

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
 Data File : BF093488.D
 Acq On : 9 Mar 2017 21:12
 Operator : SJ/MA
 Sample : I2195-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-9-COMP-0-12FT

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:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.967	5	7	19	rVB	98059	197056	3.07%	0.353%
2	4.241	204	206	221	rBV	68820	156161	2.44%	0.280%
3	4.916	262	265	280	rBV	731895	1444670	22.53%	2.590%
4	5.350	301	303	327	rBV	5145585	6001516	93.61%	10.759%
5	5.750	335	338	345	rVB	52610	81358	1.27%	0.146%
6	6.402	392	395	398	rBV	4274751	6410863	100.00%	11.493%
7	6.516	403	405	408	rVV	4287859	5650356	88.14%	10.129%
8	6.745	423	425	428	rBV	1273881	1204828	18.79%	2.160%
9	6.905	436	439	441	rBV	4502006	4551214	70.99%	8.159%
10	7.327	473	476	478	rBV	2923077	4213236	65.72%	7.553%
11	8.036	535	538	540	rBV	1523663	1595318	24.88%	2.860%
12	9.111	629	632	634	rBV	5629193	5793204	90.37%	10.385%
13	9.511	664	667	669	rBV	1116379	1013990	15.82%	1.818%
14	9.716	682	685	686	rBV	62415	75766	1.18%	0.136%
15	9.785	689	691	693	rVB	1878536	1781947	27.80%	3.194%
16	10.208	727	728	730	rVB	75155	84829	1.32%	0.152%
17	10.574	757	760	763	rBV2	2540949	3405409	53.12%	6.105%
18	10.688	768	770	777	rVB2	121212	184657	2.88%	0.331%
19	11.134	806	809	810	rBV	110427	105738	1.65%	0.190%
20	11.271	819	821	823	rBV	1900068	1857479	28.97%	3.330%
21	11.556	844	846	848	rBV	94516	79128	1.23%	0.142%
22	11.797	865	867	871	rBV2	45082	81162	1.27%	0.145%
23	12.859	957	960	962	rBV	4165224	5589758	87.19%	10.021%
