

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
 Data File : BF098842.D
 Acq On : 26 Sep 2017 19:50
 Operator : SJ/JU
 Sample : I5321-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20170530-LOC-6

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-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	2.193	14	18	29	rVB	200072	273765	5.89%	0.839%
2	5.134	515	518	529	rVB	180019	204929	4.41%	0.628%
3	5.528	581	585	588	rBV	2271743	2078139	44.71%	6.371%
4	6.533	751	756	759	rBV	1727486	1481043	31.86%	4.540%
5	6.681	776	781	785	rBV	3337755	3491864	75.12%	10.705%
6	6.916	817	821	824	rBV	1001369	900303	19.37%	2.760%
7	6.969	826	830	833	rBV	54671	48694	1.05%	0.149%
8	7.069	843	847	851	rBV	3134314	3136120	67.47%	9.614%
9	7.480	911	917	919	rBV	2365044	2627749	56.53%	8.056%
10	8.192	1034	1038	1042	rVB	1356811	1252183	26.94%	3.839%
11	9.274	1216	1222	1225	rBV	4498499	4648101	100.00%	14.250%
12	9.657	1284	1287	1291	rBV	254031	202762	4.36%	0.622%
13	9.951	1333	1337	1341	rBV	1624972	1385054	29.80%	4.246%
14	10.374	1403	1409	1411	rVB2	53640	62817	1.35%	0.193%
15	10.739	1466	1471	1475	rBV	2301003	2468255	53.10%	7.567%
16	10.845	1486	1489	1494	rBV	73721	84225	1.81%	0.258%
17	11.439	1586	1590	1593	rBV	1593590	1336629	28.76%	4.098%
18	11.815	1651	1654	1657	rVB	85519	63735	1.37%	0.195%
19	12.827	1822	1826	1829	rBV	449185	371575	7.99%	1.139%
20	13.027	1854	1860	1863	rBV	3753431	3845029	82.72%	11.788%
21	13.904	2006	2009	2017	rBV	139976	137324	2.95%	0.421%
22	14.074	2034	2038	2042	rVB	1140038	1015420	21.85%	3.113%
23	14.698	2140	2144	2148	rBV	352970	345591	7.44%	1.059%
24	15.568	2286	2292	2301	rBV	780240	980300	21.09%	3.005%
