

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081817\
 Data File : BF097850.D
 Acq On : 18 Aug 2017 23:25
 Operator : SJ/JU
 Sample : I4646-06
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-L10-ESW

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-BF081517.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	4.316	375	379	385	rVB	32805	40816	1.98%	0.194%
2	4.957	484	488	495	rVB	254432	300483	14.60%	1.427%
3	5.369	554	558	562	rBV	1911687	1938500	94.19%	9.204%
4	6.398	728	733	739	rBV	2188501	2057970	100.00%	9.771%
5	6.534	752	756	760	rBV	2068915	1955705	95.03%	9.286%
6	6.769	792	796	800	rBV	921275	724089	35.18%	3.438%
7	6.928	819	823	826	rVB	1628603	1423916	69.19%	6.761%
8	7.328	887	891	895	rBV	1262100	1232708	59.90%	5.853%
9	7.416	902	906	910	rVB2	30675	28873	1.40%	0.137%
10	8.051	1010	1014	1018	rBV	1079353	946898	46.01%	4.496%
11	9.128	1193	1197	1201	rBV	2171973	1899519	92.30%	9.019%
12	9.522	1261	1264	1268	rBV	425686	341967	16.62%	1.624%
13	9.804	1308	1312	1316	rBV	1126112	998327	48.51%	4.740%
14	10.222	1378	1383	1385	rBV4	19777	28734	1.40%	0.136%
15	10.245	1385	1387	1390	rVB	53919	40584	1.97%	0.193%
16	10.463	1421	1424	1427	rBV	29615	29255	1.42%	0.139%
17	10.592	1441	1446	1449	rBV	1403774	1270072	61.71%	6.030%
18	10.716	1464	1467	1476	rVB2	101088	127154	6.18%	0.604%
19	11.163	1540	1543	1546	rBV	76995	63554	3.09%	0.302%
20	11.192	1546	1548	1555	rVB2	32362	34062	1.66%	0.162%
21	11.286	1560	1564	1567	rVV	1177685	1053203	51.18%	5.001%
22	11.357	1571	1576	1579	rVB5	22447	27804	1.35%	0.132%
23	11.592	1613	1616	1619	rBV	43312	35506	1.73%	0.169%
24	11.998	1682	1685	1688	rBV	33366	29481	1.43%	0.140%
25	12.704	1802	1805	1807	rBV	213373	164809	8.01%	0.783%
26	12.780	1816	1818	1821	rVB2	43973	34735	1.69%	0.165%
27	12.874	1830	1834	1837	rBV	2052828	1852610	90.02%	8.796%
28	13.410	1921	1925	1928	rBV	147583	115667	5.62%	0.549%
