

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
 Data File : VX021228.D
 Acq On : 16 Mar 2021 03:04
 Operator : JC/MD
 Sample : M1665-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30821

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\82X031521W.M

Title : SW846 8260

Signal : TIC: VX021228.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	62	66	78	rBV	102473	111953	10.04%	2.766%
2	5.464	732	744	756	rBV	55742	158183	14.19%	3.908%
3	5.629	759	772	785	rBV2	82868	237567	21.30%	5.869%
4	6.029	829	840	852	rBV	63436	169150	15.17%	4.179%
5	6.188	859	867	879	rVB4	3861	11357	1.02%	0.281%
6	6.829	965	976	990	rBV	143127	339248	30.42%	8.381%
7	8.694	1286	1293	1301	rBV	305814	466386	41.82%	11.521%
8	10.094	1525	1531	1548	rVB	325151	431637	38.71%	10.663%
9	10.347	1569	1574	1582	rBV2	8508	12185	1.09%	0.301%
10	11.118	1700	1705	1717	rVB	248771	331402	29.72%	8.187%
11	11.606	1783	1788	1800	rBV	950202	1115103	100.00%	27.547%
12	11.865	1826	1832	1837	rBV	105344	129516	11.61%	3.200%
13	11.924	1837	1842	1853	rVB2	54092	69360	6.22%	1.713%
14	12.059	1860	1865	1874	rVB	314419	392886	35.23%	9.706%
15	12.142	1874	1879	1884	rVB2	35568	46666	4.18%	1.153%
16	13.771	2151	2156	2160	rBV	11446	13595	1.22%	0.336%
17	13.818	2160	2164	2168	rVB2	9284	11809	1.06%	0.292%

