

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
 Data File : BF104673.D
 Acq On : 20 Apr 2018 14:48
 Operator : JU/SJ
 Sample : J2460-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MDP-B-1-0-6

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-BF040618.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	5.004	492	496	506	rBV	58486	75684	4.48%	0.443%
2	5.422	562	567	580	rBV	1650500	1690281	100.00%	9.903%
3	6.439	735	740	756	rBV	1731944	1564742	92.57%	9.168%
4	6.575	759	763	766	rBV	1915783	1689446	99.95%	9.898%
5	6.804	798	802	805	rBV	757304	606192	35.86%	3.552%
6	6.957	824	828	832	rBV	1626295	1362387	80.60%	7.982%
7	7.369	893	898	901	rBV	1015703	950403	56.23%	5.568%
8	8.086	1017	1020	1025	rBV	856801	690563	40.85%	4.046%
9	8.669	1116	1119	1123	rBV	28357	24499	1.45%	0.144%
10	9.163	1199	1203	1213	rBV	1710949	1588265	93.96%	9.306%
11	9.233	1213	1215	1218	rVB	37210	31474	1.86%	0.184%
12	9.557	1266	1270	1278	rVB	98215	100644	5.95%	0.590%
13	9.763	1300	1305	1310	rVB	43713	40996	2.43%	0.240%
14	9.839	1315	1318	1322	rVV	744061	671552	39.73%	3.935%
15	9.874	1322	1324	1327	rVB	23172	20645	1.22%	0.121%
16	10.045	1348	1353	1357	rBV3	16747	22729	1.34%	0.133%
17	10.239	1383	1386	1388	rBV	15561	19199	1.14%	0.112%
18	10.269	1388	1391	1393	rVB	50296	43957	2.60%	0.258%
19	10.480	1424	1427	1433	rVB4	15918	22162	1.31%	0.130%
20	10.633	1449	1453	1463	rVB	937092	893560	52.86%	5.235%
21	10.739	1468	1471	1479	rVB	42908	53650	3.17%	0.314%
22	11.221	1549	1553	1557	rVB3	18920	35352	2.09%	0.207%
23	11.327	1568	1571	1574	rBV	688311	628452	37.18%	3.682%
24	11.351	1574	1575	1582	rVB	107365	81053	4.80%	0.475%
25	11.663	1625	1628	1633	rBV	19840	22325	1.32%	0.131%
26	11.851	1653	1660	1664	rBV4	52106	87917	5.20%	0.515%
27	11.945	1672	1676	1678	rBV2	29548	33855	2.00%	0.198%
28	12.063	1694	1696	1699	rBV	23451	19270	1.14%	0.113%
29	12.127	1705	1707	1709	rBV3	21406	23956	1.42%	0.140%
30	12.157	1710	1712	1716	rVB2	24807	27833	1.65%	0.163%
