

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
 Data File : BF104281.D
 Acq On : 5 Apr 2018 20:34
 Operator : JU/SJ
 Sample : J2183-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ES-4-DWS-2-SW@5

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-BF032818.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	2.287	29	34	44	rVB	122590	184809	4.92%	0.554%
2	5.198	525	529	548	rBV	48796	108068	2.88%	0.324%
3	5.581	591	594	634	rBV	1283532	2831553	75.43%	8.490%
4	6.586	761	765	784	rBV	1329749	2937706	78.26%	8.808%
5	6.716	784	787	824	rVV	2042190	3753839	100.00%	11.256%
6	6.951	824	827	848	rVV	180232	660359	17.59%	1.980%
7	7.098	848	852	889	rVB	1665063	2560490	68.21%	7.677%
8	7.510	919	922	945	rBV	835169	1897971	50.56%	5.691%
9	8.227	1040	1044	1078	rBV	388536	877328	23.37%	2.631%
10	9.298	1222	1226	1254	rBV	2542841	3715554	98.98%	11.141%
11	9.686	1287	1292	1303	rBV	232821	300195	8.00%	0.900%
12	9.886	1323	1326	1330	rVB	59510	48800	1.30%	0.146%
13	9.980	1338	1342	1346	rBV	790678	888917	23.68%	2.665%
14	10.386	1409	1411	1414	rBV	83907	61657	1.64%	0.185%
15	10.539	1431	1437	1442	rBV4	34094	72850	1.94%	0.218%
16	10.604	1442	1448	1460	rVB5	34874	89847	2.39%	0.269%
17	10.780	1474	1478	1489	rBV	1560891	2371864	63.19%	7.112%
18	10.857	1489	1491	1502	rVB	108259	195515	5.21%	0.586%
