

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
 Data File : BF090470.D
 Acq On : 8 Oct 2016 6:27
 Operator : UM/SJ
 Sample : H5136-01
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 100516-01

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-BF100516.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	3.057	60	63	68	rVB	54644	91447	1.14%	0.126%
2	5.194	247	250	255	rBV	1272525	1683667	20.95%	2.320%
3	5.606	283	286	288	rBV	5451533	5827887	72.53%	8.030%
4	6.577	368	371	372	rBV	62386	80993	1.01%	0.112%
5	6.623	372	375	377	rVB	5544864	6285955	78.23%	8.661%
6	6.760	384	387	389	rBV	6572311	6700917	83.40%	9.233%
7	6.989	404	407	409	rBV	1507897	1529228	19.03%	2.107%
8	7.149	418	421	423	rVB	4467806	5202991	64.75%	7.169%
9	7.549	453	456	458	rBV	3888245	4036897	50.24%	5.562%
10	7.640	461	464	467	rVB	136348	181482	2.26%	0.250%
11	7.994	491	495	498	rBV3	51274	100097	1.25%	0.138%
12	8.269	517	519	522	rBV	1590467	1932378	24.05%	2.663%
13	9.355	611	614	616	rBV	7406701	7135711	88.81%	9.832%
14	9.743	646	648	650	rBV	1647475	2253740	28.05%	3.105%
15	10.040	671	674	676	rVB	2149038	2363110	29.41%	3.256%
16	10.463	707	711	713	rBV	109487	136554	1.70%	0.188%
17	10.829	740	743	745	rBV	4756038	4642576	57.78%	6.397%
18	10.943	749	753	758	rBV	166514	230544	2.87%	0.318%
19	11.389	790	792	794	rBV	104982	98860	1.23%	0.136%
20	11.526	801	804	806	rBV	2890920	2389702	29.74%	3.293%
21	11.743	821	823	826	rBV	595291	732134	9.11%	1.009%
22	12.052	848	850	859	rBV	1279438	1392990	17.34%	1.919%
23	12.566	893	895	898	rBV	2811395	3151606	39.22%	4.343%
24	12.761	909	912	914	rBV2	68742	148282	1.85%	0.204%
