

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098807.D
 Acq On : 26 Sep 2017 2:46
 Operator : SJ/JU
 Sample : I5395-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4-(0-5)

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	2.234	21	25	38	rVB	74111	117435	2.23%	0.269%
2	5.157	517	522	536	rVB	633930	1031166	19.57%	2.360%
3	5.545	581	588	591	rBV	4148827	4989530	94.68%	11.422%
4	6.545	751	758	761	rBV	3981190	5209006	98.85%	11.924%
5	6.687	777	782	785	rBV	4383992	5079354	96.39%	11.627%
6	6.916	817	821	824	rVB	1190184	945592	17.94%	2.165%
7	7.075	843	848	851	rBV	3999680	3718263	70.56%	8.511%
8	7.481	911	917	920	rBV	3043975	3252367	61.72%	7.445%
9	8.198	1034	1039	1042	rBV	1444634	1283671	24.36%	2.938%
10	9.275	1216	1222	1225	rBV	5180180	5269640	100.00%	12.063%
11	9.657	1284	1287	1291	rBV	582360	530062	10.06%	1.213%
12	9.816	1311	1314	1316	rBV2	72698	69445	1.32%	0.159%
13	9.863	1319	1322	1326	rVB2	100871	114256	2.17%	0.262%
14	9.951	1332	1337	1340	rBV2	1601206	1412164	26.80%	3.233%
15	10.357	1403	1406	1411	rBV3	149193	215345	4.09%	0.493%
