

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
 Data File : BF093800.D
 Acq On : 21 Mar 2017 16:09
 Operator : SJ/MA
 Sample : I2314-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SGS47-9-11

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-BF032017.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	2.081	13	17	21	rVB2	76179	110301	2.68%	0.263%
2	4.996	269	272	275	rBV	728504	952009	23.15%	2.266%
3	5.430	307	310	312	rBV	3280645	3803790	92.48%	9.055%
4	5.830	342	345	348	rBV	80836	72009	1.75%	0.171%
5	6.459	397	400	402	rBV	3577029	3872907	94.16%	9.219%
6	6.596	409	412	414	rBV	3642152	3939249	95.77%	9.377%
7	6.824	430	432	434	rBV	1429754	1178772	28.66%	2.806%
8	6.984	443	446	448	rVB	3299142	2959130	71.94%	7.044%
9	7.385	478	481	483	rBV	2402756	2286975	55.60%	5.444%
10	7.476	487	489	498	rVB	34606	44390	1.08%	0.106%
11	8.116	542	545	547	rBV	1130713	1590959	38.68%	3.787%
12	9.190	636	639	641	rBV	4385879	4113236	100.00%	9.791%
13	9.579	671	673	675	rBV	650596	536772	13.05%	1.278%
14	9.865	695	698	700	rBV	1876999	1758997	42.76%	4.187%
15	10.276	732	734	736	rBV	33023	47448	1.15%	0.113%
16	10.311	736	737	738	rVB	87770	60238	1.46%	0.143%
17	10.528	753	756	759	rBV	32538	48114	1.17%	0.115%
