

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062618\
 Data File : BF106823.D
 Acq On : 26 Jun 2018 15:28
 Operator : JU/SJ
 Sample : J3676-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-5-8

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.201	483	487	496	rBB	82928	100446	2.58%	0.656%
2	5.607	551	556	568	rBV	848090	861237	22.16%	5.627%
3	6.601	721	725	741	rVB	813474	871129	22.41%	5.692%
4	6.737	744	748	751	rBV	966885	889470	22.88%	5.811%
5	6.960	783	786	789	rBV	331484	255573	6.58%	1.670%
6	7.119	809	813	816	rBV	820126	712714	18.34%	4.657%
7	7.525	877	882	885	rBV	609081	542894	13.97%	3.547%
8	8.242	1000	1004	1007	rBV	366202	311182	8.01%	2.033%
9	9.319	1182	1187	1190	rBV	968254	951707	24.49%	6.218%
10	9.707	1250	1253	1260	rVB	161368	129914	3.34%	0.849%
11	10.001	1300	1303	1307	rBV2	360393	309950	7.97%	2.025%
12	10.795	1434	1438	1444	rBV	628476	568371	14.62%	3.714%
13	11.495	1553	1557	1559	rBV	356316	307777	7.92%	2.011%
14	11.519	1559	1561	1565	rVB	318707	237162	6.10%	1.550%
15	11.572	1565	1570	1573	rBV	71642	58669	1.51%	0.383%
16	12.024	1645	1647	1651	rVB2	48253	39250	1.01%	0.256%
17	12.113	1658	1662	1664	rBV2	54729	61361	1.58%	0.401%
18	12.713	1760	1764	1767	rBV	392565	328777	8.46%	2.148%
19	12.948	1796	1804	1809	rBV	307673	376160	9.68%	2.458%
20	13.077	1815	1826	1829	rBV	1060061	976085	25.11%	6.377%
21	13.271	1852	1859	1865	rBV2	68815	111115	2.86%	0.726%
22	13.754	1938	1941	1944	rBV	85124	74479	1.92%	0.487%
23	13.960	1972	1976	1981	rVV4	152876	183328	4.72%	1.198%
24	14.107	1998	2001	2004	rVV	48327	48431	1.25%	0.316%
