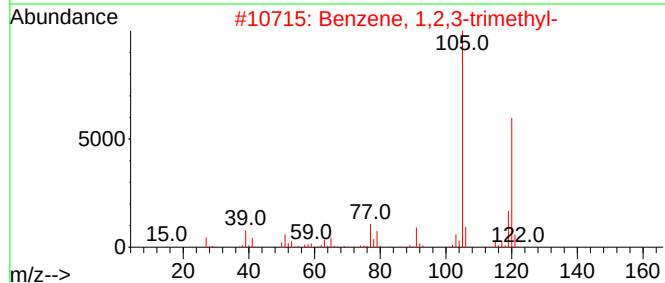
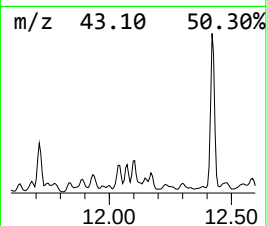
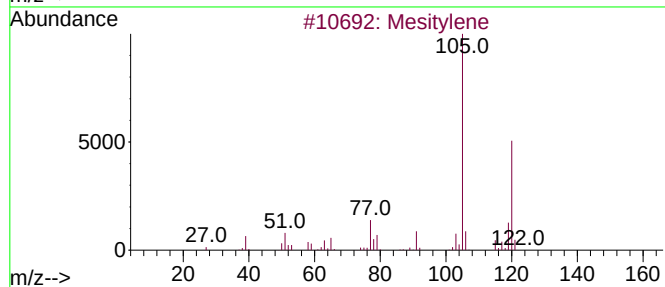
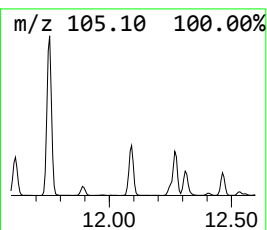
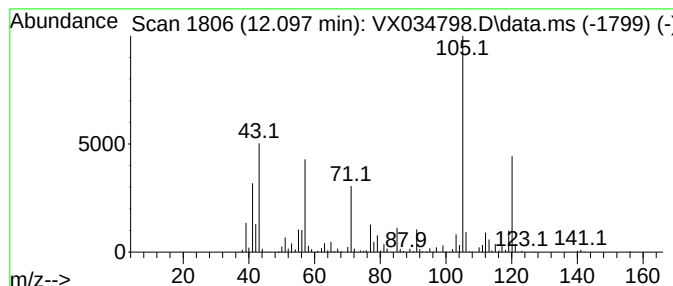
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	32.90 ug/l	1132760	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	93
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	92
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	83
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	60
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

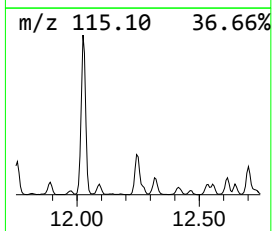
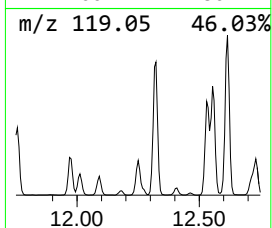
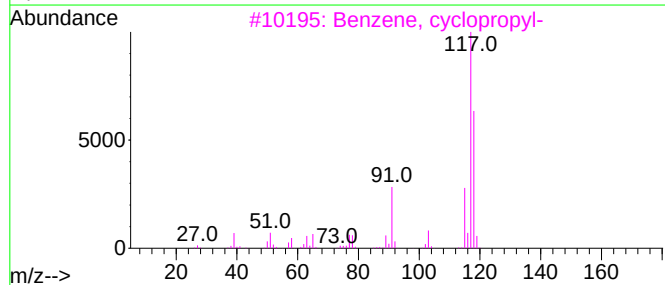
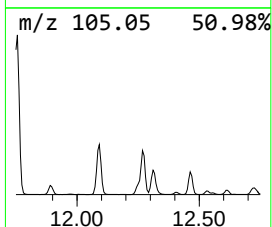
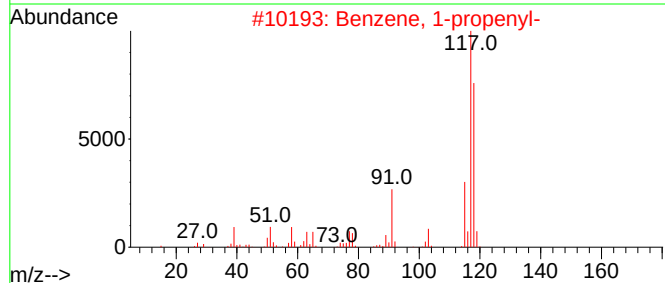
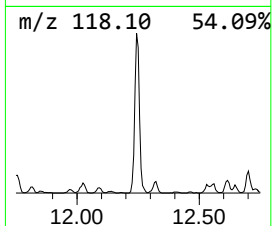
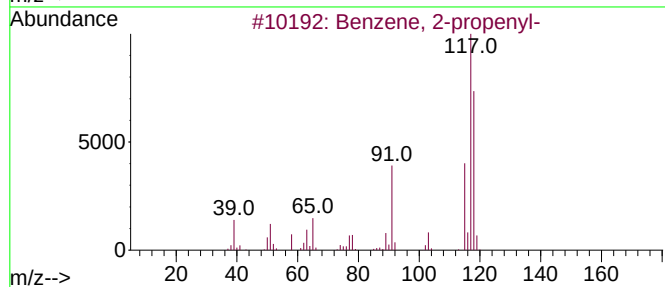
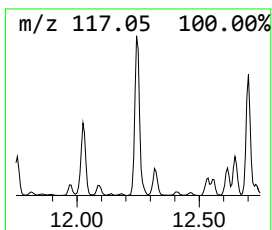
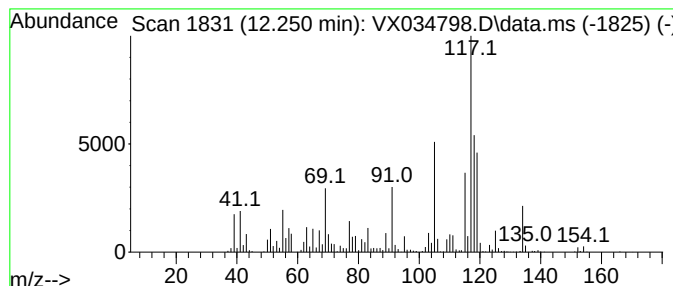