19	11.086	1521	1530	1533	rBV8	19654	43423	1.16%	0.130%
20	11.310	1564	1568	1570	rBV2	48532	48727	1.30%	0.146%
21	11.480	1593	1597	1599	rBV	669376	780569	20.79%	2.340%
22	11.504	1599	1601	1608	rVV	412867	653870	17.42%	1.961%
23	11.563	1608	1611	1628	rVB	93367	252368	6.72%	0.757%
24	11.980	1679	1682	1685	rBV	93511	121766	3.24%	0.365%
25	12.015	1685	1688	1693	rVB	61460	102839	2.74%	0.308%
26	12.092	1698	1701	1708	rVB3	57432	122975	3.28%	0.369%
27	12.527	1772	1775	1779	rBV	42593	54808	1.46%	0.164%
28	12.621	1788	1791	1800	rVB5	23524	46821	1.25%	0.140%
29	12.698	1800	1804	1812	rBV	250808	373460	9.95%	1.120%
30	12.927	1837	1843	1849	rBV2	241152	392632	10.46%	1.177%
31	12.974	1849	1851	1858	rVB2	33499	51544	1.37%	0.155%
32	13.062	1861	1866	1877	rVV	2691800	3414745	90.97%	10.239%
33	13.145	1877	1880	1886	rVB5	43405	84298	2.25%	0.253%
34	13.257	1892	1899	1904	rVB2	48135	93884	2.50%	0.282%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.362	1913	1917	1924	rVB3	32206	62794	1.67%	0.188%
36	13.492	1935	1939	1948	rVB5	22796	47021	1.25%	0.141%
37	13.904	2003	2009	2010	rBV4	30971	40974	1.09%	0.123%
38	13.927	2010	2013	2022	rVB	337502	409720	10.91%	1.229%
39	14.133	2041	2048	2064	rBV2	712650	1316485	35.07%	3.947%
40	14.868	2170	2173	2181	rBV2	143193	192692	5.13%	0.578%
41	15.221	2227	2233	2247	rBV4	64611	187403	4.99%	0.562%