25	12.841	917	919	926	rVV	1042309	1035808	12.89%	1.427%
26	12.932	926	927	930	rVB	111653	112683	1.40%	0.155%
27	13.126	941	944	946	rBV	6157808	8034919	100.00%	11.071%
28	13.321	959	961	966	rBV	162552	210999	2.63%	0.291%
29	13.561	980	982	984	rBV	366155	375373	4.67%	0.517%
30	13.652	987	990	998	rVB4	82928	245876	3.06%	0.339%
31	14.018	1019	1022	1025	rBV	459340	676886	8.42%	0.933%
32	14.166	1031	1035	1038	rBV2	1289373	1945227	24.21%	2.680%
33	15.047	1109	1112	1114	rBV	109184	152662	1.90%	0.210%
34	15.664	1163	1166	1169	rBV	790930	1204423	14.99%	1.660%

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Misc :
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Instrument :
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ClientSampleId :
100516-01

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.521	1231	1241	1252	rVB6	36479	249292	3.10%	0.344%
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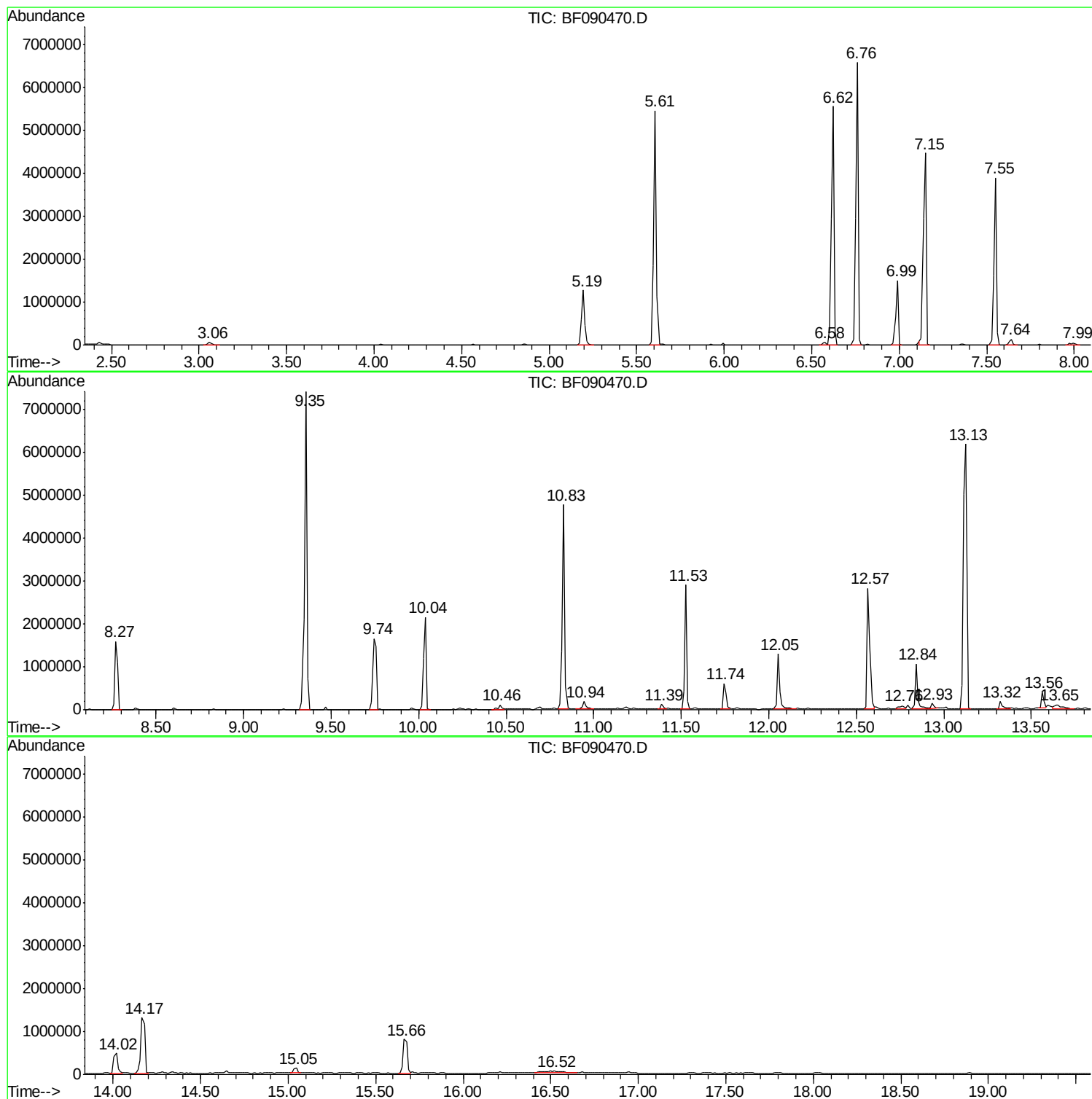
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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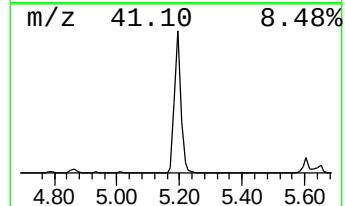
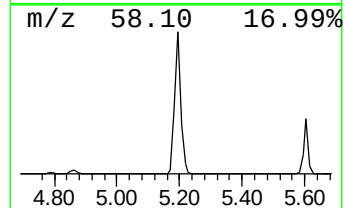
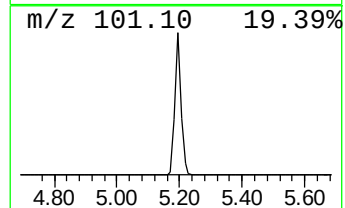
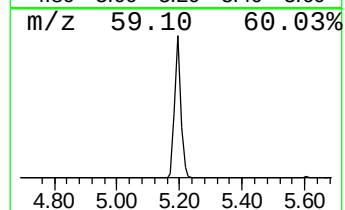
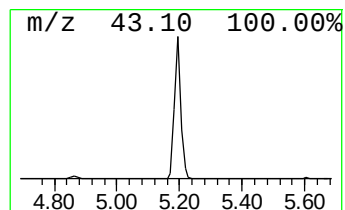
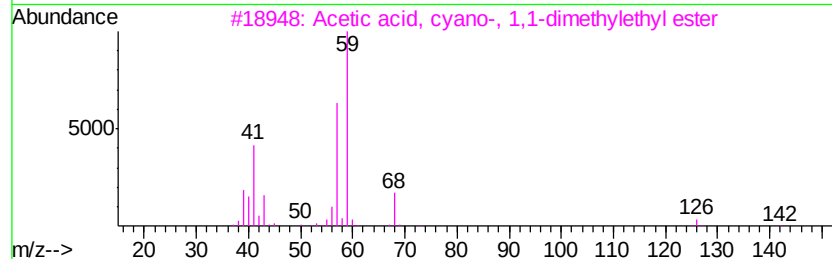
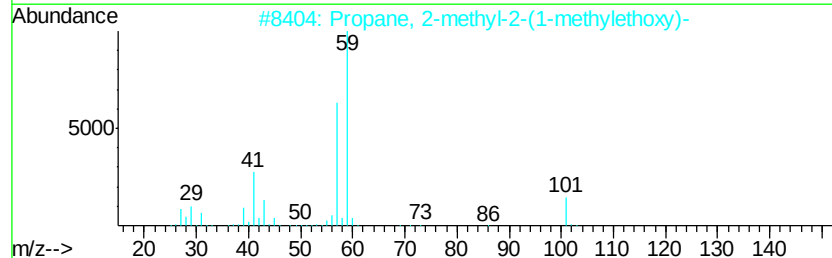
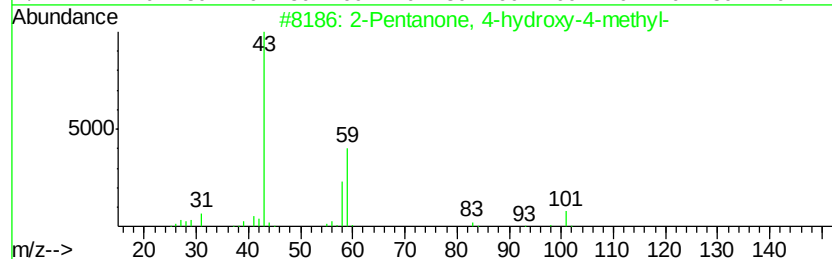
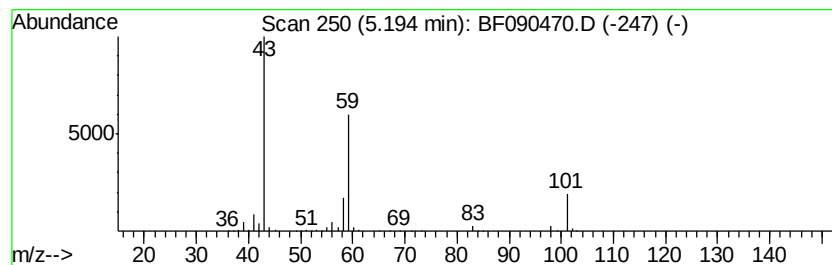
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	22.02 ng	1683670	1,4-Dichlorobenzene-d4	6.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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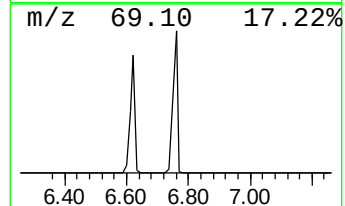