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-propenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	21.90 ug/l	753934	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	90
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	55
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	55
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	55
5			Deltacyclene	118	C9H10	007785-10-6	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

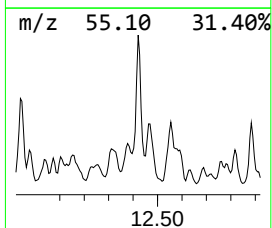
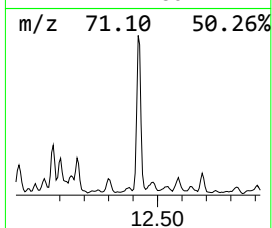
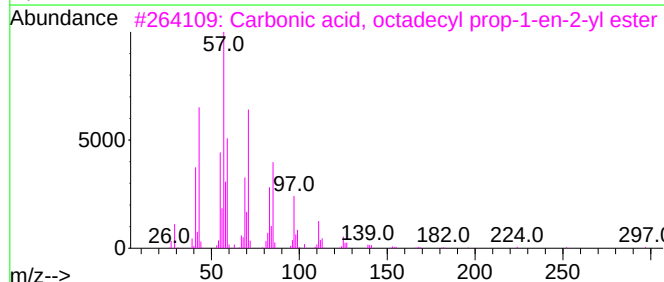
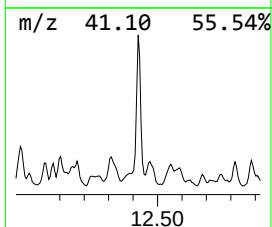
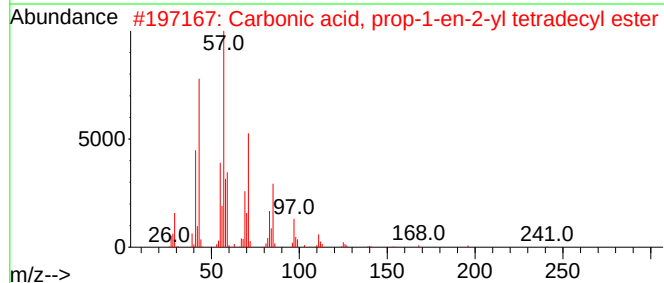
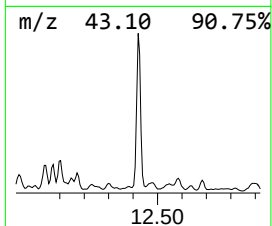
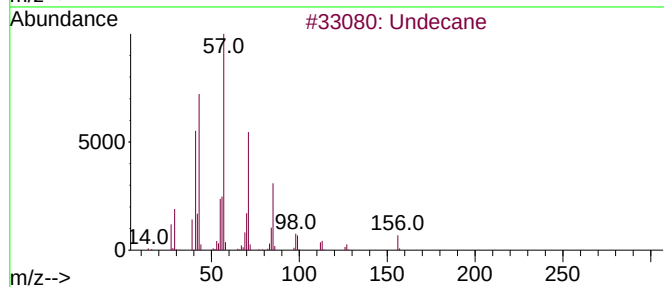
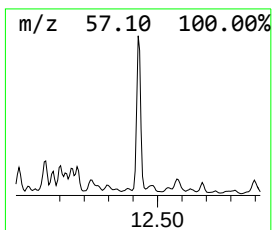
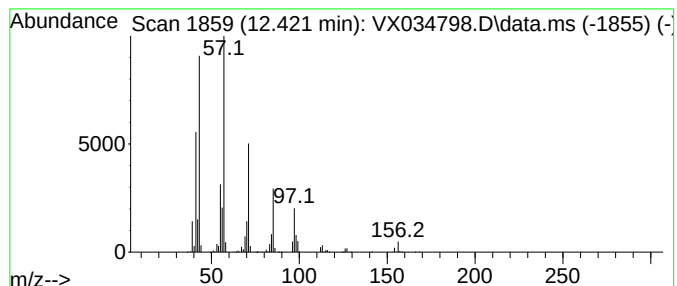
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Quant Title : SW846 8260

