

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
 Data File : BF098805.D
 Acq On : 26 Sep 2017 1:49
 Operator : SJ/JU
 Sample : I5362-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-2-A-COMP

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-BF092317.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	2.205	16	20	25	rVB	48049	60604	1.79%	0.169%
2	5.140	515	519	527	rBV	514343	618179	18.24%	1.719%
3	5.534	580	586	589	rBV	3072990	2987744	88.14%	8.309%
4	6.540	751	757	761	rBV	2781124	3100280	91.46%	8.622%
5	6.681	776	781	784	rBV	3262765	3150813	92.95%	8.762%
6	6.916	817	821	824	rVB	1013551	891309	26.29%	2.479%
7	7.069	843	847	850	rBV	2707967	2379936	70.21%	6.619%
8	7.475	911	916	919	rBV	2123933	1948377	57.48%	5.418%
9	7.539	924	927	933	rVB2	39738	43997	1.30%	0.122%
10	8.192	1035	1038	1041	rBV	1407548	1238844	36.55%	3.445%
11	8.216	1041	1042	1045	rVB	132175	67627	2.00%	0.188%
12	8.904	1156	1159	1162	rBV	70203	53673	1.58%	0.149%
13	9.004	1172	1176	1180	rBV	56886	46780	1.38%	0.130%
14	9.269	1215	1221	1224	rBV	3781551	3389711	100.00%	9.427%
15	9.345	1231	1234	1236	rBV	37085	36644	1.08%	0.102%
16	9.528	1262	1265	1269	rBV	33509	41295	1.22%	0.115%
17	9.604	1275	1278	1281	rBV	56708	56765	1.67%	0.158%
18	9.657	1284	1287	1291	rVB	508360	401943	11.86%	1.118%
19	9.810	1308	1313	1316	rBV	84950	78504	2.32%	0.218%
20	9.875	1320	1324	1327	rVV	55296	56345	1.66%	0.157%
21	9.951	1330	1337	1340	rVV	1609475	1360112	40.12%	3.782%
22	9.980	1340	1342	1345	rVB2	60985	49194	1.45%	0.137%
23	10.151	1366	1371	1374	rVB2	76907	84121	2.48%	0.234%
24	10.192	1374	1378	1382	rBV4	37510	38423	1.13%	0.107%
25	10.263	1386	1390	1392	rBV3	40913	41114	1.21%	0.114%
26	10.351	1402	1405	1406	rBV	42495	44636	1.32%	0.124%
27	10.375	1406	1409	1411	rVB	102780	95494	2.82%	0.266%
28	10.492	1426	1429	1435	rVB2	71483	83509	2.46%	0.232%
29	10.592	1442	1446	1452	rBV4	38099	58839	1.74%	0.164%
30	10.739	1464	1471	1474	rBV	1978954	1818149	53.64%	5.056%
31	10.845	1486	1489	1494	rBV2	147172	204353	6.03%	0.568%
32	11.039	1518	1522	1525	rBV4	39586	54915	1.62%	0.153%
33	11.169	1540	1544	1546	rBV3	41045	44135	1.30%	0.123%
34	11.292	1561	1565	1567	rBV2	114332	101238	2.99%	0.282%