42	15.615	2294	2300	2304	rVV2	43931	92447	2.46%	0.277%
43	15.662	2304	2308	2334	rVB	354007	756797	20.16%	2.269%
44	16.145	2385	2390	2394	rBV5	25037	48605	1.29%	0.146%

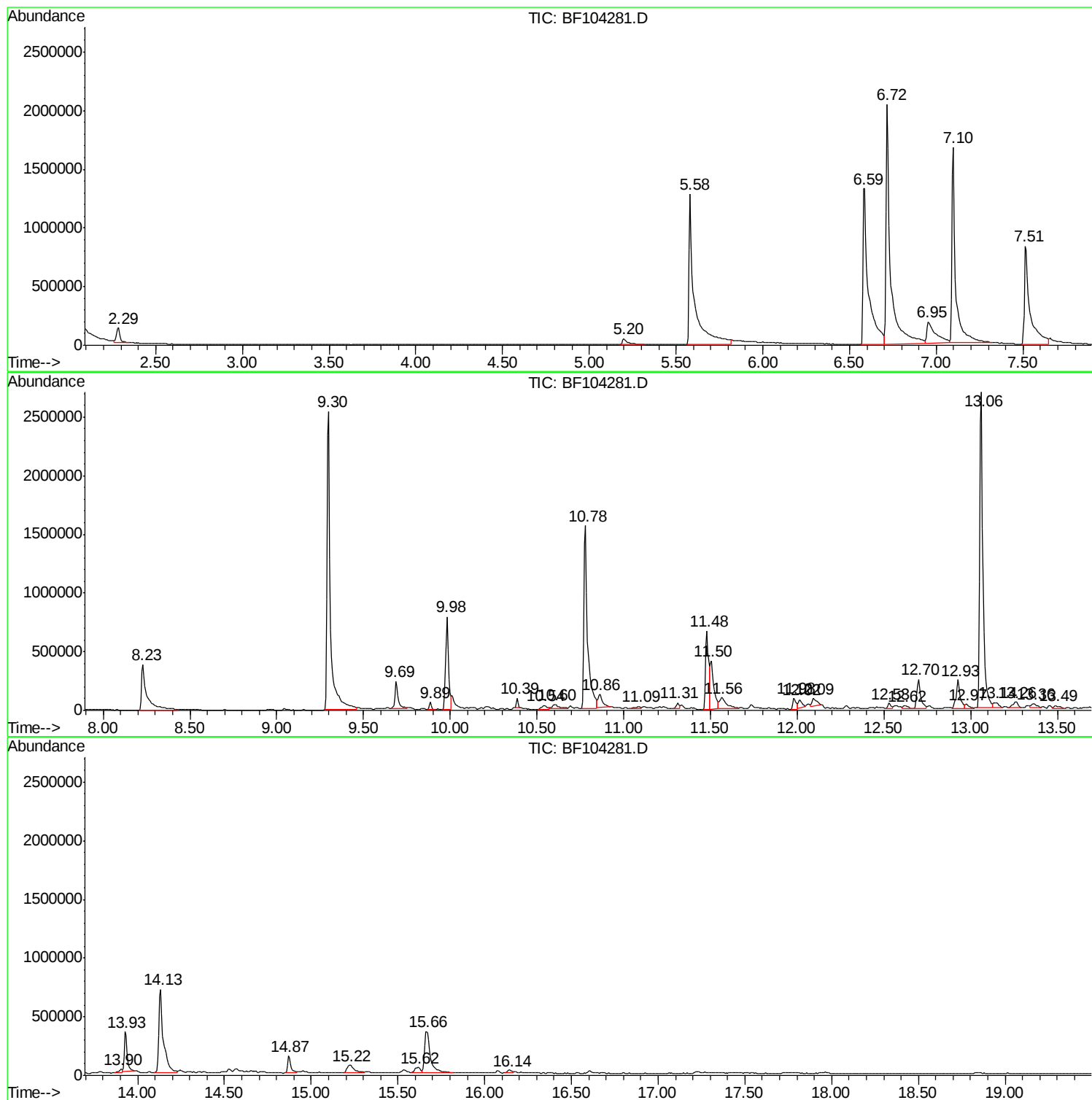
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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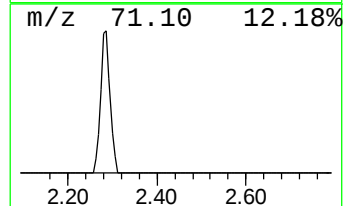
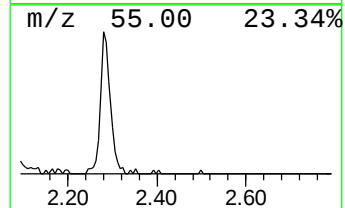
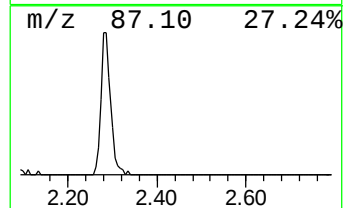
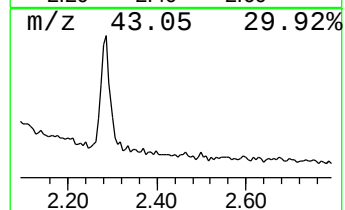
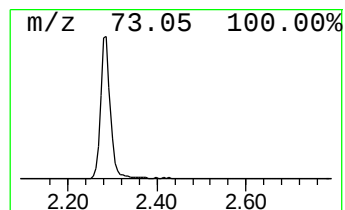
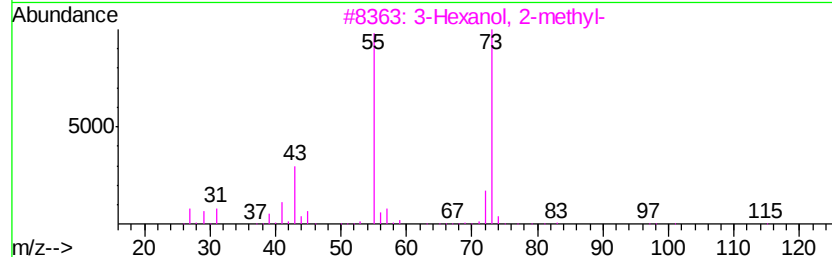
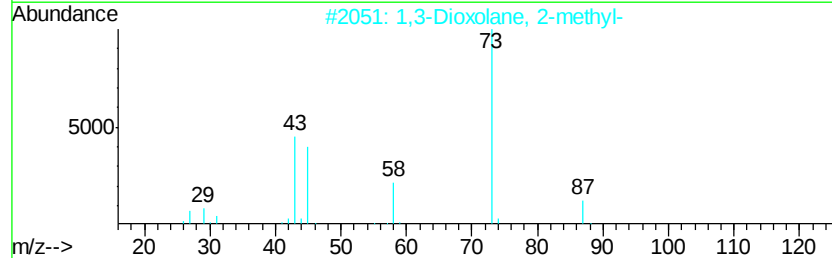
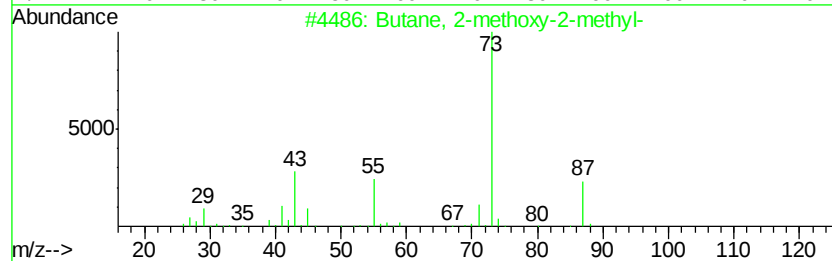
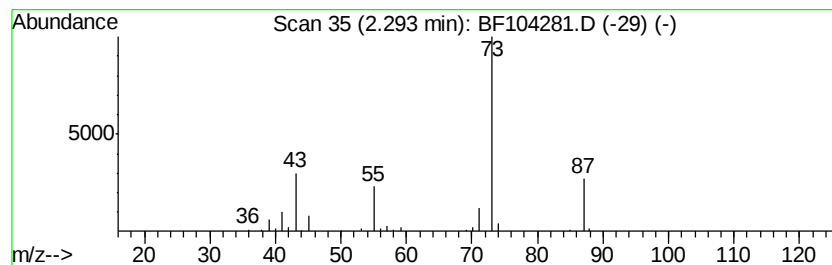
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	5.60 ng	184809	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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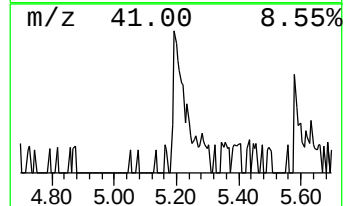
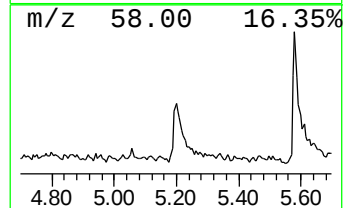
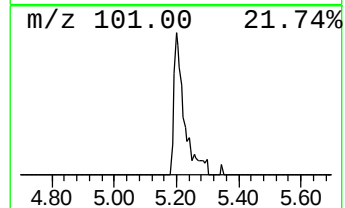
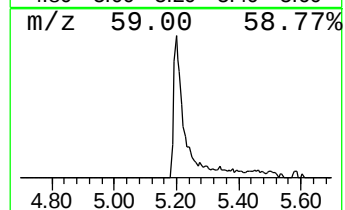
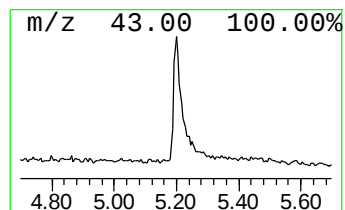
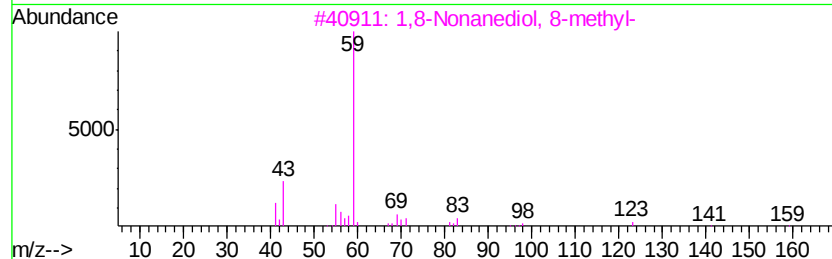
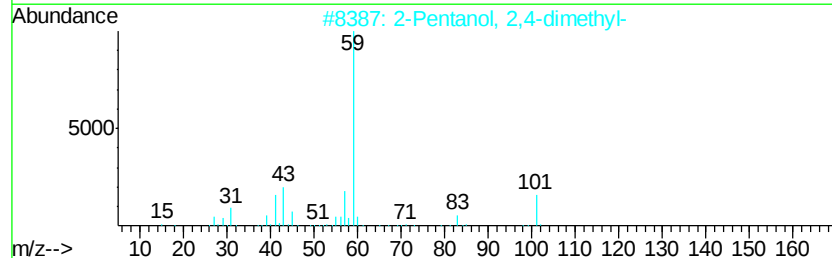
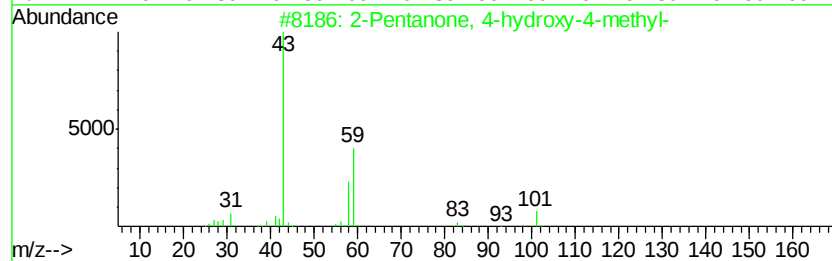
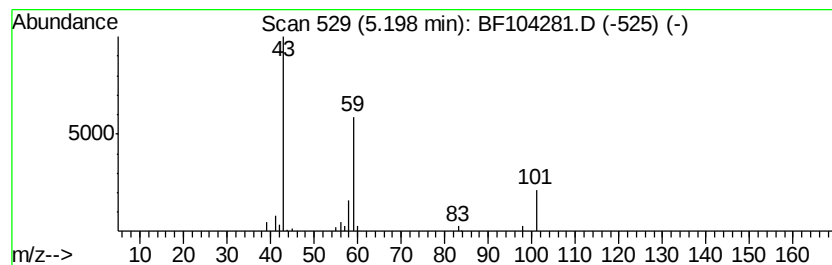
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.27 ng	108068	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4			3-Pentanol	88	C5H12O	000584-02-1	23
