

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082615\
 Data File : BF081232.D
 Acq On : 27 Aug 2015 1:24
 Operator : UM/IZ
 Sample : G3404-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF081715.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	3.063	113	116	119	rVB	11076	20414	1.24%	0.162%
2	3.829	181	183	188	rBV	15286	28416	1.73%	0.225%
3	4.606	248	251	268	rVB	282002	416708	25.35%	3.304%
4	5.074	289	292	294	rBV	739537	750490	45.65%	5.951%
5	5.497	327	329	332	rBV	29245	30983	1.88%	0.246%
6	6.160	385	387	391	rBV	549902	478717	29.12%	3.796%
7	6.274	395	397	400	rVV	1029526	1217496	74.06%	9.654%
8	6.377	403	406	408	rVB	27118	29890	1.82%	0.237%
9	6.515	416	418	420	rBV	389651	333248	20.27%	2.643%
10	6.675	429	432	434	rBV	1106929	1226741	74.62%	9.728%
11	7.086	465	468	470	rBV	1025682	995466	60.56%	7.894%
12	7.223	476	480	483	rVB	28320	30693	1.87%	0.243%
13	7.726	523	524	528	rBV	25111	32148	1.96%	0.255%
14	7.795	528	530	533	rVB	309647	391314	23.80%	3.103%
15	8.880	622	625	627	rBV	1804878	1643890	100.00%	13.036%
16	9.018	634	637	639	rBV	192256	190358	11.58%	1.509%
17	9.280	658	660	662	rVB	55340	45467	2.77%	0.361%
18	9.543	681	683	685	rBV	508322	453733	27.60%	3.598%
19	10.321	749	751	754	rBV2	749637	989315	60.18%	7.845%