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 Integrator: RTE
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 Sampling : 1
 Start Thrs: 0.2
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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-BF092317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.327	1567	1571	1576	rVB3	50180	85505	2.52%	0.238%
36	11.439	1586	1590	1592	rBV	1388208	1238100	36.53%	3.443%
37	11.457	1592	1593	1597	rVV	387976	325691	9.61%	0.906%
38	11.510	1600	1602	1605	rVB	134486	99786	2.94%	0.278%
39	11.663	1626	1628	1635	rBV3	30397	46576	1.37%	0.130%
40	11.722	1635	1638	1643	rVB2	61640	67248	1.98%	0.187%
41	11.939	1672	1675	1676	rBV	83314	91700	2.71%	0.255%
42	11.963	1676	1679	1684	rVB2	146057	198476	5.86%	0.552%
43	12.051	1690	1694	1696	rBV2	131650	151458	4.47%	0.421%
44	12.074	1696	1698	1701	rVB2	83675	71551	2.11%	0.199%
45	12.127	1704	1707	1711	rBV	65851	63576	1.88%	0.177%
46	12.233	1722	1725	1727	rBV	72452	59479	1.75%	0.165%
47	12.292	1732	1735	1741	rVB2	89756	80505	2.37%	0.224%
48	12.380	1748	1750	1753	rVB	49244	36513	1.08%	0.102%
49	12.486	1765	1768	1771	rBV	96227	92544	2.73%	0.257%
50	12.516	1771	1773	1776	rVV3	81502	82203	2.43%	0.229%
51	12.574	1780	1783	1788	rBV5	46689	73334	2.16%	0.204%
52	12.651	1792	1796	1799	rVV	790645	630345	18.60%	1.753%
53	12.692	1800	1803	1805	rVV2	44433	49482	1.46%	0.138%
54	12.739	1809	1811	1814	rVV	37616	40106	1.18%	0.112%
55	12.880	1829	1835	1841	rBV	726127	742501	21.90%	2.065%
56	13.021	1855	1859	1862	rVB	2585678	2221867	65.55%	6.179%
57	13.092	1868	1871	1875	rBV3	61132	90596	2.67%	0.252%
58	13.204	1888	1890	1894	rVB	110579	92661	2.73%	0.258%
59	13.245	1894	1897	1899	rBV2	60351	65220	1.92%	0.181%
60	13.269	1899	1901	1905	rVV	85138	98417	2.90%	0.274%
61	13.310	1905	1908	1911	rVB2	81310	84896	2.50%	0.236%
62	13.433	1927	1929	1932	rBV	47548	49346	1.46%	0.137%
63	13.904	2006	2009	2015	rVB4	235577	264719	7.81%	0.736%
64	14.074	2033	2038	2041	rBV2	955543	1122099	33.10%	3.121%
65	14.098	2041	2042	2049	rVB	279263	245145	7.23%	0.682%
66	14.533	2114	2116	2122	rVB3	119681	145348	4.29%	0.404%
67	14.998	2192	2195	2198	rVB2	135091	136672	4.03%	0.380%
68	15.127	2213	2217	2220	rBV	290259	447725	13.21%	1.245%
69	15.192	2225	2228	2230	rBV	123743	139215	4.11%	0.387%
70	15.439	2267	2270	2276	rVB	202008	240880	7.11%	0.670%
71	15.504	2277	2281	2287	rVV	253670	351934	10.38%	0.979%

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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-BF092317.M
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72	15.568	2288	2292	2303	rVB2	596509	955100	28.18%	2.656%
73	16.033	2368	2371	2375	rVB	124370	152681	4.50%	0.425%