25	14.154	2004	2009	2012	rVV2	459243	565251	14.54%	3.693%
26	14.183	2012	2014	2020	rVB	156385	141649	3.64%	0.925%
27	14.424	2053	2055	2061	rVB5	37584	49798	1.28%	0.325%
28	14.624	2085	2089	2096	rVV7	69341	155141	3.99%	1.014%
29	15.212	2163	2189	2199	rBV6	642671	3886701	100.00%	25.394%
30	15.324	2206	2208	2212	rVB2	40406	47677	1.23%	0.312%
31	15.577	2247	2251	2256	rVB	70720	99469	2.56%	0.650%
32	15.642	2258	2262	2267	rBV	93570	133247	3.43%	0.871%
33	15.712	2269	2274	2277	rBV	192462	250617	6.45%	1.637%
34	16.430	2393	2396	2401	rVB2	40879	59166	1.52%	0.387%

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ClientSampleId :
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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

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35	17.289	2538	2542	2547	rBV2	33664	61022	1.57%	0.399%
36	17.606	2590	2596	2609	rVB3	138020	366395	9.43%	2.394%
37	17.771	2620	2624	2630	rBV	26214	64686	1.66%	0.423%
38	17.971	2654	2658	2665	rVB7	53725	117460	3.02%	0.767%

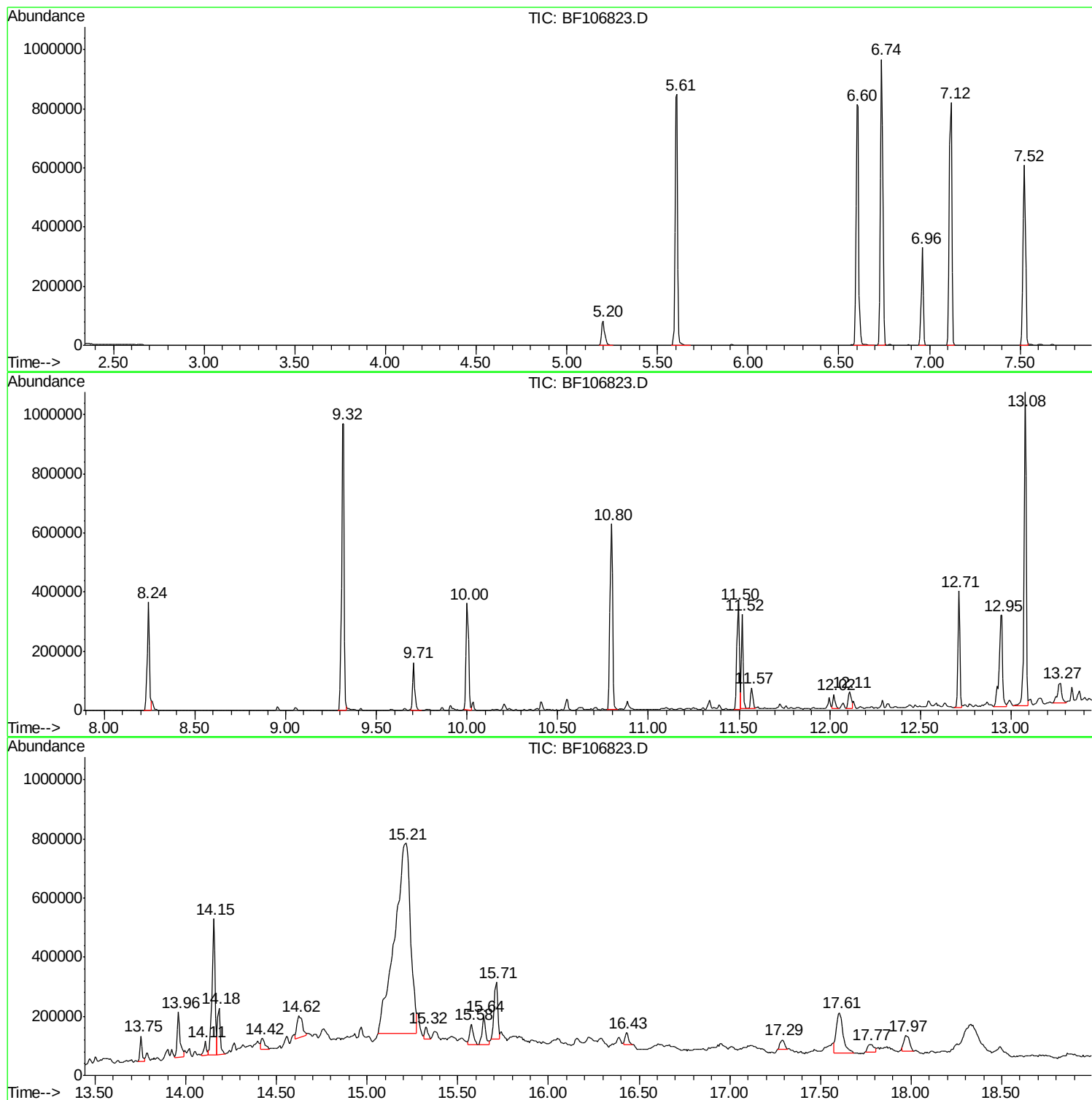
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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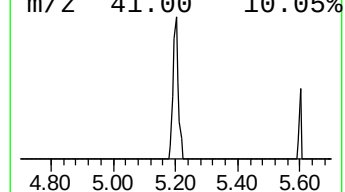
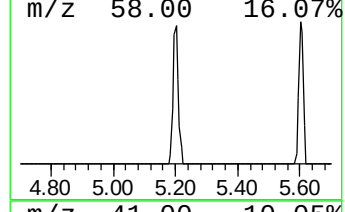
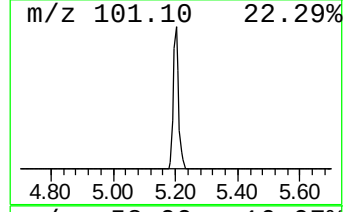
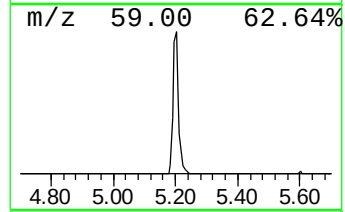
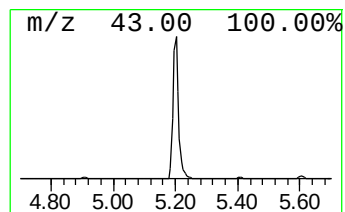
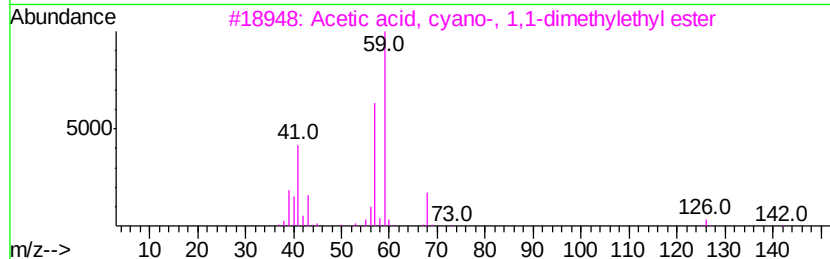
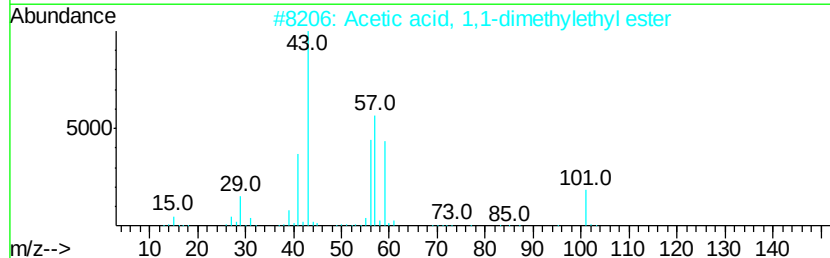
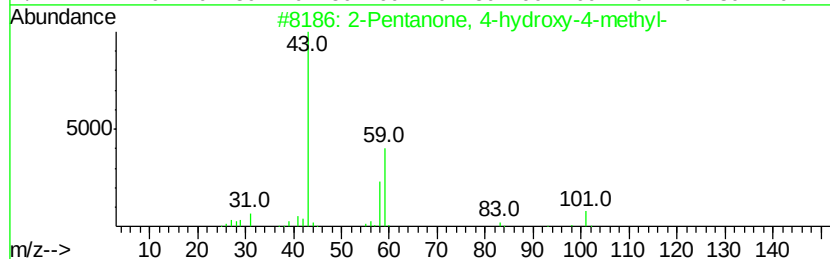
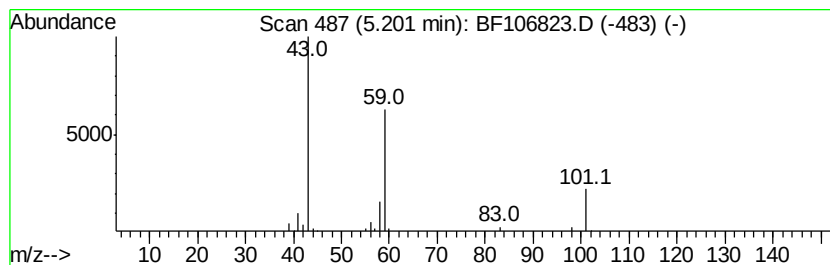
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	7.86 ng	100446	1,4-Dichlorobenzene-d4	6.96

