

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
 Data File : BF092210.D
 Acq On : 12 Jan 2017 16:13
 Operator : UM/SJ
 Sample : I1029-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-003

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.990	182	184	189	rBV	76853	142411	2.57%	0.301%
2	4.733	245	249	264	rVB	1447841	2740922	49.41%	5.788%
3	5.190	287	289	292	rBV	3487642	5211528	93.95%	11.005%
4	6.264	380	383	390	rBV	4846555	5547230	100.00%	11.714%
5	6.367	390	392	395	rVB	5086230	5000579	90.15%	10.560%
6	6.596	410	412	414	rBV	1107037	1082377	19.51%	2.286%
7	6.745	423	425	428	rBV	2571394	3495863	63.02%	7.382%
8	7.167	459	462	464	rBV	2869181	3024981	54.53%	6.388%
9	7.876	522	524	527	rBV	1107483	1247837	22.49%	2.635%
10	8.962	616	619	621	rBV	4751549	4768484	85.96%	10.070%
11	9.362	652	654	656	rBV	337637	306256	5.52%	0.647%
12	9.625	675	677	680	rBV	1391488	1399519	25.23%	2.955%
13	10.082	713	717	718	rBV	45561	67844	1.22%	0.143%
14	10.425	744	747	749	rBV2	2101160	3096451	55.82%	6.539%
15	10.551	756	758	762	rBV	98766	130094	2.35%	0.275%
16	10.996	795	797	798	rBV2	79036	78188	1.41%	0.165%
17	11.099	804	806	809	rBV	1037715	1419465	25.59%	2.997%
18	11.659	853	855	859	rBV2	371091	351490	6.34%	0.742%
19	12.437	921	923	928	rBV	113597	132651	2.39%	0.280%
20	12.539	928	932	934	rVB	42750	66096	1.19%	0.140%
21	12.699	943	946	948	rBV	3061633	4250174	76.62%	8.975%
22	13.602	1022	1025	1034	rBV	150838	226841	4.09%	0.479%
23	13.728	1034	1036	1039	rBV	961928	1092031	19.69%	2.306%
24	14.231	1076	1080	1086	rBV2	43932	105477	1.90%	0.223%
25	14.814	1129	1131	1132	rBV	65208	80187	1.45%	0.169%
26	14.837	1132	1133	1138	rVB	41062	64994	1.17%	0.137%
27	15.088	1153	1155	1158	rBV	692456	840951	15.16%	1.776%
