

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
 Data File : VX023308.D
 Acq On : 15 Jul 2021 18:46
 Operator : JC/MD
 Sample : M3059-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 210714107-02-VOA

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\82X070221W.M
 Title : SW846 8260

Signal : TIC: VX023308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	54	rVB	154356	437998	5.30%	0.965%
2	2.392	206	214	228	rVB2	53619	105281	1.27%	0.232%
3	2.977	297	310	328	rBV	3285014	7264303	87.93%	16.008%
4	4.599	560	576	622	rBV	2525979	8261458	100.00%	18.206%
5	5.013	634	644	664	rVB	611784	1869509	22.63%	4.120%
6	5.397	694	707	721	rBV	142839	410041	4.96%	0.904%
7	5.562	721	734	751	rVB	241810	692872	8.39%	1.527%
8	5.964	789	800	808	rBV	149522	398796	4.83%	0.879%
9	6.086	808	820	831	rBV5	73095	289415	3.50%	0.638%
10	6.239	838	845	856	rVB3	79739	231641	2.80%	0.510%
11	6.769	920	932	946	rVB	367268	866512	10.49%	1.910%
12	8.580	1221	1229	1234	rBV2	72931	133026	1.61%	0.293%
13	8.653	1234	1241	1247	rVV	764709	1166613	14.12%	2.571%
14	8.720	1247	1252	1261	rVB	63066	105404	1.28%	0.232%
15	8.805	1261	1266	1271	rBV	65597	106229	1.29%	0.234%
16	10.055	1460	1471	1483	rBV	761667	1108498	13.42%	2.443%
17	10.201	1490	1495	1501	rBV2	45326	100472	1.22%	0.221%
18	10.305	1508	1512	1518	rVB	136992	195363	2.36%	0.431%
19	10.384	1518	1525	1534	rVB3	38906	95022	1.15%	0.209%
20	10.647	1563	1568	1572	rBV	85037	125104	1.51%	0.276%
21	10.951	1613	1618	1627	rVB4	58988	123469	1.49%	0.272%
22	11.085	1634	1640	1646	rBV	620313	819059	9.91%	1.805%
23	11.482	1698	1705	1707	rVV3	78876	153600	1.86%	0.338%
24	11.506	1707	1709	1715	rVB	115690	129707	1.57%	0.286%
25	11.756	1746	1750	1752	rVV2	75749	102535	1.24%	0.226%
26	11.890	1765	1772	1777	rVB2	112362	155237	1.88%	0.342%
27	12.024	1788	1794	1801	rBV2	784109	1168808	14.15%	2.576%
28	12.244	1824	1830	1836	rBV4	76195	139133	1.68%	0.307%
29	12.427	1854	1860	1864	rBV	199123	255329	3.09%	0.563%
30	12.524	1872	1876	1883	rBV3	88612	205899	2.49%	0.454%
31	12.579	1883	1885	1889	rVB2	103401	116853	1.41%	0.258%
32	12.671	1896	1900	1906	rVB4	49757	88724	1.07%	0.196%
33	12.768	1908	1916	1920	rVV	529829	736916	8.92%	1.624%
34	12.908	1928	1939	1943	rBV	1908105	2457099	29.74%	5.415%
35	12.969	1943	1949	1958	rVB4	198371	437311	5.29%	0.964%
36	13.170	1977	1982	1985	rBV3	60576	100436	1.22%	0.221%

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37	13.268	1995	1998	2008	rVB3	176977	301869	3.65%	0.665%
38	13.384	2008	2017	2020	rBV2	72845	144496	1.75%	0.318%
39	13.426	2020	2024	2027	rVV4	65592	111189	1.35%	0.245%
40	13.475	2027	2032	2035	rVV2	429768	631455	7.64%	1.392%
41	13.512	2035	2038	2046	rVB	1479625	1862364	22.54%	4.104%
42	13.591	2046	2051	2060	rBV	599947	831911	10.07%	1.833%
43	13.774	2077	2081	2088	rVB2	486145	639776	7.74%	1.410%
44	13.847	2088	2093	2096	rBV2	62505	113722	1.38%	0.251%
45	13.957	2109	2111	2116	rVB	199928	223357	2.70%	0.492%
46	14.042	2121	2125	2128	rVB	155118	164295	1.99%	0.362%
47	14.097	2128	2134	2138	rBV	319331	427901	5.18%	0.943%
48	14.323	2167	2171	2176	rBV3	66603	89153	1.08%	0.196%
49	14.414	2182	2186	2194	rBV2	68511	158571	1.92%	0.349%
50	14.640	2214	2223	2231	rVB	509414	787863	9.54%	1.736%
51	14.719	2231	2236	2240	rBV	890596	1119710	13.55%	2.467%
52	14.756	2240	2242	2244	rVV	337173	392631	4.75%	0.865%
53	14.780	2244	2246	2252	rVB	389714	480931	5.82%	1.060%
54	15.213	2309	2317	2321	rBV2	213715	329545	3.99%	0.726%
55	15.353	2333	2340	2348	rBV2	283495	595501	7.21%	1.312%
56	15.487	2355	2362	2376	rBV2	1193491	2064756	24.99%	4.550%
57	15.615	2378	2383	2387	rVV	190435	318198	3.85%	0.701%
58	15.652	2387	2389	2395	rVB	95134	127672	1.55%	0.281%
59	15.725	2397	2401	2411	rVB3	54161	142181	1.72%	0.313%
60	15.841	2412	2420	2425	rBV2	56420	161808	1.96%	0.357%
61	16.091	2456	2461	2468	rBV4	89560	183194	2.22%	0.404%
62	16.188	2470	2477	2481	rBV3	91017	188092	2.28%	0.414%
63	16.328	2494	2500	2507	rBV	603412	1142837	13.83%	2.518%
64	16.688	2550	2559	2567	rVB	205126	490237	5.93%	1.080%

