

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
 Data File : VX035570.D
 Acq On : 08 May 2023 19:08
 Operator : JC/MD
 Sample : 02658-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 509

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.160	163	176	183	rBV2	53884	251325	1.04%	0.163%
2	2.386	206	213	231	rBV	2444488	4647890	19.18%	3.008%
3	2.593	231	247	283	rBV	469313	2824255	11.66%	1.828%
4	3.111	323	332	347	rVB	266999	611345	2.52%	0.396%
5	5.385	693	705	714	rBV	147212	429798	1.77%	0.278%
6	5.550	723	732	750	rVB	260301	753746	3.11%	0.488%
7	5.958	786	799	804	rBV	156293	417630	1.72%	0.270%
8	6.037	804	812	825	rVB	1760718	4637815	19.14%	3.002%
9	6.763	922	931	949	rVB	400867	958890	3.96%	0.621%
10	8.580	1221	1229	1236	rBV	8299553	13704728	56.56%	8.870%
11	8.653	1236	1241	1246	rVV	792453	1211075	5.00%	0.784%
12	8.726	1246	1253	1259	rVV	14903339	24231086	100.00%	15.682%
13	9.031	1296	1303	1320	rBV	722591	1212292	5.00%	0.785%
14	10.055	1460	1471	1476	rBV	849571	1146827	4.73%	0.742%
15	10.195	1488	1494	1501	rBV	3863387	4878828	20.13%	3.158%
16	10.305	1505	1512	1522	rBV	12601355	17557133	72.46%	11.363%
17	10.640	1562	1567	1582	rVB	8813694	11859596	48.94%	7.675%
18	10.963	1614	1620	1623	rBV	360876	456638	1.88%	0.296%