16	10.745	1467	1472	1475	rBV	2596209	2620616	49.73%	5.999%
17	10.857	1487	1491	1494	rBV	181420	244863	4.65%	0.561%
18	11.439	1586	1590	1593	rBV	1497332	1303918	24.74%	2.985%
19	11.463	1593	1594	1599	rVB	196997	113572	2.16%	0.260%
20	12.651	1793	1796	1802	rVB	159279	137663	2.61%	0.315%
21	12.880	1833	1835	1838	rVB	115954	89632	1.70%	0.205%
22	13.027	1855	1860	1863	rVB	3699765	3678832	69.81%	8.421%
23	13.451	1929	1932	1935	rBV	182047	159047	3.02%	0.364%
24	13.480	1935	1937	1943	rVB3	78432	91841	1.74%	0.210%
25	13.904	2006	2009	2014	rBV	204341	186613	3.54%	0.427%
26	14.074	2034	2038	2041	rBV	918024	866012	16.43%	1.982%
27	14.539	2114	2117	2123	rVB4	57153	71482	1.36%	0.164%
28	15.568	2287	2292	2304	rVB	655222	883919	16.77%	2.023%

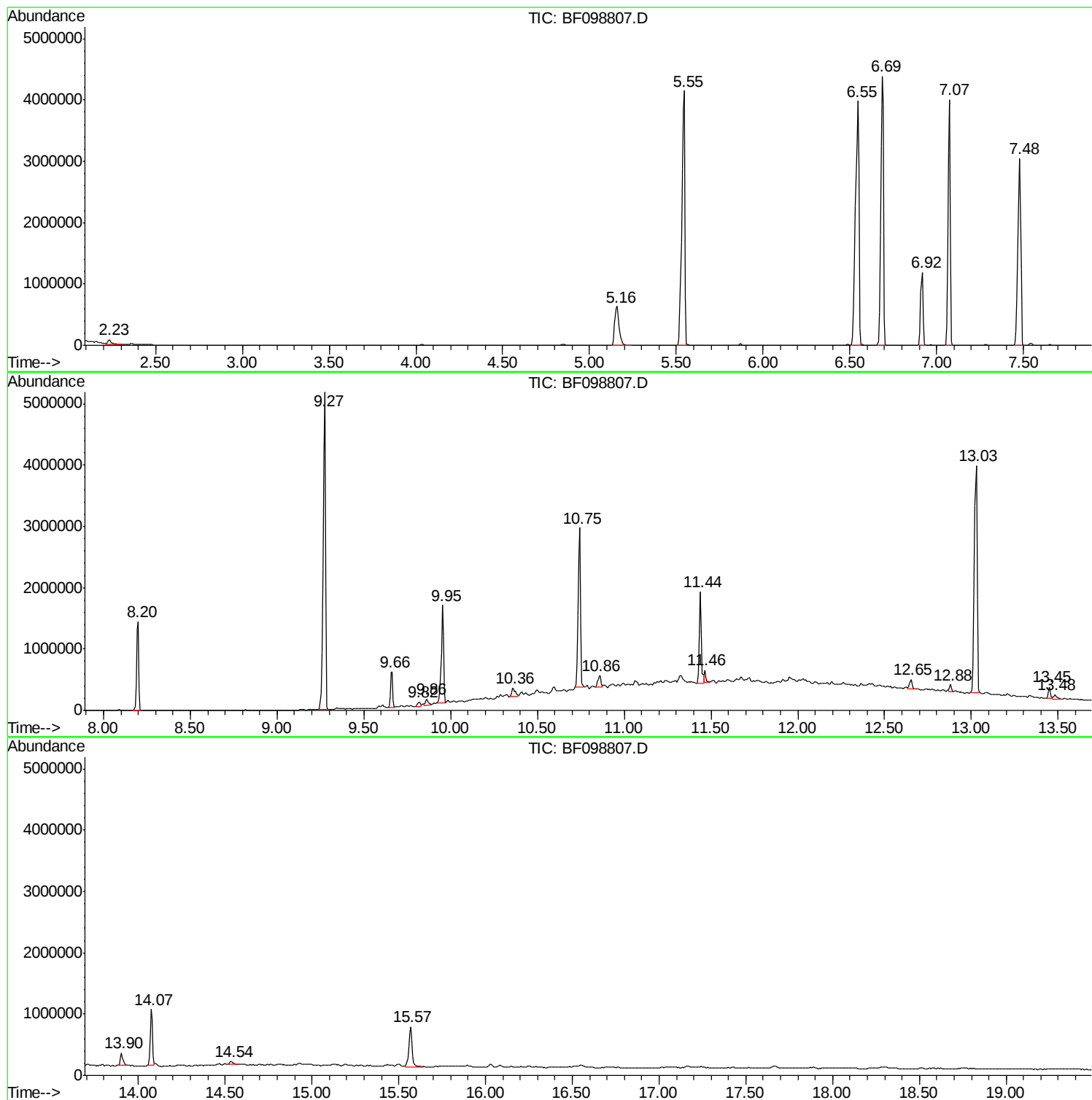
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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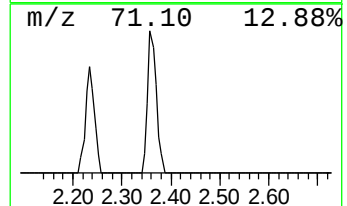
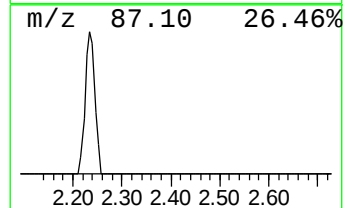
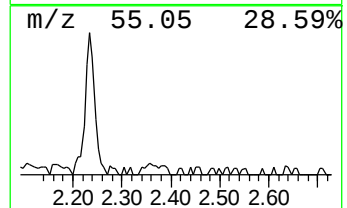
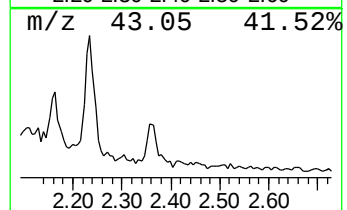