31	12.257	1727	1729	1731	rBV	38262	34192	2.02%	0.200%
32	12.304	1735	1737	1739	rBV2	34848	31872	1.89%	0.187%
33	12.380	1747	1750	1752	rBV	45380	43866	2.60%	0.257%
34	12.545	1775	1778	1781	rBV	91995	95012	5.62%	0.557%

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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	12.727	1805	1809	1812	rVB	887793	763898	45.19%	4.476%
36	12.774	1814	1817	1824	rVB	104773	137198	8.12%	0.804%
37	12.915	1837	1841	1848	rVB	1580162	1414687	83.70%	8.289%
38	13.774	1984	1987	1991	rBV	112857	132270	7.83%	0.775%
39	13.974	2018	2021	2024	rBV	663659	569052	33.67%	3.334%
40	14.604	2126	2128	2132	rVB	177877	147507	8.73%	0.864%
41	15.445	2268	2271	2278	rVB	442094	575316	34.04%	3.371%

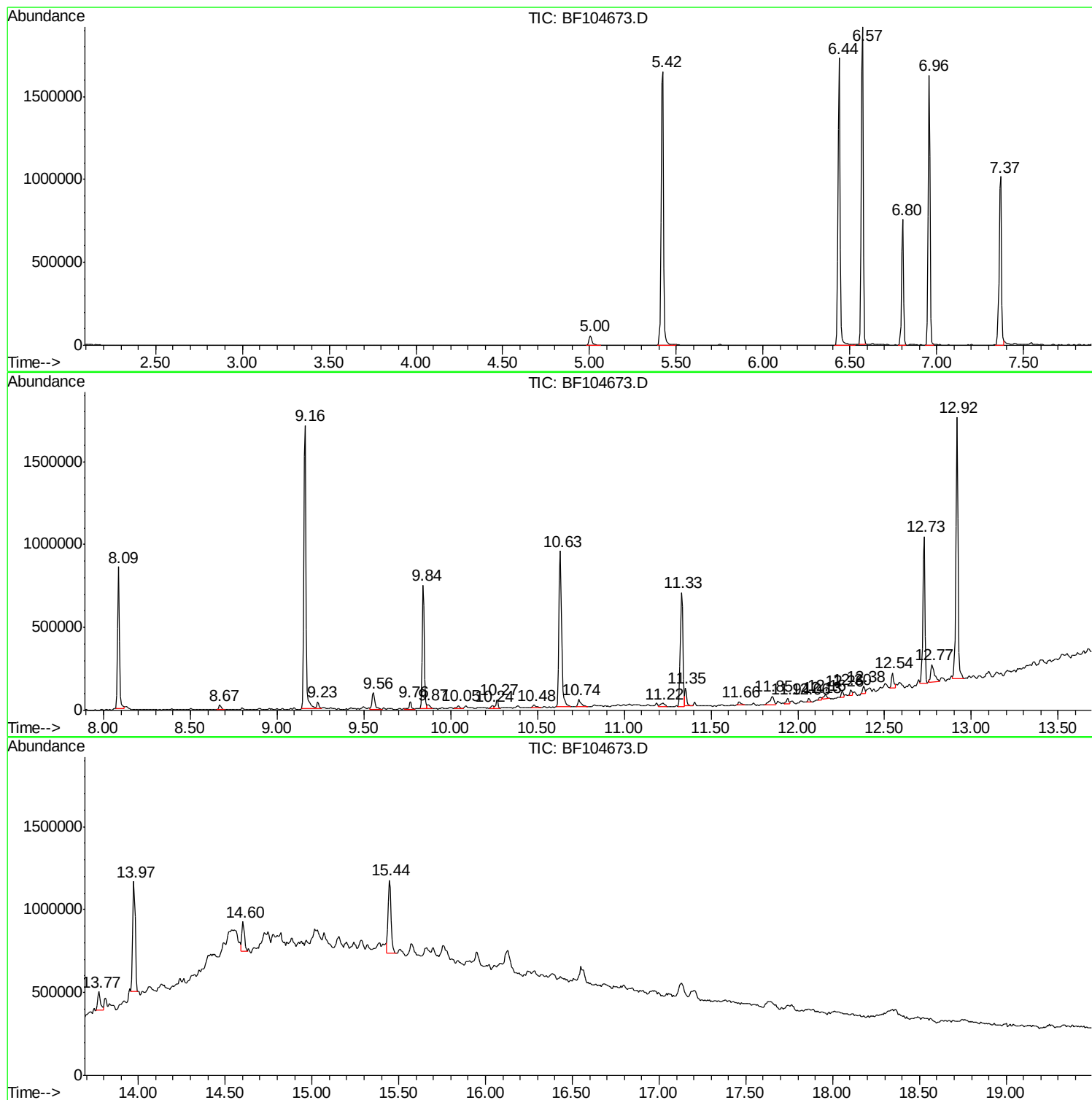
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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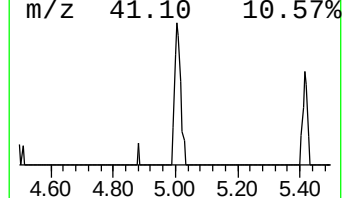
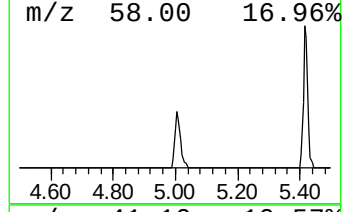
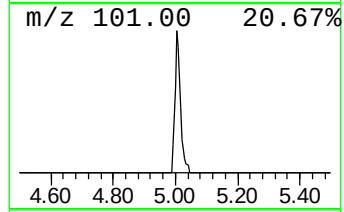