28	15.500	1188	1191	1193	rBV	63918	91850	1.66%	0.194%
29	16.163	1245	1249	1252	rBV	173629	321184	5.79%	0.678%
30	16.345	1261	1265	1268	rBV4	23318	59236	1.07%	0.125%
31	16.448	1271	1274	1280	rVV2	127168	309330	5.58%	0.653%
32	16.551	1280	1283	1284	rVV	70274	137772	2.48%	0.291%
33	16.586	1284	1286	1291	rVB	89153	171298	3.09%	0.362%
34	16.814	1302	1306	1311	rBV3	54912	138737	2.50%	0.293%

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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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.328	1347	1351	1354	rBV	38897	89226	1.61%	0.188%
36	17.648	1375	1379	1388	rBV5	20383	66096	1.19%	0.140%

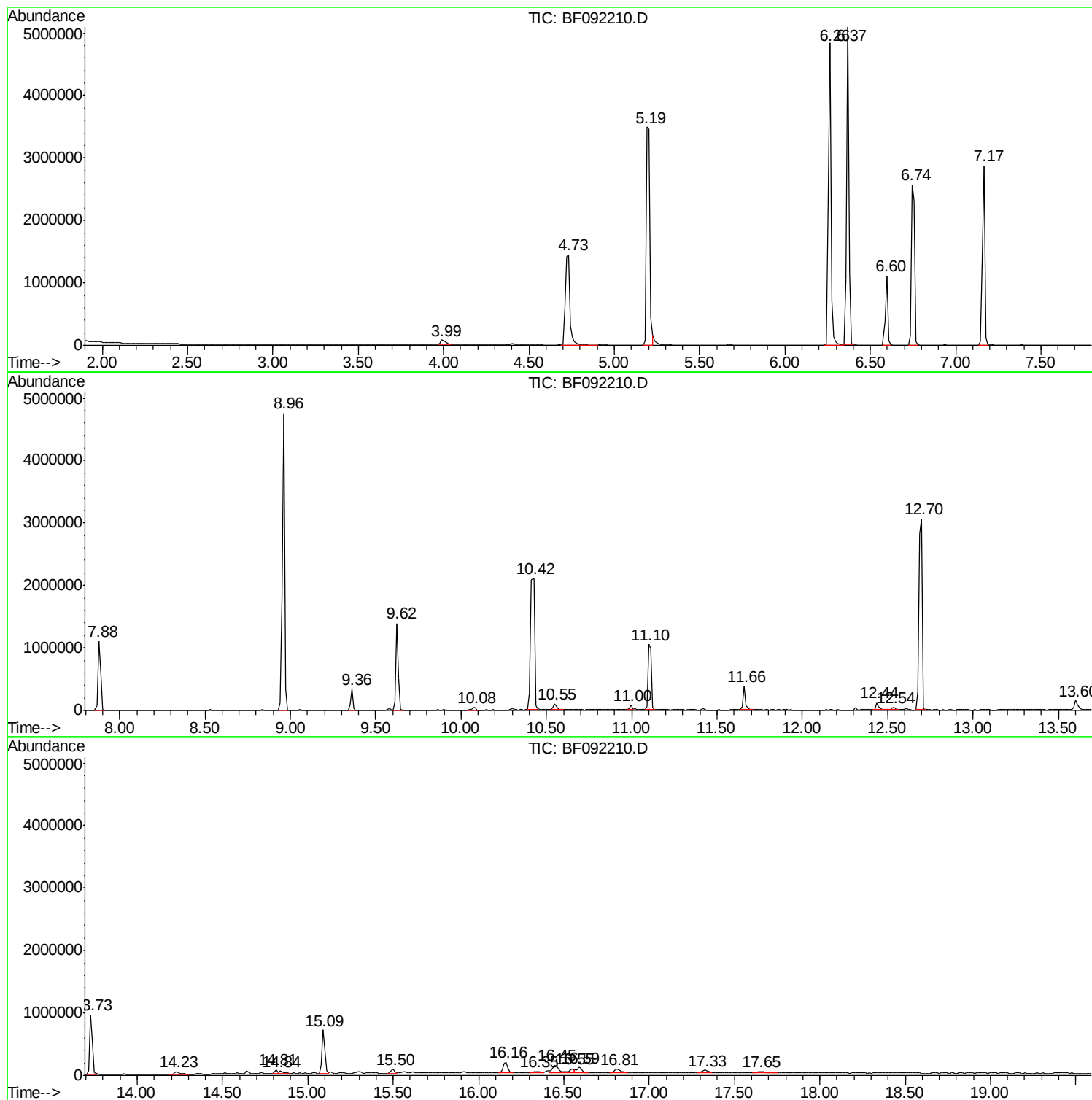
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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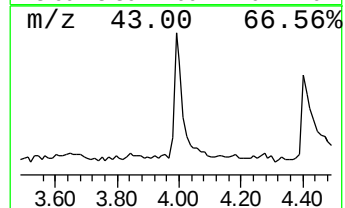
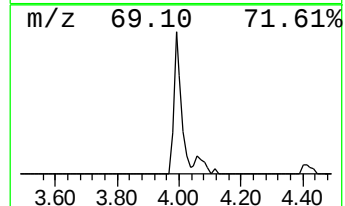
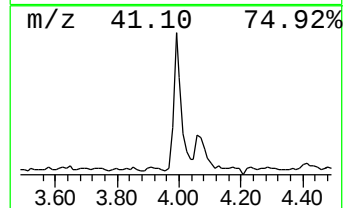
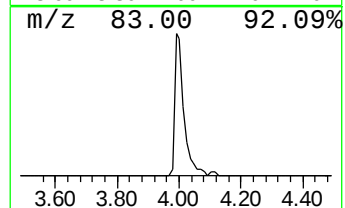
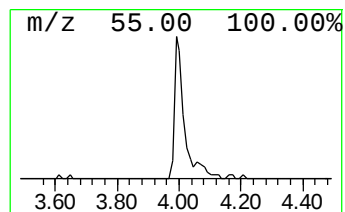
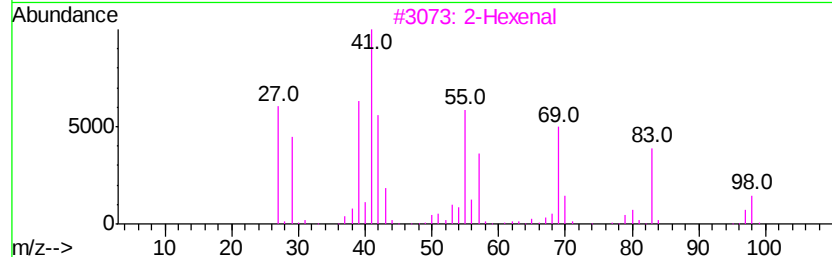
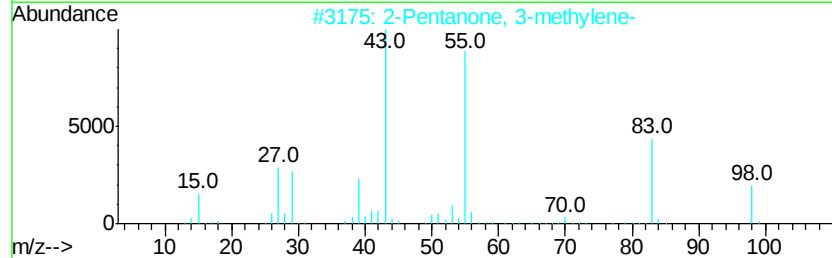
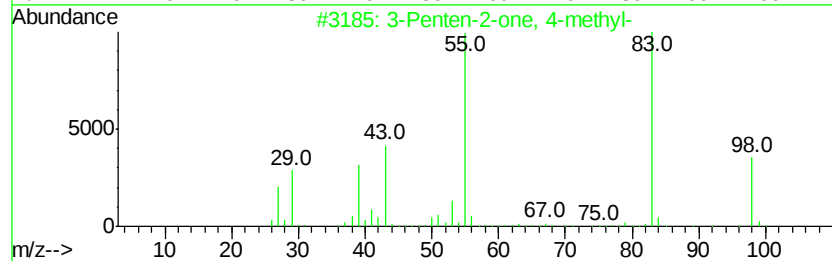
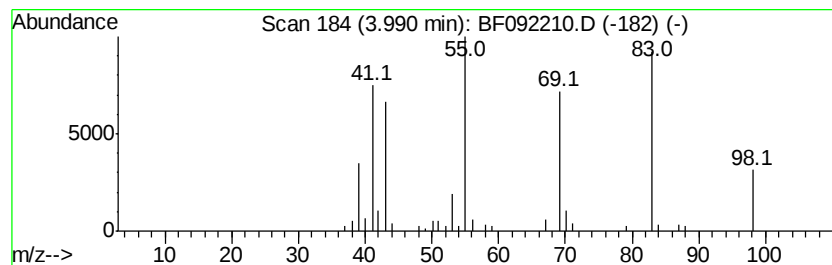
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	2.63 ng	142411	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	74
2			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	64
3			2-Hexenal	98	C6H10O	000505-57-7	59
4			3-Hexen-2-one	98	C6H10O	000763-93-9	53
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	53



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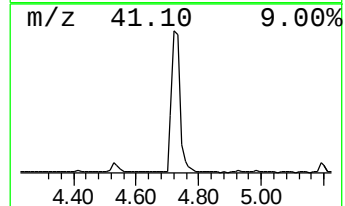
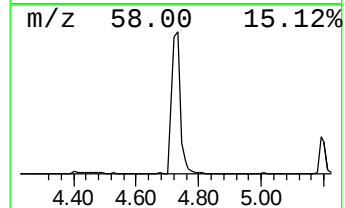
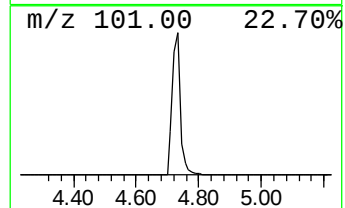
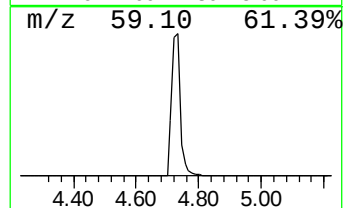
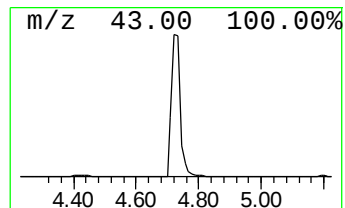