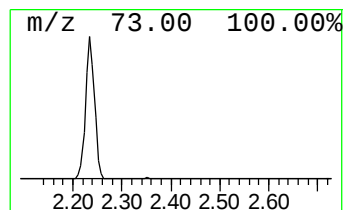
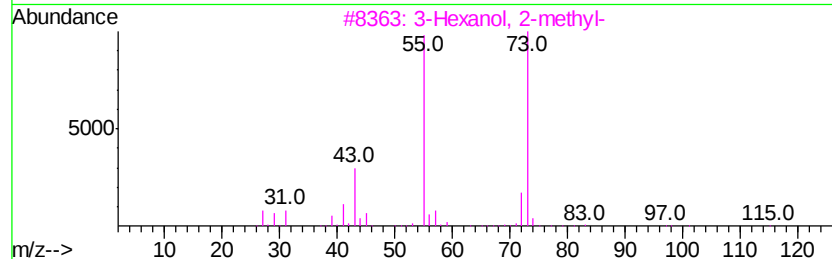
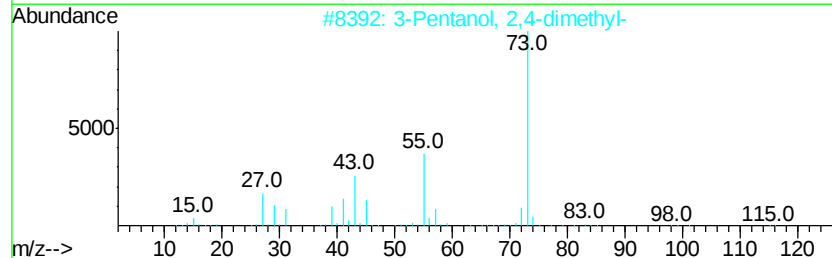
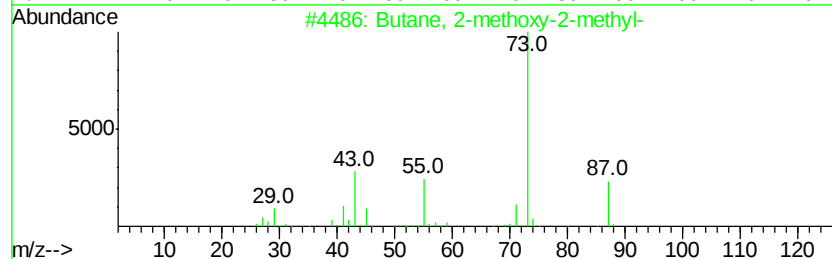
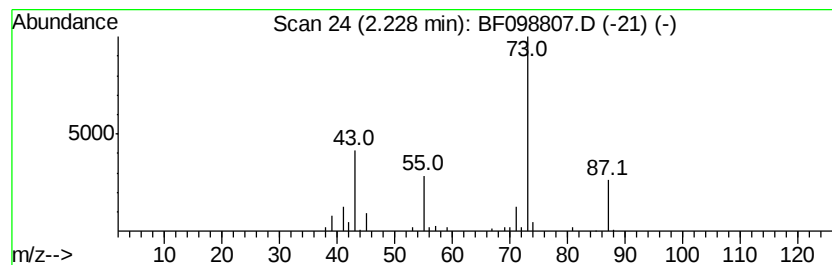
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	2.48 ng	117435	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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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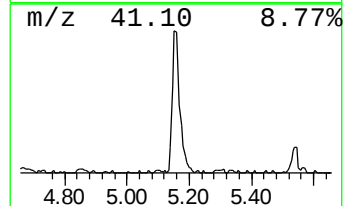
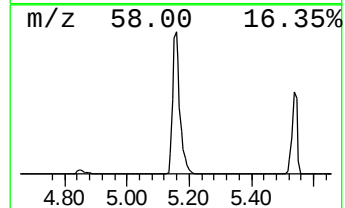
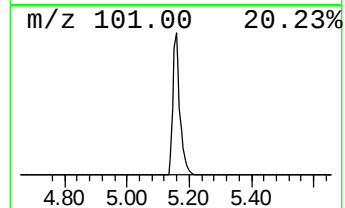
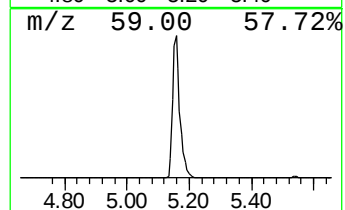
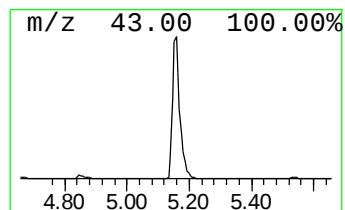
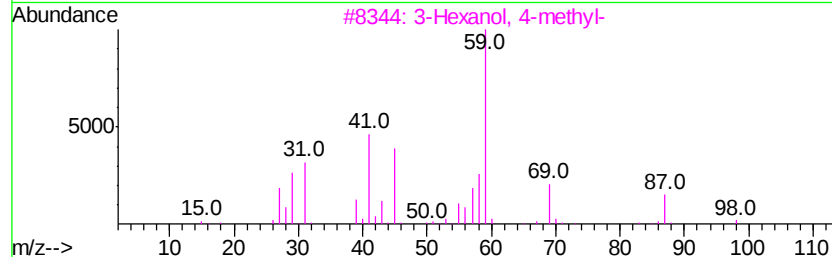
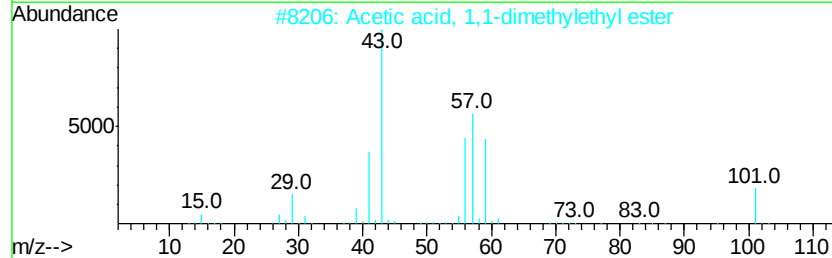
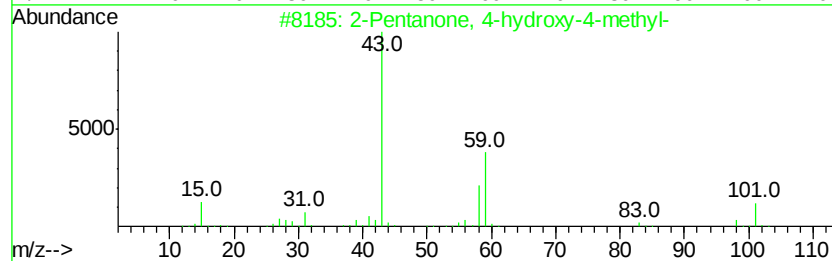
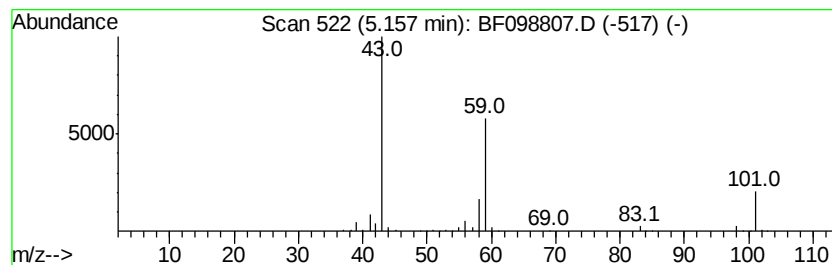
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	21.81 ng	1031170	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	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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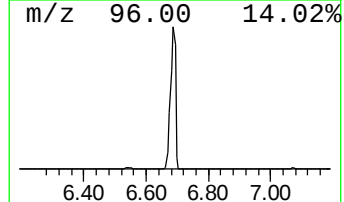
