

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
 Data File : VX023010.D
 Acq On : 29 Jun 2021 17:53
 Operator : JC/MD
 Sample : M2875-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X062321W.M
 Title : SW846 8260

Signal : TIC: VX023010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.751	103	109	119	rVB	285156	383624	3.72%	0.694%
2	2.782	260	278	281	rBV	104987	232112	2.25%	0.420%
3	2.831	281	286	291	rVB	159172	290784	2.82%	0.526%
4	3.105	321	331	348	rBV2	276043	658062	6.37%	1.191%
5	3.739	427	435	443	rVB	53909	125969	1.22%	0.228%
6	4.312	520	529	540	rVB	194884	548830	5.32%	0.993%
7	5.196	646	674	687	rBV7	36481	172909	1.67%	0.313%
8	5.397	693	707	713	rBV3	53245	170839	1.65%	0.309%
9	5.489	713	722	729	rBV5	72594	260507	2.52%	0.471%
10	5.629	740	745	766	rVB4	73015	257394	2.49%	0.466%
11	5.836	766	779	791	rBV2	83884	260695	2.53%	0.472%
12	5.970	791	801	805	rVV2	61632	157240	1.52%	0.285%
13	6.049	805	814	825	rVV	610321	1641038	15.90%	2.970%
14	6.171	825	834	843	rVV5	75086	335390	3.25%	0.607%
15	6.263	843	849	855	rVV3	112673	343016	3.32%	0.621%
16	6.342	855	862	878	rVB5	156526	571483	5.54%	1.034%
17	6.769	921	932	938	rBV	141393	357494	3.46%	0.647%
18	6.848	939	945	958	rVB3	102850	323360	3.13%	0.585%
19	7.177	991	999	1007	rVB	72933	155152	1.50%	0.281%
20	7.385	1019	1033	1044	rBV3	183027	519625	5.03%	0.940%
21	7.988	1123	1132	1144	rVB2	57630	158362	1.53%	0.287%