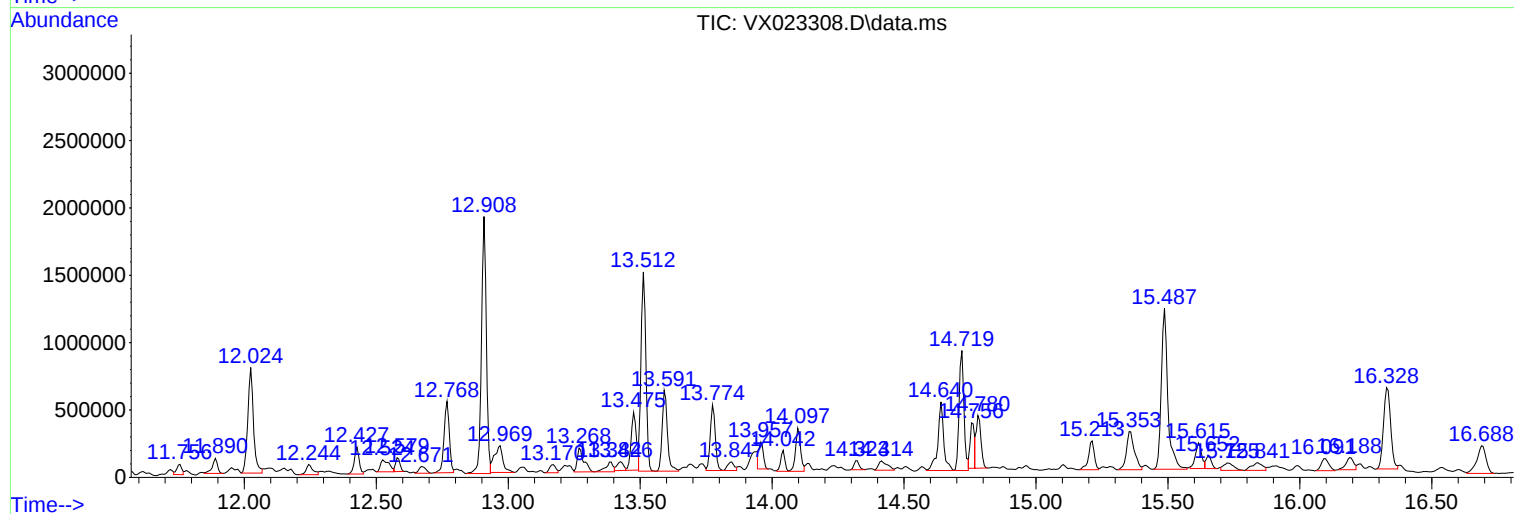
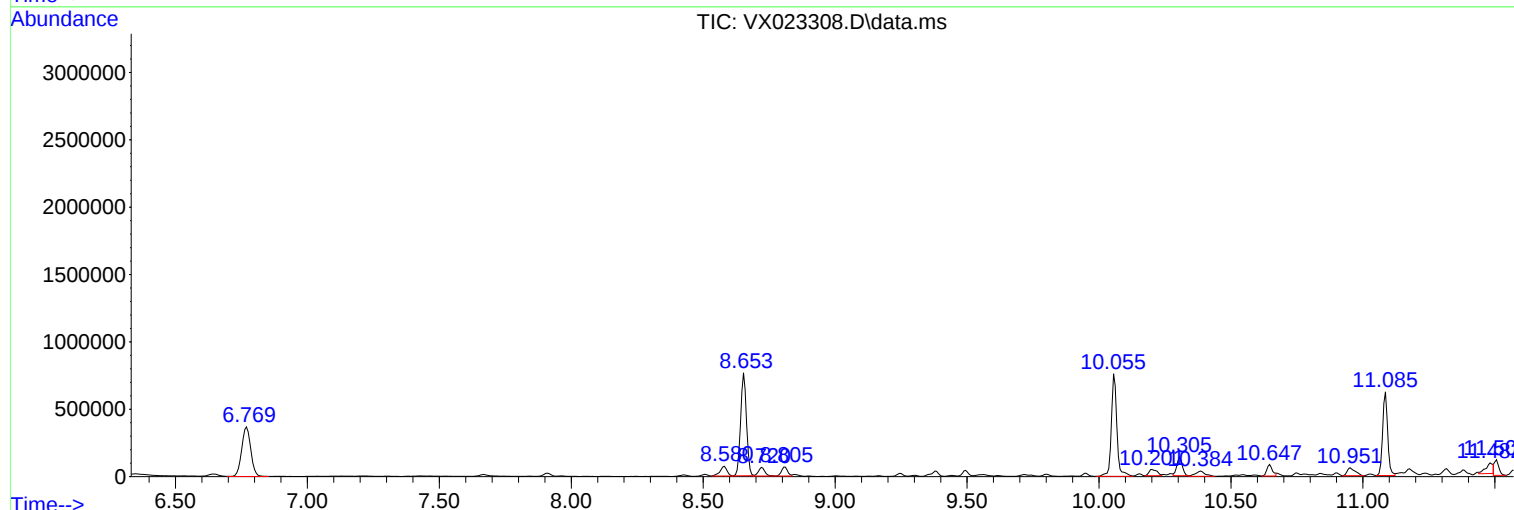
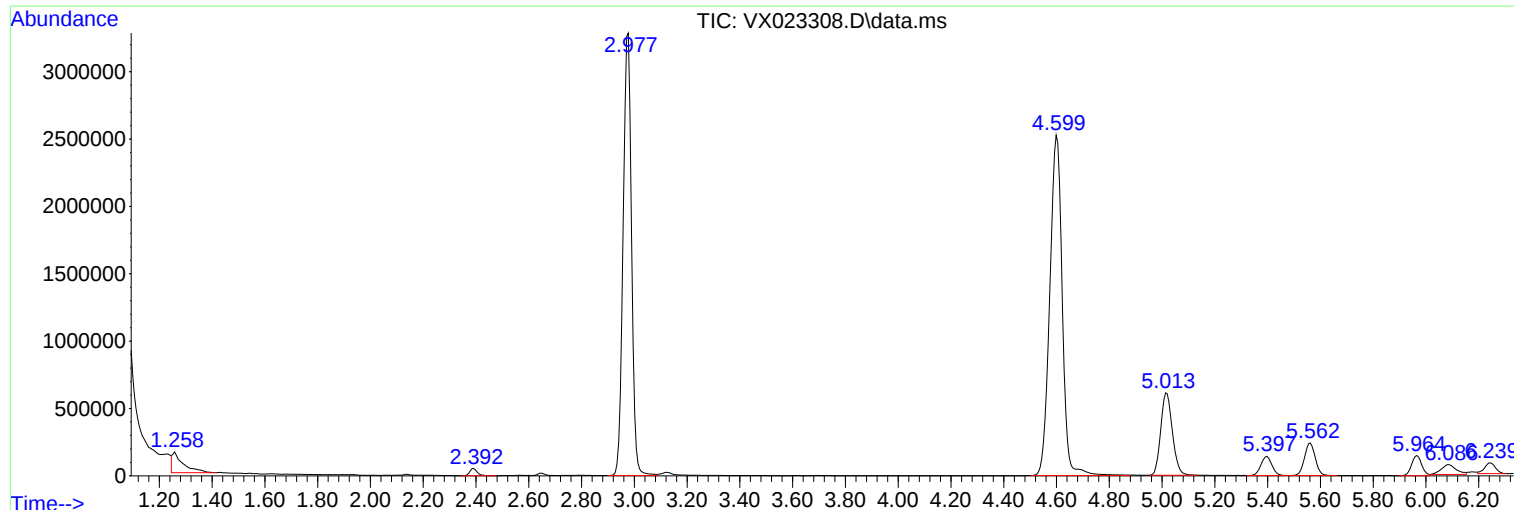
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
210714107-02-VOA

