

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN123024\
 Data File : VN085357.D
 Acq On : 30 Dec 2024 20:03
 Operator : JC\MD
 Sample : P5386-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MOO-24-00397

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M

Title : SW846 8260

Signal : TIC: VN085357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	16	21	29	rVB2	10670	17228	2.12%	0.326%
2	2.289	50	57	61	rBV3	7559	13579	1.67%	0.257%
3	2.477	83	89	94	rBV2	14925	25513	3.14%	0.483%
4	2.665	115	121	127	rVB2	4731	8859	1.09%	0.168%
5	3.789	307	312	323	rVB4	4044	11064	1.36%	0.210%
6	4.430	411	421	435	rBV	33311	98985	12.17%	1.875%
7	7.488	932	941	952	rVB	22116	56614	6.96%	1.072%
8	8.165	1046	1056	1061	rBV	117734	285353	35.08%	5.404%
9	8.224	1061	1066	1077	rVB	191942	410070	50.41%	7.766%
10	8.577	1115	1126	1136	rBV	131896	299216	36.79%	5.667%
11	8.965	1185	1192	1202	rBV	26228	54634	6.72%	1.035%
12	9.100	1204	1215	1223	rBV	296814	597068	73.40%	11.308%
13	9.176	1223	1228	1236	rVB3	6449	14155	1.74%	0.268%
14	9.524	1279	1287	1294	rBV4	12174	29534	3.63%	0.559%
15	9.906	1347	1352	1359	rVB2	4977	9722	1.20%	0.184%
16	10.447	1437	1444	1451	rBV2	9016	17041	2.09%	0.323%
17	10.565	1456	1464	1472	rVV	447370	813416	100.00%	15.405%
18	10.635	1472	1476	1487	rVB4	9933	28325	3.48%	0.536%
19	11.059	1543	1548	1557	rVB3	6833	14775	1.82%	0.280%
20	11.194	1564	1571	1580	rVB2	9888	17487	2.15%	0.331%
21	11.865	1674	1685	1693	rBV	389936	687746	84.55%	13.025%
22	11.935	1693	1697	1705	rVB3	6832	14783	1.82%	0.280%
23	12.382	1766	1773	1780	rBV5	4317	9882	1.21%	0.187%
24	12.594	1802	1809	1813	rBV5	4740	9380	1.15%	0.178%
25	12.847	1845	1852	1860	rBV	286846	478755	58.86%	9.067%
26	12.982	1871	1875	1880	rVB6	4741	8463	1.04%	0.160%
27	13.035	1880	1884	1890	rVB3	7021	10954	1.35%	0.207%
28	13.159	1901	1905	1912	rVB5	6714	11989	1.47%	0.227%
29	13.282	1919	1926	1934	rBV6	7569	18687	2.30%	0.354%
30	13.441	1949	1953	1961	rBV5	7716	17252	2.12%	0.327%
31	13.670	1987	1992	2002	rBV2	23785	50104	6.16%	0.949%
32	13.788	2005	2012	2018	rVV	346072	589488	72.47%	11.164%
33	13.859	2018	2024	2035	rVB4	87755	197617	24.29%	3.743%
34	14.059	2052	2058	2063	rVB6	6767	14095	1.73%	0.267%
35	14.453	2116	2125	2134	rBV7	22696	77383	9.51%	1.466%
36	14.523	2134	2137	2142	rBV4	7796	11902	1.46%	0.225%

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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

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37	14.582	2143	2147	2150	rBV3	6890	10326	1.27%	0.196%
38	14.629	2150	2155	2159	rBV2	38046	59444	7.31%	1.126%
39	14.735	2169	2173	2177	rBV3	22532	34330	4.22%	0.650%
40	14.770	2177	2179	2183	rVB4	9374	10818	1.33%	0.205%
41	15.323	2266	2273	2285	rBV2	40416	84218	10.35%	1.595%
42	15.435	2285	2292	2294	rBV4	12342	25054	3.08%	0.474%
43	15.458	2294	2296	2303	rVB4	15021	24834	3.05%	0.470%