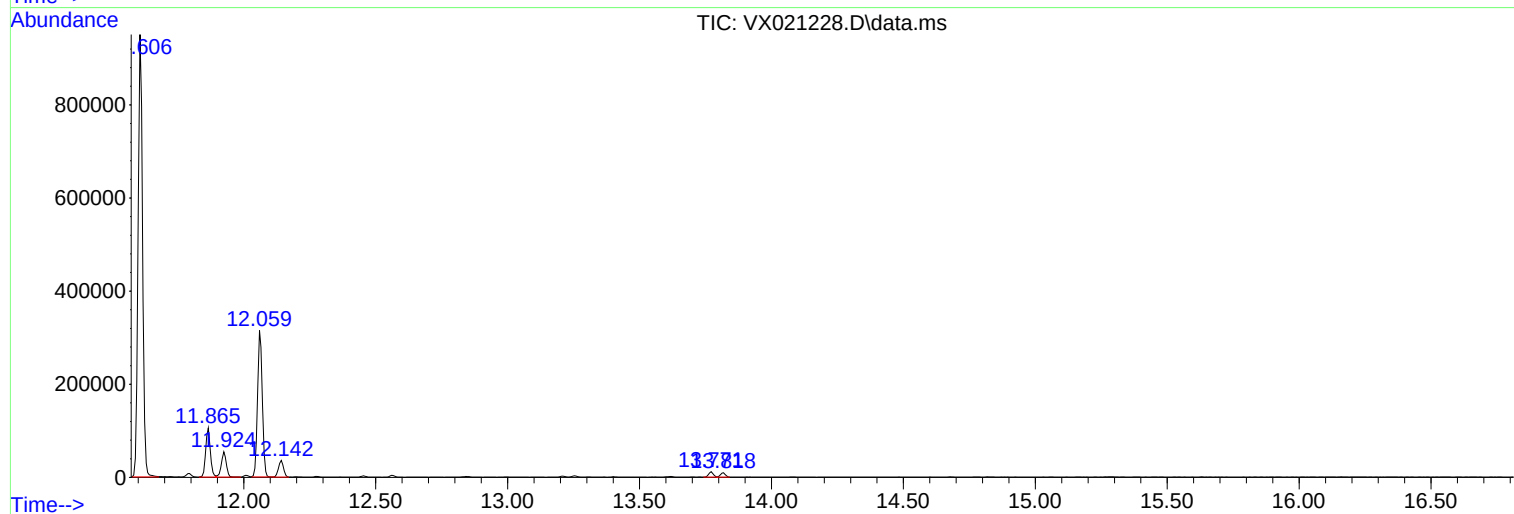
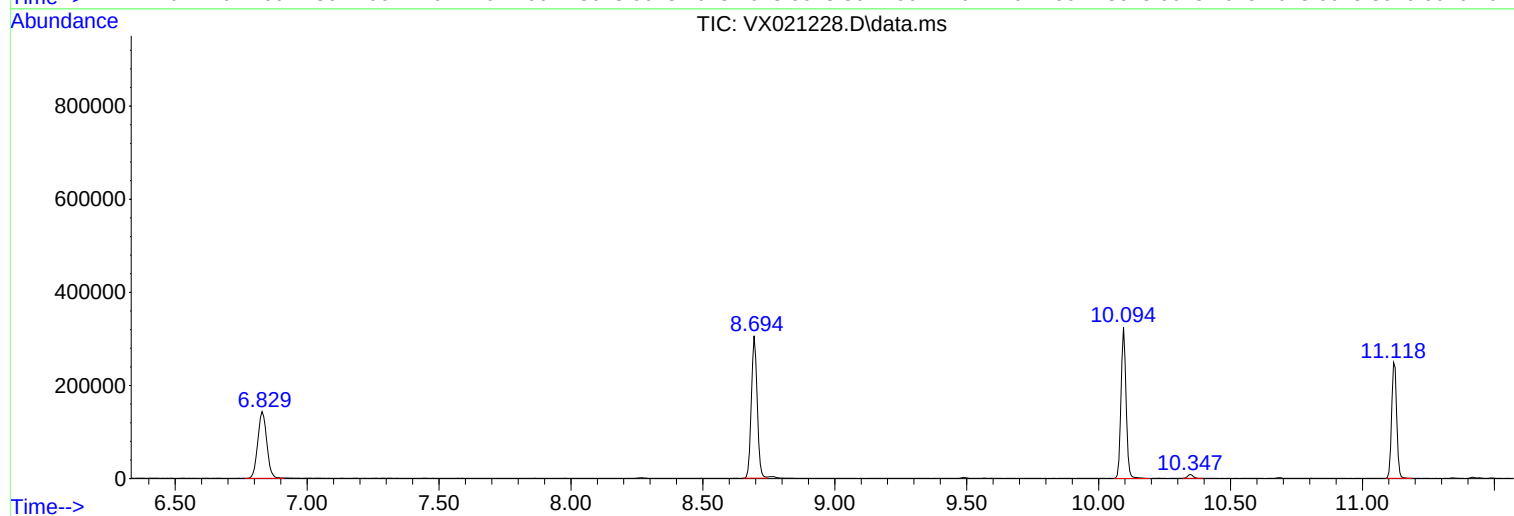
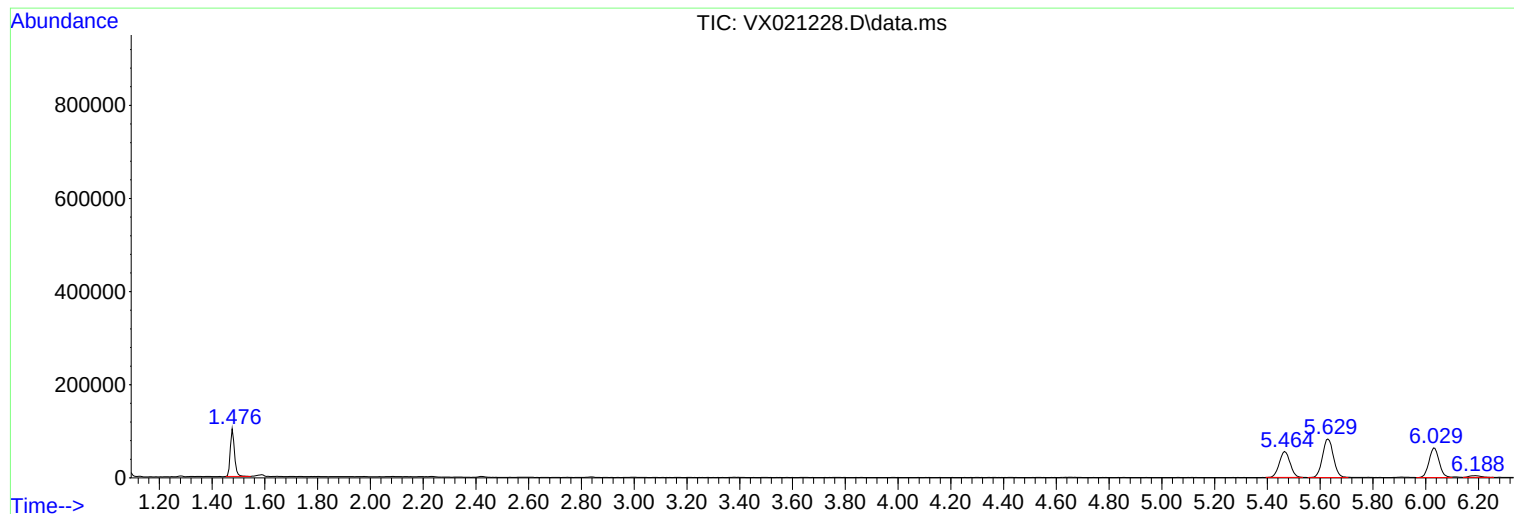
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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