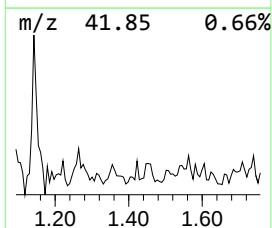
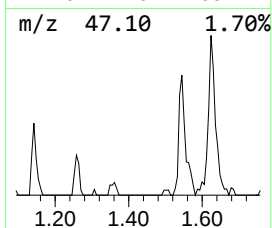
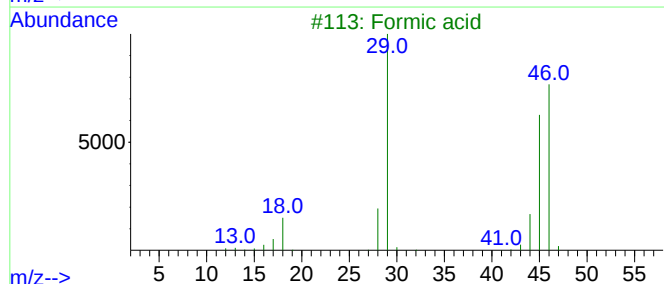
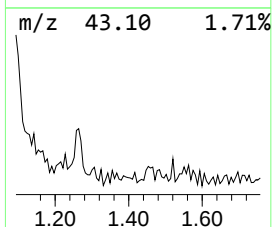
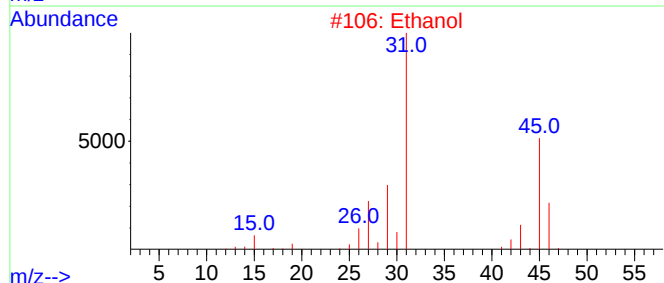
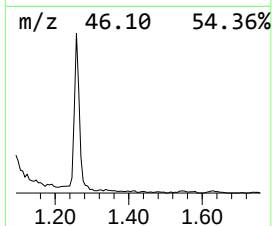
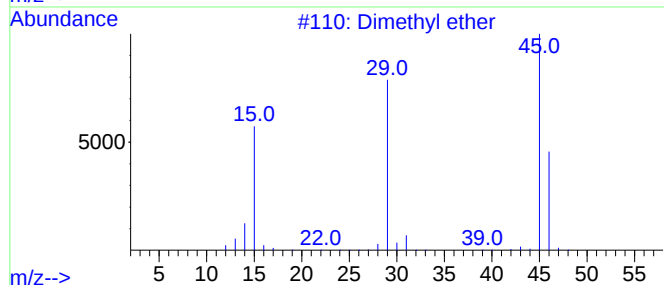
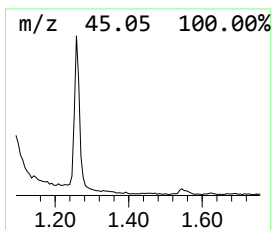
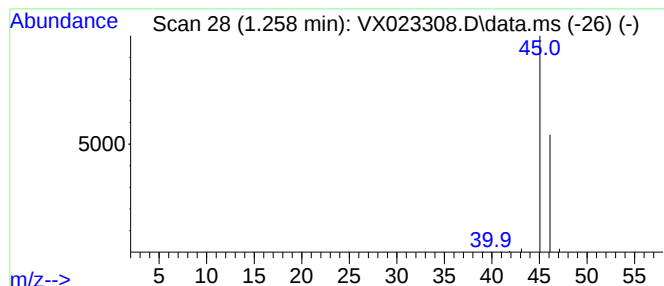
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	31.61 ug/l	437998	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	74
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Ethene, fluoro-	46	C2H3F	000075-02-5	4
5			Hydrazine, methyl-	46	CH6N2	000060-34-4	4



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Instrument :
MSVOA_X
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210714107-02-VOA