19	11.006	1623	1627	1635	rVV	200318	379864	1.57%	0.246%
20	11.079	1635	1639	1650	rVB	733298	953059	3.93%	0.617%
21	11.305	1668	1676	1681	rBV	661745	810825	3.35%	0.525%
22	11.378	1683	1688	1696	rVV	3687486	6135862	25.32%	3.971%
23	11.451	1696	1700	1711	rVB	1772061	2123912	8.77%	1.375%
24	11.610	1721	1726	1737	rVB	2005898	2567405	10.60%	1.662%
25	11.756	1744	1750	1755	rBV	8782743	11243673	46.40%	7.277%
26	12.024	1789	1794	1799	rVB	905270	1157049	4.78%	0.749%
27	12.085	1799	1804	1810	rBV	3785626	4788402	19.76%	3.099%
28	12.244	1822	1830	1838	rBV2	3540232	4985235	20.57%	3.226%
29	12.317	1838	1842	1851	rVV2	701717	1042325	4.30%	0.675%
30	12.414	1852	1858	1862	rVV2	191780	278170	1.15%	0.180%
31	12.463	1862	1866	1872	rVB	222845	265183	1.09%	0.172%
32	12.530	1872	1877	1879	rBV	680107	810940	3.35%	0.525%
33	12.555	1879	1881	1886	rVV	534355	574564	2.37%	0.372%
34	12.615	1886	1891	1894	rVV	952372	1172707	4.84%	0.759%
35	12.701	1900	1905	1912	rVV2	733089	1045940	4.32%	0.677%
36	12.798	1912	1921	1925	rVV3	130459	305643	1.26%	0.198%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.847	1925	1929	1935	rVB	408267	496792	2.05%	0.322%
38	12.920	1935	1941	1944	rBV	864590	1014767	4.19%	0.657%