5			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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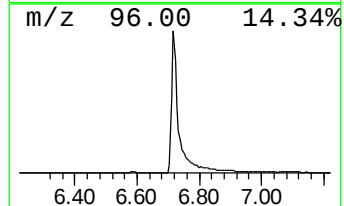
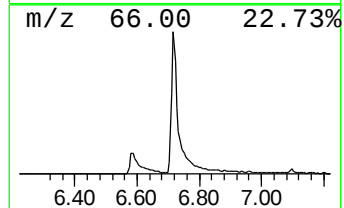
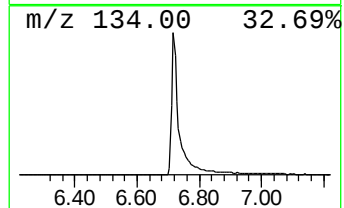
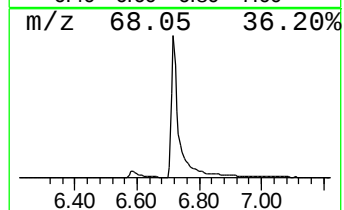
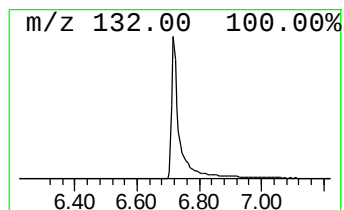
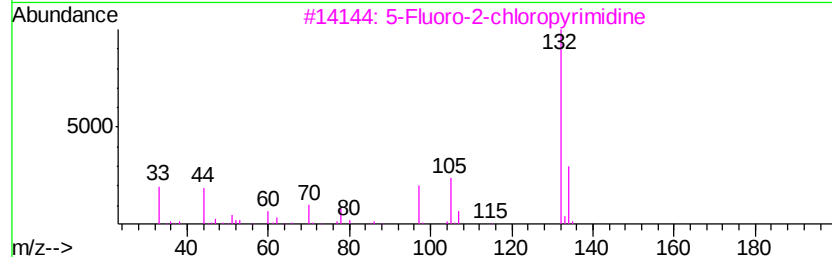
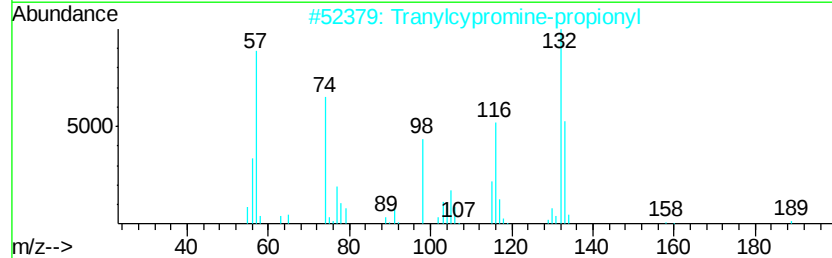
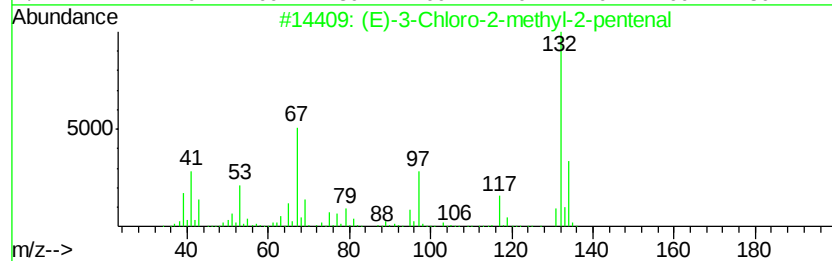
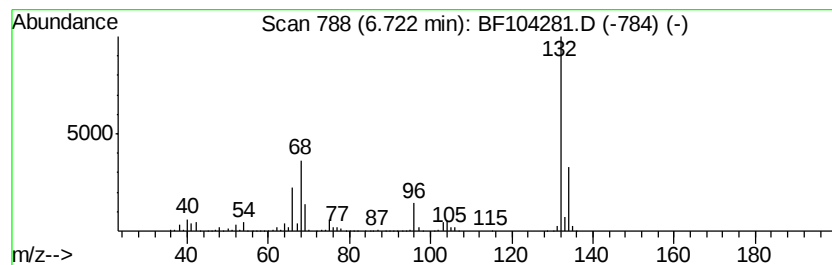
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	113.69 ng	3753840	1,4-Dichlorobenzene-d4	6.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	
5	5-Aminoindole	132	C8H8N2	005192-03-0	9	



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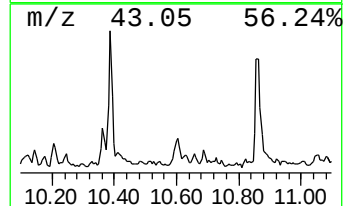
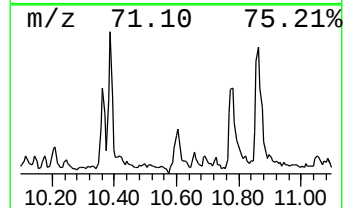
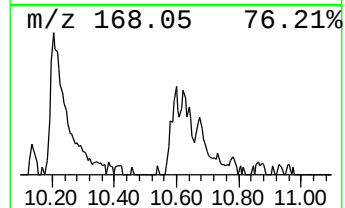
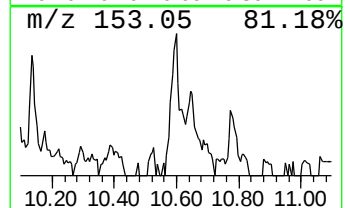
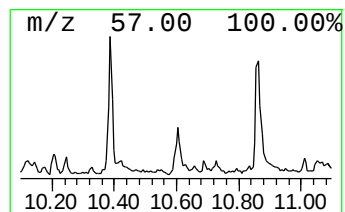
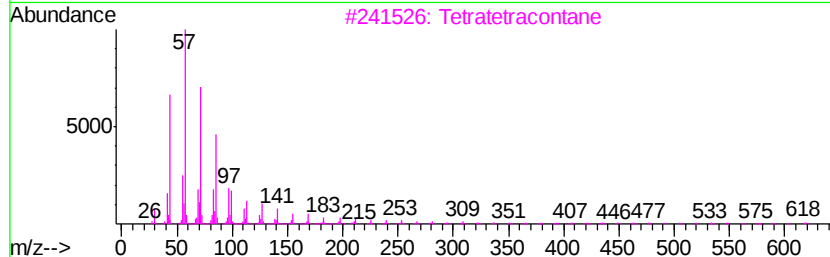
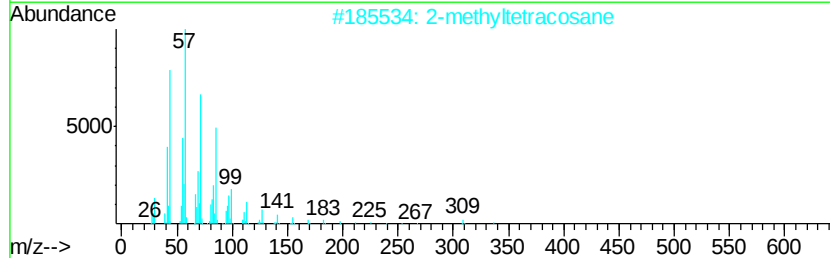
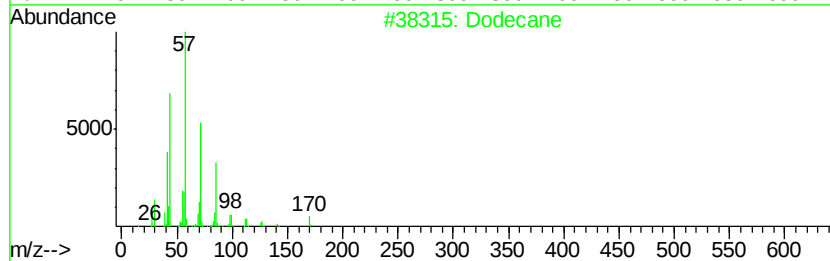
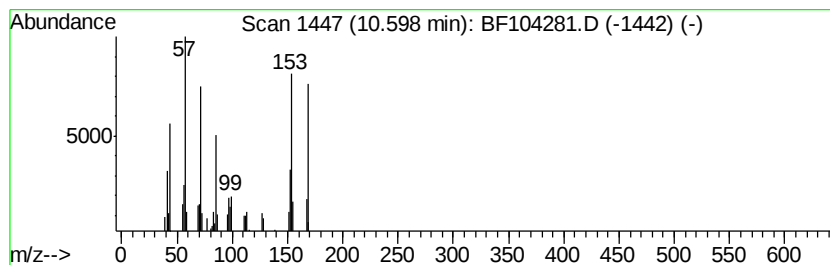
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.02 ng	89847	Acenaphthene-d10	9.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane		170 C12H26	000112-40-3 55