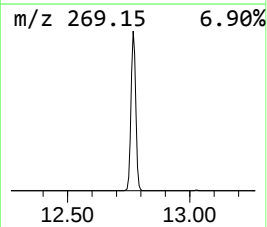
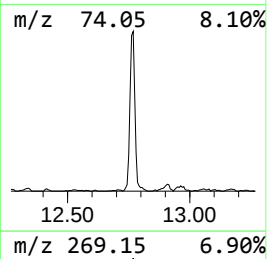
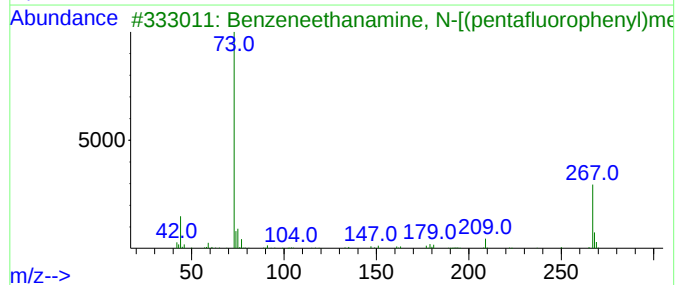
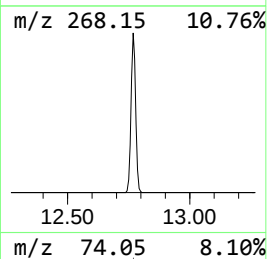
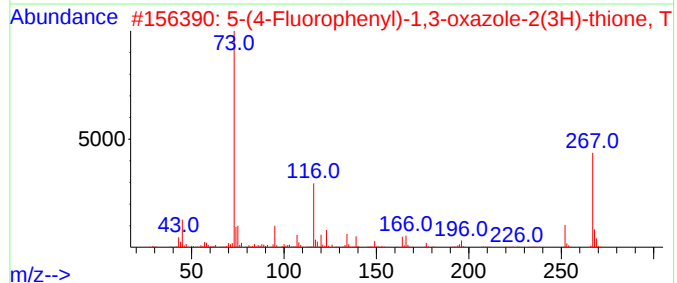
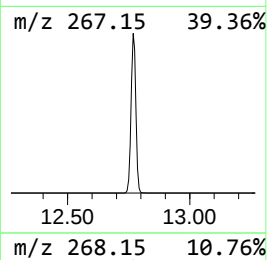
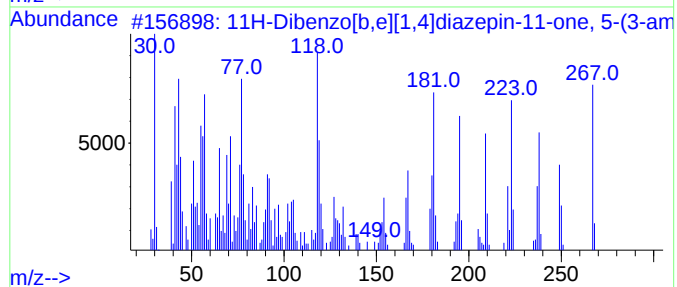
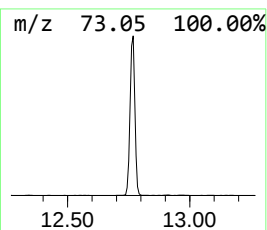
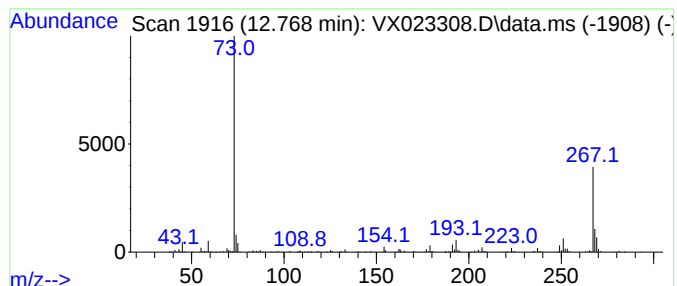
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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

Peak Number 3 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	31.52 ug/l	736916	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	90
2			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	59
3			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	59
4			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	59
5			Benzeneethanamine, N-methyl-.bet...	311	C15H29NO2Si2	029522-18-7	45



