

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
 Data File : BF099176.D
 Acq On : 7 Oct 2017 5:11
 Operator : SJ/JU
 Sample : I5542-02
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OWL-C2-GW

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.152	6	11	19	rVB	584773	741072	19.27%	2.772%
2	3.951	312	317	323	rVB	30643	38837	1.01%	0.145%
3	5.087	507	510	522	rVB	221423	263258	6.84%	0.985%
4	5.487	573	578	581	rBV	1831063	1720065	44.72%	6.435%
5	6.487	744	748	757	rBV	1153263	1089303	28.32%	4.075%
6	6.634	768	773	776	rBV	3012890	2887325	75.07%	10.802%
7	6.863	808	812	815	rBV	1008718	816776	21.24%	3.056%
8	7.022	834	839	842	rBV	2890708	2656249	69.07%	9.937%
9	7.428	903	908	911	rBV	2051025	2180977	56.71%	8.159%
10	8.145	1026	1030	1032	rBV	1313887	1130695	29.40%	4.230%
11	8.163	1032	1033	1036	rVB	124861	81681	2.12%	0.306%
12	8.704	1119	1125	1128	rBV2	31053	39516	1.03%	0.148%
13	8.951	1161	1167	1171	rBV4	22666	46106	1.20%	0.172%
14	9.222	1207	1213	1216	rBV	3931635	3846008	100.00%	14.388%
15	9.898	1324	1328	1332	rBV2	1464558	1231642	32.02%	4.608%
16	10.104	1360	1363	1368	rBV3	37627	53703	1.40%	0.201%
17	10.510	1429	1432	1436	rBV	195956	178436	4.64%	0.668%
18	10.692	1458	1463	1466	rBV	1951320	2012929	52.34%	7.531%
19	11.022	1516	1519	1526	rVB2	74394	78761	2.05%	0.295%
20	11.227	1549	1554	1558	rBV2	36852	75070	1.95%	0.281%
21	11.386	1577	1581	1584	rBV	1334016	1093601	28.43%	4.091%
22	12.780	1814	1818	1821	rVB	79294	73226	1.90%	0.274%
23	12.969	1845	1850	1853	rBV	2947393	2953820	76.80%	11.050%