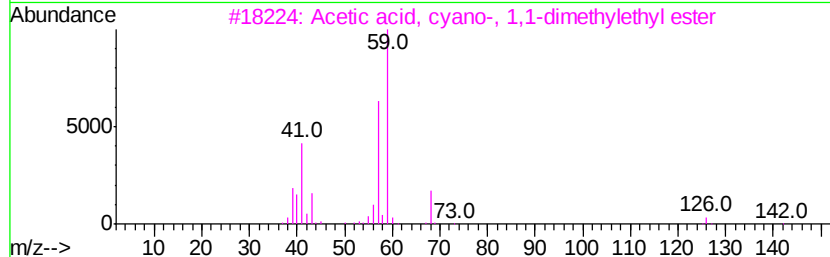
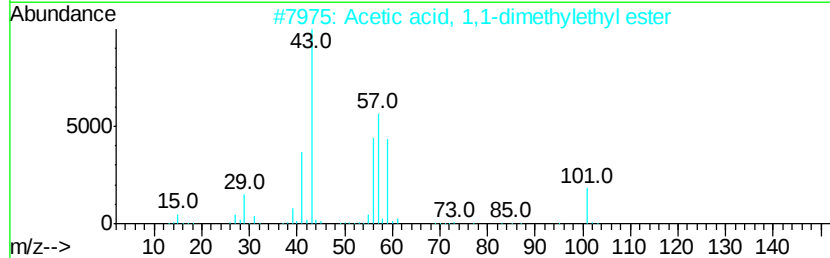
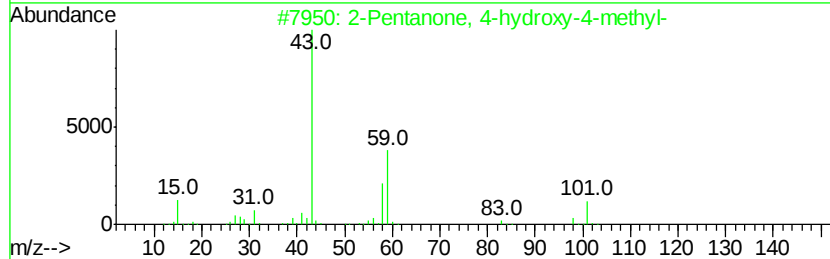
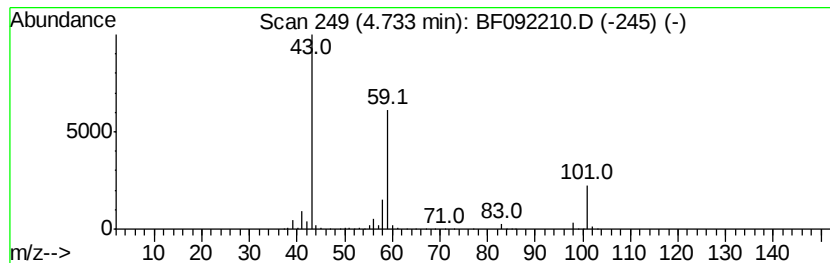
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	50.65 ng	2740920	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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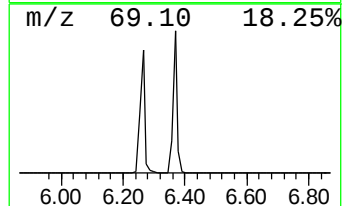
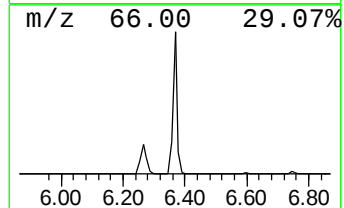
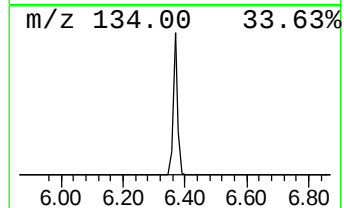
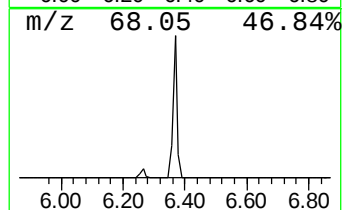
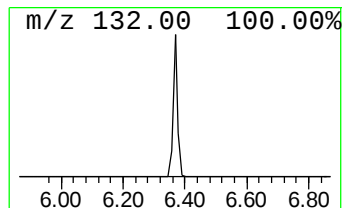
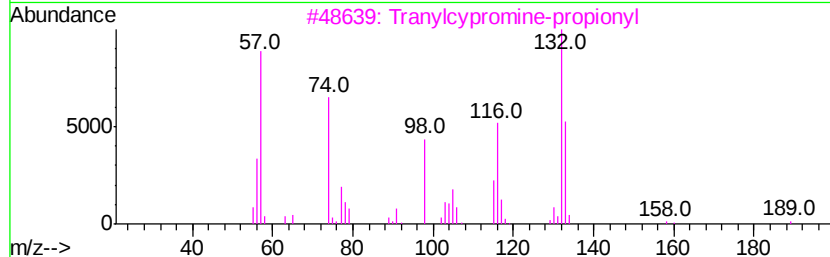
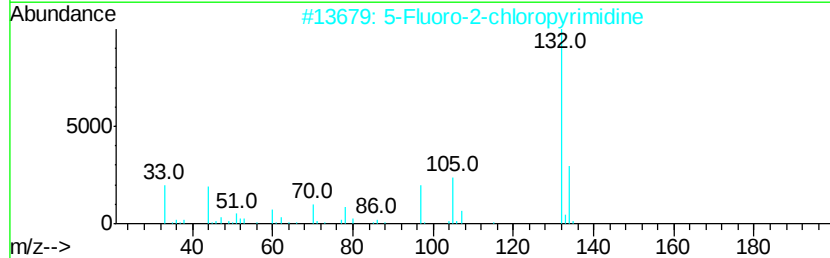
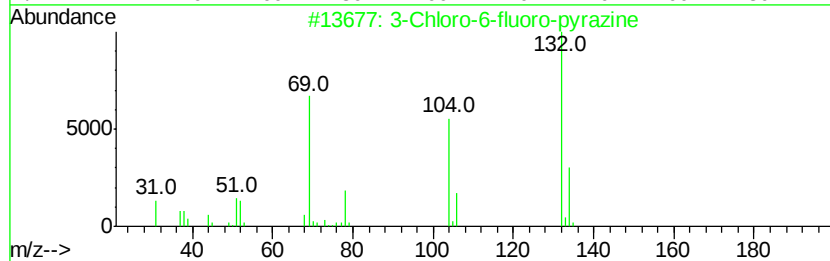
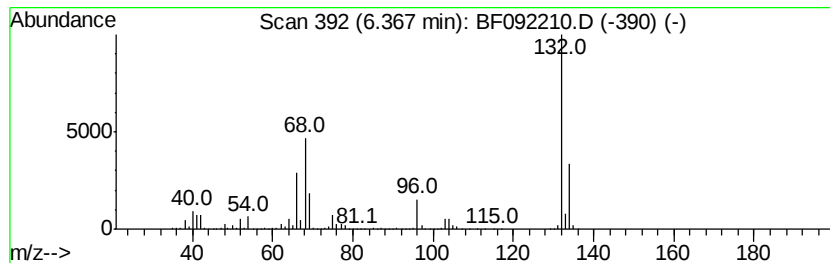
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	92.40 ng	5000580	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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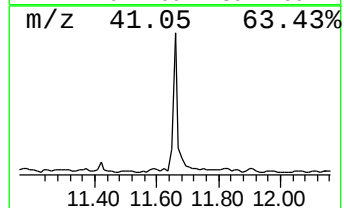
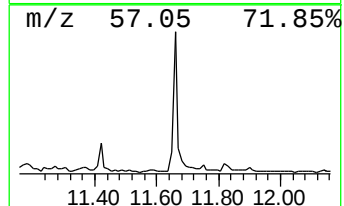
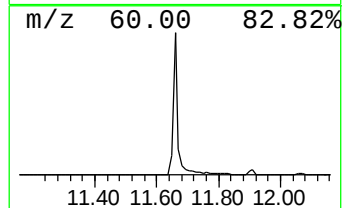
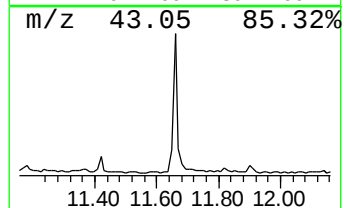
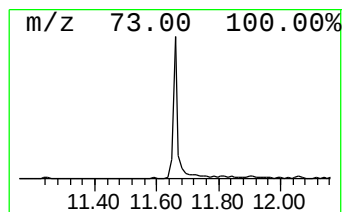
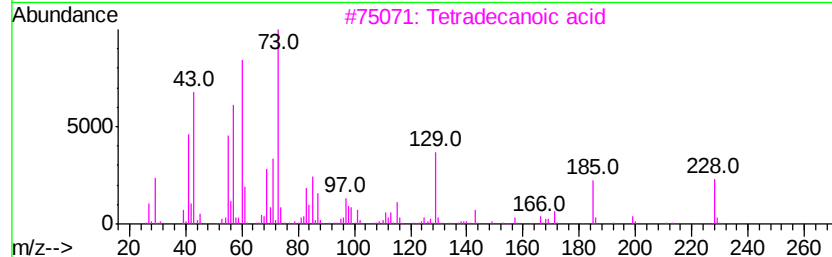
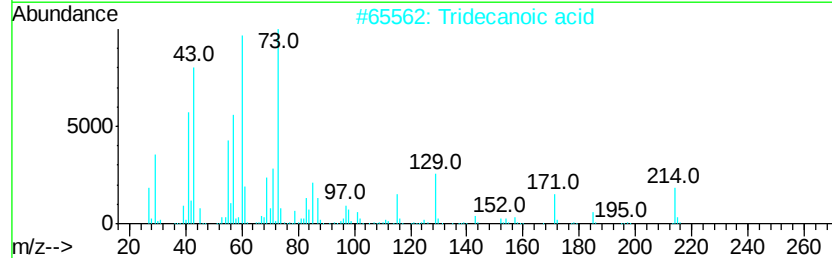
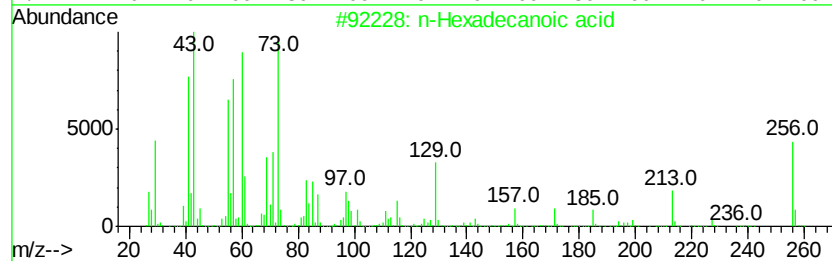
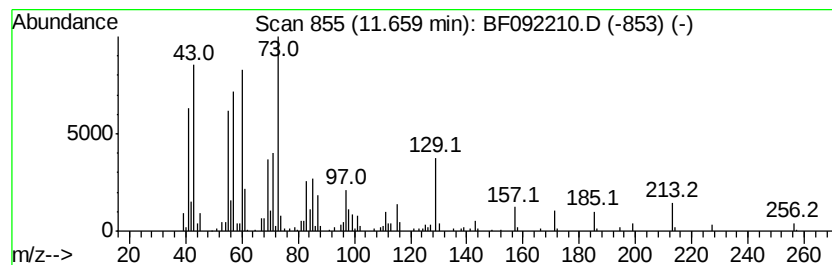
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	4.95 ng	351490	Phenanthrene-d10	11.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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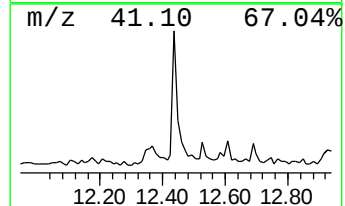
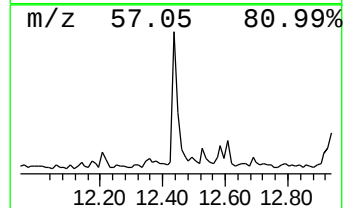
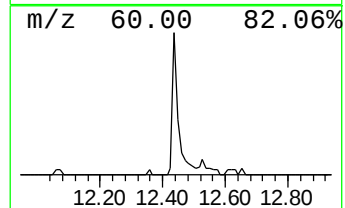
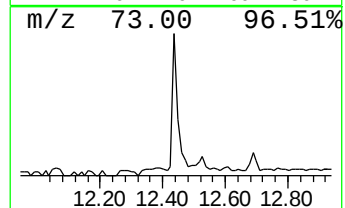
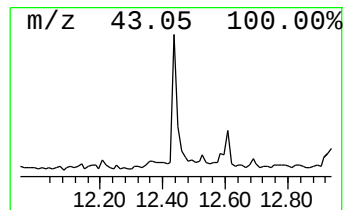
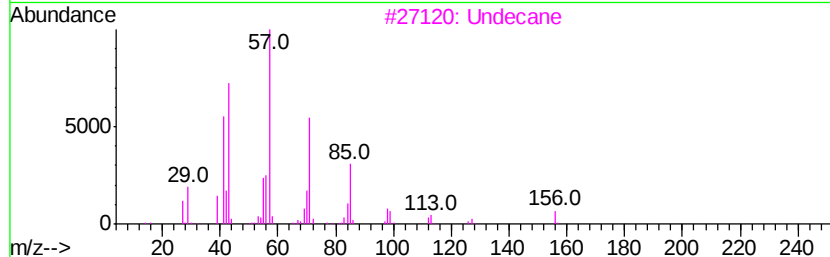
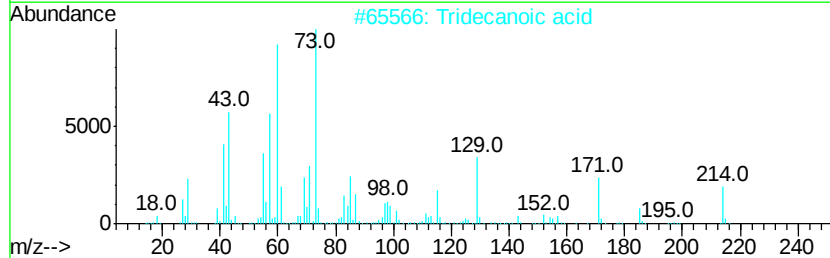