29	13.457	1928	1933	1935	rBV2	21867	22683	1.10%	0.108%
30	13.774	1983	1987	1995	rBV2	124017	148574	7.22%	0.705%
31	13.921	2008	2012	2016	rBV	1112400	1006776	48.92%	4.780%
32	14.104	2039	2043	2047	rBV	30136	30451	1.48%	0.145%
33	14.410	2089	2095	2100	rBV	27218	32487	1.58%	0.154%
34	14.704	2142	2145	2150	rVB	28590	26860	1.31%	0.128%

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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-BF081517.M
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35	15.033	2197	2201	2204	rBV2	31652	34441	1.67%	0.164%
36	15.351	2249	2255	2260	rBV	626581	734580	35.69%	3.488%
37	15.398	2260	2263	2270	rVB2	34151	42442	2.06%	0.202%
38	15.821	2331	2335	2339	rBV2	27486	37174	1.81%	0.176%
39	16.304	2412	2417	2423	rBV3	22840	35310	1.72%	0.168%
40	16.874	2509	2514	2519	rBV3	15349	27867	1.35%	0.132%
41	17.315	2582	2589	2597	rBV7	21410	56708	2.76%	0.269%
42	17.539	2625	2627	2635	rVB5	15333	28417	1.38%	0.135%

