

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
 Data File : BF092371.D
 Acq On : 20 Jan 2017 14:24
 Operator : UM/SJ
 Sample : I1271-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-02

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	4.633	246	249	265	rBV	978401	1773020	27.00%	3.597%
2	5.101	288	290	293	rBV	2587063	3888007	59.21%	7.889%
3	6.187	383	385	388	rBV	3425216	4351183	66.26%	8.828%
4	6.290	392	394	397	rVV	4056825	4008650	61.04%	8.133%
5	6.519	412	414	418	rVB	1214097	1082707	16.49%	2.197%
6	6.679	425	428	430	rBV	2988833	3247503	49.45%	6.589%
7	7.102	462	465	467	rBV	2171575	2768293	42.16%	5.617%
8	7.319	480	484	488	rVB2	32351	66617	1.01%	0.135%
9	7.810	524	527	529	rBV	2050458	1996674	30.41%	4.051%
10	8.096	547	552	555	rBV4	32612	95491	1.45%	0.194%
11	8.256	563	566	570	rBV2	84609	170270	2.59%	0.345%
12	8.439	578	582	583	rBV3	27817	79791	1.22%	0.162%
13	8.507	586	588	590	rVB2	41793	67312	1.03%	0.137%
14	8.622	596	598	600	rBV2	37898	66669	1.02%	0.135%
15	8.725	603	607	609	rBV3	36594	79136	1.21%	0.161%
16	8.850	615	618	619	rBV	122703	145444	2.21%	0.295%
17	8.896	619	622	624	rVV	5164305	6566921	100.00%	13.324%
18	8.987	626	630	632	rVV4	40680	101612	1.55%	0.206%
19	9.033	632	634	637	rVB2	38811	66249	1.01%	0.134%
20	9.147	642	644	649	rBV3	47092	113876	1.73%	0.231%
21	9.227	649	651	652	rBV	63031	76654	1.17%	0.156%
22	9.262	652	654	655	rVB2	61296	74394	1.13%	0.151%
23	9.296	655	657	660	rBV	509119	570018	8.68%	1.157%
24	9.513	674	676	677	rBV	68981	79894	1.22%	0.162%
25	9.559	677	680	682	rBV	1963496	2148530	32.72%	4.359%
26	9.673	687	690	692	rVB2	49845	85752	1.31%	0.174%
27	9.765	696	698	700	rVV	84358	98145	1.49%	0.199%
28	9.810	700	702	703	rVV	42901	68525	1.04%	0.139%
29	9.879	706	708	710	rBV2	55422	82726	1.26%	0.168%
30	9.959	713	715	718	rBV4	45708	114481	1.74%	0.232%
31	10.005	718	719	721	rVB	139512	122979	1.87%	0.250%
32	10.222	736	738	740	rBV	137513	172682	2.63%	0.350%