2	2-methyltetracosane		352 C25H52	1000376-72-6 46
3	Tetratetracontane		619 C44H90	007098-22-8 46
4	2-methyloctacosane		408 C29H60	1000376-72-8 46
5	Tridecane		184 C13H28	000629-50-5 43



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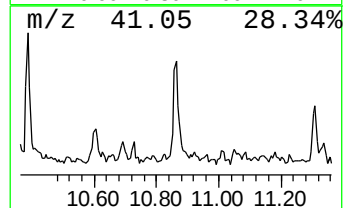
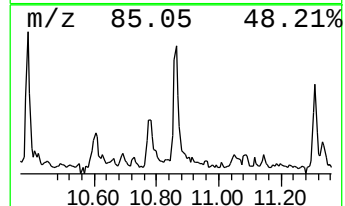
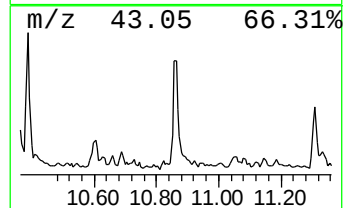
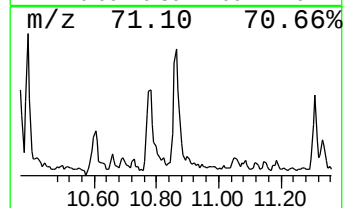
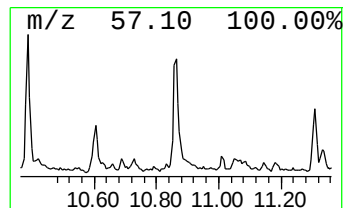
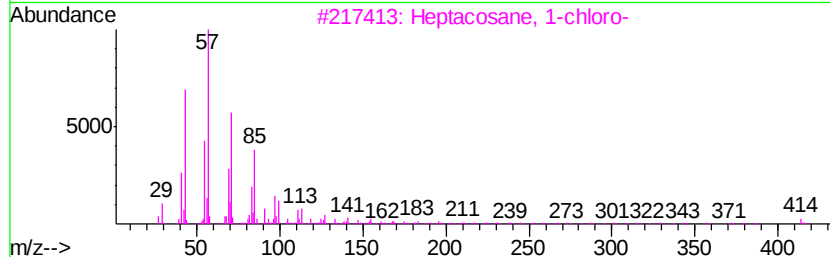
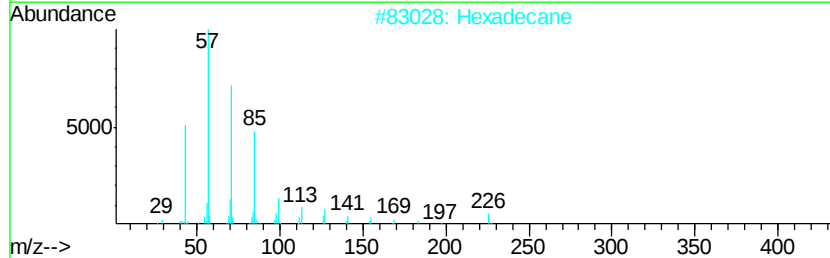
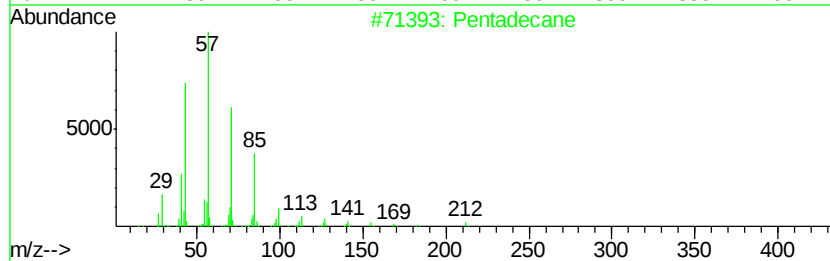
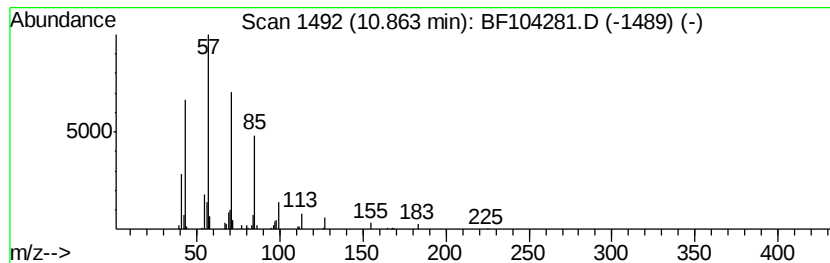
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.86	5.01 ng	195515	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
Data File : BF104281.D
Acq On : 5 Apr 2018 20:34
Operator : JU/SJ
Sample : J2183-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ES-4-DWS-2-SW@5

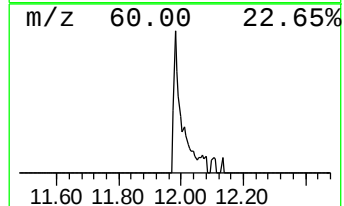
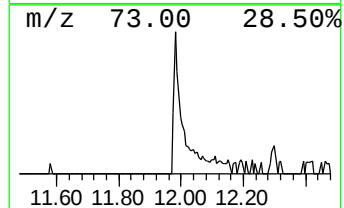
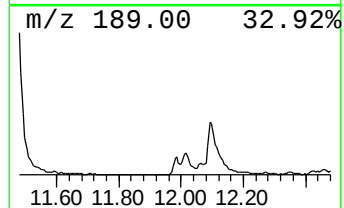
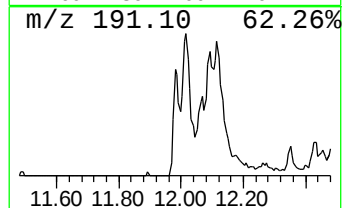
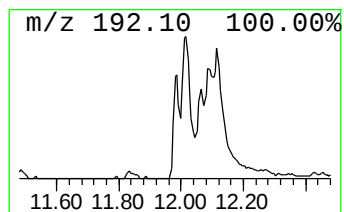
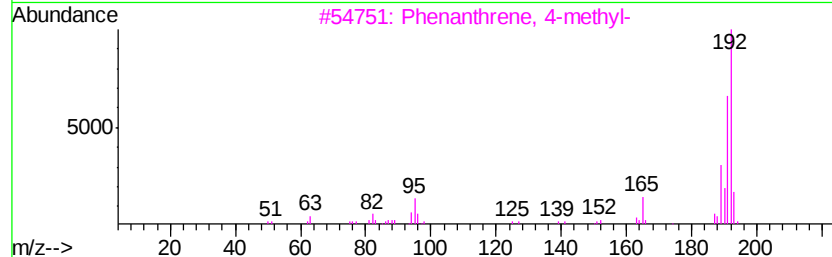
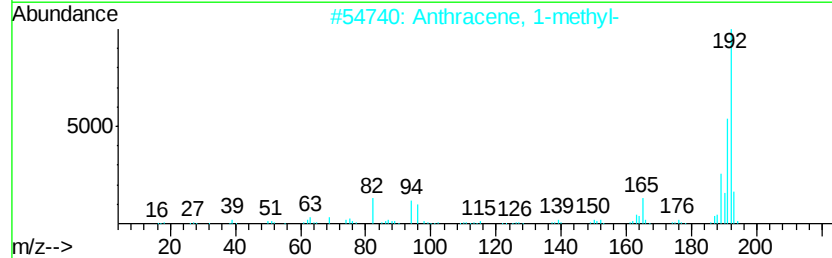
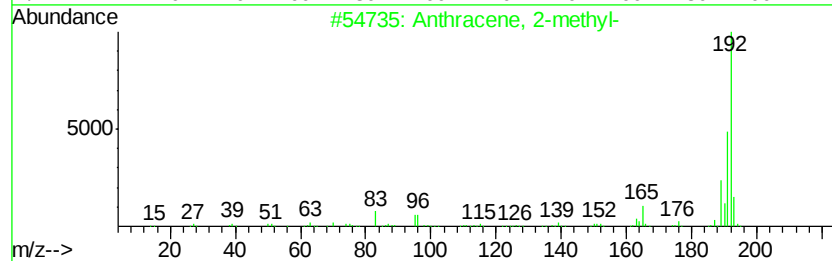
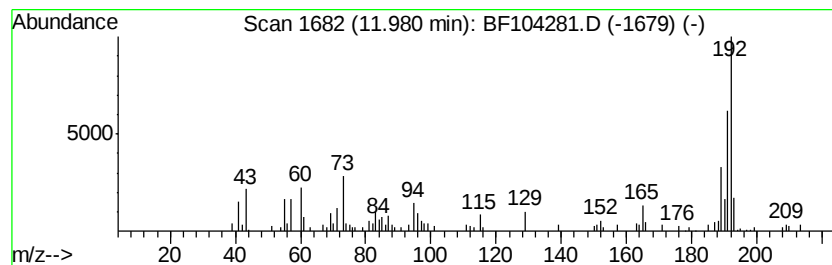