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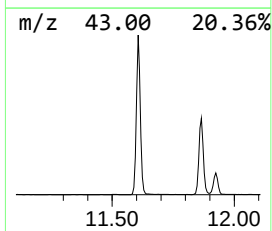
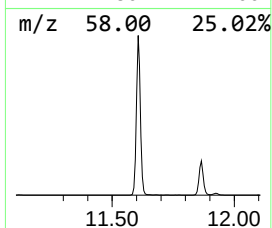
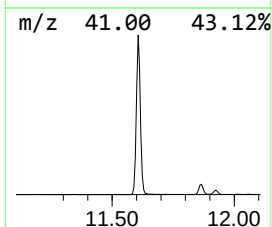
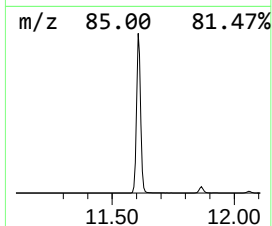
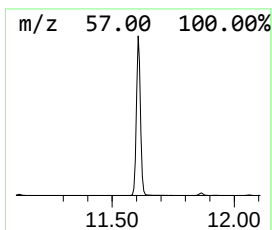
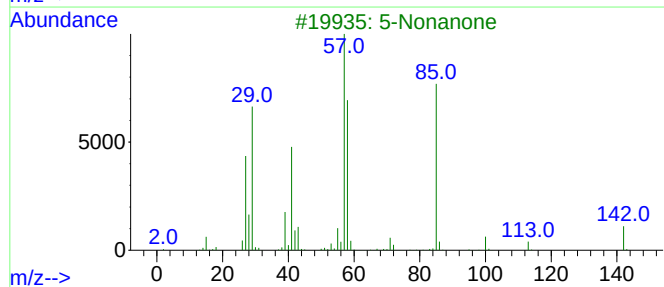
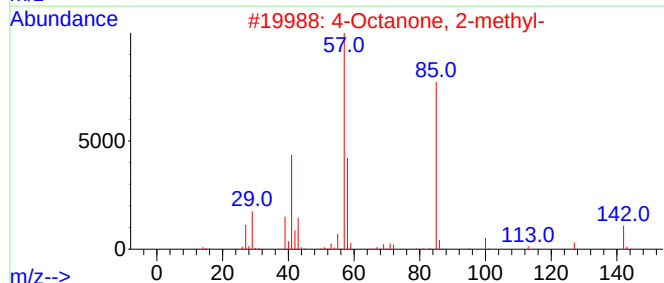
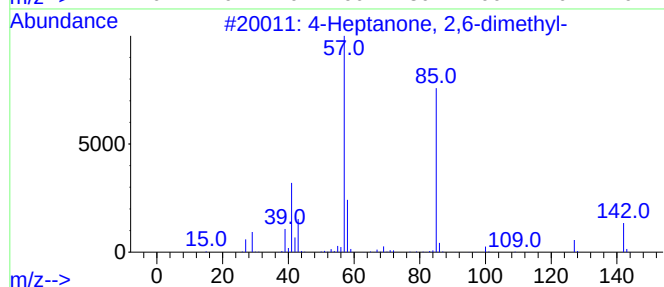
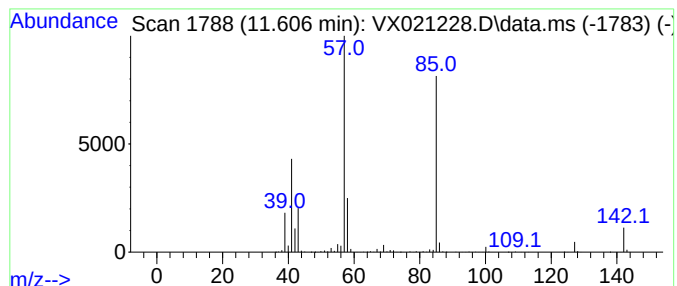
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	141.91 ug/l	1115100	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5			Allyl isovalerate	142	C8H14O2	002835-39-4	50



