

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092280.D
 Acq On : 14 Jan 2017 12:55
 Operator : UM/SJ
 Sample : I1162-14
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08-COMP

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-BF122116.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	4.702	252	255	270	rBV	1516139	2553229	44.27%	5.415%
2	5.170	294	296	313	rBV	4649251	5127177	88.90%	10.873%
3	6.245	387	390	397	rBV	4791984	5767095	100.00%	12.230%
4	6.347	397	399	402	rVB	5512738	5173847	89.71%	10.972%
5	6.576	416	419	421	rBV	1302898	1346942	23.36%	2.856%
6	6.725	430	432	435	rBV	3312767	4367117	75.72%	9.261%
7	7.147	466	469	471	rBV	3362025	3297413	57.18%	6.993%
8	7.856	529	531	534	rBV	1202276	1552861	26.93%	3.293%
9	8.942	623	626	629	rBV	4948493	4729408	82.01%	10.030%
10	9.342	659	661	664	rBV	703260	603560	10.47%	1.280%
11	9.605	682	684	687	rBV	1317404	1514027	26.25%	3.211%
12	10.062	720	724	725	rBV	120694	136649	2.37%	0.290%
13	10.279	740	743	745	rBV2	55532	86274	1.50%	0.183%
14	10.393	751	753	756	rBV2	1644619	2386888	41.39%	5.062%
15	10.531	763	765	769	rVB	167022	190874	3.31%	0.405%
16	10.976	802	804	805	rBV	123302	109963	1.91%	0.233%
17	11.091	811	814	816	rBV	1042953	1287428	22.32%	2.730%
18	11.399	839	841	844	rVB	69900	60689	1.05%	0.129%
19	11.639	861	862	866	rBV2	71659	78076	1.35%	0.166%
20	12.291	917	919	922	rBV	101203	94259	1.63%	0.200%
21	12.508	936	938	941	rBV2	147889	203964	3.54%	0.433%
22	12.668	950	952	955	rBV	2809943	3019599	52.36%	6.404%
23	13.217	997	1000	1002	rBV	67981	74864	1.30%	0.159%
24	13.605	1029	1034	1041	rBV3	87495	248353	4.31%	0.527%
25	13.708	1041	1043	1046	rBV	1022672	1245680	21.60%	2.642%
26	14.200	1082	1086	1088	rBV3	29520	60205	1.04%	0.128%