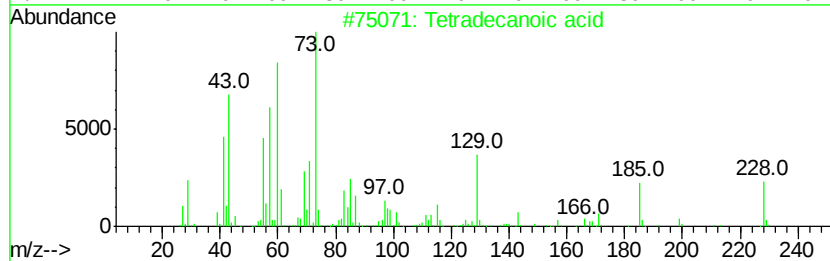
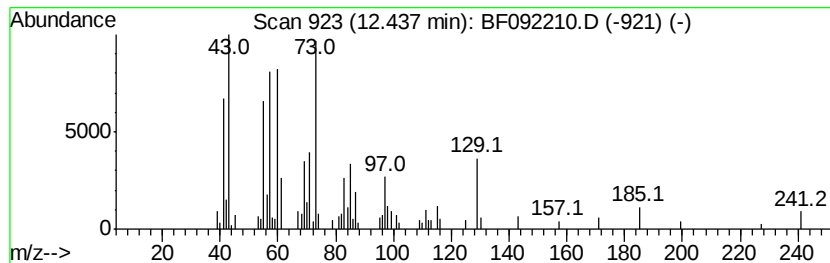
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	2.43 ng	132651	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Undecane	156	C11H24	001120-21-4	11
4		Decane	142	C10H22	000124-18-5	11
5		Tridecane	184	C13H28	000629-50-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092210.D
Acq On : 12 Jan 2017 16:13
Operator : UM/SJ
Sample : I1029-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMP-003

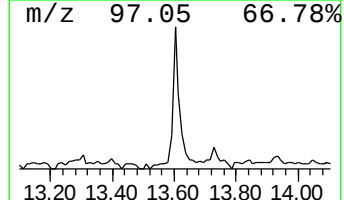
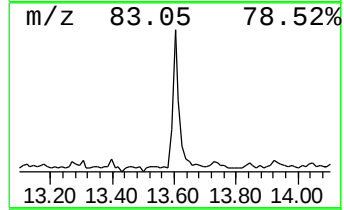
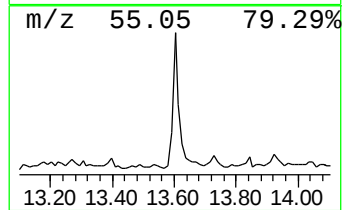
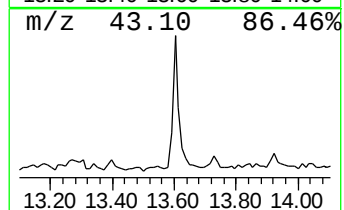
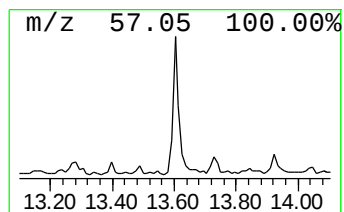
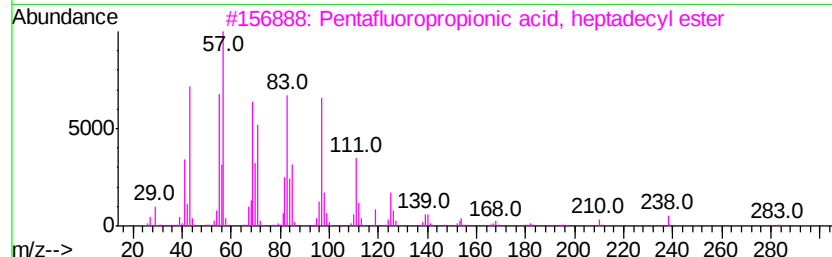
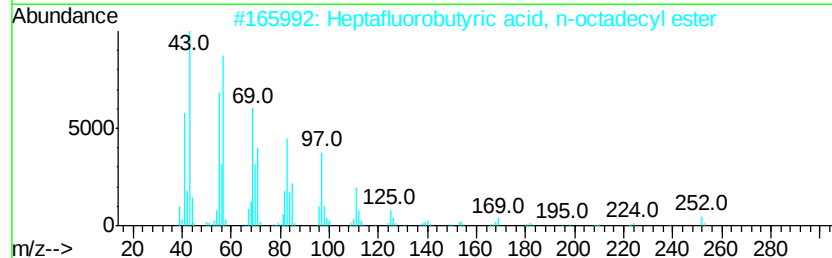
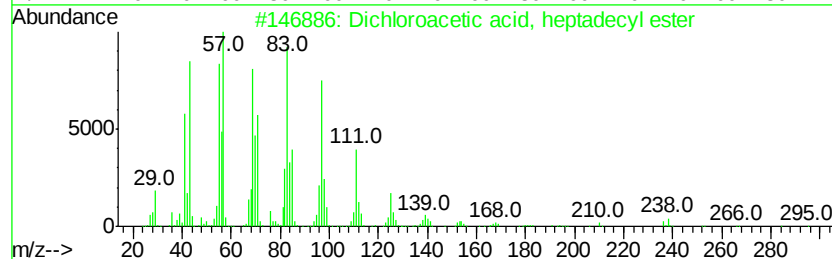
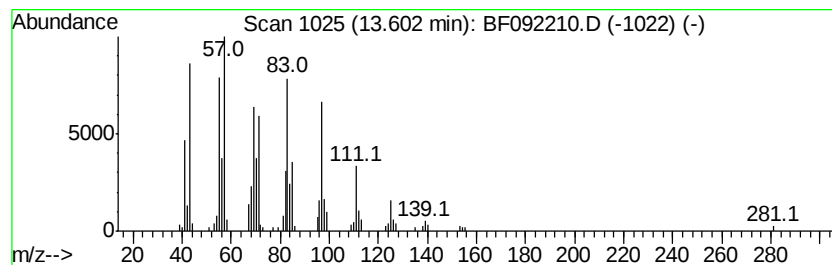
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	4.15 ng	226841	Chrysene-d12	13.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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Acq On : 12 Jan 2017 16:13
Operator : UM/SJ
Sample : I1029-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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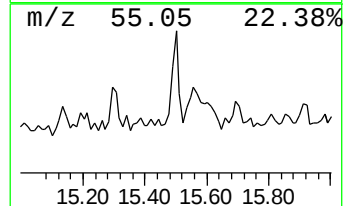
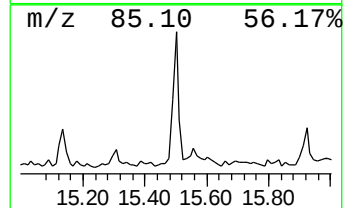
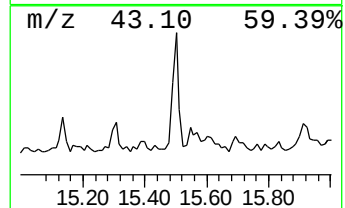
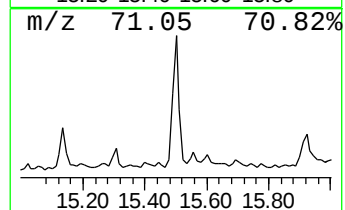
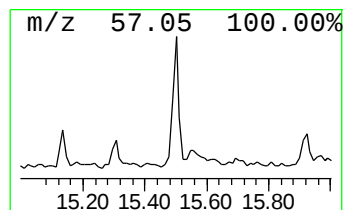
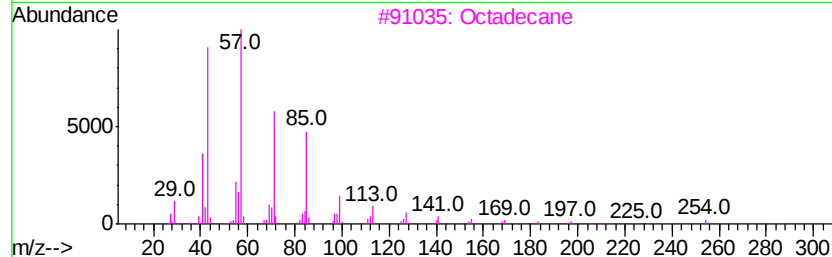
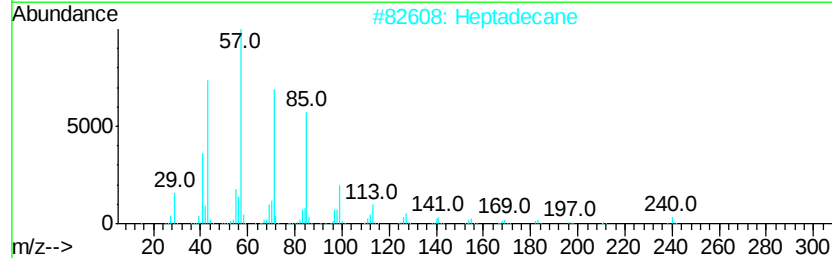
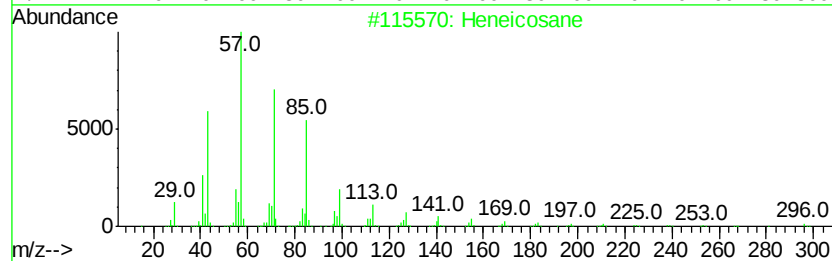
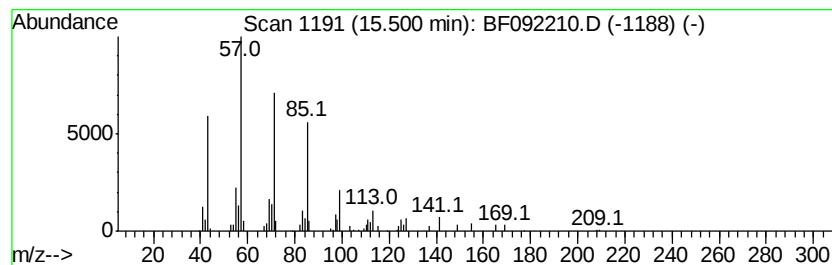
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	2.18 ng	91850	Perylene-d12	15.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane		240	C17H36	000629-78-7	90