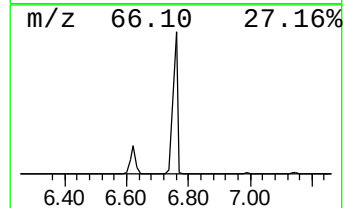
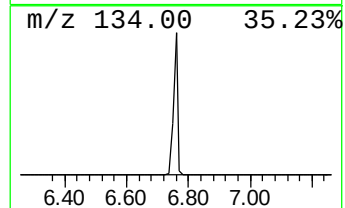
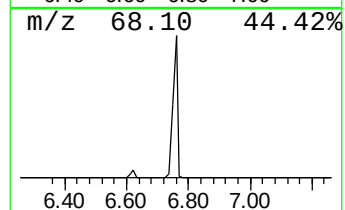
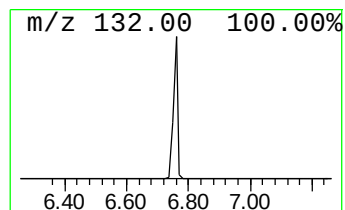
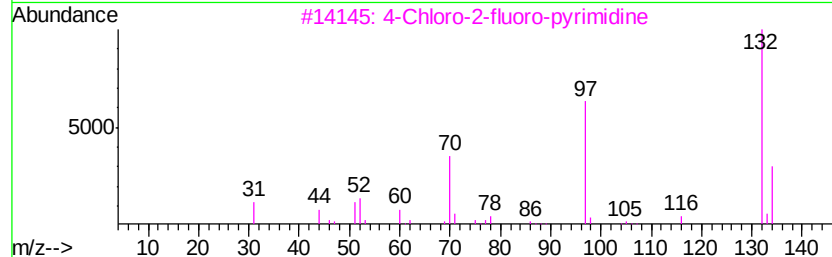
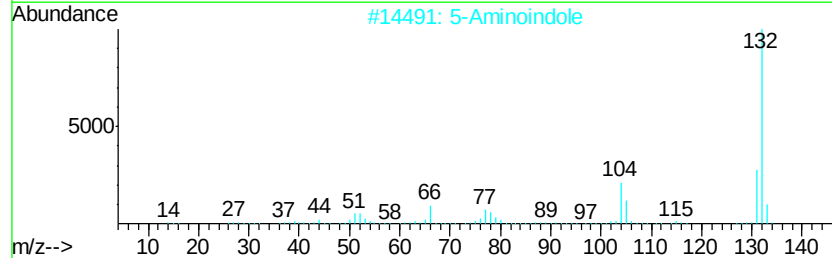
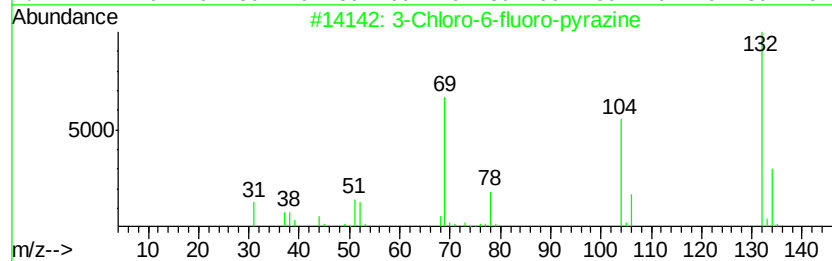
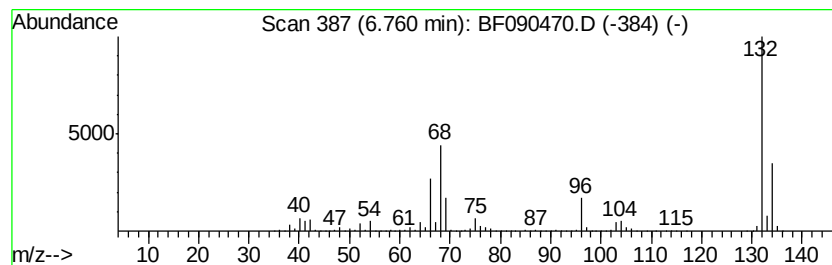
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	87.64 ng	6700920	1,4-Dichlorobenzene-d4	6.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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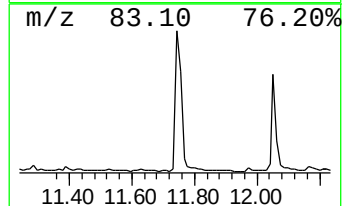
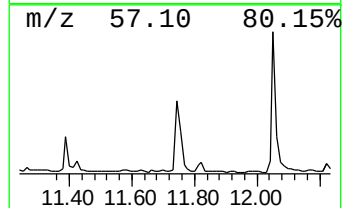
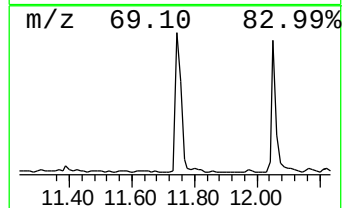
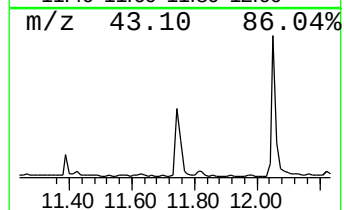
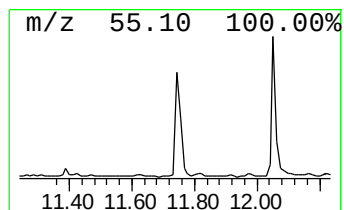
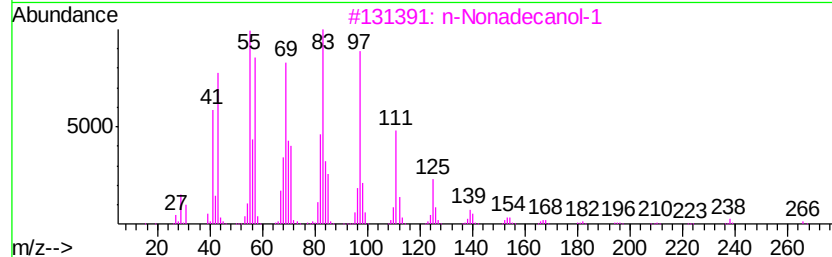
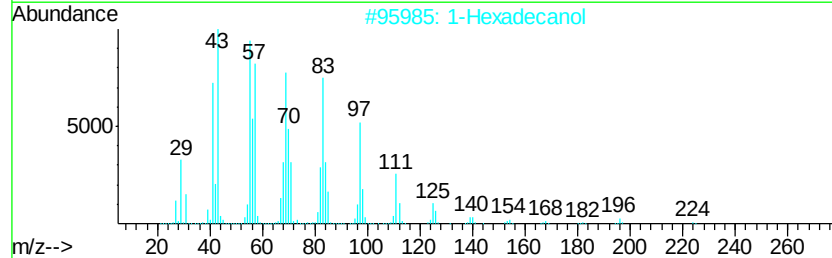
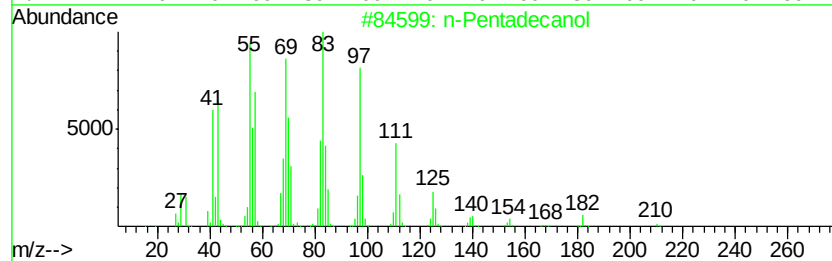
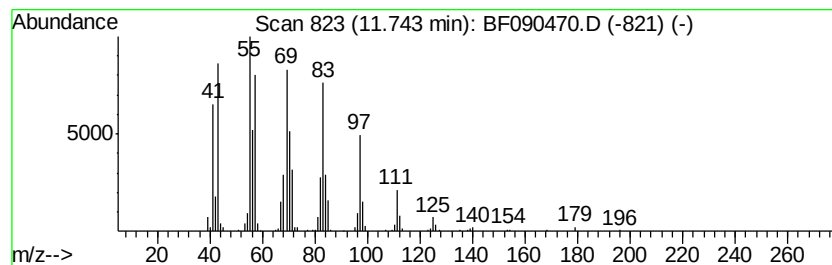
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Pentadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.74	6.13 ng	732134	Phenanthrene-d10	11.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Pentadecanol	228	C15H32O	000629-76-5	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Tetradecanol	214	C14H30O	000112-72-1	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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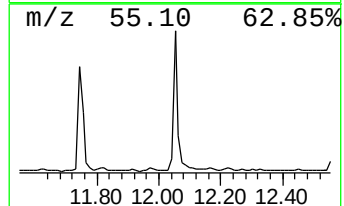
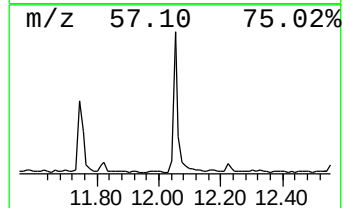
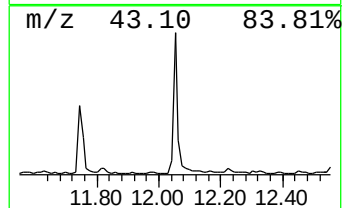
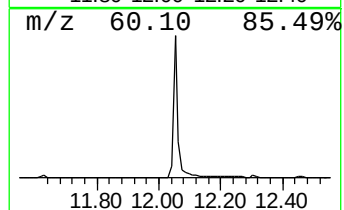
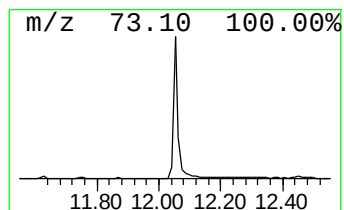
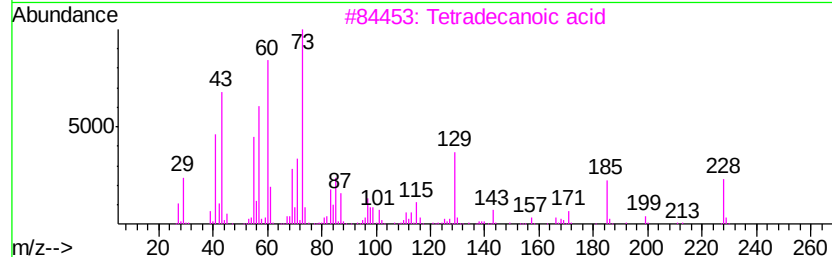
