

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN123124\
 Data File : VN085365.D
 Acq On : 31 Dec 2024 11:42
 Operator : JC\MD
 Sample : P5386-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 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: VN085365.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	17	21	30	rVB2	14126	21580	2.63%	0.414%
2	2.283	51	56	66	rBV2	12729	24898	3.04%	0.477%
3	2.477	83	89	93	rBV2	17388	30990	3.78%	0.594%
4	2.807	140	145	150	rBV5	4358	9932	1.21%	0.190%
5	3.795	307	313	323	rVB2	3834	8619	1.05%	0.165%
6	4.430	411	421	435	rBV	31154	94219	11.50%	1.806%
7	7.483	931	940	953	rVB	21396	55181	6.73%	1.058%
8	8.165	1046	1056	1060	rBV	123232	276809	33.79%	5.306%
9	8.224	1060	1066	1076	rVB	190807	433245	52.88%	8.305%
10	8.577	1115	1126	1138	rBV	133716	305005	37.23%	5.846%
11	8.965	1183	1192	1200	rBV2	25206	55022	6.72%	1.055%
12	9.100	1206	1215	1224	rBV	302963	604209	73.75%	11.582%
13	9.177	1224	1228	1233	rVB3	5060	9127	1.11%	0.175%
14	9.524	1278	1287	1299	rBB3	10925	27469	3.35%	0.527%
15	10.447	1435	1444	1451	rBV3	8232	16246	1.98%	0.311%
16	10.565	1455	1464	1471	rVV	453705	819319	100.00%	15.705%
17	10.630	1471	1475	1488	rVB6	10292	29932	3.65%	0.574%
18	11.059	1541	1548	1559	rVB3	6682	13726	1.68%	0.263%
19	11.194	1563	1571	1577	rBV2	9749	16505	2.01%	0.316%
20	11.865	1677	1685	1693	rBV	394069	684504	83.55%	13.121%
21	11.935	1693	1697	1705	rVB4	5918	12785	1.56%	0.245%
22	12.065	1713	1719	1722	rBV4	5771	9944	1.21%	0.191%
23	12.382	1766	1773	1781	rBV7	4576	10896	1.33%	0.209%
24	12.847	1845	1852	1860	rVB	274664	463110	56.52%	8.877%
25	13.041	1880	1885	1890	rVB3	6452	10947	1.34%	0.210%
26	13.159	1901	1905	1910	rVB4	5879	10457	1.28%	0.200%
27	13.282	1920	1926	1936	rVB5	6529	15698	1.92%	0.301%