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-dimethyl...	141	C7H11NO2	001116-98-9	23
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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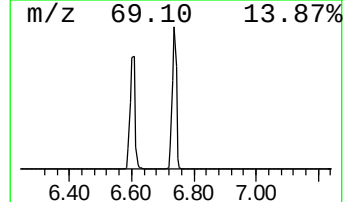
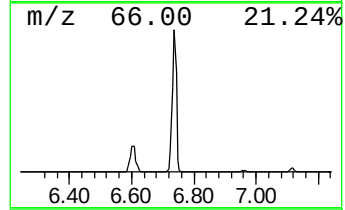
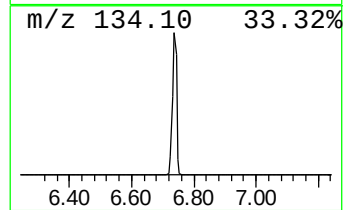
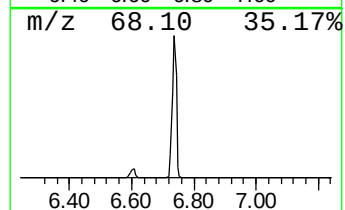
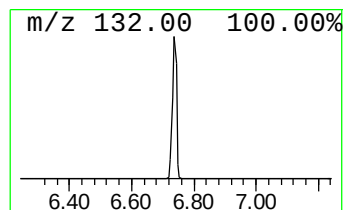
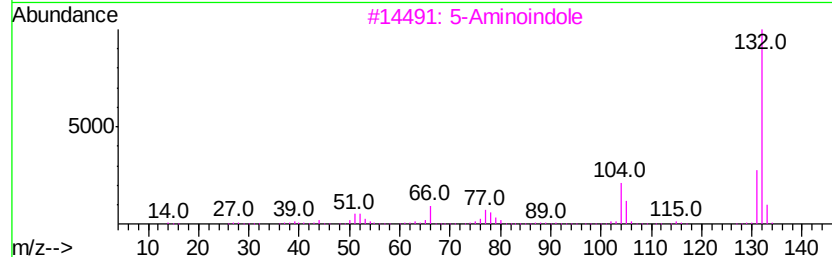
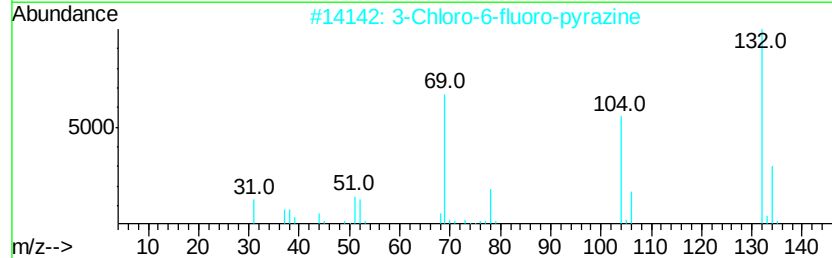
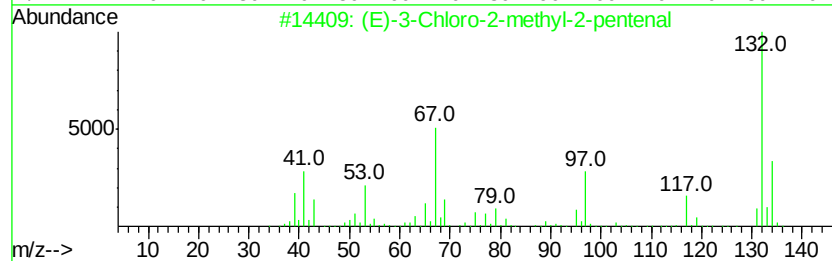
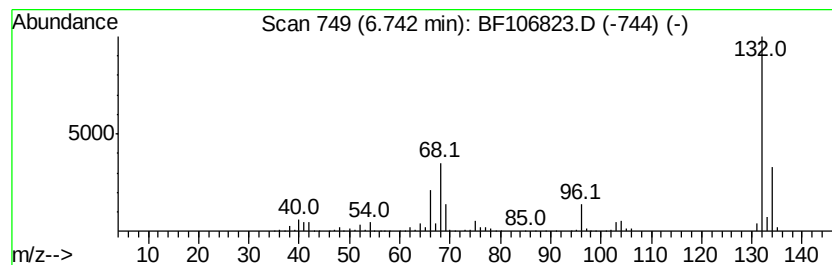
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.61 ng	889470	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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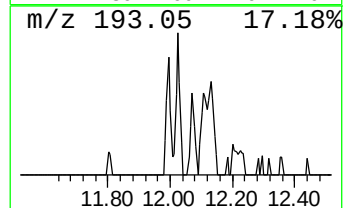
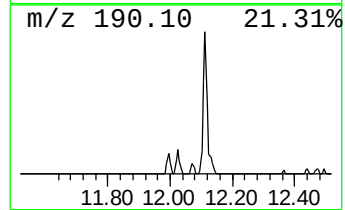
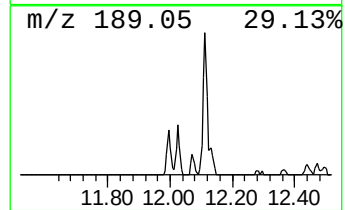
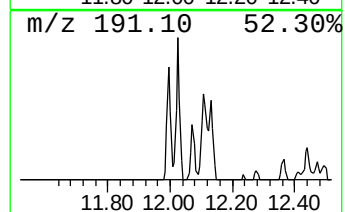
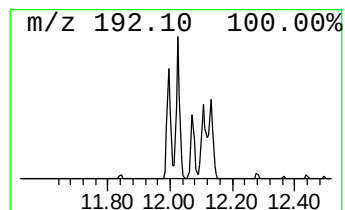
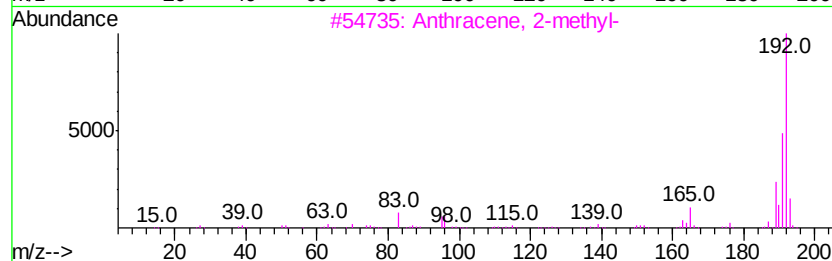
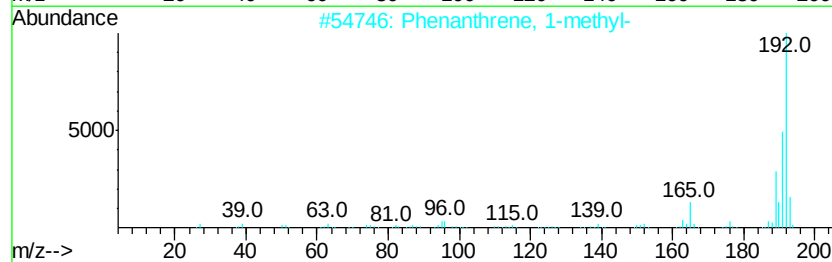
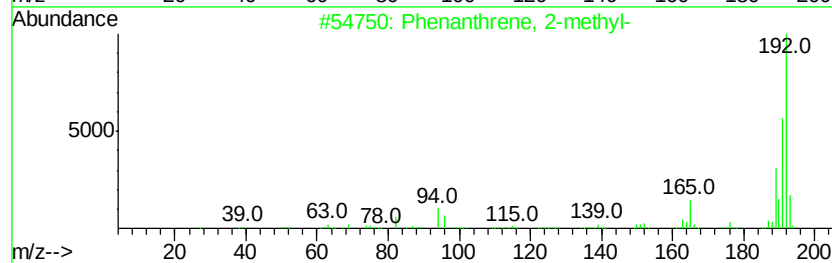
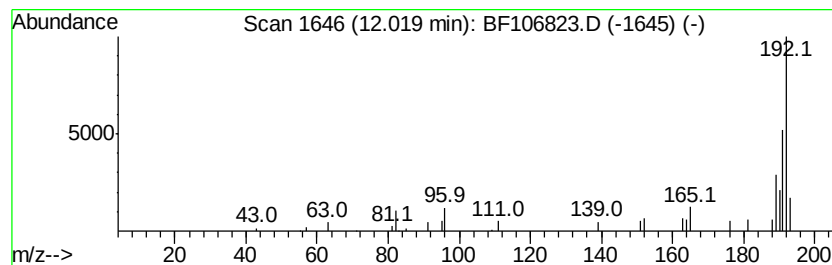
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.55 ng	39250	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4		1H-Cyclopropa[1,1]phenanthrene, 1a, ...	192	C15H12	000949-41-7	94
5		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93



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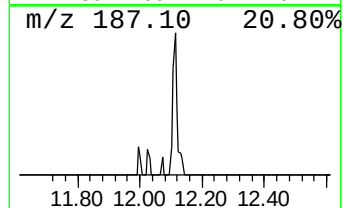
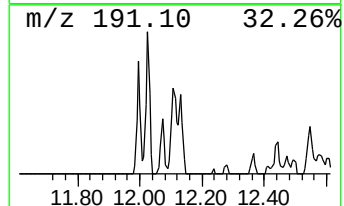
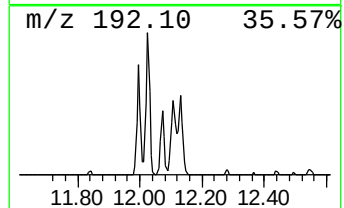
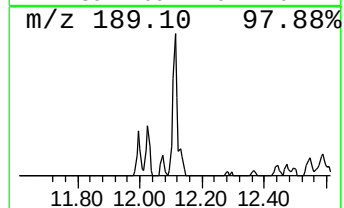
