

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060415\
 Data File : BF079726.D
 Acq On : 5 Jun 2015 4:43
 Operator : TP/IZ
 Sample : G2443-08
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-027

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-BF060415.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	2.261	92	94	108	rVB	136191	357793	10.85%	0.980%
2	2.455	108	111	125	rVV2	589413	1425146	43.22%	3.902%
3	2.661	125	129	141	rVB	68481	212764	6.45%	0.582%
4	2.924	149	152	156	rVB	224616	332646	10.09%	0.911%
5	6.124	430	432	435	rBV	2290737	2068037	62.72%	5.662%
6	7.107	515	518	520	rBV	1952504	2274990	68.99%	6.228%
7	7.279	530	533	535	rBV	2405938	2343216	71.06%	6.415%
8	7.507	551	553	555	rVB	607538	499633	15.15%	1.368%
9	7.667	565	567	569	rBV	2151669	1776138	53.86%	4.862%
10	8.067	599	602	604	rBV	1035449	1254925	38.06%	3.436%
11	8.799	664	666	670	rBV	832724	716403	21.73%	1.961%
12	9.873	758	760	763	rVB	3402212	2740754	83.12%	7.503%
13	10.262	792	794	795	rBV	625818	575706	17.46%	1.576%
14	10.582	820	822	823	rBV	638073	785300	23.82%	2.150%
15	11.371	888	891	894	rBV	1940948	1695377	51.42%	4.641%