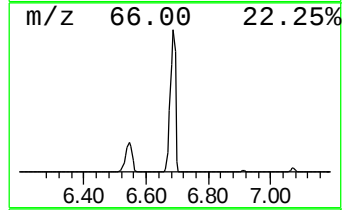
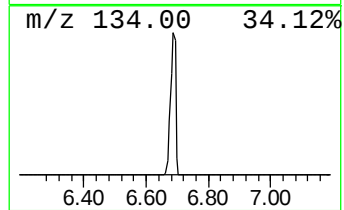
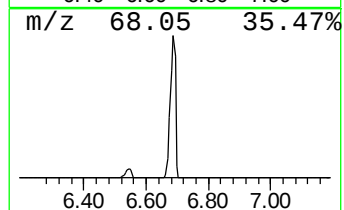
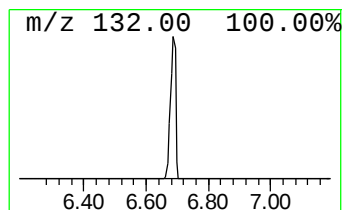
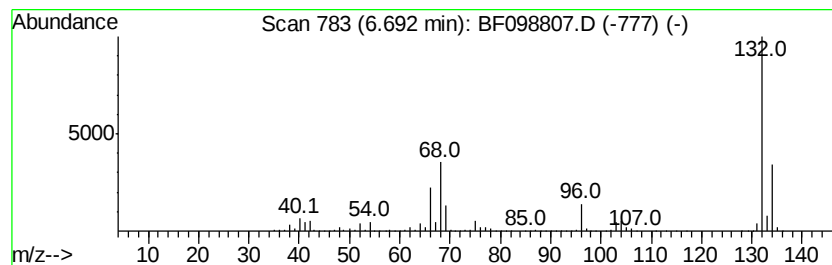
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	107.43 ng	5079350	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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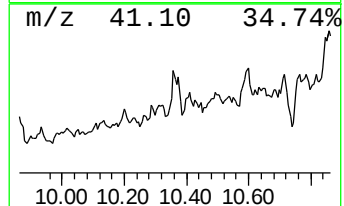
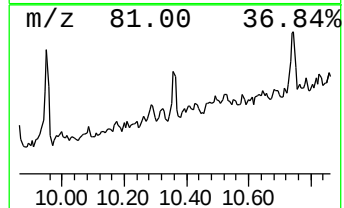
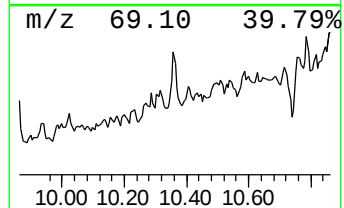
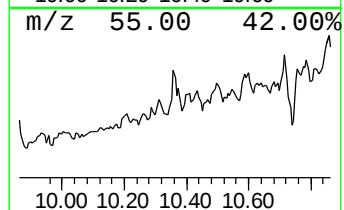
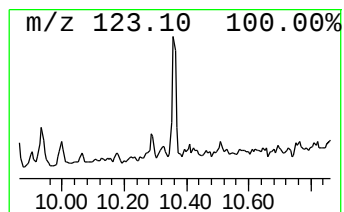
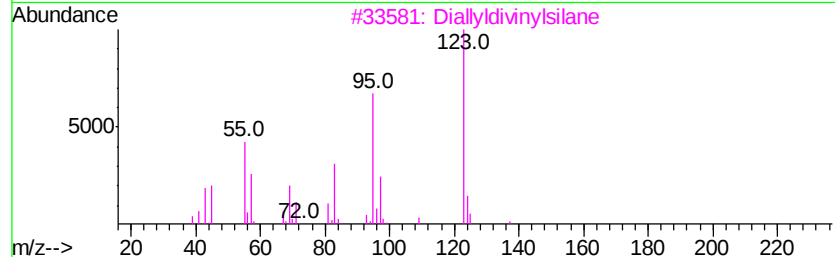
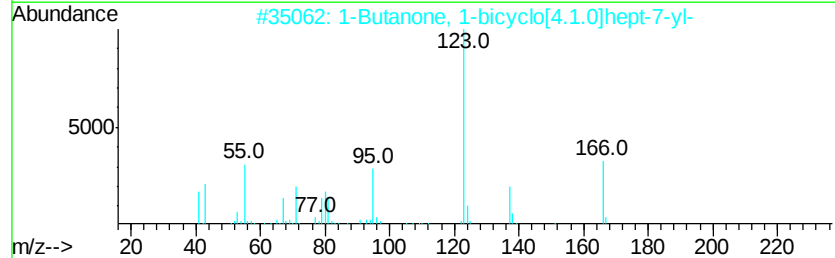
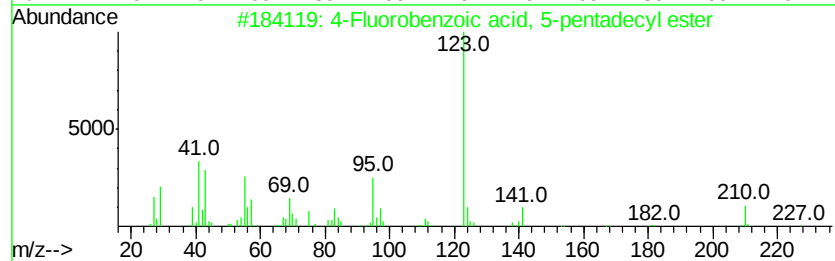
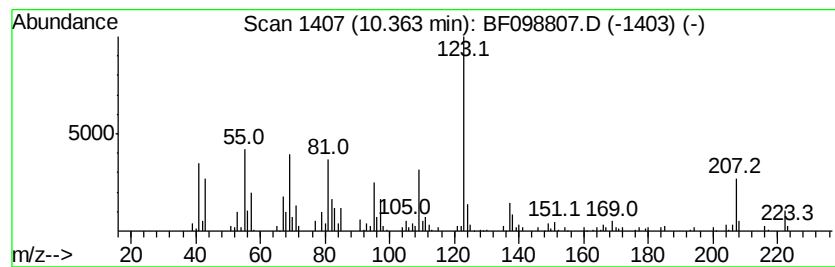
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Fluorobenzoic acid, 5-pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.36	3.05 ng	215345	Acenaphthene-d10	9.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluorobenzoic acid, 5-pentadec...	350	C22H35F02	1000280-68-6	52