27	14.565	1116	1118	1121	rBV2	78032	111444	1.93%	0.236%
28	14.714	1128	1131	1136	rBV	49962	97788	1.70%	0.207%
29	14.794	1136	1138	1140	rBV2	43257	63268	1.10%	0.134%
30	14.851	1140	1143	1146	rBV4	31989	77846	1.35%	0.165%
31	15.068	1159	1162	1164	rBV	1055546	1167156	20.24%	2.475%
32	15.103	1164	1165	1168	rVB	48321	64958	1.13%	0.138%
33	15.468	1195	1197	1201	rVB	59827	79830	1.38%	0.169%
34	15.571	1201	1206	1210	rBV6	31399	101437	1.76%	0.215%

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ClientSampleId :
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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.880	1231	1233	1238	rVB2	36228	74267	1.29%	0.157%
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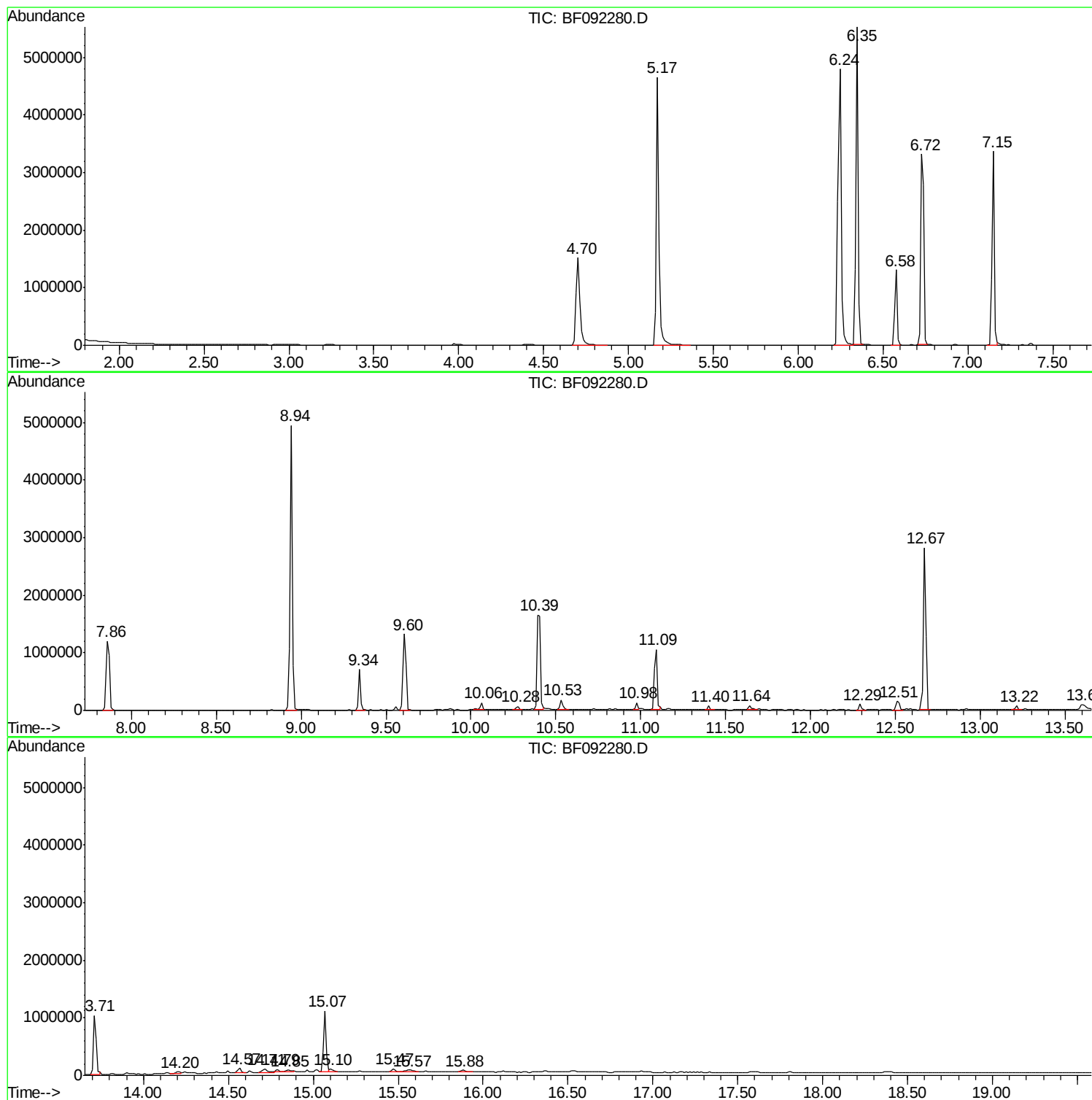
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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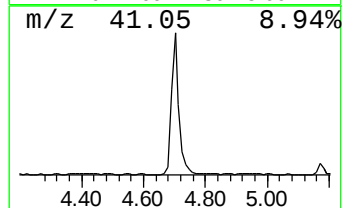