Sum of corrected areas: 5280142

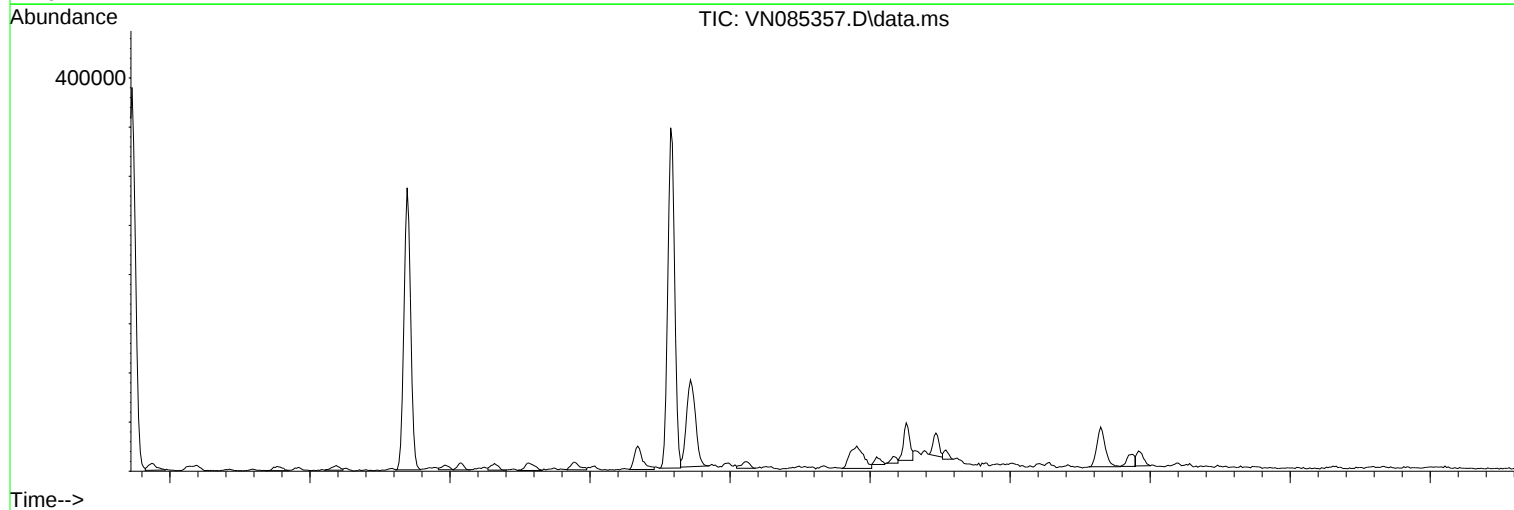
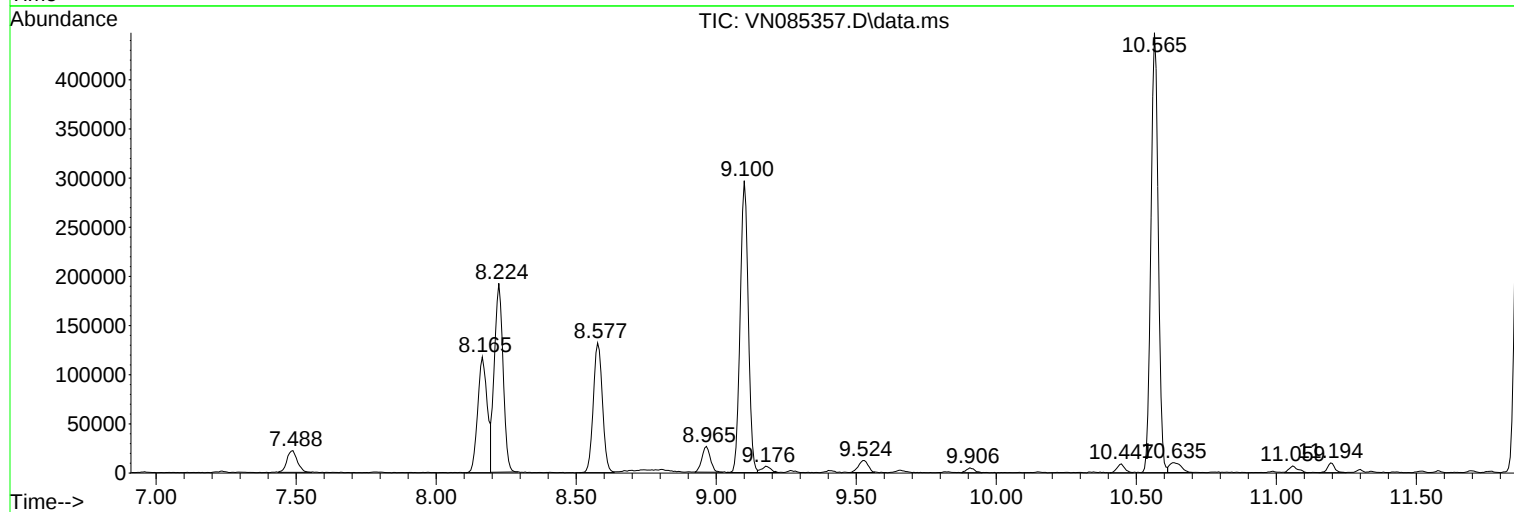
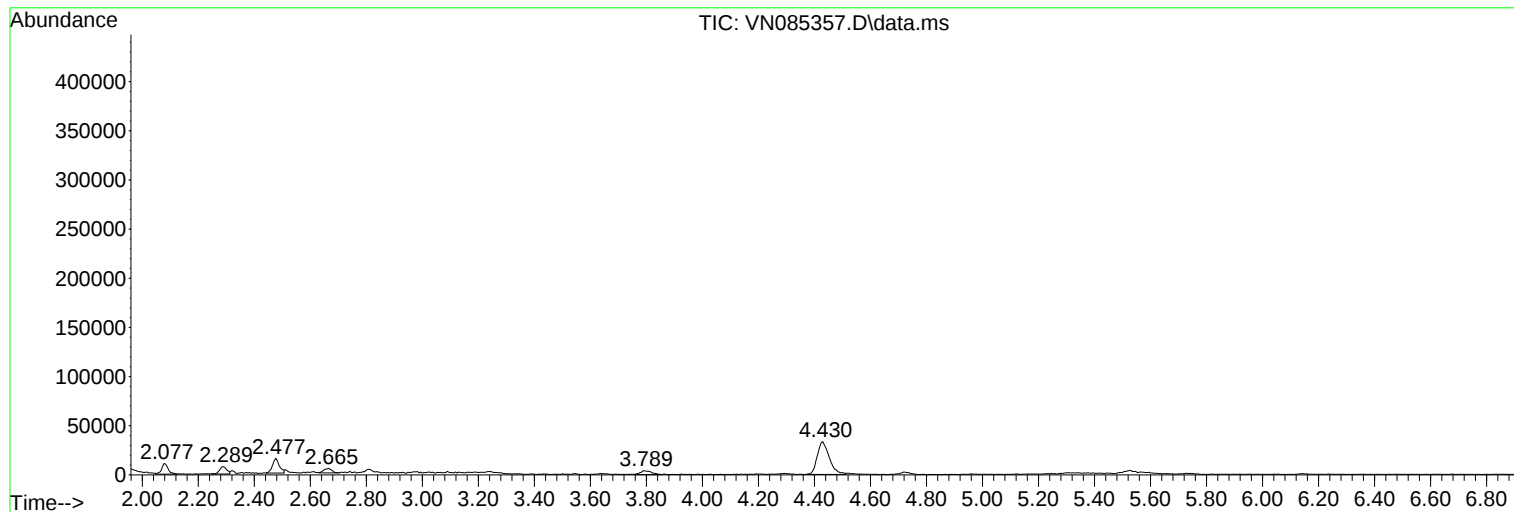
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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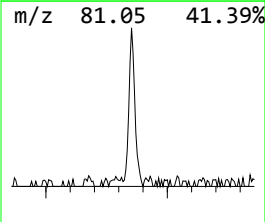
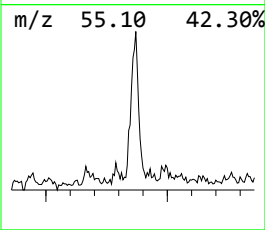