3	Octadecane		254	C18H38	000593-45-3	86
4	Hexadecane		226	C16H34	000544-76-3	86
5	Octacosane		394	C28H58	000630-02-4	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092210.D
Acq On : 12 Jan 2017 16:13
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Sample : I1029-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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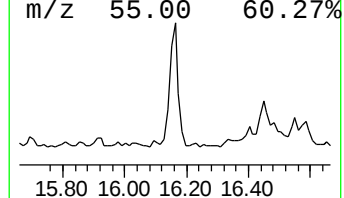
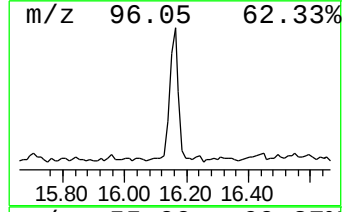
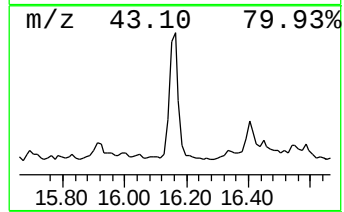
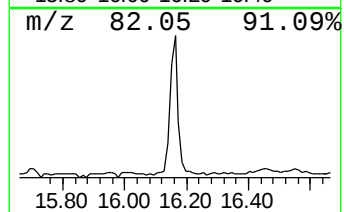
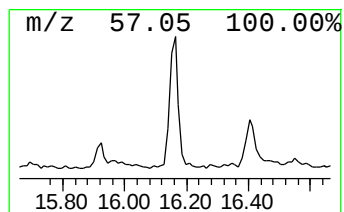
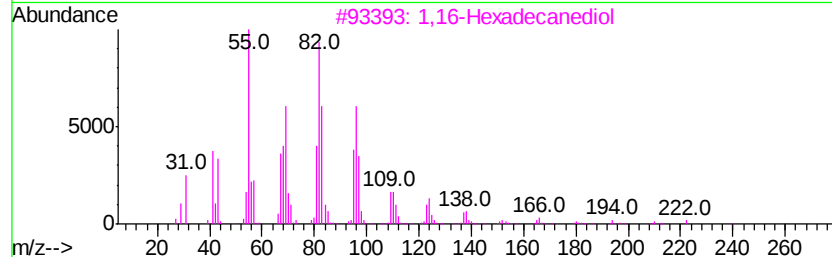
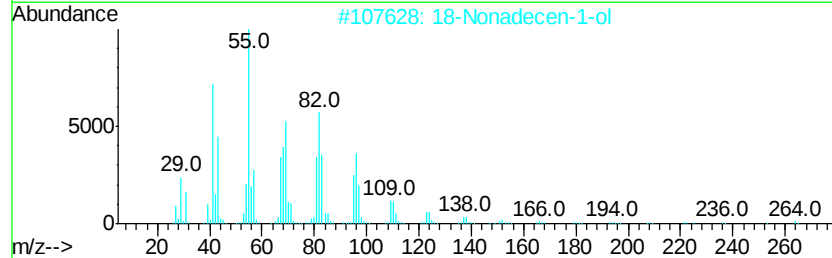
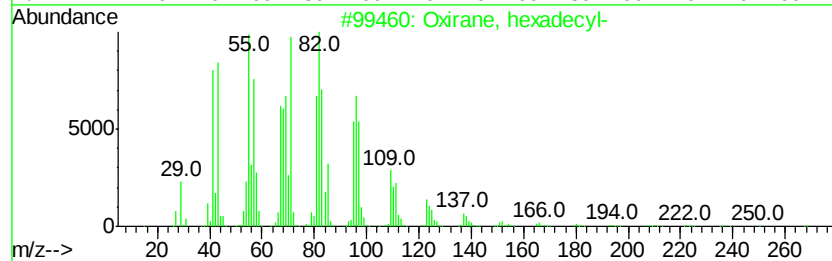
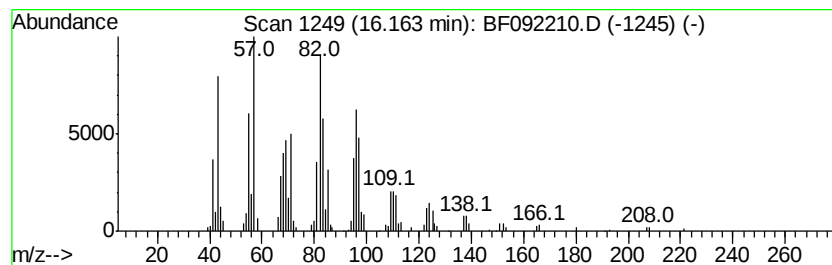
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	7.64 ng	321184	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	74
3		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	72
4		1,19-Eicosadiene	278	C20H38	014811-95-1	64
5		trans-11-Tetradecenyl acetate	254	C16H30O2	033189-72-9	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092210.D
Acq On : 12 Jan 2017 16:13
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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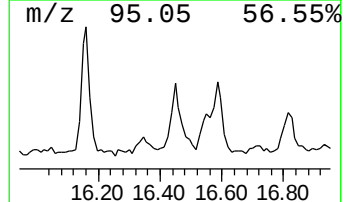
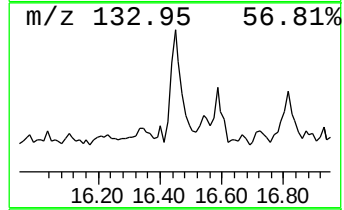
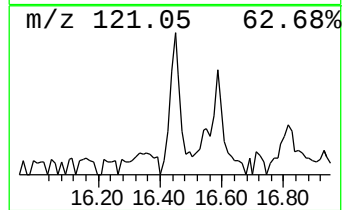
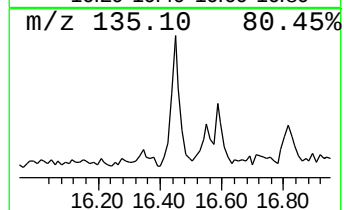
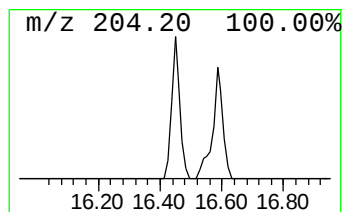
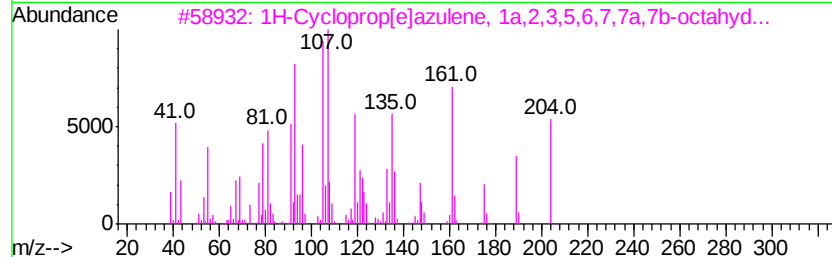
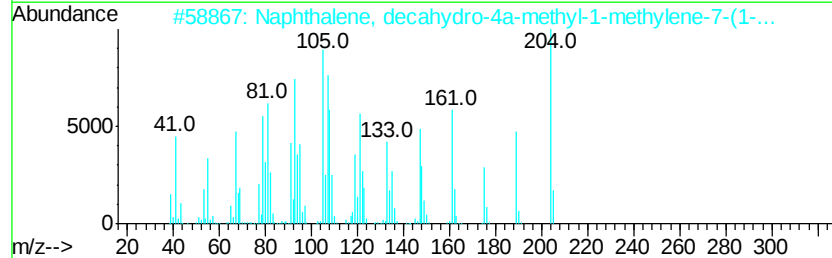
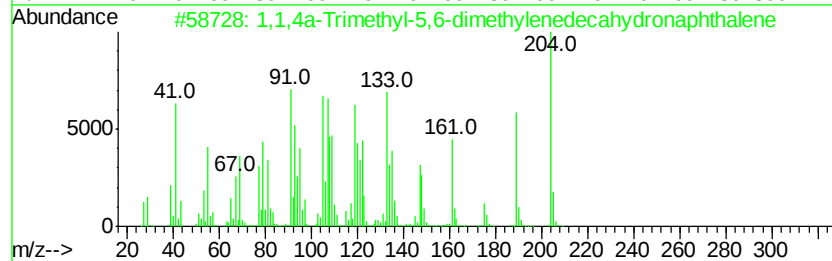
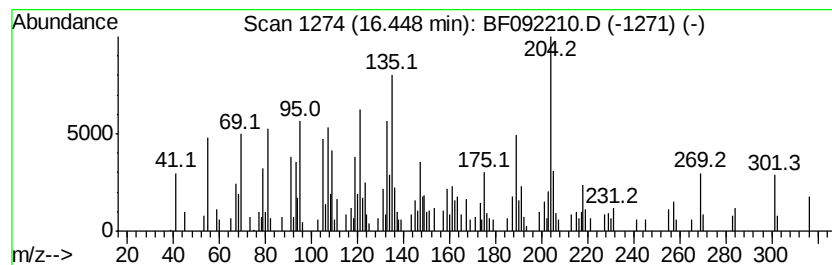
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	7.36 ng	309330	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	68