20	10.469	762	764	767	rVB	25946	26680	1.62%	0.212%
21	10.538	767	770	773	rBV3	17072	41025	2.50%	0.325%
22	10.698	783	784	786	rVB	19074	19149	1.16%	0.152%
23	10.915	799	803	804	rBV	21670	32752	1.99%	0.260%
24	11.006	809	811	813	rVB	459429	428461	26.06%	3.398%
25	11.281	832	835	838	rVB	13571	25938	1.58%	0.206%
26	11.418	845	847	849	rBV	41891	48832	2.97%	0.387%
27	11.566	858	860	864	rBV	145808	148235	9.02%	1.175%
28	12.344	926	928	932	rBV	56050	63956	3.89%	0.507%
29	12.595	947	950	953	rBV	1536622	1507274	91.69%	11.952%
30	13.509	1028	1030	1034	rVB	21152	27861	1.69%	0.221%
31	13.624	1038	1040	1042	rBV	331552	381440	23.20%	3.025%
32	14.412	1105	1109	1111	rBV2	31128	39145	2.38%	0.310%
33	14.870	1143	1149	1152	rBV5	6167	17904	1.09%	0.142%
34	14.950	1153	1156	1158	rVV	235283	274305	16.69%	2.175%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	14.995	1158	1160	1163	rVB	68825	99854	6.07%	0.792%
36	15.738	1221	1225	1229	rBV	39951	65320	3.97%	0.518%
37	16.733	1309	1312	1315	rBV	16545	31633	1.92%	0.251%
38	18.116	1426	1433	1441	rBV3	6588	25508	1.55%	0.202%

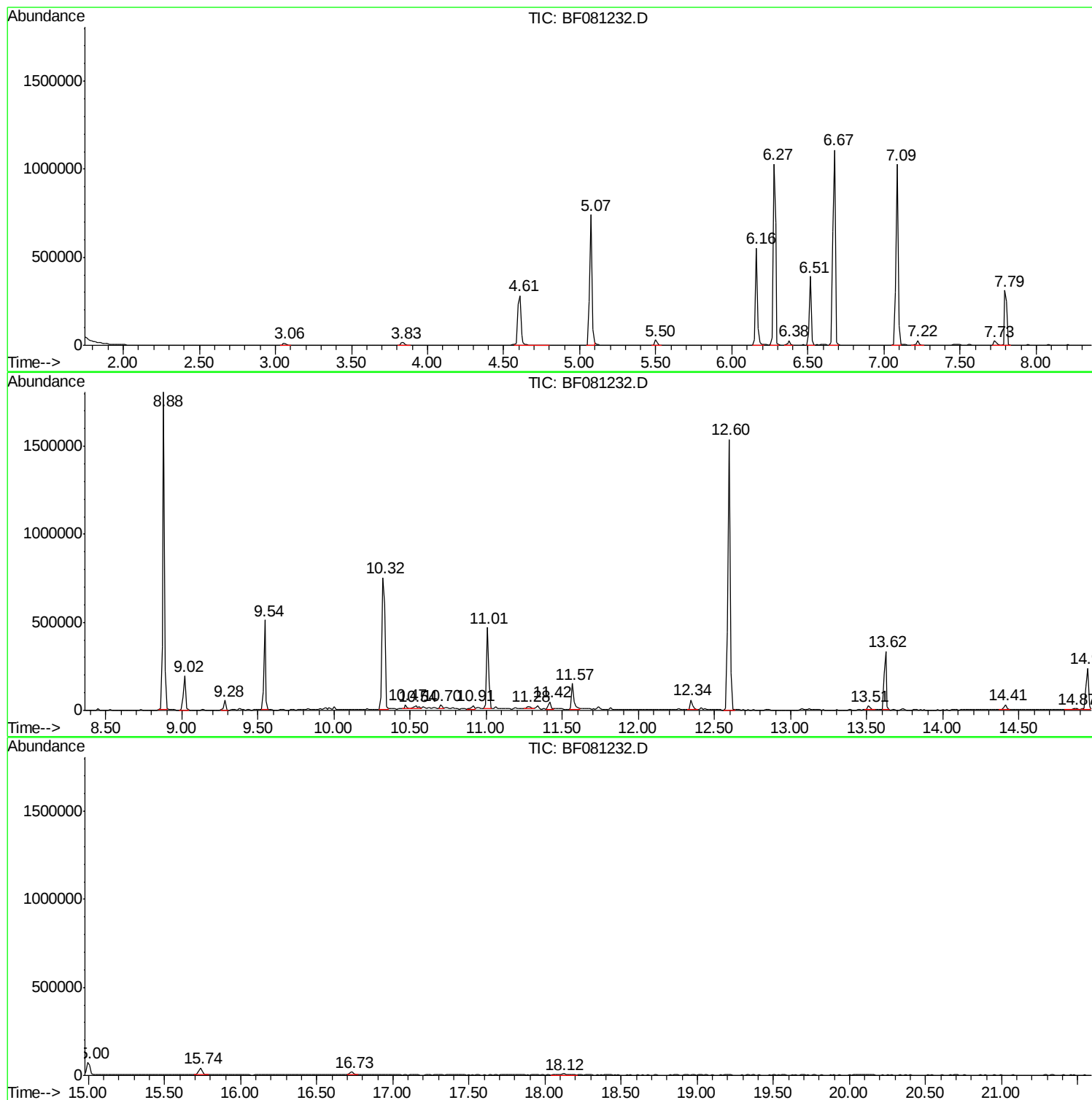
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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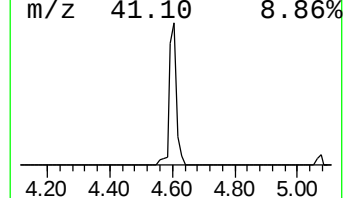