28	13.447	1948	1954	1958	rBV4	6920	12480	1.52%	0.239%
29	13.665	1986	1991	1999	rBV	20973	40510	4.94%	0.777%
30	13.788	2005	2012	2018	rBV	345784	581719	71.00%	11.151%
31	13.859	2018	2024	2034	rVB4	84787	188558	23.01%	3.614%
32	14.053	2053	2057	2062	rVB5	9033	14778	1.80%	0.283%
33	14.453	2116	2125	2133	rBV6	18739	66745	8.15%	1.279%
34	14.523	2133	2137	2142	rBV3	7056	10852	1.32%	0.208%
35	14.594	2142	2149	2150	rBV5	7593	13409	1.64%	0.257%
36	14.629	2150	2155	2159	rBV2	33970	53686	6.55%	1.029%

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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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Title : SW846 8260

37	14.735	2169	2173	2177	rBV3	22951	31810	3.88%	0.610%
38	14.806	2183	2185	2191	rVB6	7036	11111	1.36%	0.213%
39	15.323	2263	2273	2281	rBV2	36150	75364	9.20%	1.445%
40	15.429	2286	2291	2294	rVV5	10757	19045	2.32%	0.365%
41	15.465	2294	2297	2301	rVB6	10716	15559	1.90%	0.298%
42	15.629	2323	2325	2333	rVB3	6495	10896	1.33%	0.209%

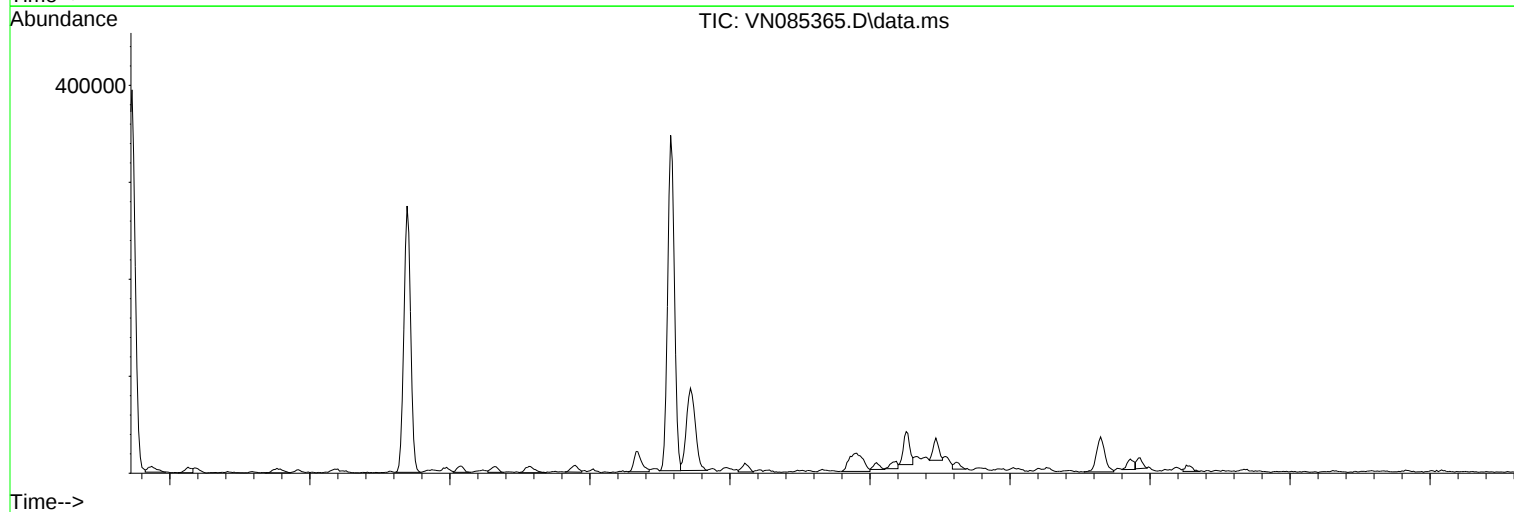
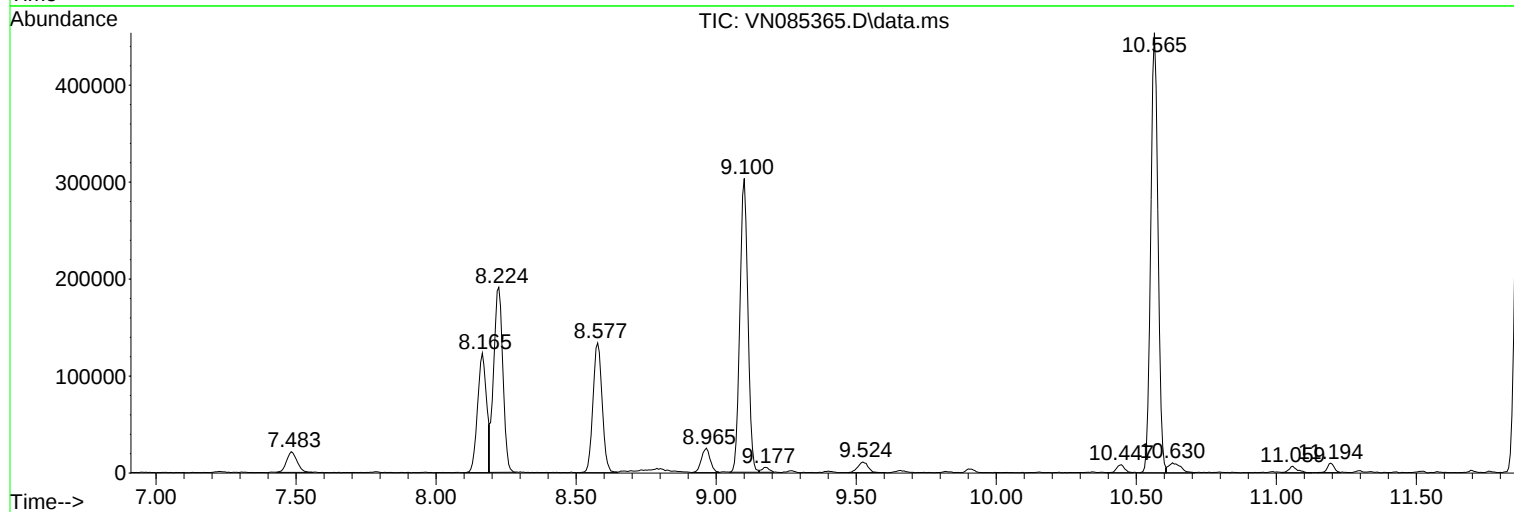
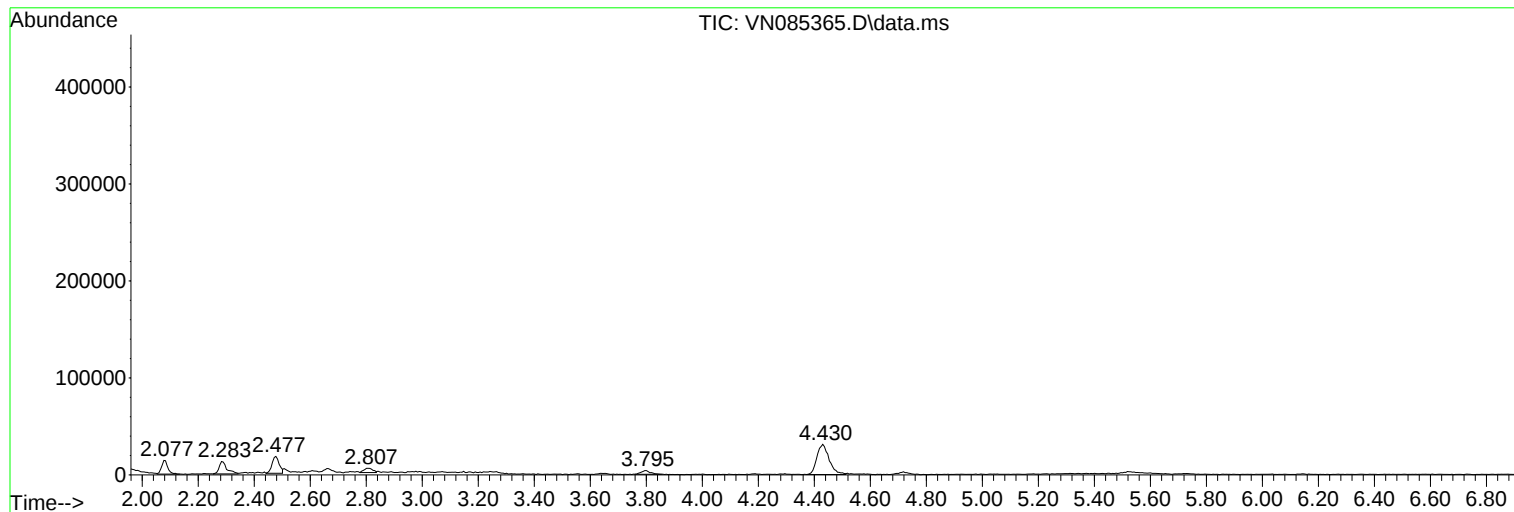
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

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



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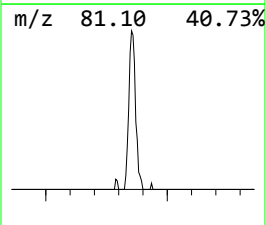
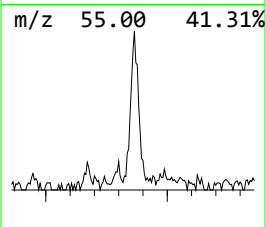
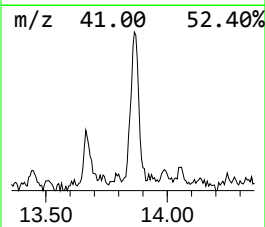
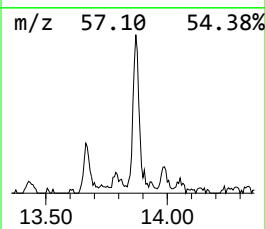
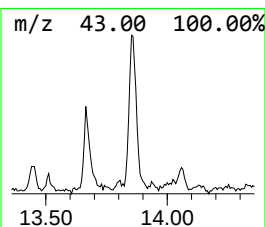
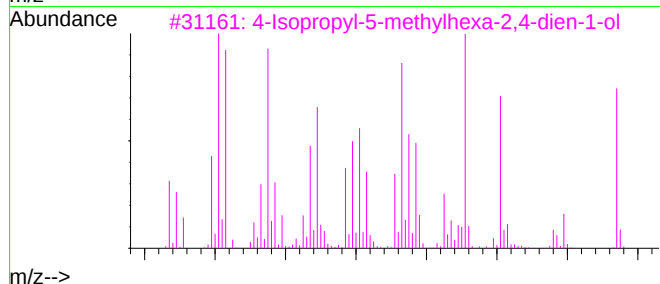
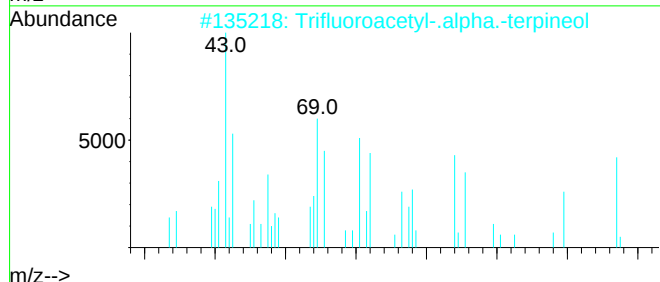
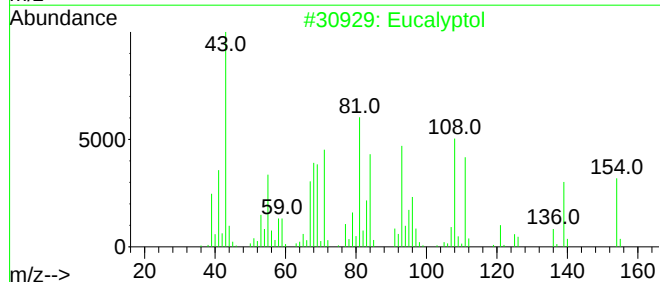
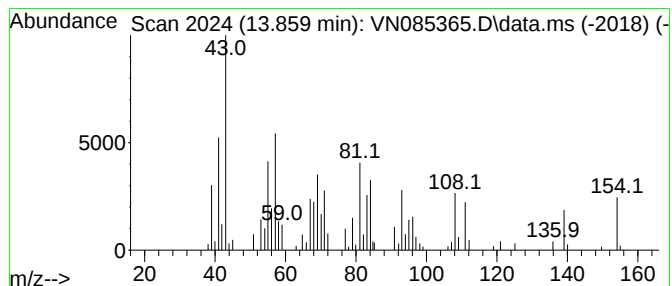
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
Quant Title : SW846 8260

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.