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

Peak Number 6 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	71.16 ug/l	2449870	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	80
3	Carbonic acid, octadecyl prop-1-...			354	C22H42O3	1000383-11-5	72
4	Tetradecane			198	C14H30	000629-59-4	64
5	Tridecane			184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

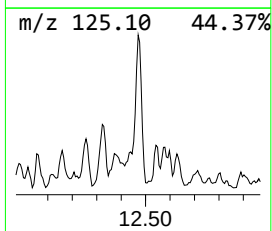
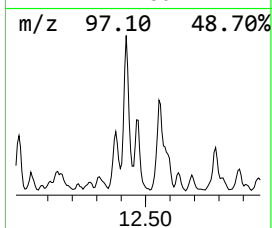
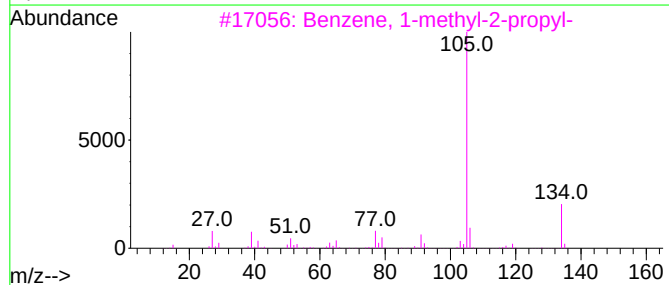
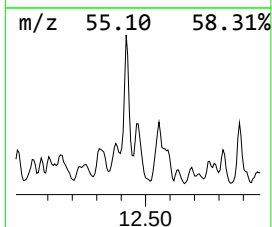
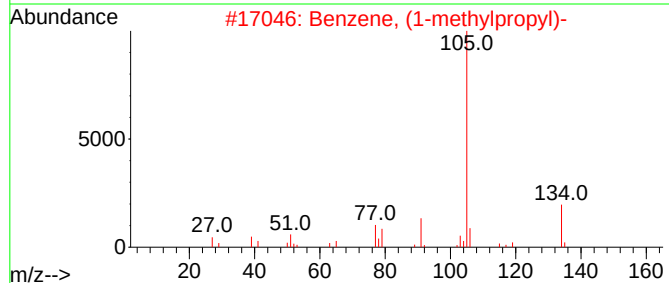
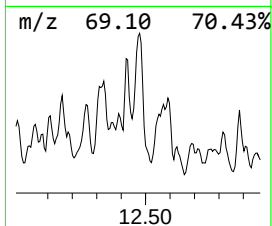
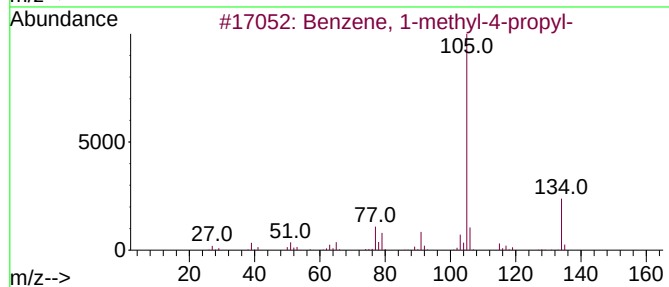
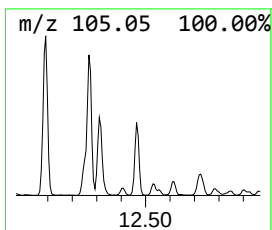
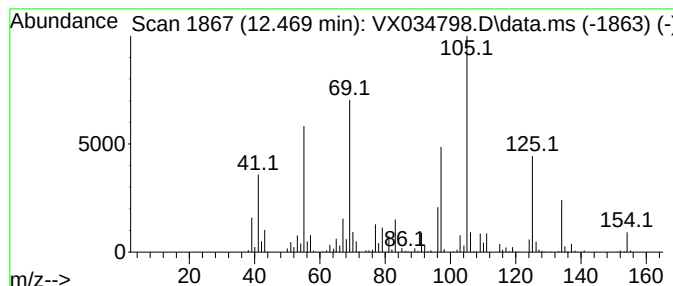
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-4-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	28.89 ug/l	994825	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	56