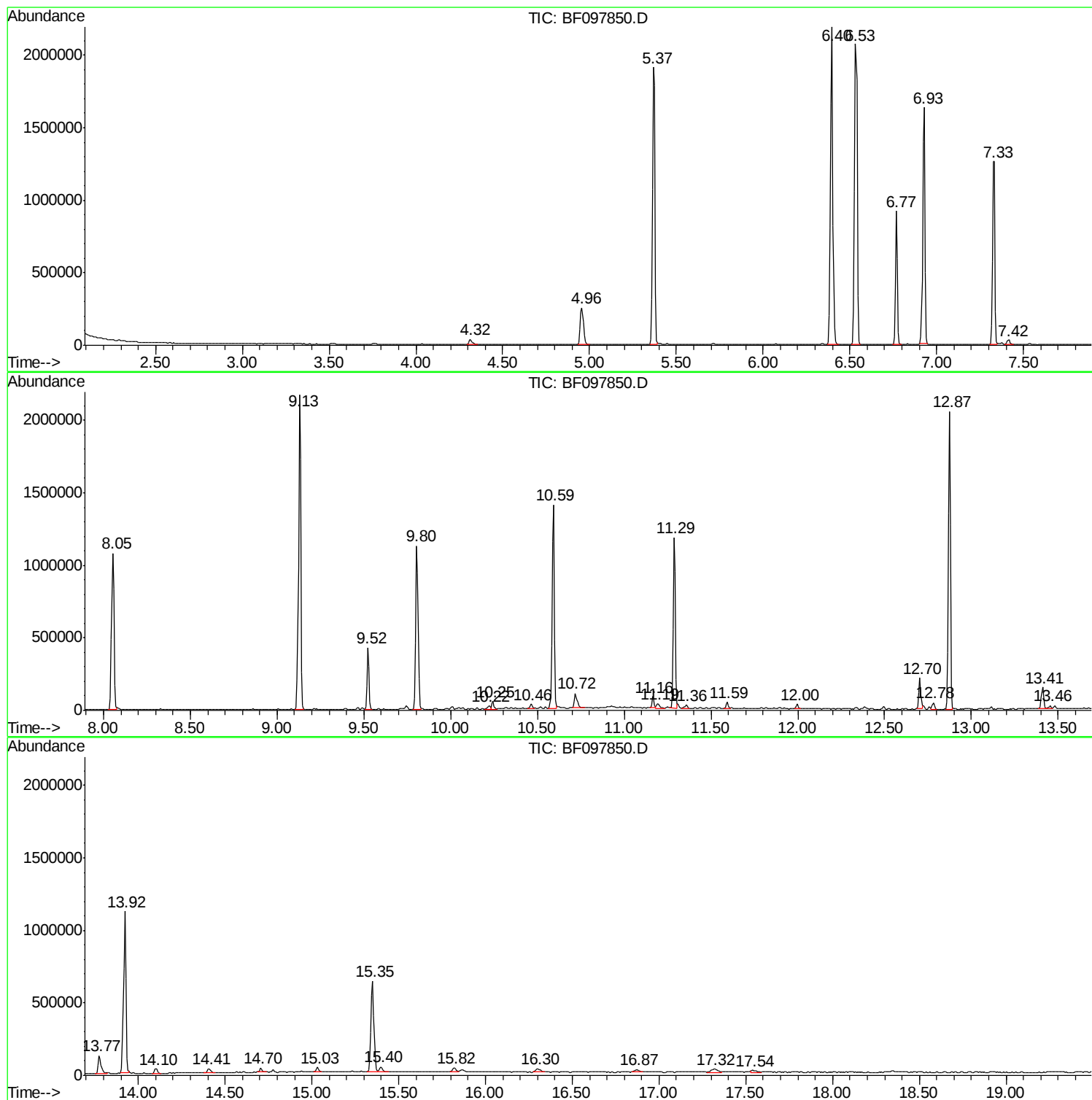
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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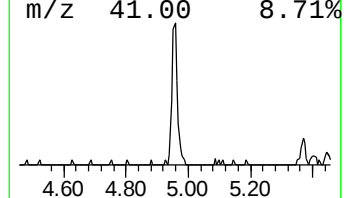
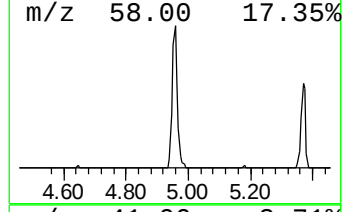
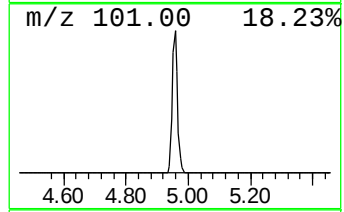
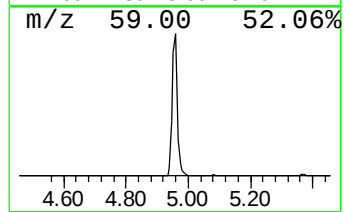
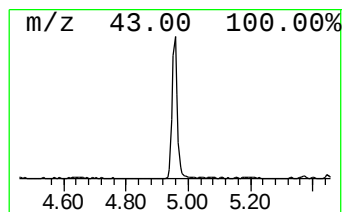
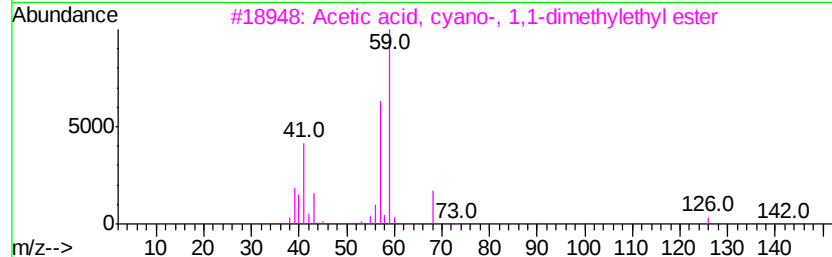
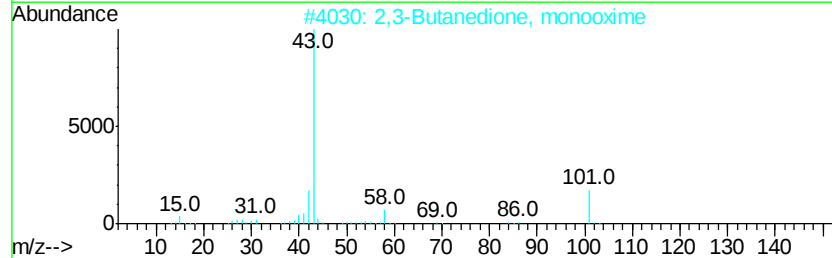
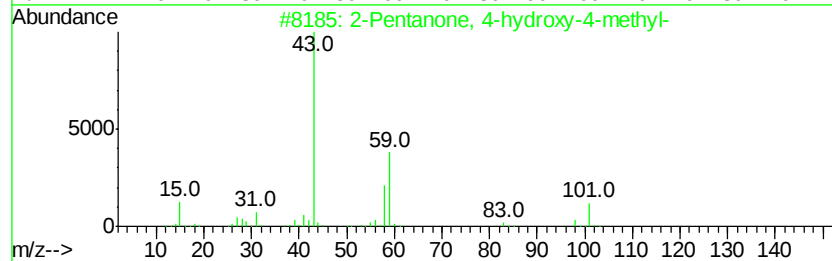
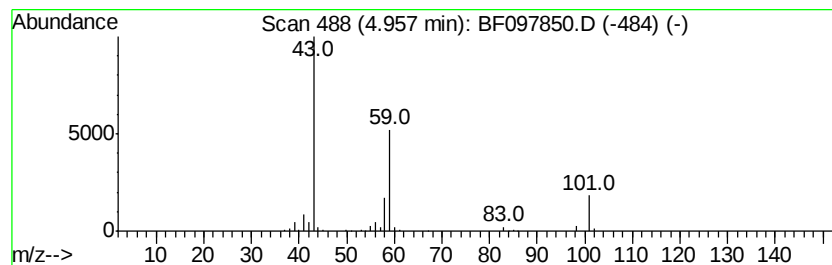
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.30 ng	300483	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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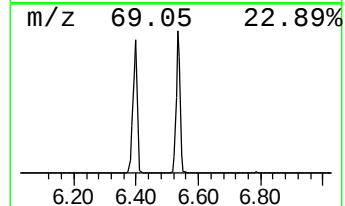
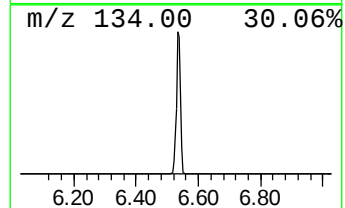
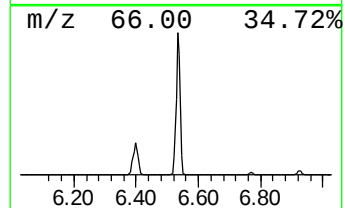
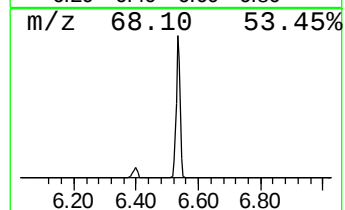
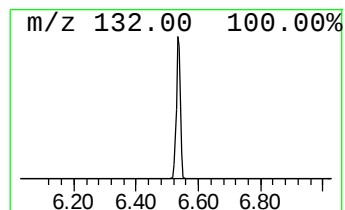
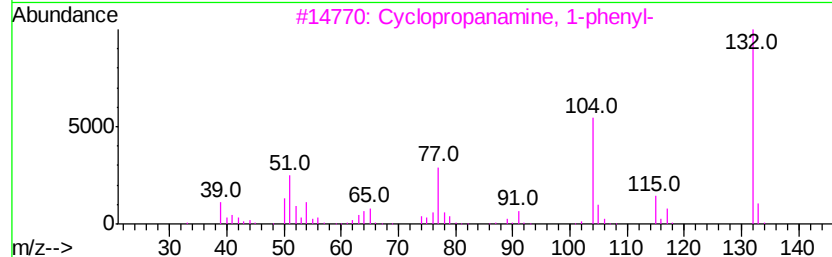