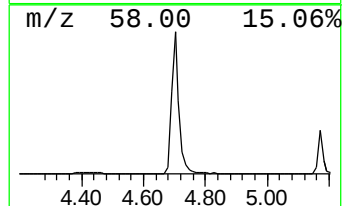
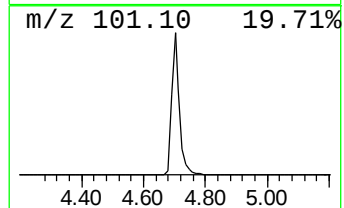
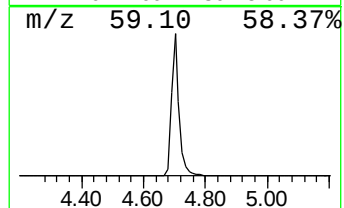
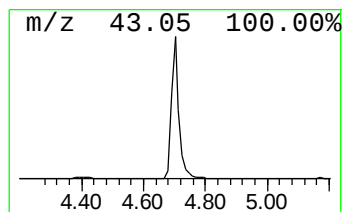
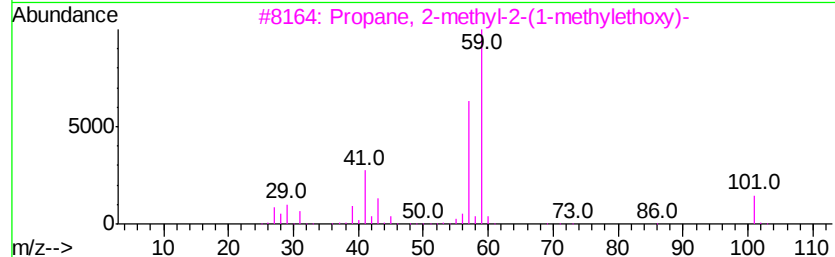
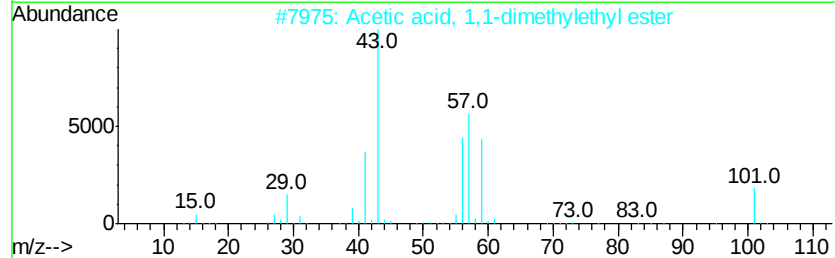
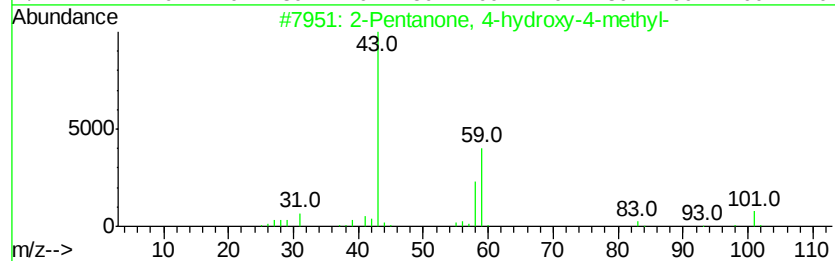
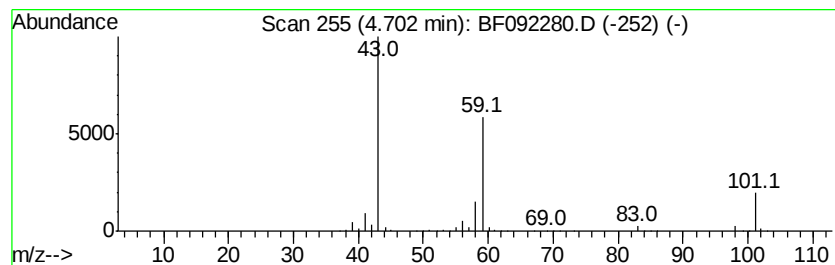
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	37.91 ng	2553230	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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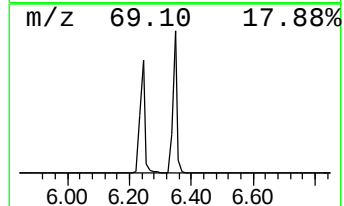
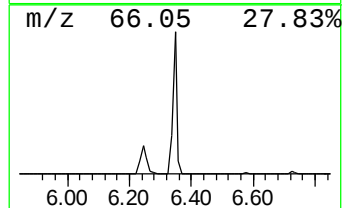
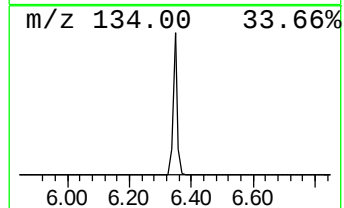
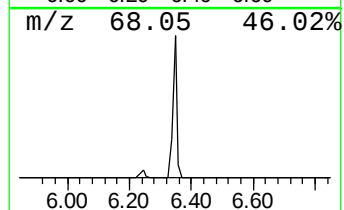
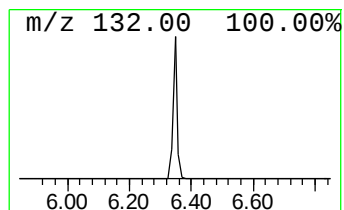
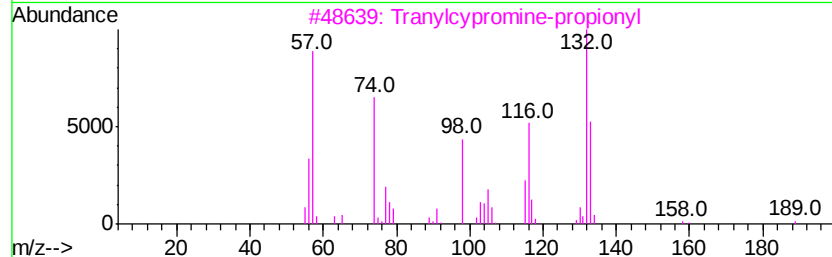
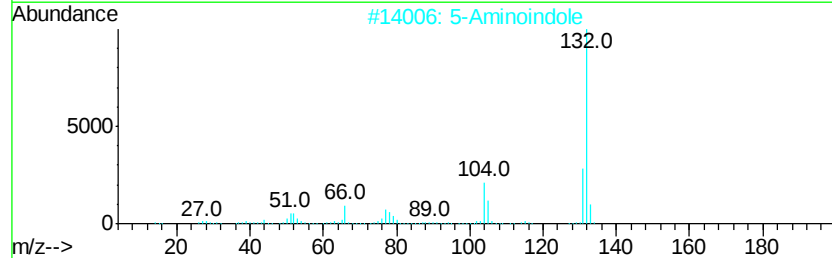
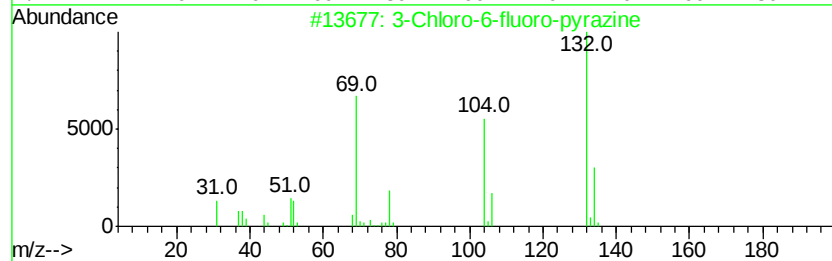