2			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	25
3			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	25
4			Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	22
5			2-Tolylloxirane	134	C9H10O	002783-26-8	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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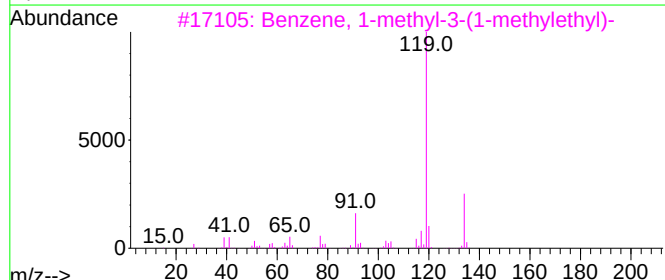
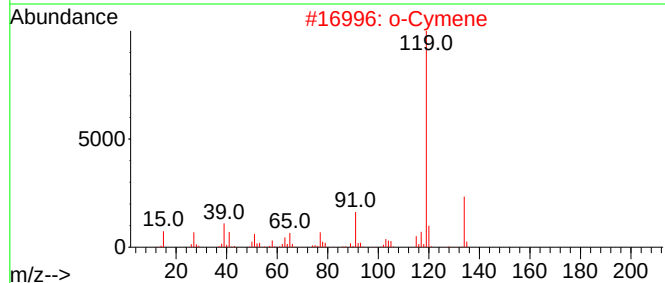
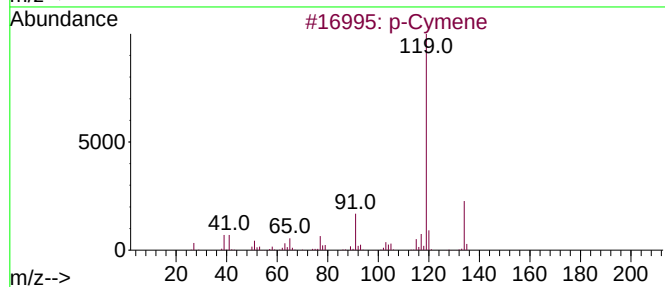
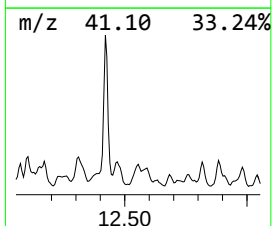
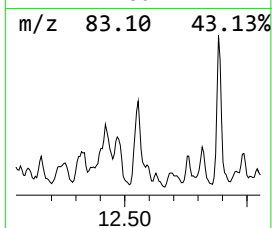
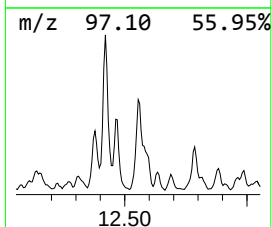
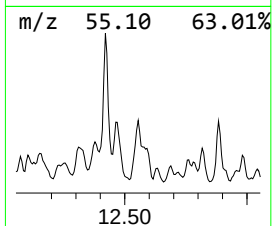
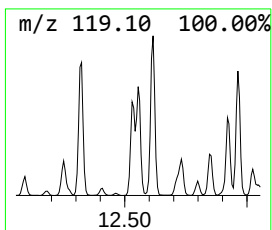
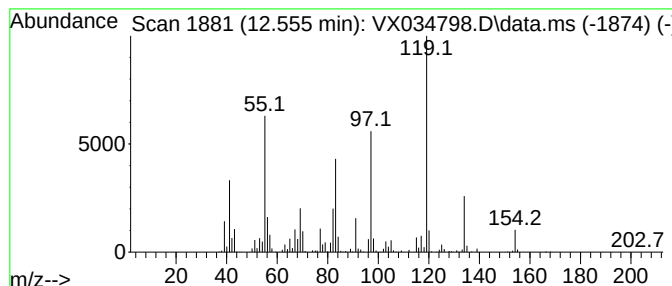
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Quant Title : SW846 8260

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

Peak Number 8 p-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.555	34.94 ug/l	1202820	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	90