2	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	50
3	Diallyldivinylsilane	164	C10H16Si	119901-88-1	50
4	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	49
5	4-Fluorobenzoic acid, 3-methylbu...	208	C12H13F02	1000299-15-1	49



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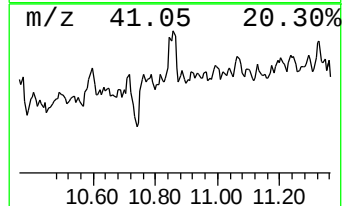
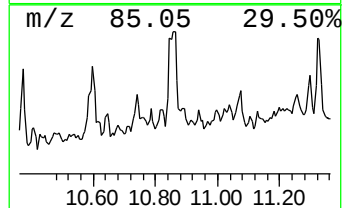
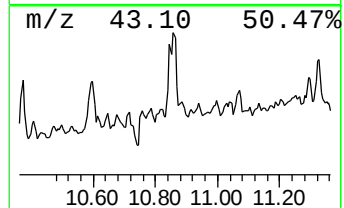
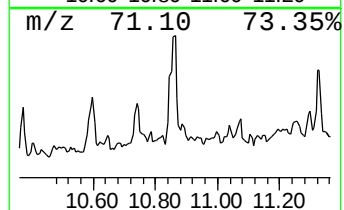
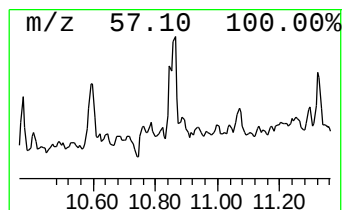
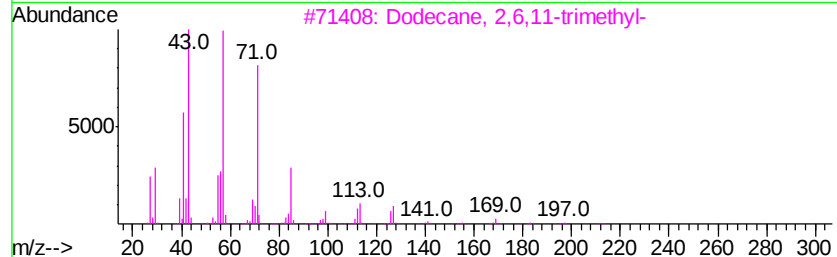
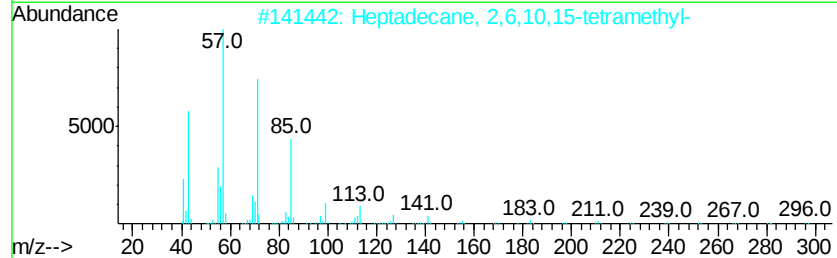
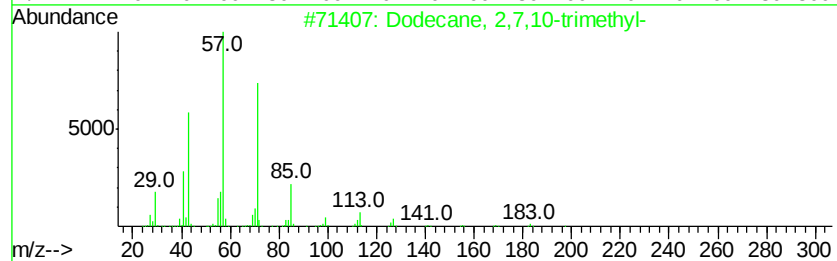
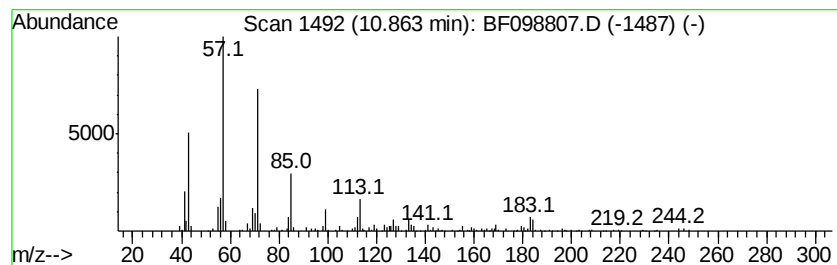
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane, 2,7,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	3.76 ng	244863	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5		Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	80



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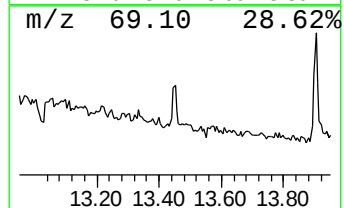