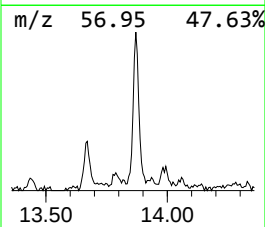
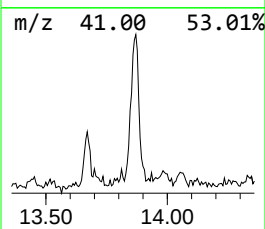
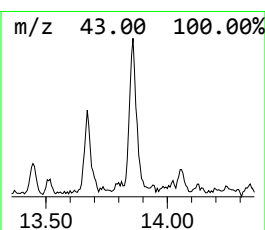
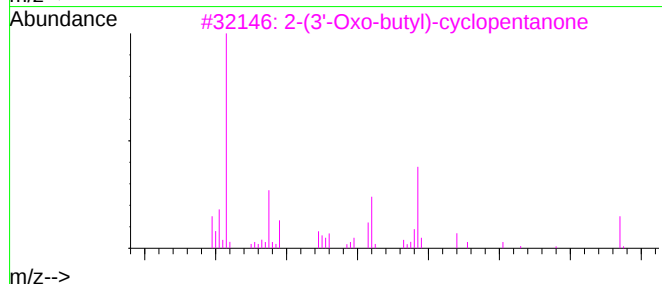
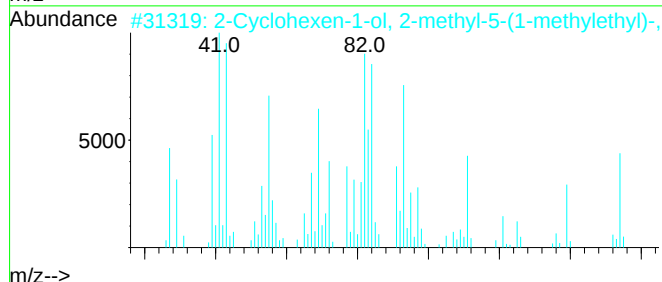
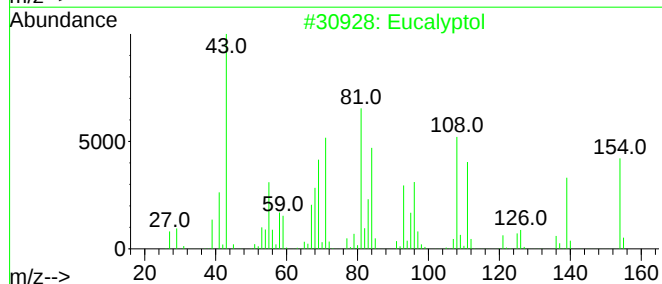
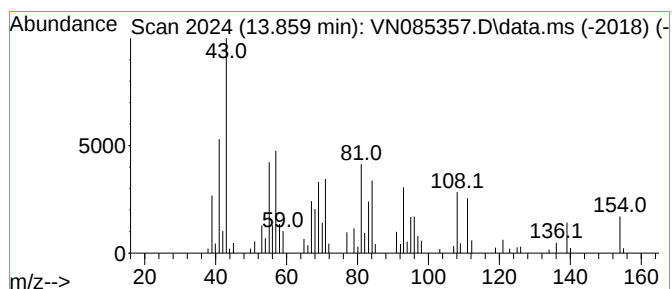
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.858	16.76 ug/l	197617	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	93
2	2-Cyclohexen-1-ol, 2-methyl-5-(1...	154	C10H18O	000536-30-1	49
3	2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	27
4	1-Heptanol, 2,4-dimethyl-,	144	C9H20O	098982-97-9	12
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	12