16	12.091	952	954	955	rBV	945384	1001826	30.38%	2.743%
17	12.114	955	956	958	rVV	946695	690180	20.93%	1.889%
18	12.171	958	961	962	rVV	154738	206189	6.25%	0.564%
19	12.731	1008	1010	1013	rBV2	167337	284444	8.63%	0.779%
20	13.382	1064	1067	1069	rBV	1405182	1338444	40.59%	3.664%
21	13.645	1085	1090	1092	rBV	951761	1545046	46.86%	4.230%
22	13.782	1099	1102	1104	rBV	3246919	3297400	100.00%	9.027%
23	13.885	1108	1111	1115	rBV3	88251	207873	6.30%	0.569%
24	14.011	1115	1122	1124	rBV	150643	347084	10.53%	0.950%
25	14.754	1183	1187	1188	rBV2	101545	179453	5.44%	0.491%
26	14.822	1191	1193	1195	rBV2	326327	389346	11.81%	1.066%
27	15.062	1211	1214	1216	rBV2	1075572	1904969	57.77%	5.215%
28	15.097	1216	1217	1222	rVB	648120	614516	18.64%	1.682%
29	15.657	1264	1266	1271	rBV5	75609	216179	6.56%	0.592%
30	16.183	1309	1312	1315	rBV2	164122	263643	8.00%	0.722%
31	16.445	1332	1335	1340	rBV	511856	1330768	40.36%	3.643%
32	16.857	1368	1371	1375	rVB	342906	569081	17.26%	1.558%
33	16.937	1375	1378	1382	rBV	417536	730491	22.15%	2.000%
34	17.028	1383	1386	1388	rVV	669234	1039831	31.53%	2.847%