22	8.110	1144	1152	1155	rBV2	81667	170336	1.65%	0.308%
23	8.147	1155	1158	1163	rVB	113779	169249	1.64%	0.306%
24	8.512	1212	1218	1227	rVB3	135050	291755	2.83%	0.528%
25	8.610	1227	1234	1236	rBV3	59415	108269	1.05%	0.196%
26	8.653	1236	1241	1247	rVB	290346	474972	4.60%	0.860%
27	8.720	1247	1252	1258	rBV	117600	198982	1.93%	0.360%
28	9.165	1321	1325	1335	rVB	104181	172500	1.67%	0.312%
29	10.055	1467	1471	1476	rVB	249123	339850	3.29%	0.615%
30	10.201	1490	1495	1501	rVB	1702658	2323142	22.50%	4.204%
31	10.311	1505	1513	1519	rVB	7362154	10323845	100.00%	18.684%
32	10.646	1562	1568	1578	rVB	1081808	1377253	13.34%	2.492%
33	10.963	1614	1620	1628	rBV	277345	358004	3.47%	0.648%
34	11.085	1635	1640	1644	rBV	224232	280293	2.72%	0.507%
35	11.305	1672	1676	1682	rVB	456630	574524	5.57%	1.040%
36	11.384	1683	1689	1696	rVV	1290781	2438530	23.62%	4.413%

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37	11.457	1696	1701	1711	rVB	1037869	1314040	12.73%	2.378%
38	11.616	1721	1727	1736	rBV	1308733	1572545	15.23%	2.846%
39	11.756	1745	1750	1755	rVB	4265406	4982531	48.26%	9.017%
40	12.024	1789	1794	1798	rBV	292854	370469	3.59%	0.670%
41	12.091	1798	1805	1810	rVB	2002904	2407130	23.32%	4.356%
42	12.250	1825	1831	1838	rBV	2916640	3860229	37.39%	6.986%
43	12.323	1838	1843	1849	rVB3	402043	594582	5.76%	1.076%
44	12.414	1852	1858	1862	rBV2	253725	332573	3.22%	0.602%