2			o-Cymene	134	C10H14	000527-84-4	90
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	89
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	89
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	89



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

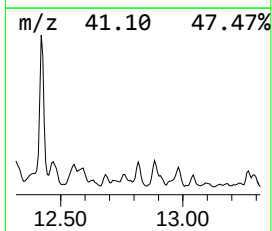
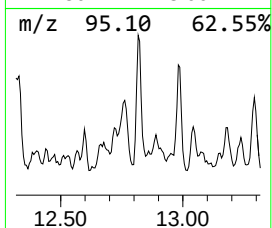
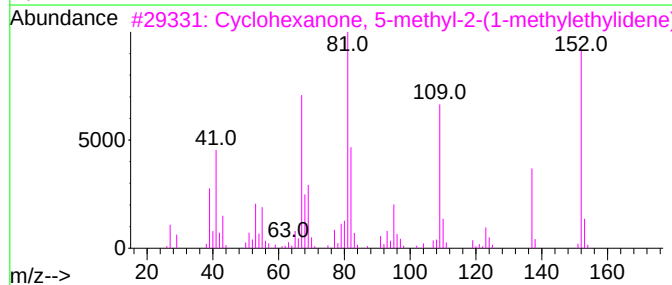
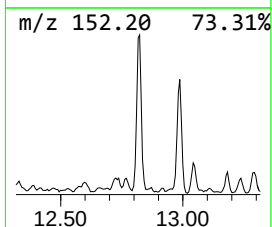
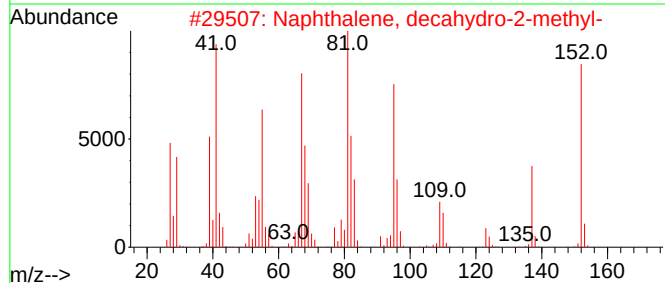
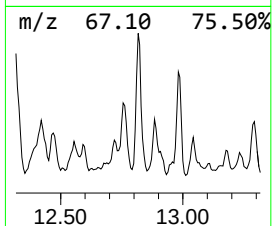
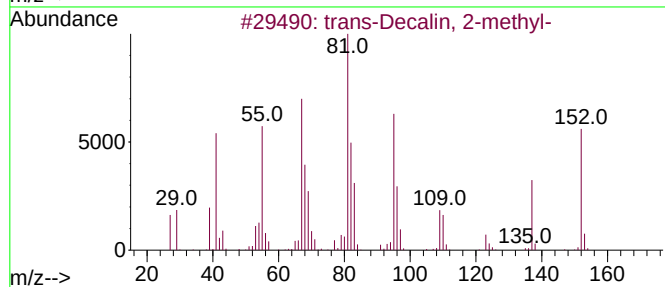
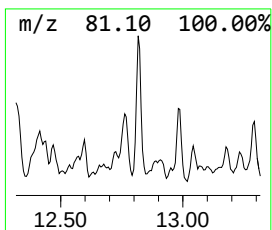
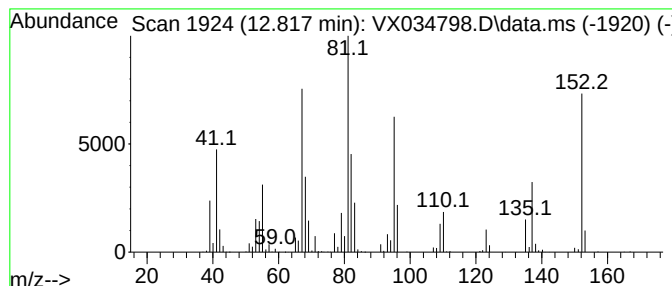
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Quant Title : SW846 8260

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

Peak Number 9 trans-Decalin, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	22.93 ug/l	789599	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	96