39	12.963	1944	1948	1953	rVB	1377989	1593110	6.57%	1.031%
40	13.170	1977	1982	1986	rVB	1017842	1196699	4.94%	0.774%
41	13.292	1997	2002	2007	rVB2	2262260	3031195	12.51%	1.962%
42	13.420	2019	2023	2032	rVB	392744	507347	2.09%	0.328%
43	13.585	2046	2050	2056	rVV2	227024	441263	1.82%	0.286%
44	13.664	2060	2063	2068	rVB2	192334	297835	1.23%	0.193%
45	13.774	2076	2081	2087	rBV	6036903	7645422	31.55%	4.948%
46	14.219	2149	2154	2160	rBV2	192582	346683	1.43%	0.224%
47	14.633	2215	2222	2228	rBV	2545974	3283198	13.55%	2.125%
48	14.780	2240	2246	2251	rBV	1639406	1930225	7.97%	1.249%
49	15.615	2375	2383	2386	rBV	187093	296866	1.23%	0.192%

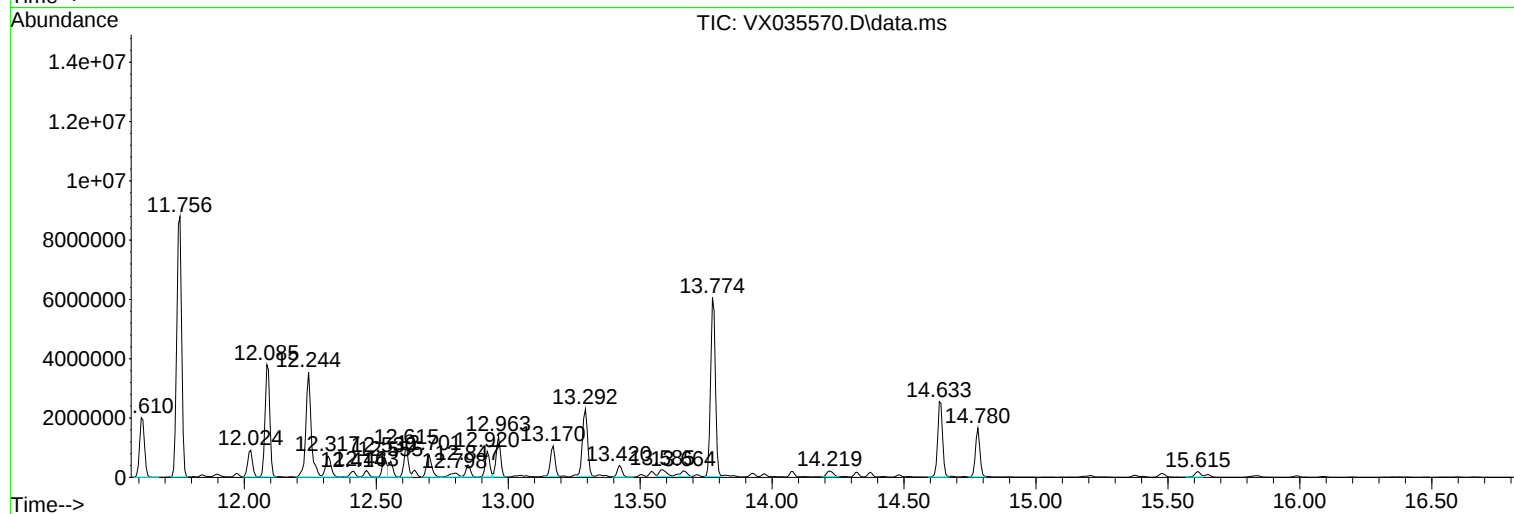
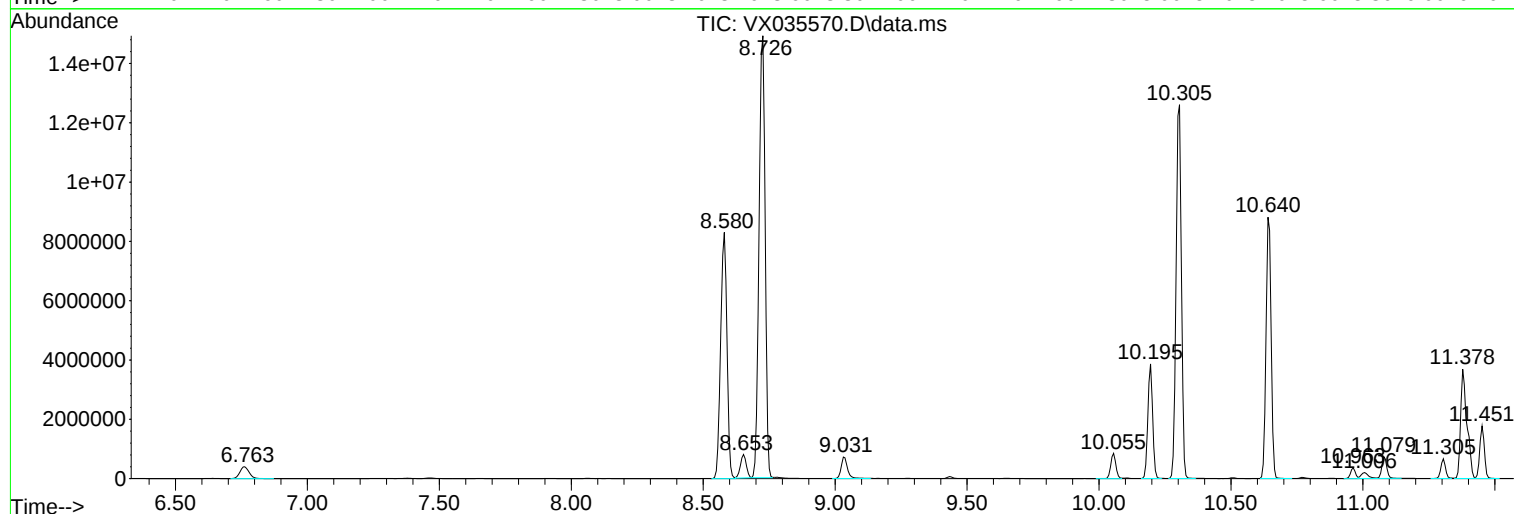
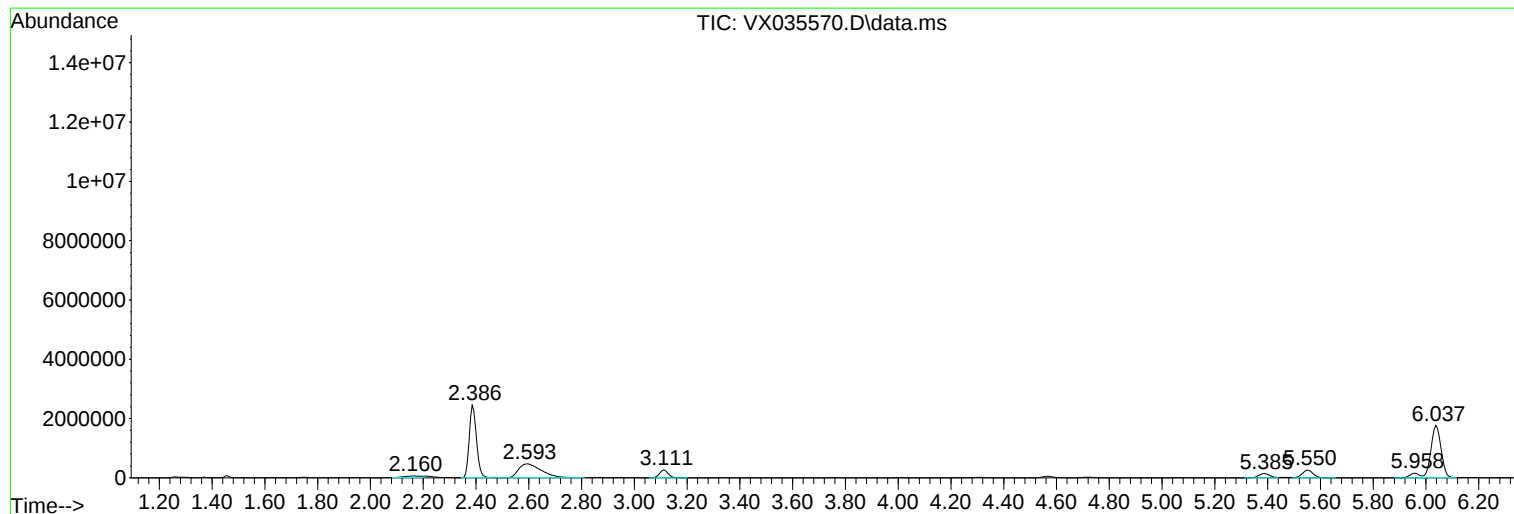
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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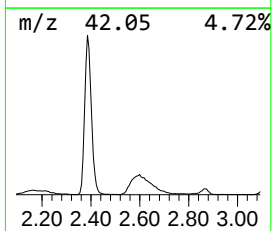
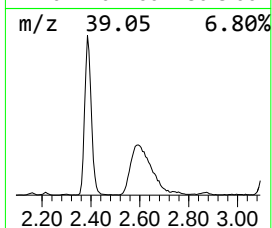
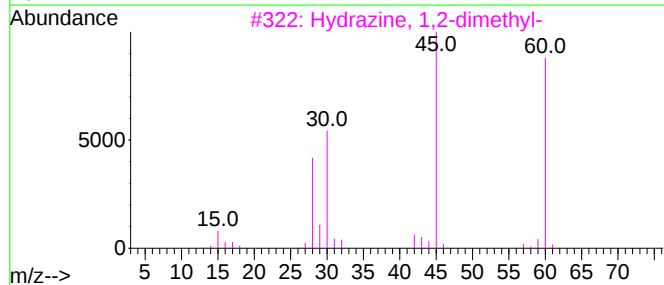
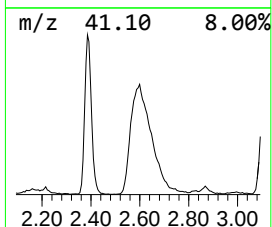
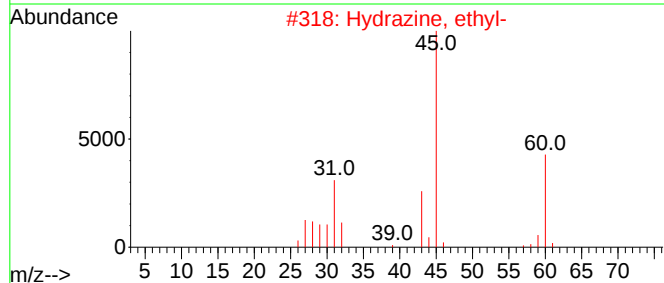
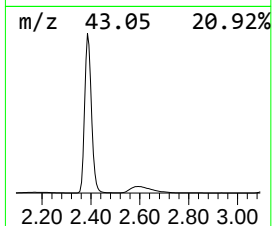
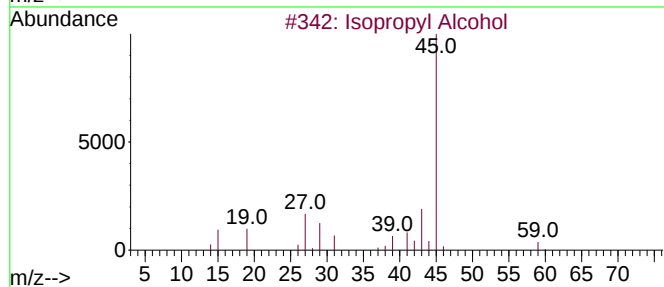
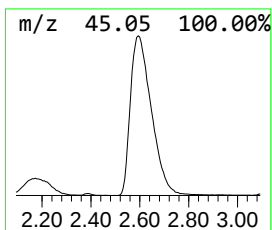
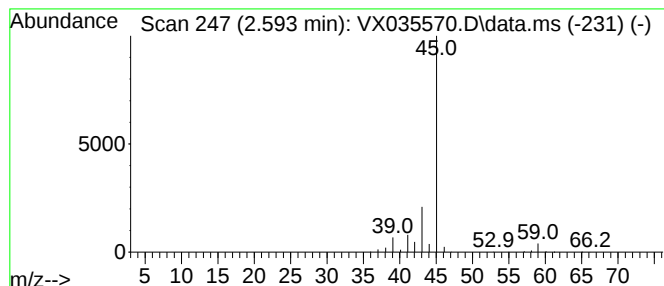