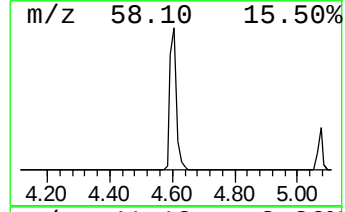
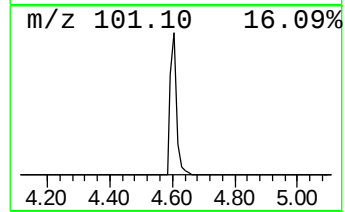
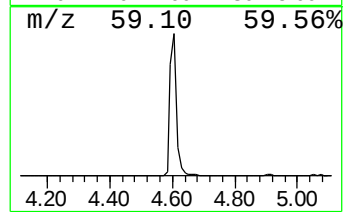
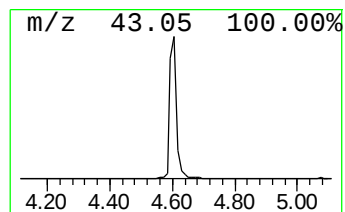
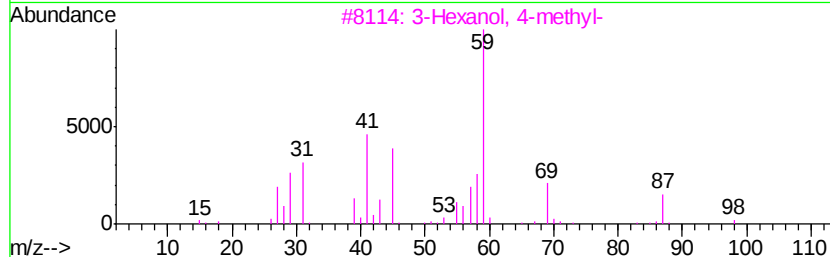
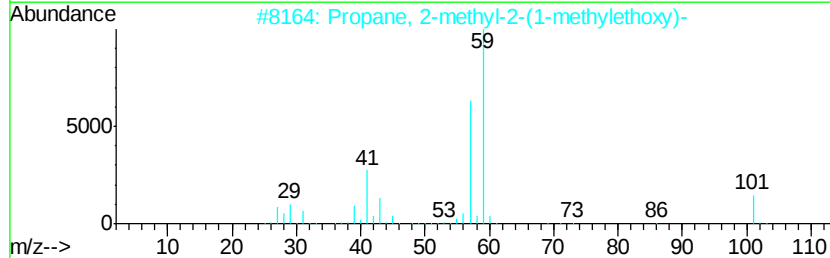
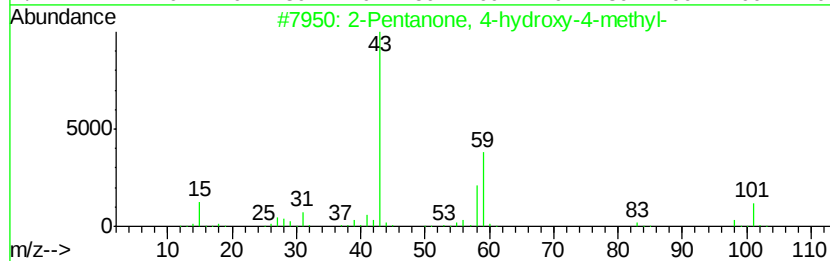
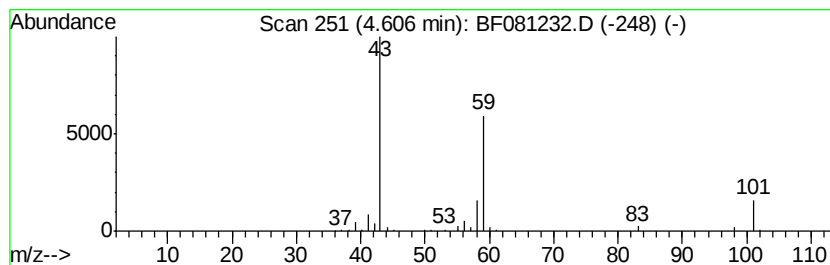
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.61	25.01 ng	416708	1,4-Dichlorobenzene-d4	6.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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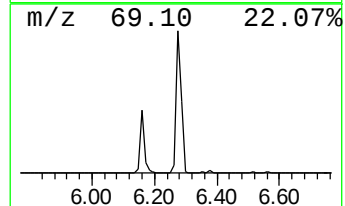
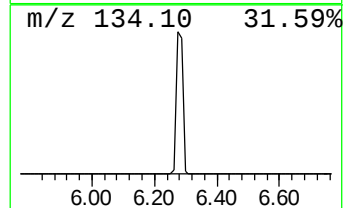
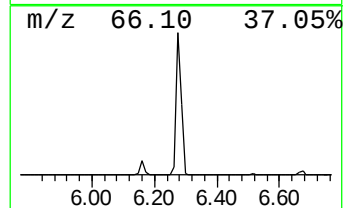
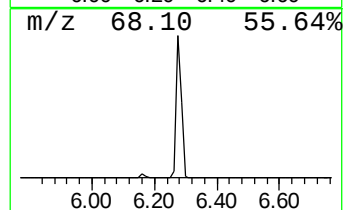
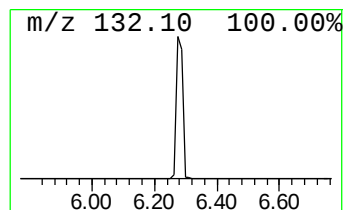
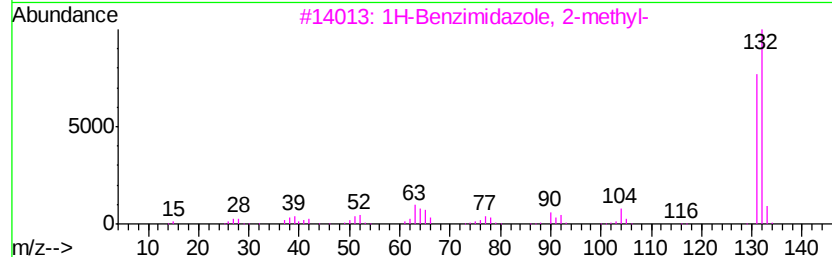
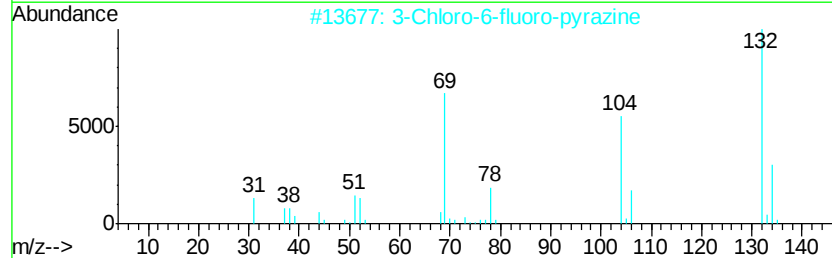
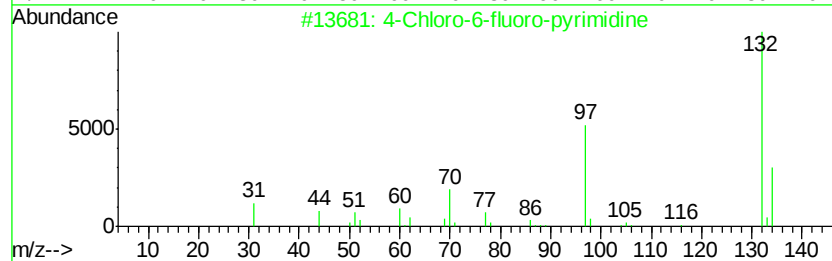
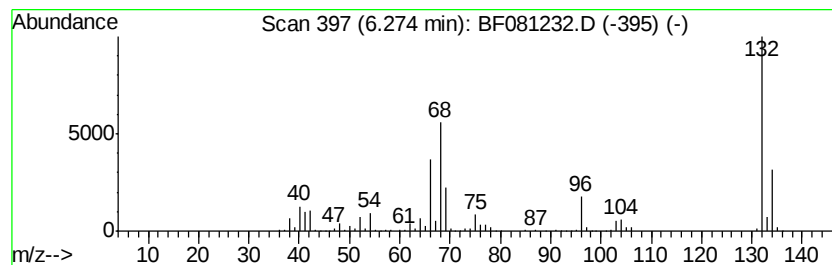
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	73.07 ng	1217500	1,4-Dichlorobenzene-d4	6.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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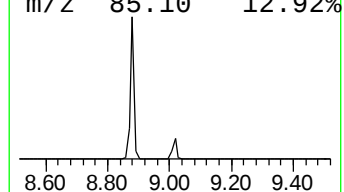
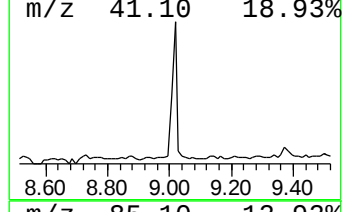
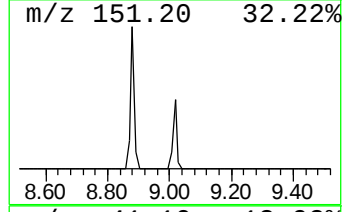