2		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	52
3		1H-Cycloprop[elazulene, 1a,2,3,5...	204	C15H24	021747-46-6	50
4		Labda-7,14-dien-13(R)-ol-.alpha....	436	C26H44O5	1000292-93-1	50
5		Aciphyllene	204	C15H24	087745-31-1	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092210.D
Acq On : 12 Jan 2017 16:13
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Misc :
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ClientSampleId :
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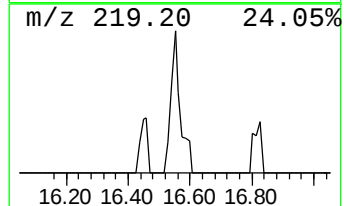
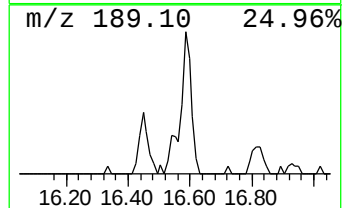
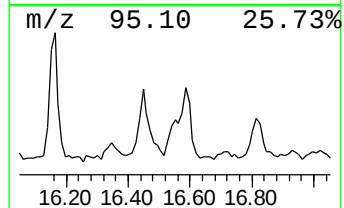
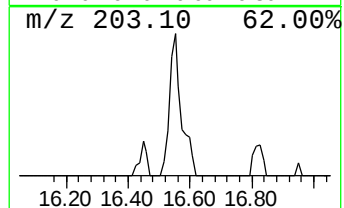
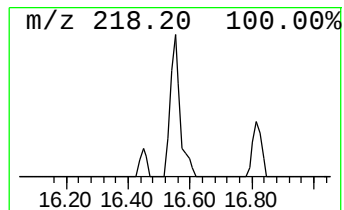
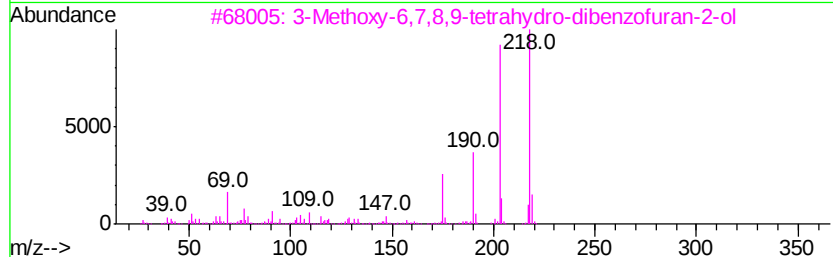
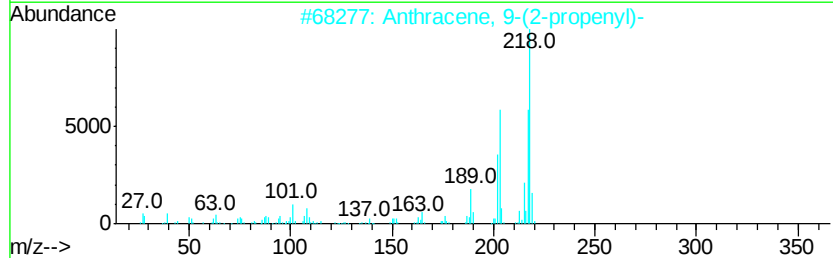
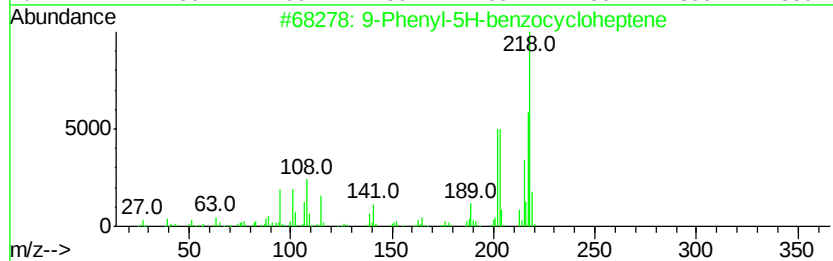
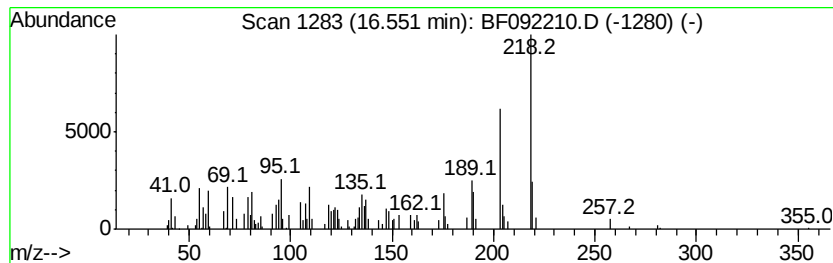
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Phenyl-5H-benzocycloheptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	3.28 ng	137772	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	58
2		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	52
3		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	50
4		5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	50
5		1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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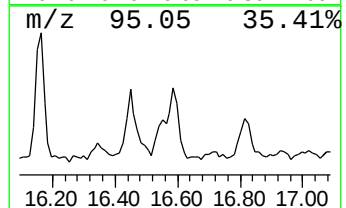
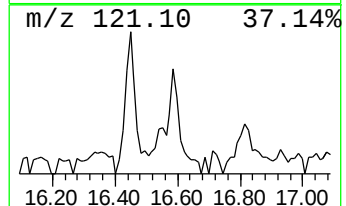
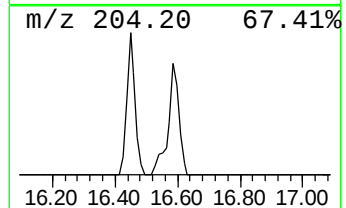
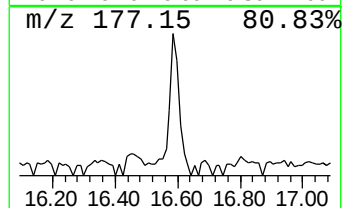
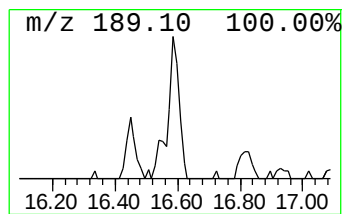
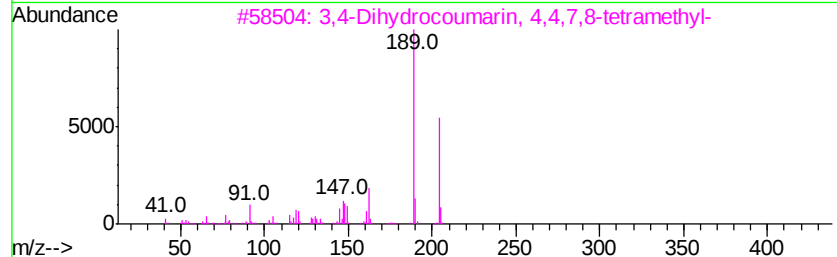
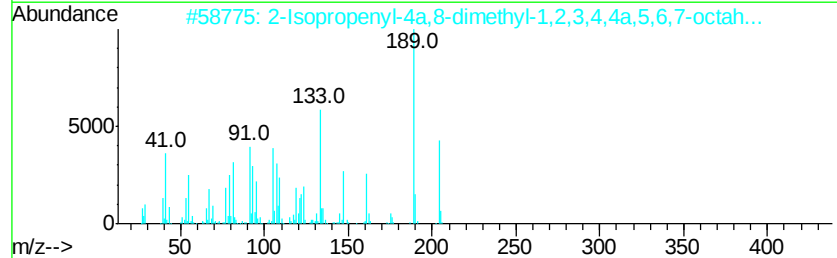
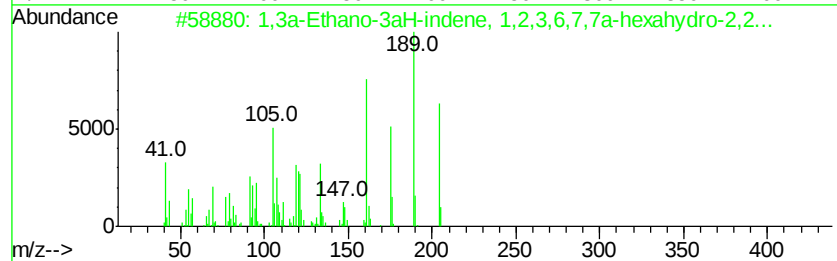