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	3.12 ng	121766	Phenanthrene-d10	11.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	83
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	83
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
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Sample : J2183-09
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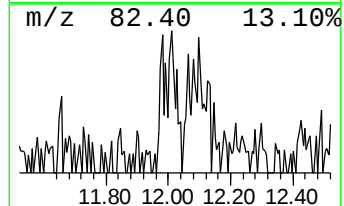
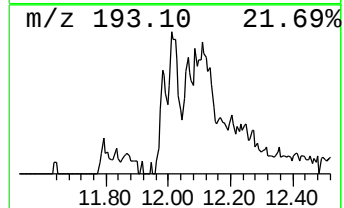
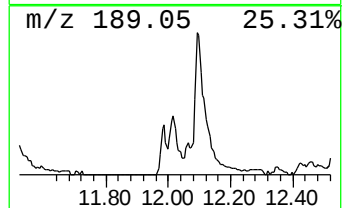
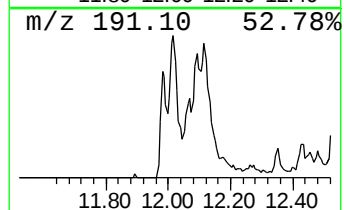
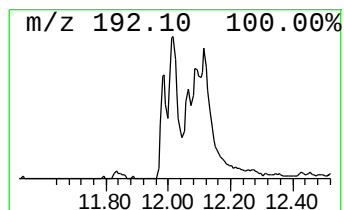
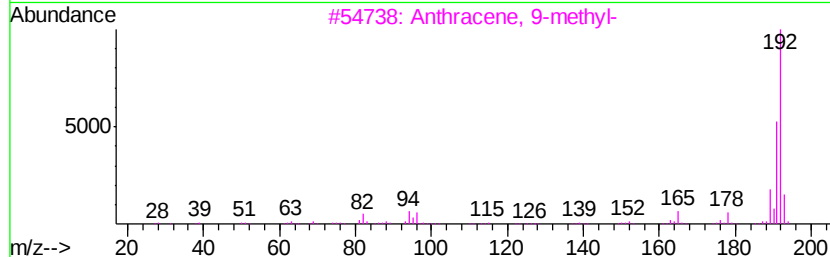
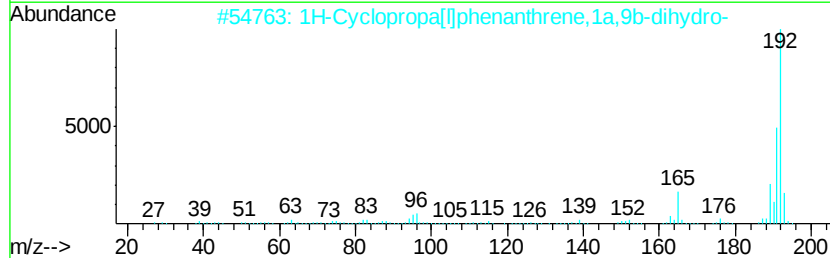
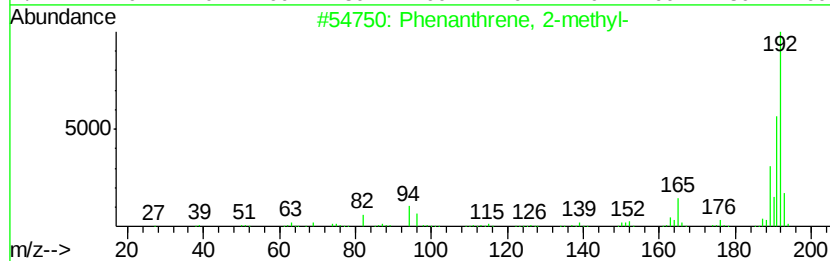
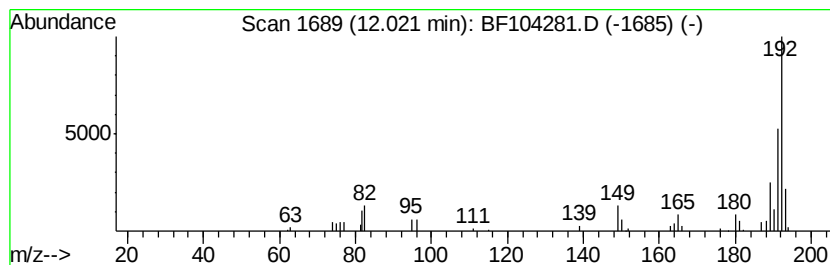
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.02	2.63 ng	102839	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
2	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	83
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	76
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	70
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
Data File : BF104281.D
Acq On : 5 Apr 2018 20:34
Operator : JU/SJ
Sample : J2183-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ES-4-DWS-2-SW@5

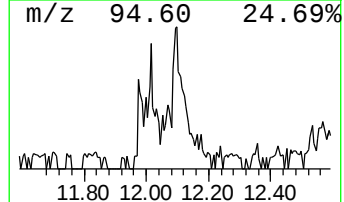
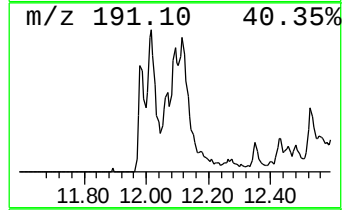