33	10.279	740	743	744	rVB3	36030	69466	1.06%	0.141%
34	10.348	746	749	751	rBV	3302722	3483402	53.04%	7.068%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.485	758	761	764	rVB2	232537	408906	6.23%	0.830%
36	10.919	798	799	801	rBV	106938	148261	2.26%	0.301%
37	10.953	801	802	805	rVB	145184	128445	1.96%	0.261%
38	11.033	807	809	811	rBV	2066893	1915727	29.17%	3.887%
39	11.353	835	837	839	rBV	69649	95591	1.46%	0.194%
40	11.536	848	853	855	rBV3	27867	69448	1.06%	0.141%
41	11.593	855	858	861	rVV3	212820	302307	4.60%	0.613%
42	11.651	861	863	868	rVB3	35977	80549	1.23%	0.163%
43	12.371	924	926	932	rVB	64425	81055	1.23%	0.164%
44	12.622	945	948	950	rBV	4725660	5119182	77.95%	10.387%
45	13.559	1026	1030	1037	rBV2	83505	297001	4.52%	0.603%
46	13.662	1037	1039	1042	rBV	1235365	1331008	20.27%	2.701%
47	15.011	1154	1157	1164	rVB	864335	1165015	17.74%	2.364%
48	15.800	1223	1226	1231	rVB2	43175	89330	1.36%	0.181%