24	13.480	1934	1937	1941	rVB	50472	44219	1.15%	0.165%
25	13.851	1996	2000	2006	rBV	40437	41995	1.09%	0.157%
26	14.021	2025	2029	2037	rVB	765867	675864	17.57%	2.528%
27	15.492	2274	2279	2287	rBV	535135	679156	17.66%	2.541%

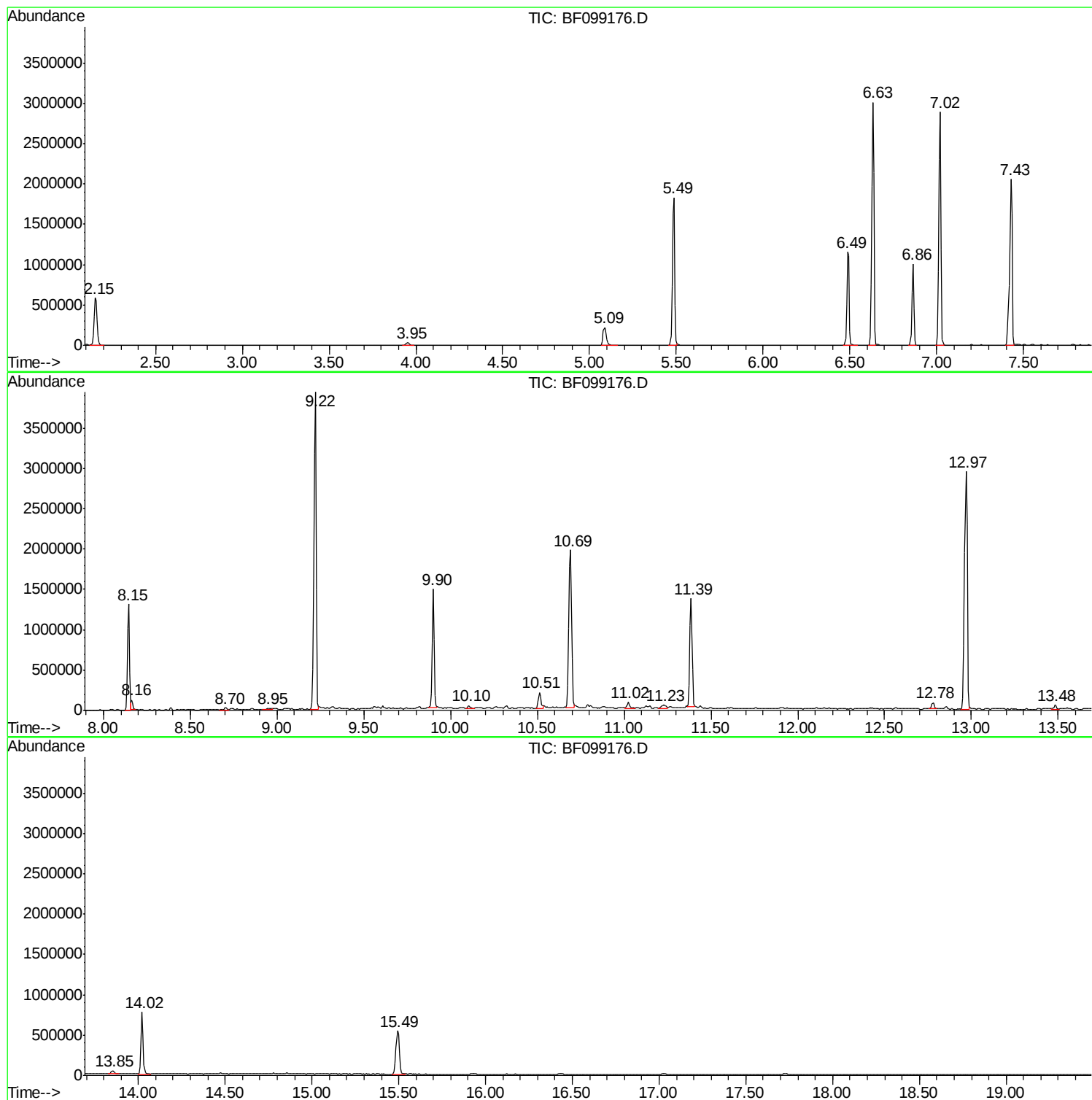
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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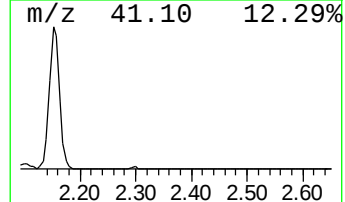
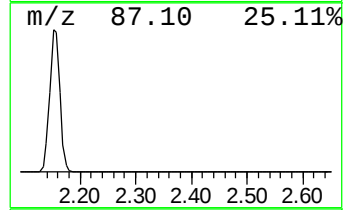
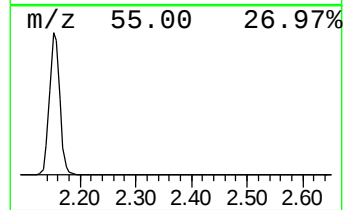
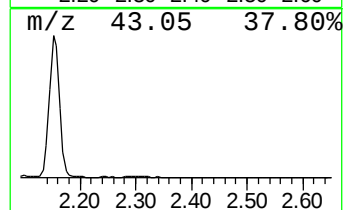
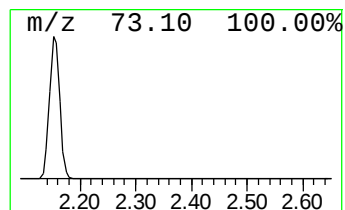
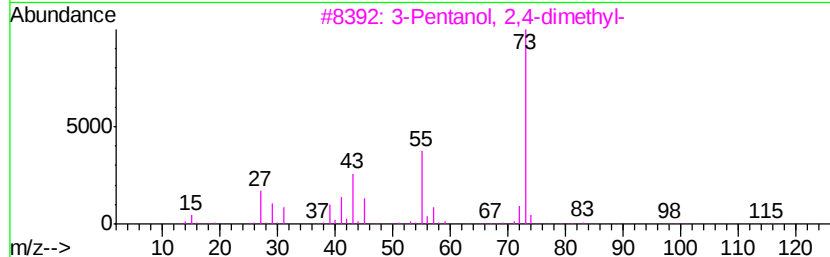
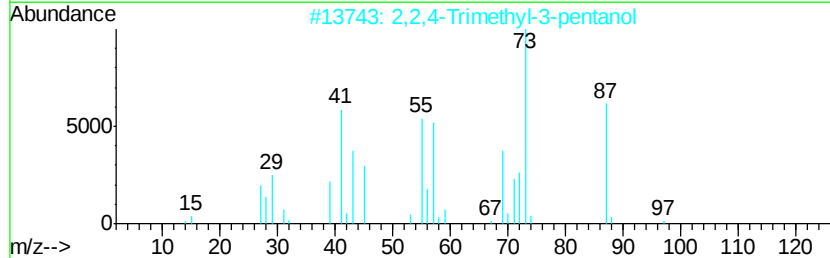
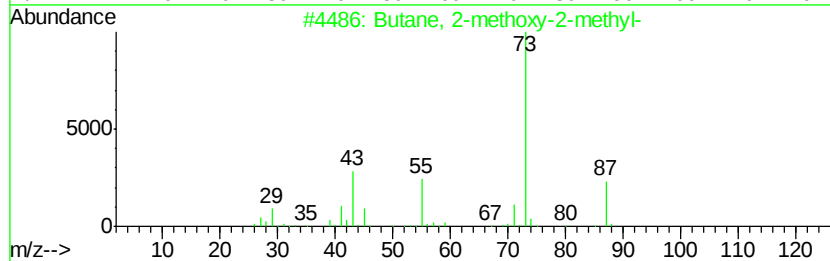
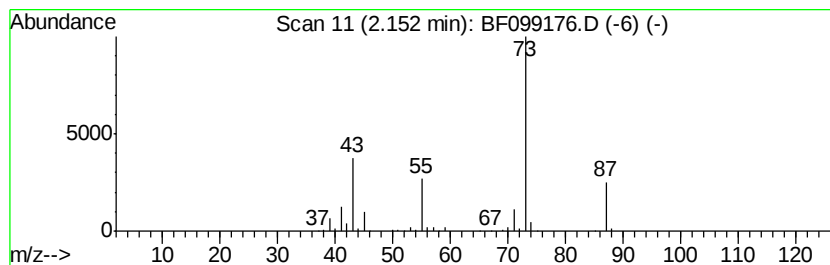