24	13.751	1035	1038	1047	rBV	336398	606577	9.46%	1.087%
25	13.877	1047	1049	1050	rBV	72005	71583	1.12%	0.128%
26	13.911	1050	1052	1054	rVV	1705773	1726262	26.93%	3.095%
27	15.317	1172	1175	1184	rVB	1226717	1557295	24.29%	2.792%
28	15.694	1205	1208	1211	rVB	59881	91495	1.43%	0.164%
29	15.808	1212	1218	1220	rBV5	29653	103831	1.62%	0.186%
30	16.151	1245	1248	1255	rVB3	27983	65761	1.03%	0.118%

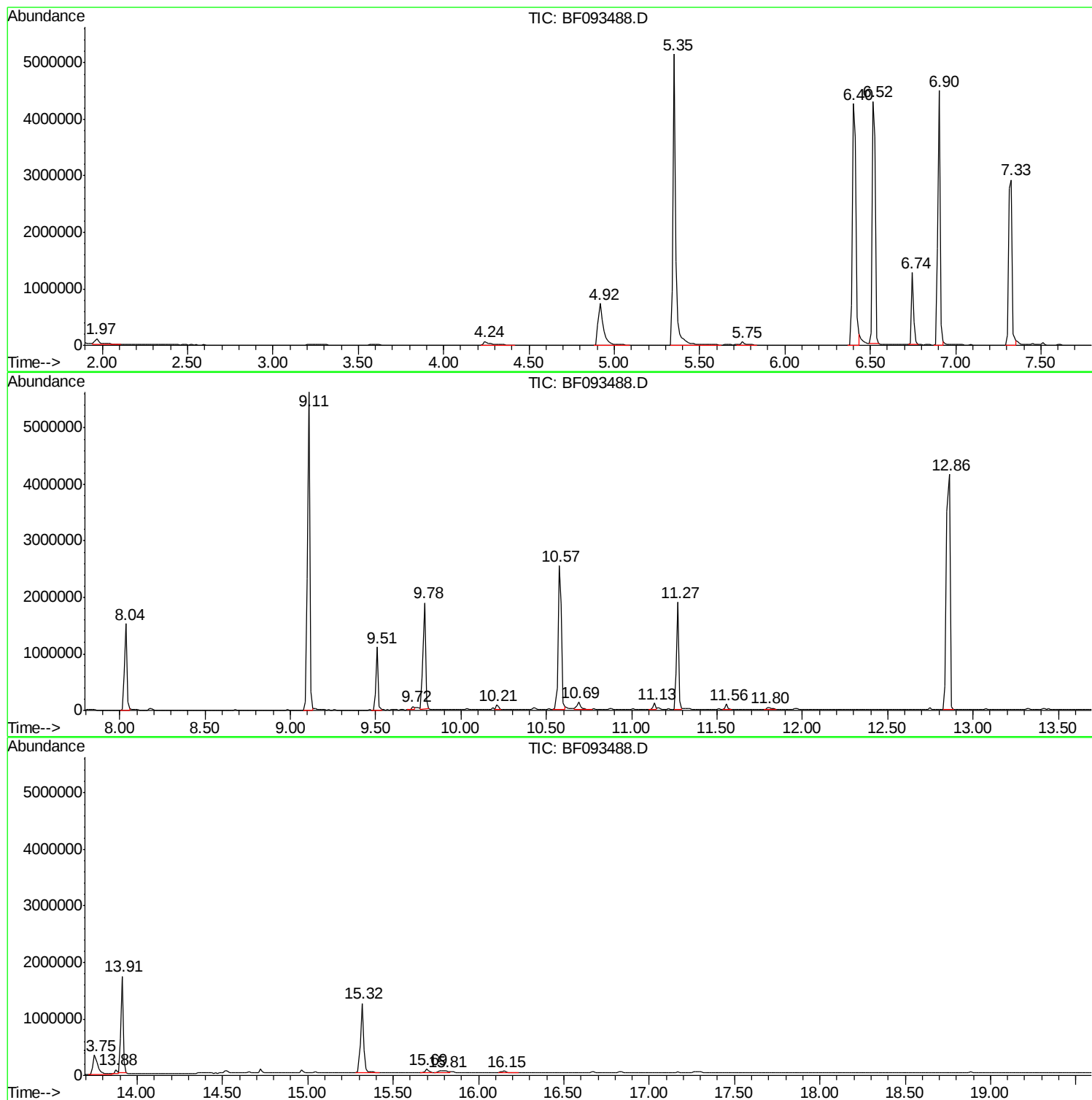
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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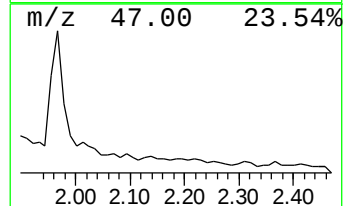
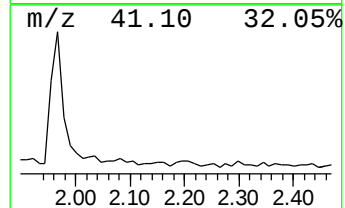
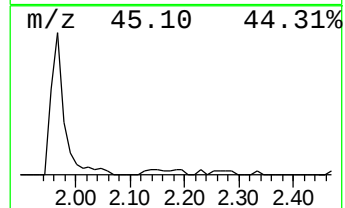
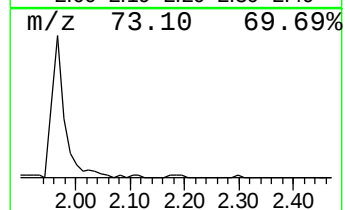
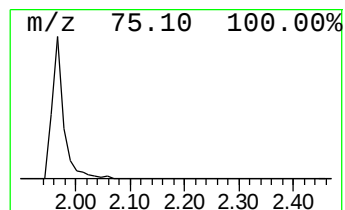
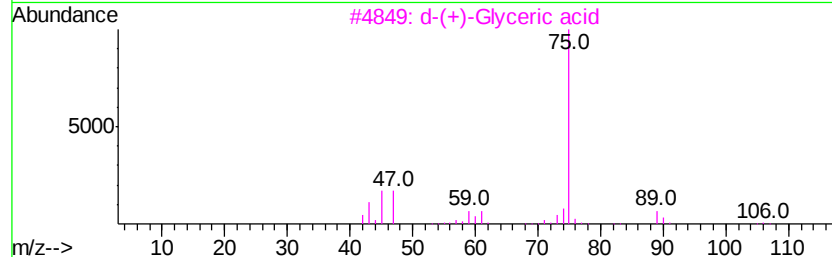