13.859	16.21 ug/l	188558	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	91
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	74
3	4-Isopropyl-5-methylhexa-2,4-die...	154	C10H18O	1000191-04-3	41
4	Ketone, methyl 2,2,3-trimethylcy...	154	C10H18O	017983-22-1	27
5	1-Cyclopentene-1-methanol, .alph...	154	C10H18O	056666-68-3	22



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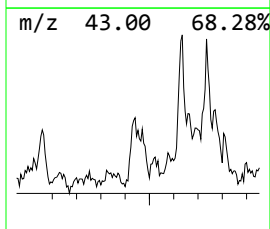
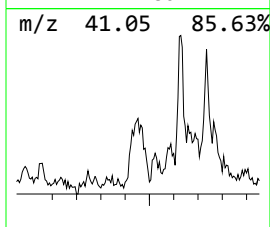
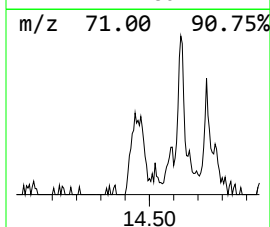
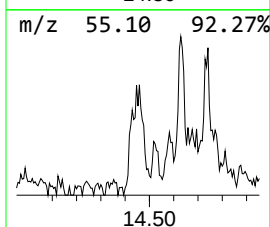
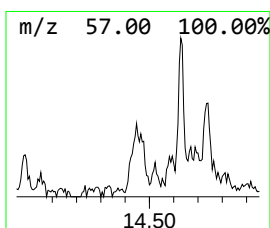
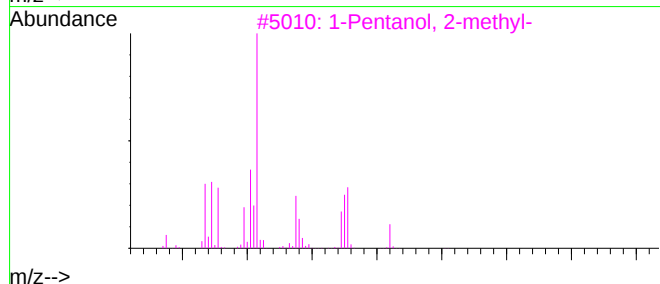
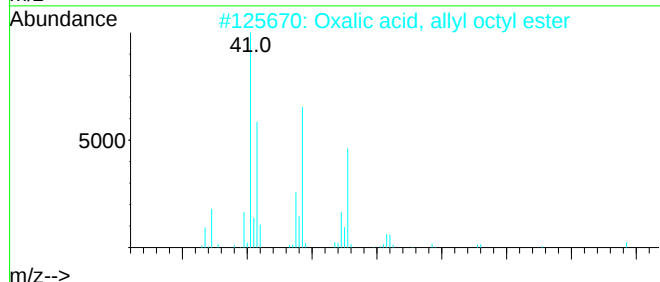
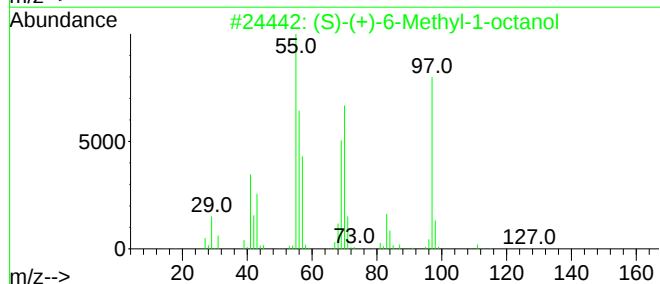
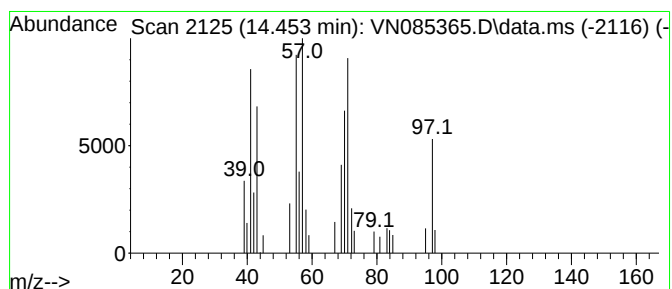
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122724W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.453 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.453	5.74 ug/l	66745	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	27
2	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	25