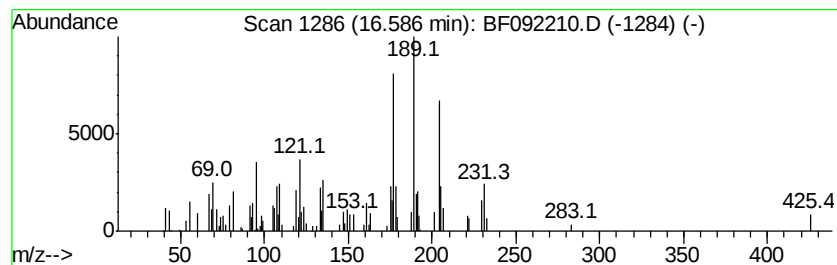
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	4.07 ng	171298	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	41
2		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	41
3		3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	38
4		2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	38
5		Cedrene-V6	204	C15H24	1000162-76-8	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
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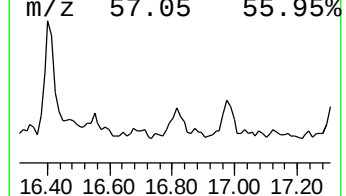
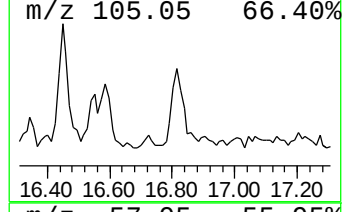
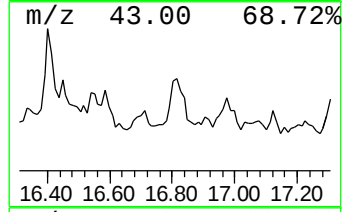
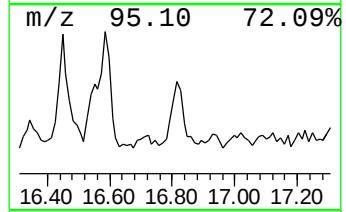
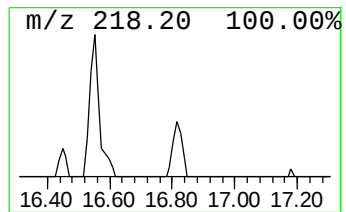
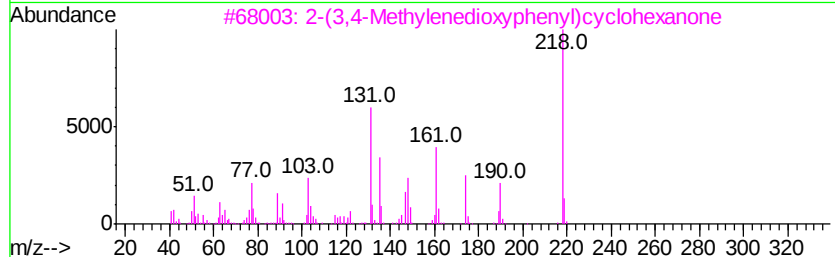
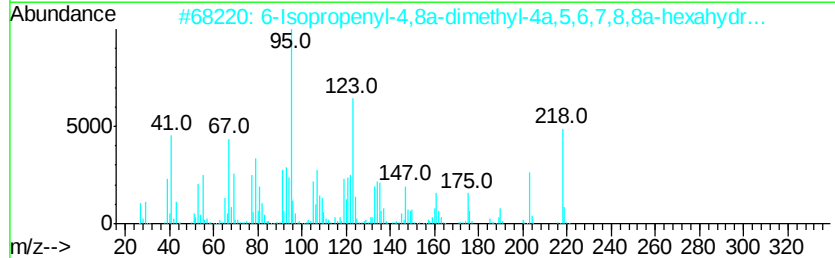
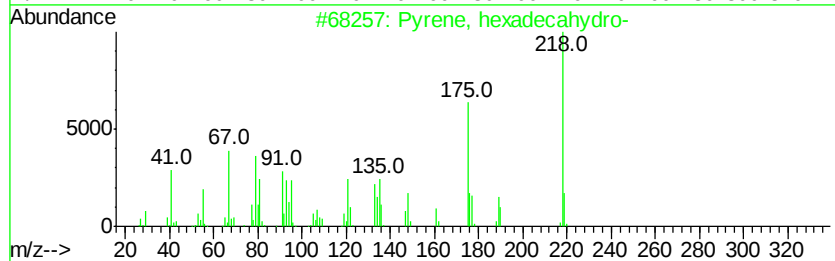
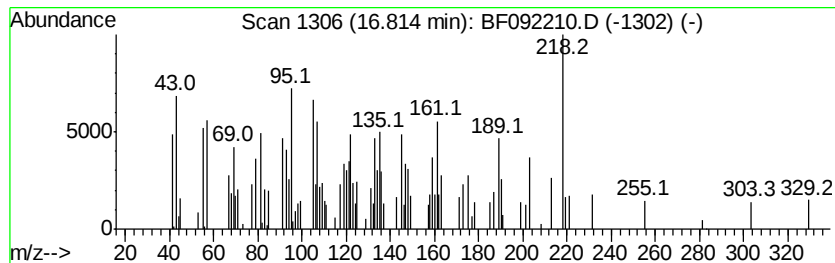
Instrument :
BNA_F
ClientSampleId :
COMP-003

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

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

Peak Number 13 unknown16.81 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	3.30 ng	138737	Perylene-d12	15.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, hexadecahydro-	218 C16H26	002435-85-0 45
2		6-Isopropenyl-4,8a-dimethyl-4a,5...	218 C15H220	086917-79-5 45
3		2-(3,4-Methylenedioxyphenyl)cycl...	218 C13H1403	042866-86-4 42
4		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218 C15H220	006754-66-1 38
5		1s,4R,7R,11R-1,3,4,7-Tetramethyl...	218 C15H220	137235-42-8 38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092210.D
Acq On : 12 Jan 2017 16:13
Operator : UM/SJ
Sample : I1029-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-003

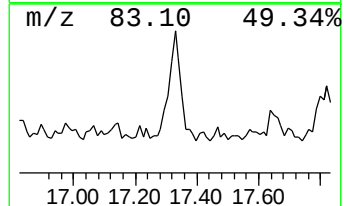