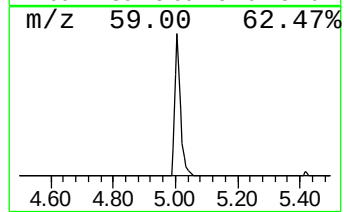
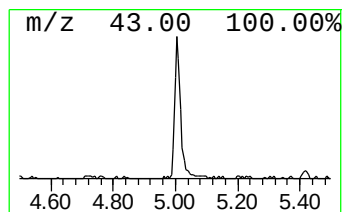
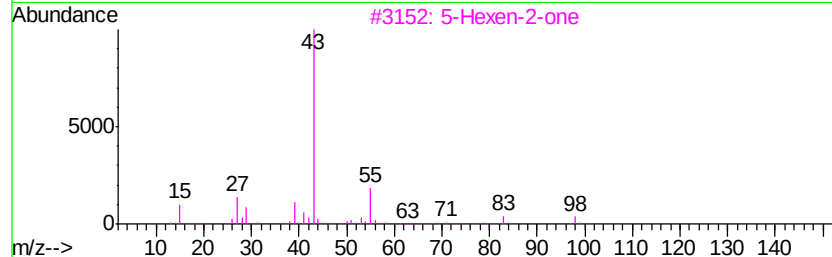
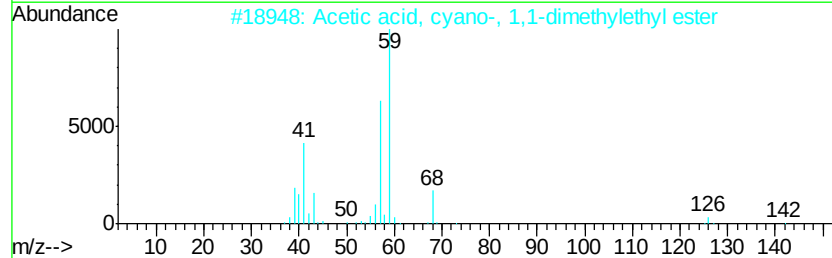
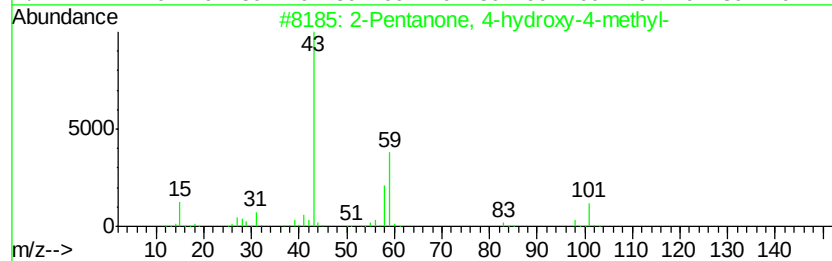
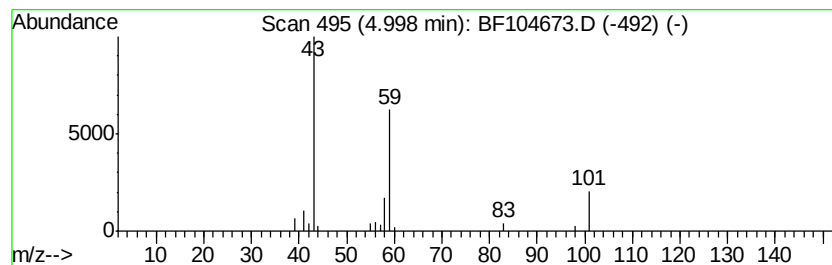
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.50 ng	75684	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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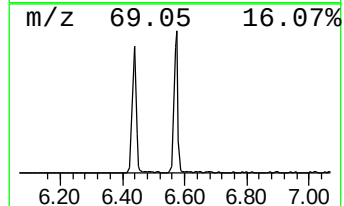
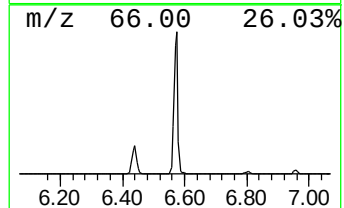
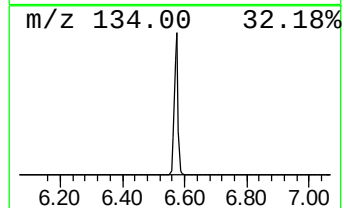
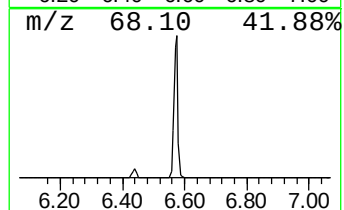
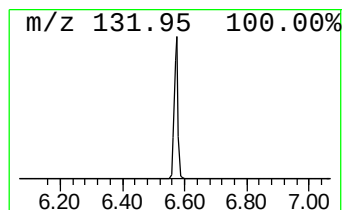
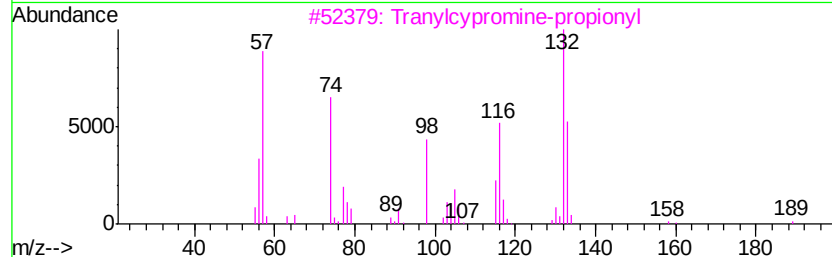
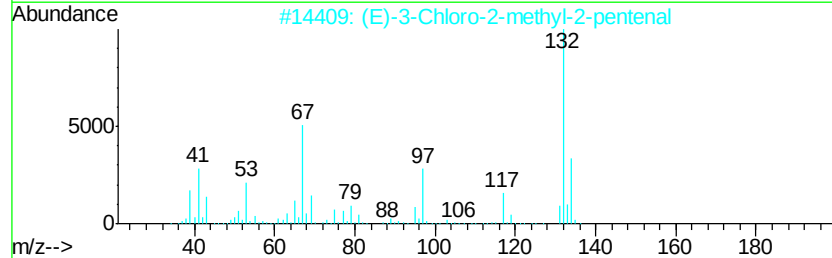
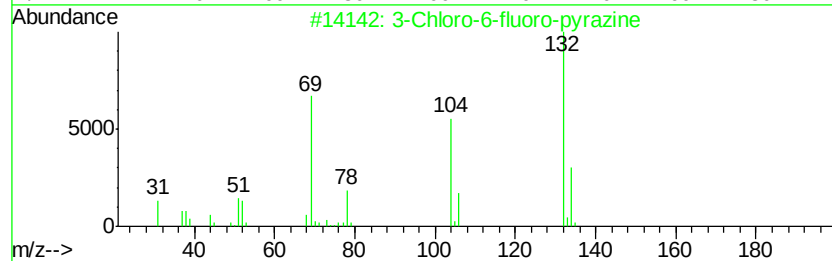
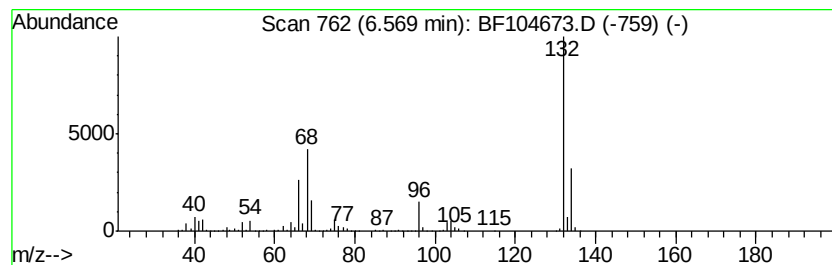
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	55.74 ng	1689450	1,4-Dichlorobenzene-d4	6.80

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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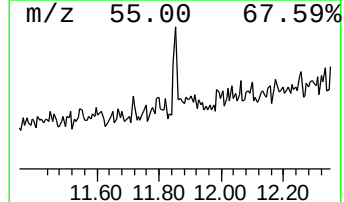