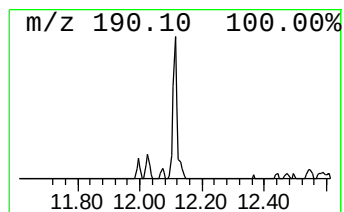
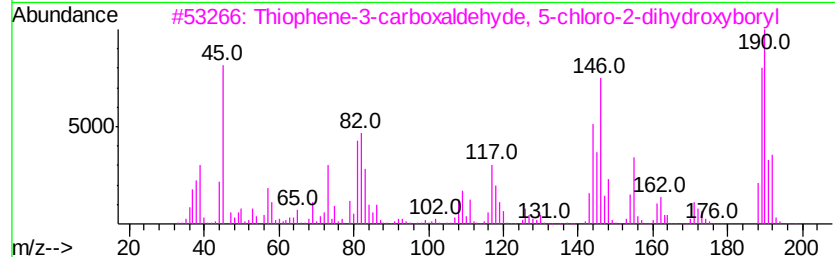
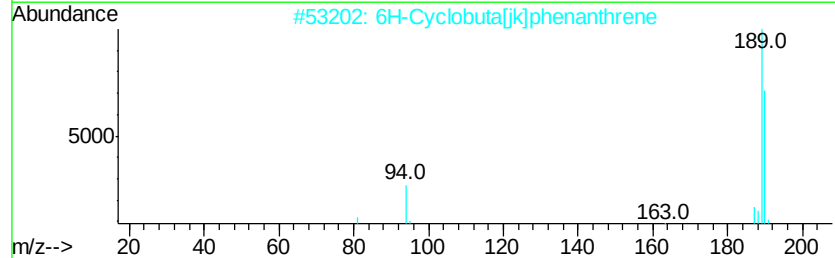
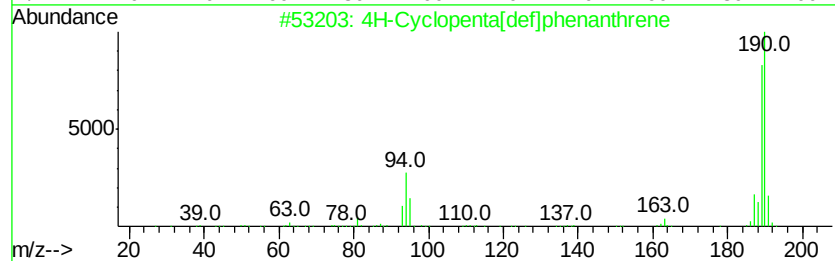
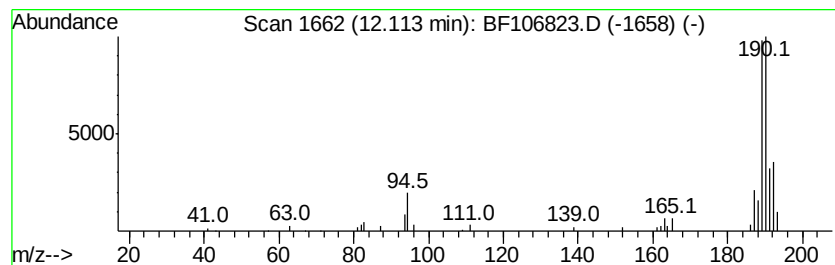
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	3.99 ng	61361	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2		6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	64
3		Thiophene-3-carboxaldehyd, 5-ch...	190	C5H4BClO3S	036155-87-0	49
4		Methyl diselenide	190	C2H6Se2	007101-31-7	43
5		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42



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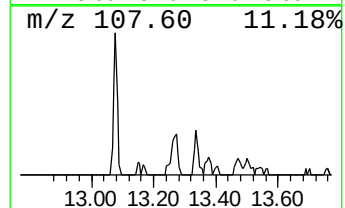
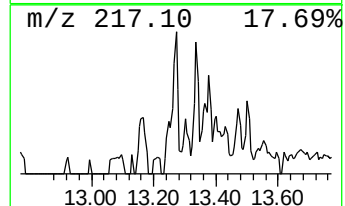
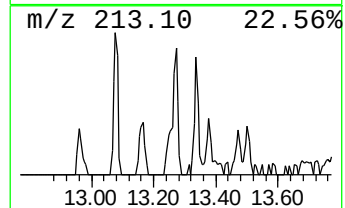
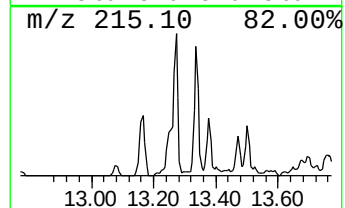
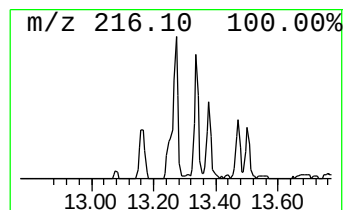
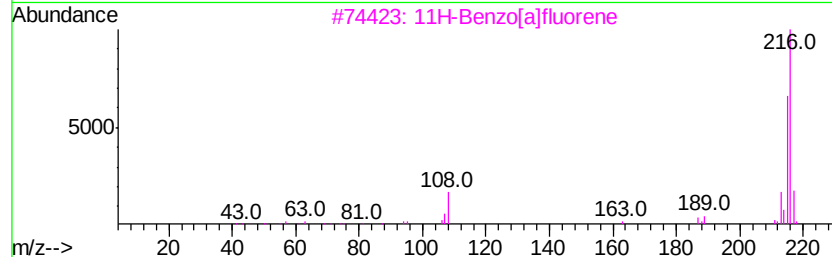
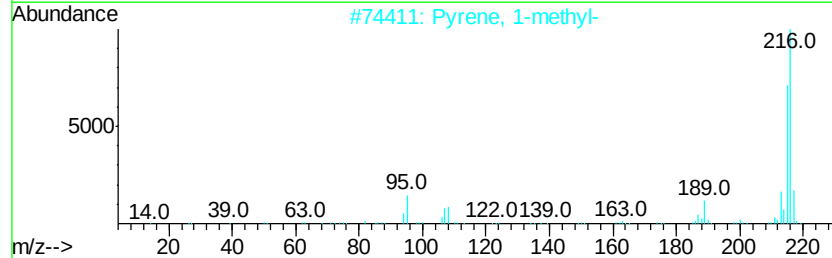
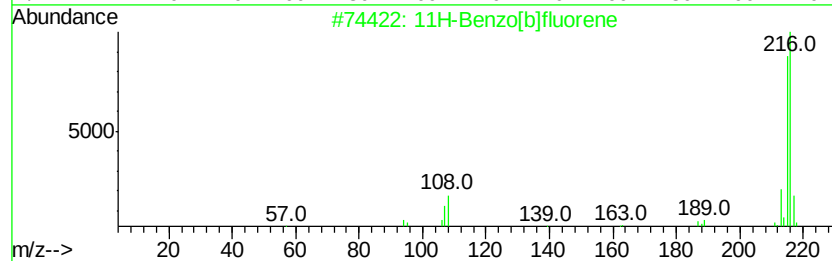
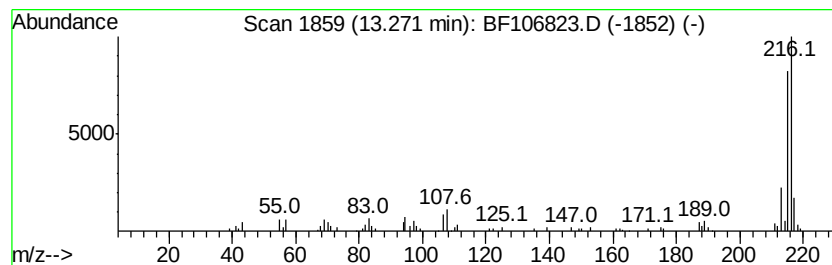
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	3.93 ng	111115	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81



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Data File : BF106823.D
Acq On : 26 Jun 2018 15:28
Operator : JU/SJ
Sample : J3676-05
Misc :
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Instrument :
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ClientSampleId :
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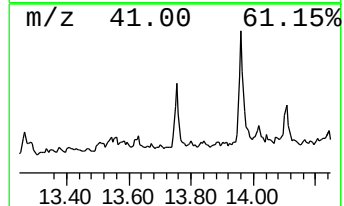
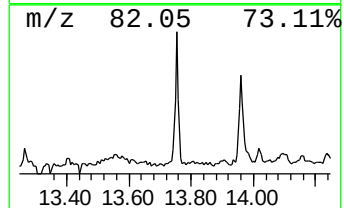
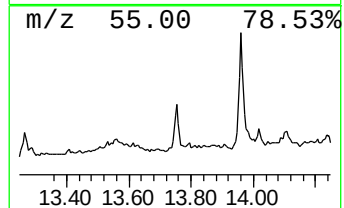