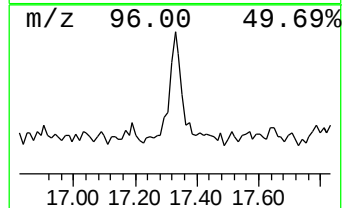
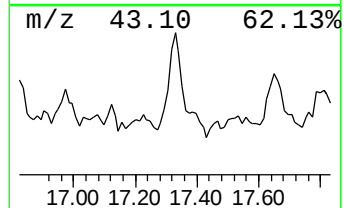
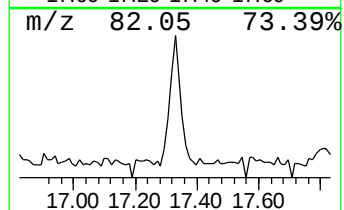
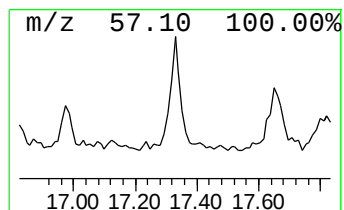
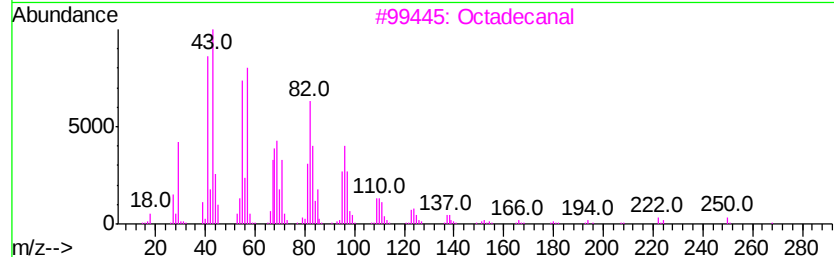
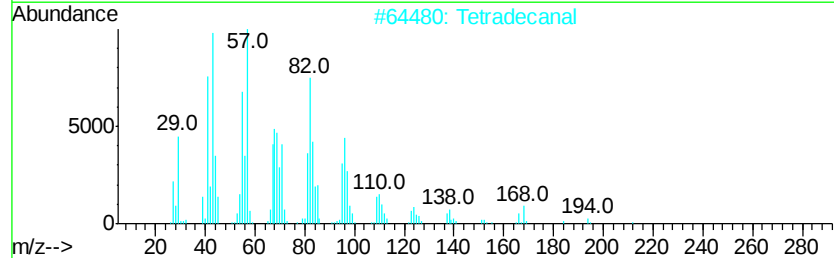
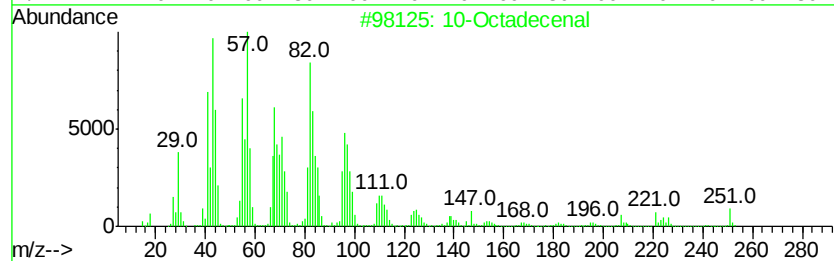
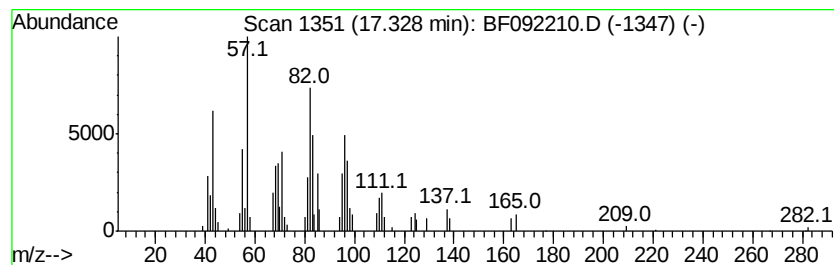
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 10-Octadecenal Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	2.12 ng	89226	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Octadecenal	266	C18H34O	056554-92-8	86
2		Tetradecanal	212	C14H28O	000124-25-4	78
3		Octadecanal	268	C18H36O	000638-66-4	78
4		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74
5		Dodecane, 2-cyclohexyl-	252	C18H36	013151-82-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
 Data File : BF092210.D
 Acq On : 12 Jan 2017 16:13
 Operator : UM/SJ
 Sample : I1029-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-003

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.99	2.6	ng	142411	1	6.60	1082380	20.0
2-Pentanone, 4-hy...	4.73	50.6	ng	2740920	1	6.60	1082380	20.0
unknown6.37	6.37	92.4	ng	5000580	1	6.60	1082380	20.0
n-Hexadecanoic acid	11.66	5.0	ng	351490	4	11.11	1419470	20.0
Tetradecanoic acid	12.44	2.4	ng	132651	5	13.73	1092030	20.0
Dichloroacetic ac...	13.60	4.2	ng	226841	5	13.73	1092030	20.0
Heneicosane	15.50	2.2	ng	91850	6	15.09	840951	20.0
Oxirane, hexadecyl-	16.16	7.6	ng	321184	6	15.09	840951	20.0
1,1,4a-Trimethyl-...	16.45	7.4	ng	309330	6	15.09	840951	20.0
9-Phenyl-5H-benzo...	16.55	3.3	ng	137772	6	15.09	840951	20.0
unknown16.59	16.59	4.1	ng	171298	6	15.09	840951	20.0
unknown16.81	16.81	3.3	ng	138737	6	15.09	840951	20.0
10-Octadecenal	17.33	2.1	ng	89226	6	15.09	840951	20.0