45	12.469	1862	1867	1873	rVB2	261226	356117	3.45%	0.644%
46	12.536	1873	1878	1880	rBV	286095	388127	3.76%	0.702%
47	12.560	1880	1882	1886	rVB	208679	206851	2.00%	0.374%
48	12.615	1886	1891	1894	rBV	872403	1028451	9.96%	1.861%
49	12.646	1894	1896	1900	rVV	198457	227430	2.20%	0.412%
50	12.701	1900	1905	1913	rVV	834334	1135907	11.00%	2.056%
51	12.853	1924	1930	1934	rVB2	166898	219875	2.13%	0.398%
52	12.926	1934	1942	1945	rBV	613403	748831	7.25%	1.355%
53	12.963	1945	1948	1954	rVB	479635	602427	5.84%	1.090%
54	13.030	1954	1959	1965	rBV3	56942	124685	1.21%	0.226%
55	13.170	1978	1982	1988	rVB	619612	717970	6.95%	1.299%
56	13.292	1998	2002	2008	rVB2	1225420	1626460	15.75%	2.943%
57	13.426	2020	2024	2033	rVB	260574	326169	3.16%	0.590%
58	13.548	2040	2044	2047	rVV	162206	204185	1.98%	0.370%
59	13.585	2047	2050	2056	rVB3	136689	205252	1.99%	0.371%
60	13.670	2061	2064	2069	rVB2	145553	217183	2.10%	0.393%
61	13.780	2075	2082	2091	rBV	2065916	2509595	24.31%	4.542%
62	13.871	2091	2097	2101	rVB	95391	133696	1.30%	0.242%
63	14.079	2126	2131	2137	rBV	110866	138645	1.34%	0.251%
64	14.219	2149	2154	2159	rBV	92320	151857	1.47%	0.275%
65	14.639	2219	2223	2234	rVB	476120	584218	5.66%	1.057%
66	14.780	2241	2246	2256	rBV	333608	442629	4.29%	0.801%

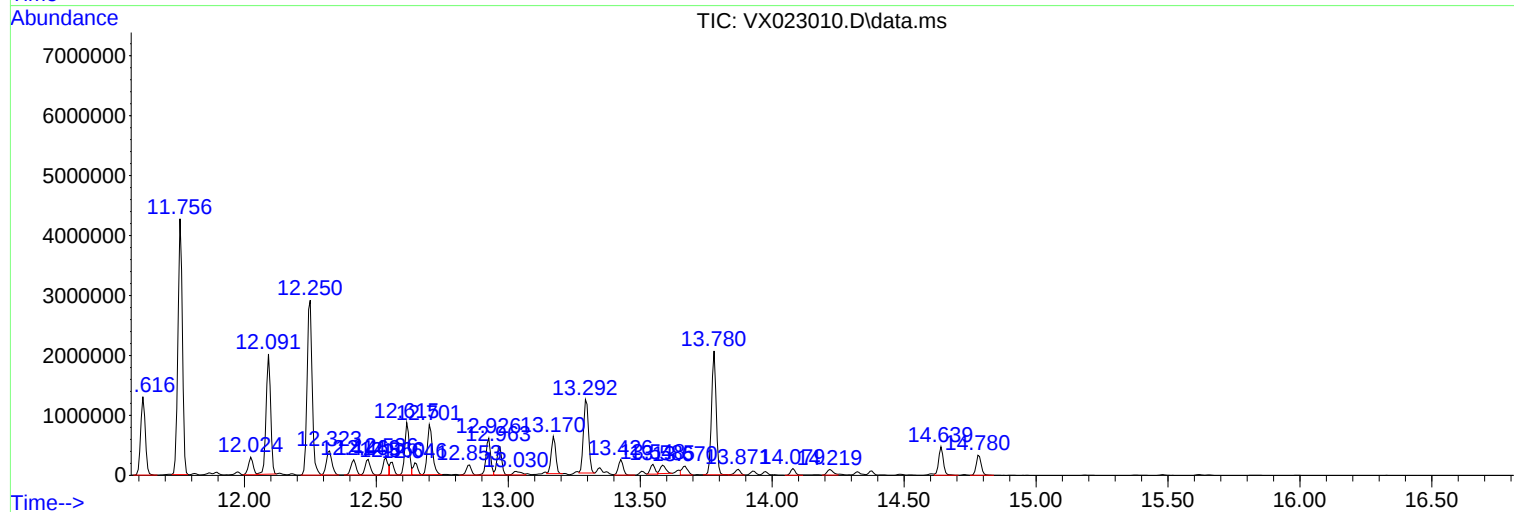
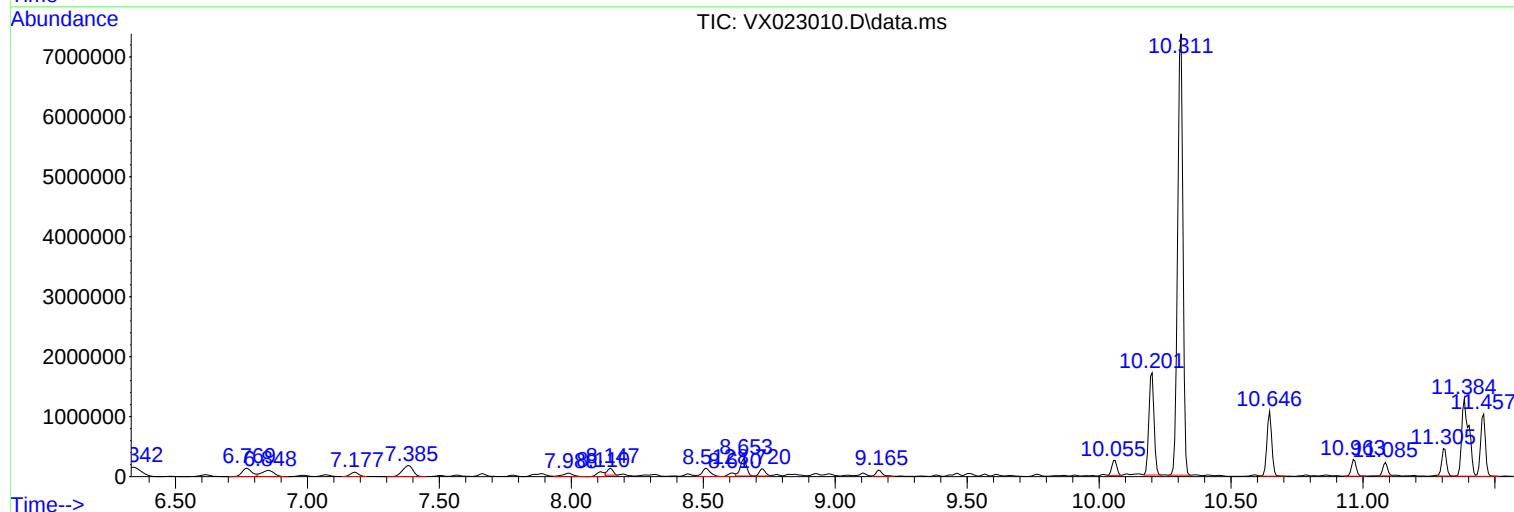
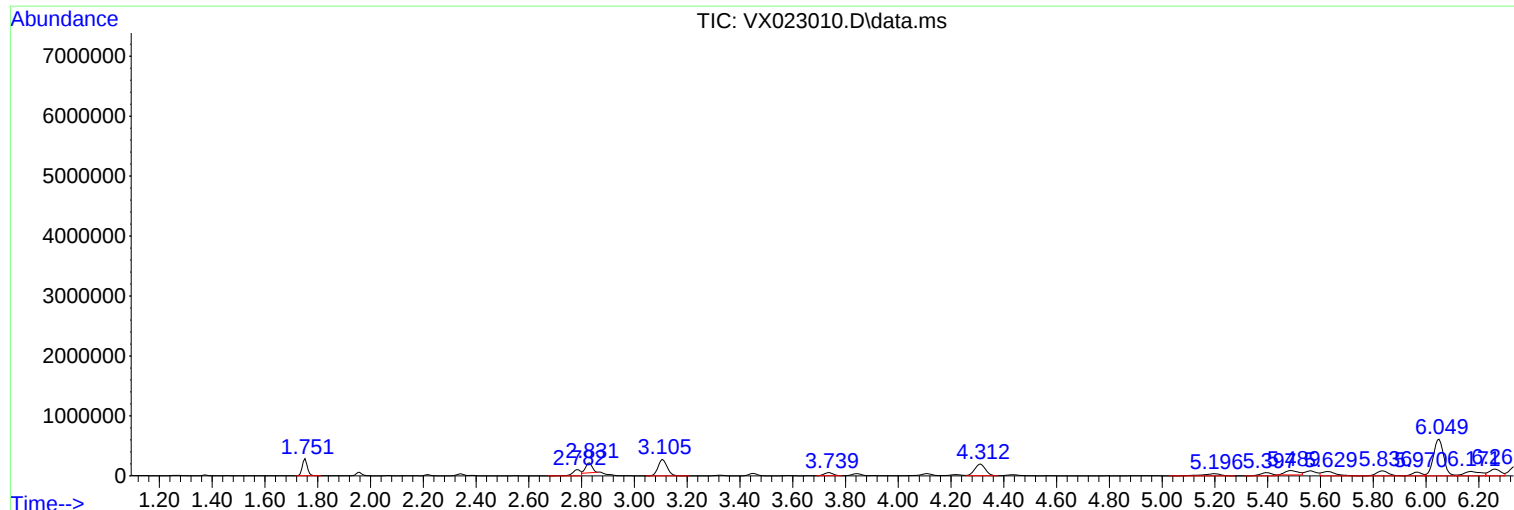