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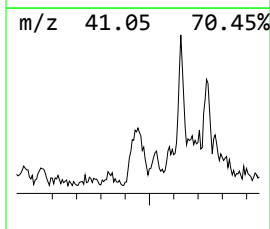
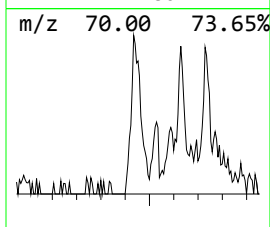
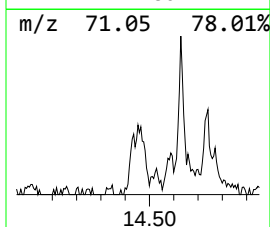
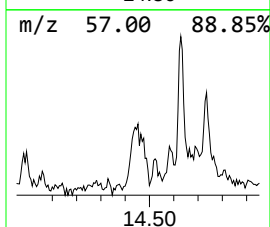
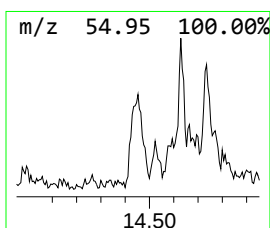
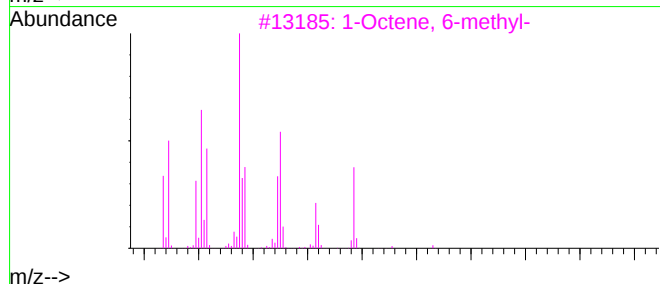
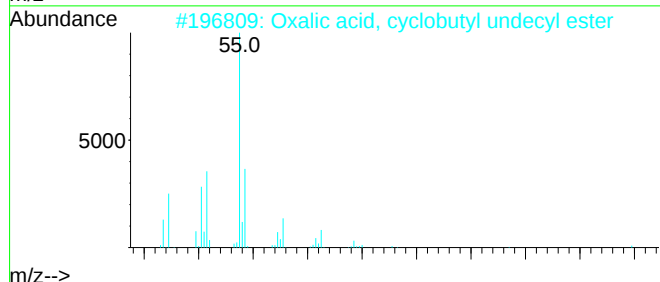
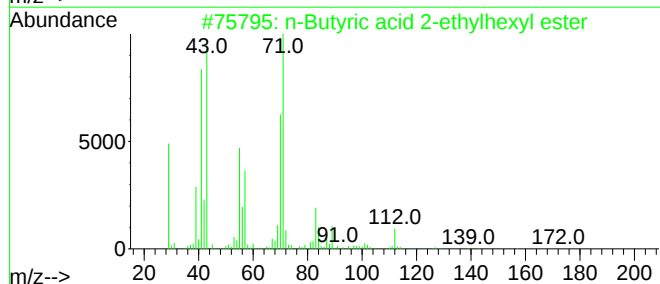
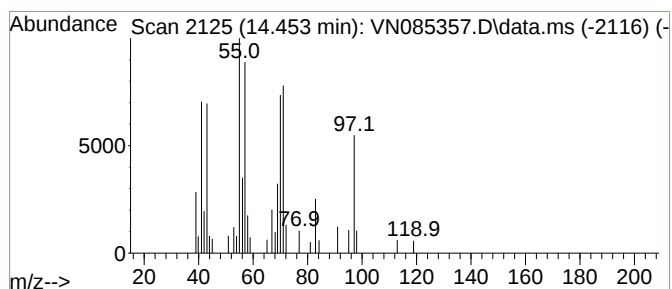
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.453 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.453	6.56 ug/l	77383	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	47
2	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	43
3	1-Octene, 6-methyl-	126	C9H18	013151-10-5	38
4	Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	38
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	37