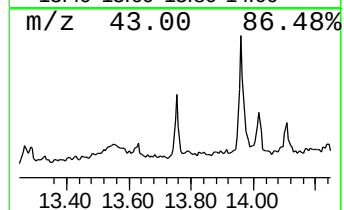
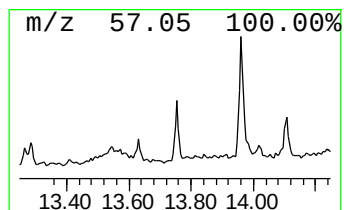
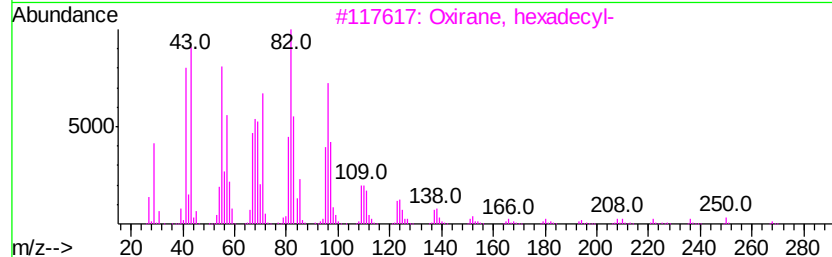
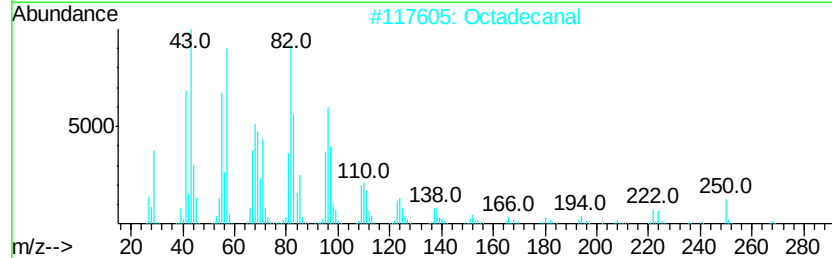
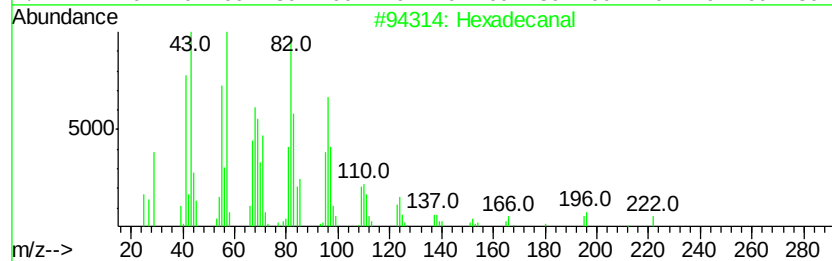
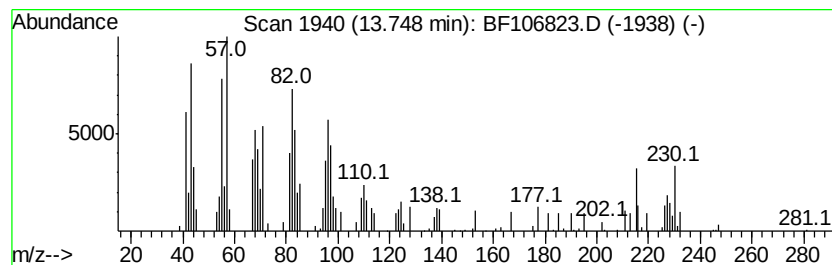
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.64 ng	74479	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	93
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4	Heptadecanal	254	C17H34O	1000376-70-0	87
5	17-Octadecenal	266	C18H34O	056554-86-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106823.D
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ClientSampleId :
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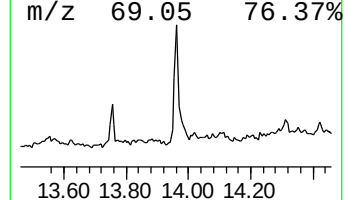
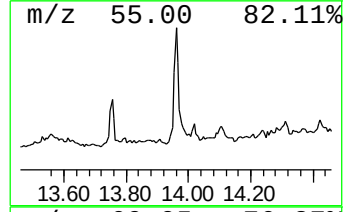
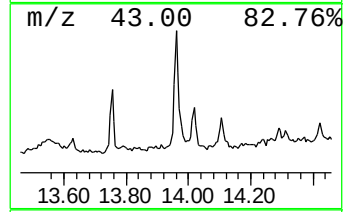
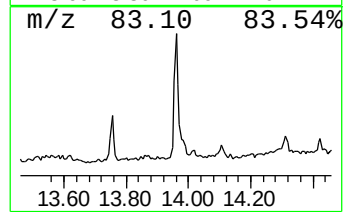
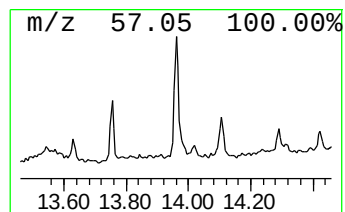
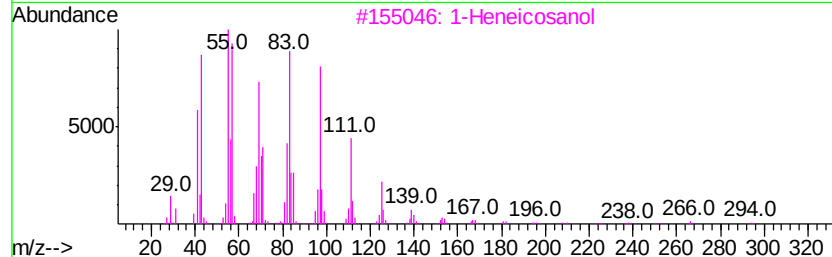
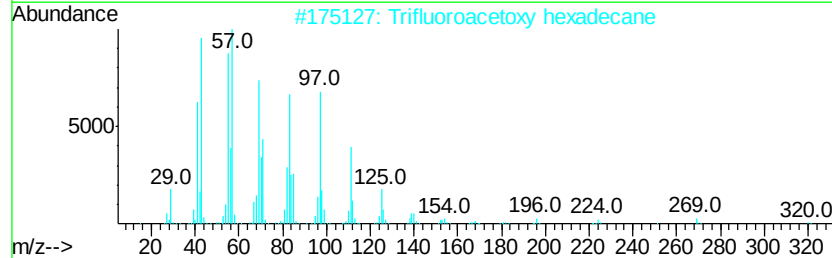
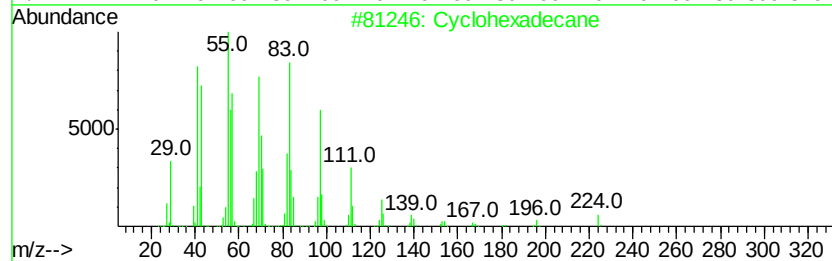
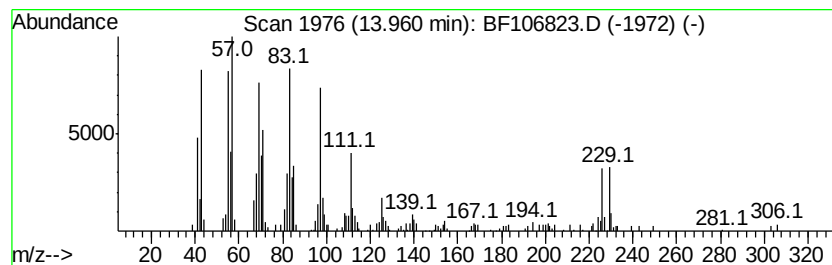
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	6.49 ng	183328	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	97
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106823.D
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Sample : J3676-05
Misc :
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Instrument :
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ClientSampleId :
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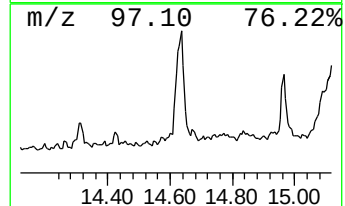
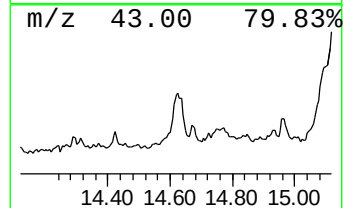