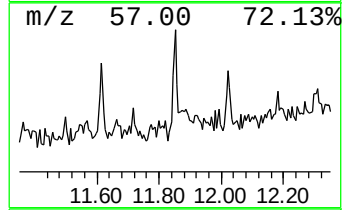
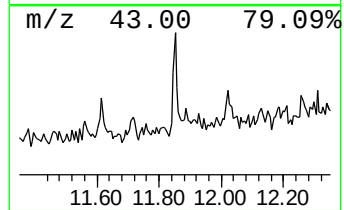
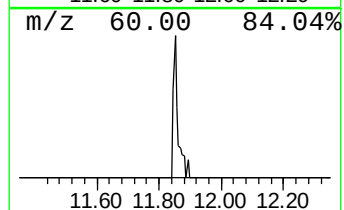
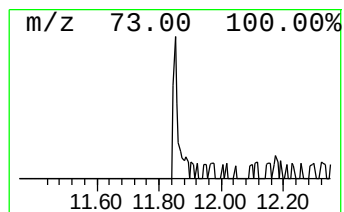
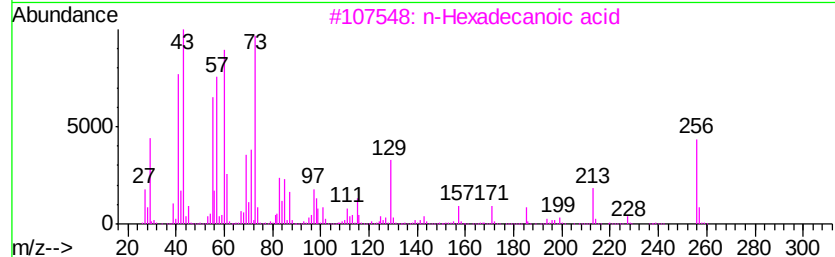
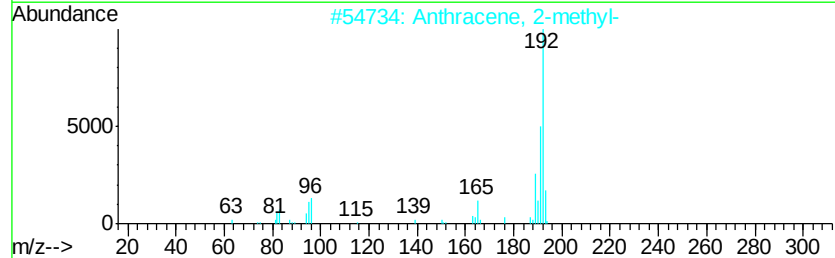
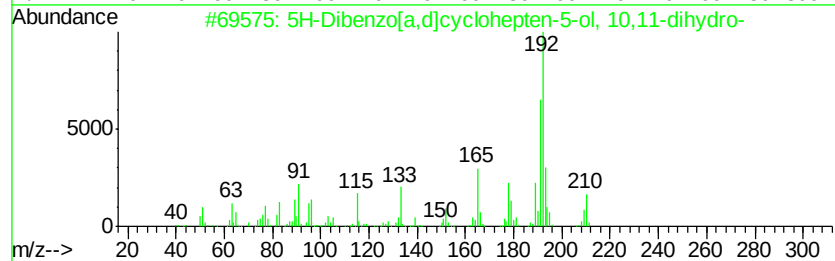
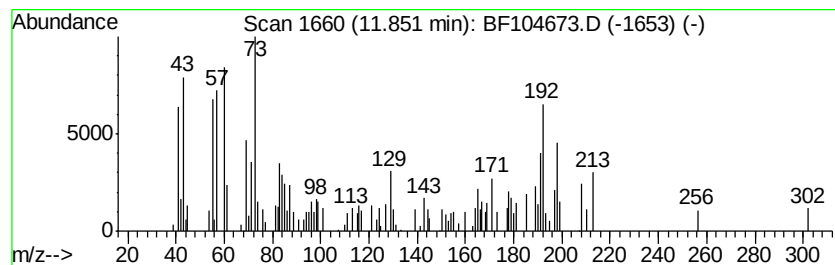
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.85 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.80 ng	87917	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cyclohepten-5-ol,...	210	C15H14O	001210-34-0	48
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	25
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	20
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	15
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	15



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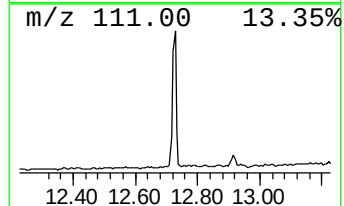
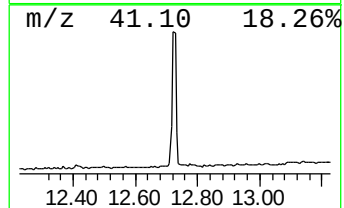
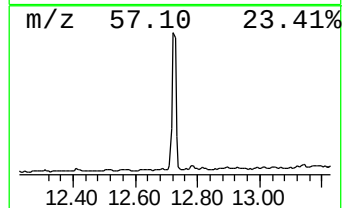