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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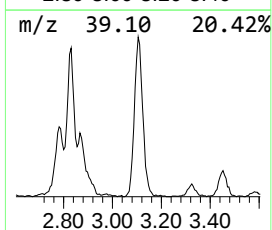
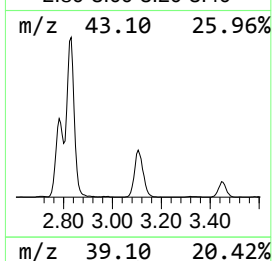
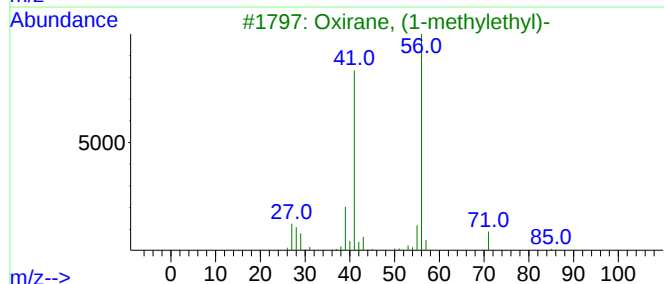
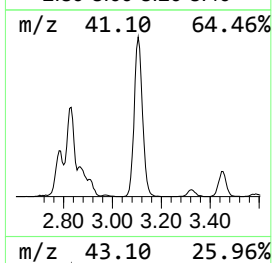
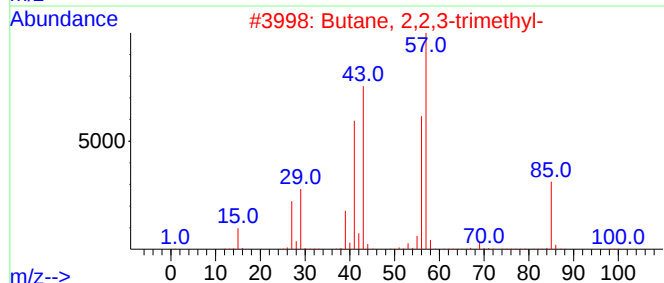
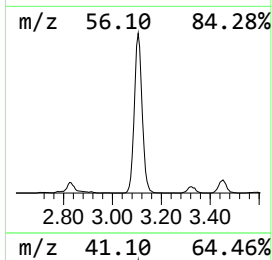
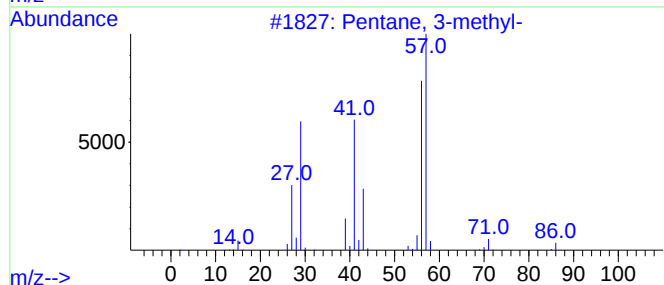
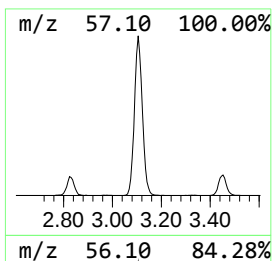
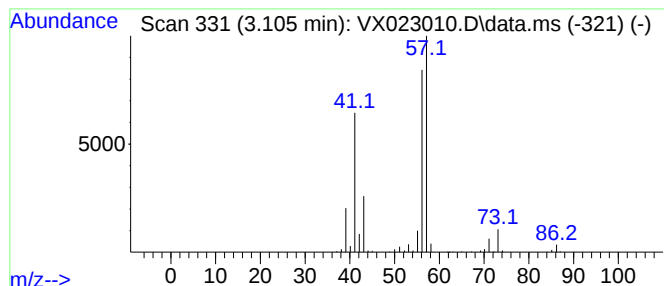
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	127.83 ug/l	658062	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	56
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42
4			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	39
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	39



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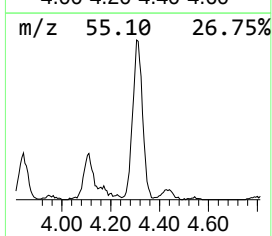
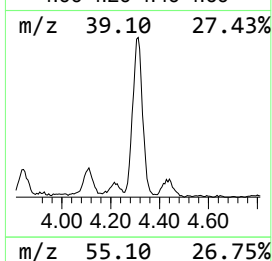
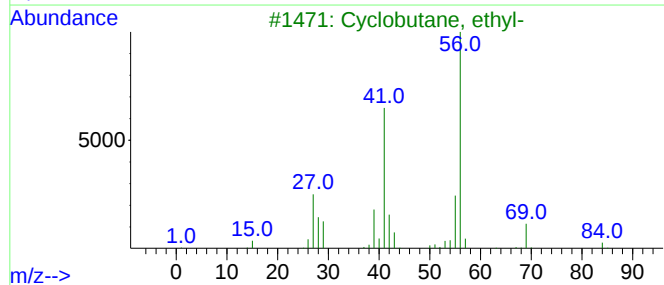
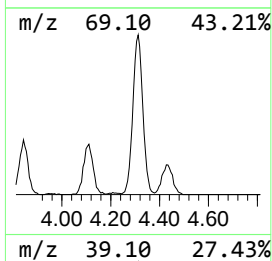
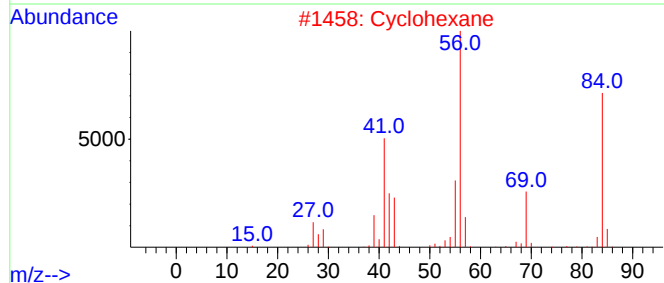
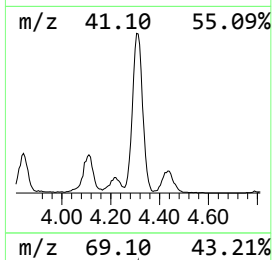
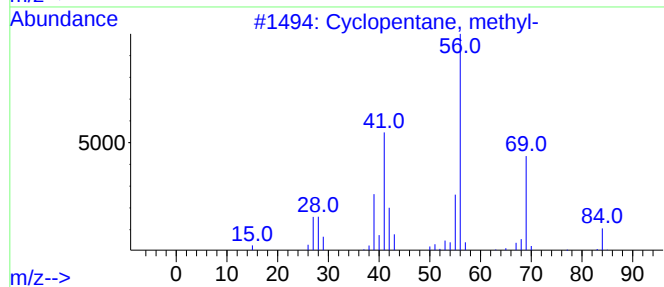
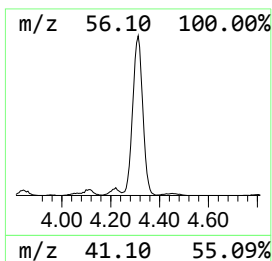
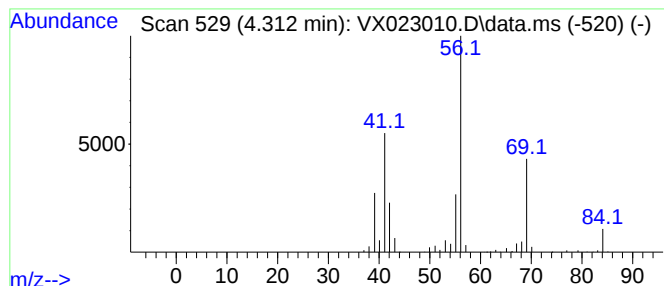
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	106.61 ug/l	548830	Pentafluorobenzene	5.562

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			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5			Cyclobutane	56	C4H8	000287-23-0	50