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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-BF060415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.074	1388	1390	1394	rVB2	133812	257076	7.80%	0.704%
36	19.040	1558	1562	1568	rVB2	223052	582357	17.66%	1.594%
37	19.646	1611	1615	1622	rVB	179679	472611	14.33%	1.294%

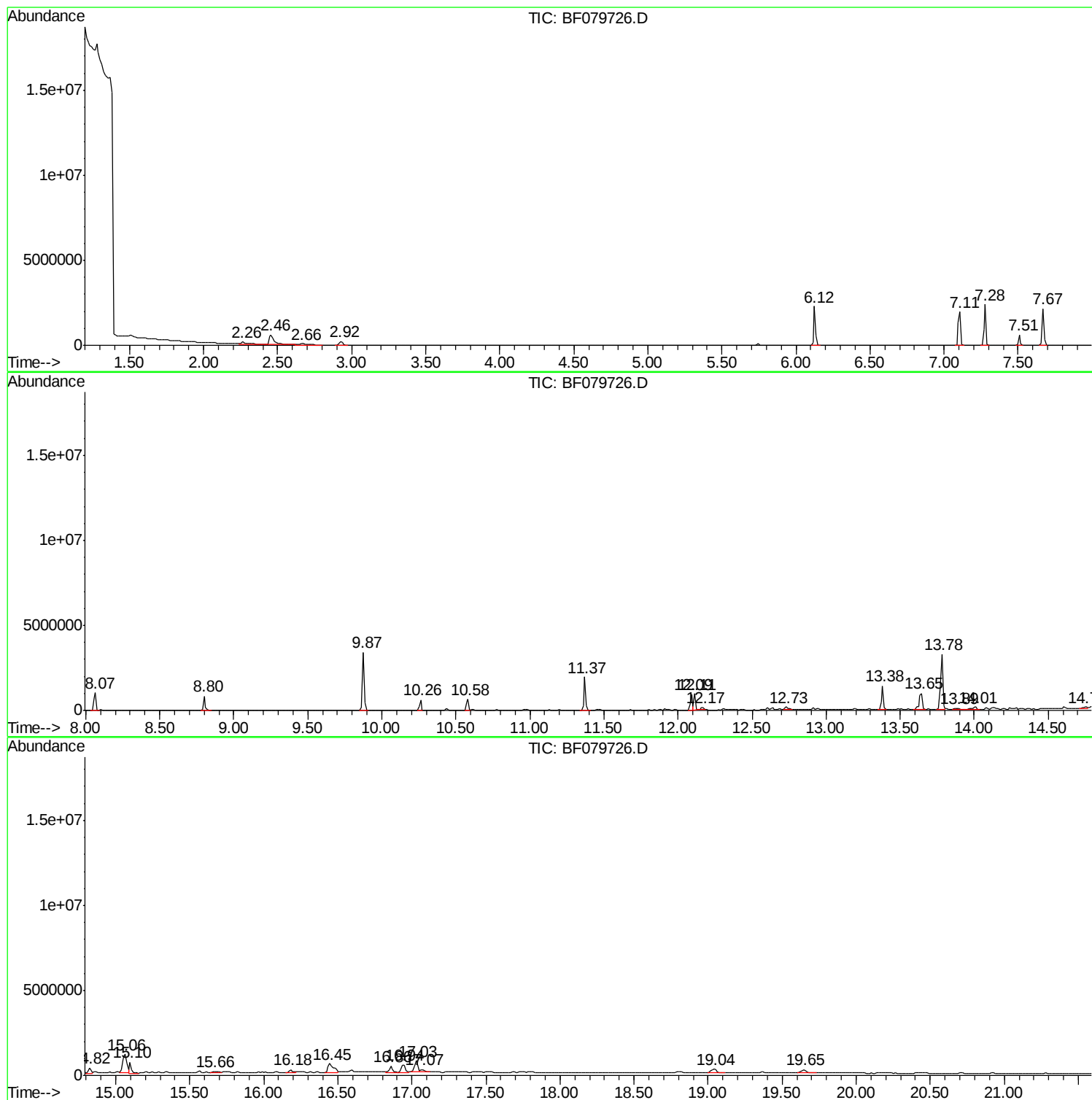
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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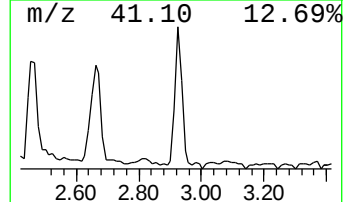
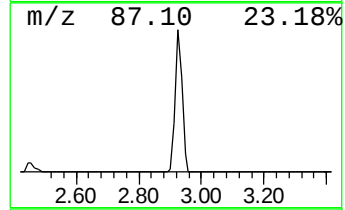
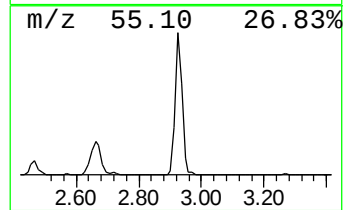
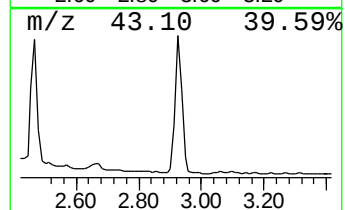
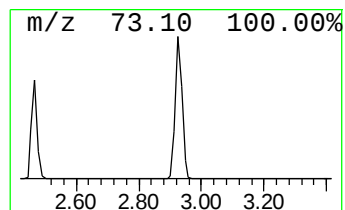
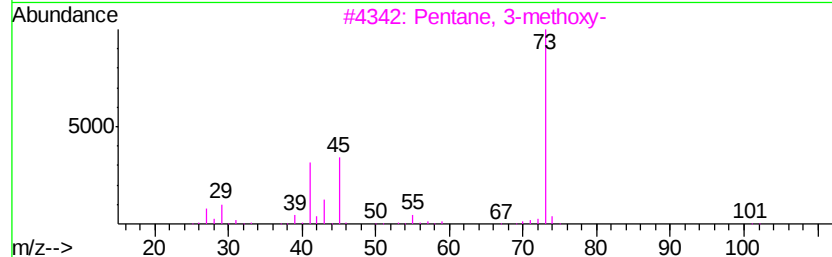
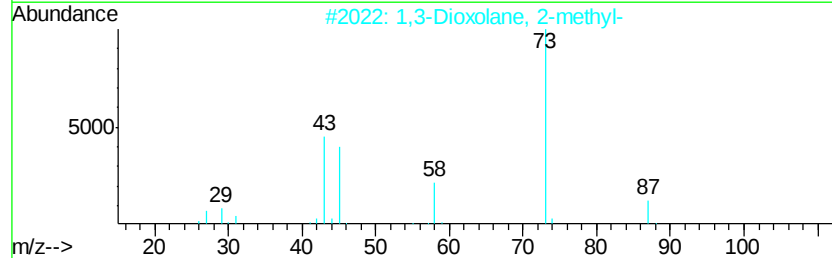
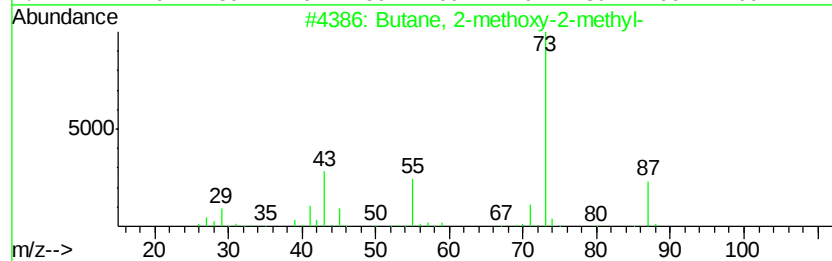
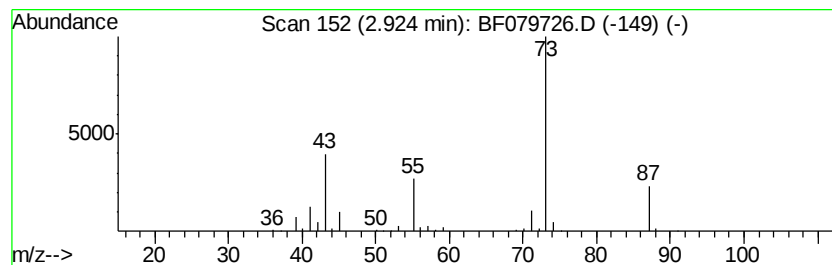
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	13.32 ng	332646	1,4-Dichlorobenzene-d4	7.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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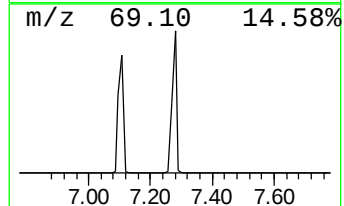
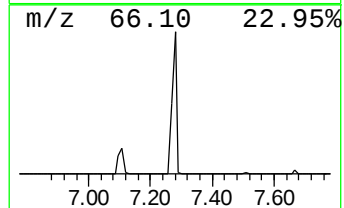
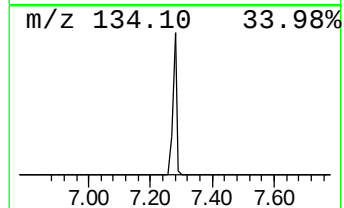