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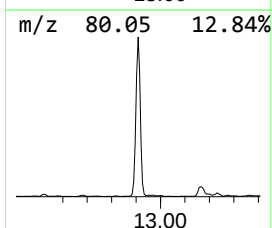
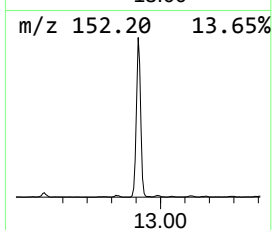
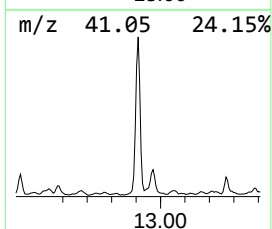
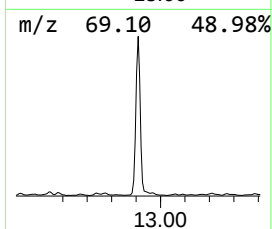
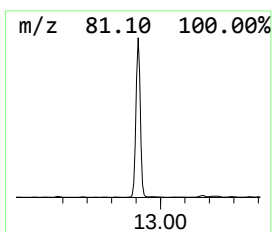
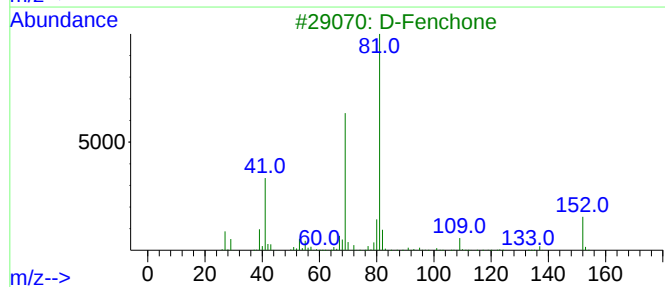
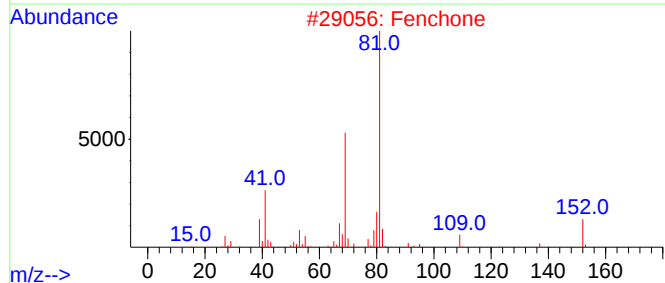
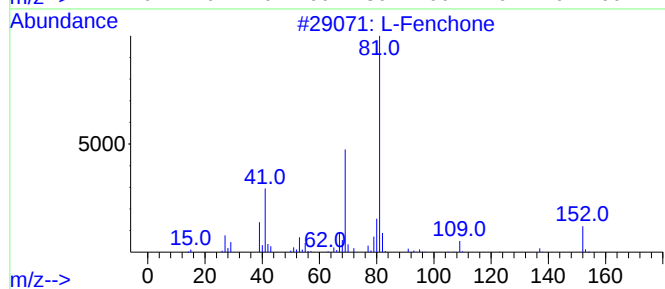
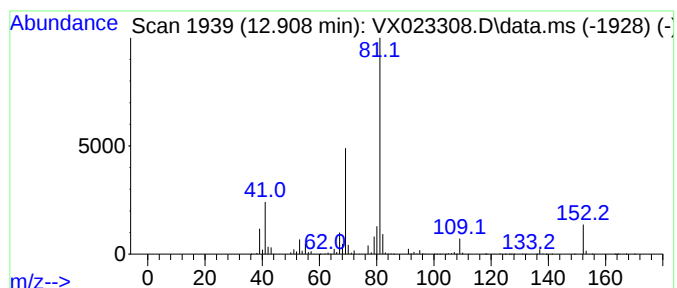
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	105.11 ug/l	2457100	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Fenchone	152	C10H16O	007787-20-4	95
2			Fenchone	152	C10H16O	001195-79-5	95
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	42



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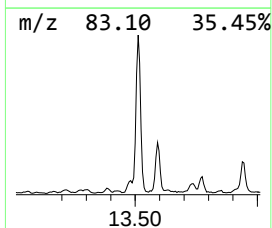
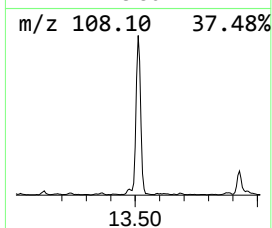
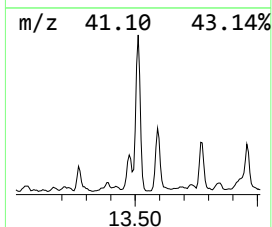
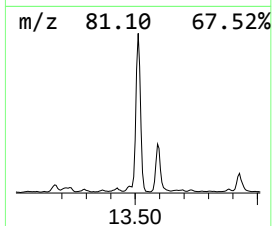
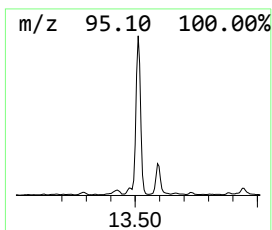
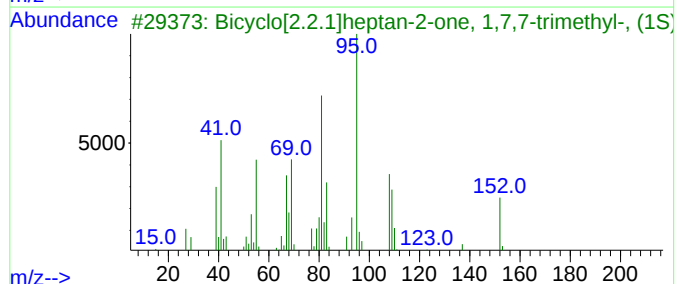
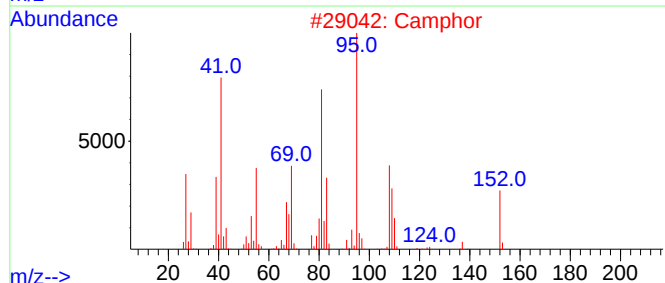
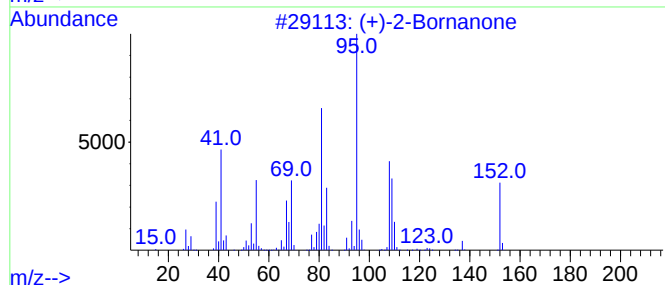
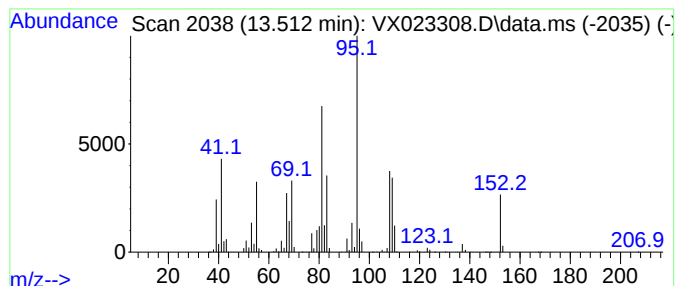
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Peak Number 5 (+)-2-Bornanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	79.67 ug/l	1862360	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2			Camphor	152	C10H16O	000076-22-2	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023308.D
Acq On : 15 Jul 2021 18:46
Operator : JC/MD
Sample : M3059-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714107-02-VOA