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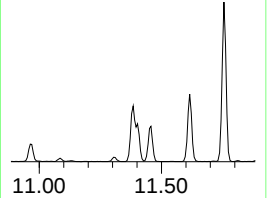
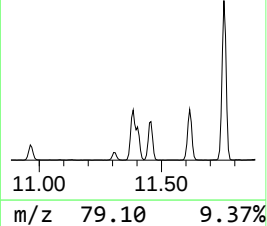
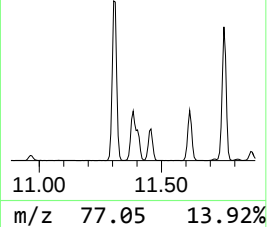
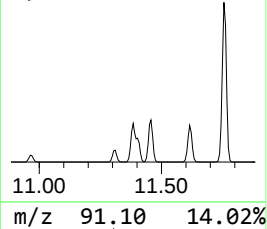
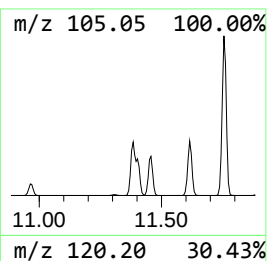
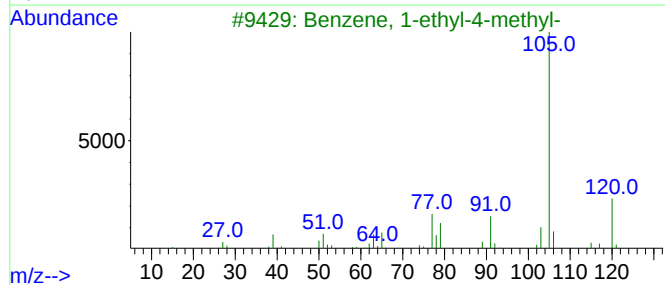
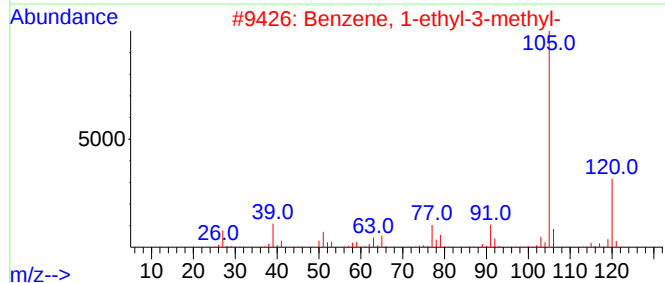
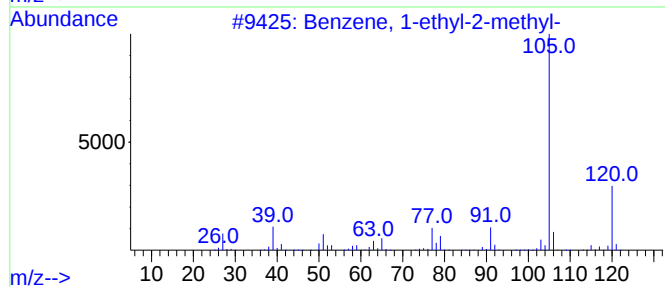
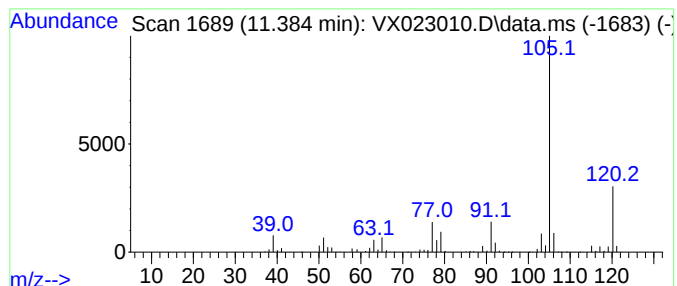
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	329.11 ug/l	2438530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
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			Mesitylene	120	C9H12	000108-67-8	91



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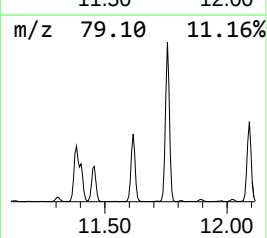
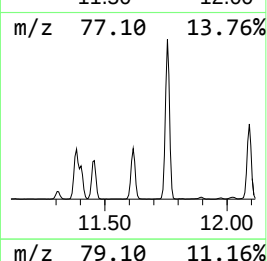
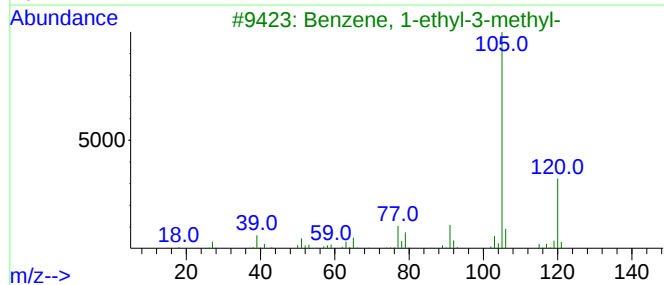
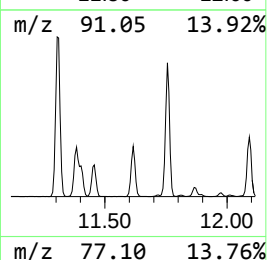
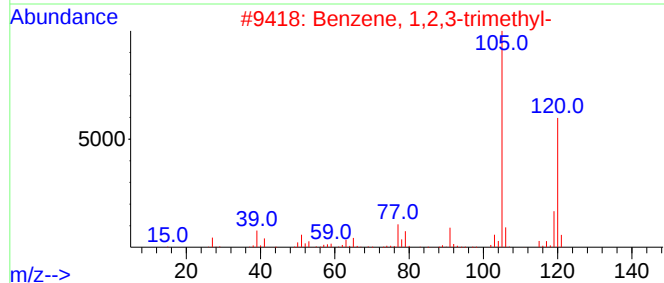
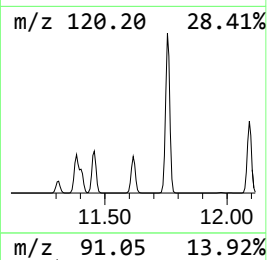
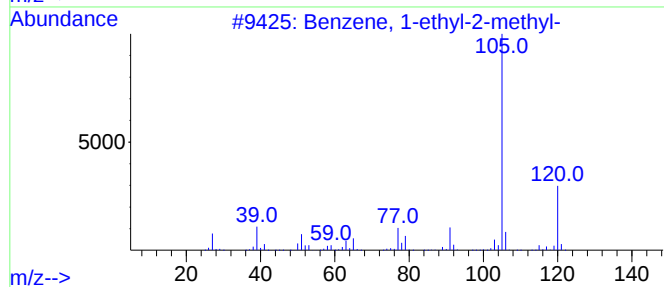
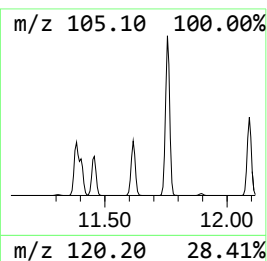
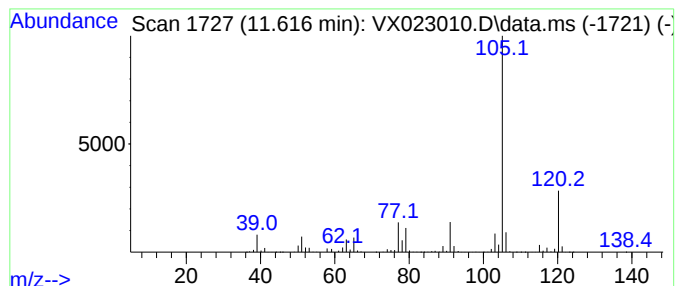
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Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	212.24 ug/l	1572550	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	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

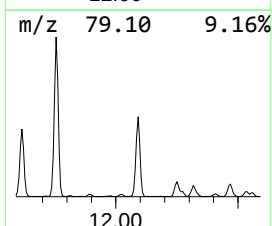
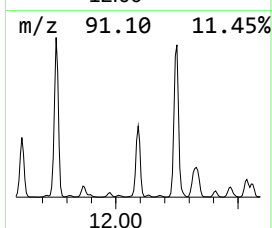