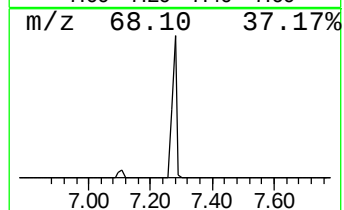
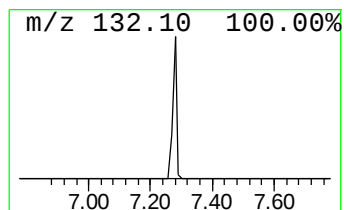
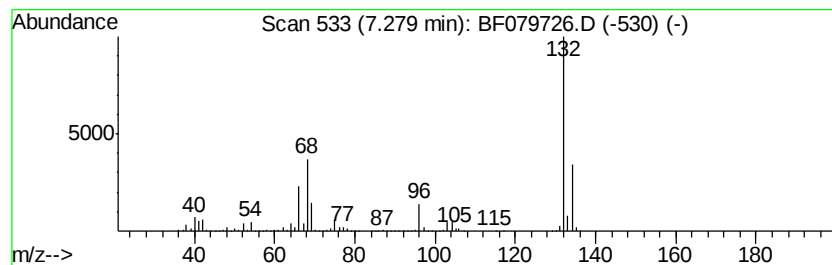
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	93.80 ng	2343220	1,4-Dichlorobenzene-d4	7.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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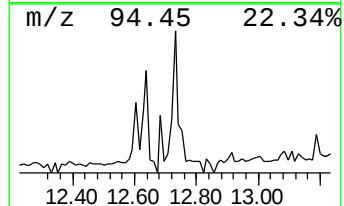
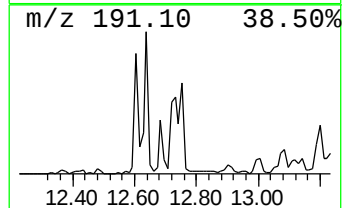
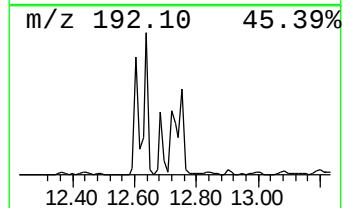
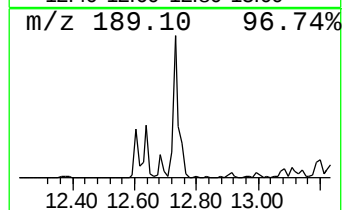
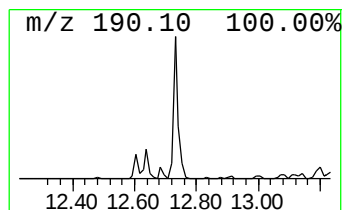
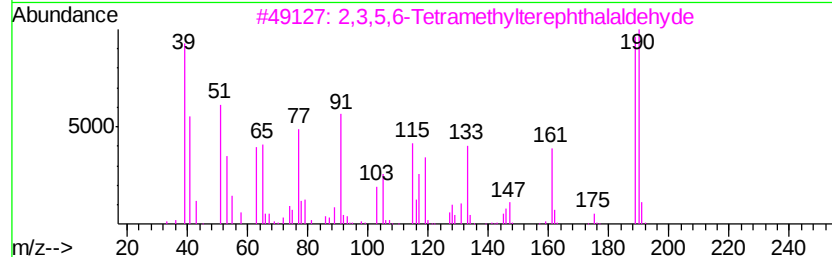
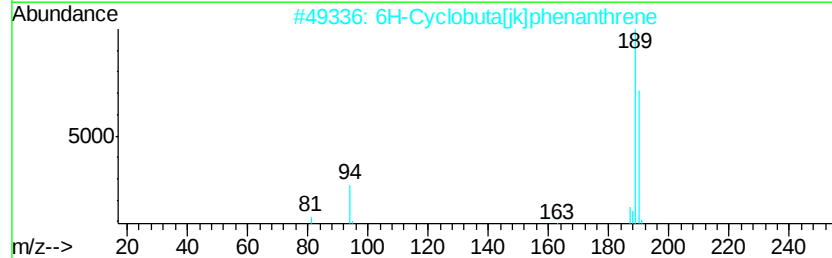
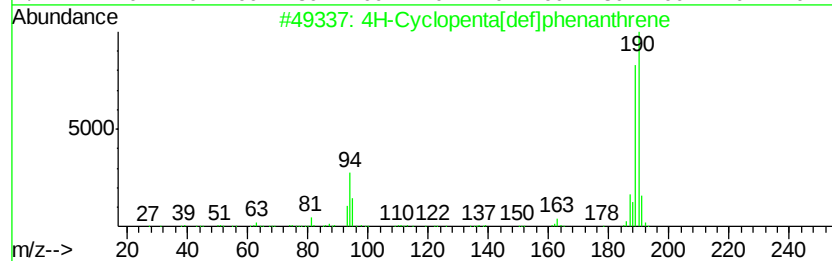
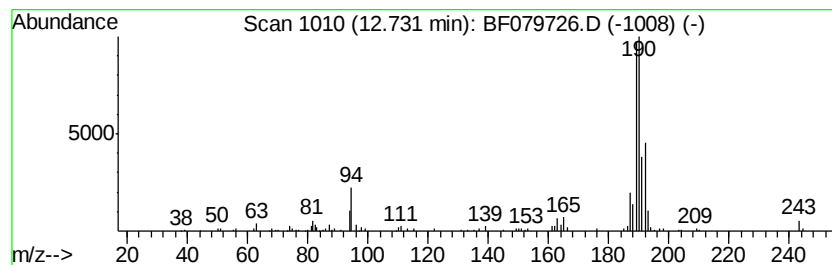
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.73	5.68 ng	284444	Phenanthrene-d10	12.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25



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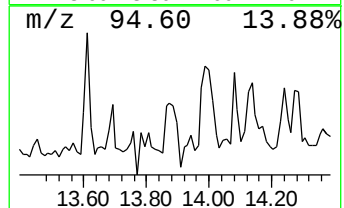
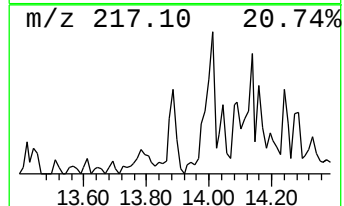
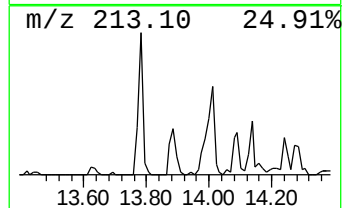
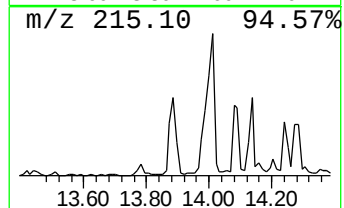
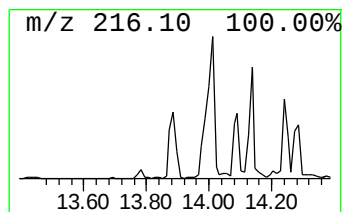
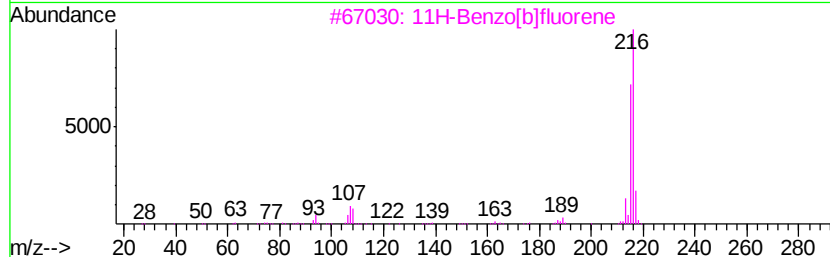