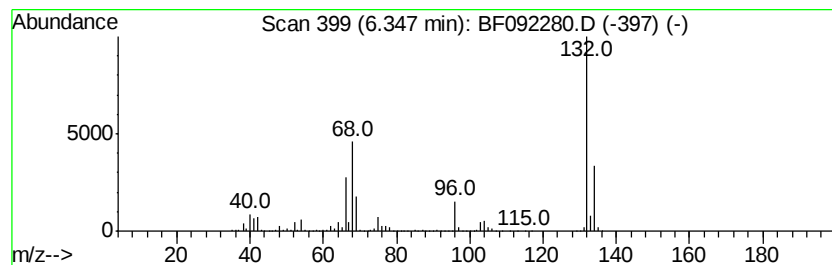
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	76.82 ng	5173850	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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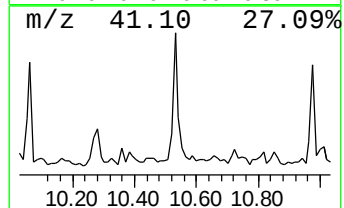
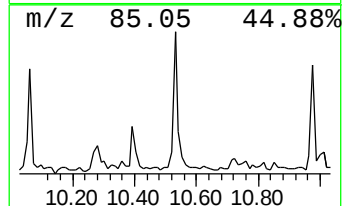
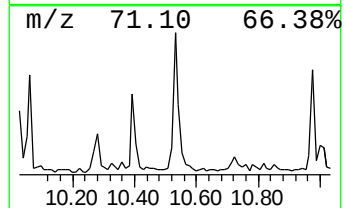
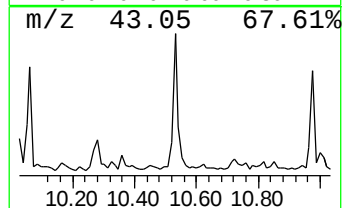
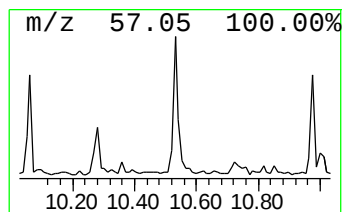
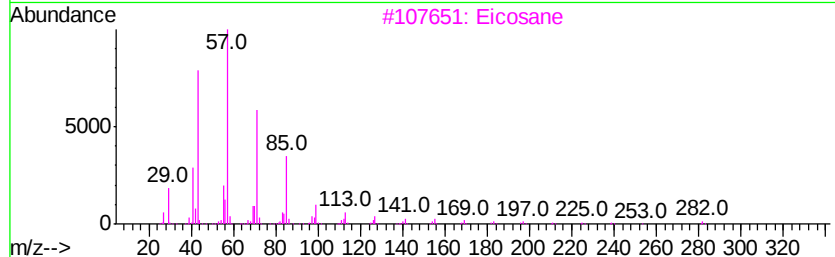
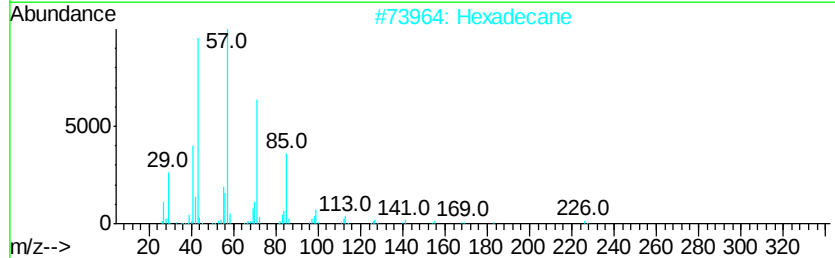
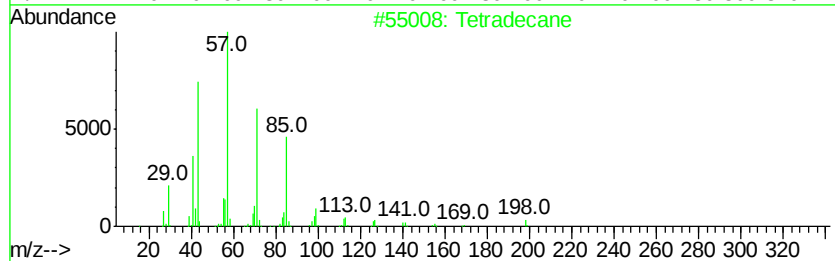
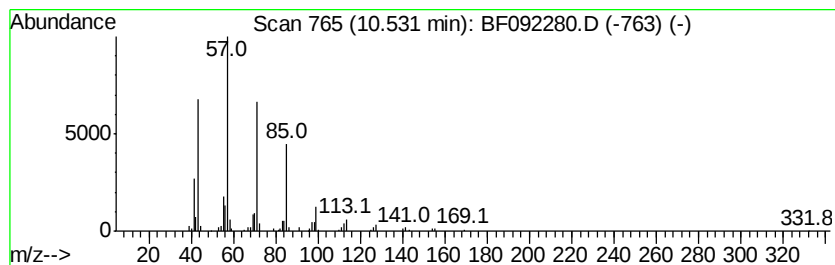
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	2.97 ng	190874	Phenanthrene-d10	11.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	86
2		Hexadecane	226	C16H34	000544-76-3	72
3		Eicosane	282	C20H42	000112-95-8	59
4		Tridecane	184	C13H28	000629-50-5	59