18	10.642	763	766	769	rVV2	1945688	2241622	54.50%	5.336%
19	10.779	776	778	782	rBV	128069	146593	3.56%	0.349%
20	11.225	815	817	819	rBV	121040	110965	2.70%	0.264%
21	11.339	825	827	829	rVB	1867544	1602896	38.97%	3.816%
22	11.648	852	854	857	rBV	86306	91072	2.21%	0.217%
23	11.876	872	874	876	rBV	106476	110692	2.69%	0.263%
24	12.928	963	966	968	rBV	3074358	3374582	82.04%	8.033%
25	13.831	1042	1045	1049	rBV	118337	169236	4.11%	0.403%
26	13.968	1054	1057	1059	rBV	1152767	1217378	29.60%	2.898%
27	14.174	1068	1075	1086	rBV2	127509	719724	17.50%	1.713%
28	14.380	1091	1093	1098	rVB4	37505	111223	2.70%	0.265%
29	14.562	1106	1109	1112	rVB	154671	191392	4.65%	0.456%
30	15.374	1177	1180	1183	rBV	784069	965510	23.47%	2.298%
31	15.500	1187	1191	1192	rBV4	15449	42634	1.04%	0.101%
32	15.728	1208	1211	1217	rVB	57008	127647	3.10%	0.304%
33	15.842	1218	1221	1223	rBV	27364	50062	1.22%	0.119%
34	16.311	1259	1262	1273	rVB3	52821	156110	3.80%	0.372%

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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-BF032017.M
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35	16.860	1307	1310	1314	rBV	24755	59988	1.46%	0.143%
36	17.134	1320	1334	1346	rBV2	474717	3027799	73.61%	7.207%