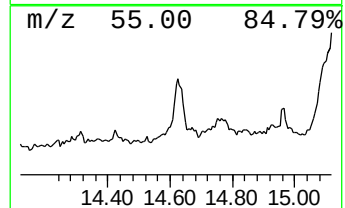
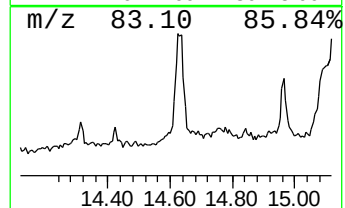
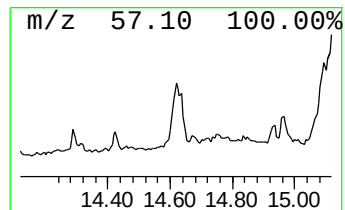
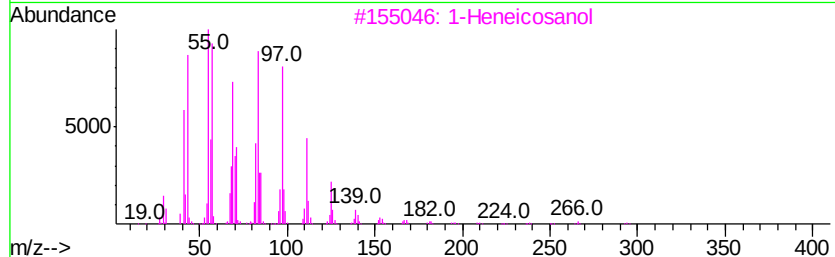
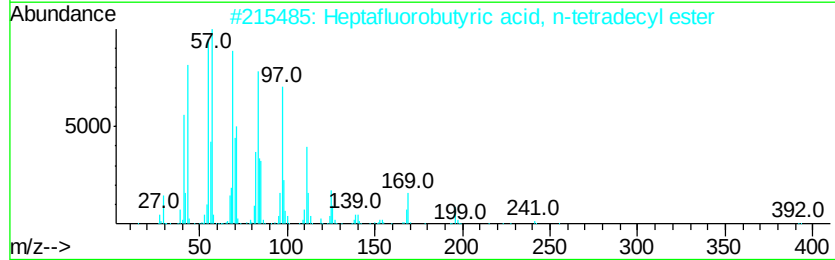
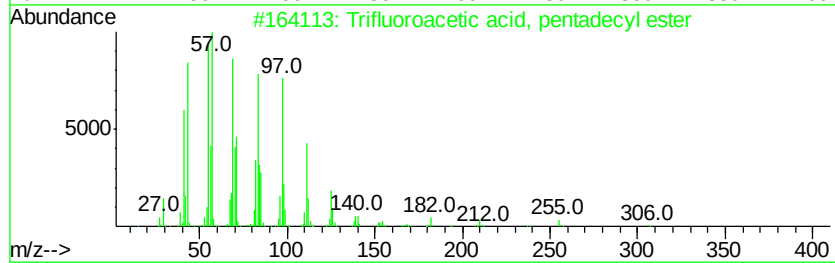
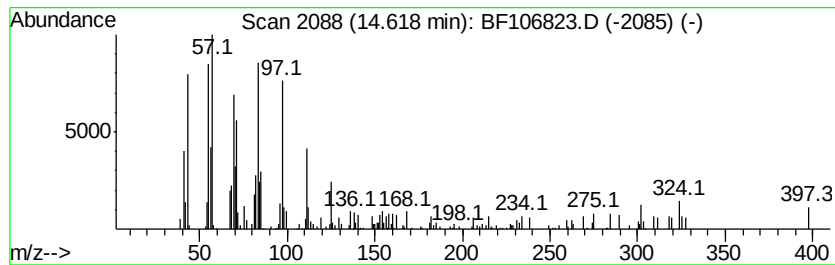
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.49 ng	155141	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	50
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	50
3		1-Heneicosanol	312	C21H44O	015594-90-8	50
4		Trifluoroacetox hexadecane	338	C18H33F3O2	006222-03-3	45
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
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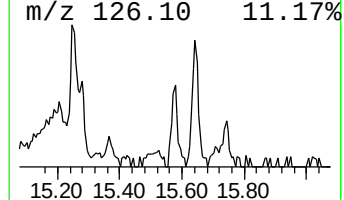
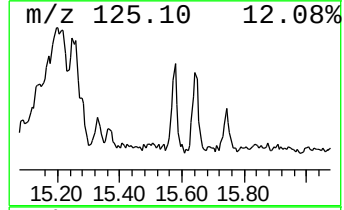
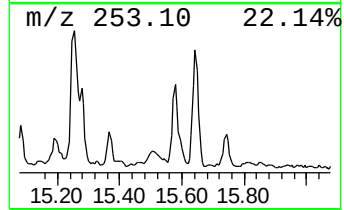
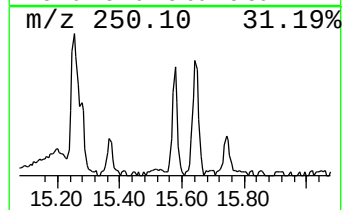
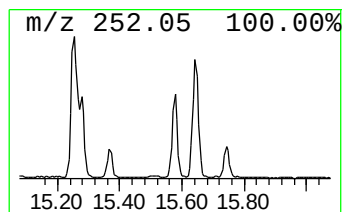
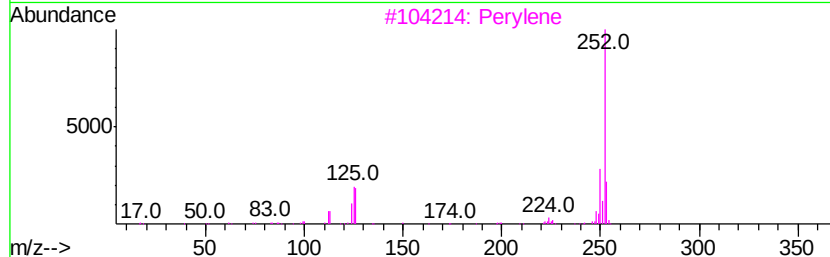
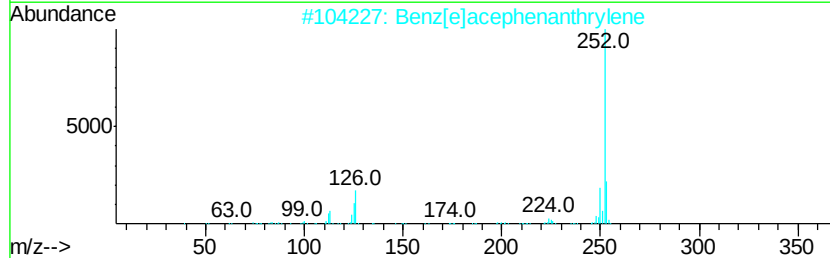
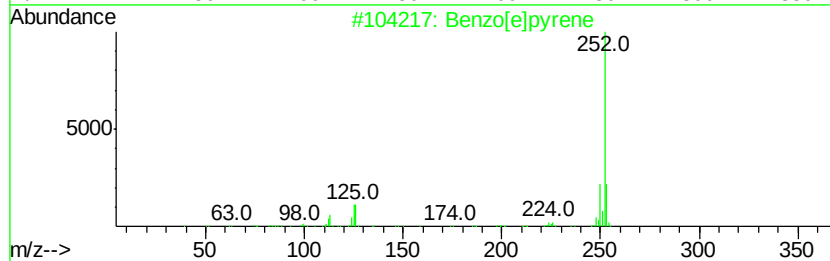
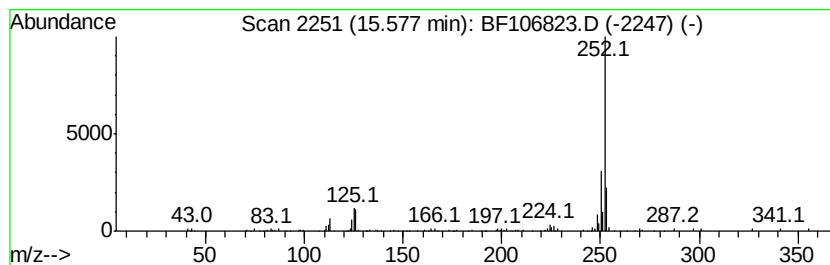
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	7.94 ng	99469	Perylene-d12	15.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
3		Perylene	252	C20H12	000198-55-0	94
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5		Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106823.D
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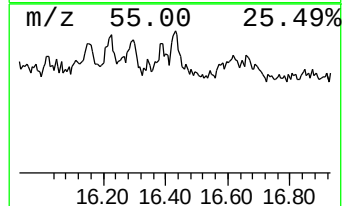
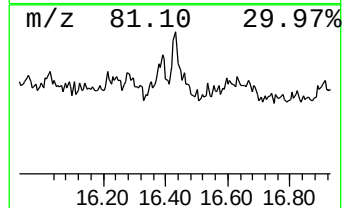
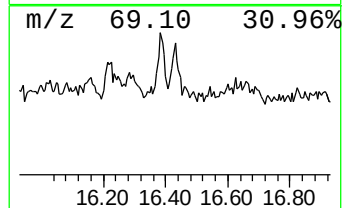
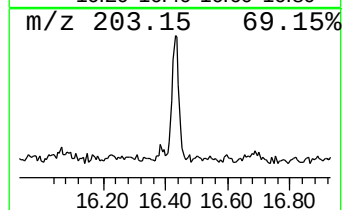
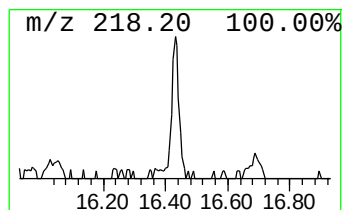