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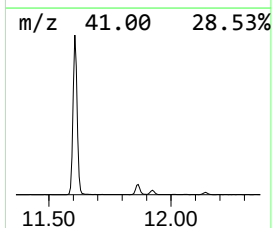
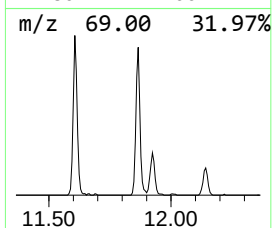
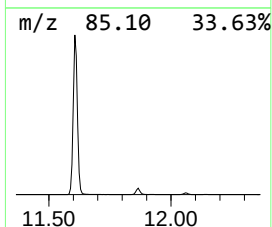
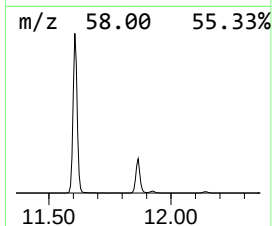
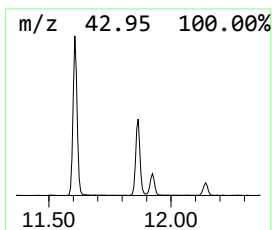
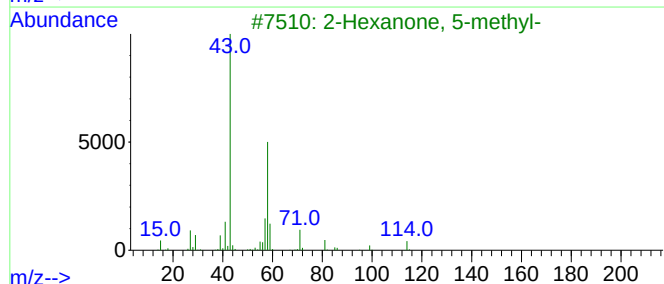
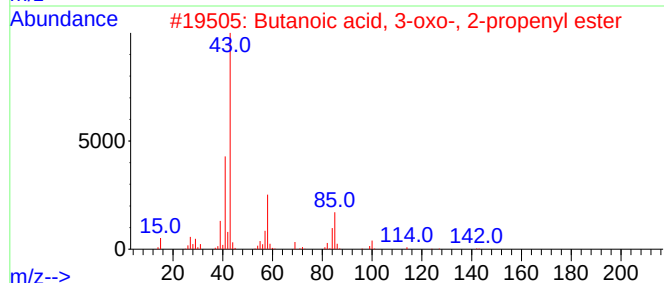
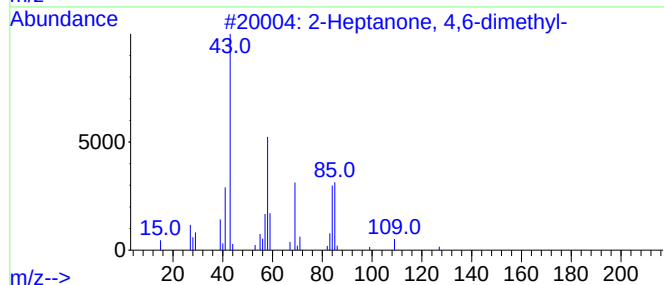
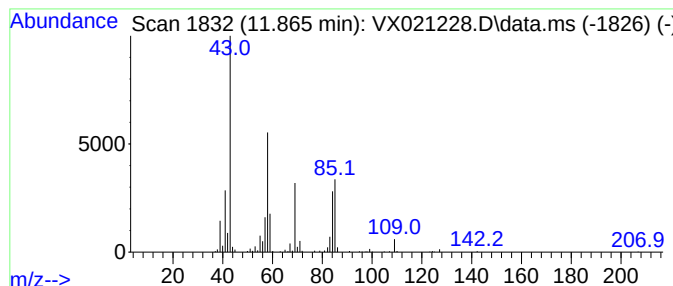
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.865	16.48 ug/l	129516	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2			Butanoic acid, 3-oxo-, 2-propeny...	142	C7H10O3	001118-84-9	64
3			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
4			Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
5			2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	40