37	17.511	1365	1367	1372	rVB3	30007	70239	1.71%	0.167%
38	18.288	1432	1435	1441	rBV7	15263	46633	1.13%	0.111%

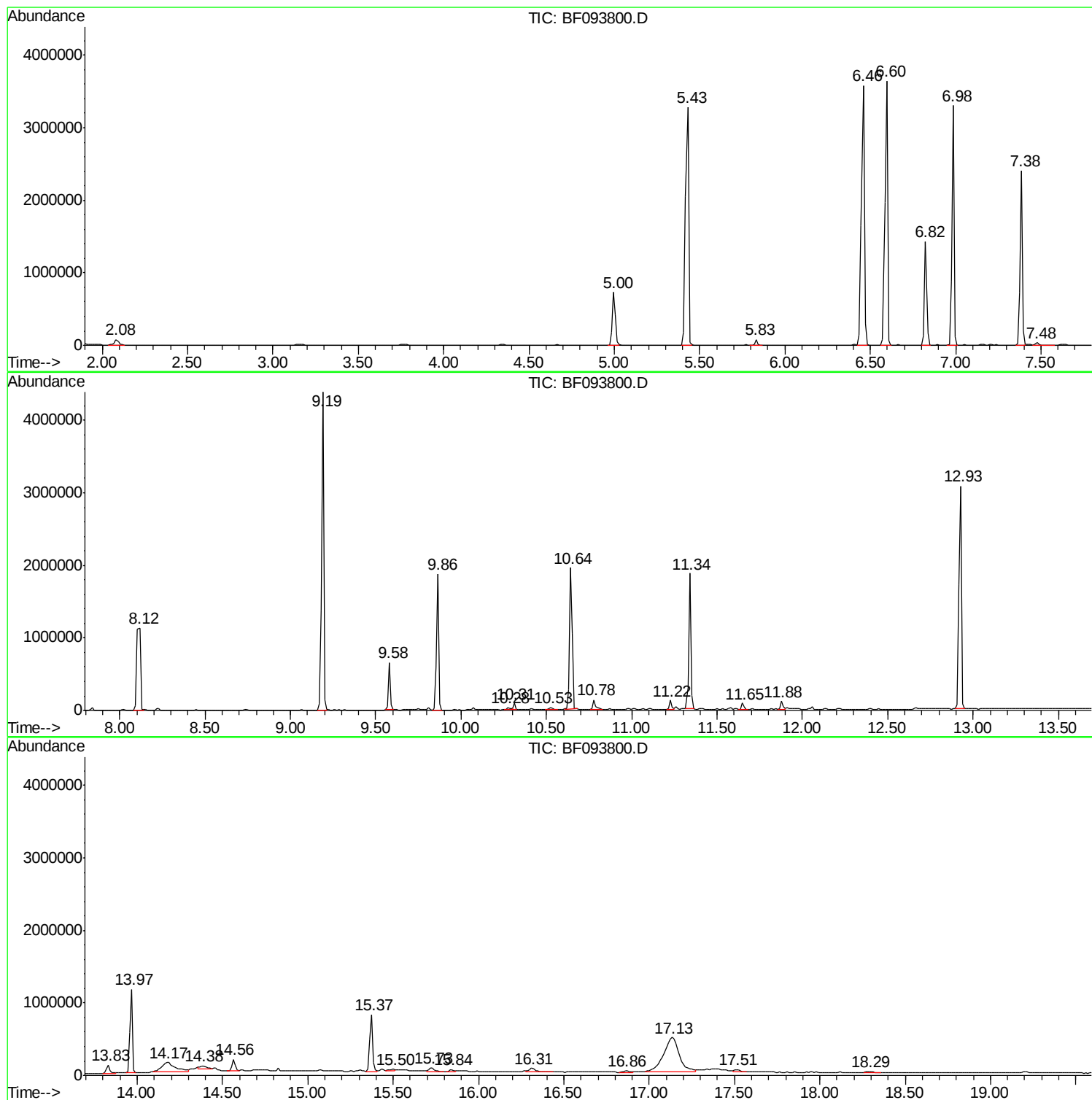
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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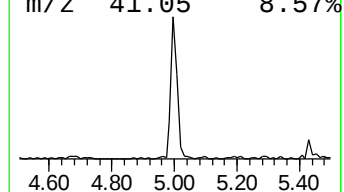
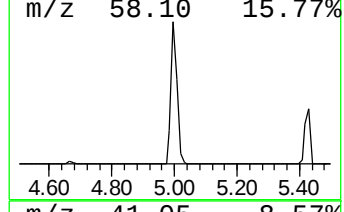
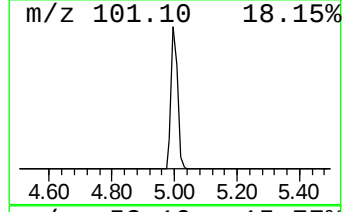
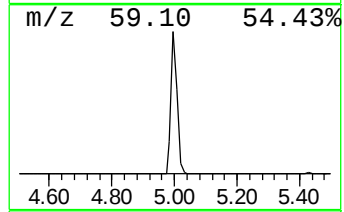
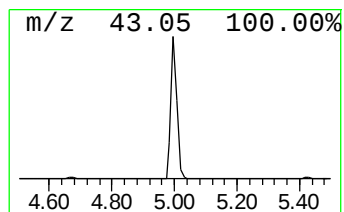
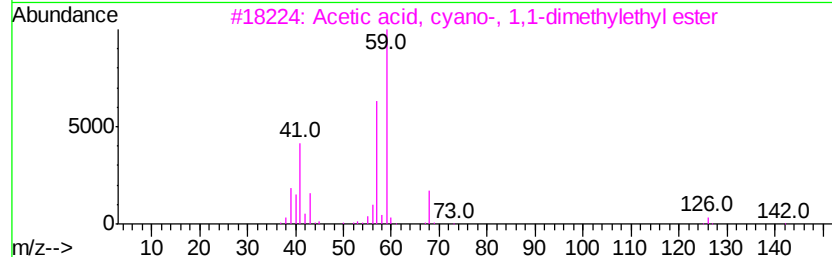
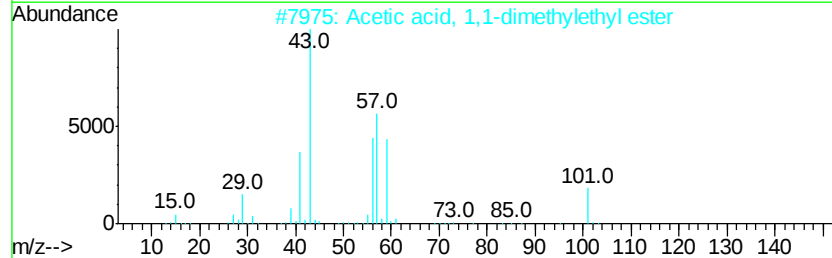
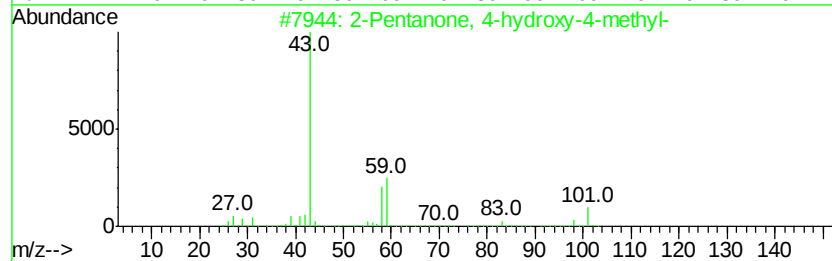
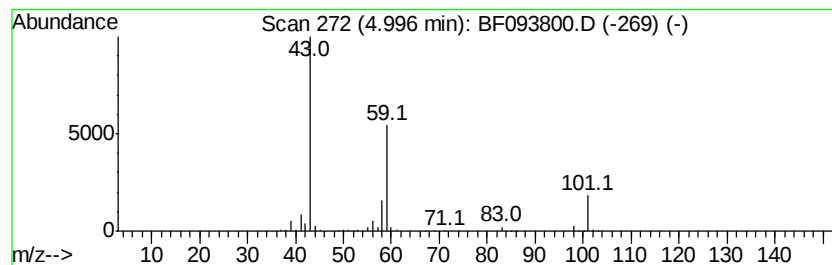
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	16.15 ng	952009	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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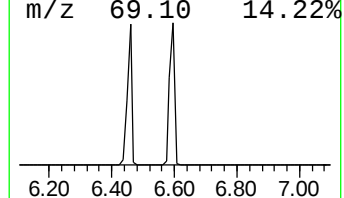
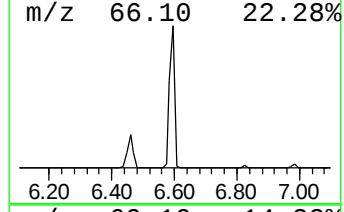
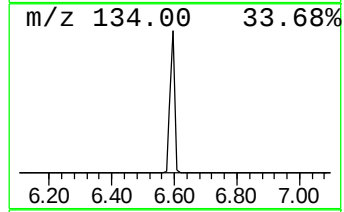
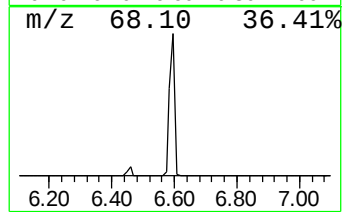
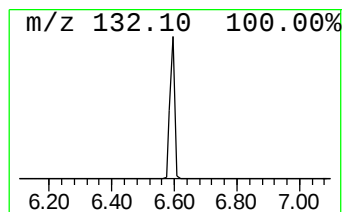
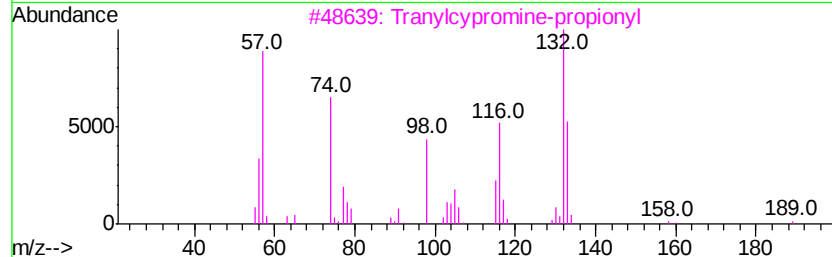
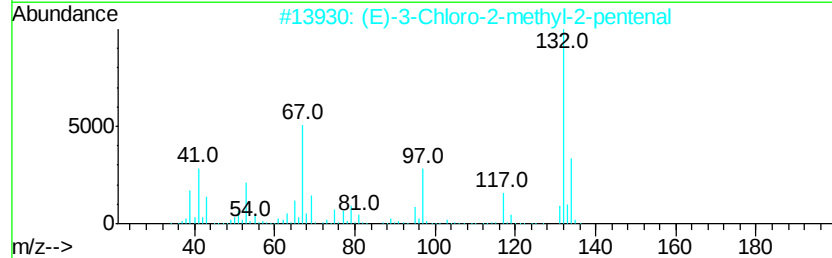
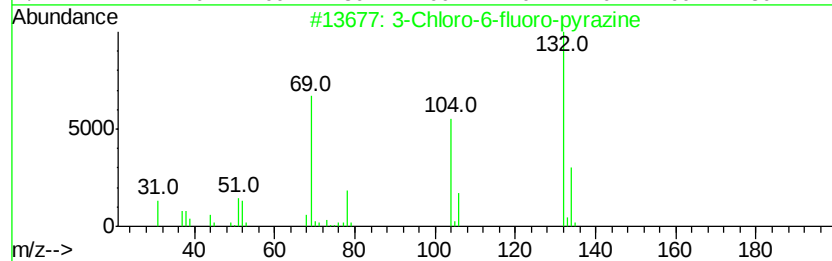
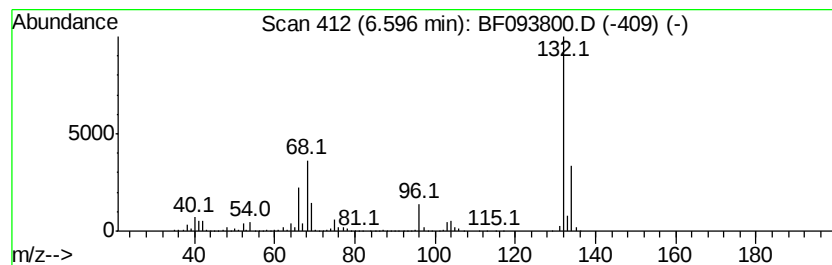