25	16.027	2365	2370	2375	rBV	43568	69250	1.49%	0.212%
26	16.545	2454	2458	2464	rBV	32580	53078	1.14%	0.163%
27	17.162	2559	2563	2571	rVB3	27265	54918	1.18%	0.168%

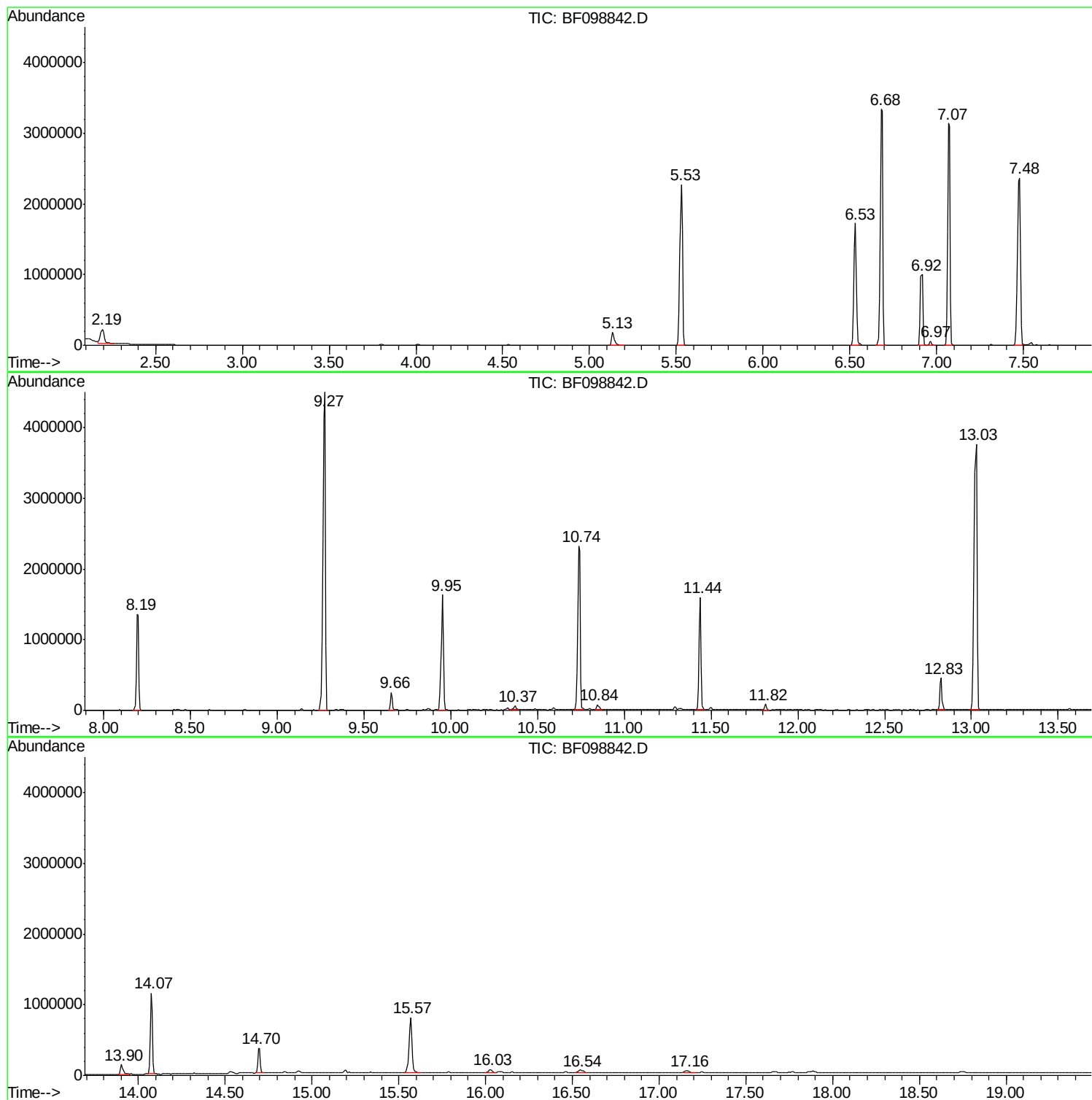
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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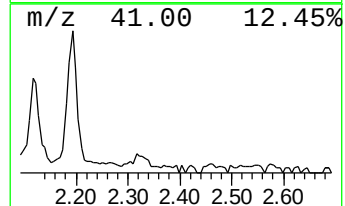
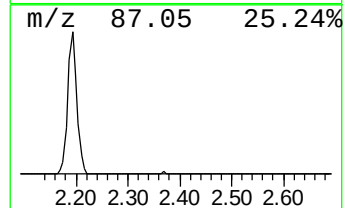
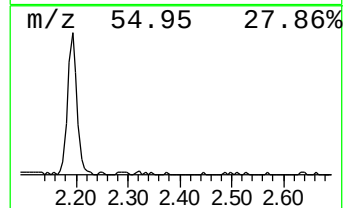
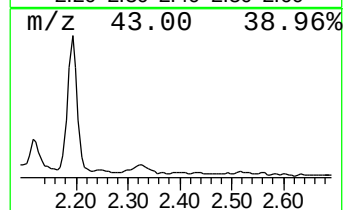
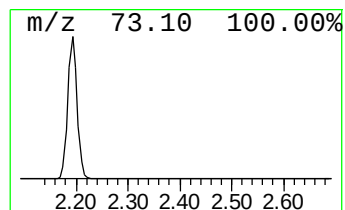
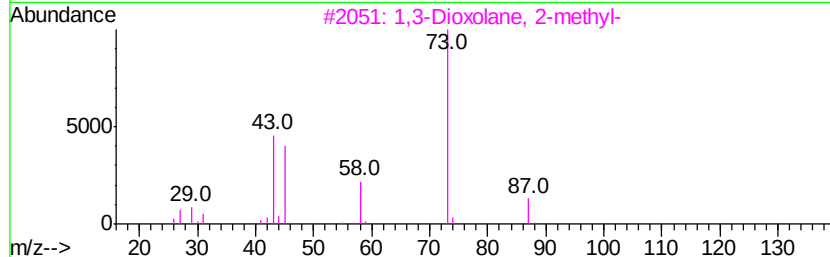
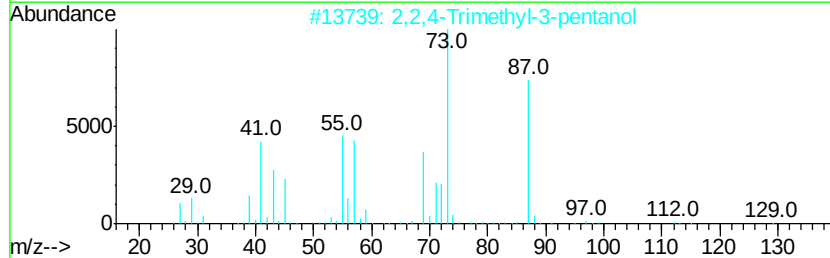
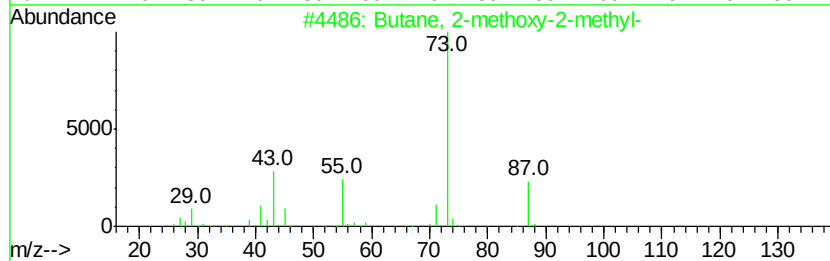
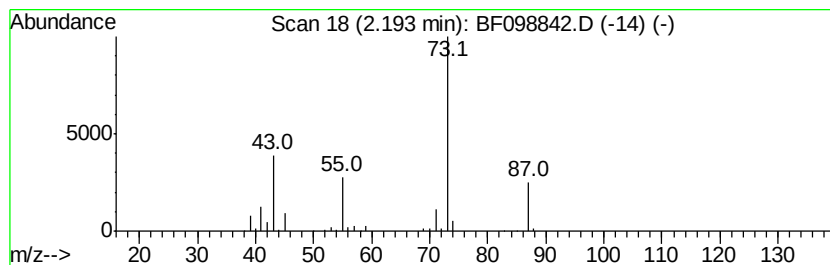
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	6.08 ng	273765	1,4-Dichlorobenzene-d4	6.92