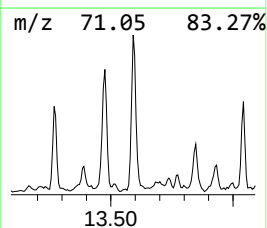
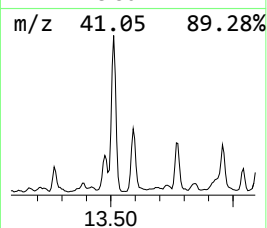
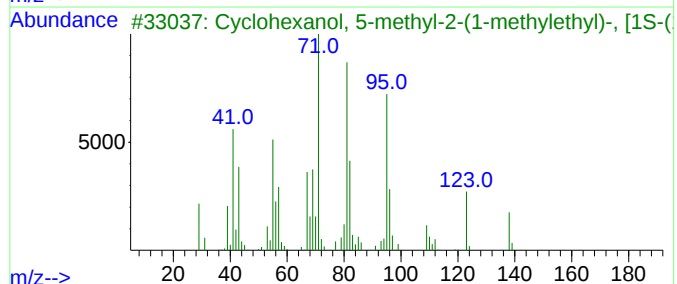
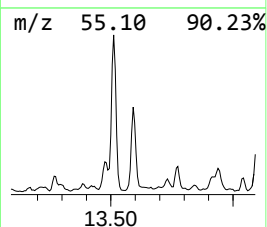
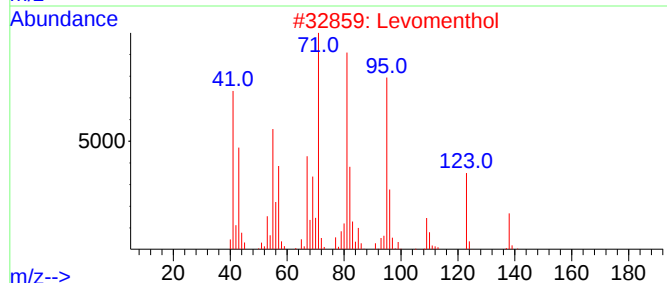
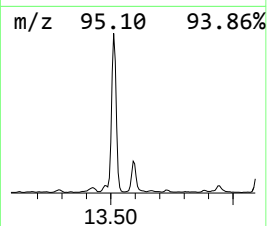
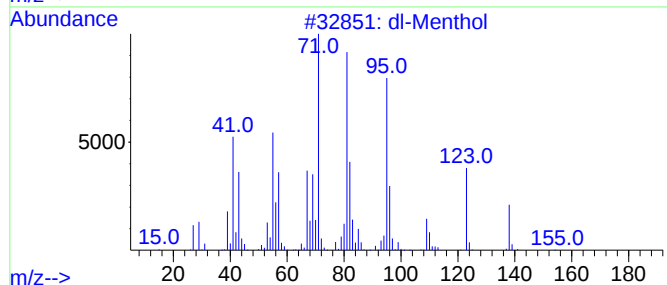
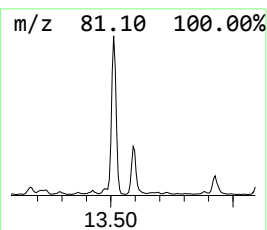
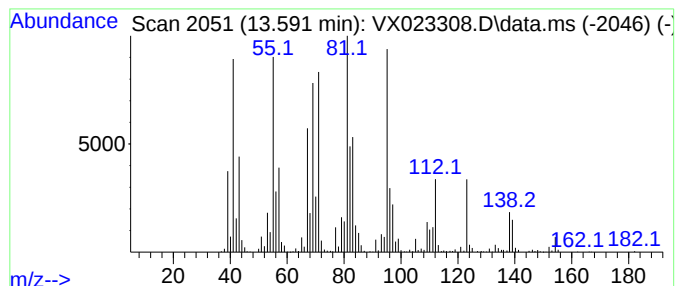
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Quant Title : SW846 8260

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

Peak Number 6 dl-Menthol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	35.59 ug/l	831911	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			dl-Menthol	156	C10H20O	000089-78-1	58
2			Levomenthol	156	C10H20O	002216-51-5	53
3			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	49
4			5-Undecyne	152	C11H20	002294-72-6	41
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023308.D
Acq On : 15 Jul 2021 18:46
Operator : JC/MD
Sample : M3059-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714107-02-VOA