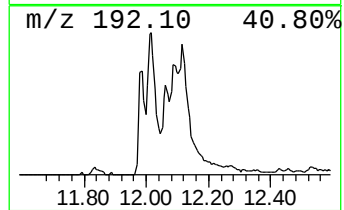
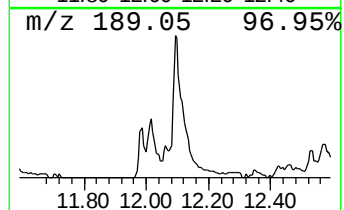
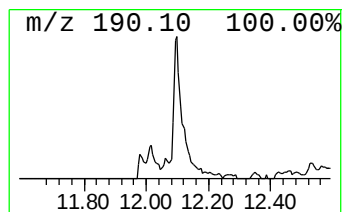
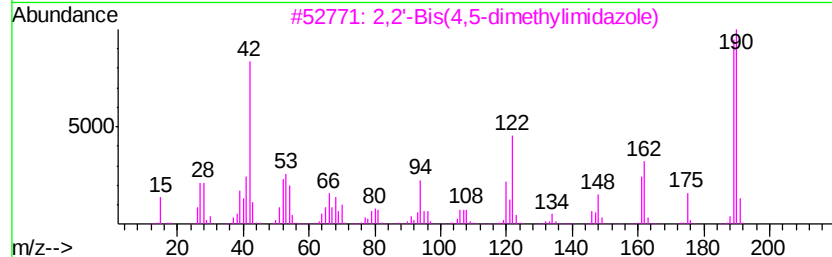
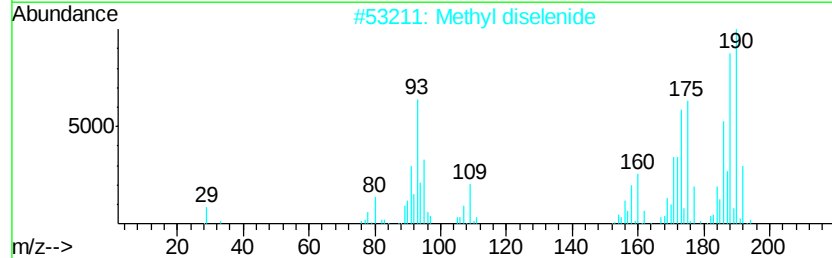
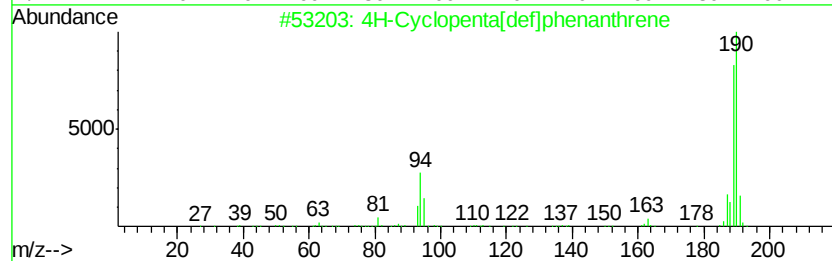
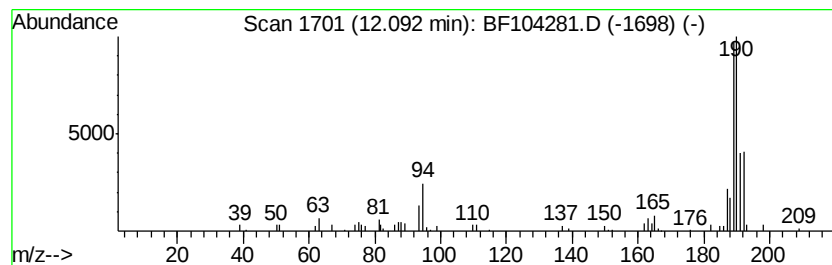
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	3.15 ng	122975	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2		Methyl diselenide	190	C2H6Se2	007101-31-7	43
3		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
4		6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	25
5		4-(4-Chlorophenyl)pyridine	189	C11H8ClN	005957-96-0	25



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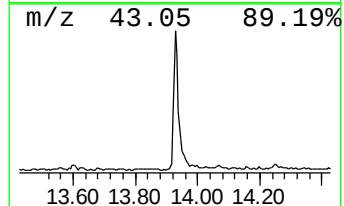
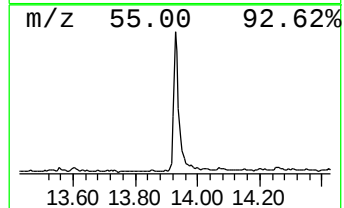
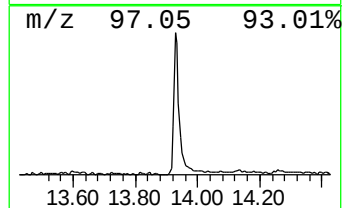
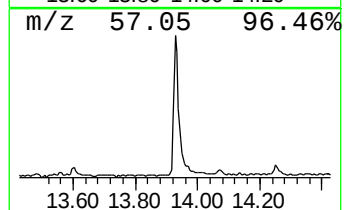
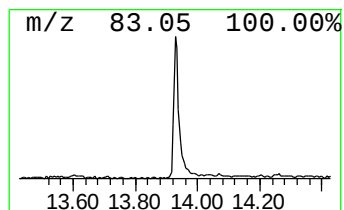
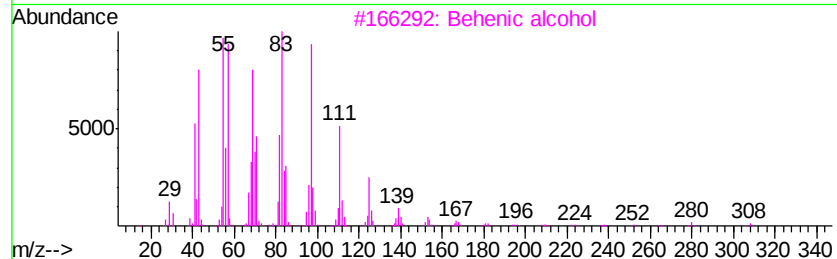
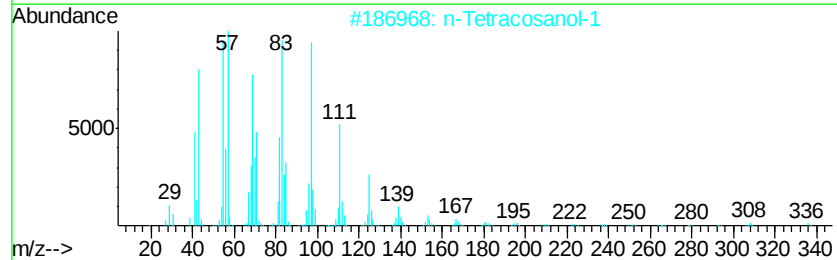
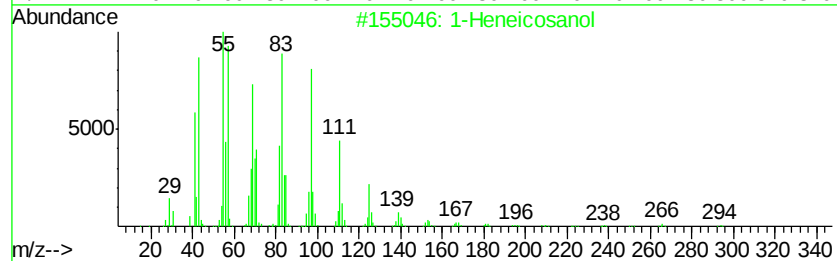
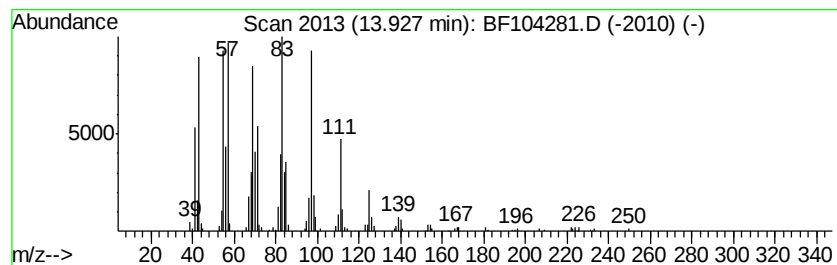
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.93	6.22 ng	409720	Chrysene-d12		14.13	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		Behenic alcohol	326	C22H46O	000661-19-8	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
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Operator : JU/SJ