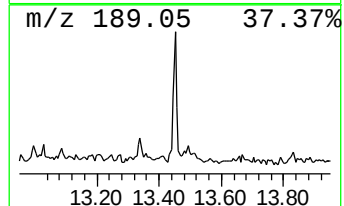
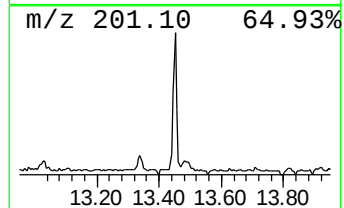
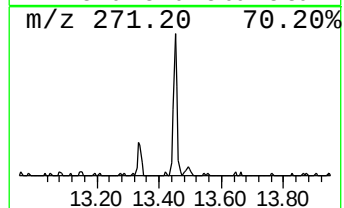
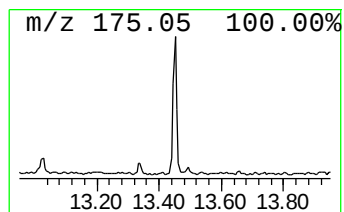
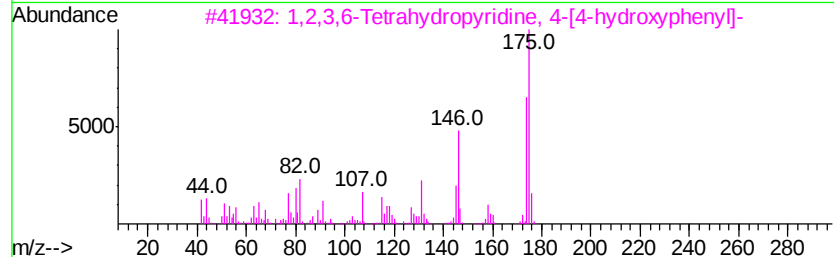
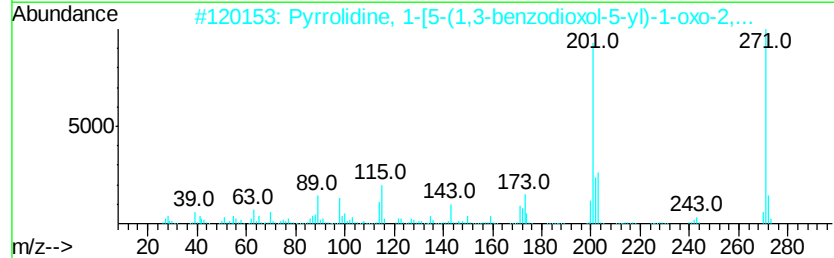
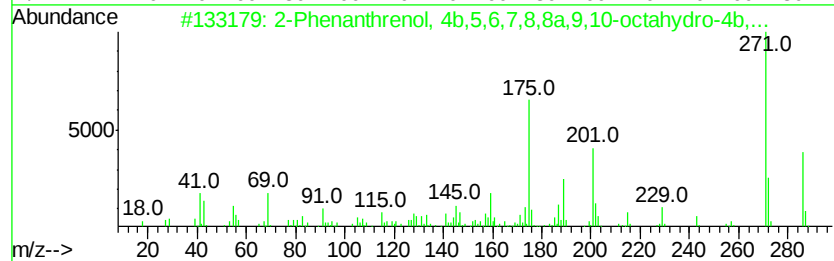
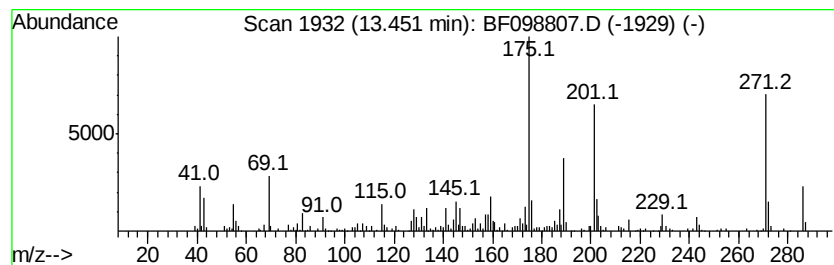
Instrument :
BNA_F
ClientSampleId :
TP-4-(0-5)

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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 8 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.45	3.67 ng	159047	Chrysene-d12	14.07		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	60	
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	30	
3	1,2,3,6-Tetrahydro-4H-pyridine, 4-[4...	175	C11H13NO	090684-15-4	25	
4	1,2-Naphthalenedione, 6-hydroxyv...	244	C15H16O3	007715-96-0	25	
5	Benzene, 1,4-dimethyl-2,5-bis(1-...	190	C14H22	010375-96-9	22	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098807.D
Acq On : 26 Sep 2017 2:46
Operator : SJ/JU
Sample : I5395-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4-(0-5)