5		Heptacosane	380	C27H56	000593-49-7	53



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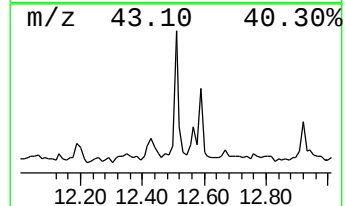
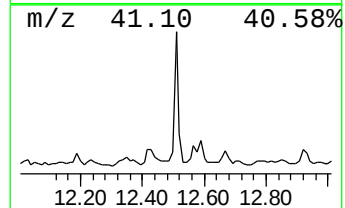
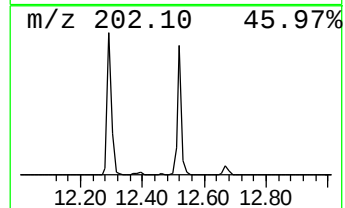
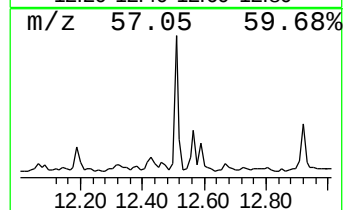
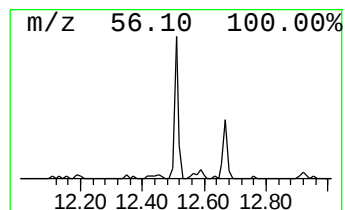
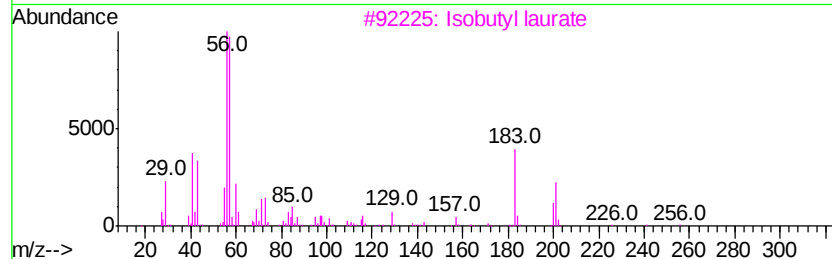
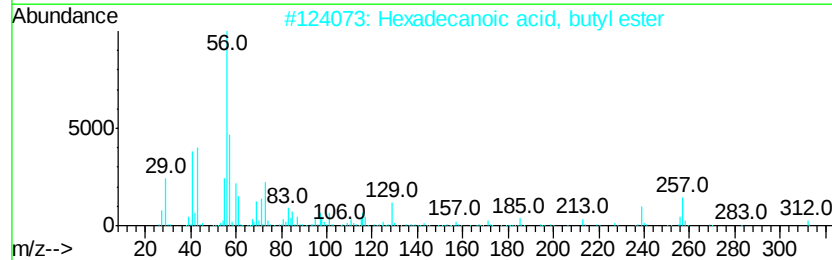
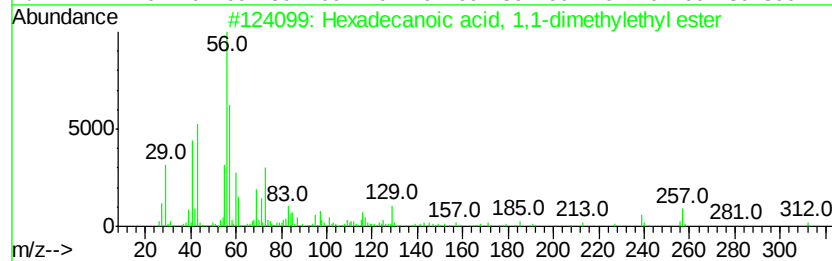
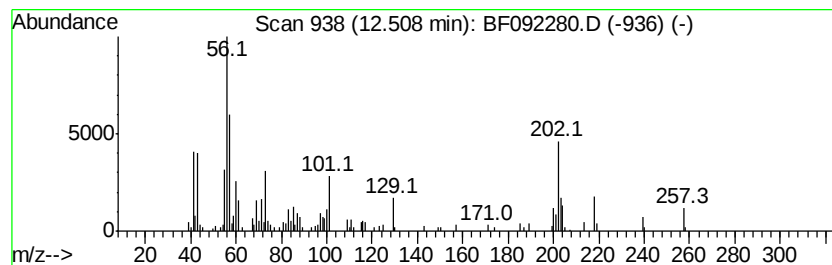
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.51 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	3.27 ng	203964	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
3		Isobutyl laurate	256	C16H32O2	037811-72-6	38
4		Dodecanoic acid tert-butyl ester	256	C16H32O2	007143-18-2	32
5		n-Butyl laurate	256	C16H32O2	000106-18-3	27



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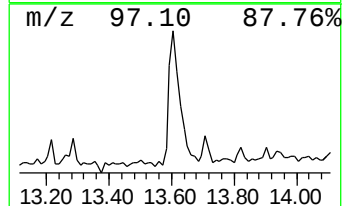