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

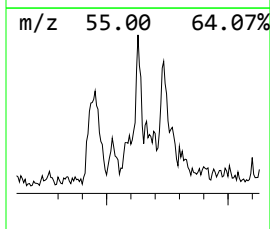
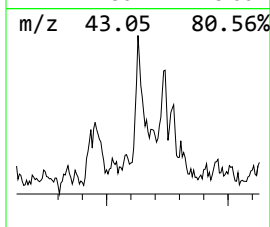
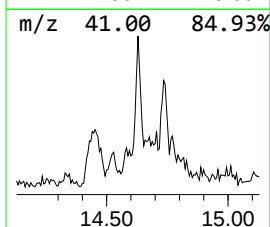
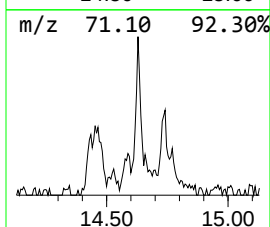
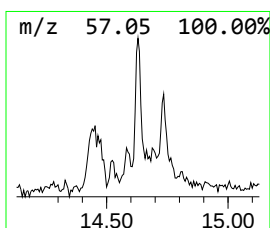
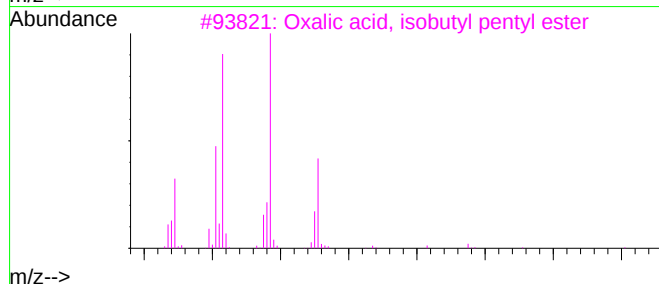
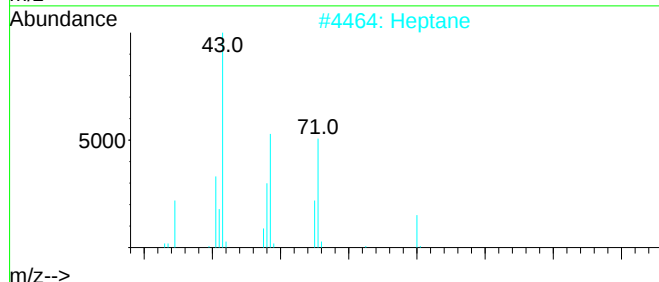
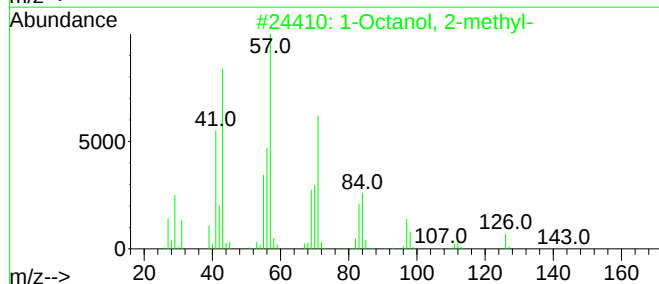
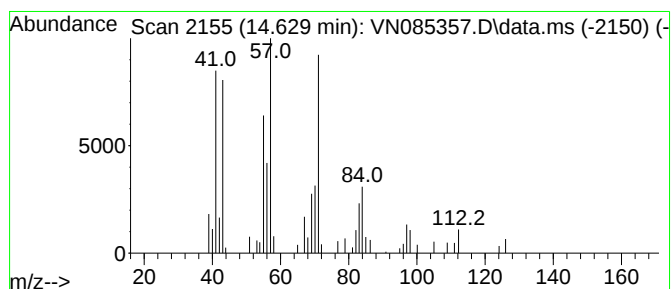
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Quant Title : SW846 8260

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

Peak Number 3 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.629	5.04 ug/l	59444	1,4-Dichlorobenzene-d4		13.788	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-		144	C9H20O	000818-81-5	72
2	Heptane		100	C7H16	000142-82-5	52
3	Oxalic acid, isobutyl pentyl ester		216	C11H20O4	1000309-37-0	47
4	1-Dodecene		168	C12H24	000112-41-4	38
5	cis-2-Nonene		126	C9H18	006434-77-1	38