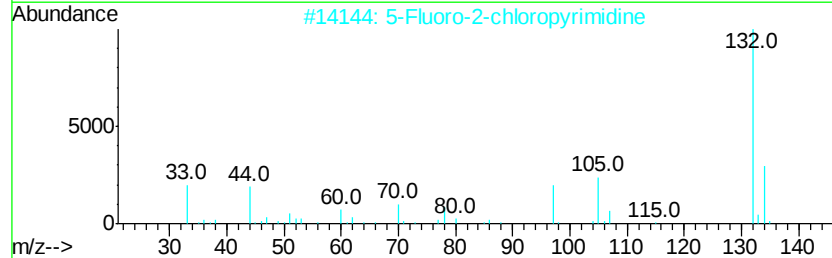
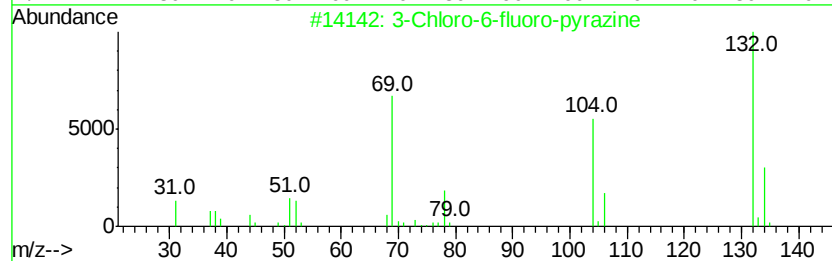
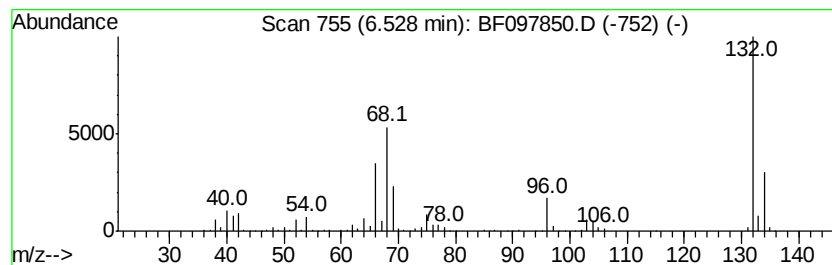
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	54.02 ng	1955710	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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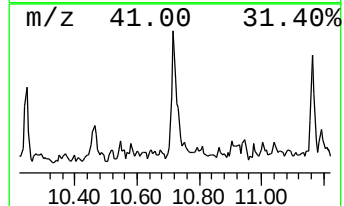
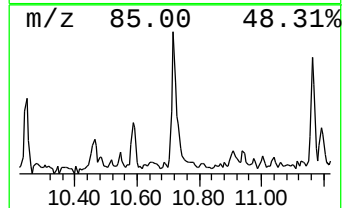
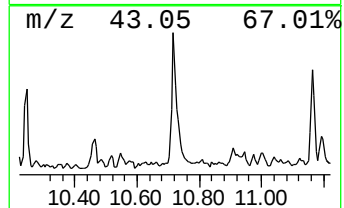
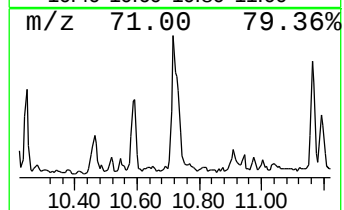
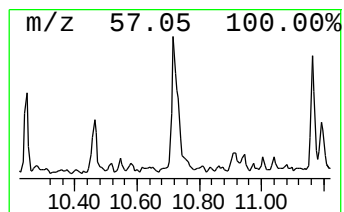
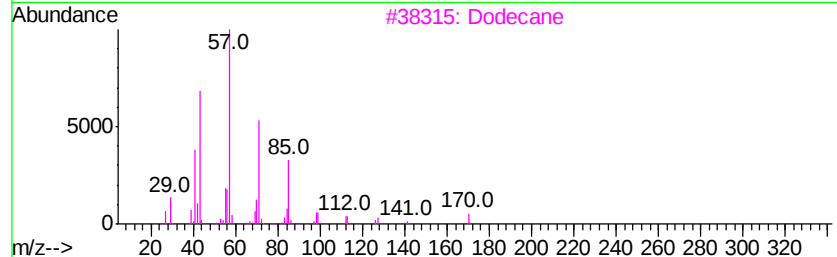
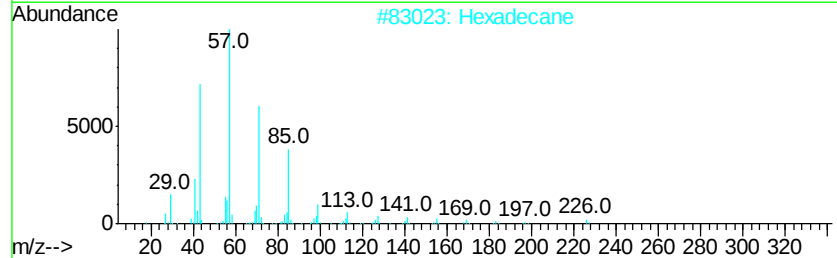
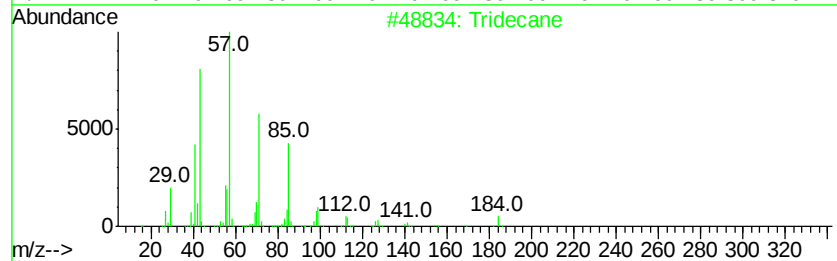
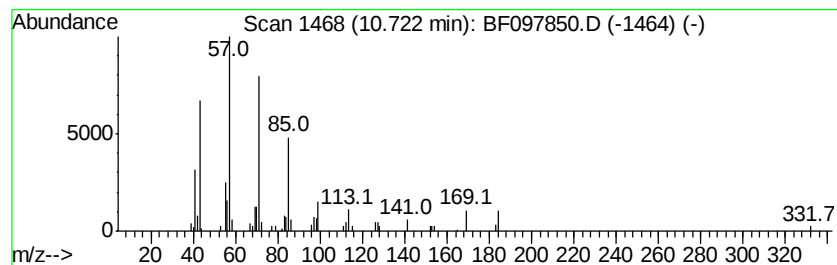
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.41 ng	127154	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Dodecane		170	C12H26	000112-40-3	87
4	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	86
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86