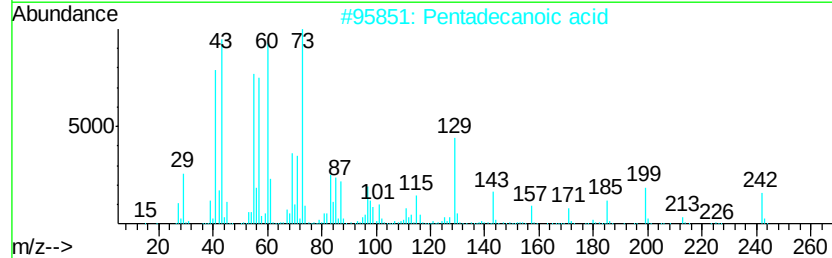
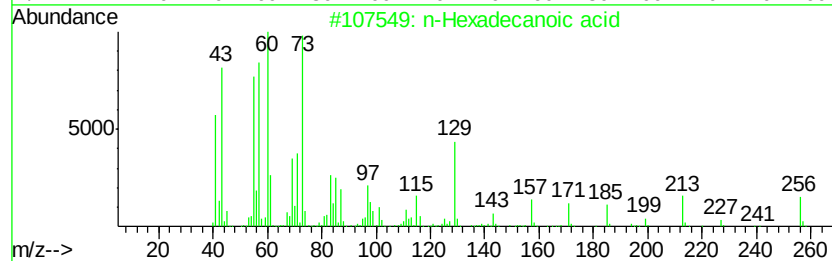
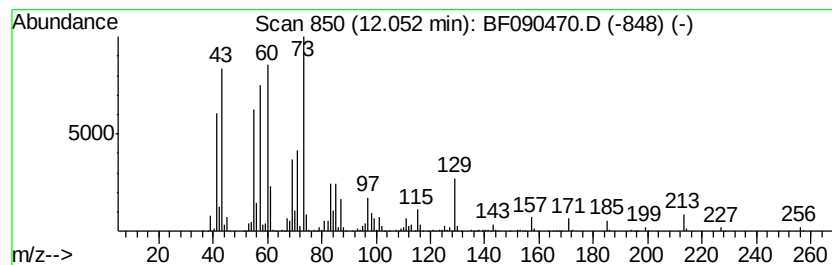
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	11.66 ng	1392990	Phenanthrene-d10	11.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	18
5		Undecane	156	C11H24	001120-21-4	18



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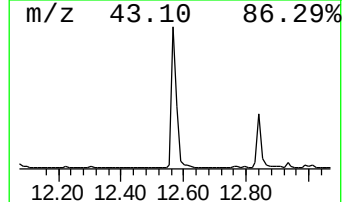
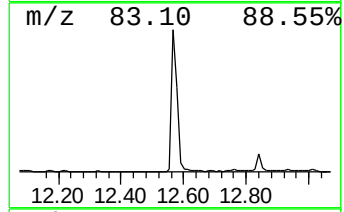
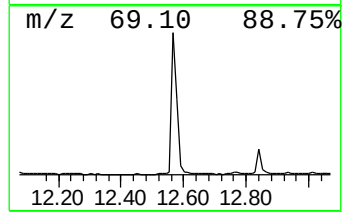
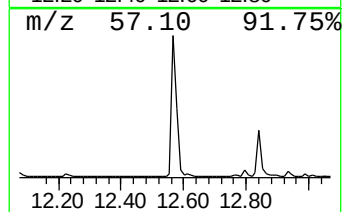
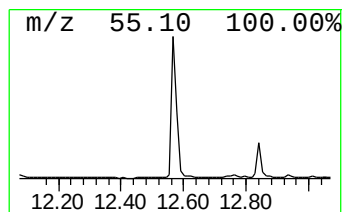
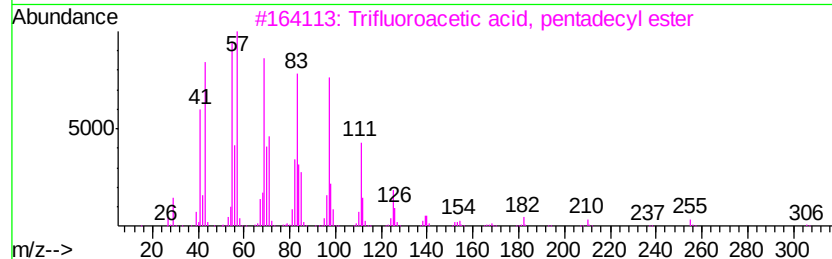
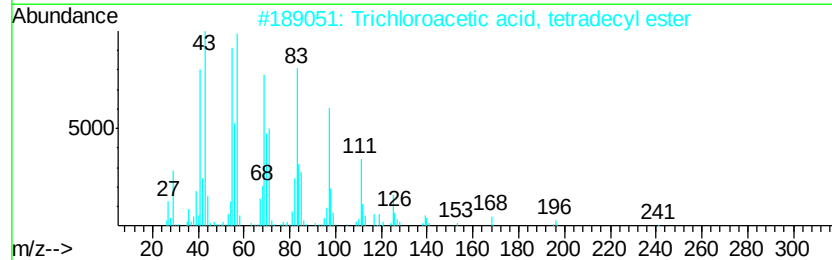
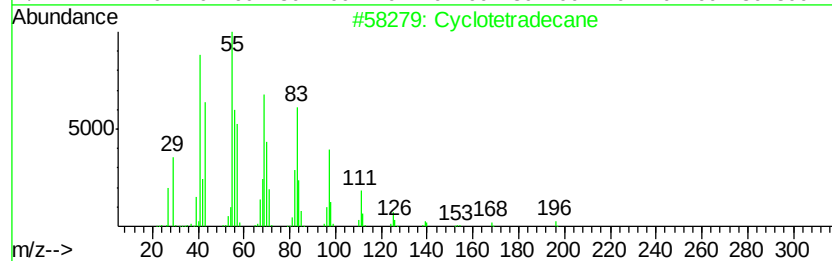
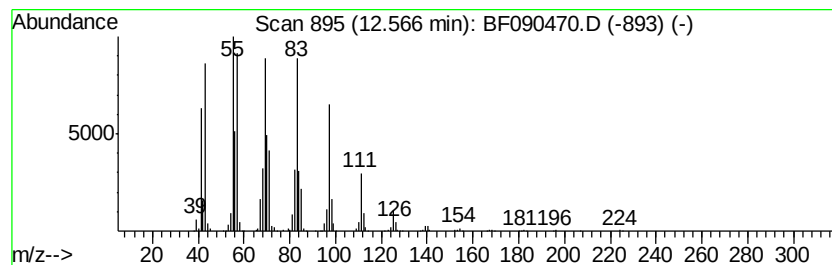
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	26.38 ng	3151610	Phenanthrene-d10	11.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetradecane	196	C14H28	000295-17-0	97
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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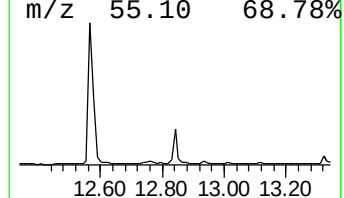
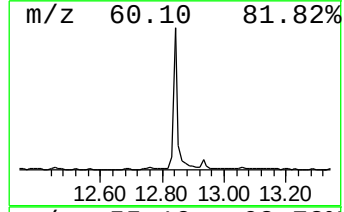
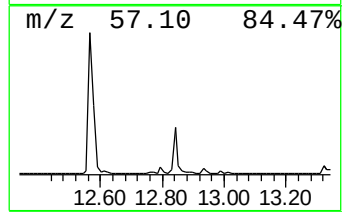
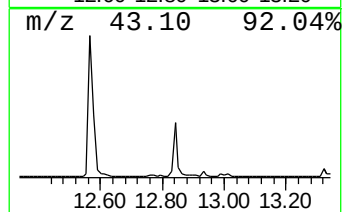
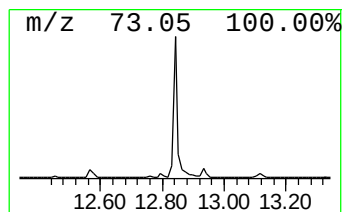
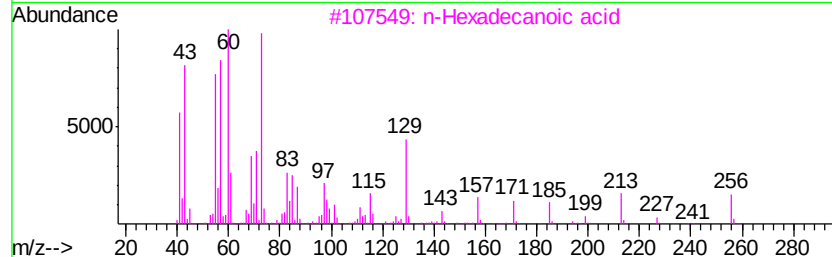
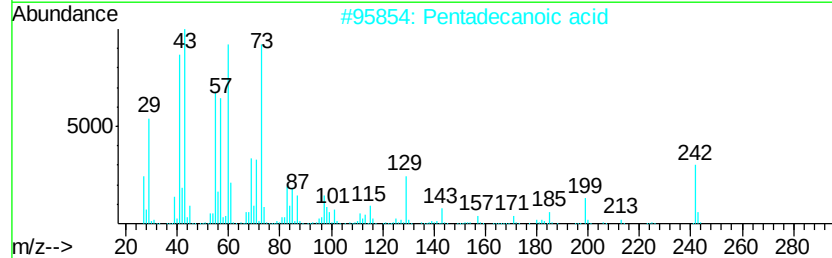
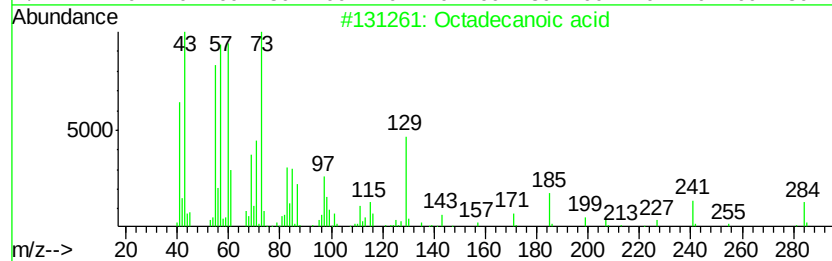
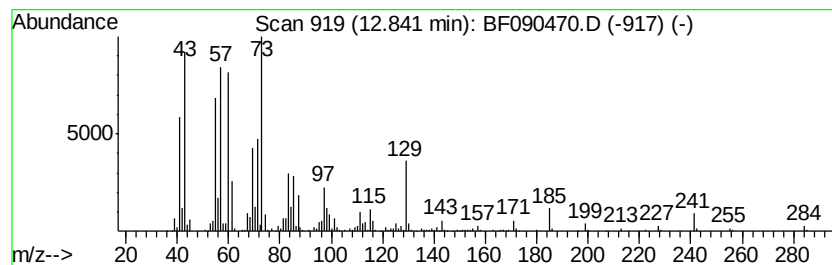
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.84	8.67 ng	1035810	Phenanthrene-d10		11.53
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090470.D
Acq On : 8 Oct 2016 6:27
Operator : UM/SJ