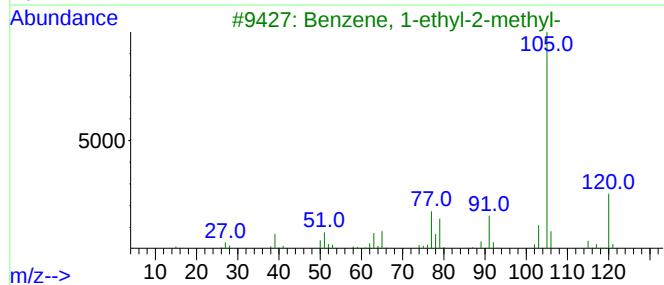
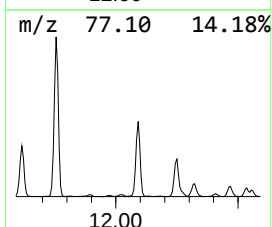
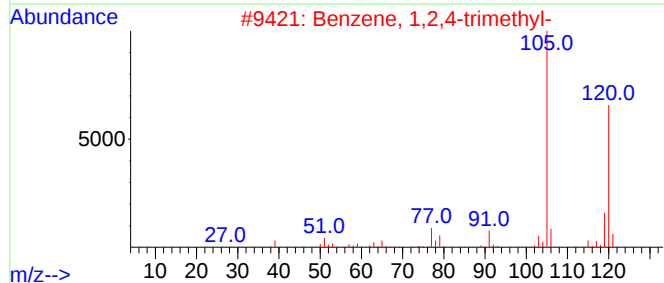
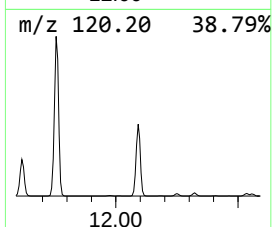
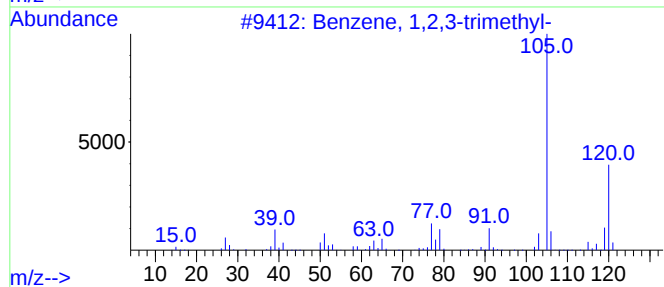
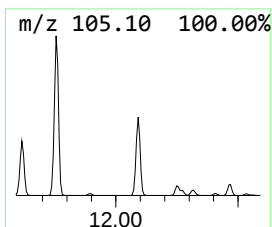
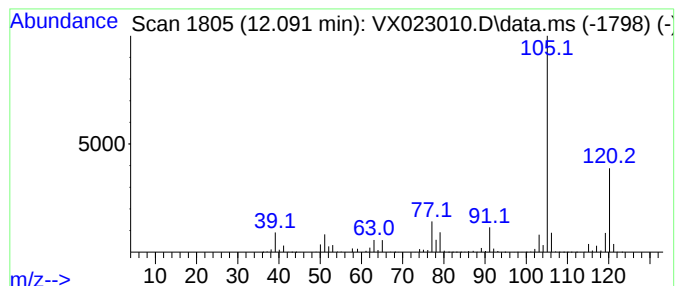
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	324.88 ug/l	2407130	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

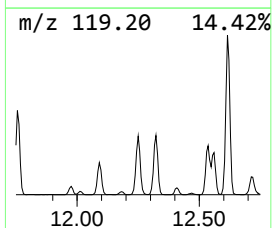
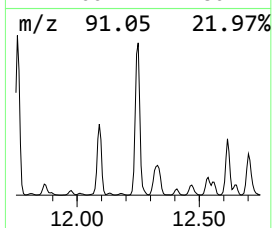
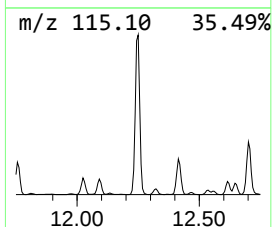
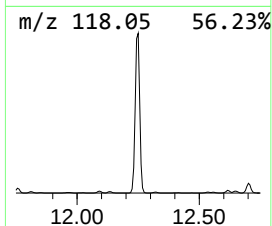
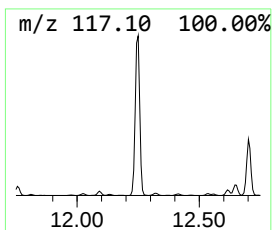
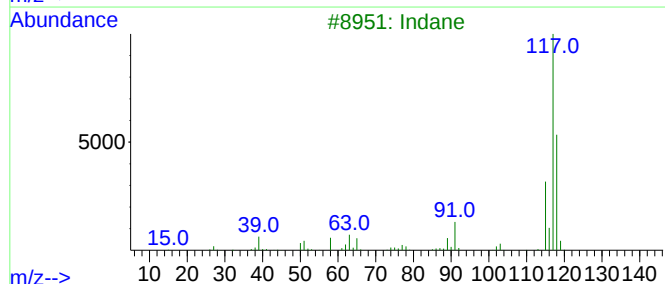
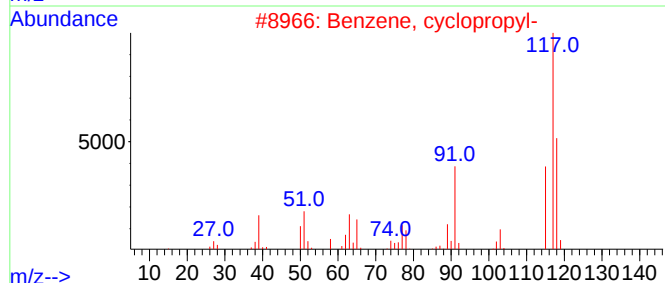
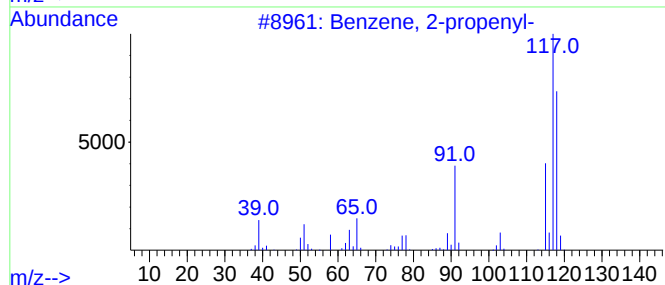
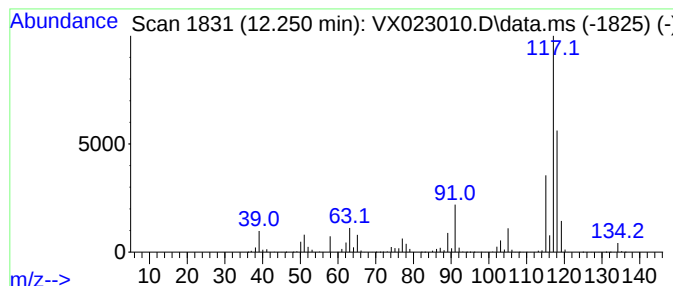
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	520.99 ug/l	3860230	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Indane	118	C9H10	000496-11-7	76
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

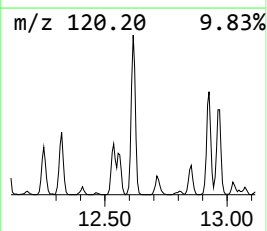
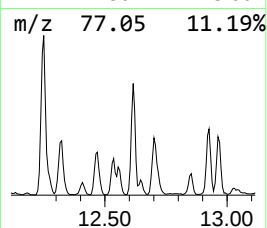
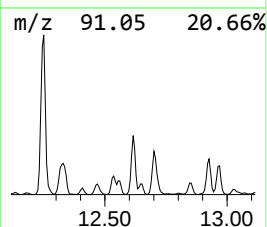
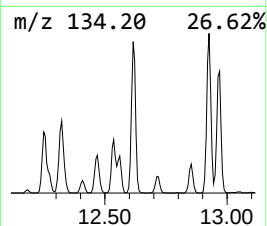
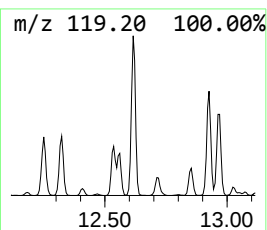
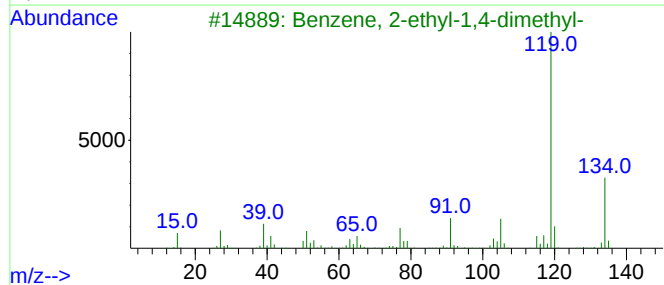
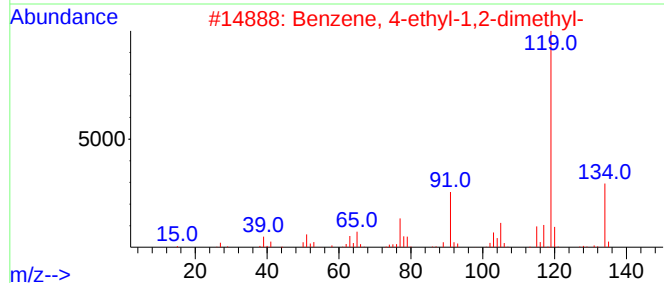
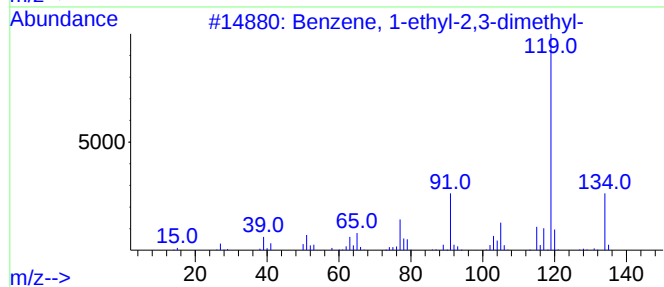
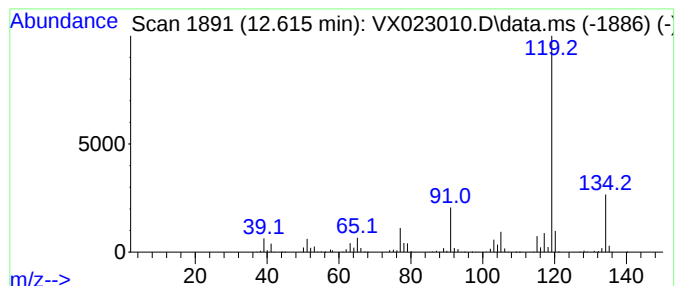