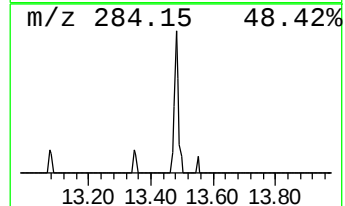
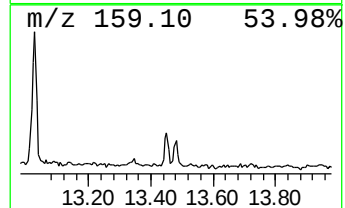
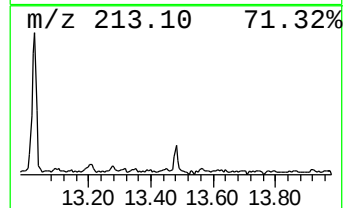
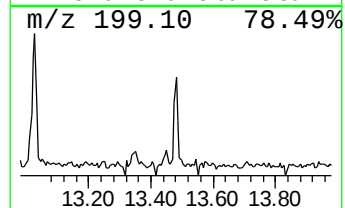
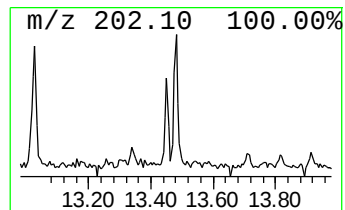
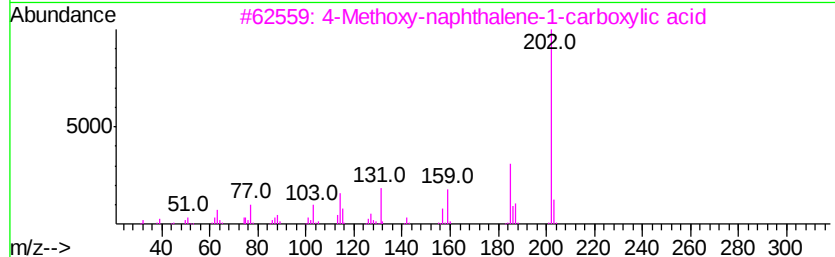
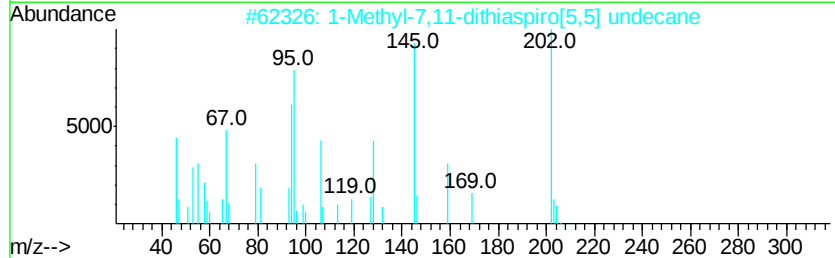
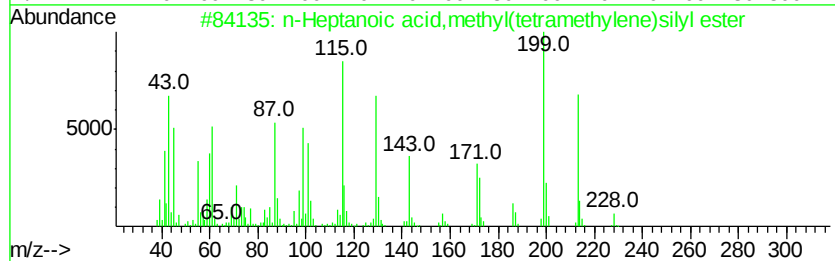
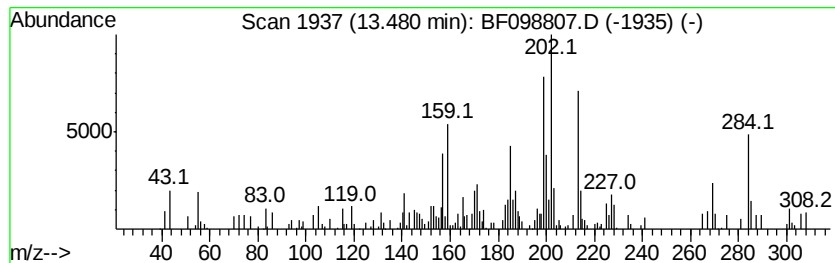
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.48 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.12 ng	91841	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Heptanoic acid,methyl(tetramet...	228	C12H24O2Si	1000217-03-6	30
2		1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	25
3		4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	22
4		Pyrimidine-2,4(3H,5H)-dione, 6-m...	242	C11H18N2O2S	105916-31-2	22
5		Ethanone, 1-(2'-fluoro[1,1'-biph...	214	C14H11FO	000345-55-1	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4-(0-5)

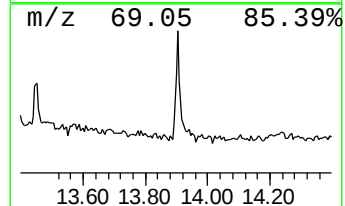
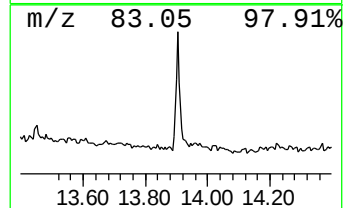