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.593	187.35 ug/l	2824260	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Formamide	45	CH3NO	000075-12-7	5
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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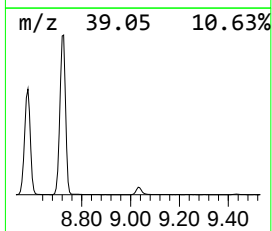
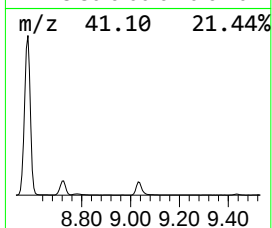
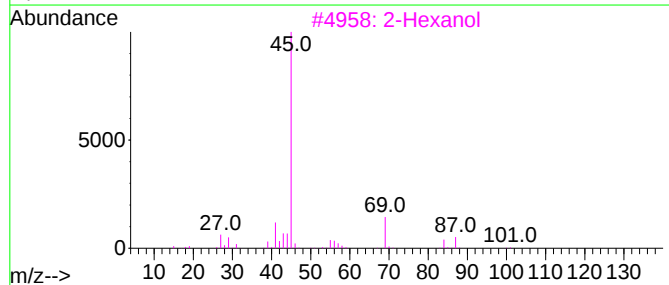
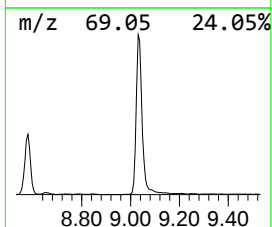
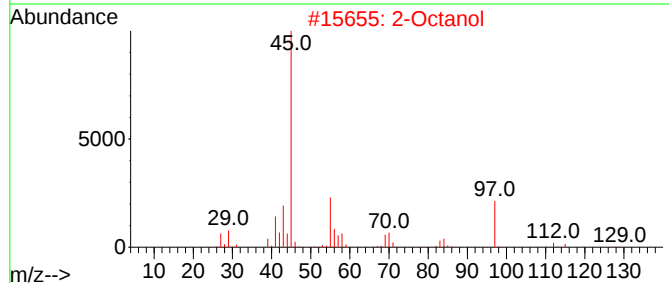
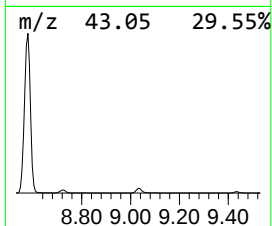
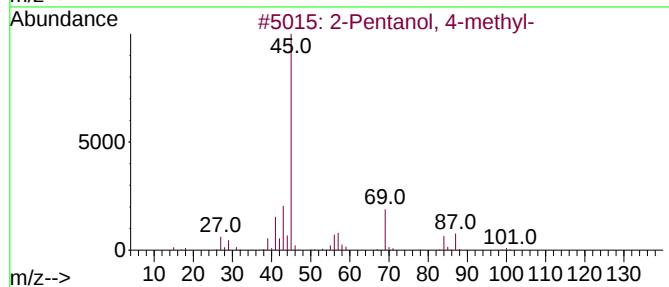
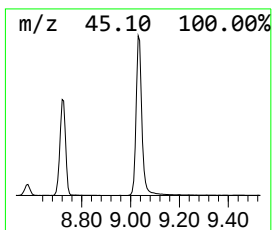
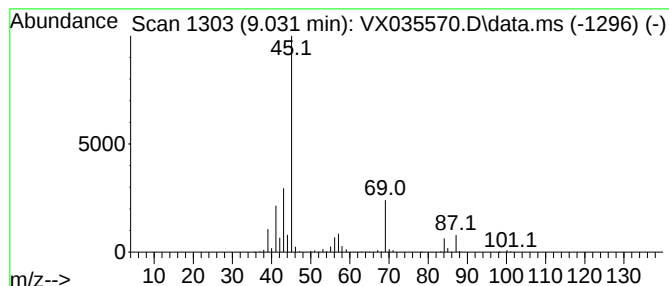
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Pentanol, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.031	52.85 ug/l	1212290	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
2			2-Octanol	130	C8H18O	000123-96-6	78
3			2-Hexanol	102	C6H14O	000626-93-7	78
4			2-Octanol, (R)-	130	C8H18O	005978-70-1	78
5			2-Octanol, (S)-	130	C8H18O	006169-06-8	64



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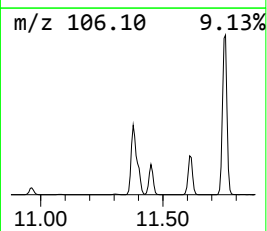
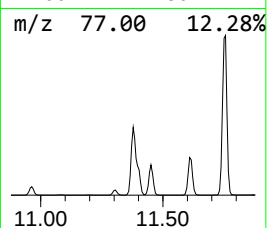
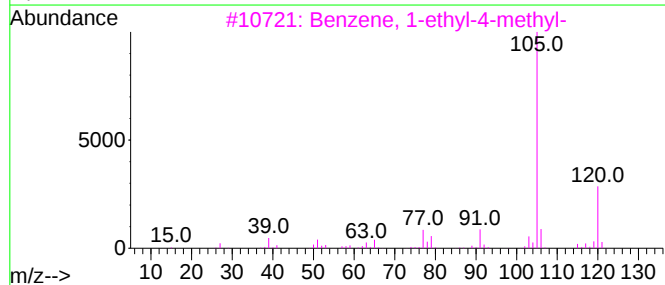
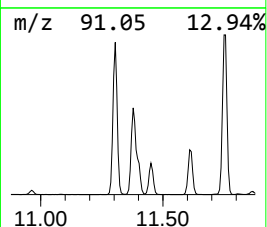