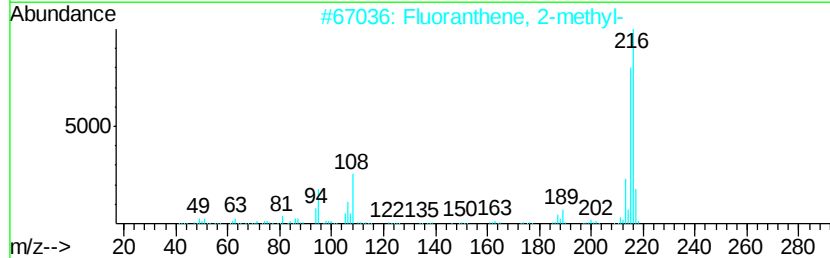
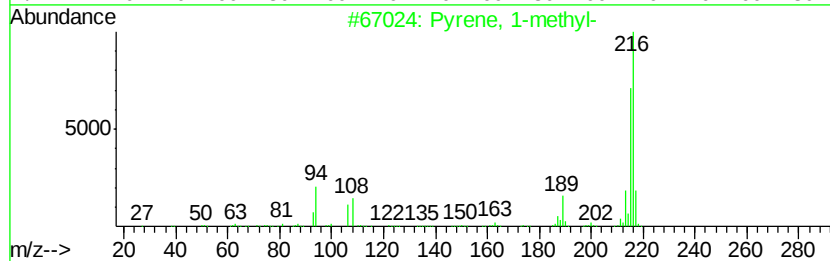
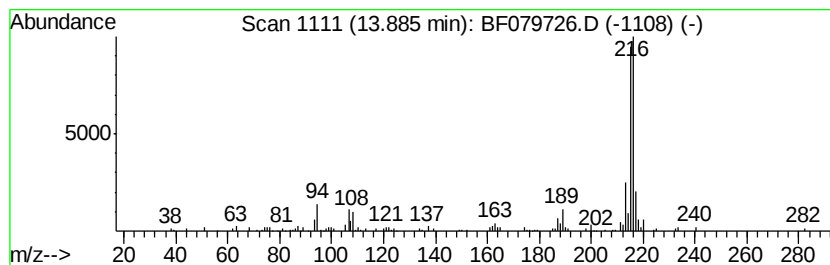
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.18 ng	207873	Chrysene-d12	15.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	86
5		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81



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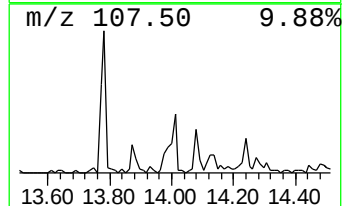
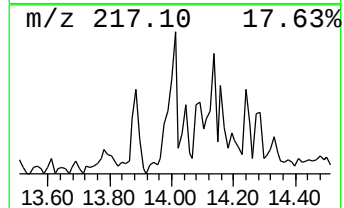
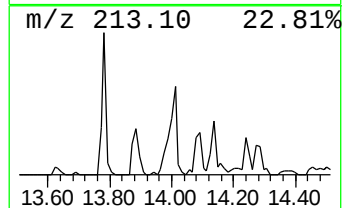
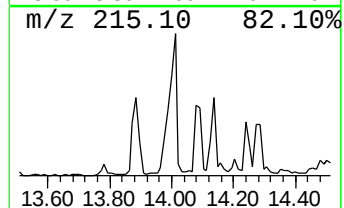
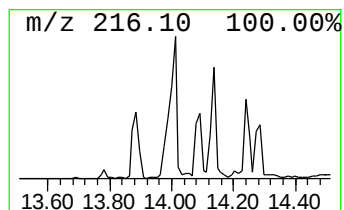
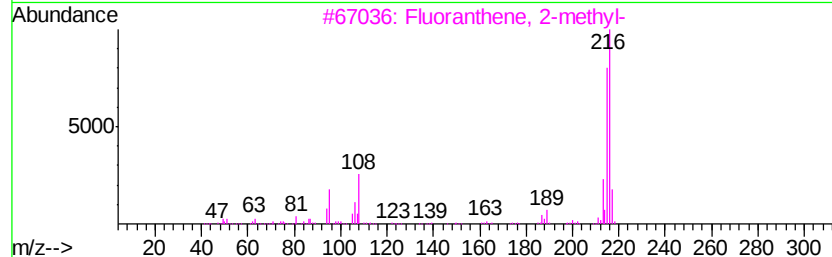
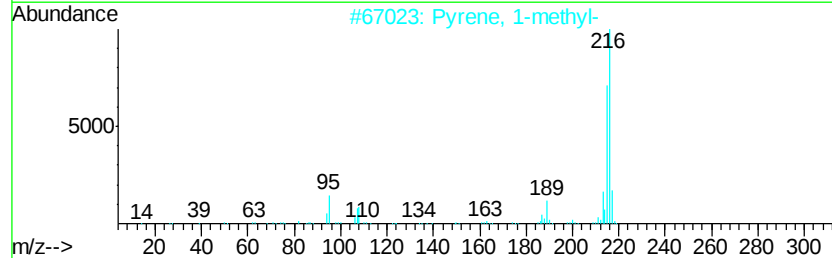
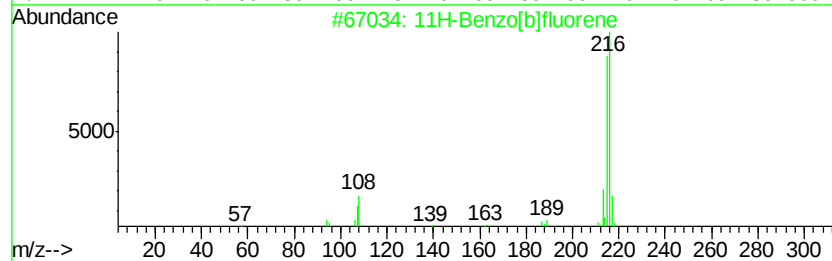
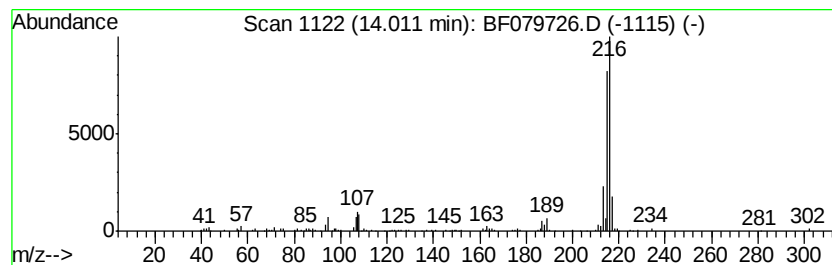
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.01	3.64 ng	347084	Chrysene-d12	15.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5		Pyridin-3-ol, 2-(4-nitrophenyl)-	216	C11H8N2O3	030820-89-4	64



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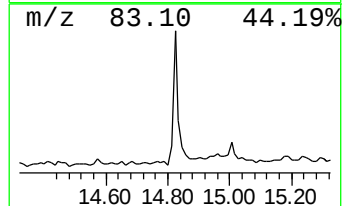
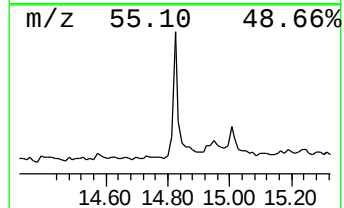
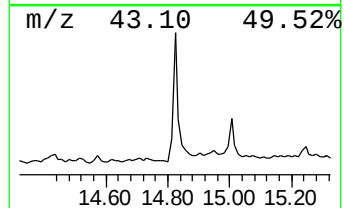