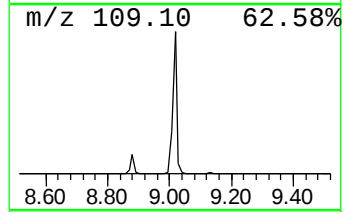
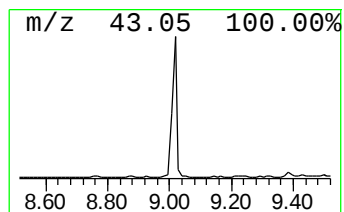
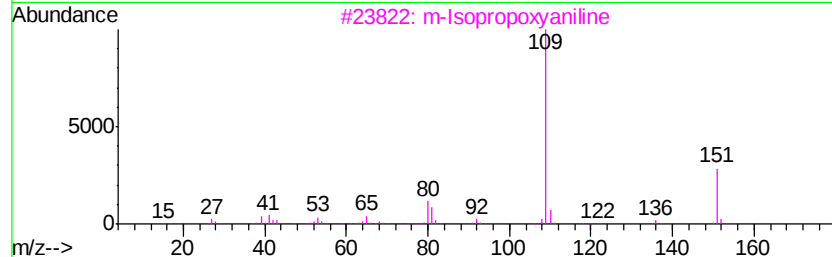
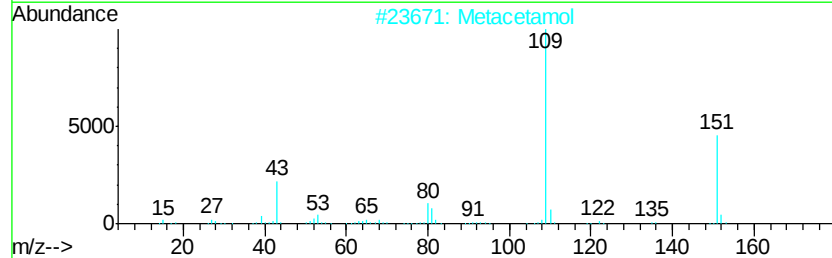
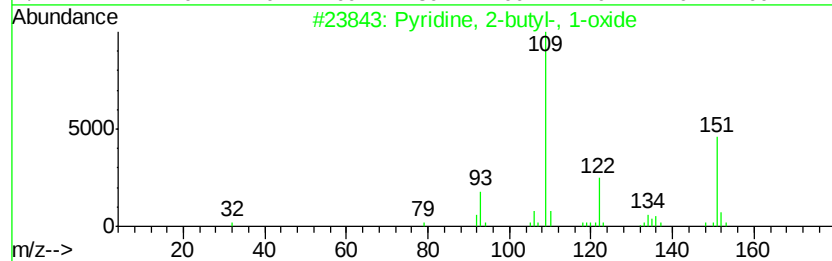
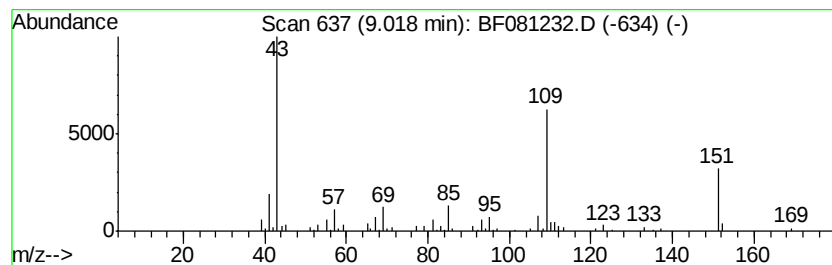
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pyridine, 2-butyl-, 1-oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	8.39 ng	190358	Acenaphthene-d10	9.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
2		Metacetamol	151	C8H9NO2	000621-42-1	47
3		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47
4		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	40
5		1-(1,2,3-Trimethyl-cyclopent-2-e...	152	C10H16O	070987-81-4	38



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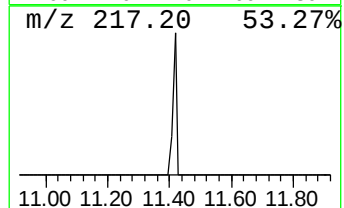
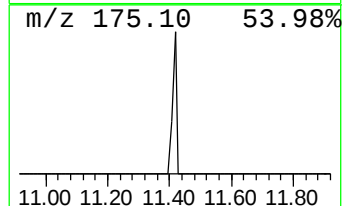
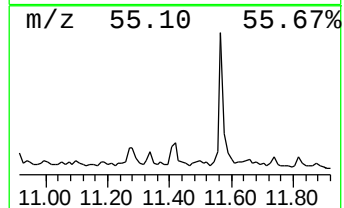
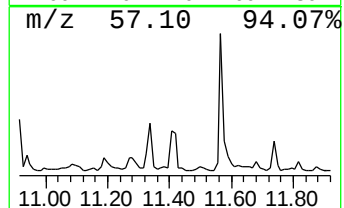
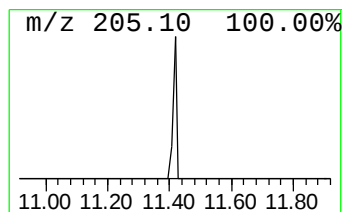
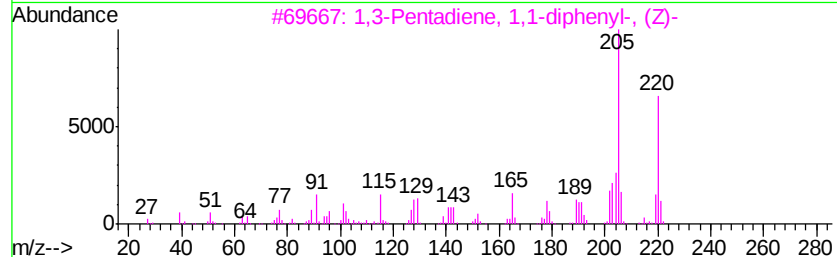
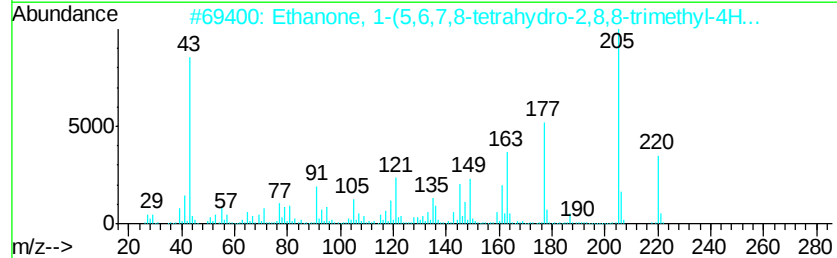
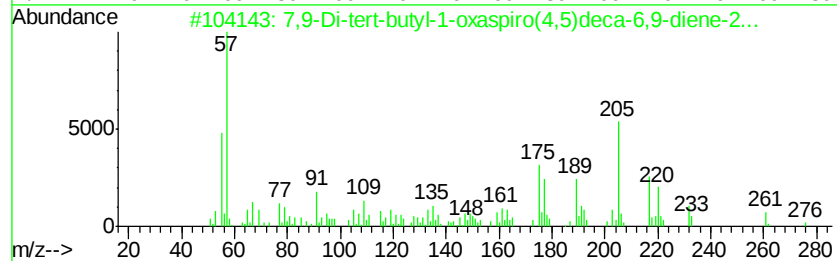
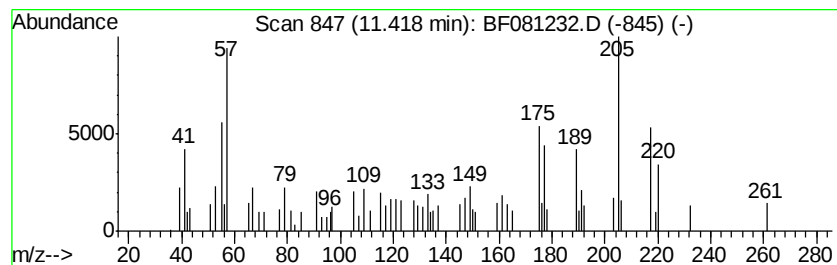
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	2.28 ng	48832	Phenanthrene-d10	11.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	91	