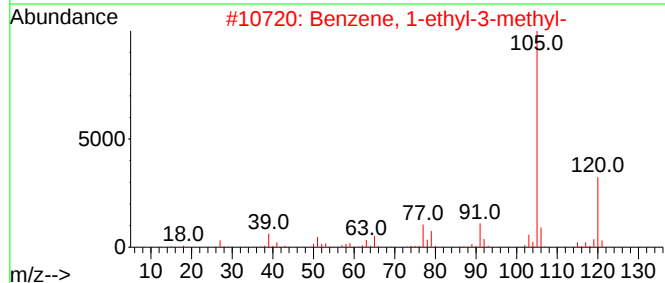
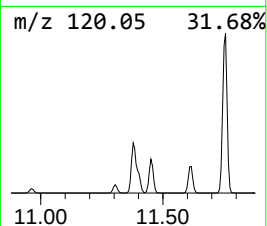
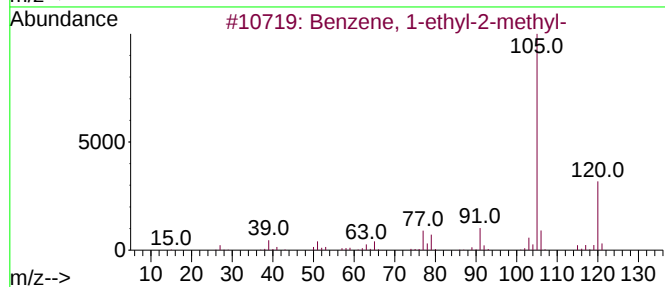
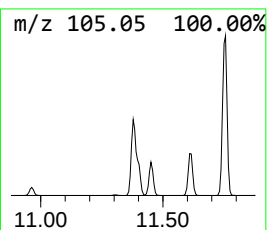
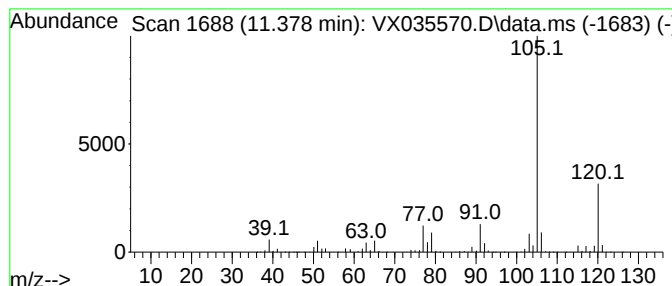
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	265.15 ug/l	6135860	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	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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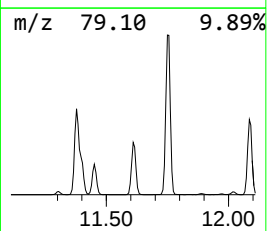
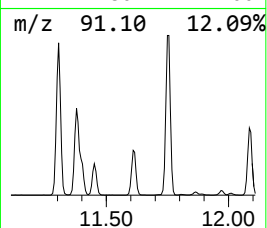
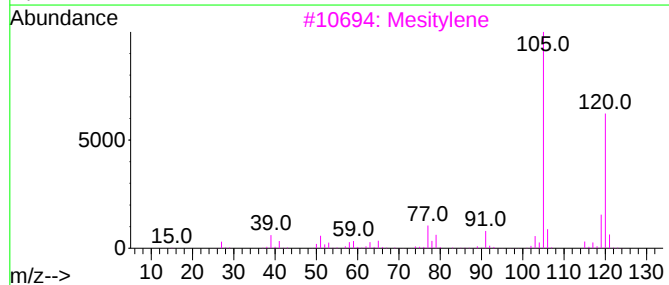
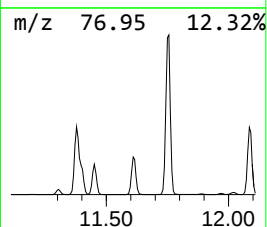
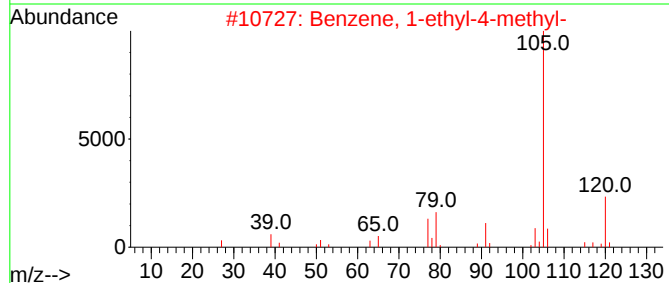
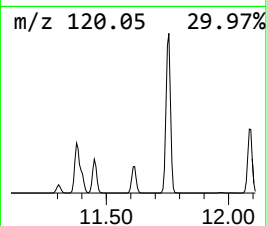
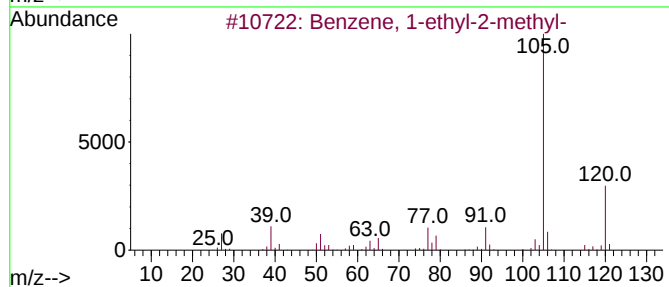
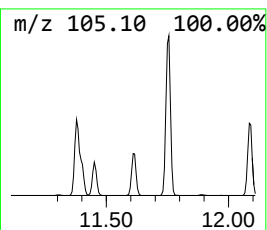
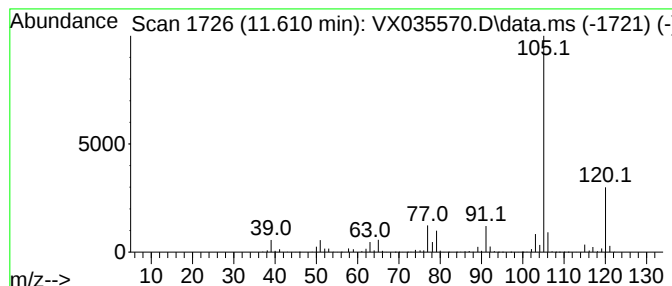
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	110.95 ug/l	2567410	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-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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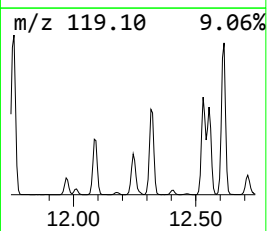
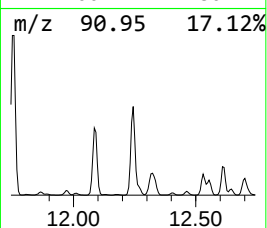
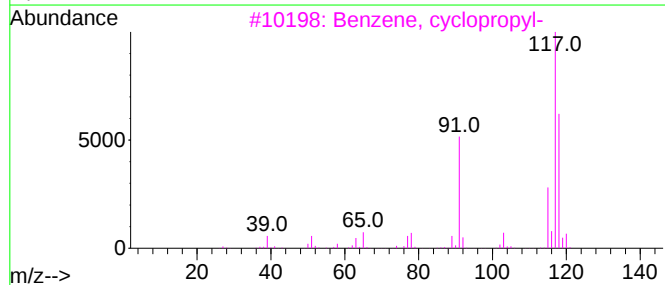
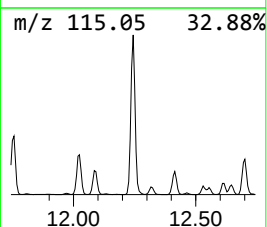
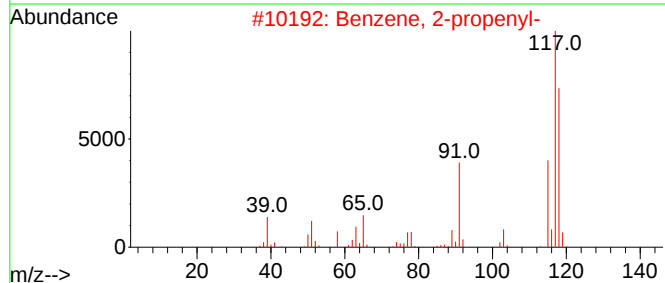