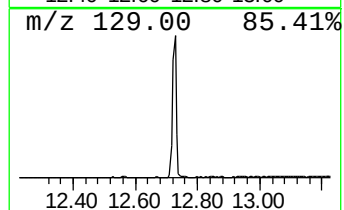
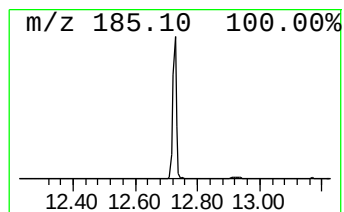
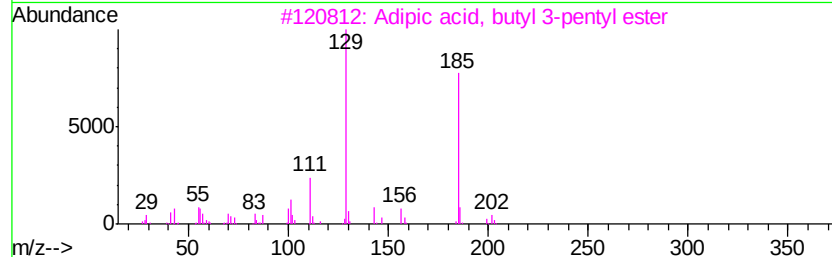
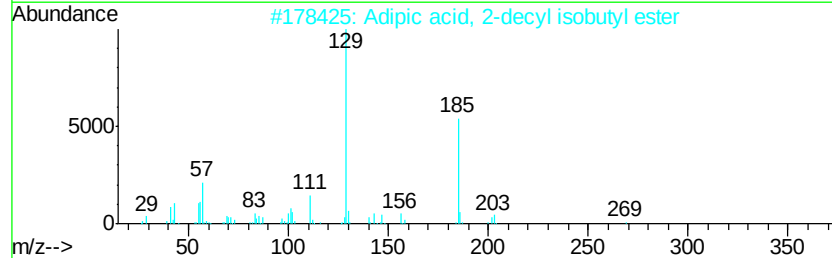
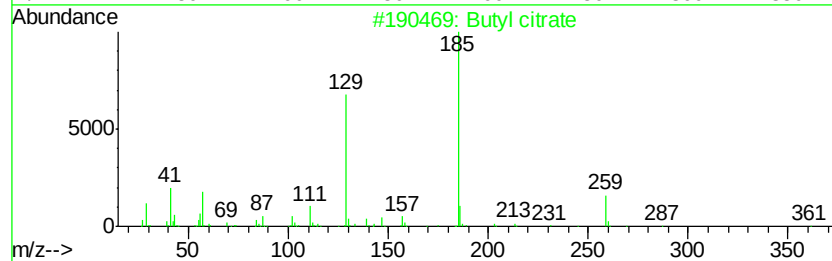
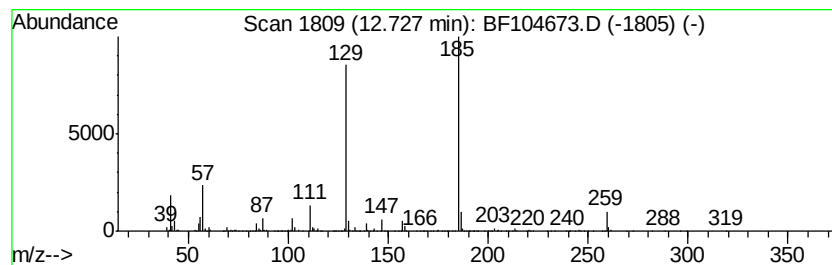
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	26.85 ng	763898	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Adipic acid, 2-decyl isobutyl ester	342 C20H38O4	1000353-59-6	64
3	Adipic acid, butyl 3-pentyl ester	272 C15H28O4	1000324-60-5	64
4	Adipic acid, isobutyl 4-methylpe...	286 C16H30O4	1000353-50-1	56
5	Adipic acid, 3,3-dimethylbut-2-y...	286 C16H30O4	1000353-66-7	56



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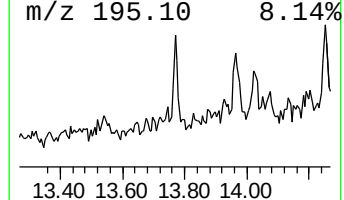
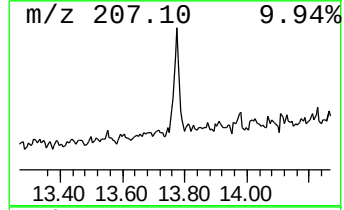
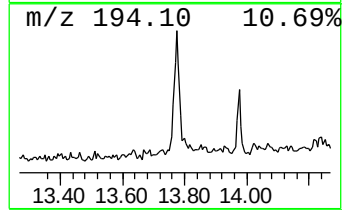
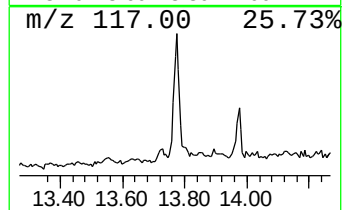
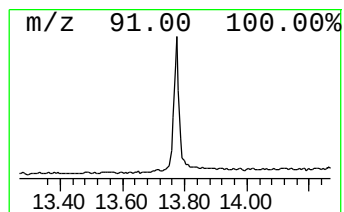
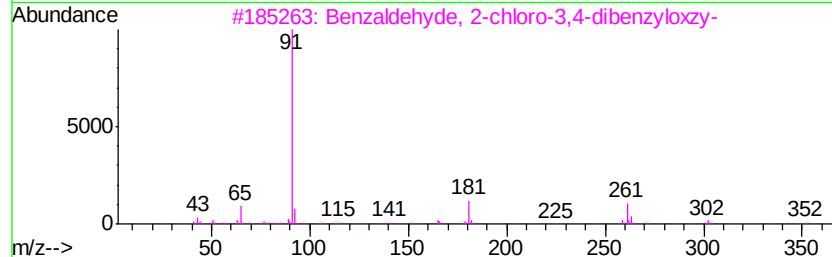
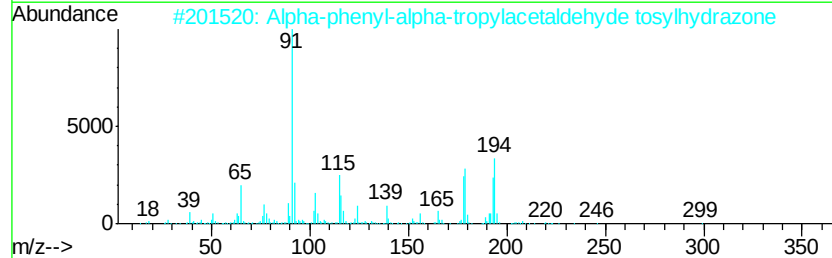