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	64	
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	42	
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42	
5	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	35	



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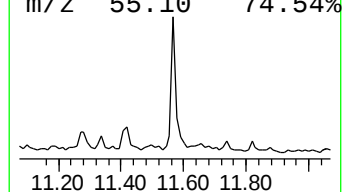
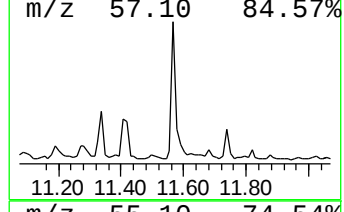
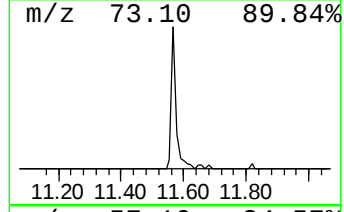
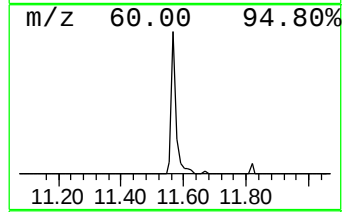
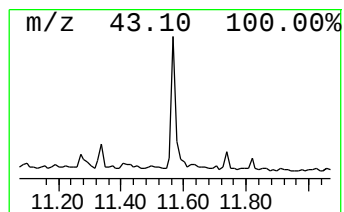
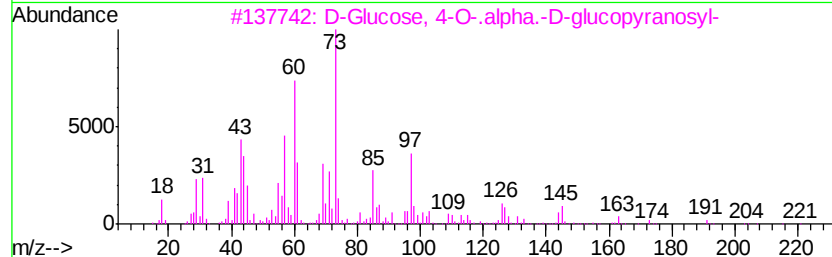
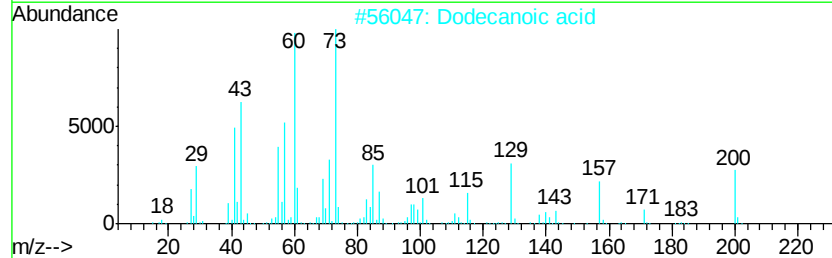
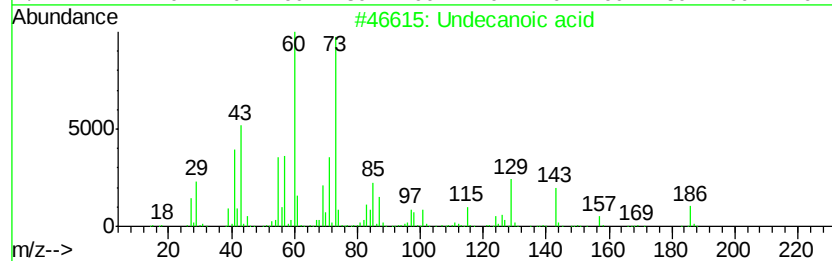
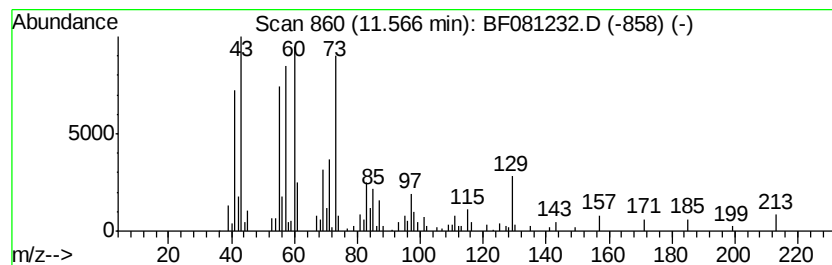
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.57	6.92 ng	148235	Phenanthrene-d10		11.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	72
2			Dodecanoic acid	200	C12H24O2	000143-07-7	53
3			D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	43
4			Heptanoic acid	130	C7H14O2	000111-14-8	35
5			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082615\
Data File : BF081232.D
Acq On : 27 Aug 2015 1:24
Operator : UM/IZ
Sample : G3404-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

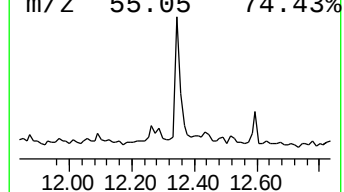
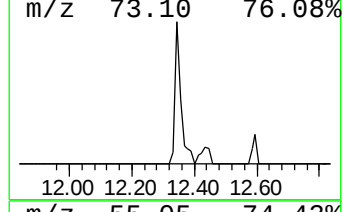