Sample : J2183-09
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ALS Vial : 11 Sample Multiplier: 1

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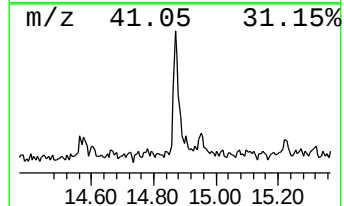
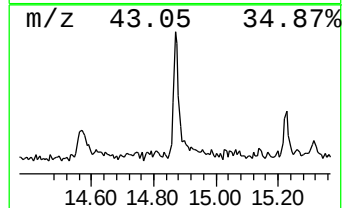
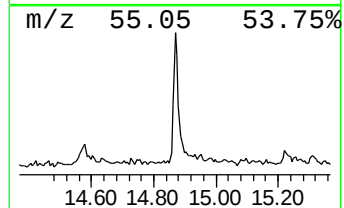
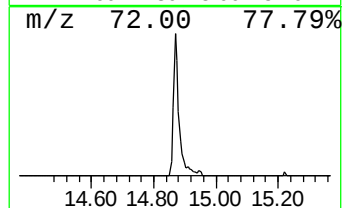
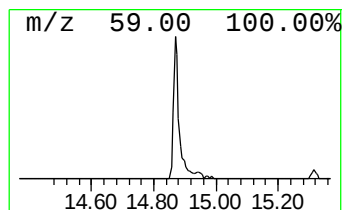
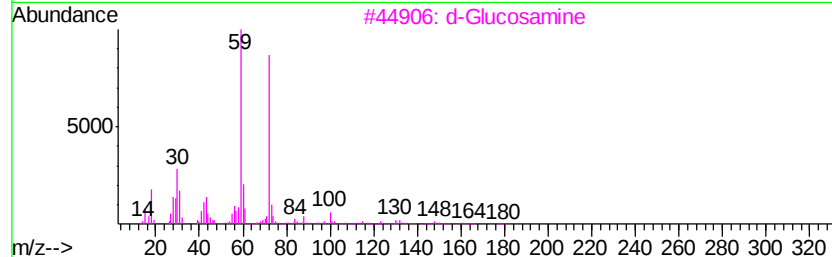
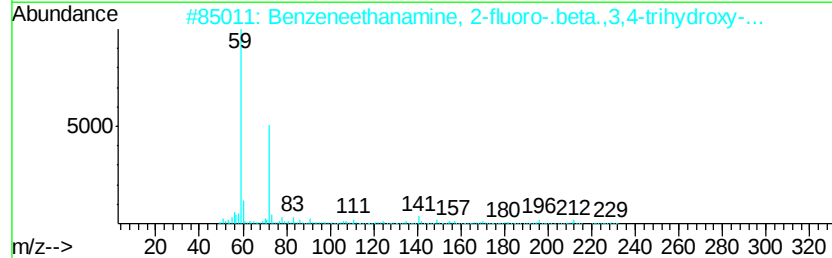
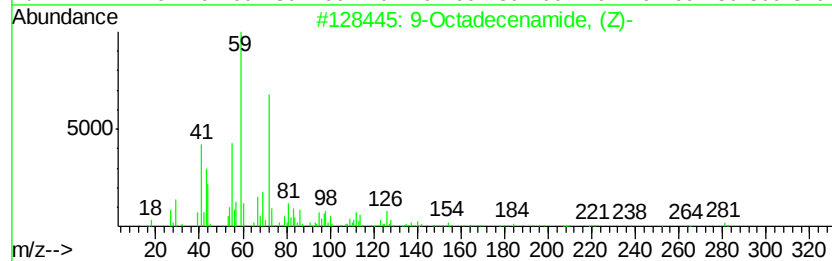
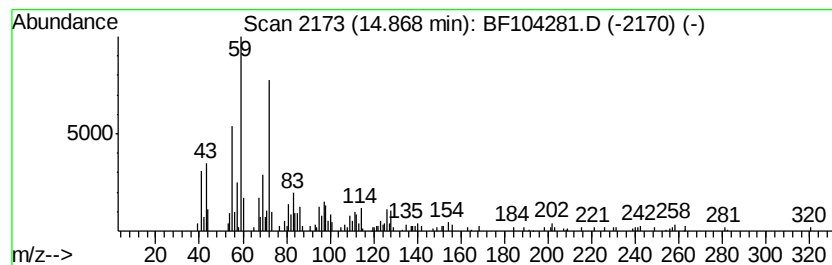
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.93 ng	192692	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
3		d-Glucosamine	179	C6H13N05	000090-77-7	50
4		Hexadecanamide	255	C16H33NO	000629-54-9	47
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.20	3.3	ng	108068	1	6.95	660359	20.0
unknown6.72	6.72	113.7	ng	3753840	1	6.95	660359	20.0
Dodecane	10.60	2.0	ng	89847	3	9.98	888917	20.0
Pentadecane	10.86	5.0	ng	195515	4	11.48	780569	20.0
Anthracene, 2-met...	11.98	3.1	ng	121766	4	11.48	780569	20.0
Phenanthrene, 2-m...	12.02	2.6	ng	102839	4	11.48	780569	20.0
4H-Cyclopenta[def...	12.09	3.1	ng	122975	4	11.48	780569	20.0
1-Heneicosanol	13.93	6.2	ng	409720	5	14.13	1316490	20.0
9-Octadecenamide, ...	14.87	2.9	ng	192692	5	14.13	1316490	20.0