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	66.84 ng	3939250	1,4-Dichlorobenzene-d4	6.82

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		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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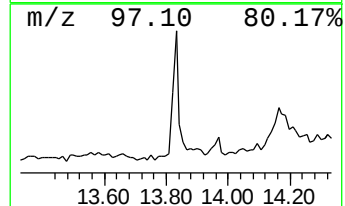
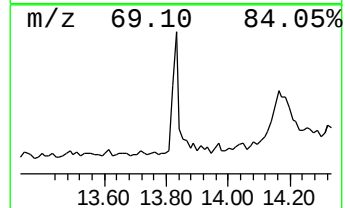
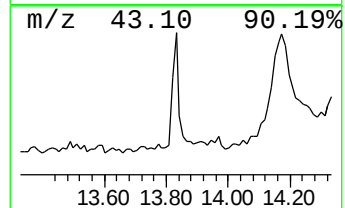
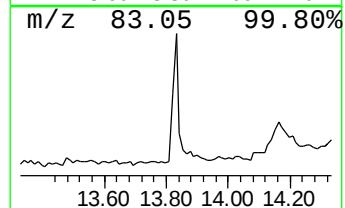
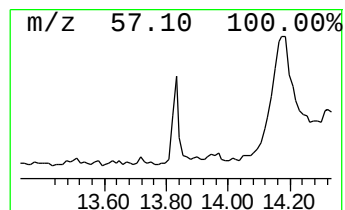
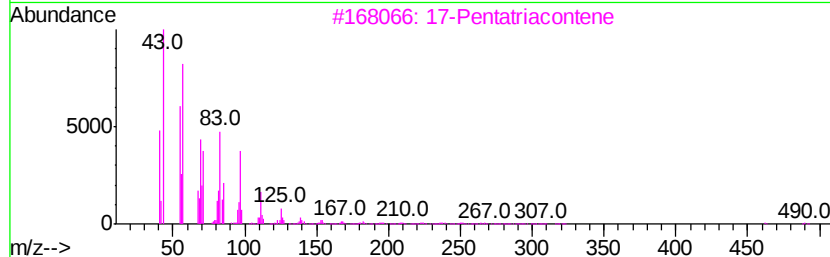
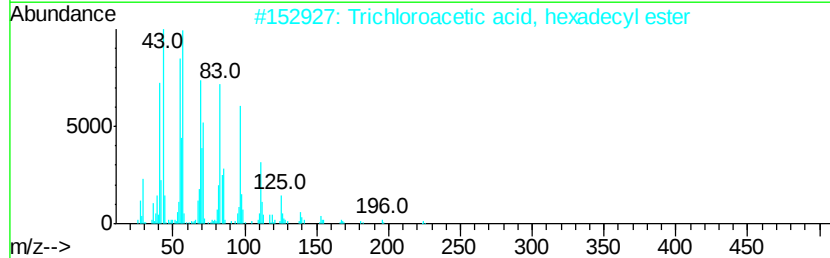
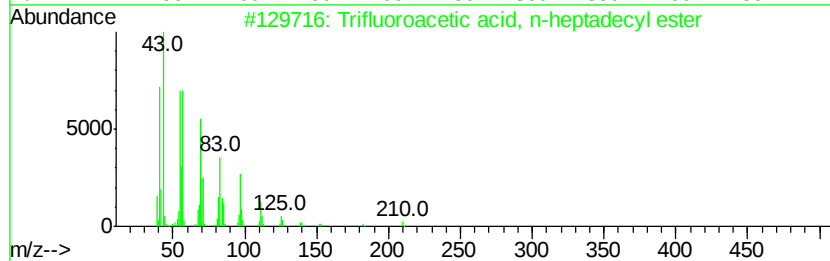
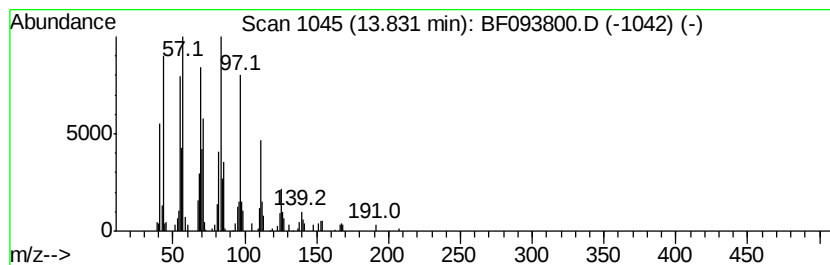
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetic acid, n-hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.78 ng	169236	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3		17-Pentatriacontene	491	C35H70	006971-40-0	86
4		Pentafluoropropionic acid, tride...	346	C16H27F5O2	1000280-07-3	80
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62



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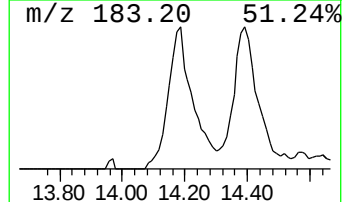
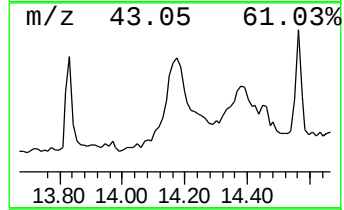
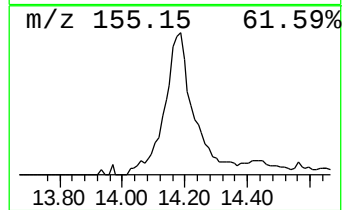
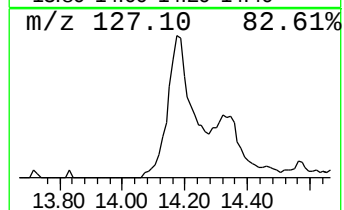
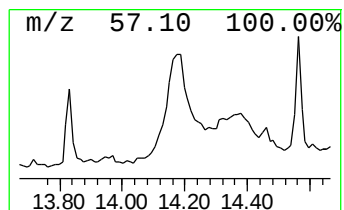