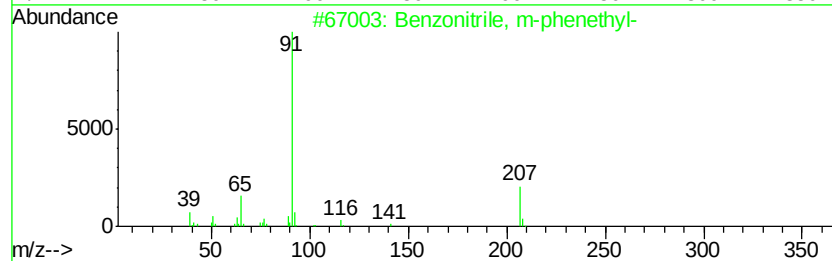
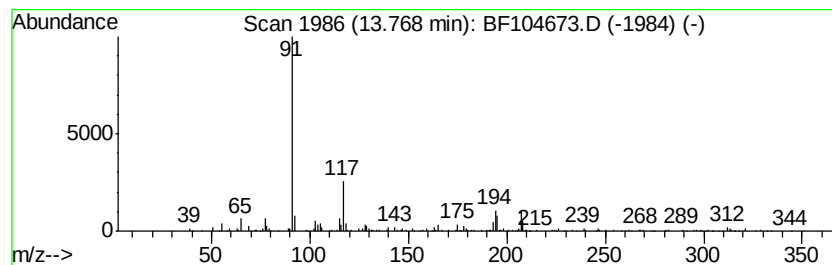
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 unknown13.77 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.65 ng	132270	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	27
2		Alpha-phenyl-alpha-trotylacetalde...	378	C22H22N2O2S	022532-16-7	14
3		Benzaldehyde, 2-chloro-3,4-diben...	352	C21H17ClO3	037687-59-5	10
4		Coumarin, 6-benzoyloxy-3,4-dihydr...	282	C18H18O3	084945-10-8	10
5		4H-1-Benzopyran-4-one, 2,3-dihyd...	254	C16H14O3	1000319-40-1	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
Data File : BF104673.D
Acq On : 20 Apr 2018 14:48
Operator : JU/SJ
Sample : J2460-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-1-0-6

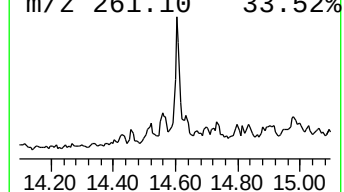
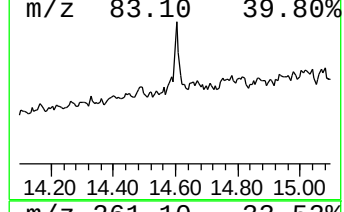
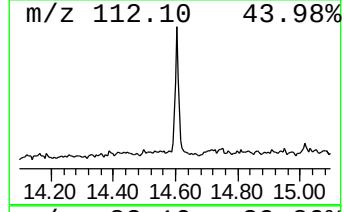
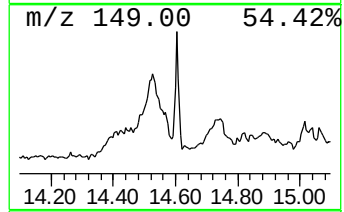
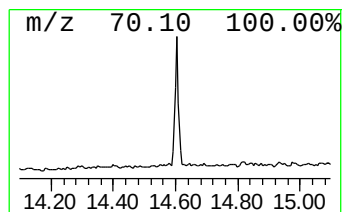
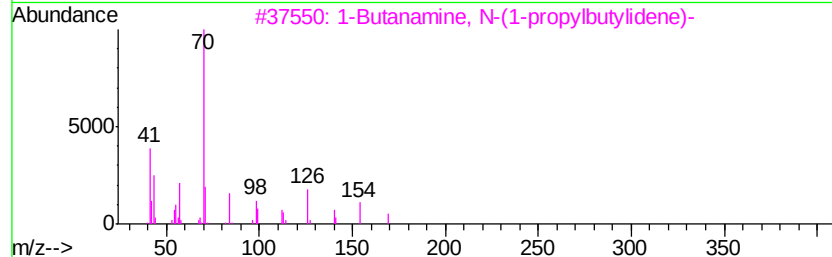