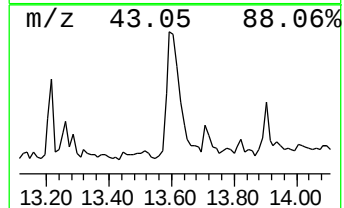
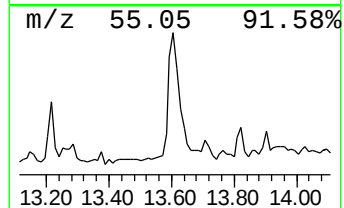
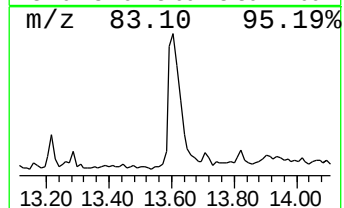
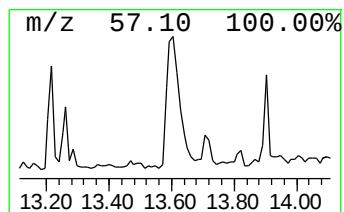
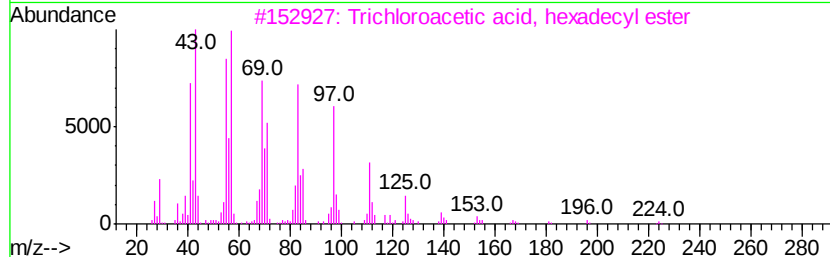
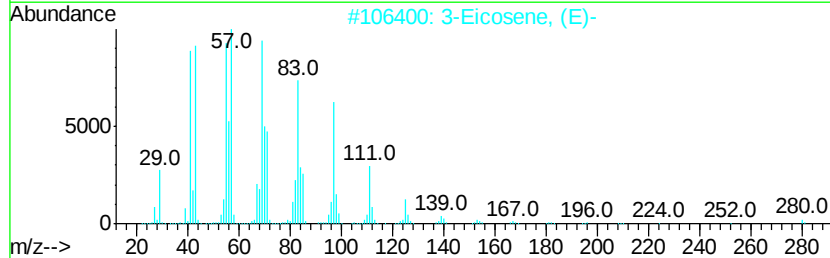
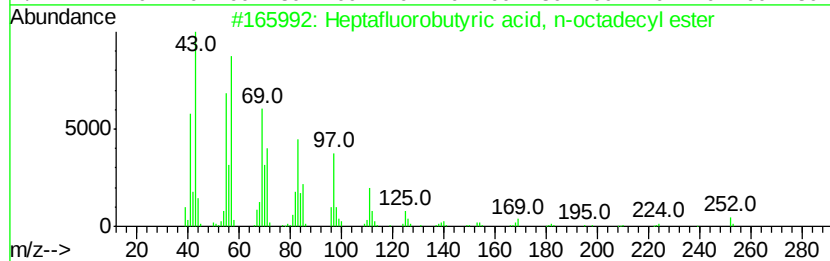
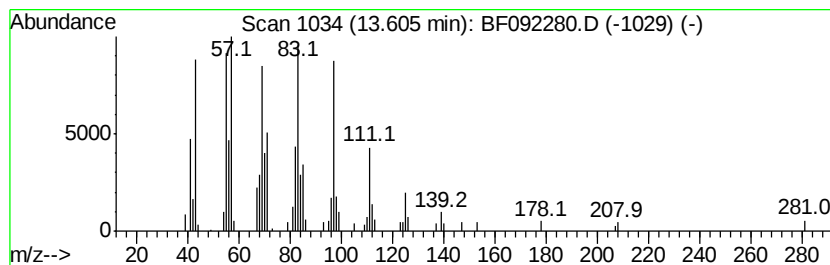
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	3.99 ng	248353	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



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ClientSampleId :
SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	37.9	ng	2553230	1	6.58	1346940	20.0
unknown6.35	6.35	76.8	ng	5173850	1	6.58	1346940	20.0
Tetradecane	10.53	3.0	ng	190874	4	11.09	1287430	20.0
unknown12.51	12.51	3.3	ng	203964	5	13.71	1245680	20.0
Heptafluorobutyri...	13.61	4.0	ng	248353	5	13.71	1245680	20.0