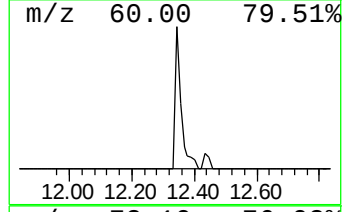
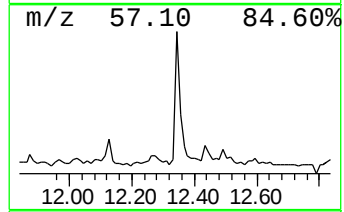
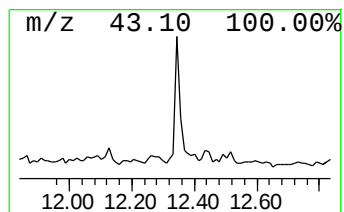
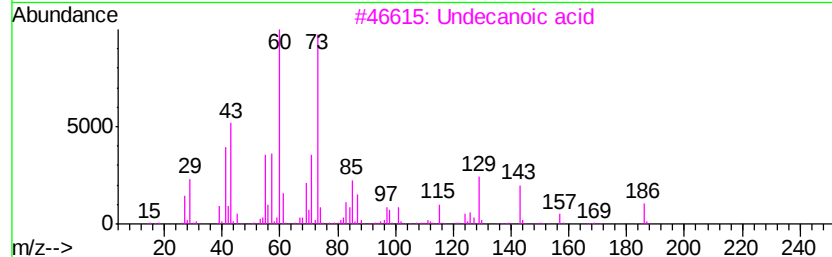
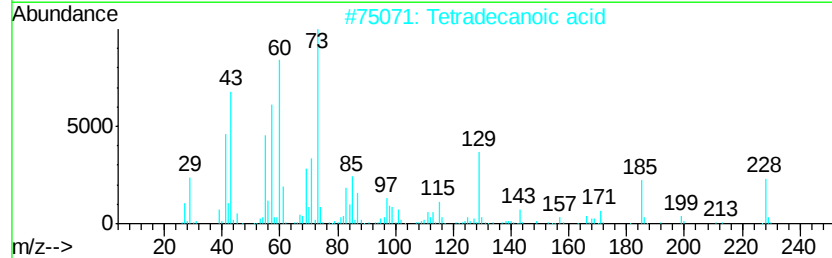
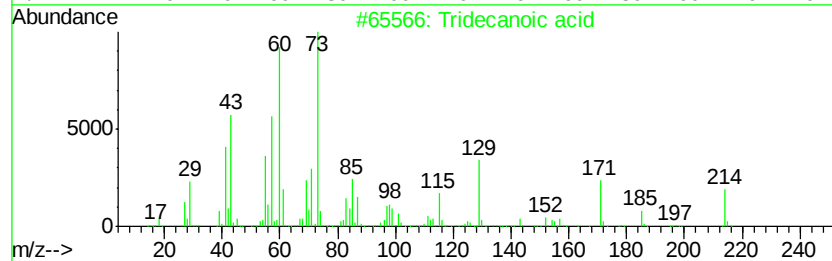
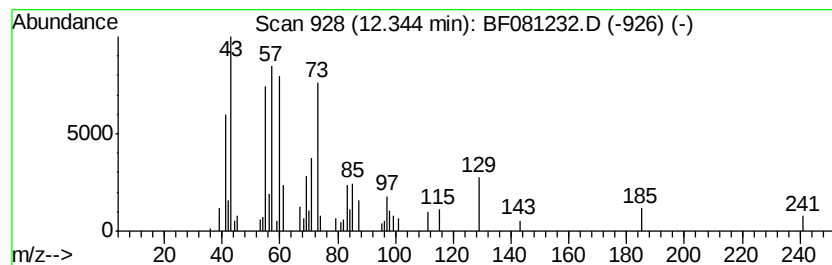
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	3.35 ng	63956	Chrysene-d12	13.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	72
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Undecanoic acid	186	C11H22O2	000112-37-8	64
4		Dodecanoic acid	200	C12H24O2	000143-07-7	59
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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Sample : G3404-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

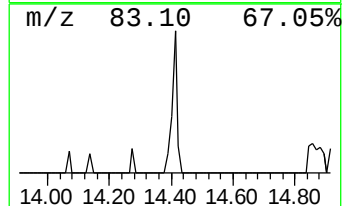
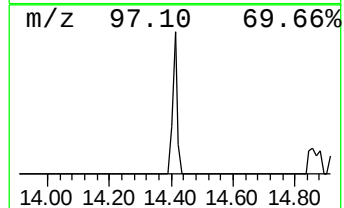
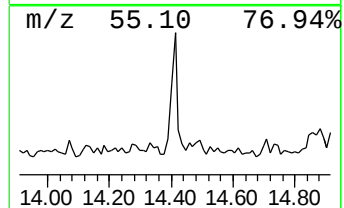
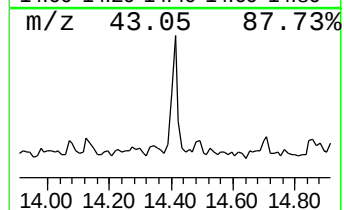
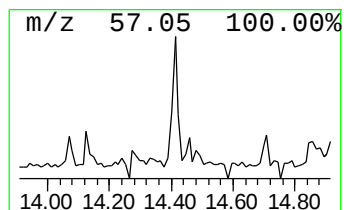
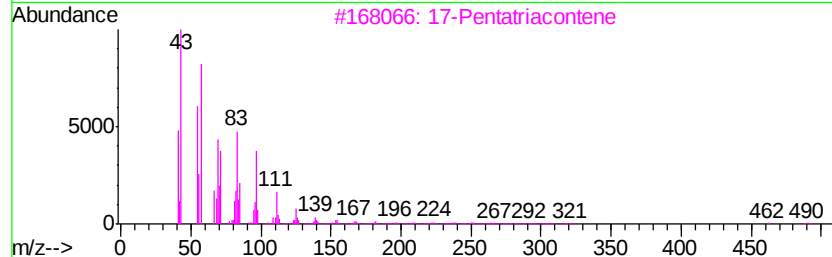
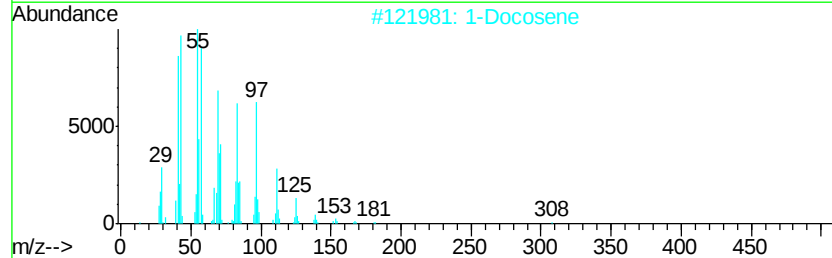
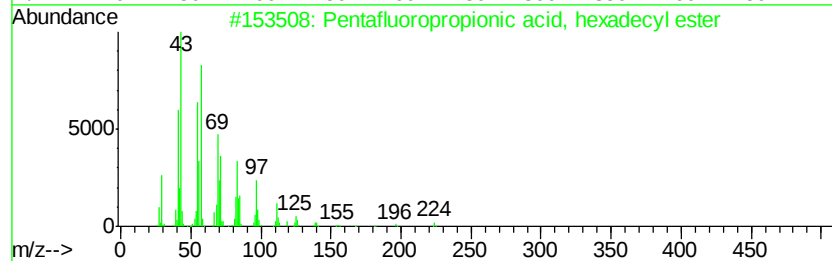
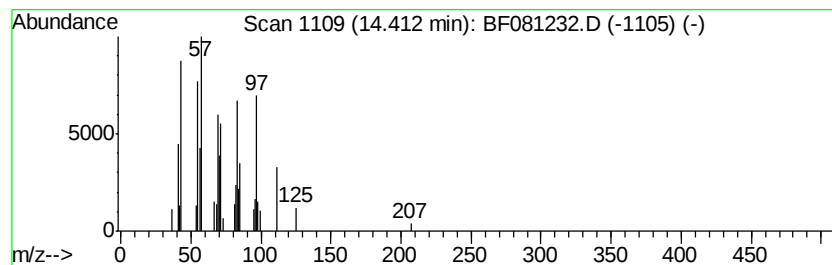
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.85 ng	39145	Perylene-d12	14.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