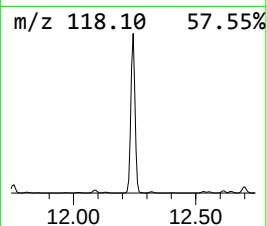
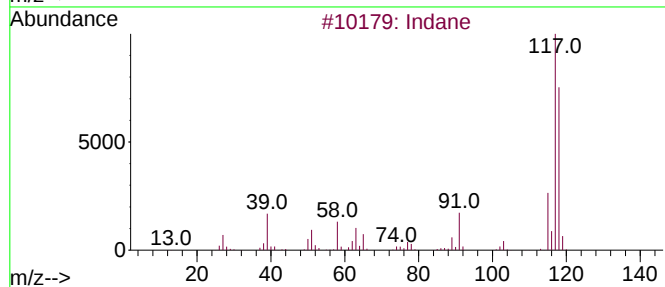
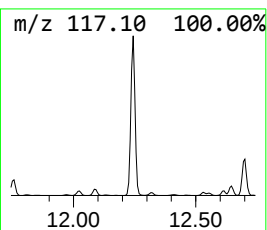
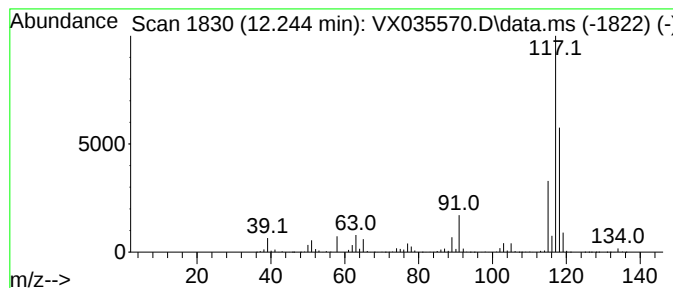
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	215.43 ug/l	4985240	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035570.D
Acq On : 08 May 2023 19:08
Operator : JC/MD
Sample : 02658-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
509

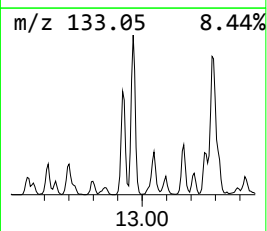
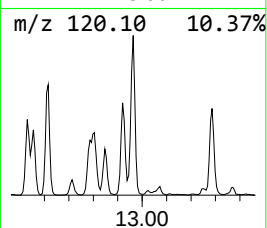
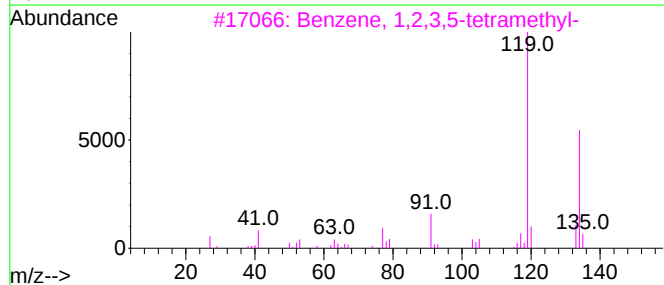
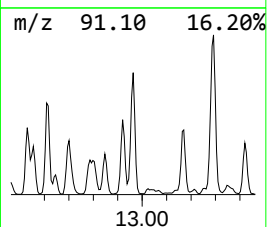
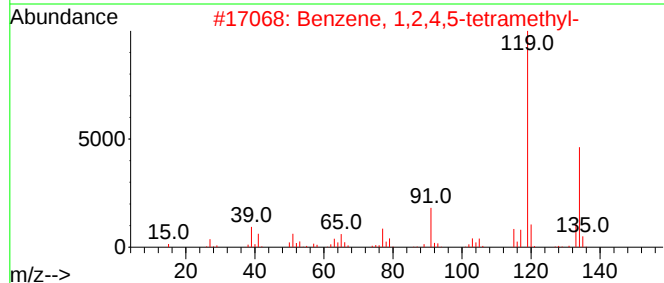
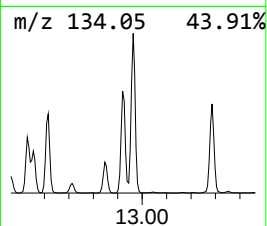
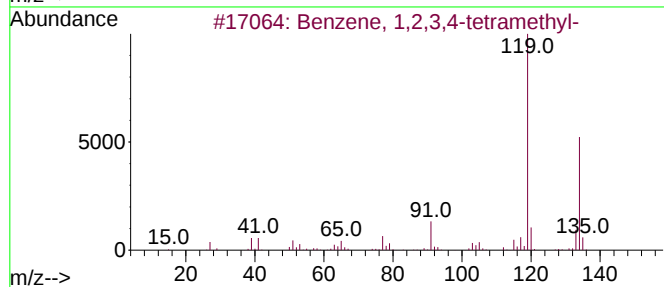
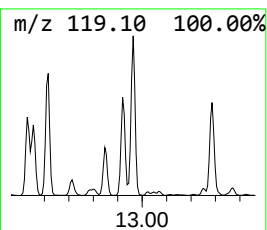
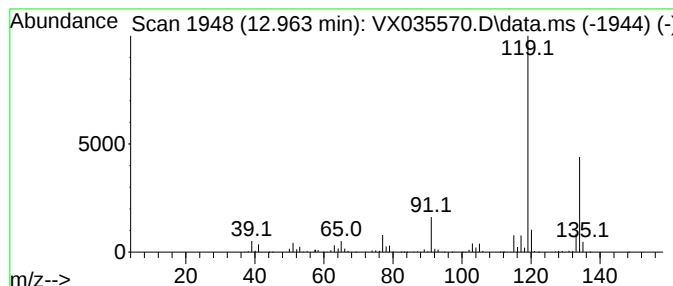
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	68.84 ug/l	1593110	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035570.D
Acq On : 08 May 2023 19:08
Operator : JC/MD
Sample : 02658-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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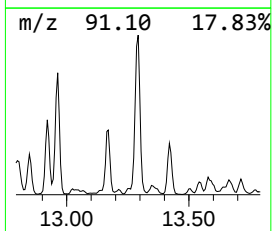
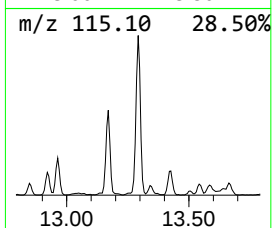
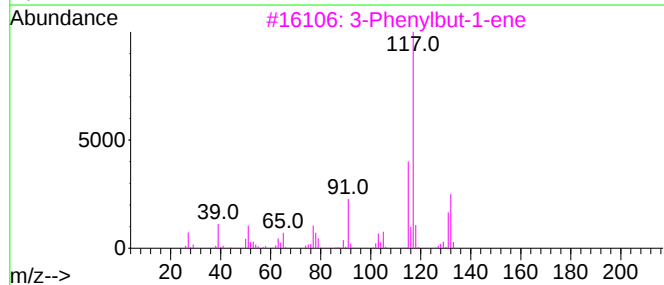