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	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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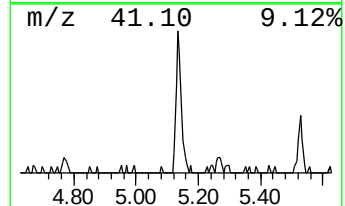
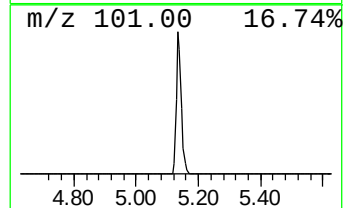
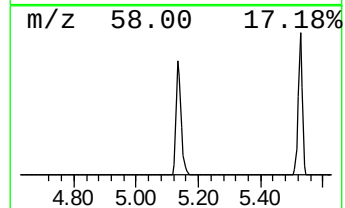
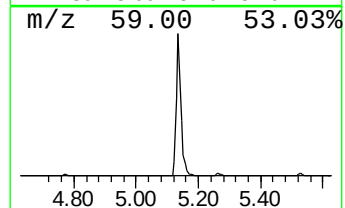
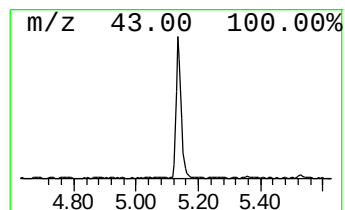
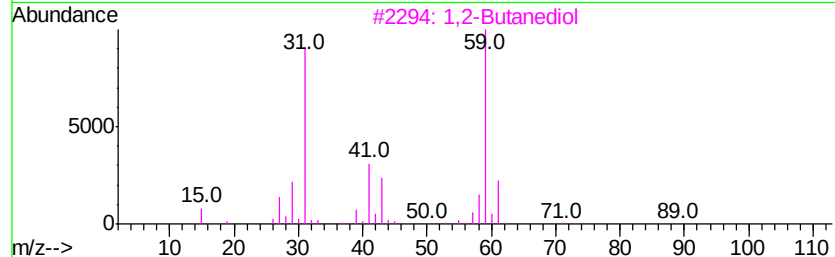
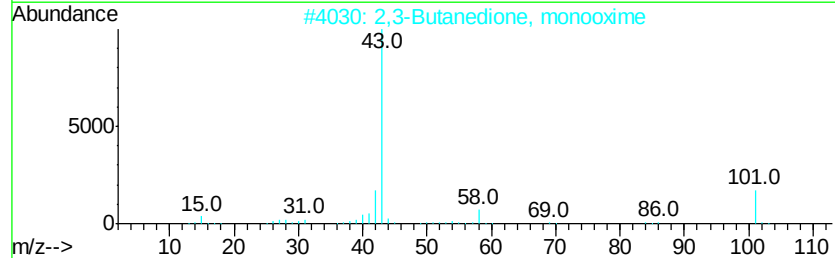
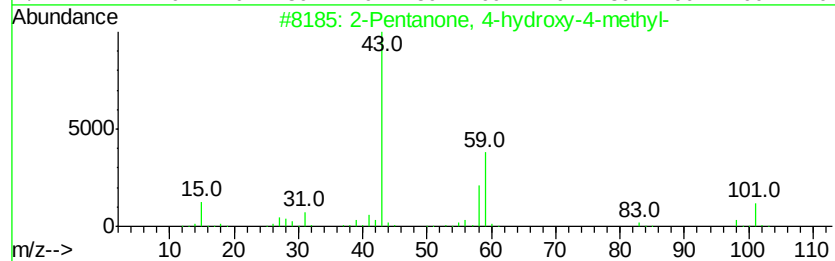
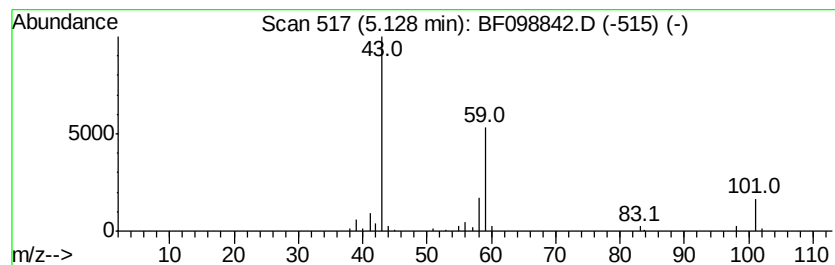
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.55 ng	204929	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		1,2-Butanediol	90	C4H10O2	000584-03-2	9
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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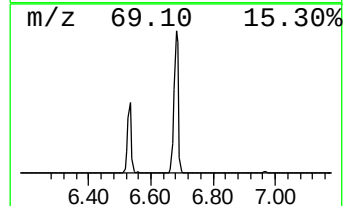