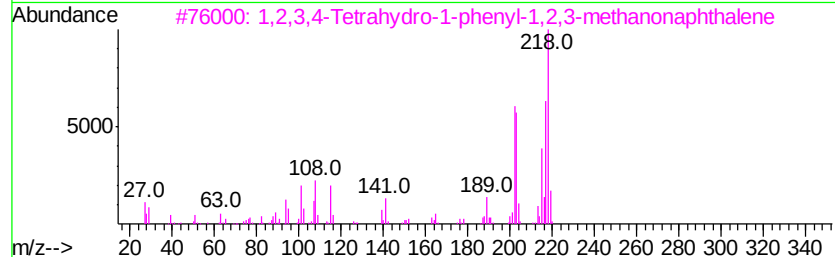
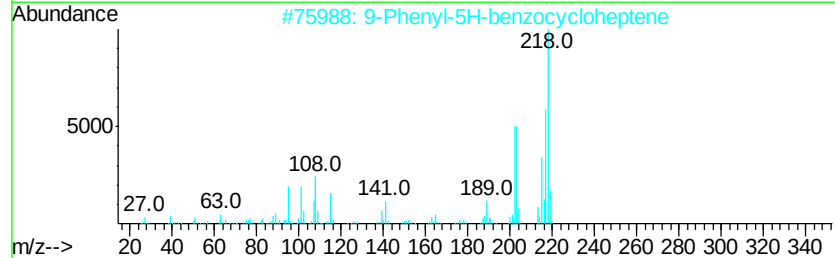
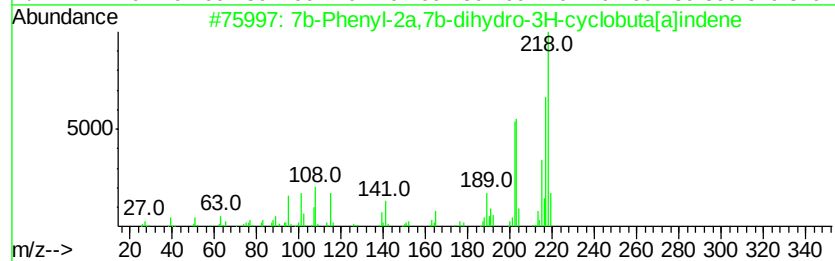
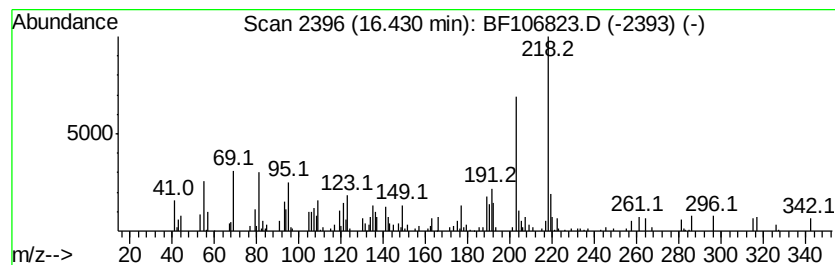
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 7b-Phenyl-2a,7b-dihydro-3H-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	4.72 ng	59166	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	58
2		9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	58
3		1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	53
4		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	50
5		Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
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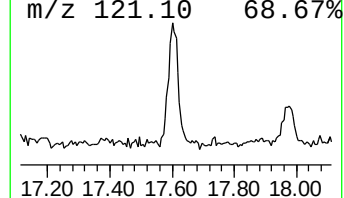
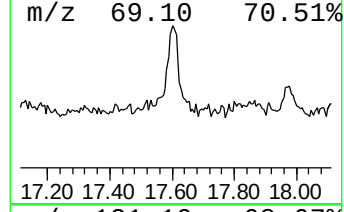
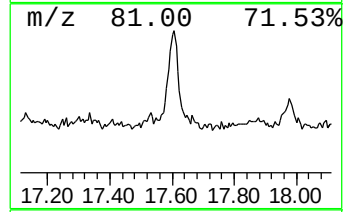
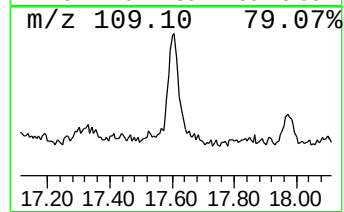
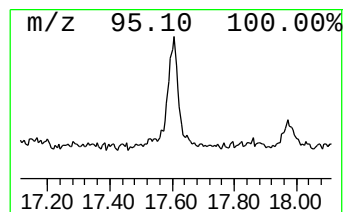
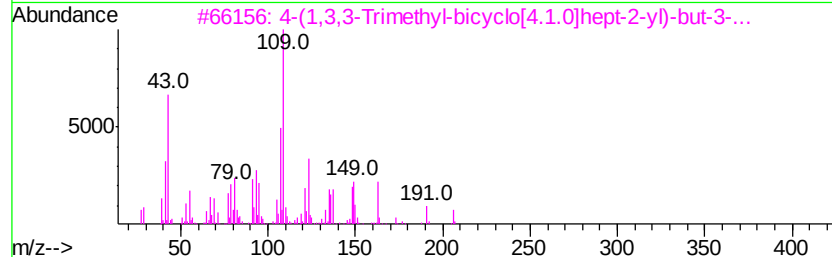
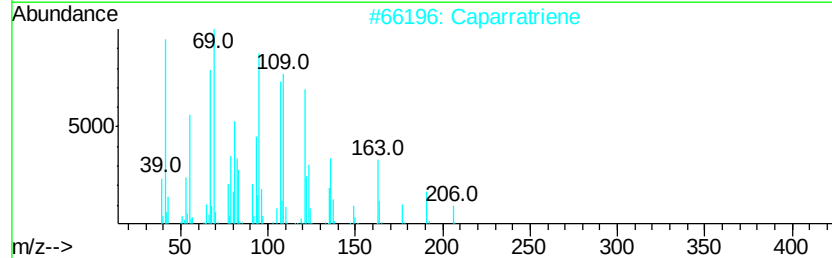
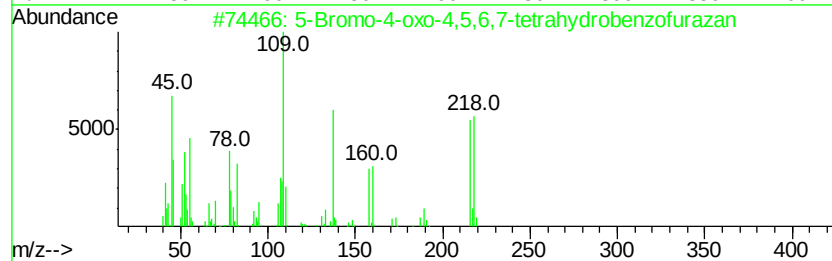
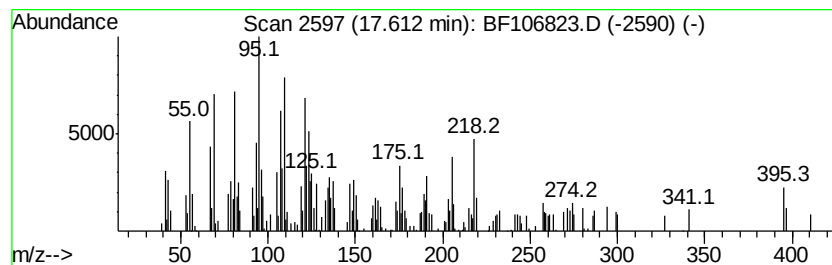
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	29.24 ng	366395	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60
2		Caparratriene	206	C15H26	1000374-08-7	43
3		4-(1,3,3-Trimethyl-bicyclo[4.1.0]hept-2-yl)-but-3-...	206	C14H22O	077143-31-8	38
4		Squalene	410	C30H50	000111-02-4	38
5		4,8,13-Cyclotetradecatriene-1,3-...	306	C20H34O2	007220-78-2	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106823.D
Acq On : 26 Jun 2018 15:28
Operator : JU/SJ
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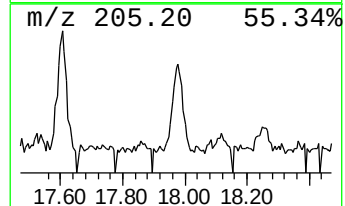