3	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	23
4	1-Octene, 6-methyl-	126	C9H18	013151-10-5	22
5	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	22



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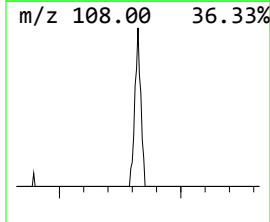
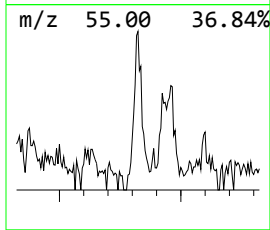
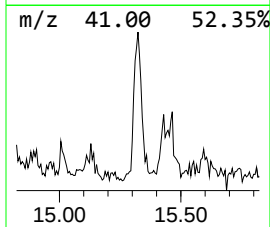
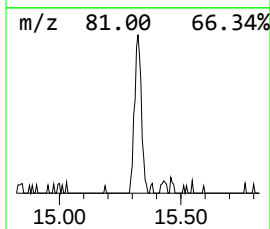
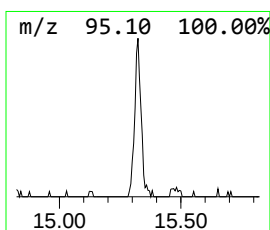
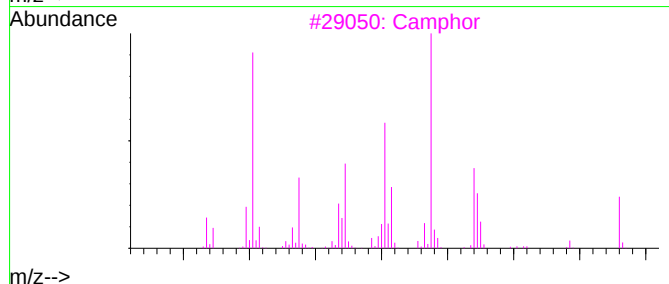
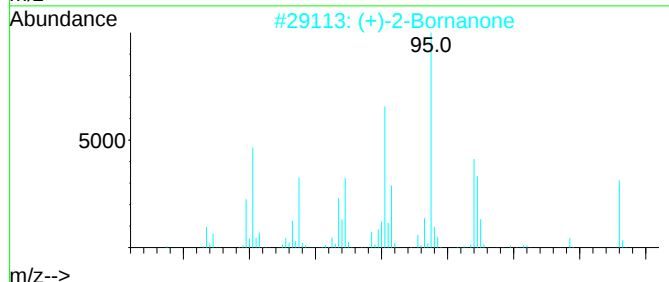
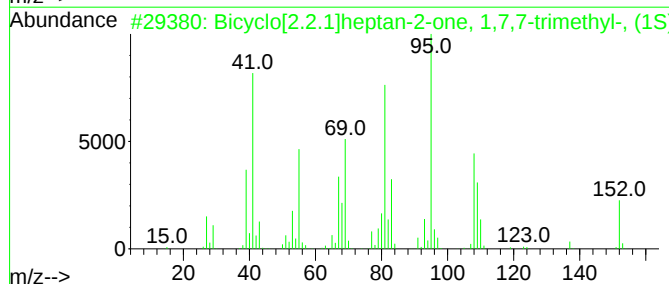
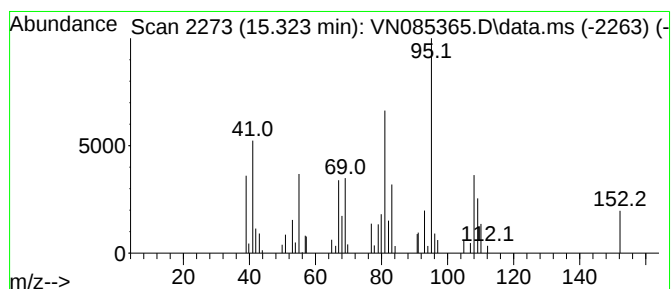
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	6.48 ug/l	75364	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	94
4	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5	.alpha.-Santoline alcohol	154	C10H18O	090823-36-2	43



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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	13.859	16.2	ug/l	188558	4	13.788	581719	50.0
unknown14.453	14.453	5.7	ug/l	66745	4	13.788	581719	50.0
Bicyclo[2.2.1]h...	15.323	6.5	ug/l	75364	4	13.788	581719	50.0