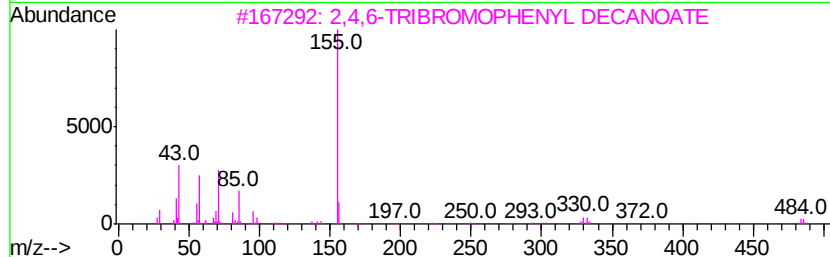
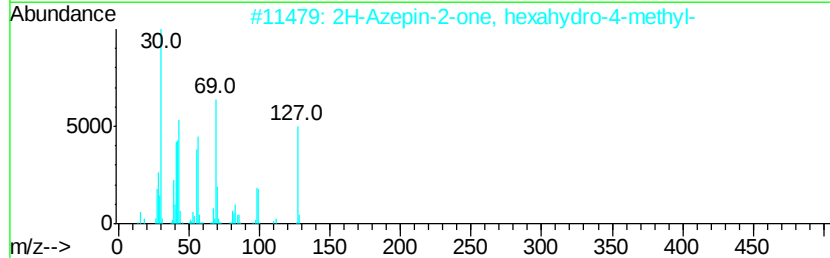
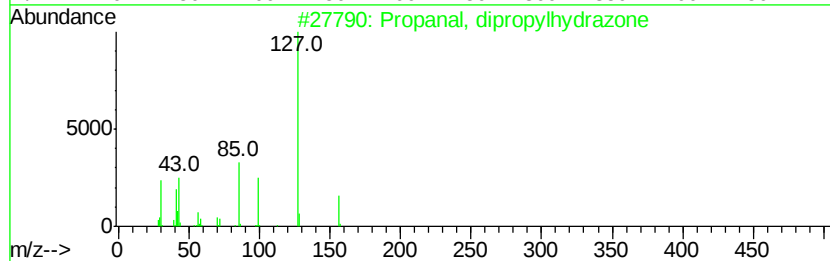
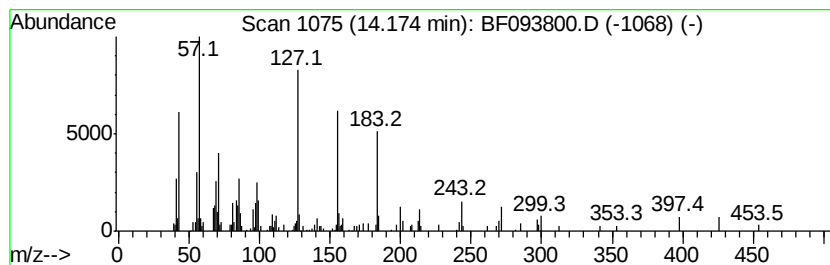
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown14.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	11.82 ng	719724	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, dipropylhydrazone	156	C9H20N2	034687-35-9	30
2		2H-Azepin-2-one, hexahydro-4-met...	127	C7H13NO	003623-05-0	27
3		2,4,6-TRIBROMOPHENYL DECANOATE	482	C16H21Br3O2	1000233-09-1	27
4		3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	25
5		2,2,7-Trimethyloctane-3,5-dione,...	184	C11H20O2	1000202-25-0	25



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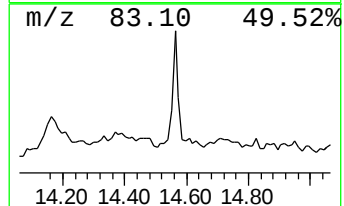
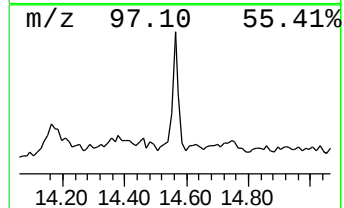
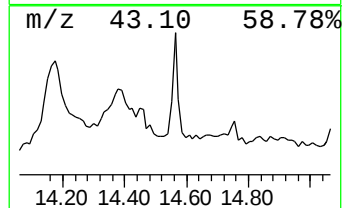
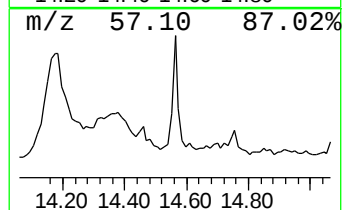
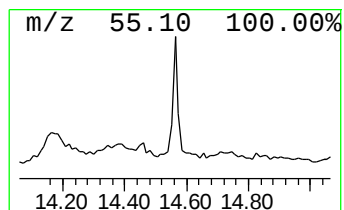
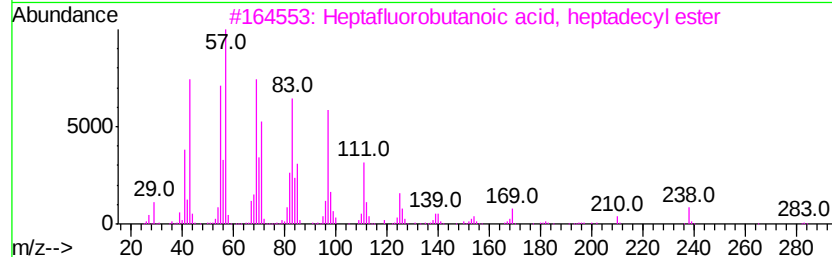
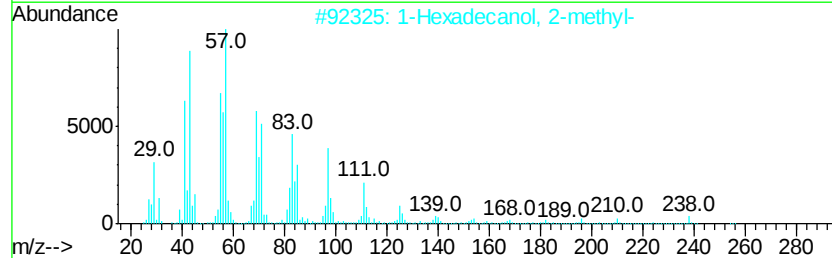
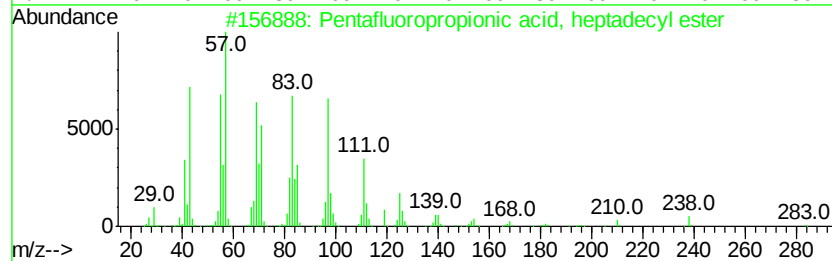
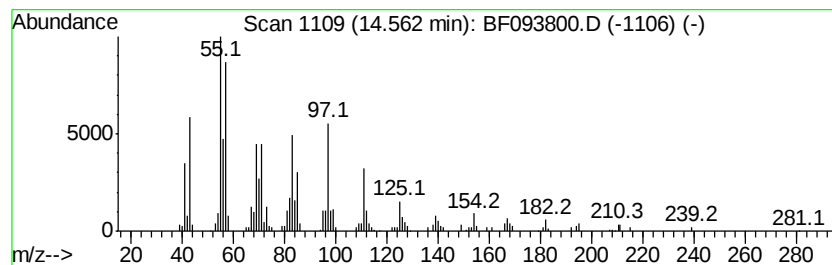
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.14 ng	191392	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
2		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	72