Sample : H5136-01
Misc :
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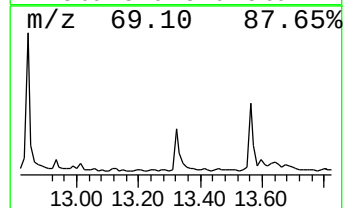
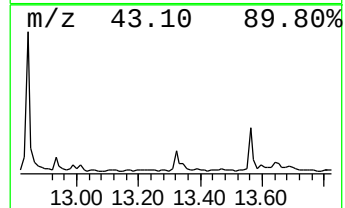
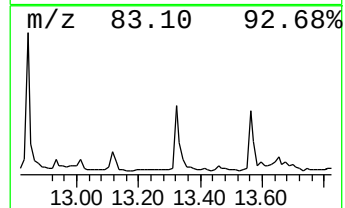
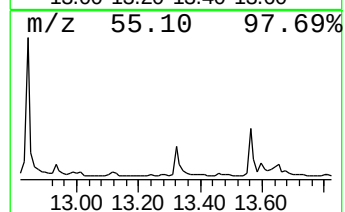
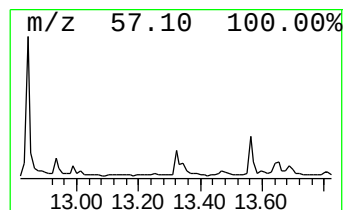
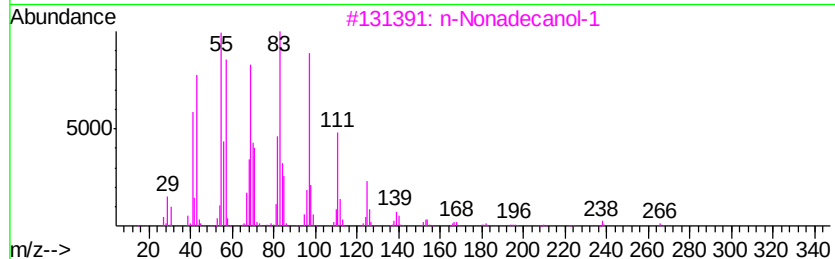
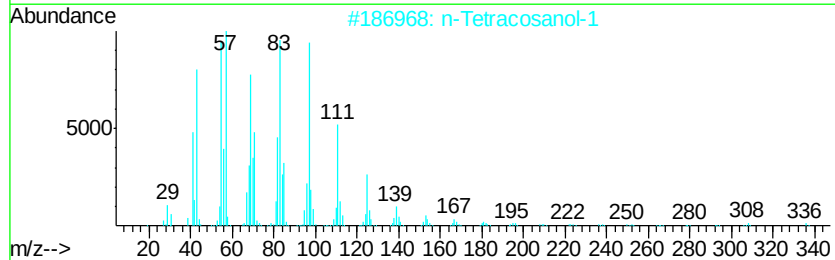
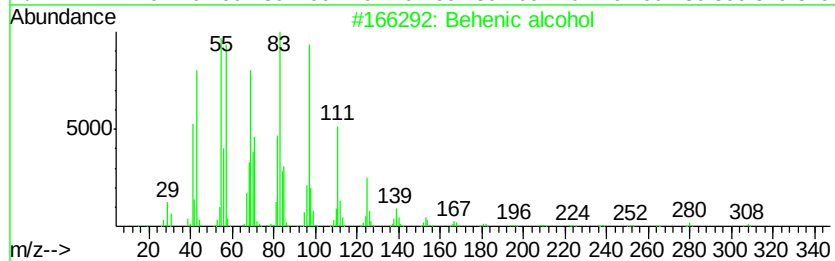
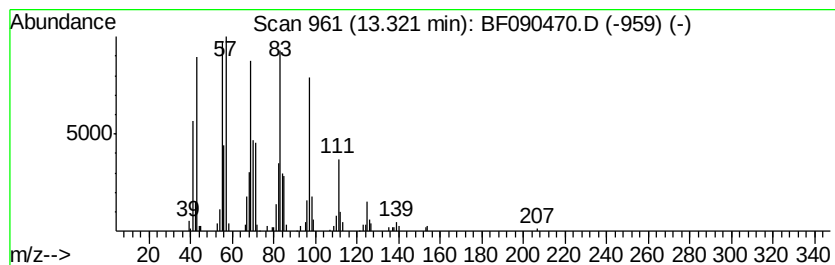
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.17 ng	210999	Chrysene-d12	14.18
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		n-Tetracosanol-1	354 C24H50O	000506-51-4 94
3		n-Nonadecanol-1	284 C19H40O	001454-84-8 94
4		1-Nonadecene	266 C19H38	018435-45-5 91
5		9-Eicosene, (E)-	280 C20H40	074685-29-3 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
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Acq On : 8 Oct 2016 6:27
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Sample : H5136-01
Misc :
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Instrument :
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ClientSampleId :
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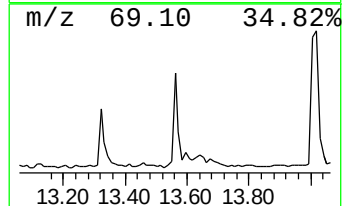
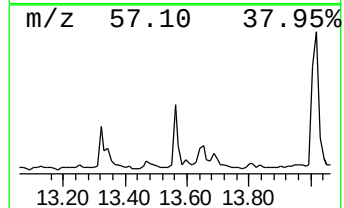
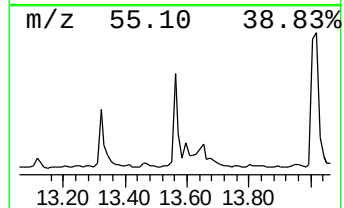
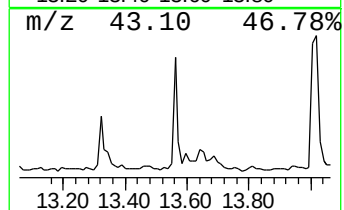
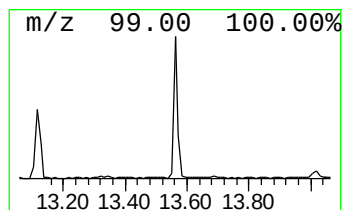
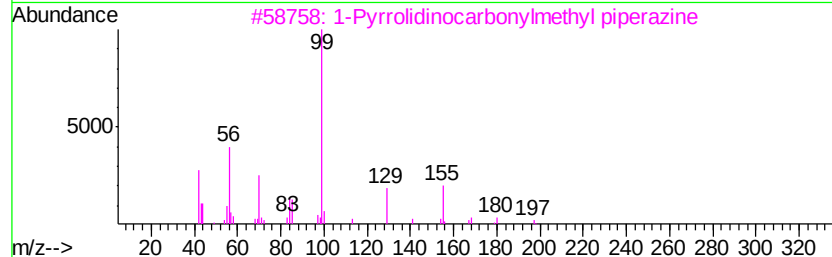
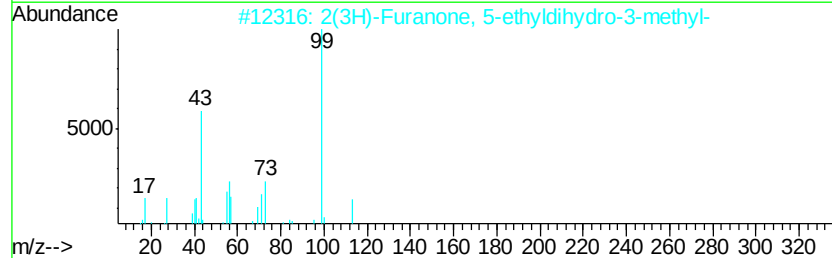
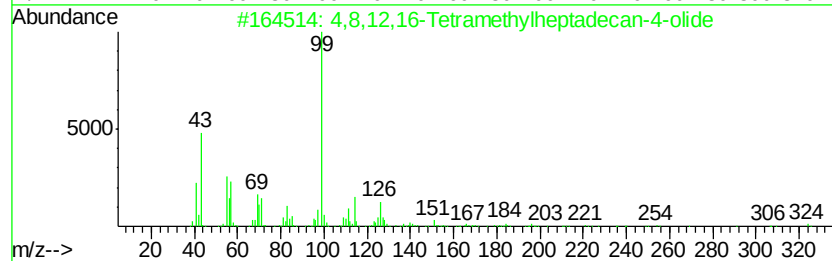
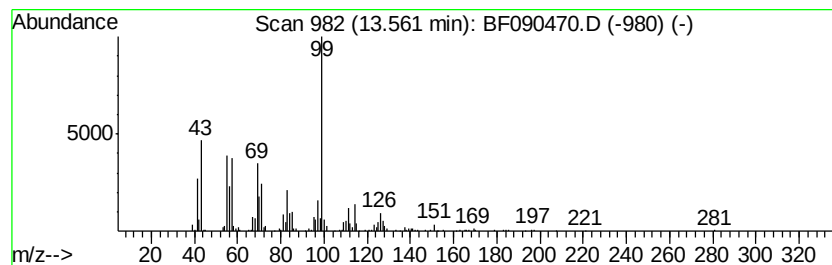