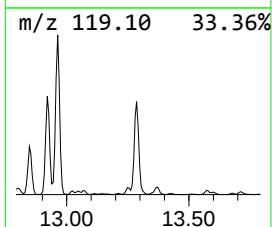
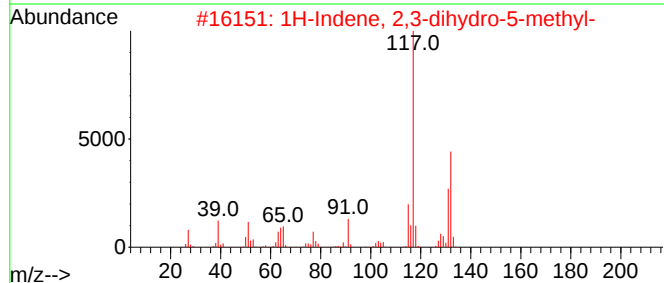
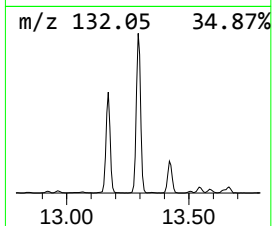
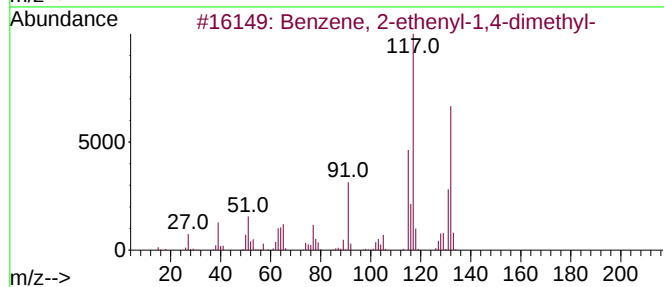
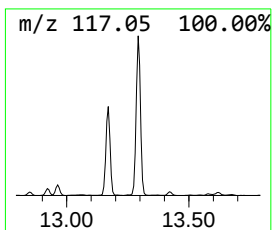
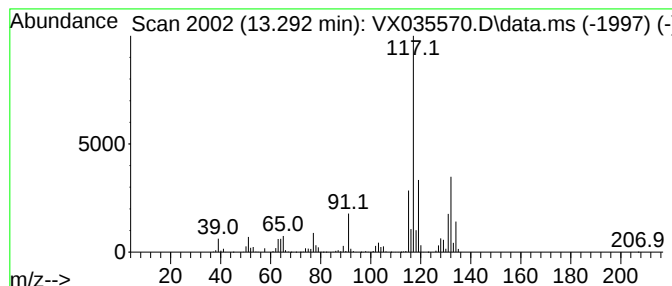
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	130.99 ug/l	3031200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035570.D
Acq On : 08 May 2023 19:08
Operator : JC/MD
Sample : 02658-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
509

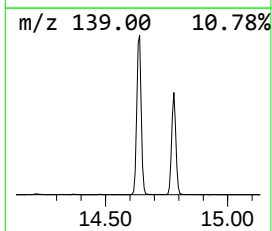
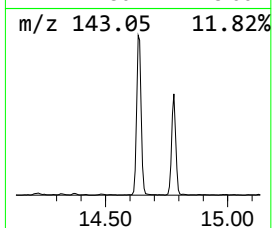
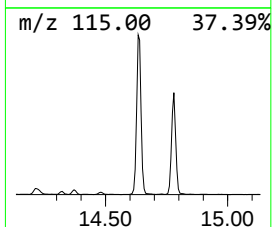
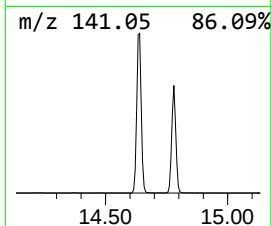
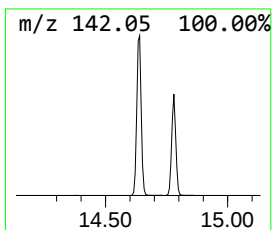
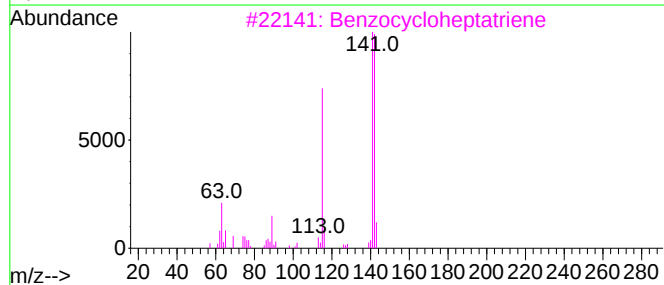
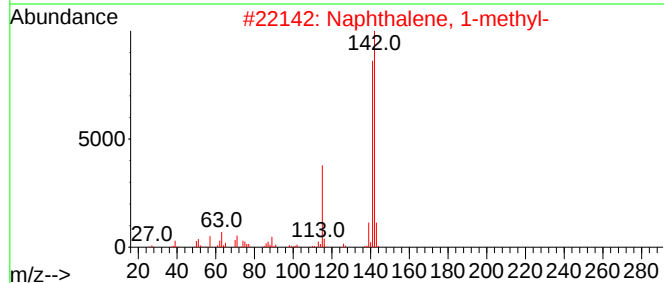
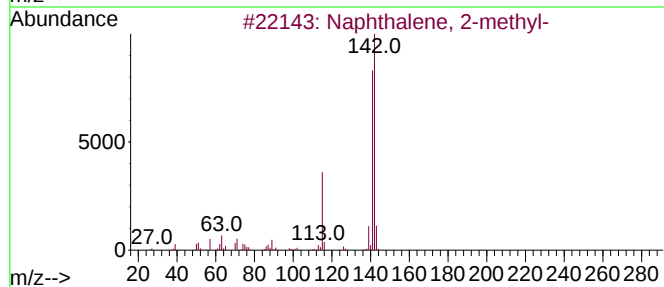
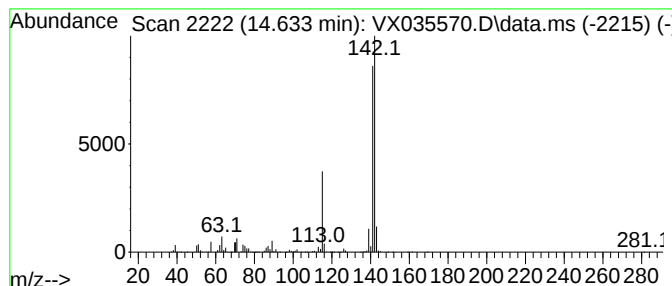
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	141.88 ug/l	3283200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX050823\
Data File : VX035570.D
Acq On : 08 May 2023 19:08
Operator : JC/MD
Sample : 02658-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
509

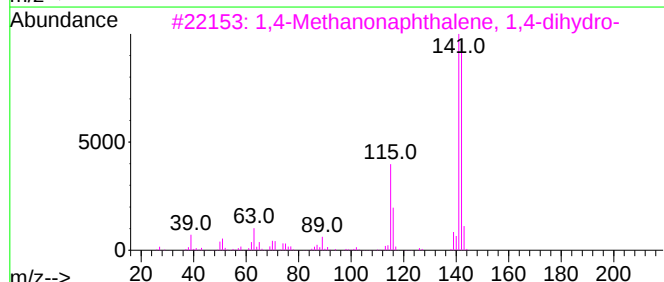
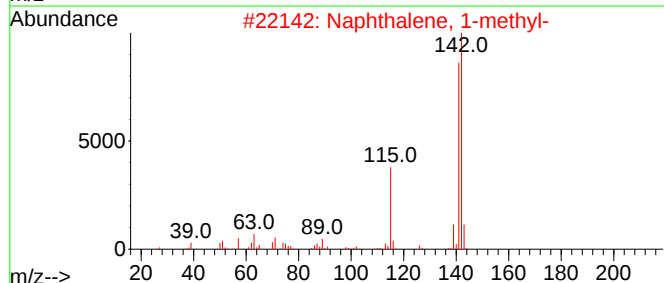
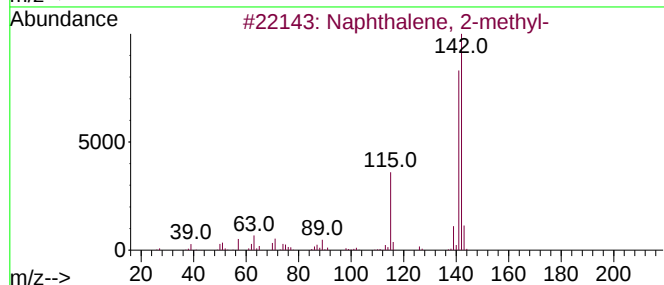