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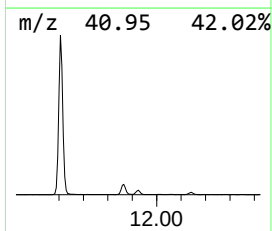
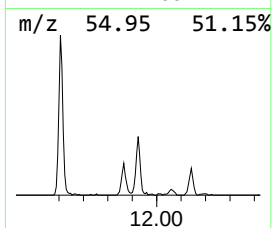
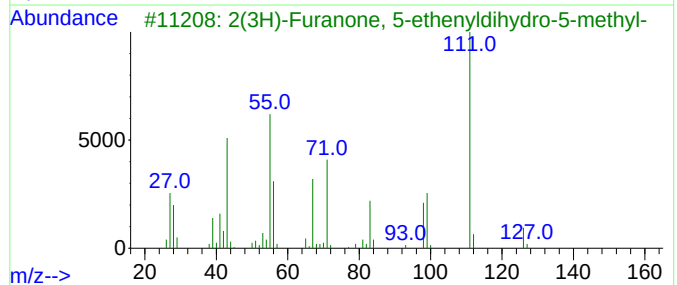
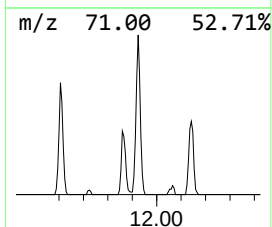
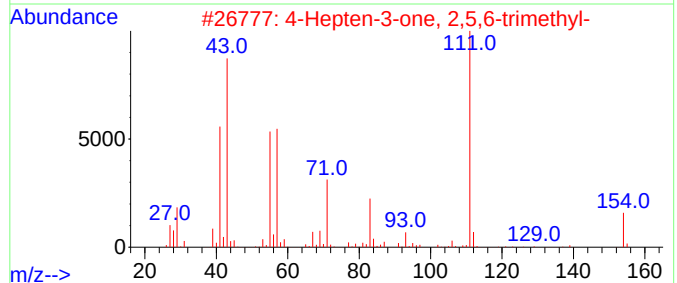
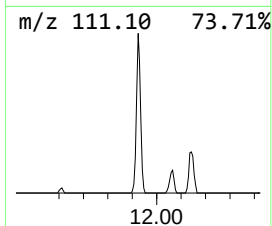
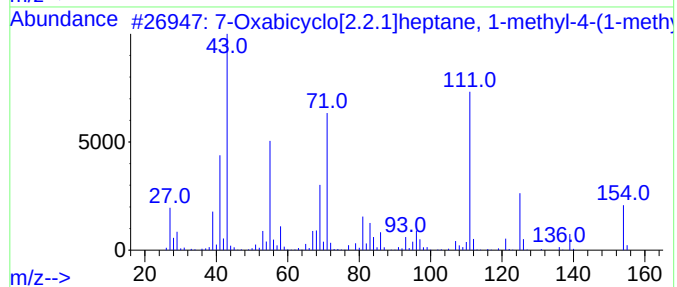
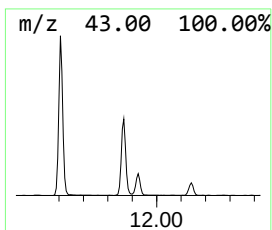
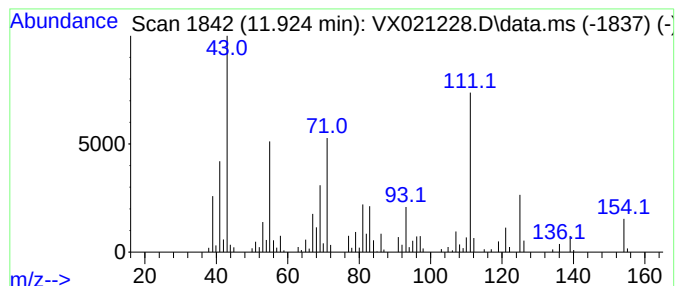
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Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.924	8.83 ug/l	69360	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	70
2			4-Hepten-3-one, 2,5,6-trimethyl-	154	C10H18O	016466-21-0	49
3			2(3H)-Furanone, 5-ethenyldihydro...	126	C7H10O2	001073-11-6	47
4			Tetrahydrocarvone	154	C10H18O	000499-70-7	41
5			1,2-Propanedione, 1-(2-thienyl)-	154	C7H6O2S	013678-69-8	38