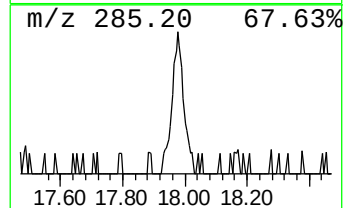
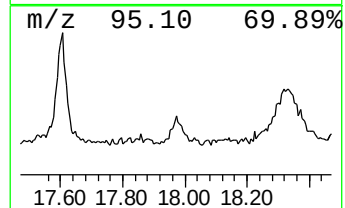
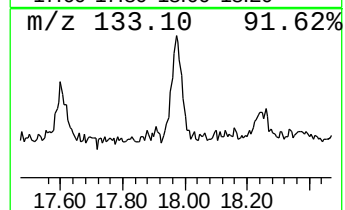
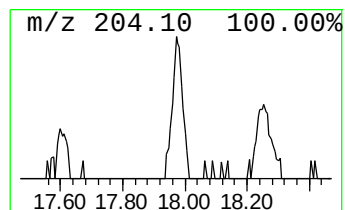
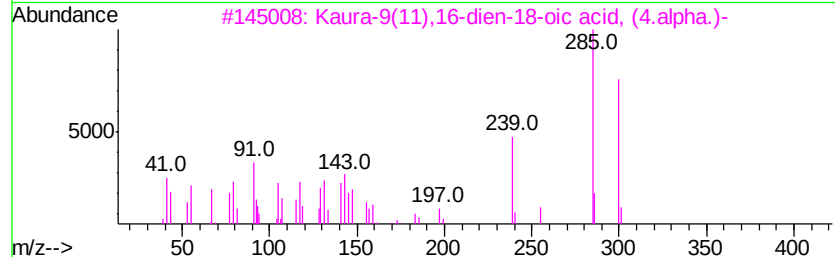
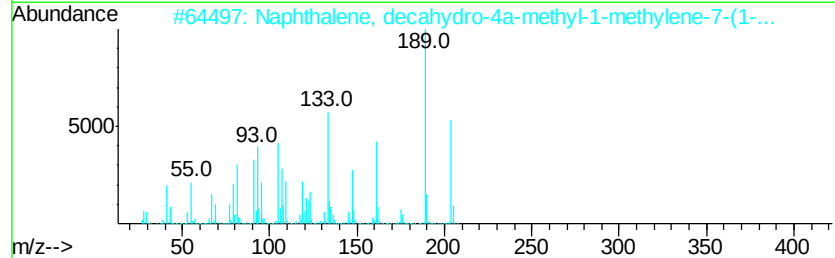
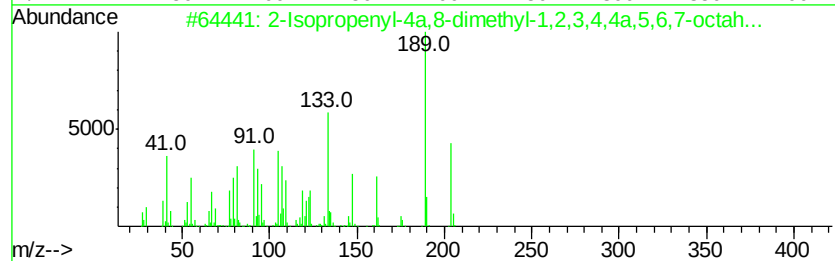
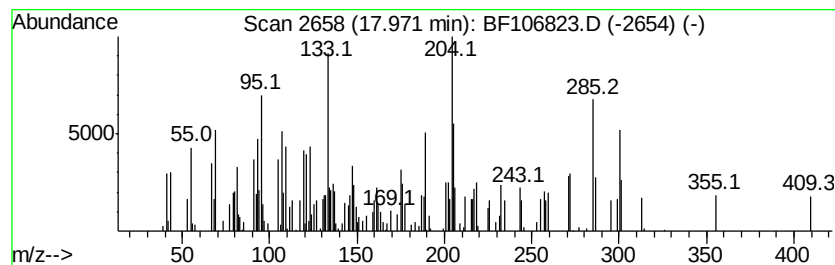
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	9.37 ng	117460	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	46
2		Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	38
3		Kaura-9(11),16-dien-18-oic acid,...	300	C20H28O2	022338-67-6	25
4		1H-Cyclopropafalnaphthalene, 1a,...	204	C15H24	000489-29-2	25
5		Aciphyllene	204	C15H24	087745-31-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062618\
Data File : BF106823.D
Acq On : 26 Jun 2018 15:28
Operator : JU/SJ
Sample : J3676-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-5-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.20	7.9	ng	100446	1	6.96	255573	20.0
unknown6.74	6.74	69.6	ng	889470	1	6.96	255573	20.0
Phenanthrene, 2-m...	12.02	2.5	ng	39250	4	11.50	307777	20.0
4H-Cyclopenta[def...	12.11	4.0	ng	61361	4	11.50	307777	20.0
11H-Benzo[b]fluorene	13.27	3.9	ng	111115	5	14.15	565251	20.0
Hexadecanal	13.75	2.6	ng	74479	5	14.15	565251	20.0
Cyclohexadecane	13.96	6.5	ng	183328	5	14.15	565251	20.0
Trifluoroacetic a...	14.62	5.5	ng	155141	5	14.15	565251	20.0
Benzo[e]pyrene	15.58	7.9	ng	99469	6	15.71	250617	20.0
7b-Phenyl-2a,7b-d...	16.43	4.7	ng	59166	6	15.71	250617	20.0
5-Bromo-4-oxo-4,5...	17.61	29.2	ng	366395	6	15.71	250617	20.0
unknown17.97	17.97	9.4	ng	117460	6	15.71	250617	20.0