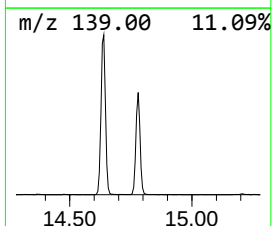
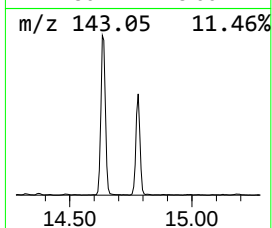
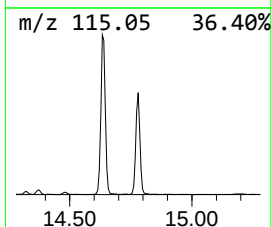
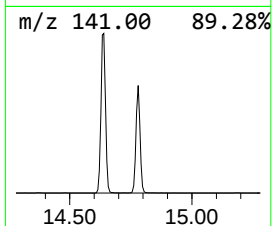
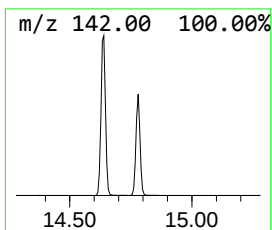
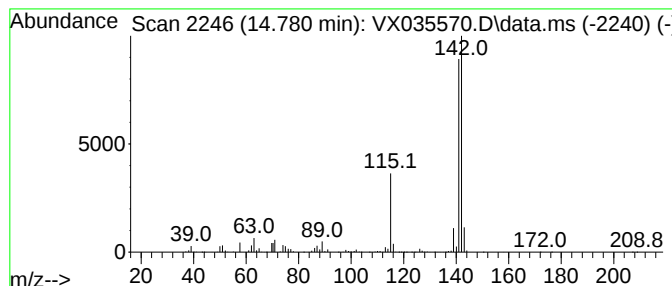
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	83.41 ug/l	1930230	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050823\
Data File : VX035570.D
Acq On : 08 May 2023 19:08
Operator : JC/MD
Sample : 02658-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
509

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.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
Isopropyl Alcohol	2.593	187.3	ug/l	2824260	1	5.556	753746	50.0
2-Pentanol, 4-m...	9.031	52.9	ug/l	1212290	3	10.055	1146830	50.0
Benzene, 1-ethy...	11.378	265.1	ug/l	6135860	4	12.024	1157050	50.0
Benzene, 1-ethy...	11.610	111.0	ug/l	2567410	4	12.024	1157050	50.0
Indane	12.244	215.4	ug/l	4985240	4	12.024	1157050	50.0
Benzene, 1,2,3,...	12.963	68.8	ug/l	1593110	4	12.024	1157050	50.0
Benzene, 2-ethe...	13.292	131.0	ug/l	3031200	4	12.024	1157050	50.0
Naphthalene, 1-...	14.633	141.9	ug/l	3283200	4	12.024	1157050	50.0
1,4-Methanonaph...	14.780	83.4	ug/l	1930230	4	12.024	1157050	50.0