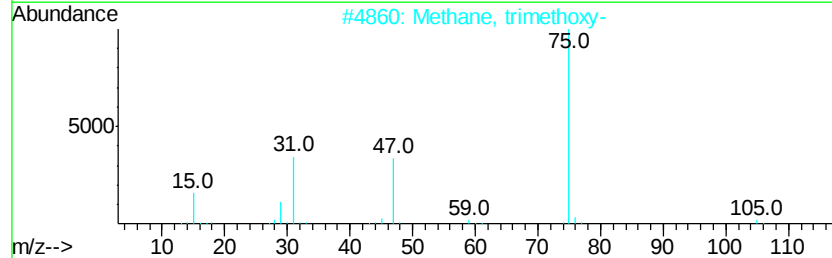
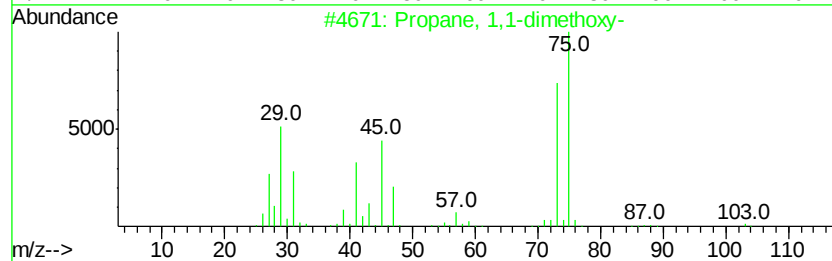
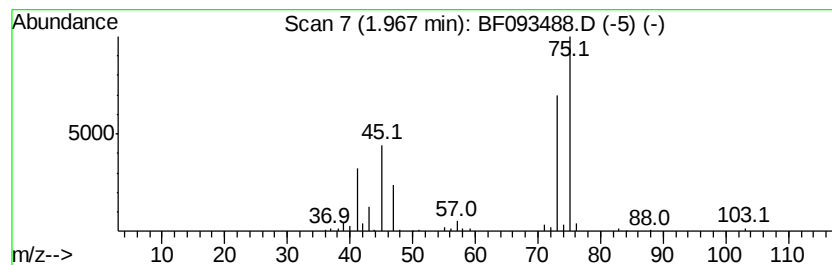
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.97	3.27 ng	197056	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Methane, trimethoxy-	106	C4H10O3	000149-73-5	33
3		d-(+)-Glyceric acid	106	C3H6O4	1000211-40-8	9
4		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9
5		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9



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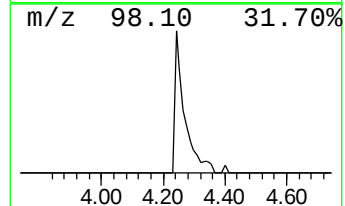
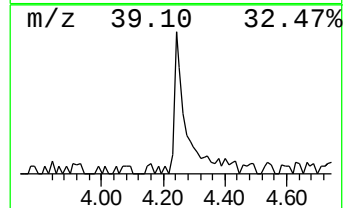
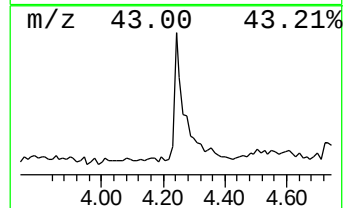
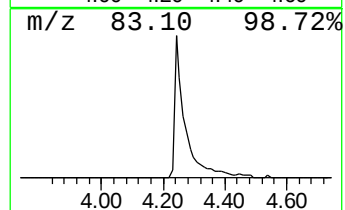
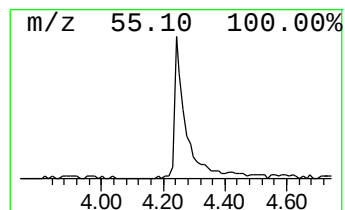
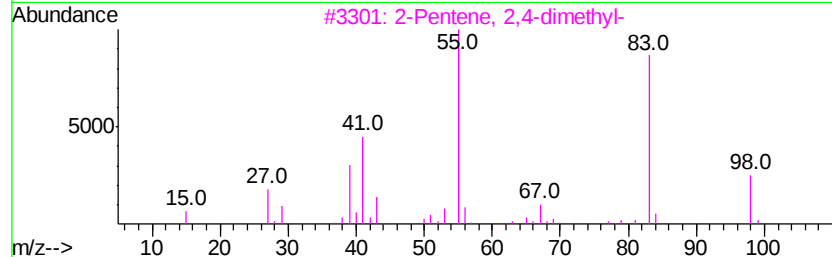