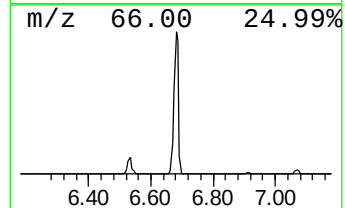
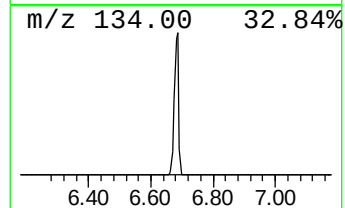
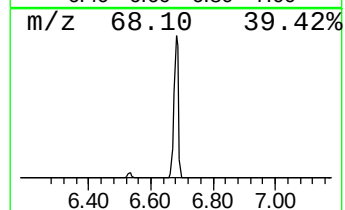
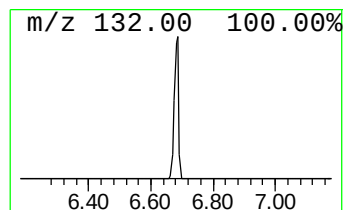
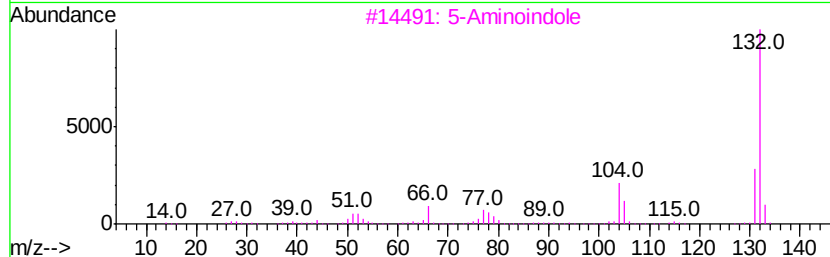
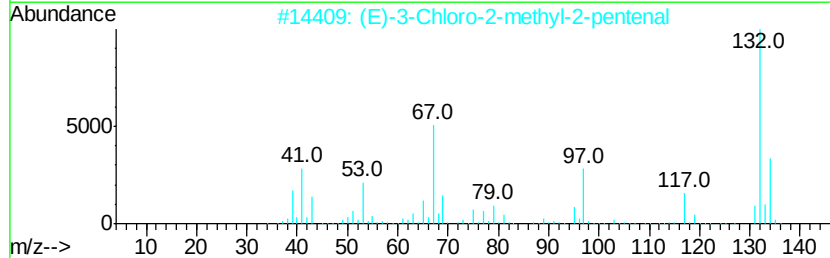
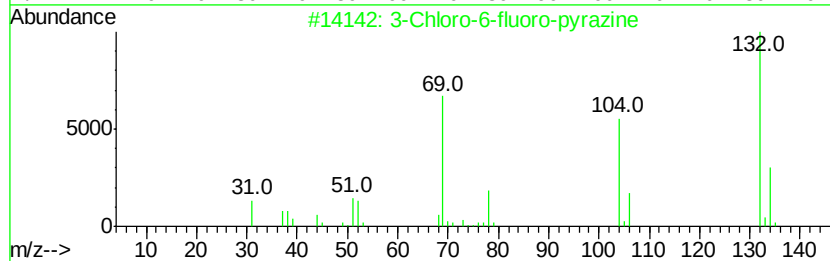
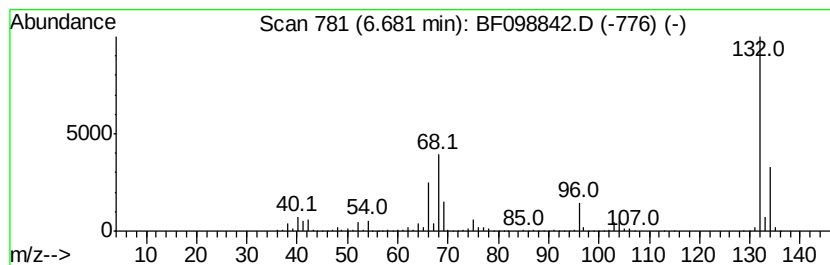
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Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	77.57 ng	3491860	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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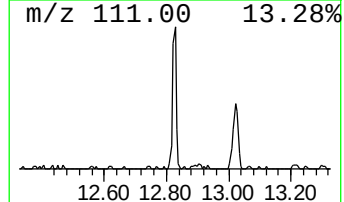
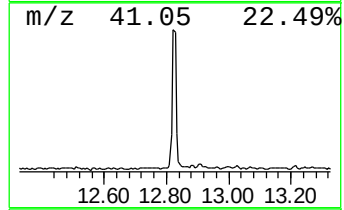
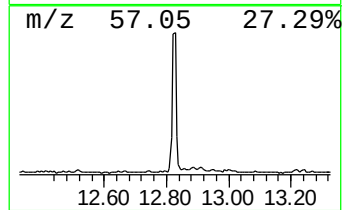
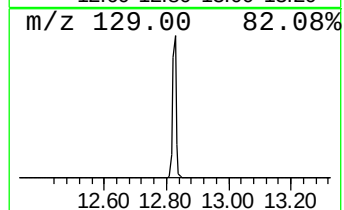
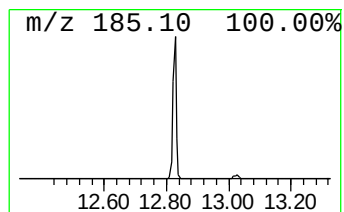
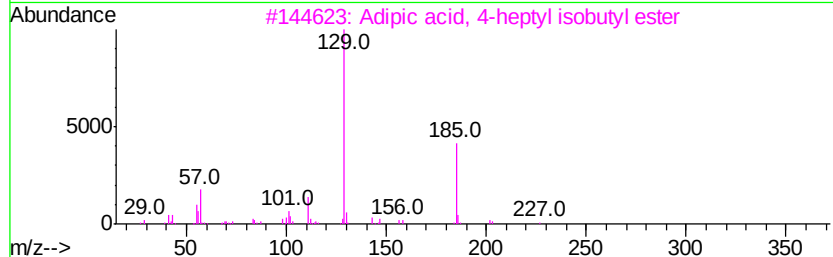