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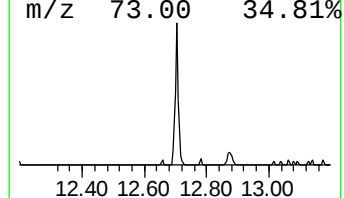
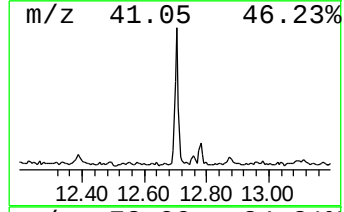
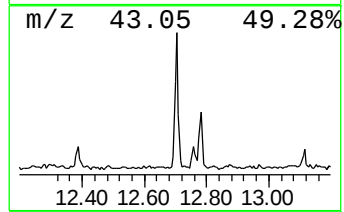
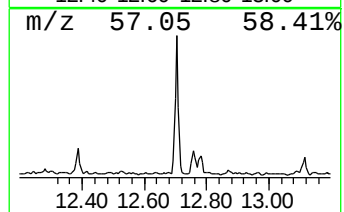
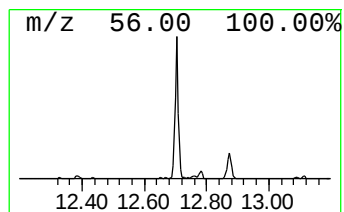
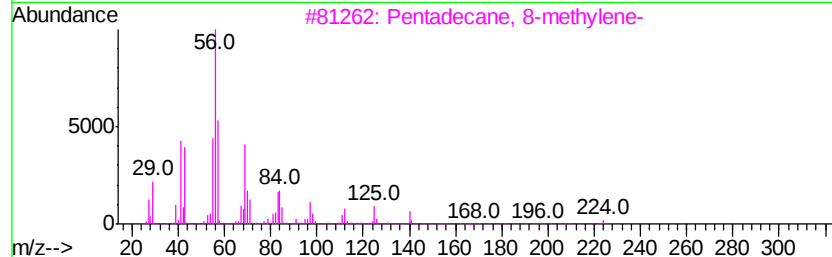
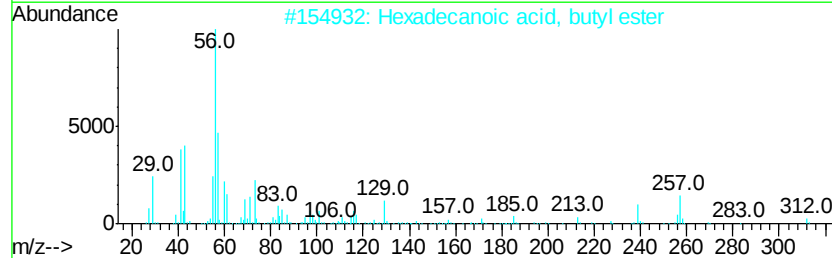
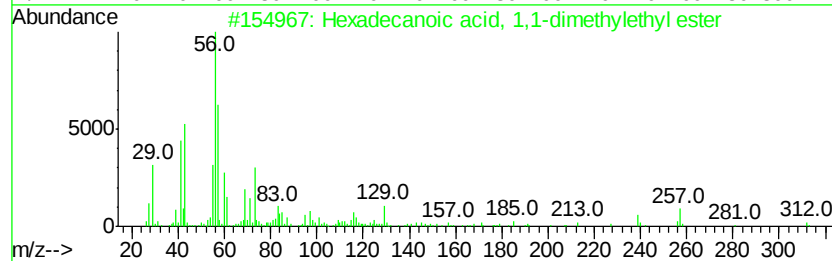
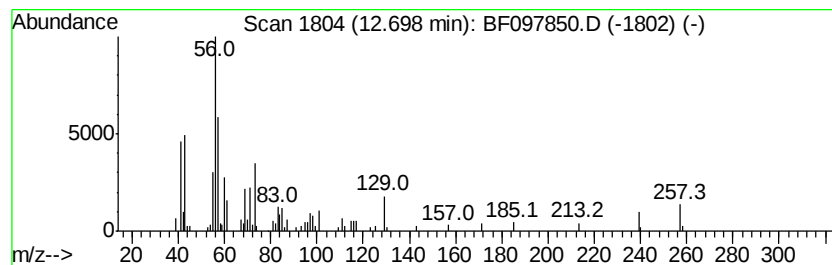
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.27 ng	164809	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	46
3		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4		5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	32
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30



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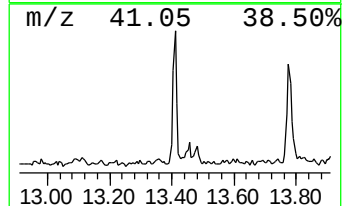
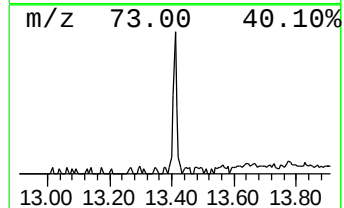
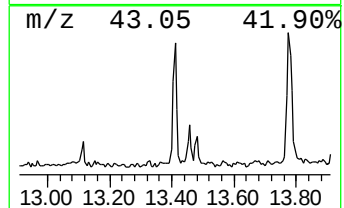
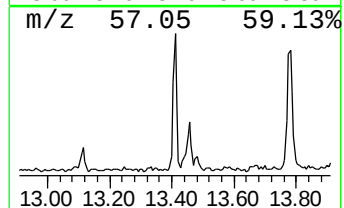
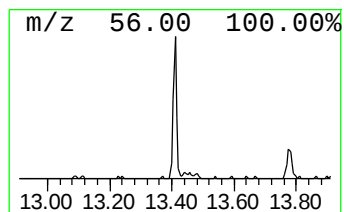