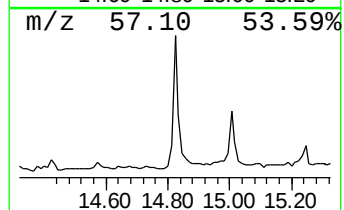
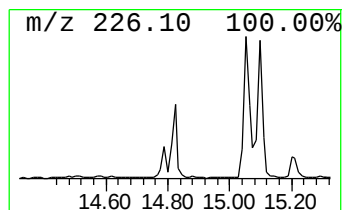
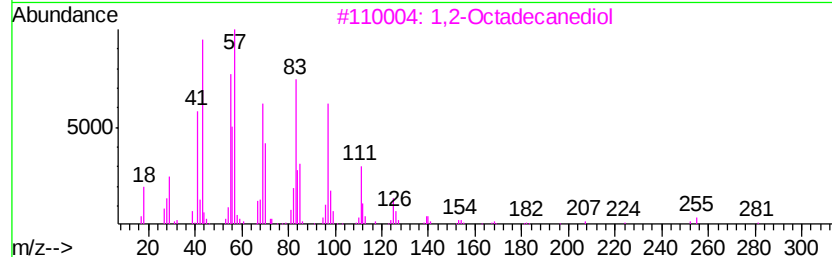
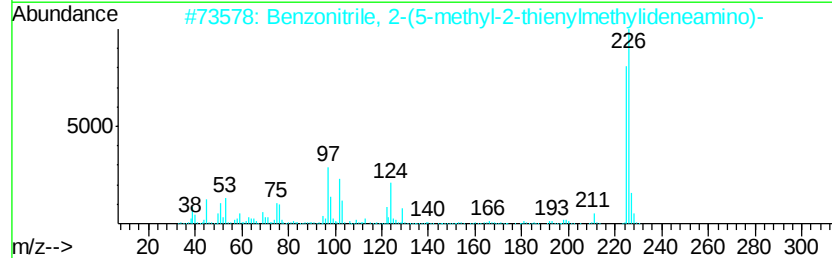
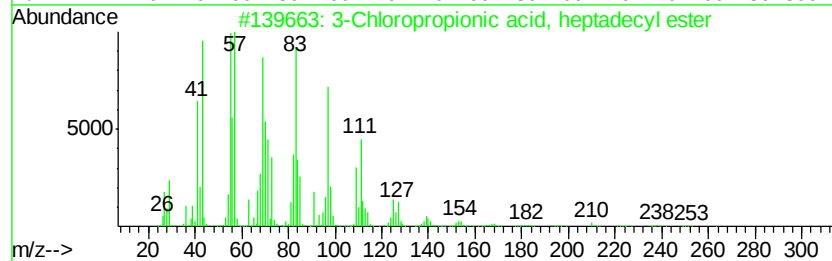
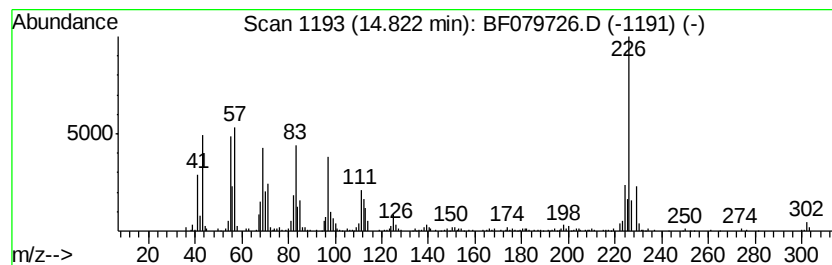
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.82 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	4.09 ng	389346	Chrysene-d12	15.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	42
2		Benzonitrile, 2-(5-methyl-2-thie...	226	C13H10N2S	315670-19-0	38
3		1,2-Octadecanediol	286	C18H38O2	020294-76-2	30
4		5(10H)-Pyrido[3,4-b]quinolone, 7...	226	C13H10N2O2	1000256-99-5	30
5		Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060415\
Data File : BF079726.D
Acq On : 5 Jun 2015 4:43
Operator : TP/IZ
Sample : G2443-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

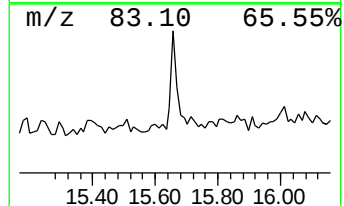
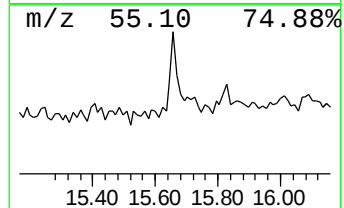
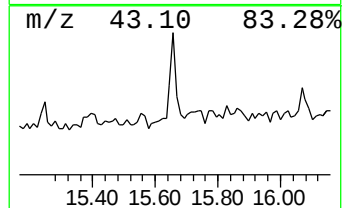
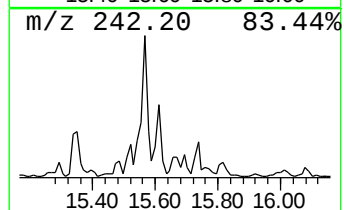
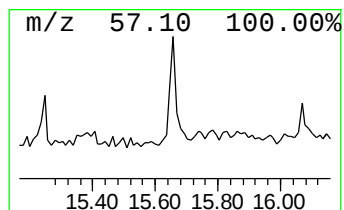
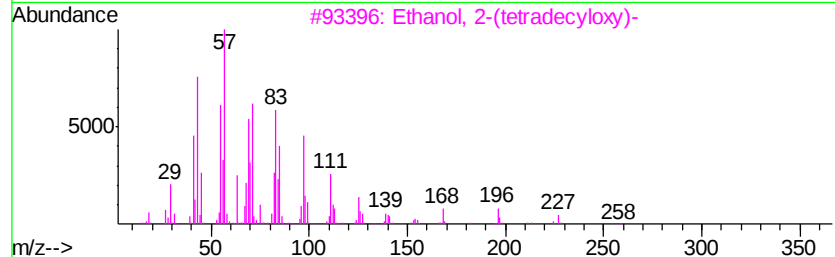
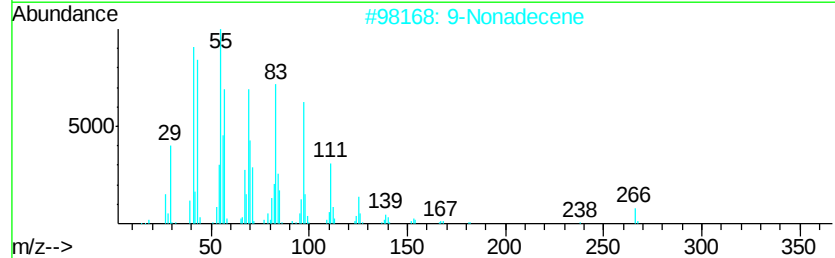
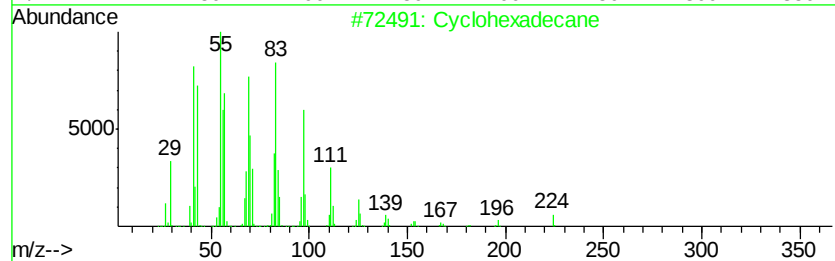