2			1-Docosene	308	C22H44	001599-67-3	90
3			17-Pentatriacontene	491	C35H70	006971-40-0	87
4			1-Nonadecene	266	C19H38	018435-45-5	87
5			11-Tricosene	322	C23H46	052078-56-5	86



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Operator : UM/IZ
Sample : G3404-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

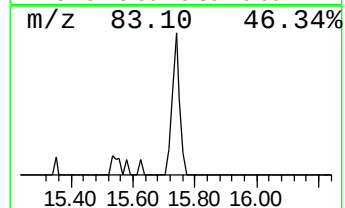
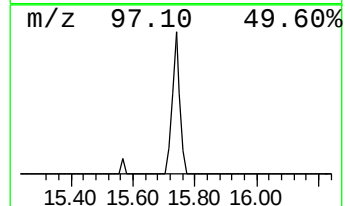
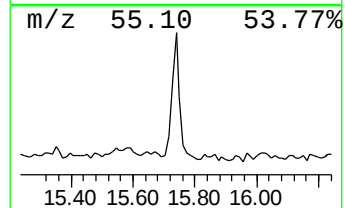
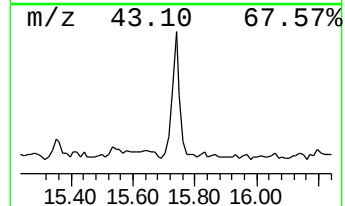
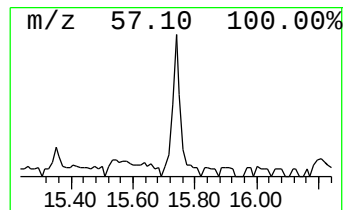
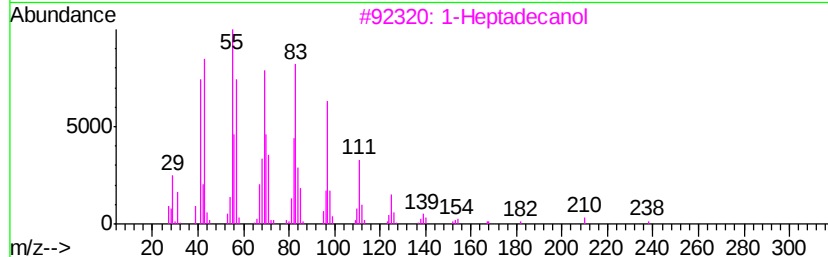
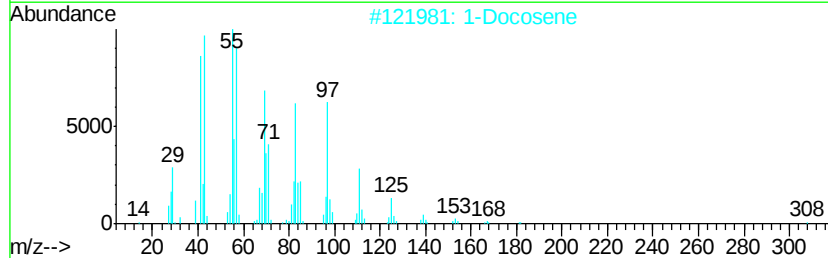
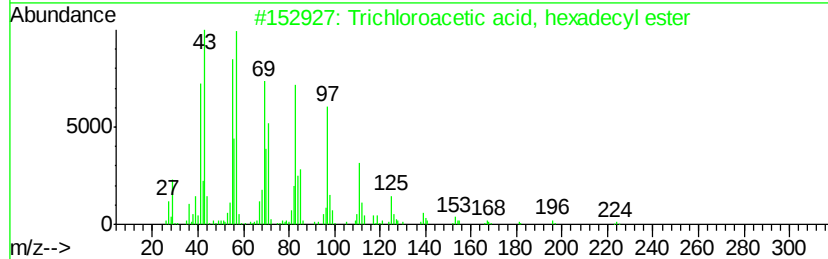
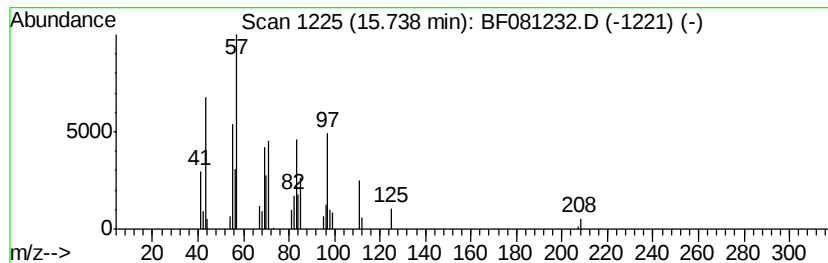
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.76 ng	65320	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	86
2		1-Docosene	308	C22H44	001599-67-3	74
3		1-Heptadecanol	256	C17H36O	001454-85-9	72
4		1-Hexacosanol	382	C26H54O	000506-52-5	72
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082615\
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Operator : UM/IZ
Sample : G3404-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

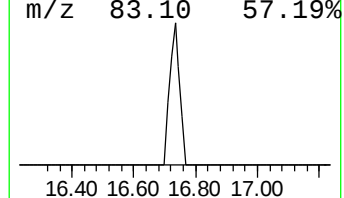
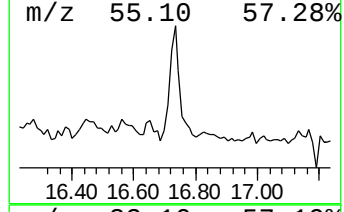