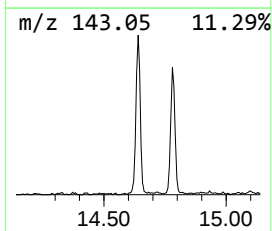
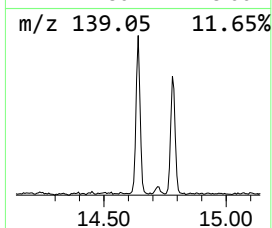
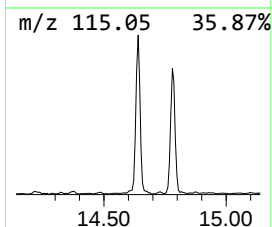
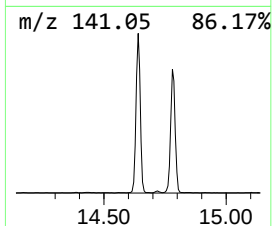
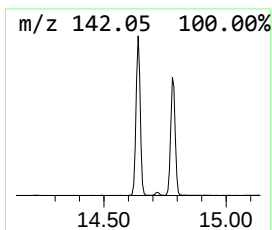
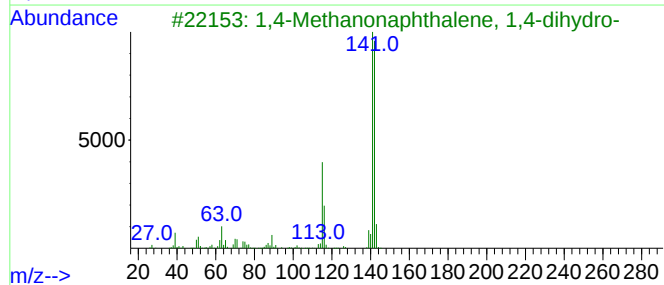
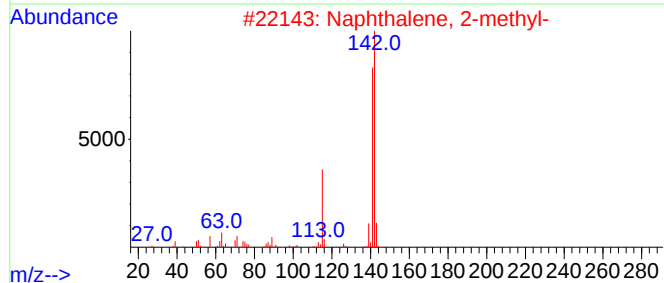
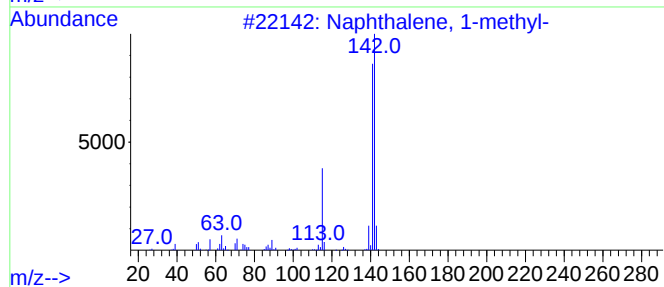
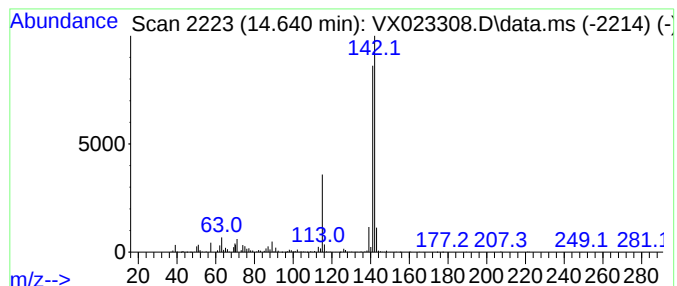
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	33.70 ug/l	787863	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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-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	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023308.D
Acq On : 15 Jul 2021 18:46
Operator : JC/MD
Sample : M3059-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714107-02-VOA

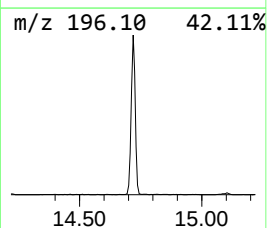
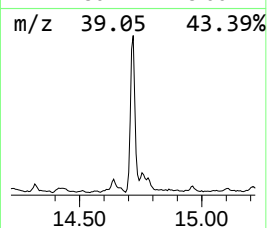
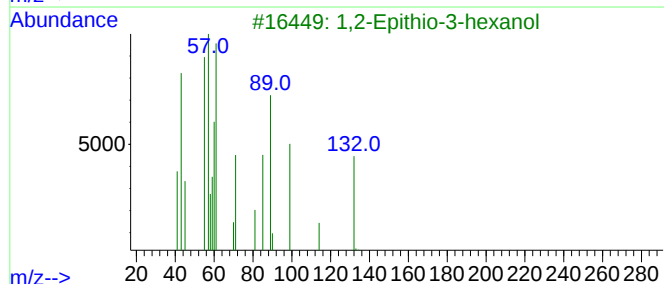
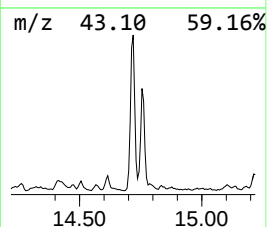
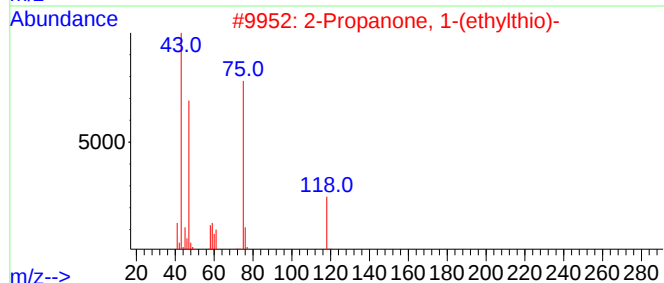
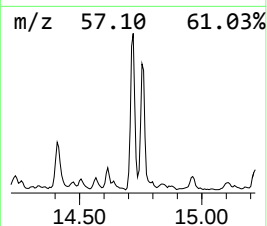
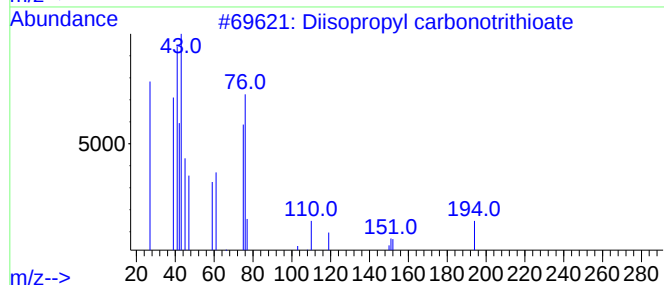
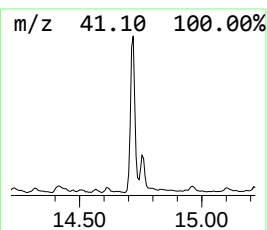
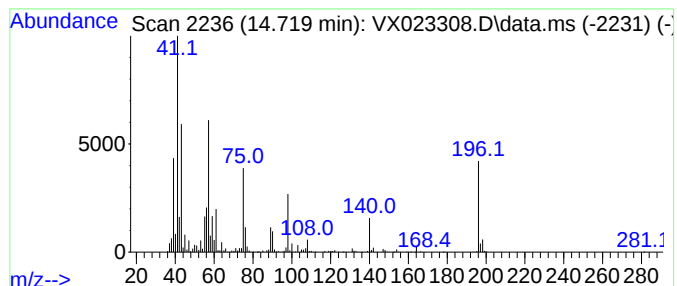
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.719 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.719	47.90 ug/l	1119710	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl carbonotrithioate	194	C7H14S3	002314-51-4	16
2			2-Propanone, 1-(ethylthio)-	118	C5H10OS	020996-62-7	12
3			1,2-Epithio-3-hexanol	132	C6H12OS	1000101-71-4	10
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	10
5			1,3-Cyclohexanedione, 2-methyl-2...	196	C11H16O3	005073-65-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023308.D
Acq On : 15 Jul 2021 18:46
Operator : JC/MD
Sample : M3059-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714107-02-VOA