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	64
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	62
5		Cyclohexanone, 3-methyl-2-(1-met...	154	C10H18O	028357-23-5	60



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093800.D
Acq On : 21 Mar 2017 16:09
Operator : SJ/MA
Sample : I2314-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SGS47-9-11

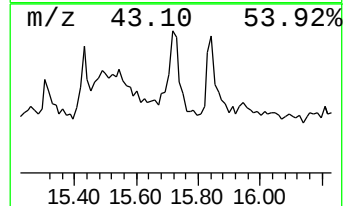
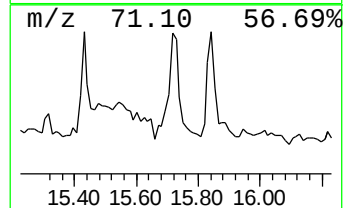
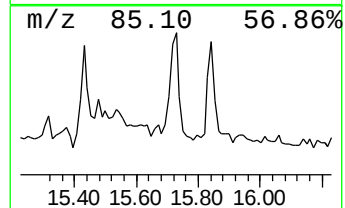
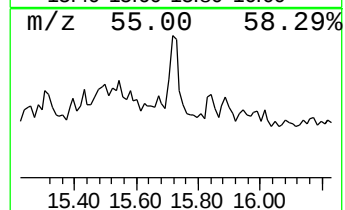
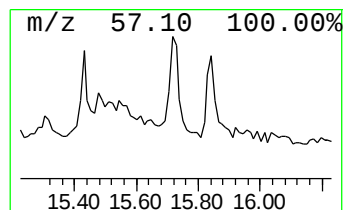
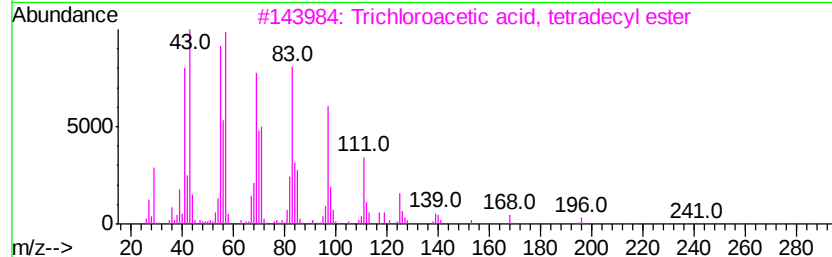
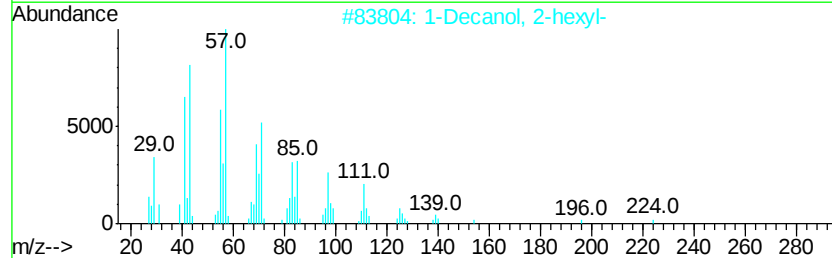
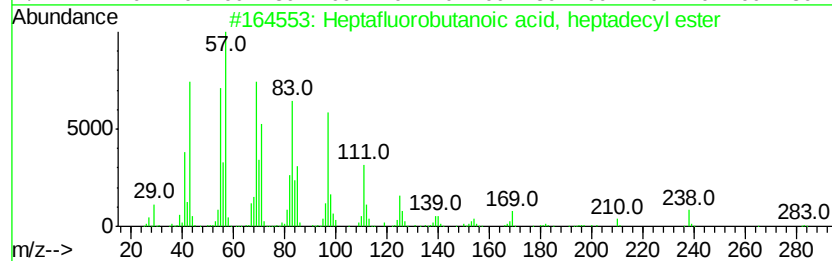
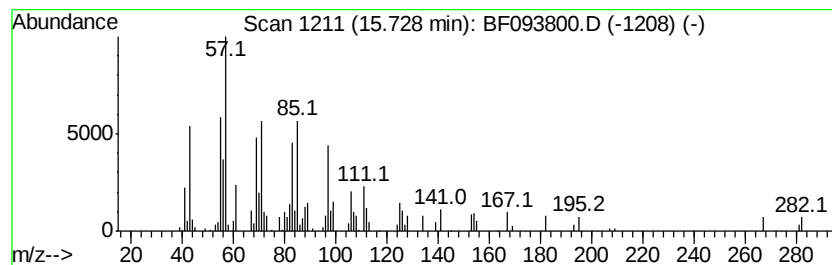
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.73 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.64 ng	127647	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	46
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	46
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	43
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	43
5		Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093800.D
Acq On : 21 Mar 2017 16:09