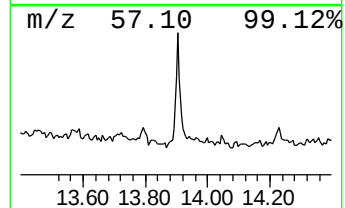
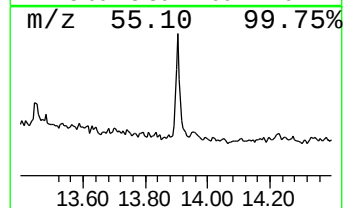
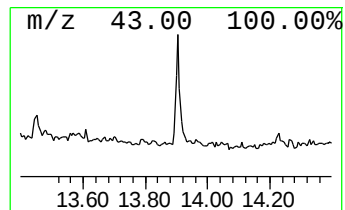
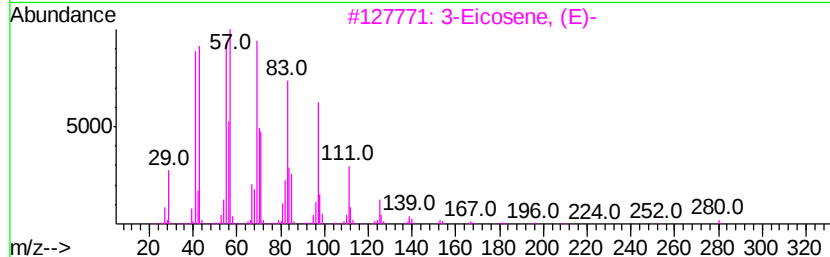
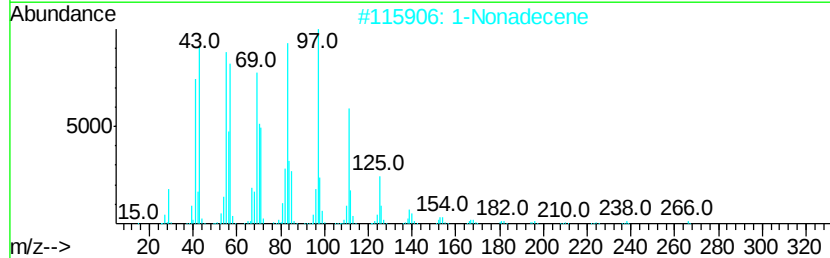
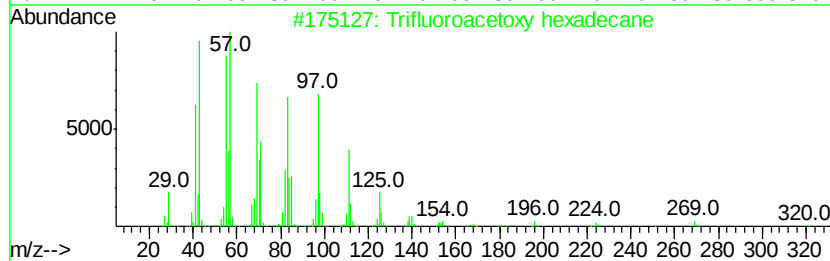
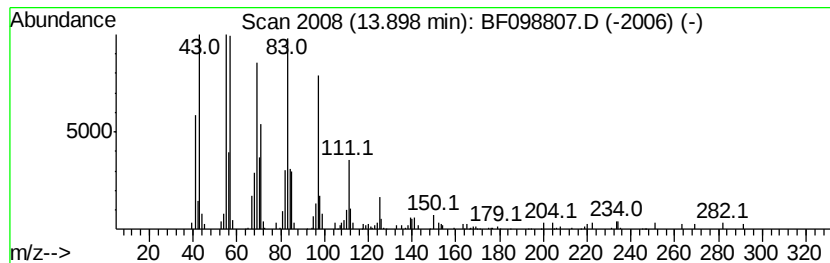
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.31 ng	186613	Chrysene-d12	14.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



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Sample : I5395-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4-(0-5)

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...	2.23	2.5	ng	117435	1	6.92	945592	20.0
2-Pentanone, 4-hy...	5.16	21.8	ng	1031170	1	6.92	945592	20.0
unknown6.69	6.69	107.4	ng	5079350	1	6.92	945592	20.0
4-Fluorobenzoic a...	10.36	3.0	ng	215345	3	9.95	1412160	20.0
Dodecane, 2,7,10-...	10.86	3.8	ng	244863	4	11.44	1303920	20.0
2-Phenanthrenol, ...	13.45	3.7	ng	159047	5	14.07	866012	20.0
unknown13.48	13.48	2.1	ng	91841	5	14.07	866012	20.0
Trifluoroacetoxy ...	13.90	4.3	ng	186613	5	14.07	866012	20.0