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	18.15 ng	741072	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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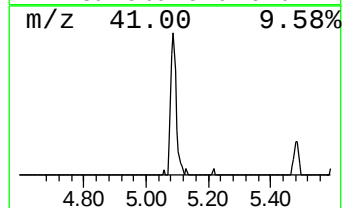
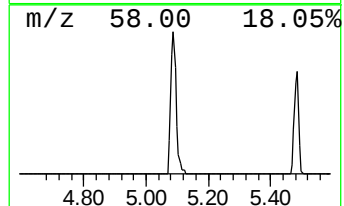
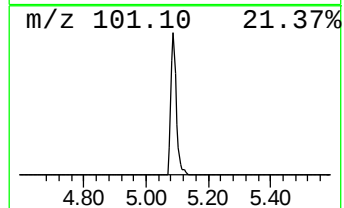
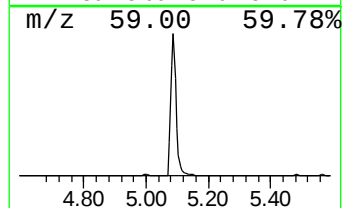
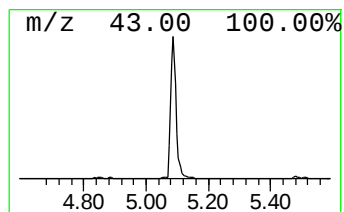
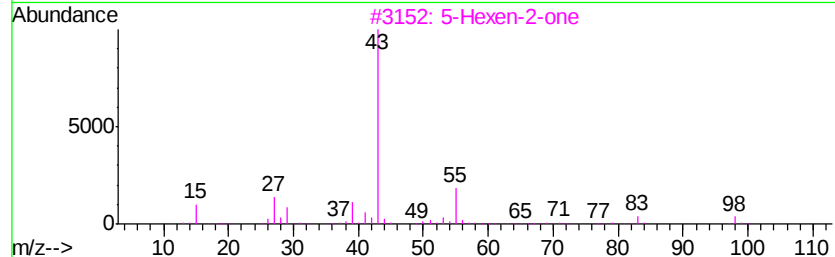
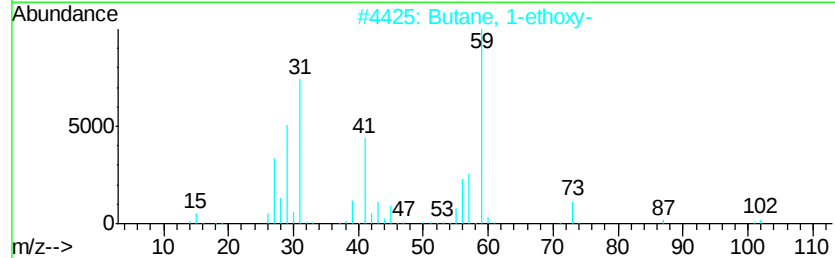
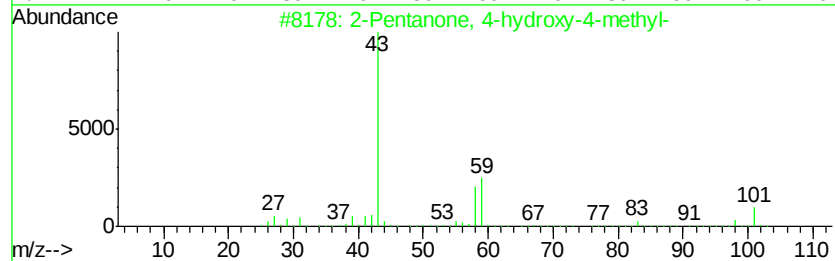
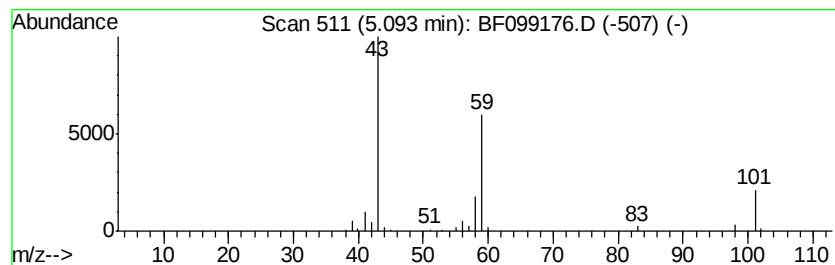
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.45 ng	263258	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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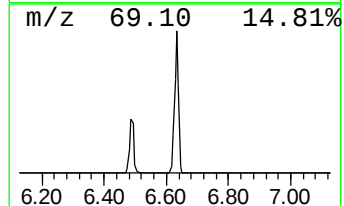