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4,8,12,16-Tetramethylheptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	3.86 ng	375373	Chrysene-d12	14.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	59
2			2(3H)-Furanone, 5-ethylidihydro-3...	128	C7H12O2	002610-98-2	50
3			1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	47
4			trans-4-Hydroxy-3-methylundecano...	198	C12H22O2	148806-10-4	47
5			Phosphonofluoridic acid, methyl-...	210	C9H20F02P	144313-52-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090470.D
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Sample : H5136-01
Misc :
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ClientSampleId :
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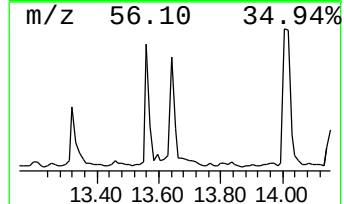
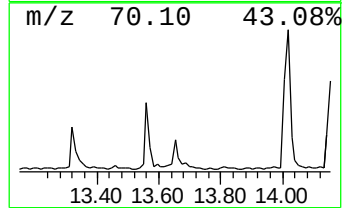
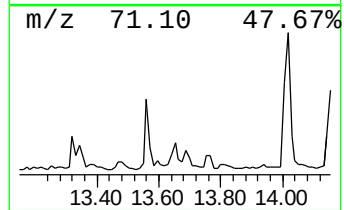
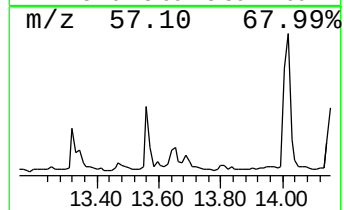
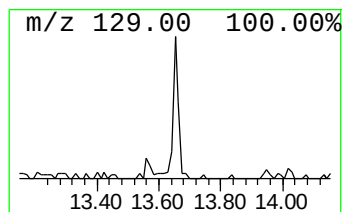
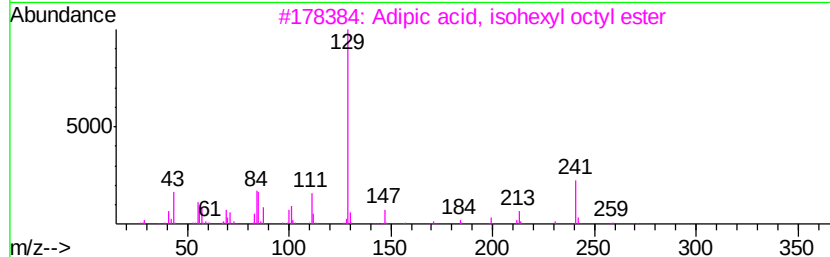
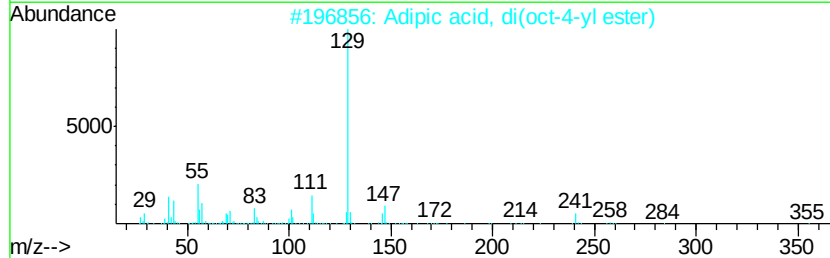
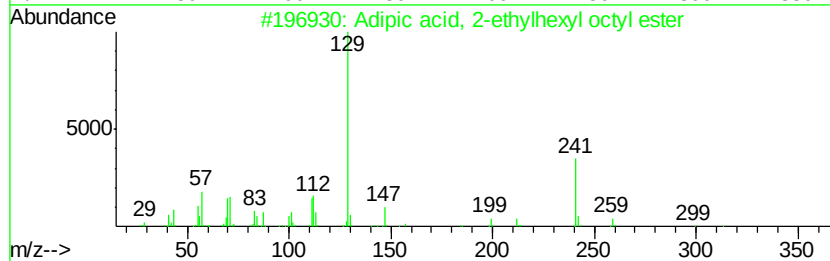
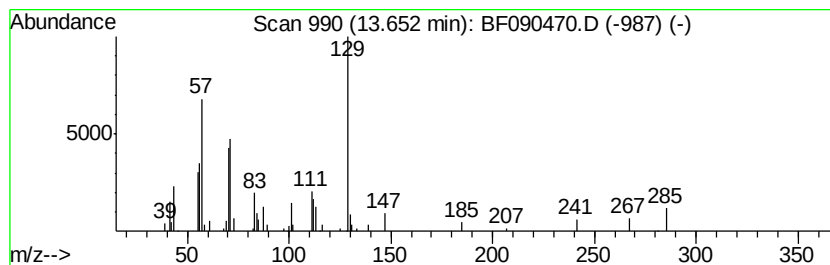
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Adipic acid, 2-ethylhexyl o... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	2.53 ng	245876	Chrysene-d12	14.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	50
2			Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	43
3			Adipic acid, isohexyl octyl ester	342	C20H38O4	1000324-47-0	43
4			Adipic acid, 2-methylbutyl octyl...	328	C19H36O4	1000324-67-7	40
5			Diisopropyl adipate	230	C12H22O4	006938-94-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090470.D
Acq On : 8 Oct 2016 6:27