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.615	138.80 ug/l	1028450	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

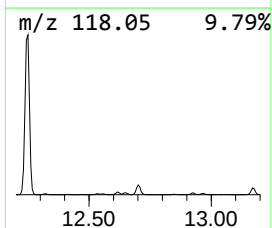
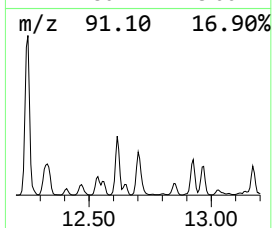
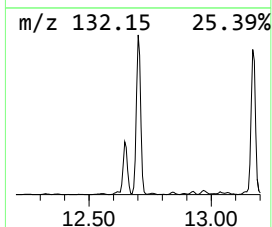
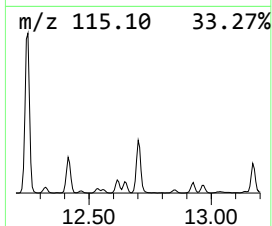
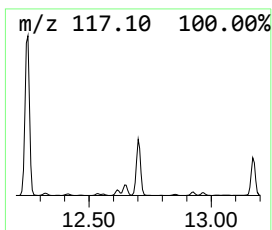
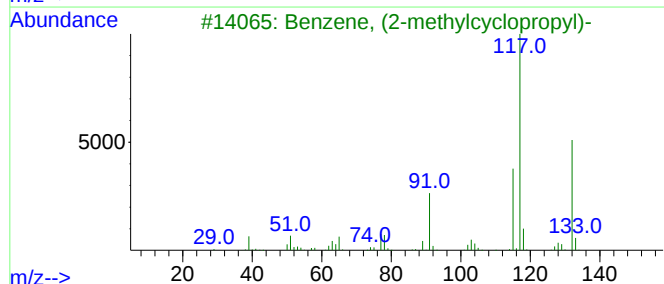
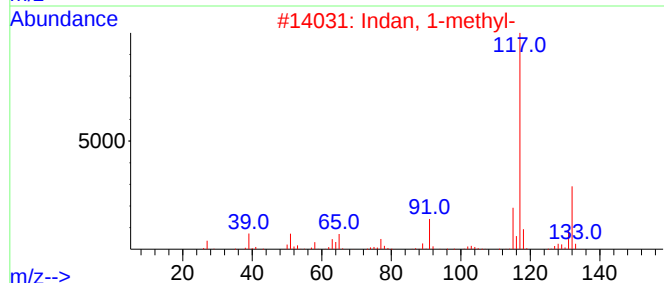
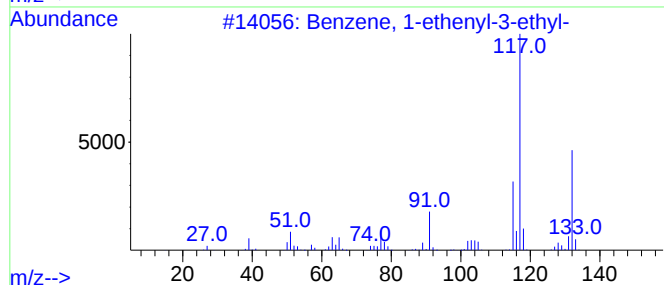
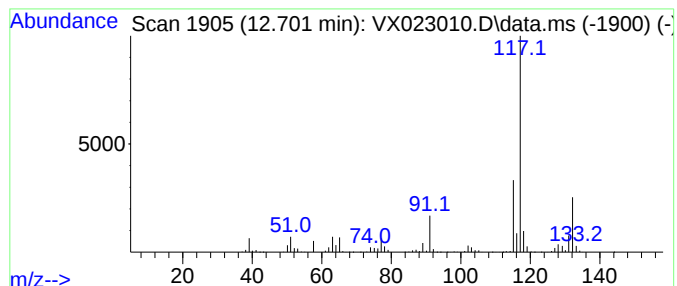
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	153.31 ug/l	1135910	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	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	90
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

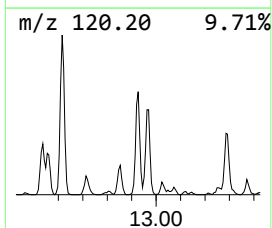
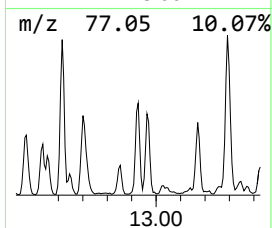
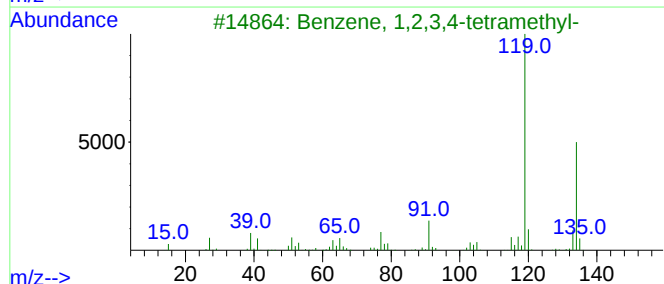
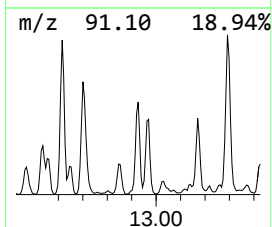
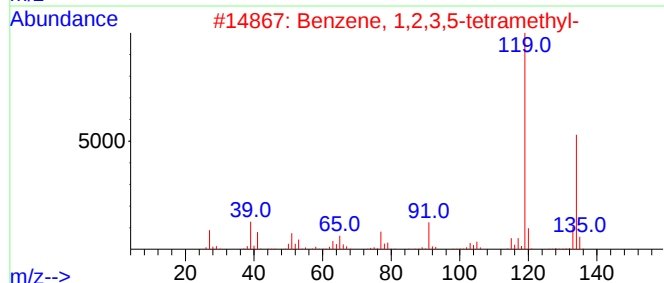
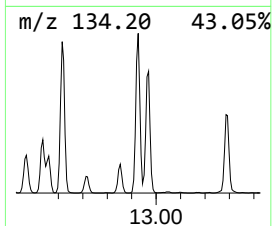
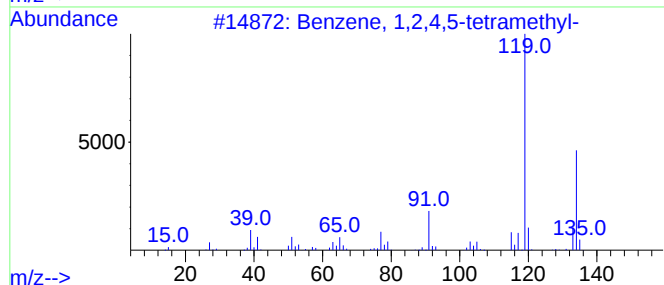
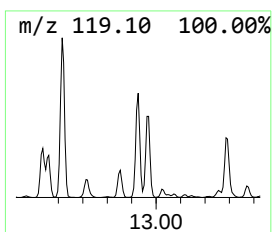
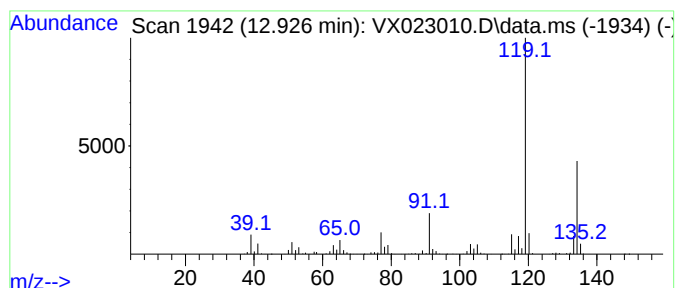
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.926	101.07 ug/l	748831	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	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5			o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

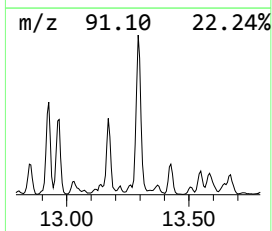