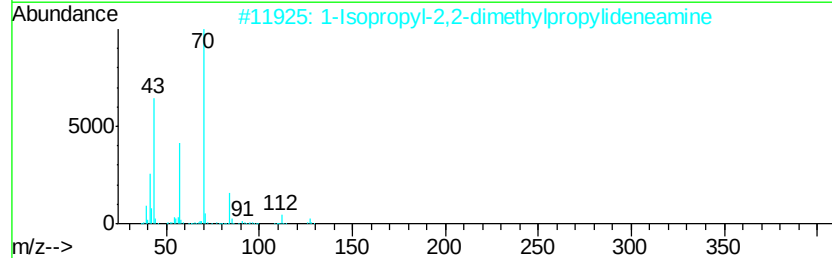
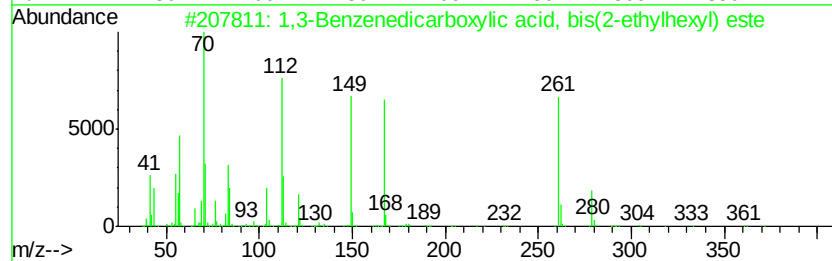
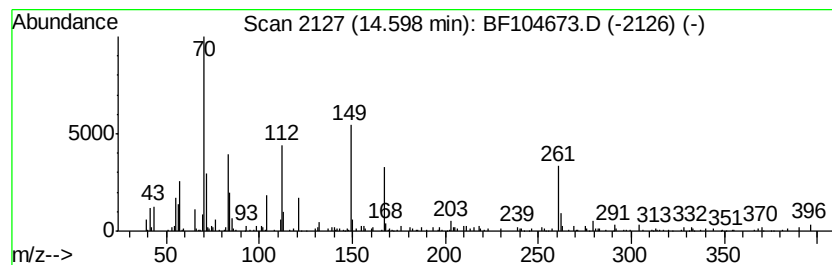
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	5.18 ng	147507	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2		1-Isopropyl-2,2-dimethylpropylid...	127	C8H17N	1000210-05-3	22
3		1-Butanamine, N-(1-propylbutylid...	169	C11H23N	010599-80-1	12
4		Di(E)-hex-3-enyl phthalate	330	C20H26O4	1000373-64-8	11
5		Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
Data File : BF104673.D
Acq On : 20 Apr 2018 14:48
Operator : JU/SJ
Sample : J2460-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-1-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	2.5	ng	75684	1	6.80	606192	20.0
unknown6.57	6.57	55.7	ng	1689450	1	6.80	606192	20.0
unknown11.85	11.85	2.8	ng	87917	4	11.33	628452	20.0
Butyl citrate	12.73	26.9	ng	763898	5	13.97	569052	20.0
unknown13.77	13.77	4.7	ng	132270	5	13.97	569052	20.0
1,3-Benzenedicarb...	14.60	5.2	ng	147507	5	13.97	569052	20.0