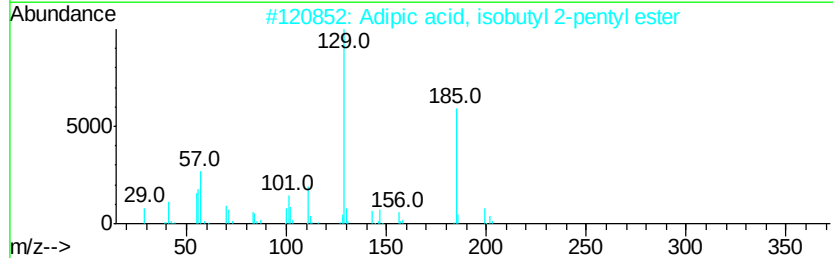
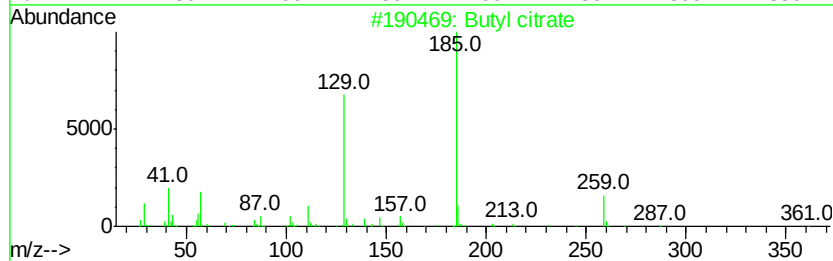
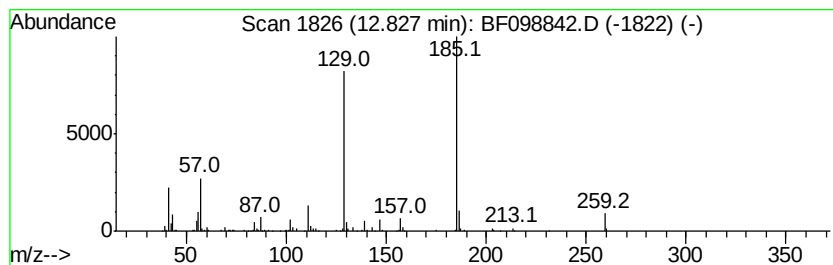
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	7.32 ng	371575	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl citrate	360	C18H32O7	000077-94-1	91
2		Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	56
3		Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	56
4		Dibutyl adipate	258	C14H26O4	000105-99-7	56
5		Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1000353-55-8	42



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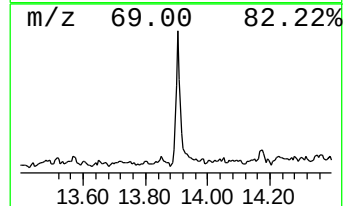
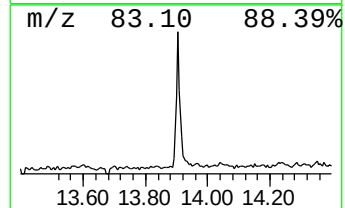
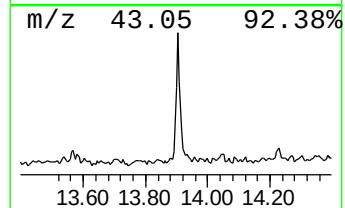
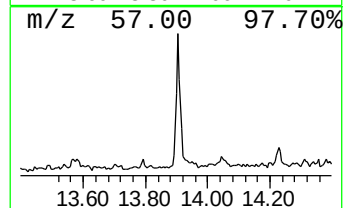
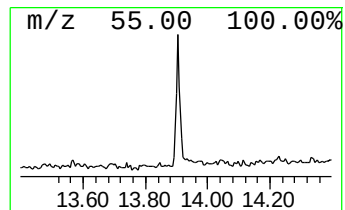