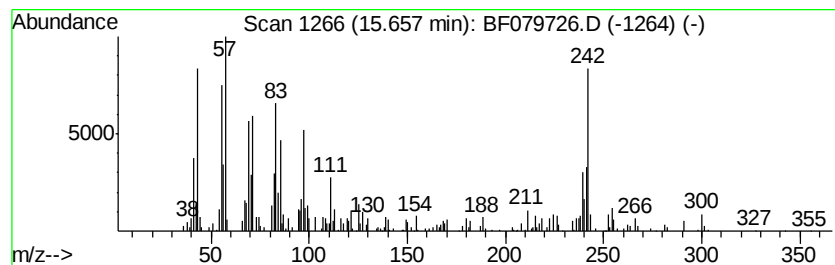
Instrument :
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ClientSampleId :
SW-027

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclohexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.27 ng	216179	Chrysene-d12	15.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 59
2		9-Nonadecene	266 C19H38	031035-07-1 56
3		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 45
4		Bromoacetic acid, hexadecyl ester	362 C18H35BrO2	005454-48-8 42
5		17-Pentatriacontene	491 C35H70	006971-40-0 42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060415\
Data File : BF079726.D
Acq On : 5 Jun 2015 4:43
Operator : TP/IZ
Sample : G2443-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-027

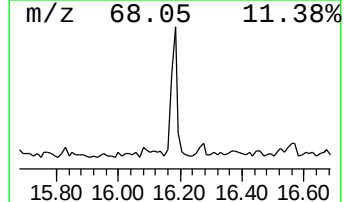
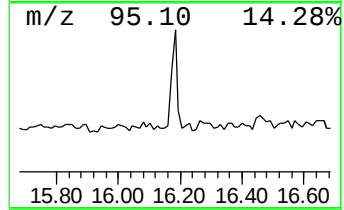
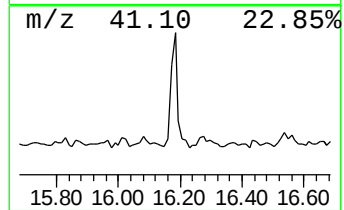
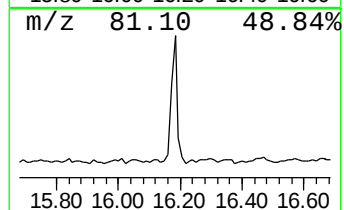
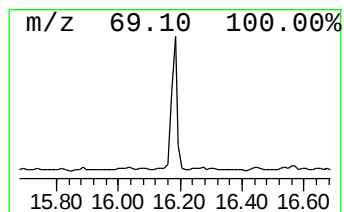
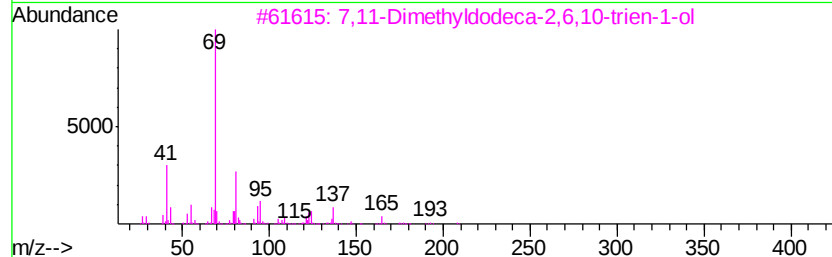
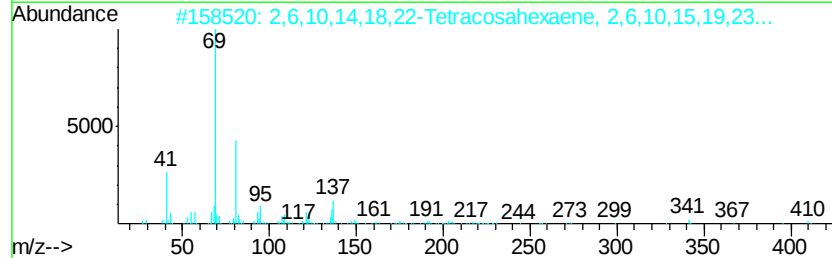
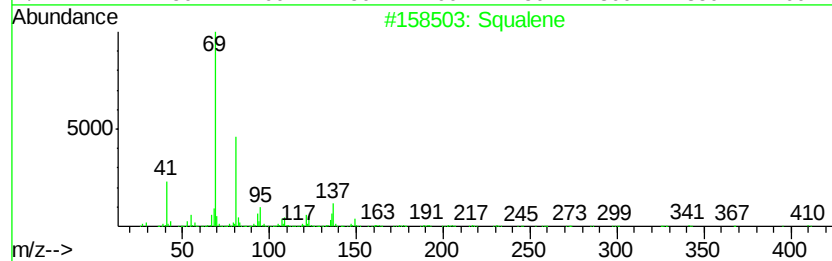
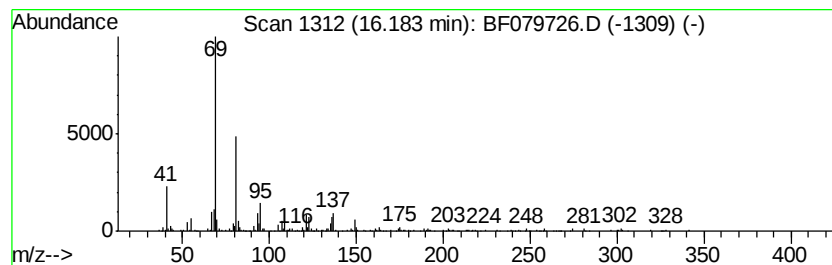
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	5.07 ng	263643	Perylene-d12	17.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	90
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H240	125529-10-4	64
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H260	000106-28-5	59
5		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H300	001117-52-8	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060415\
Data File : BF079726.D
Acq On : 5 Jun 2015 4:43
Operator : TP/IZ
Sample : G2443-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-027

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060415.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
Butane, 2-methoxy...	2.92	13.3	ng	332646	1	7.51	499633	20.0
unknown7.28	7.28	93.8	ng	2343220	1	7.51	499633	20.0
4H-Cyclopenta[def...	12.73	5.7	ng	284444	4	12.09	1001830	20.0
Pyrene, 1-methyl-	13.89	2.2	ng	207873	5	15.06	1904970	20.0
11H-Benzo[b]fluorene	14.01	3.6	ng	347084	5	15.06	1904970	20.0
unknown14.82	14.82	4.1	ng	389346	5	15.06	1904970	20.0
Cyclohexadecane	15.66	2.3	ng	216179	5	15.06	1904970	20.0
Squalene	16.18	5.1	ng	263643	6	17.03	1039830	20.0