49	16.268	1264	1267	1273	rVB2	31870	71698	1.09%	0.145%

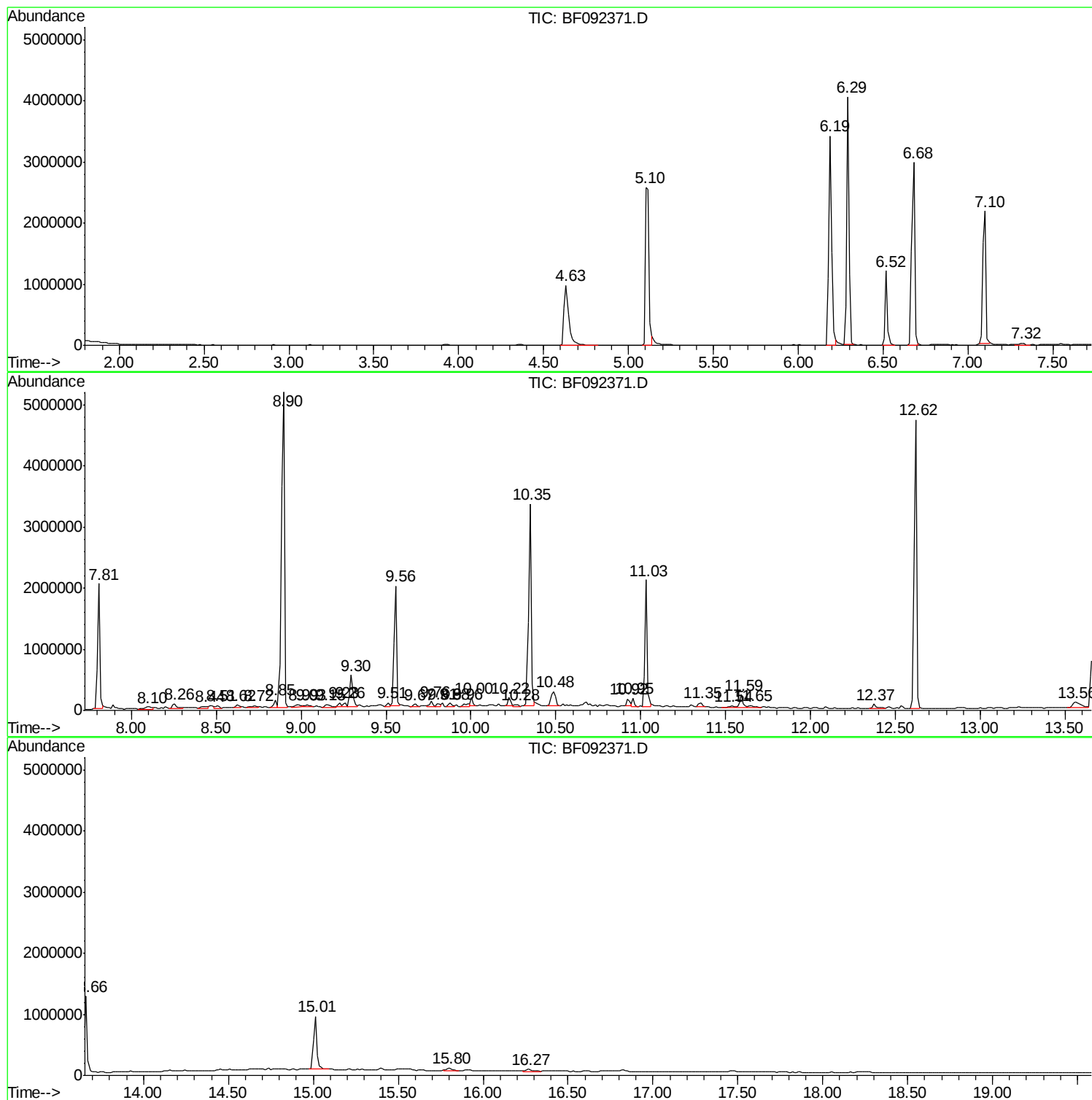
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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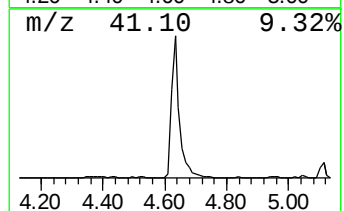
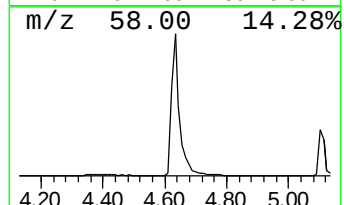
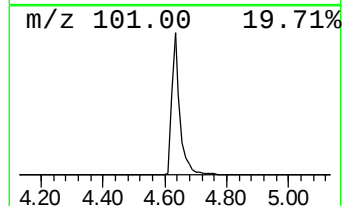
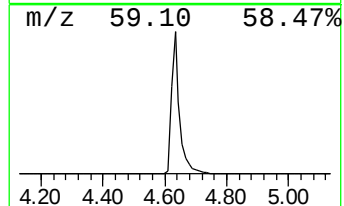
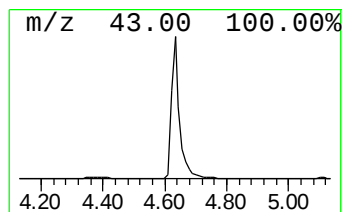
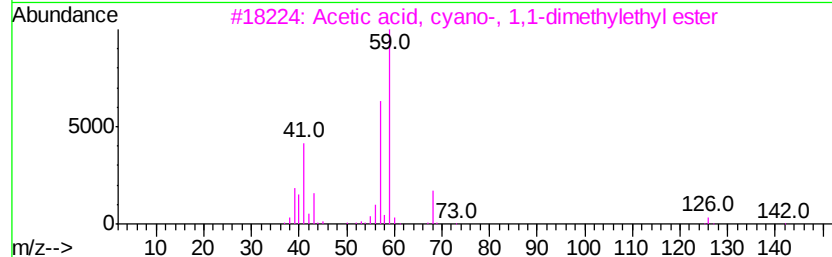
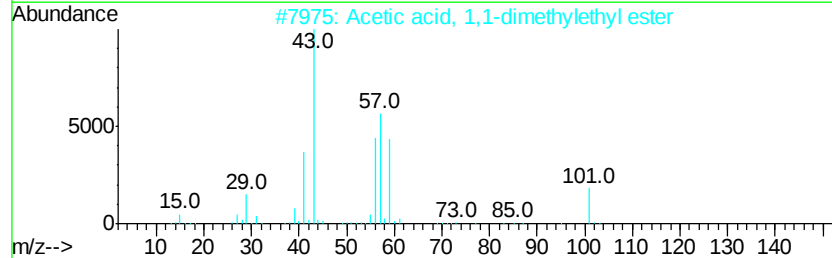
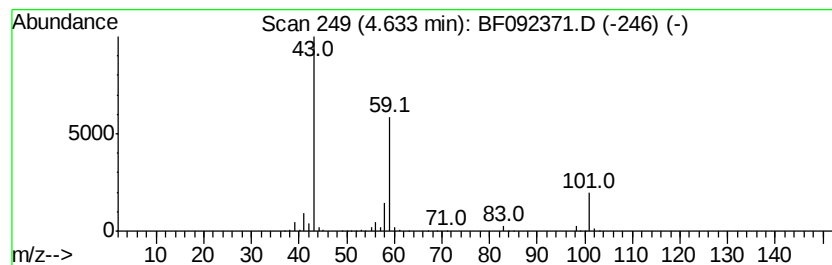
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	32.75 ng	1773020	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
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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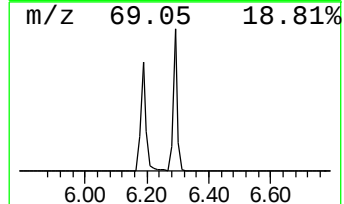
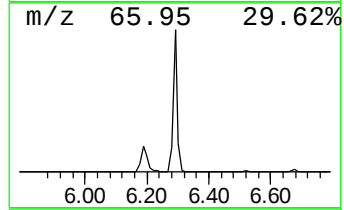
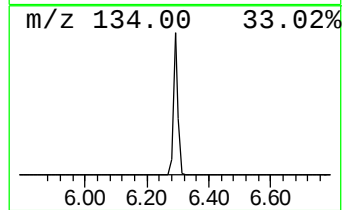
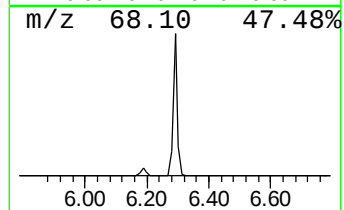
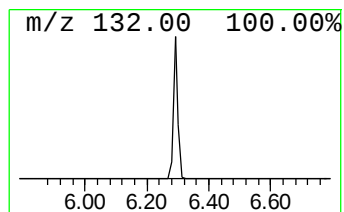