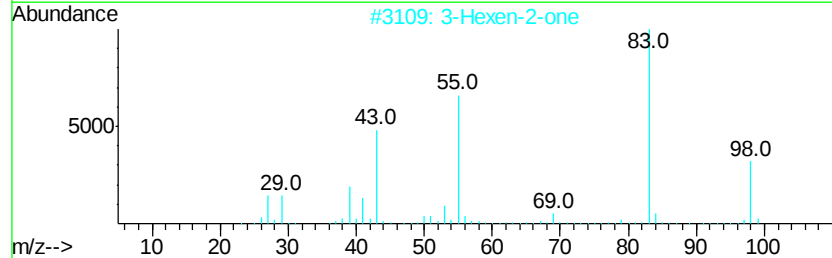
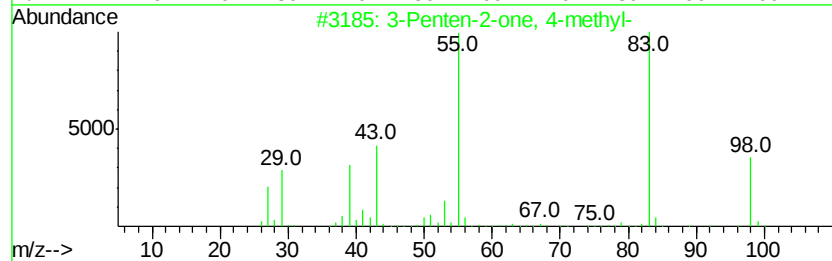
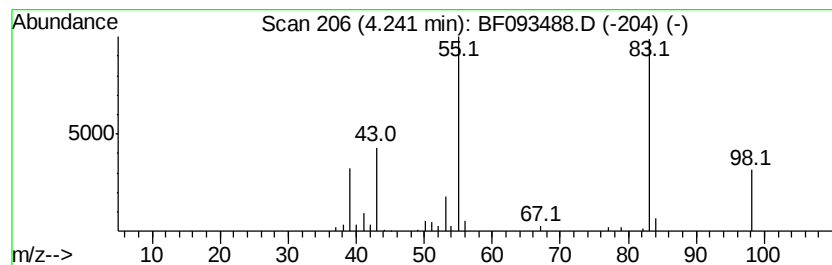
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	2.59 ng	156161	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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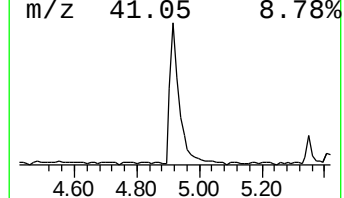
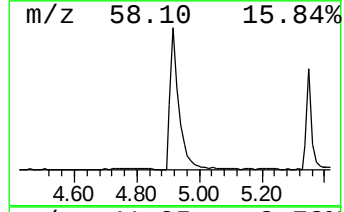
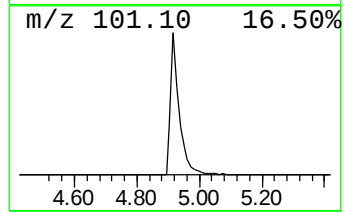
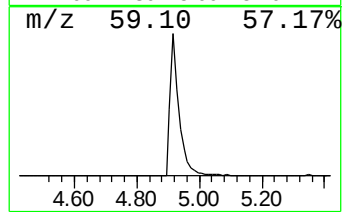
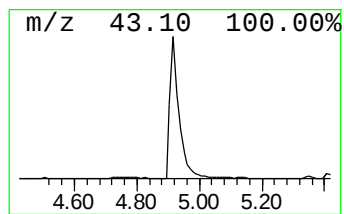
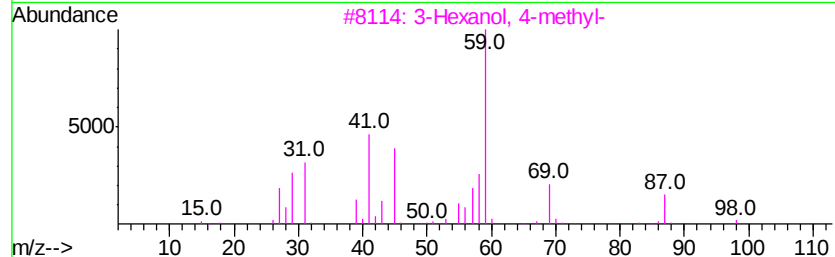
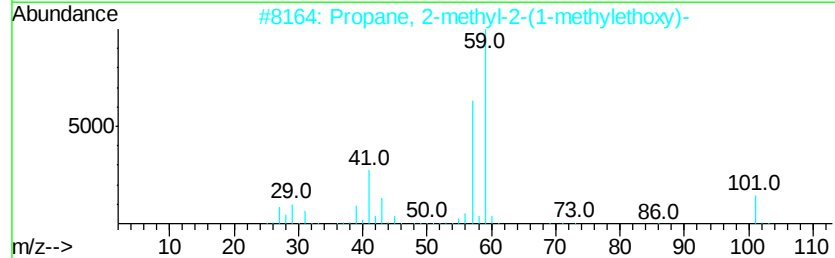
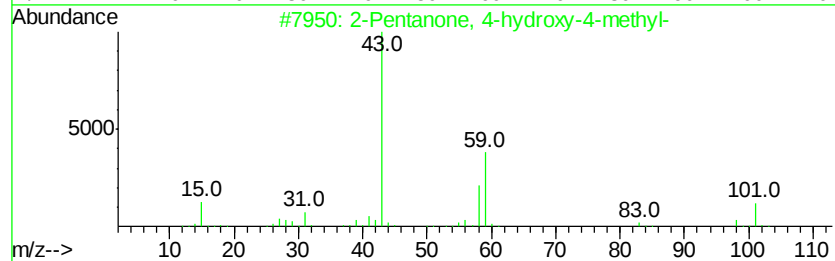
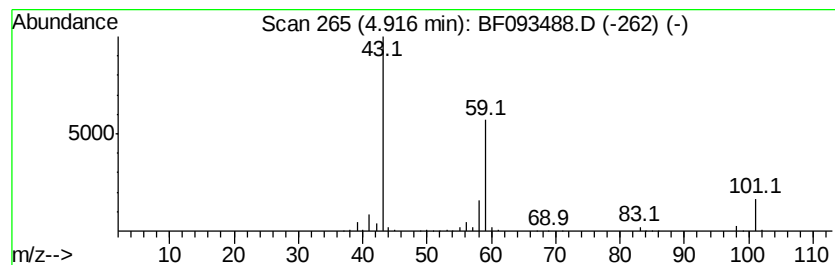
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	23.98 ng	1444670	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		3-Octanol	130	C8H18O	000589-98-0	33