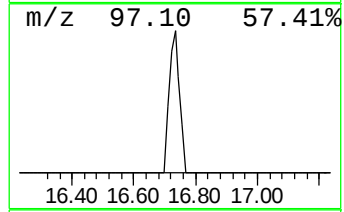
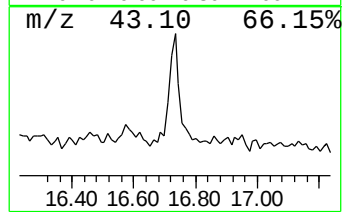
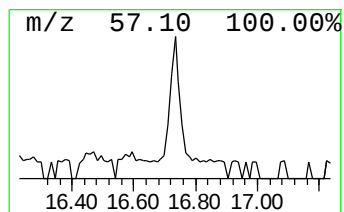
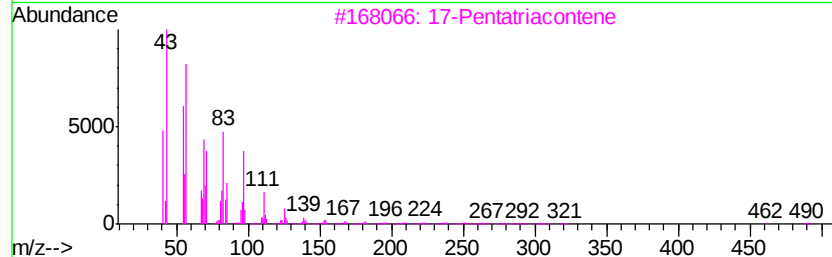
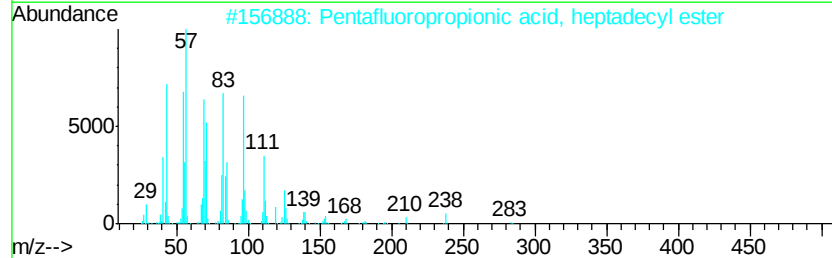
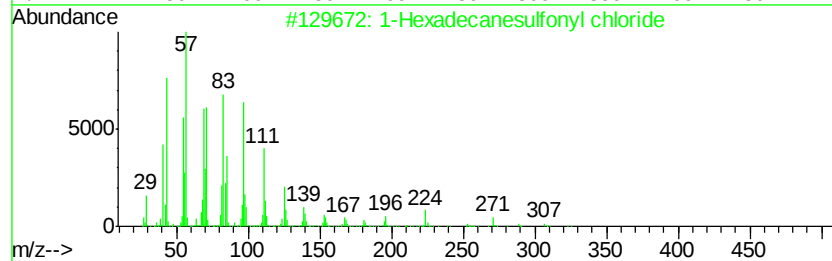
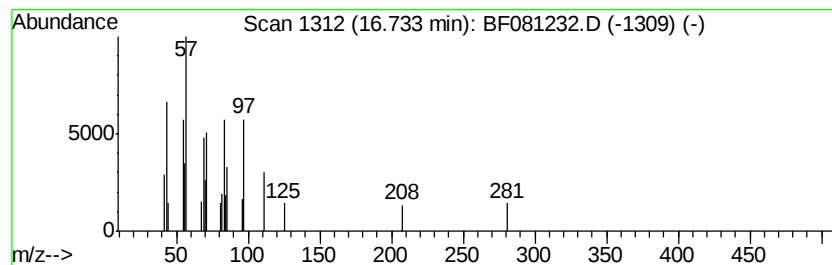
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Hexadecanesulfonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.31 ng	31633	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	86
3		17-Pentatriacontene	491	C35H70	006971-40-0	83
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	74



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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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...	4.61	25.0	ng	416708	1	6.51	333248	20.0
unknown6.27	6.27	73.1	ng	1217500	1	6.51	333248	20.0
Pyridine, 2-butyl...	9.02	8.4	ng	190358	3	9.54	453733	20.0
7,9-Di-tert-butyl...	11.42	2.3	ng	48832	4	11.01	428461	20.0
Undecanoic acid	11.57	6.9	ng	148235	4	11.01	428461	20.0
Tridecanoic acid	12.34	3.4	ng	63956	5	13.62	381440	20.0
Pentafluoropropio...	14.41	2.9	ng	39145	6	14.95	274305	20.0
Trichloroacetic a...	15.74	4.8	ng	65320	6	14.95	274305	20.0
1-Hexadecanesulfo...	16.73	2.3	ng	31633	6	14.95	274305	20.0