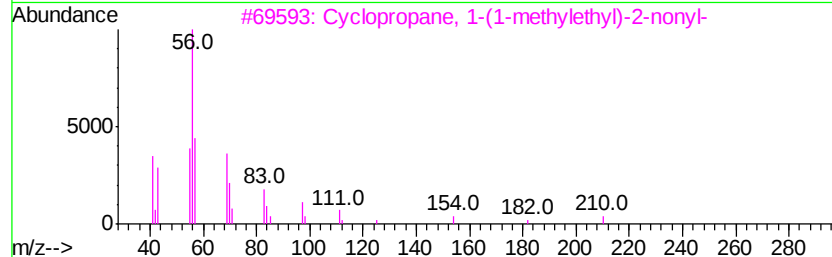
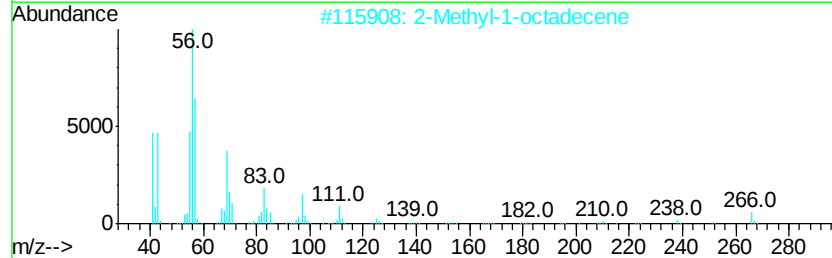
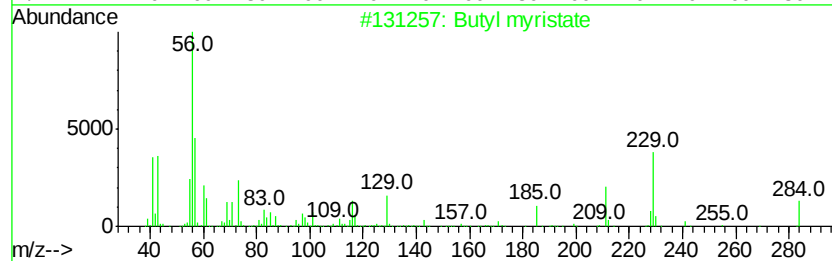
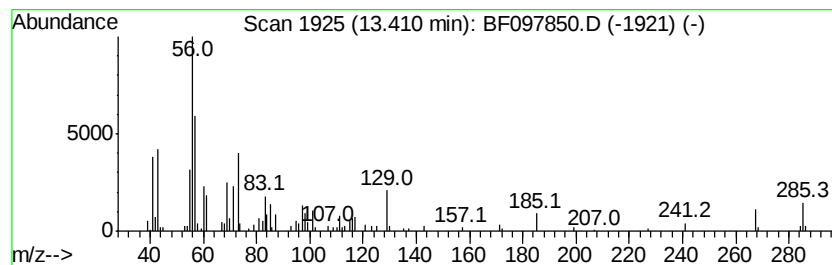
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.41 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	2.30 ng	115667	Chrysene-d12	13.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl myristate	284	C18H36O2	000110-36-1	45
2			2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
3			Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38
4			Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	38
5			1-Piperidinyloxy, 4-(hydroxyimin...	185	C9H17N2O2	003229-75-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097850.D
Acq On : 18 Aug 2017 23:25
Operator : SJ/JU
Sample : I4646-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-L10-ESW

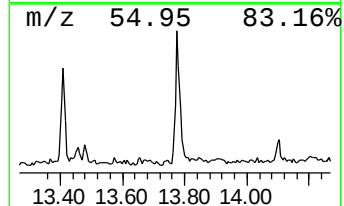
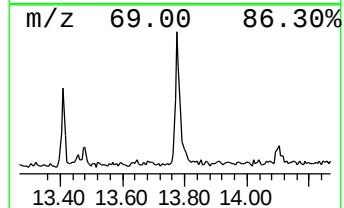