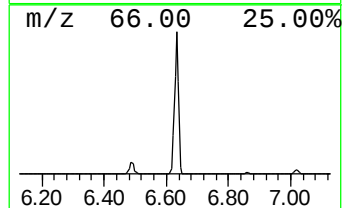
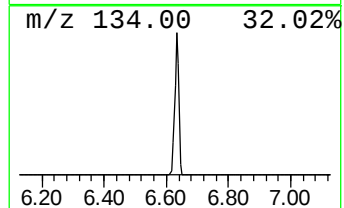
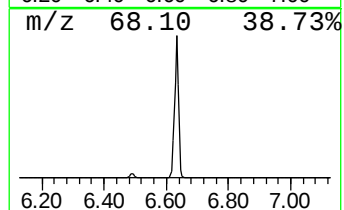
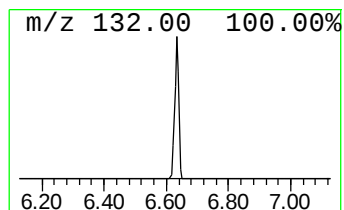
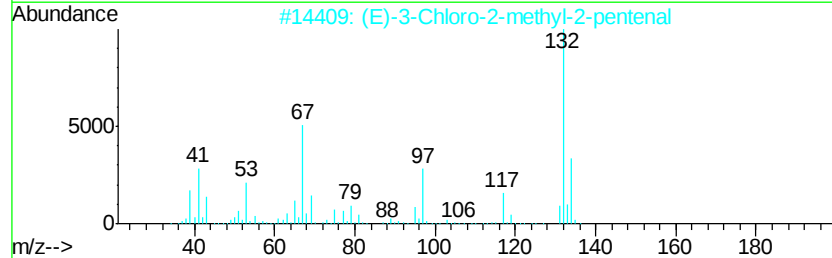
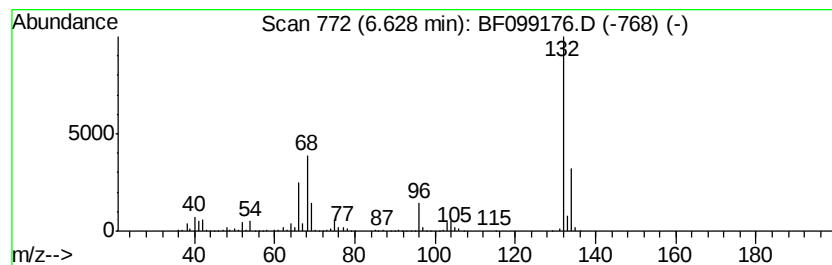
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	70.70 ng	2887330	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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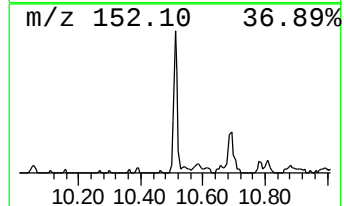
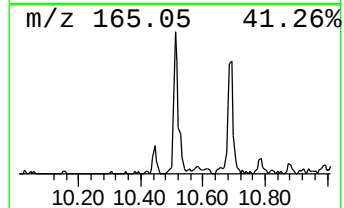
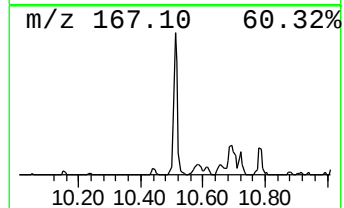
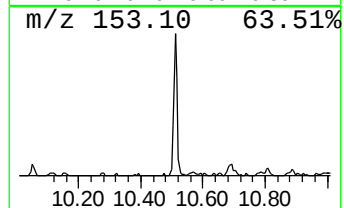
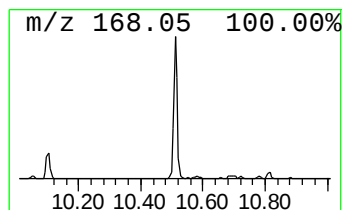
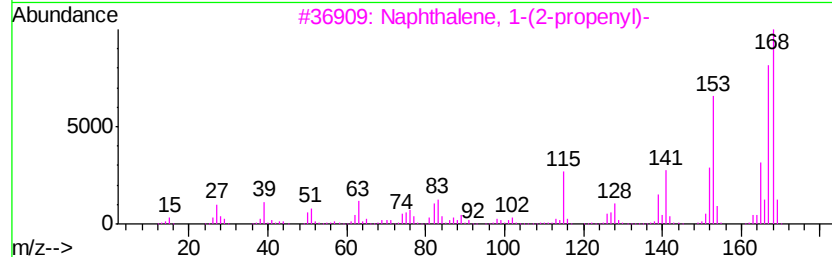
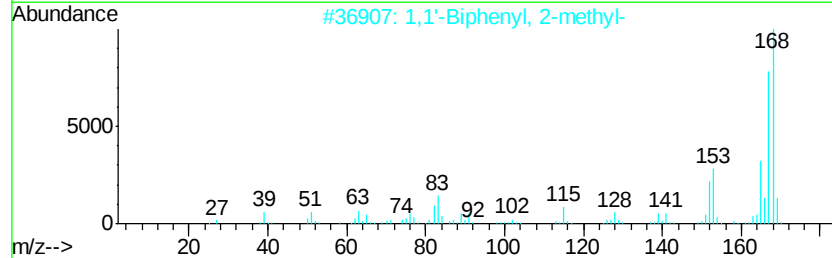
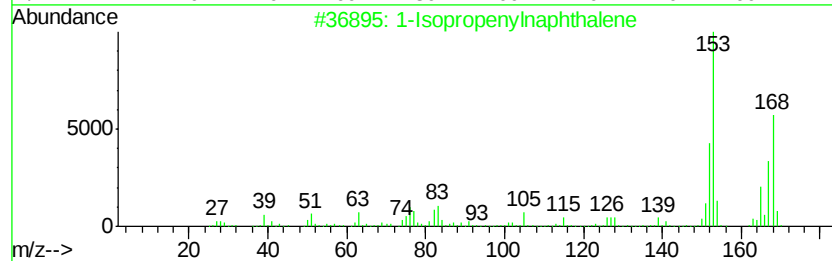