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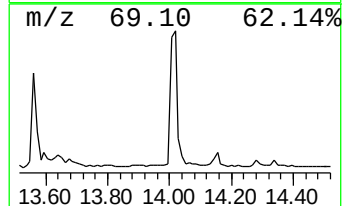
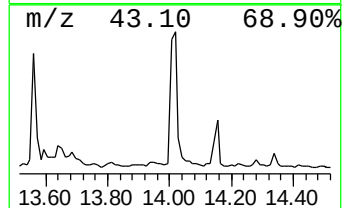
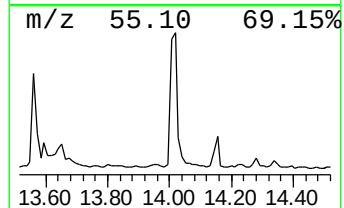
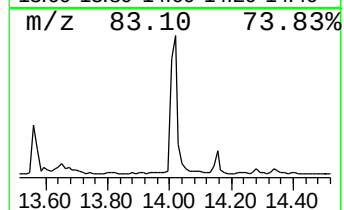
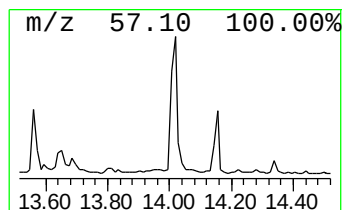
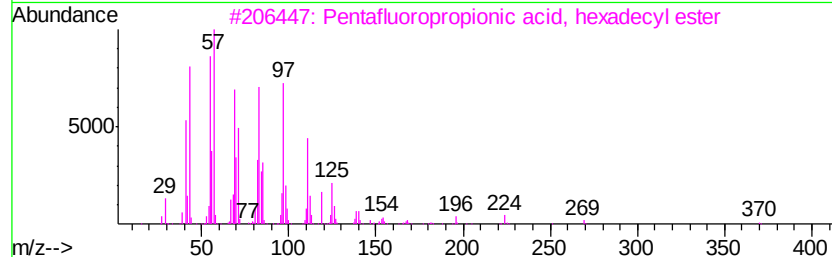
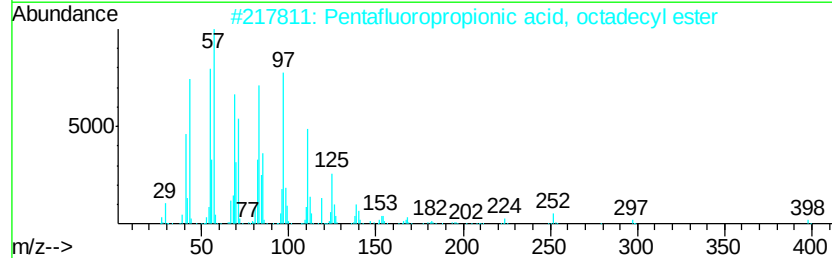
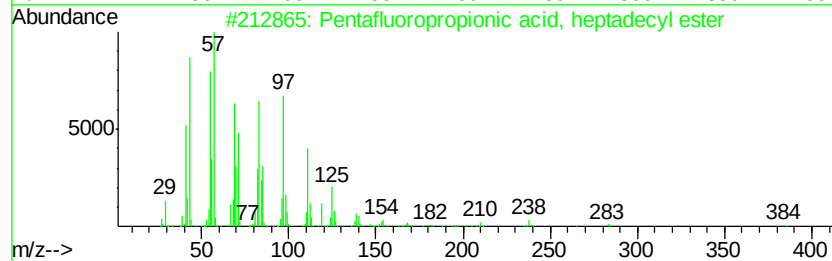
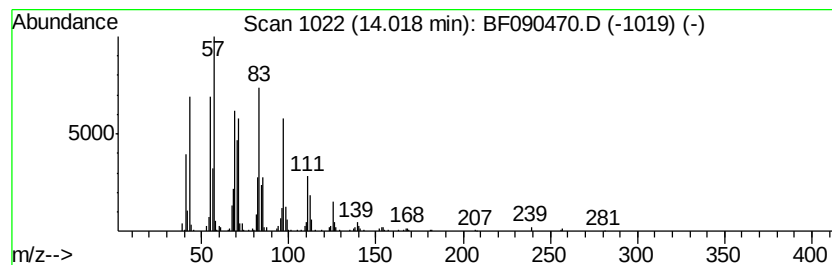
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	6.96 ng	676886	Chrysene-d12	14.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
5			1-Docosene	308	C22H44	001599-67-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
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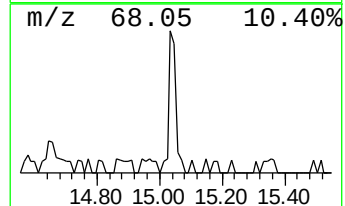
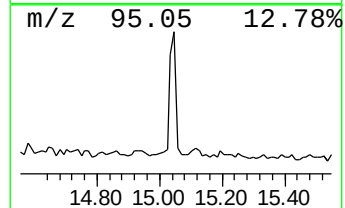
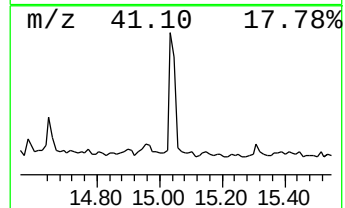
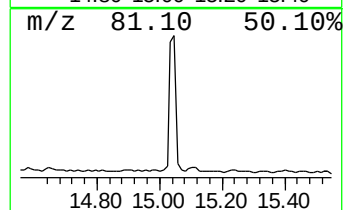
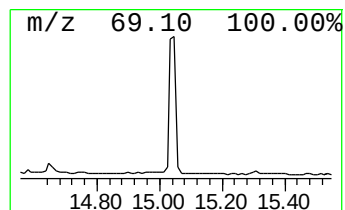
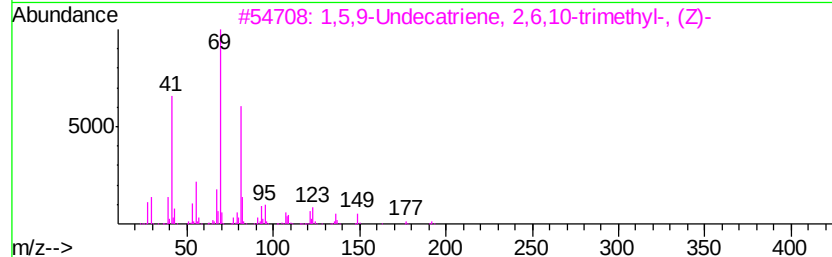
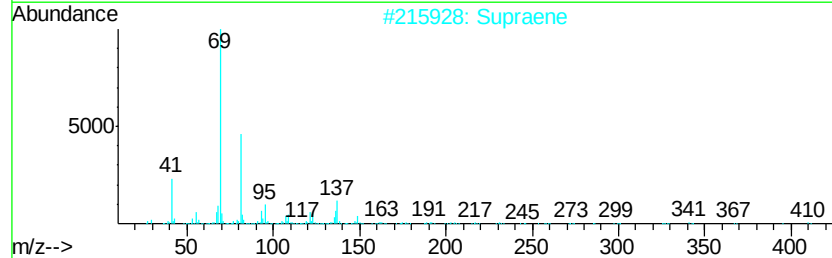
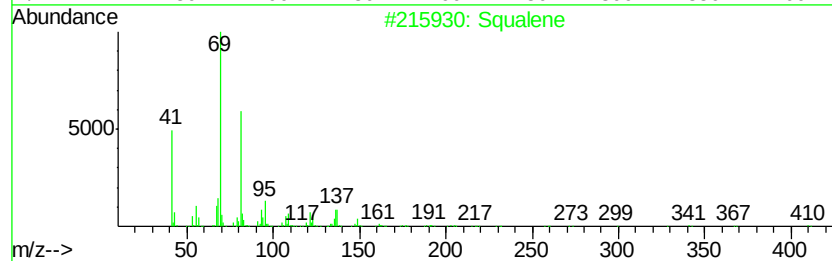
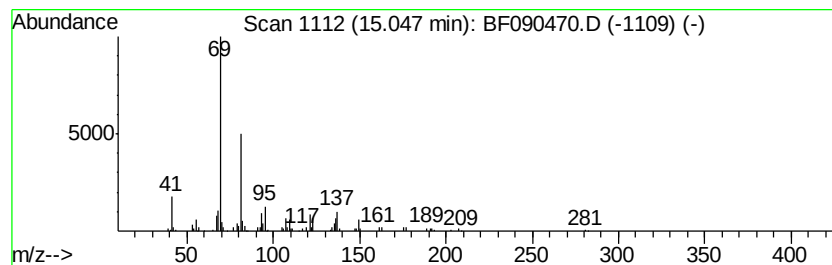
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.54 ng	152662	Perylene-d12	15.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	87
4	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	80
5	(.+/-)-Lavandulol, pentafluorop...	300 C13H17F5O2	1000352-63-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
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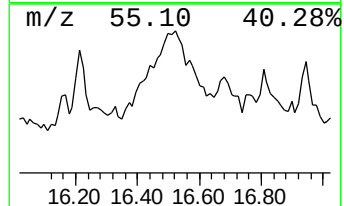
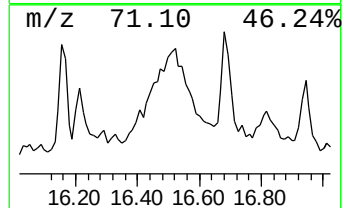
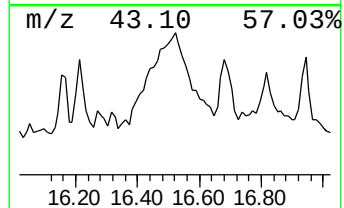
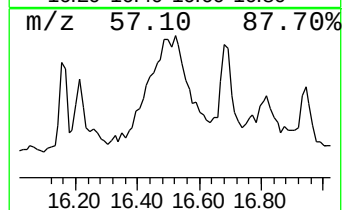
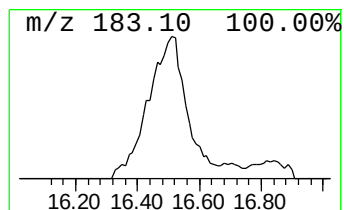