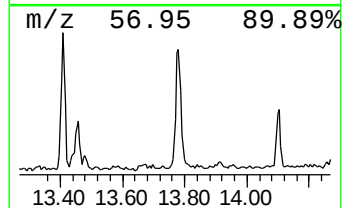
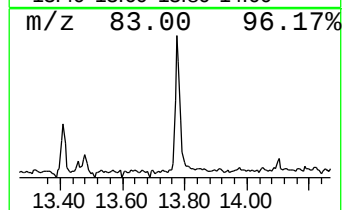
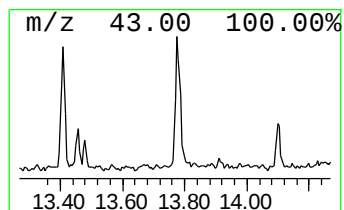
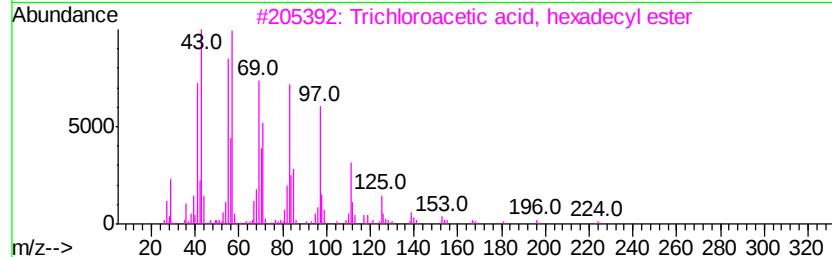
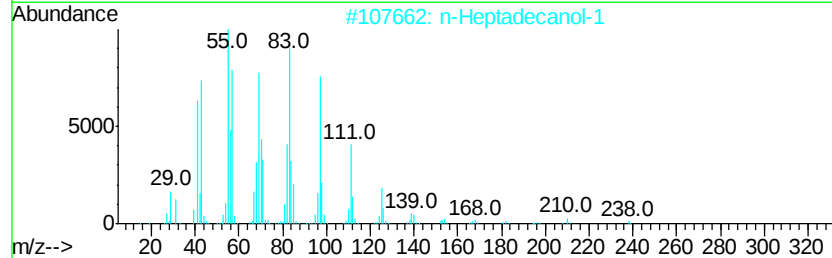
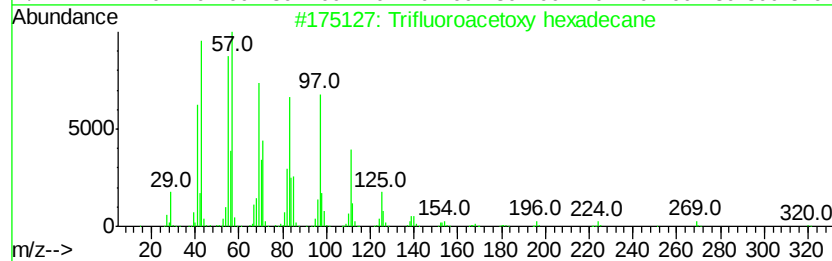
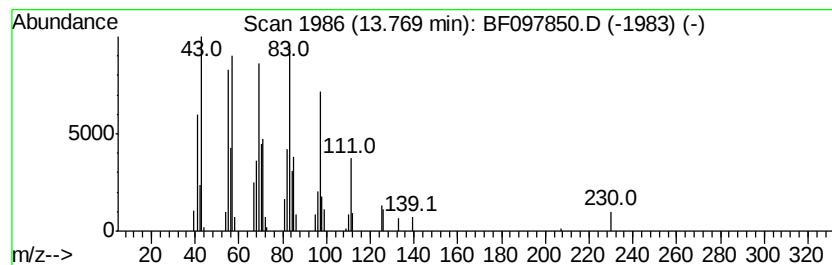
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.95 ng	148574	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	90
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097850.D
Acq On : 18 Aug 2017 23:25
Operator : SJ/JU
Sample : I4646-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-L10-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.96	8.3	ng	300483	1	6.77	724089	20.0
unknown6.53	6.53	54.0	ng	1955710	1	6.77	724089	20.0
Tridecane	10.72	2.4	ng	127154	4	11.29	1053200	20.0
Hexadecanoic acid...	12.70	3.3	ng	164809	5	13.92	1006780	20.0
unknown13.41	13.41	2.3	ng	115667	5	13.92	1006780	20.0
Trifluoroacetoxy ...	13.77	3.0	ng	148574	5	13.92	1006780	20.0