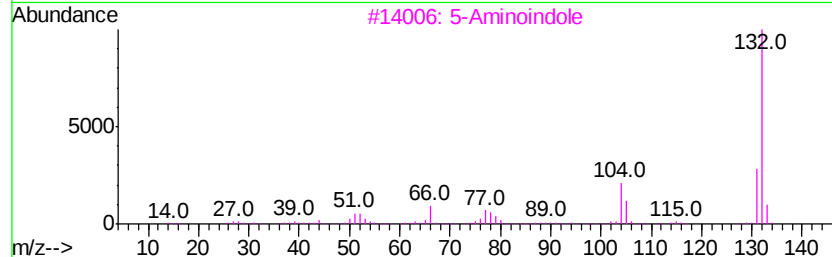
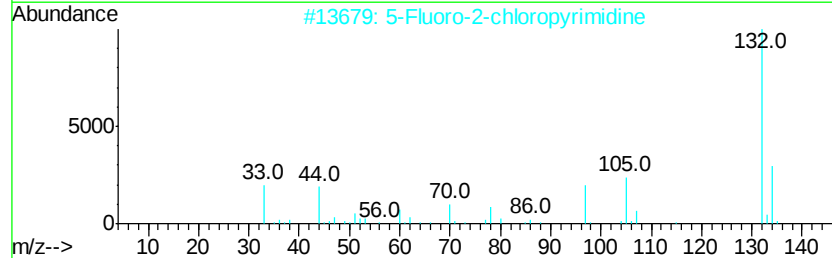
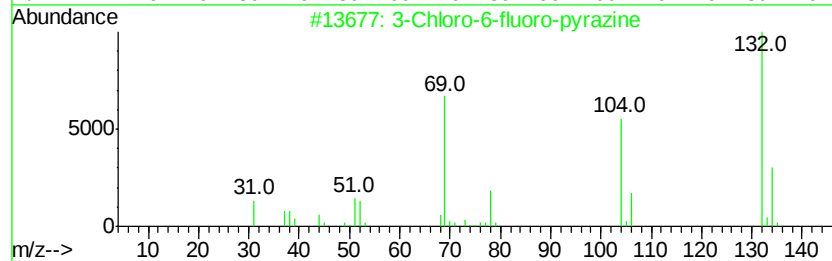
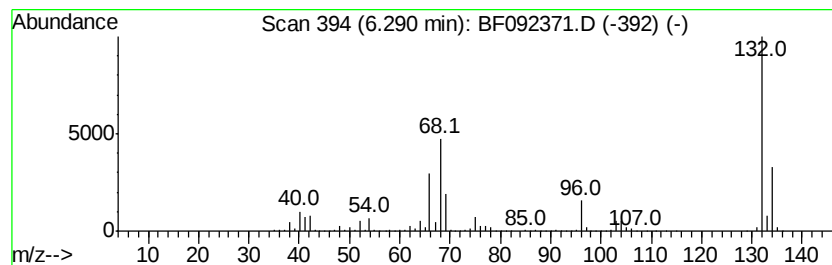
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	74.05 ng	4008650	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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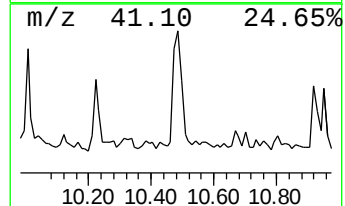
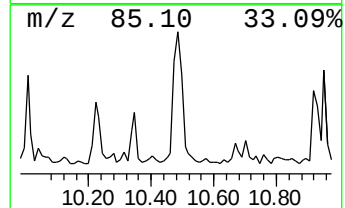
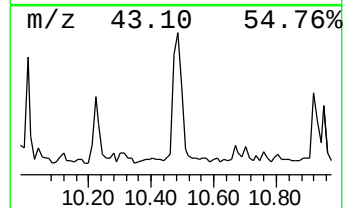
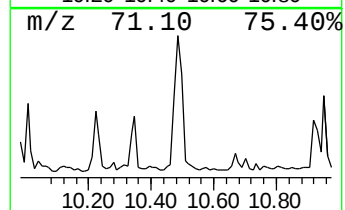
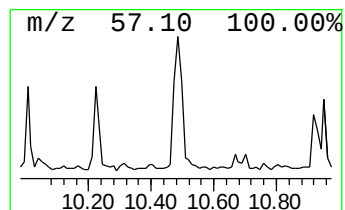
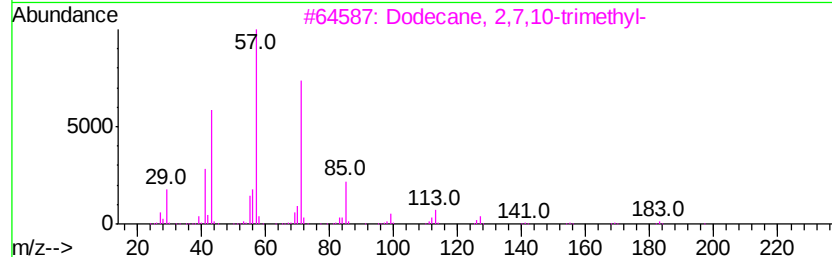
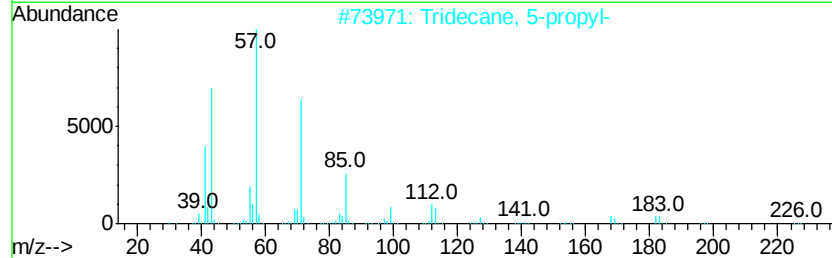
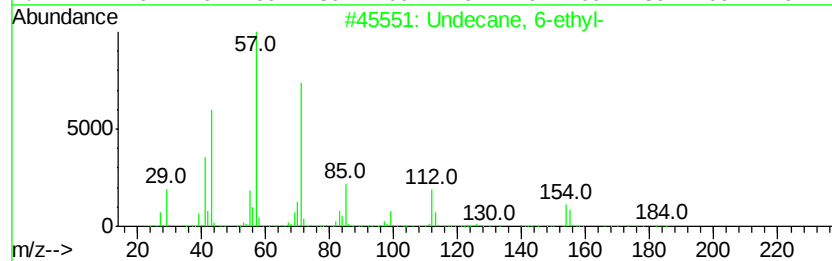
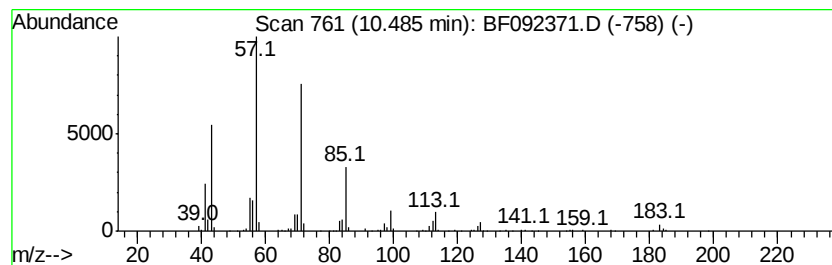
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Undecane, 6-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.48	4.27 ng	408906	Phenanthrene-d10	11.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-	184	C13H28	017312-60-6	90