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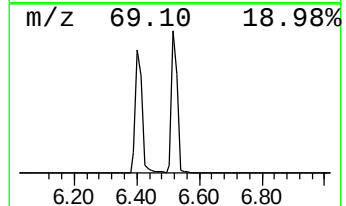
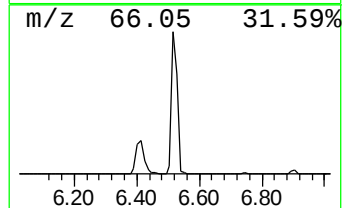
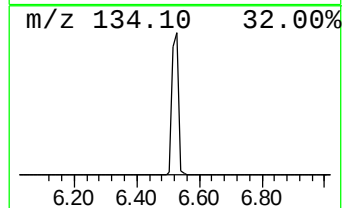
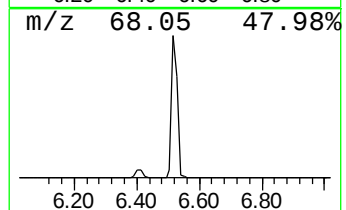
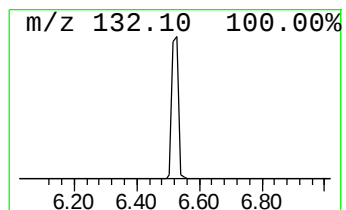
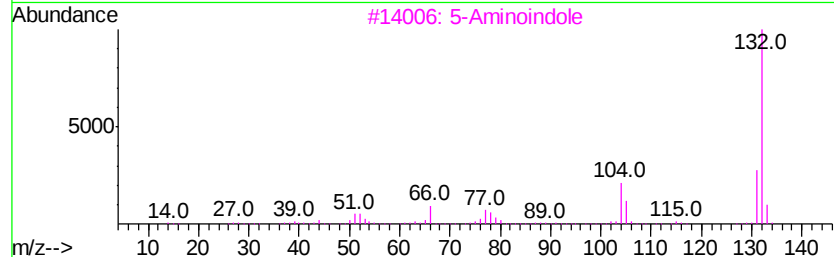
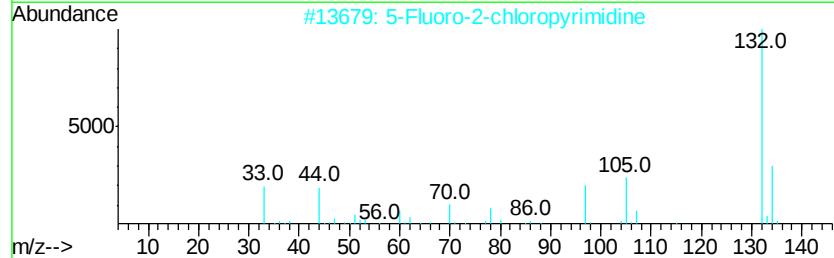
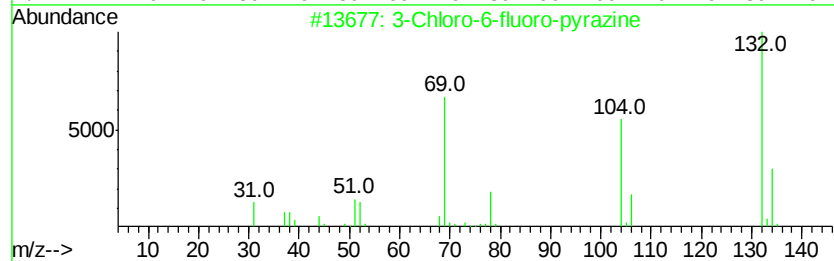
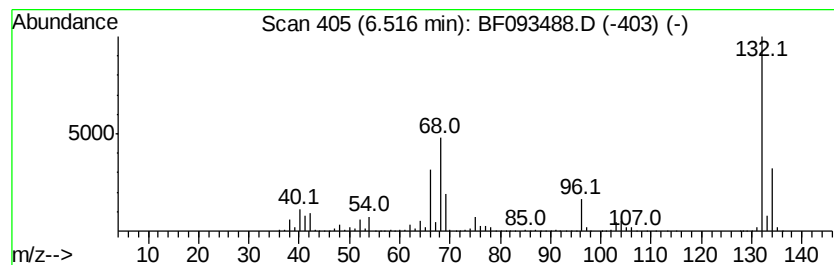
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Peak Number 4 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	93.80 ng	5650360	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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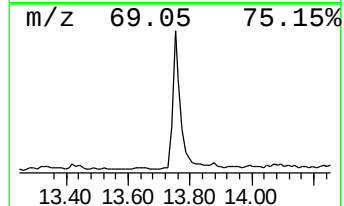