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Quant Title : SW846 8260

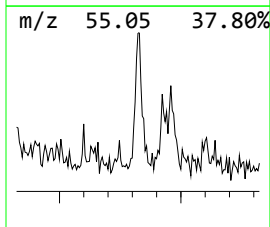
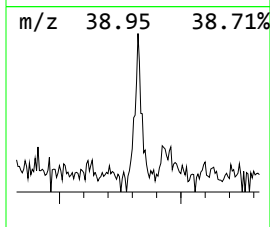
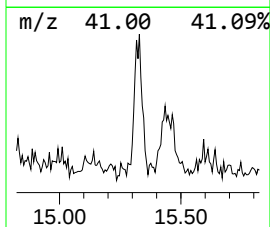
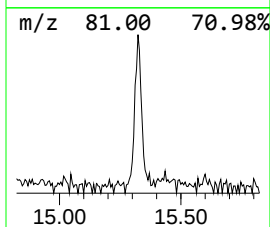
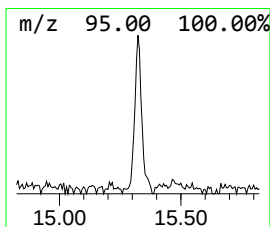
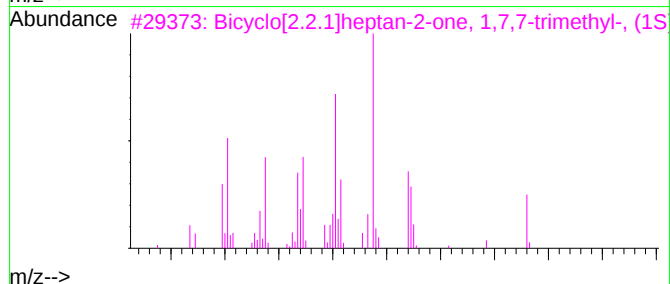
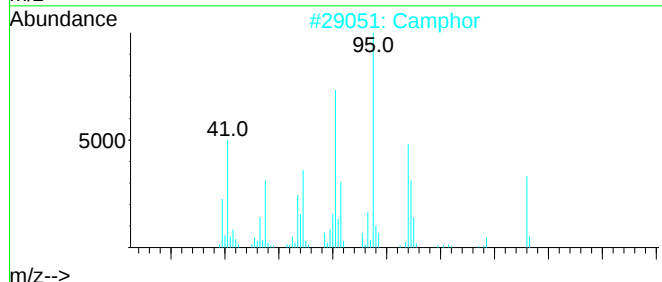
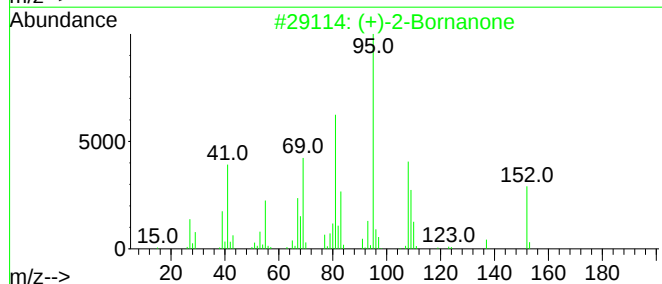
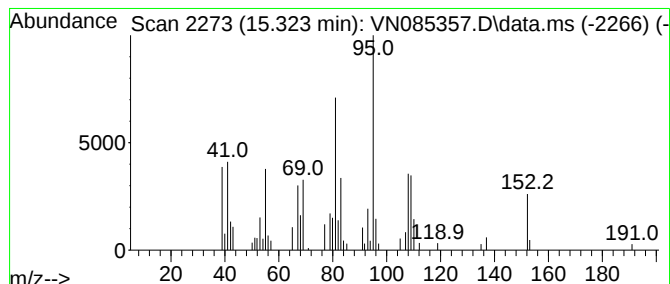
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	7.14 ug/l	84218	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	94
2	Camphor	152	C10H16O	000076-22-2	94
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	93
4	Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	49
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	47



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	13.858	16.8	ug/l	197617	4	13.788	589488	50.0
unknown14.453	14.453	6.6	ug/l	77383	4	13.788	589488	50.0
1-Octanol, 2-me...	14.629	5.0	ug/l	59444	4	13.788	589488	50.0
(+)-2-Bornanone	15.323	7.1	ug/l	84218	4	13.788	589488	50.0