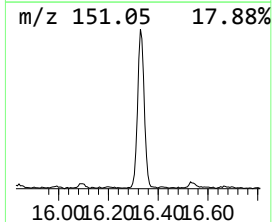
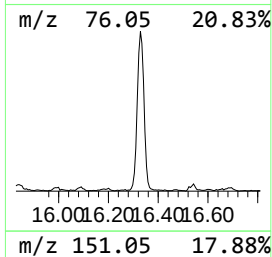
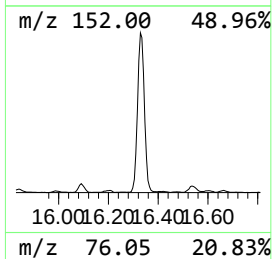
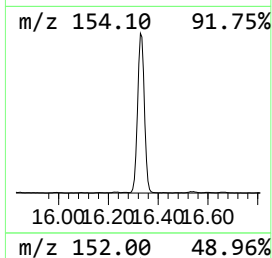
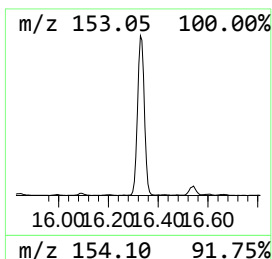
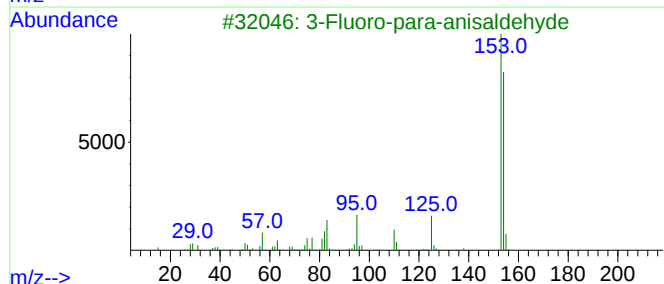
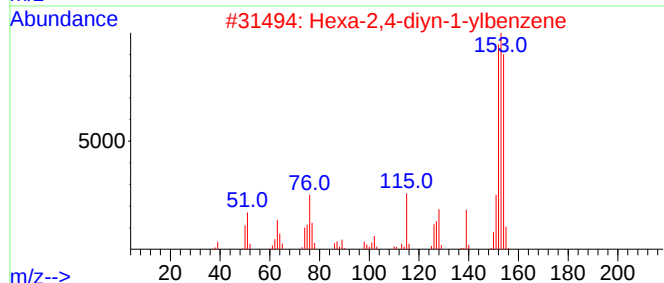
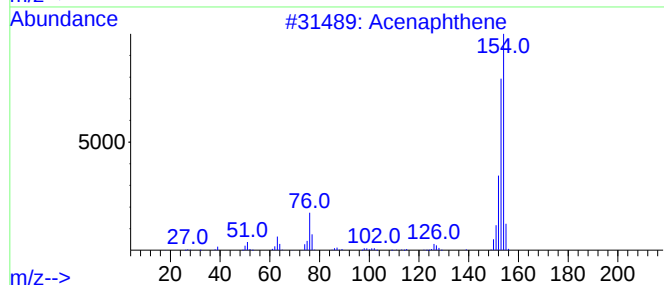
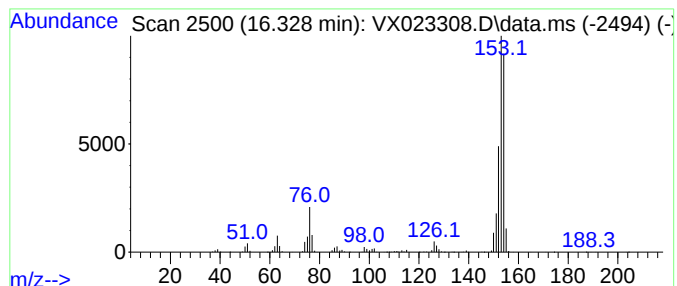
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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

Peak Number 10 Acenaphthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	48.89 ug/l	1142840	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acenaphthene	154	C12H10	000083-32-9	93
2		Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3		3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
4		1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	45
5		Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023308.D
Acq On : 15 Jul 2021 18:46
Operator : JC/MD
Sample : M3059-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.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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11H-Dibenzo[b,e...	12.768	31.5	ug/l	736916	4	12.024	1168810	50.0
L-Fenchone	12.908	105.1	ug/l	2457100	4	12.024	1168810	50.0
(+)-2-Bornanone	13.512	79.7	ug/l	1862360	4	12.024	1168810	50.0
dl-Menthol	13.591	35.6	ug/l	831911	4	12.024	1168810	50.0
Naphthalene, 1-...	14.640	33.7	ug/l	787863	4	12.024	1168810	50.0
unknown14.719	14.719	47.9	ug/l	1119710	4	12.024	1168810	50.0
Acenaphthene	16.328	48.9	ug/l	1142840	4	12.024	1168810	50.0