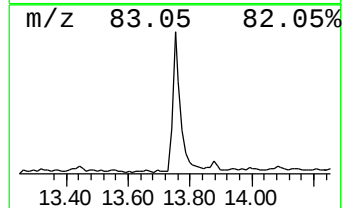
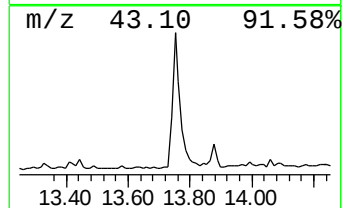
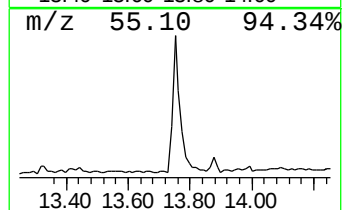
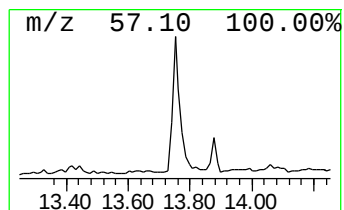
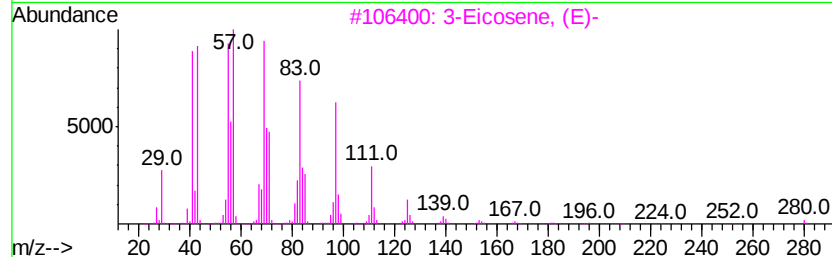
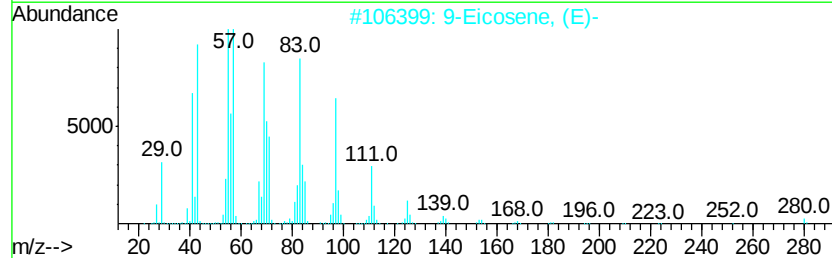
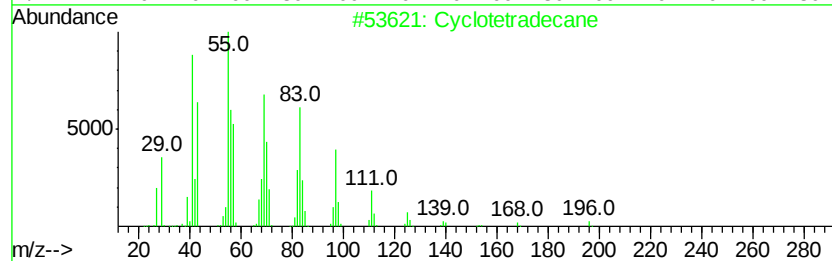
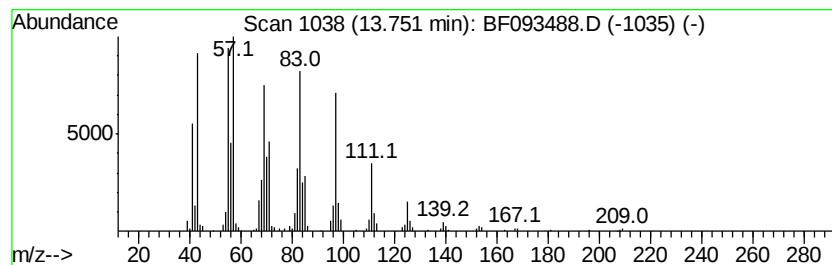
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	7.03 ng	606577	Chrysene-d12	13.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	96
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.97	3.3	ng	197056	1	6.74	1204830	20.0
3-Penten-2-one, 4...	4.24	2.6	ng	156161	1	6.74	1204830	20.0
2-Pentanone, 4-hy...	4.92	24.0	ng	1444670	1	6.74	1204830	20.0
unknown6.52	6.52	93.8	ng	5650360	1	6.74	1204830	20.0
Cyclotetradecane	13.75	7.0	ng	606577	5	13.91	1726260	20.0