Operator : SJ/MA
Sample : I2314-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SGS47-9-11

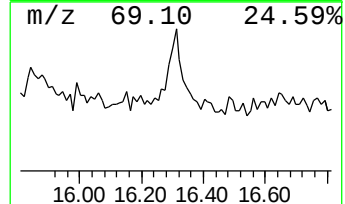
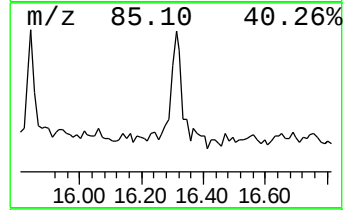
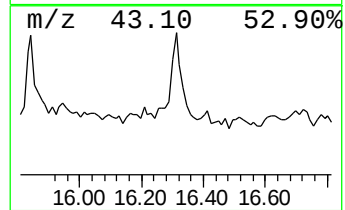
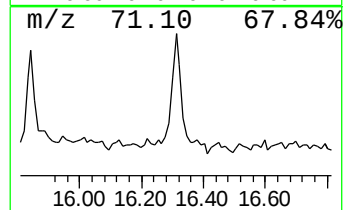
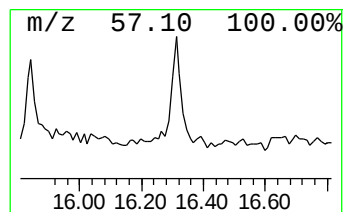
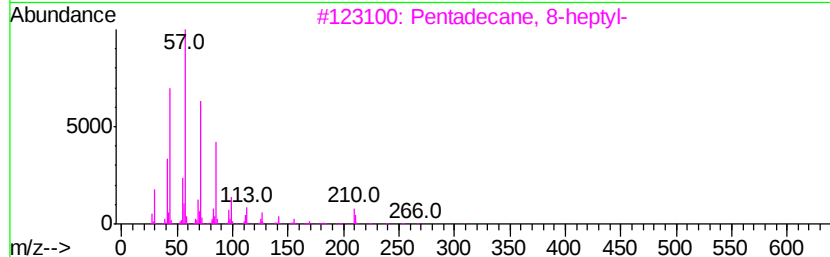
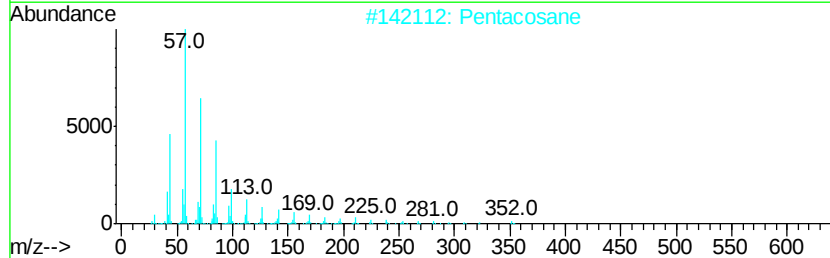
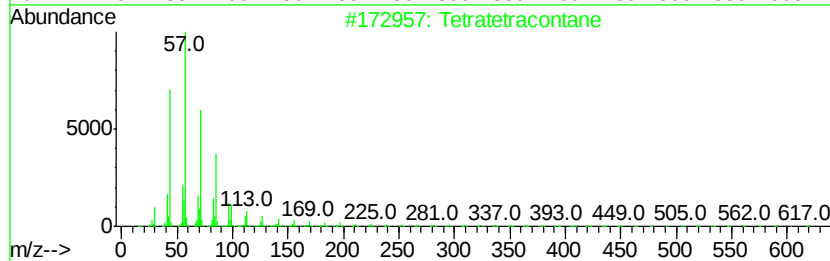
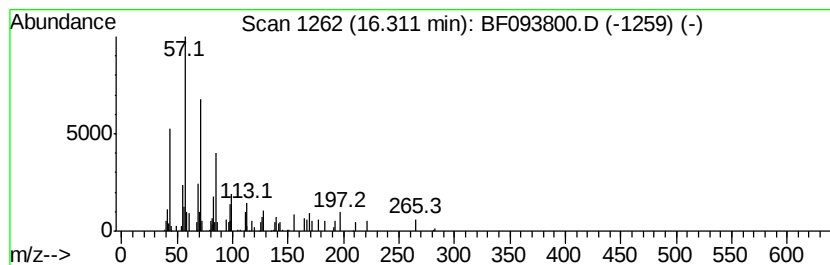
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	3.23 ng	156110	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	86
2		Pentacosane	352	C25H52	000629-99-2	80
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
4		Heptacosane	380	C27H56	000593-49-7	80
5		Hentriacontane	437	C31H64	000630-04-6	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093800.D
Acq On : 21 Mar 2017 16:09
Operator : SJ/MA
Sample : I2314-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SGS47-9-11

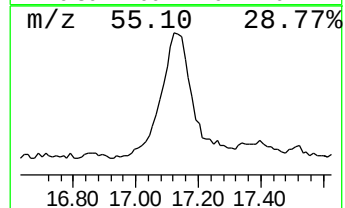
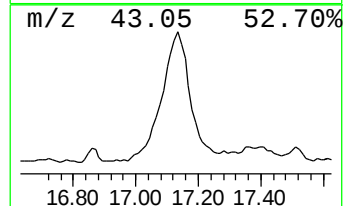
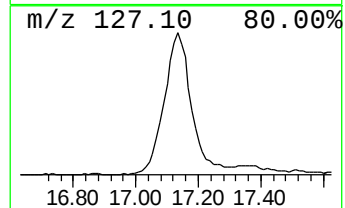
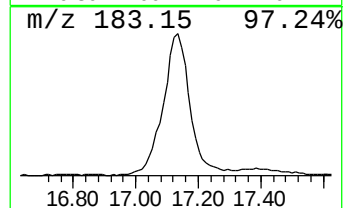
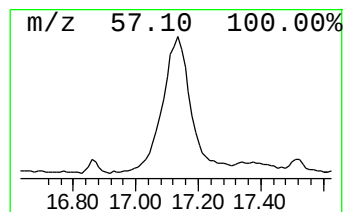
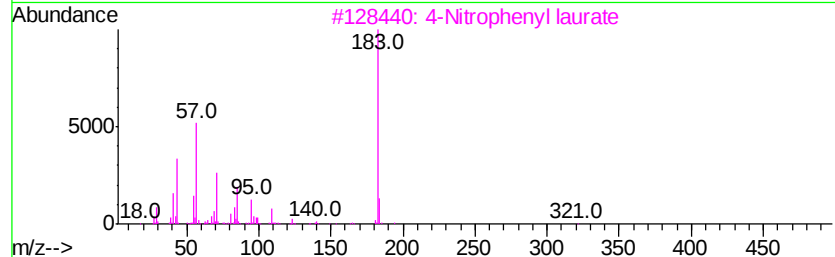
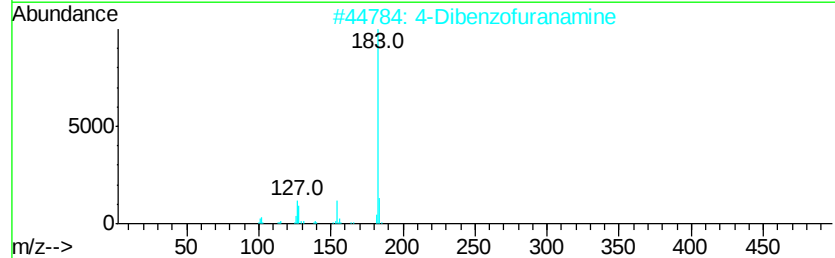