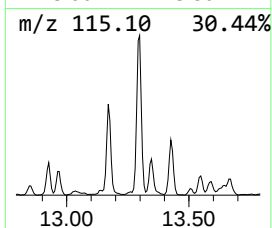
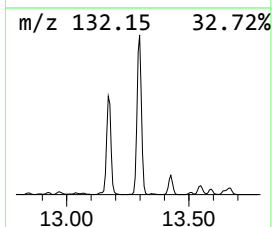
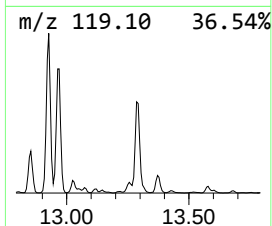
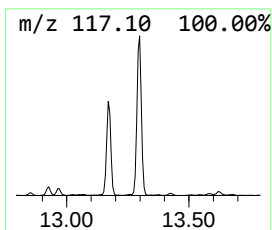
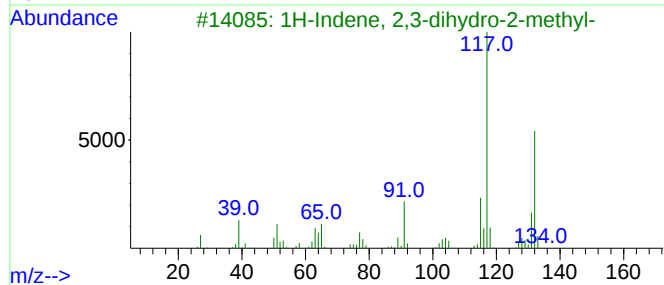
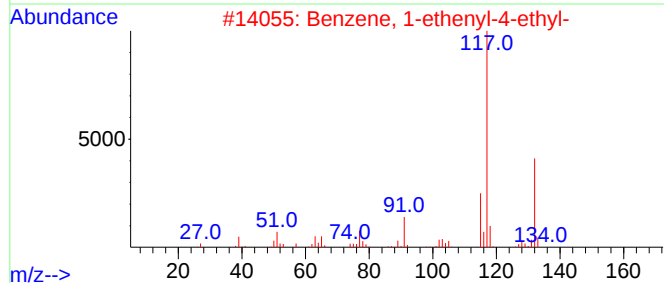
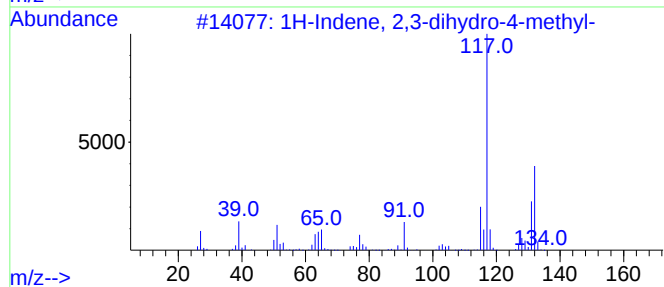
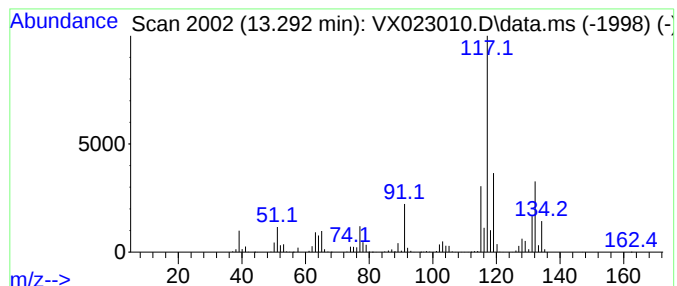
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	219.51 ug/l	1626460	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	93
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	81
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023010.D
Acq On : 29 Jun 2021 17:53
Operator : JC/MD
Sample : M2875-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.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
Pentane, 3-methyl-	3.105	127.8	ug/l	658062	1	5.562	257394	50.0
Cyclopentane, m...	4.312	106.6	ug/l	548830	1	5.562	257394	50.0
Benzene, 1-ethy...	11.384	329.1	ug/l	2438530	4	12.024	370469	50.0
Benzene, 1,2,3-...	11.616	212.2	ug/l	1572550	4	12.024	370469	50.0
Benzene, 1-ethy...	12.091	324.9	ug/l	2407130	4	12.024	370469	50.0
Benzene, 2-prop...	12.250	521.0	ug/l	3860230	4	12.024	370469	50.0
Benzene, 1-ethy...	12.615	138.8	ug/l	1028450	4	12.024	370469	50.0
Benzene, 1-ethe...	12.701	153.3	ug/l	1135910	4	12.024	370469	50.0
Benzene, 1,2,4,...	12.926	101.1	ug/l	748831	4	12.024	370469	50.0
1H-Indene, 2,3-...	13.292	219.5	ug/l	1626460	4	12.024	370469	50.0