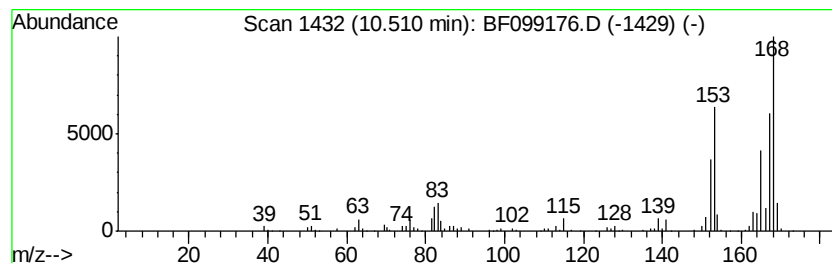
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Isopropenylnaphthalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	2.90 ng	178436	Acenaphthene-d10	9.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Isopropenylnaphthalene	168	C13H12	001855-47-6	81
2		1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	81
3		Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	58
4		1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	58
5		1,1-Diphenyl-2-propanol	212	C15H16O	029338-49-6	53



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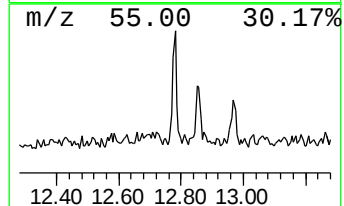
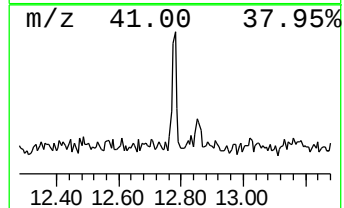
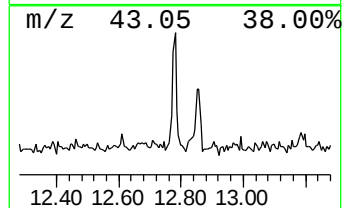
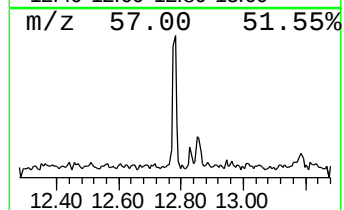