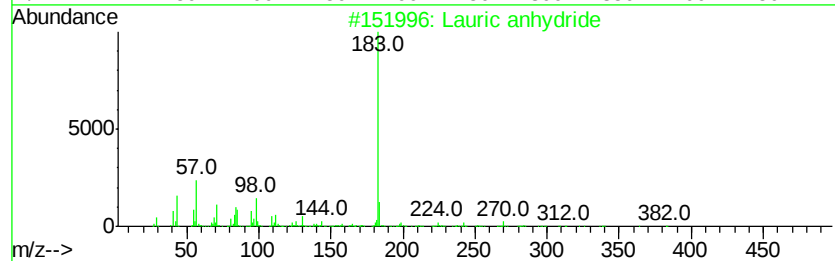
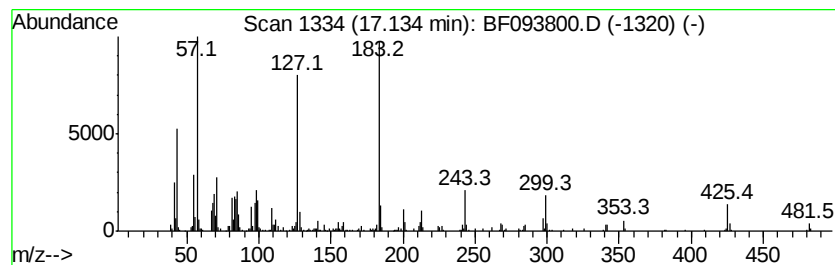
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	62.72 ng	3027800	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Lauric anhydride	382	C24H46O3	000645-66-9	41
2		4-Dibenzofuranamine	183	C12H9NO	050548-43-1	38
3		4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	35
4		3-Dibenzofuranamine	183	C12H9NO	004106-66-5	35
5		Pyrrolidine, 1-(7-oxo-2,4,6-trim...	239	C14H25NO2	1000197-25-1	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093800.D
Acq On : 21 Mar 2017 16:09
Operator : SJ/MA
Sample : I2314-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SGS47-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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...	5.00	16.1	ng	952009	1	6.82	1178770	20.0
unknown6.60	6.60	66.8	ng	3939250	1	6.82	1178770	20.0
Trifluoroacetic a...	13.83	2.8	ng	169236	5	13.97	1217380	20.0
unknown14.17	14.17	11.8	ng	719724	5	13.97	1217380	20.0
Pentafluoropropio...	14.56	3.1	ng	191392	5	13.97	1217380	20.0
unknown15.73	15.73	2.6	ng	127647	6	15.37	965510	20.0
Tetratetracontane	16.31	3.2	ng	156110	6	15.37	965510	20.0
unknown17.13	17.13	62.7	ng	3027800	6	15.37	965510	20.0