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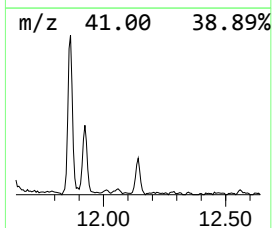
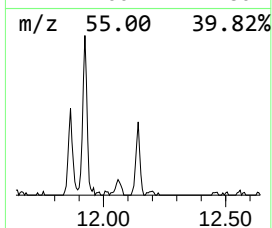
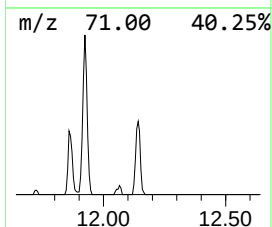
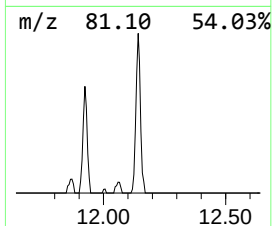
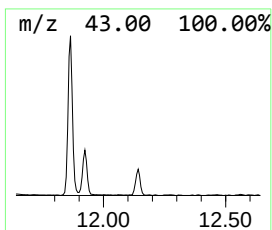
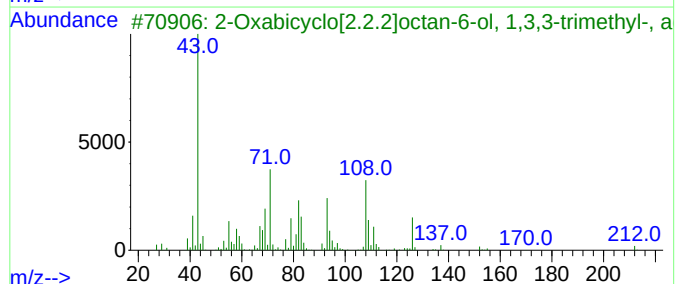
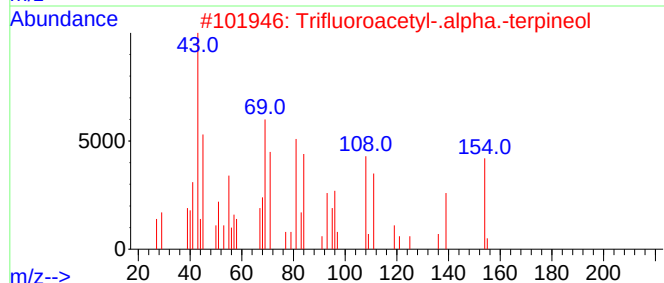
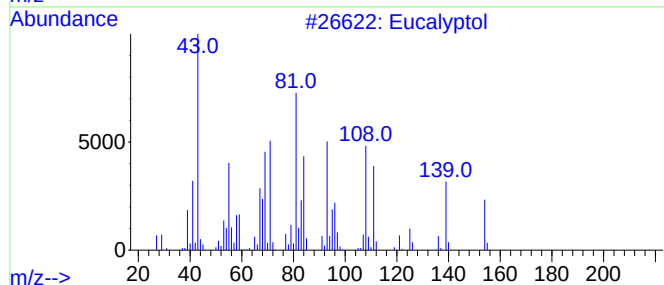
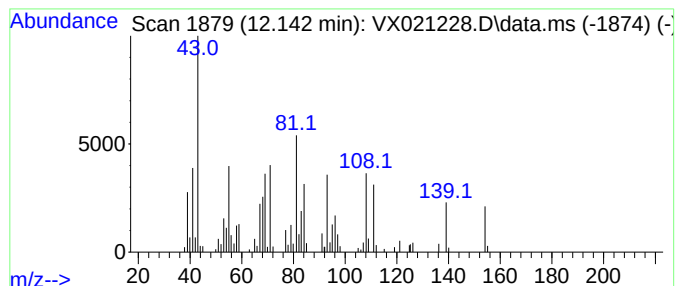
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Quant Title : SW846 8260

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

Peak Number 5 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	5.94 ug/l	46666	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	43
4			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	30
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22



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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
4-Heptanone, 2,...	11.606	141.9	ug/l	1115100	4	12.059	392886	50.0
2-Heptanone, 4,...	11.865	16.5	ug/l	129516	4	12.059	392886	50.0
7-Oxabicyclo[2....	11.924	8.8	ug/l	69360	4	12.059	392886	50.0
Eucalyptol	12.142	5.9	ug/l	46666	4	12.059	392886	50.0