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	90
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	83



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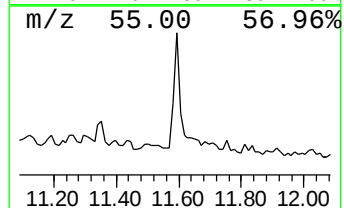
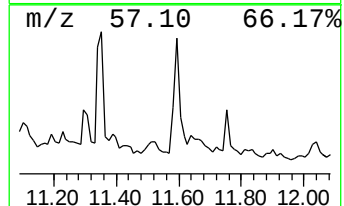
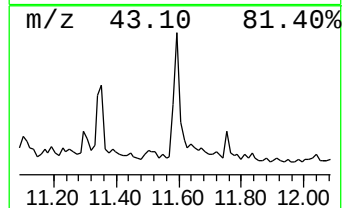
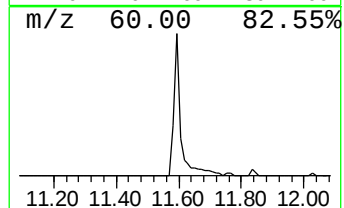
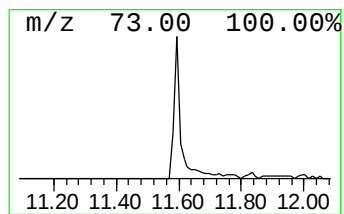
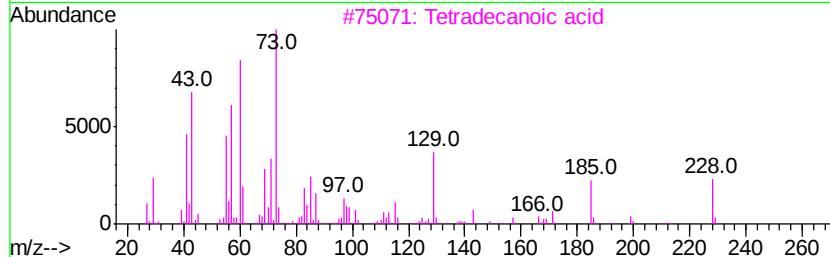
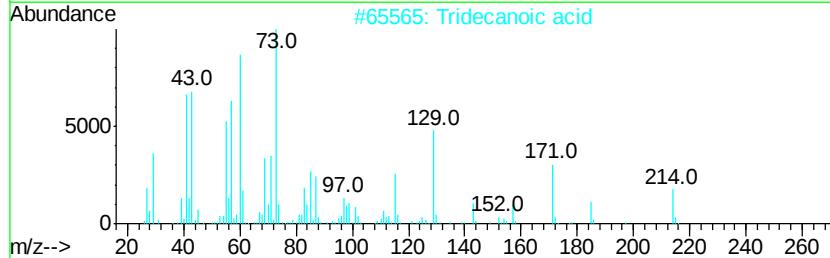
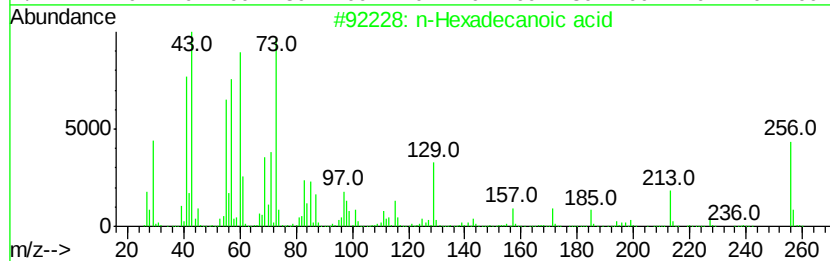
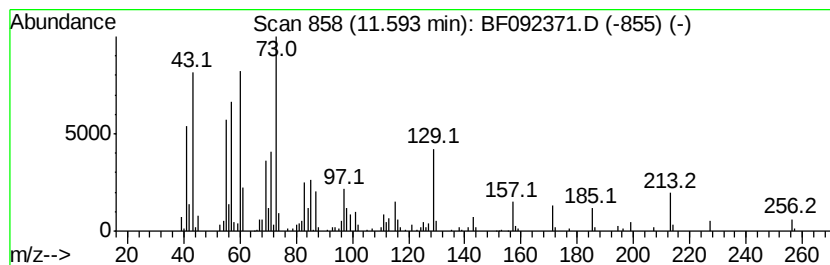
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	3.16 ng	302307	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	80



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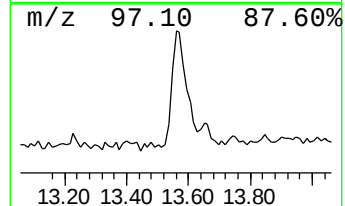
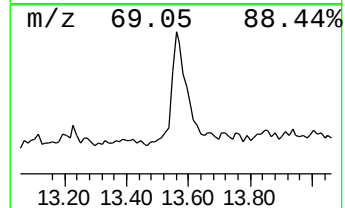
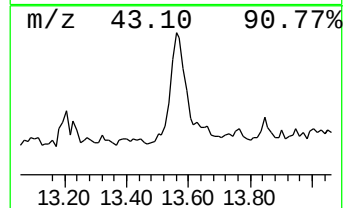
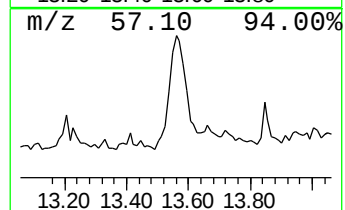
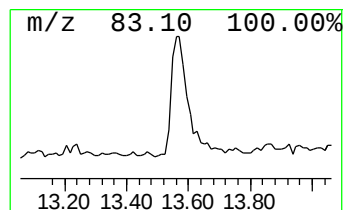
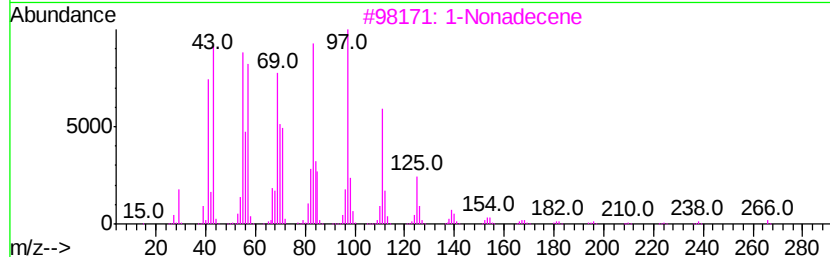