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
3			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	87
4			Pulegone	152	C10H16O	000089-82-7	81
5			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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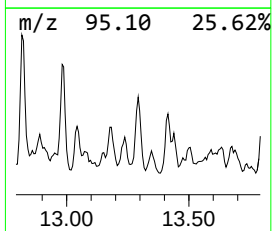
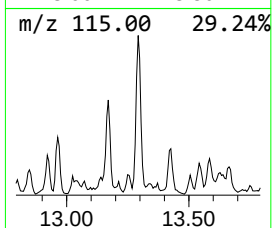
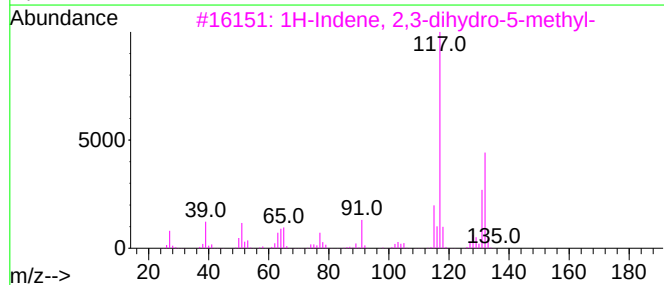
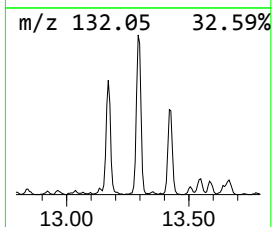
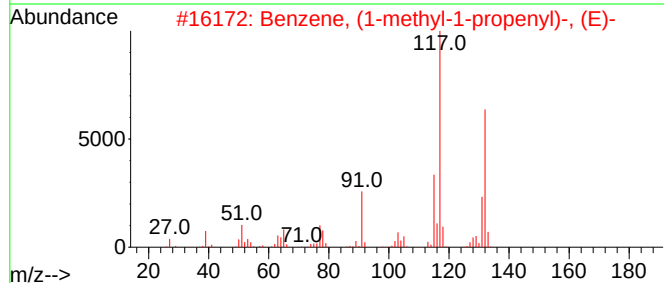
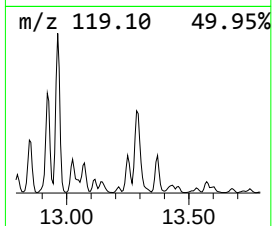
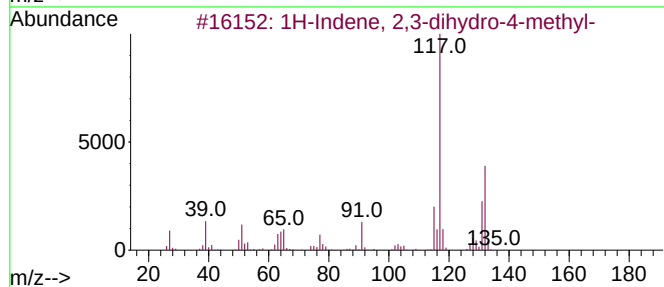
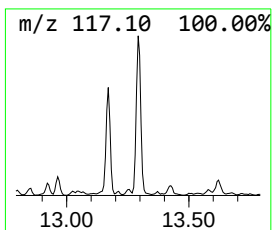
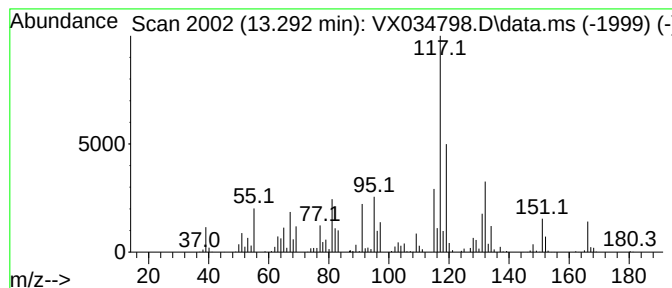
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	25.73 ug/l	885839	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	60
2		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	60
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	60
4		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	56
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034798.D
Acq On : 28 Mar 2023 17:13
Operator : JC/MD
Sample : 02065-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1161

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
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Benzene, 1-ethy...	11.378	42.4	ug/l	1458060	4	12.024	1721480	50.0
Benzene, 1-ethy...	11.616	20.7	ug/l	713777	4	12.024	1721480	50.0
Benzene, 1,2,3-...	12.097	32.9	ug/l	1132760	4	12.024	1721480	50.0
Benzene, 2-prop...	12.250	21.9	ug/l	753934	4	12.024	1721480	50.0
Undecane	12.421	71.2	ug/l	2449870	4	12.024	1721480	50.0
Benzene, 1-meth...	12.469	28.9	ug/l	994825	4	12.024	1721480	50.0
p-Cymene	12.555	34.9	ug/l	1202820	4	12.024	1721480	50.0
trans-Decalin, ...	12.817	22.9	ug/l	789599	4	12.024	1721480	50.0
1H-Indene, 2,3-...	13.292	25.7	ug/l	885839	4	12.024	1721480	50.0