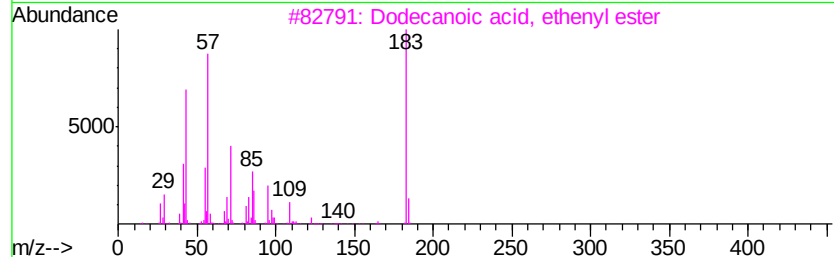
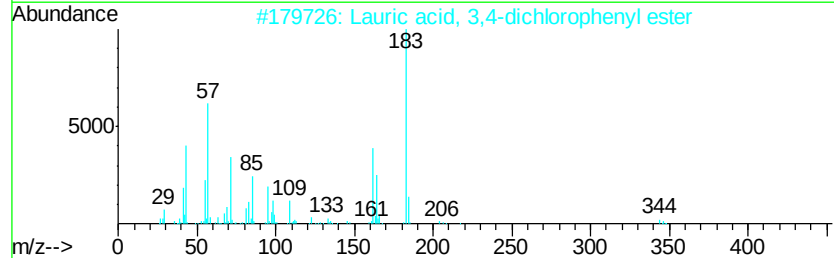
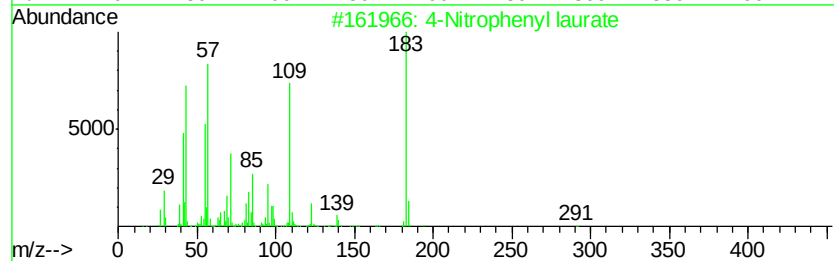
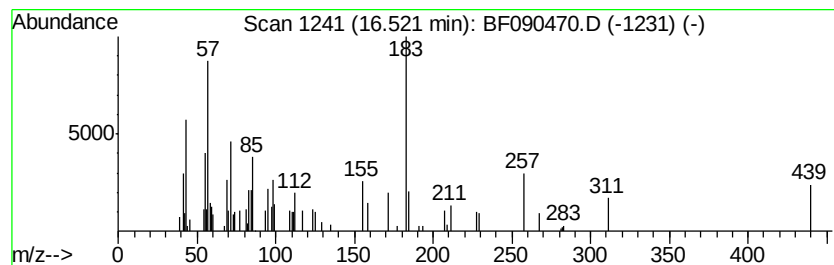
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown16.52 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.52	4.14 ng	249292	Perylene-d12		15.68	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Nitrophenyl laurate	321	C18H27N04	001956-11-2	38
2		Lauric acid, 3,4-dichlorophenyl ...	344	C18H26Cl202	1000357-92-7	35
3		Dodecanoic acid, ethenyl ester	226	C14H2602	002146-71-6	35
4		Lauric anhydride	382	C24H4603	000645-66-9	25
5		Fumaric acid, hexyl 4-octyl ester	312	C18H3204	1000339-21-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090470.D
Acq On : 8 Oct 2016 6:27
Operator : UM/SJ
Sample : H5136-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100516-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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...	5.19	22.0	ng	1683670	1	6.99	1529230	20.0
unknown6.76	6.76	87.6	ng	6700920	1	6.99	1529230	20.0
n-Pentadecanol	11.74	6.1	ng	732134	4	11.53	2389700	20.0
n-Hexadecanoic acid	12.05	11.7	ng	1392990	4	11.53	2389700	20.0
Cyclotetradecane	12.57	26.4	ng	3151610	4	11.53	2389700	20.0
Octadecanoic acid	12.84	8.7	ng	1035810	4	11.53	2389700	20.0
Behenic alcohol	13.32	2.2	ng	210999	5	14.18	1945230	20.0
4,8,12,16-Tetrame...	13.56	3.9	ng	375373	5	14.18	1945230	20.0
Adipic acid, 2-et...	13.65	2.5	ng	245876	5	14.18	1945230	20.0
Pentafluoropropio...	14.02	7.0	ng	676886	5	14.18	1945230	20.0
Squalene	15.05	2.5	ng	152662	6	15.68	1204420	20.0
unknown16.52	16.52	4.1	ng	249292	6	15.68	1204420	20.0