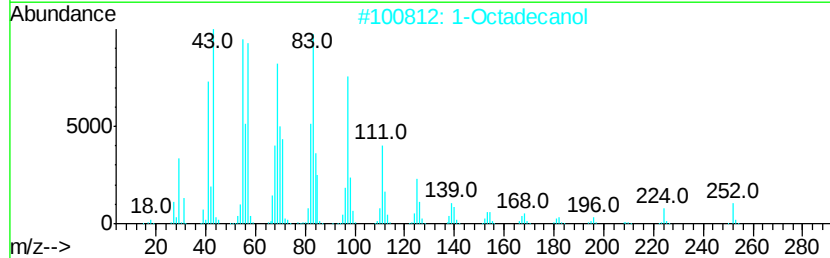
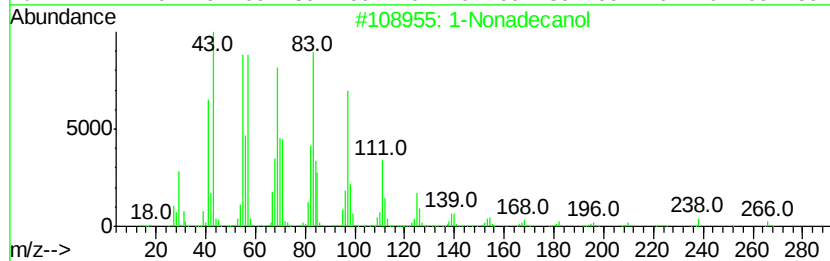
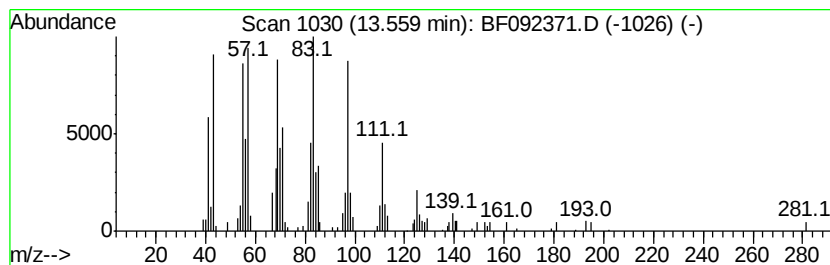
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.56	4.46 ng	297001	Chrysene-d12	13.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecanol	284	C19H40O	001454-84-8	95
2	1-Octadecanol	270	C18H38O	000112-92-5	94
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	1-Heptadecanol	256	C17H36O	001454-85-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092371.D
Acq On : 20 Jan 2017 14:24
Operator : UM/SJ
Sample : I1271-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-02

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...	4.63	32.8	ng	1773020	1	6.52	1082710	20.0
unknown6.29	6.29	74.0	ng	4008650	1	6.52	1082710	20.0
Undecane, 6-ethyl-	10.48	4.3	ng	408906	4	11.03	1915730	20.0
n-Hexadecanoic acid	11.59	3.2	ng	302307	4	11.03	1915730	20.0
1-Nonadecanol	13.56	4.5	ng	297001	5	13.66	1331010	20.0