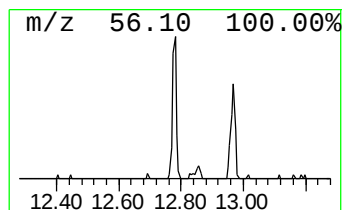
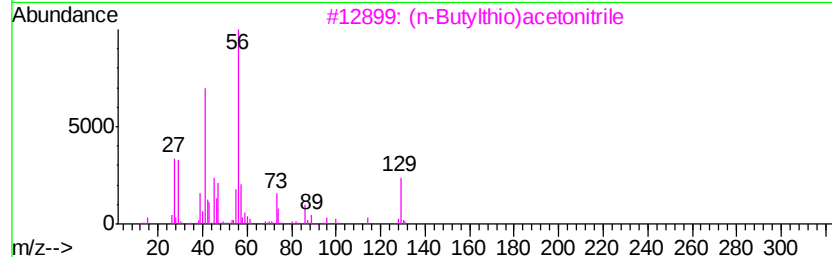
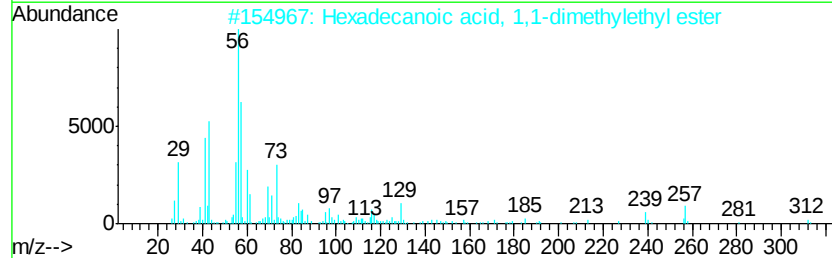
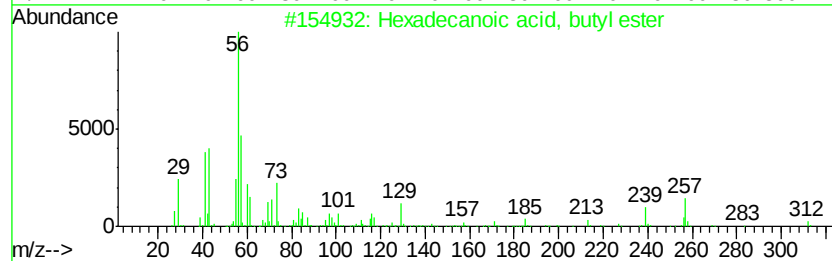
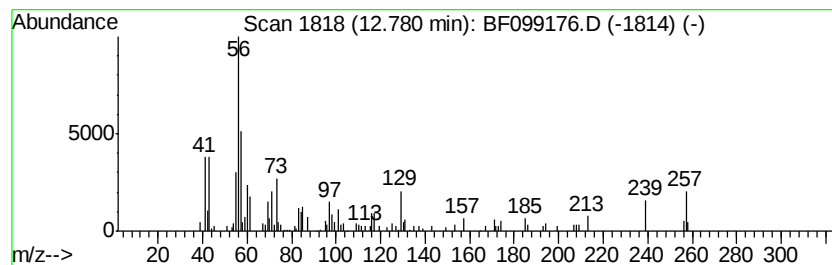
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.17 ng	73226	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3			(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	47
4			Cyclohexanamine	99	C6H13N	000108-91-8	30
5			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	18.1	ng	741072	1	6.86	816776	20.0
2-Pentanone, 4-hy...	5.09	6.5	ng	263258	1	6.86	816776	20.0
unknown6.63	6.63	70.7	ng	2887330	1	6.86	816776	20.0
1-Isopropenyl naph...	10.51	2.9	ng	178436	3	9.90	1231640	20.0
Hexadecanoic acid...	12.78	2.2	ng	73226	5	14.02	675864	20.0