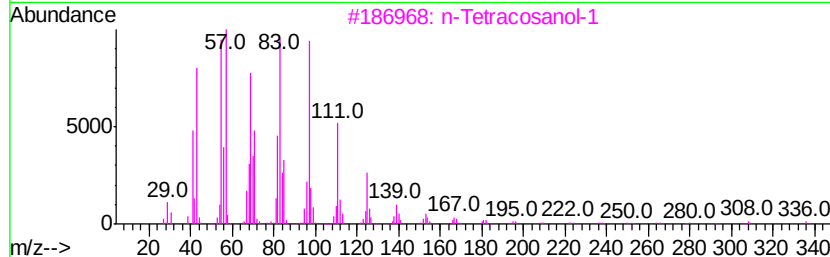
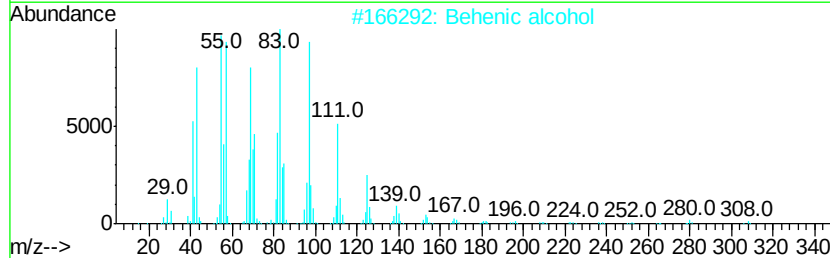
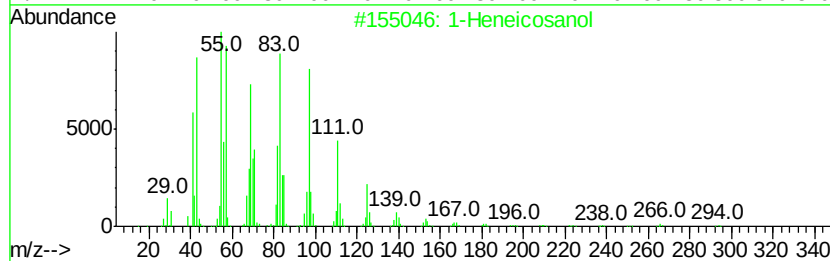
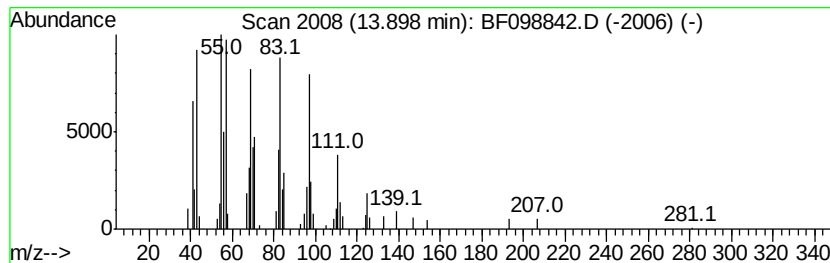
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	2.70 ng	137324	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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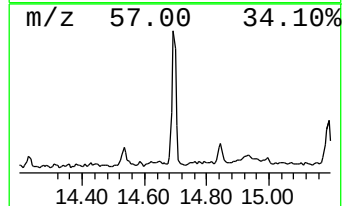
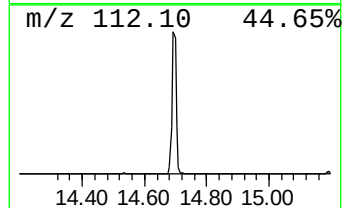
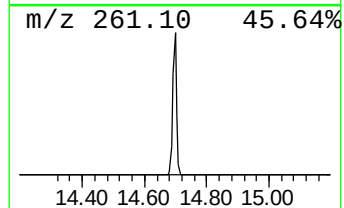
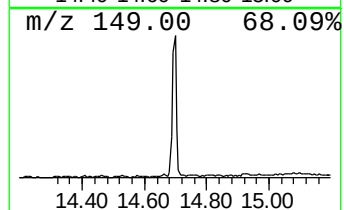
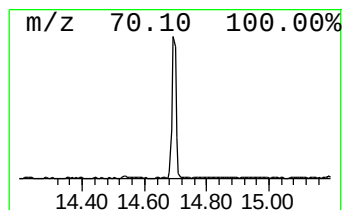
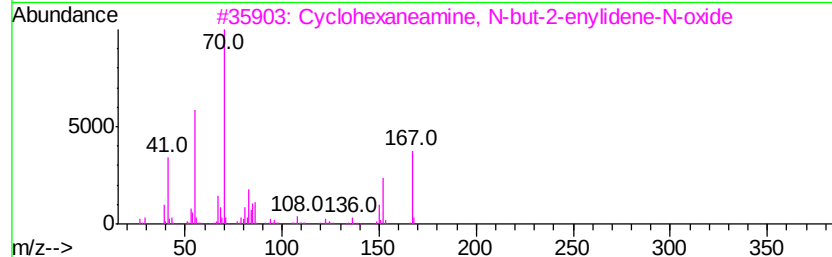
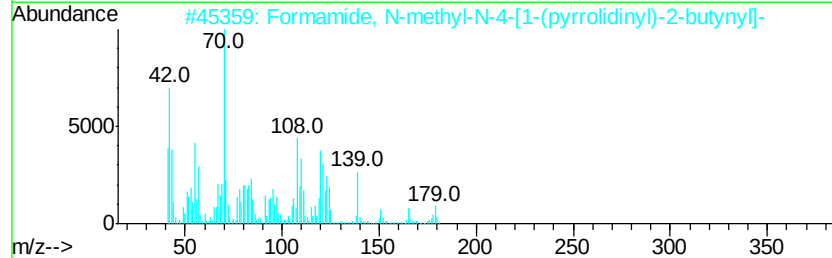
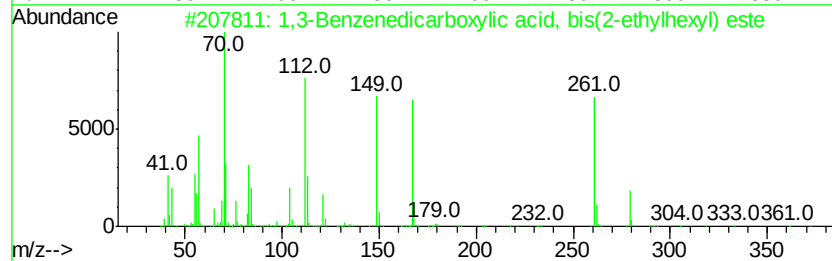
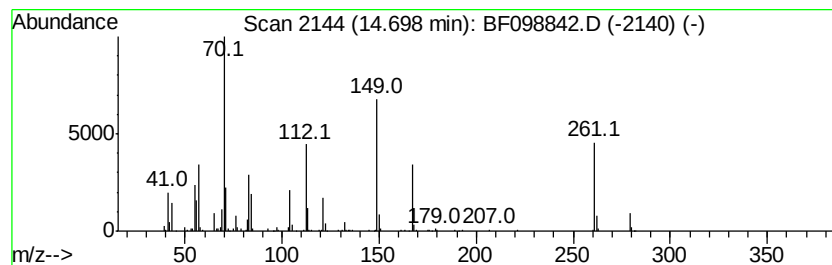
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.70 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	6.81 ng	345591	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2		Formamide, N-methyl-N-4-[1-(pyrr...	180	C10H16N2O	018327-40-7	22
3		Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	22
4		Diisooctyl phthalate	390	C24H38O4	000131-20-4	18
5		Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
Data File : BF098842.D
Acq On : 26 Sep 2017 19:50
Operator : SJ/JU
Sample : I5321-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20170530-LOC-6

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	6.1	ng	273765	1	6.92	900303	20.0
2-Pentanone, 4-hy...	5.13	4.5	ng	204929	1	6.92	900303	20.0
unknown6.68	6.68	77.6	ng	3491860	1	6.92	900303	20.0
Butyl citrate	12.83	7.3	ng	371575	5	14.07	1015420	20.0
1-Heneicosanol	13.90	2.7	ng	137324	5	14.07	1015420	20.0
unknown14.70	14.70	6.8	ng	345591	5	14.07	1015420	20.0