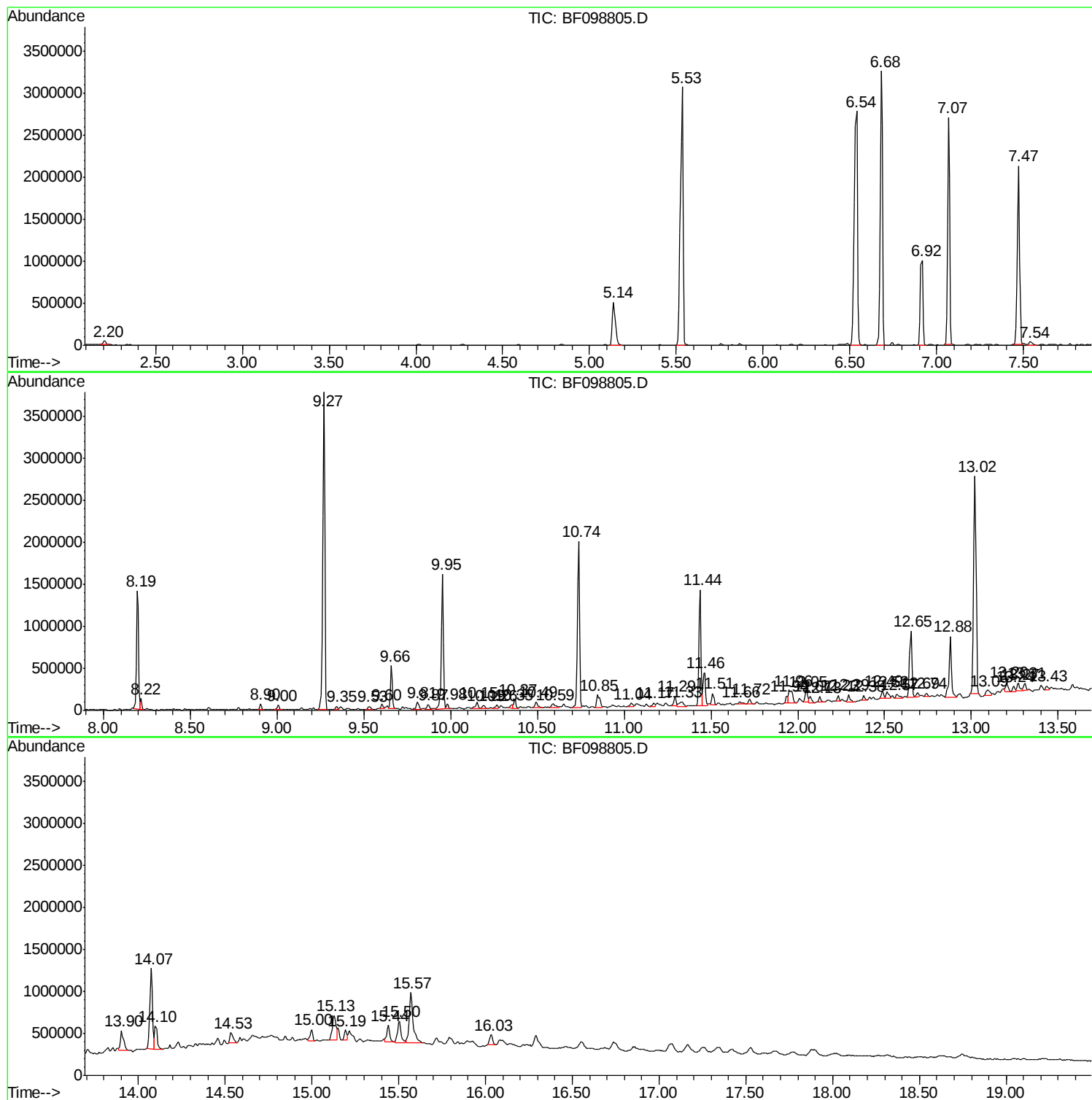
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Misc :
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Instrument :
BNA_F
ClientSampled :
SP-2-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Acq On : 26 Sep 2017 1:49
Operator : SJ/JU
Sample : I5362-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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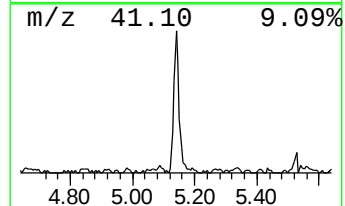
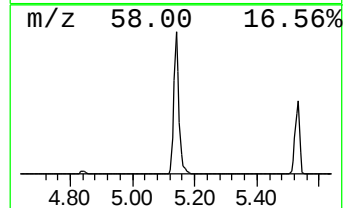
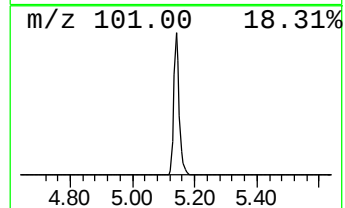
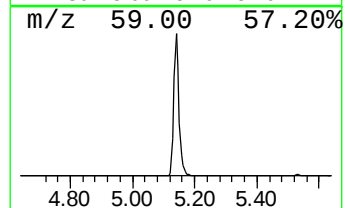
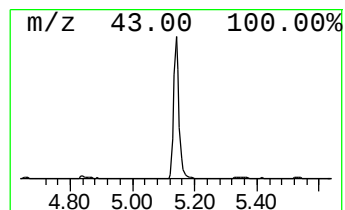
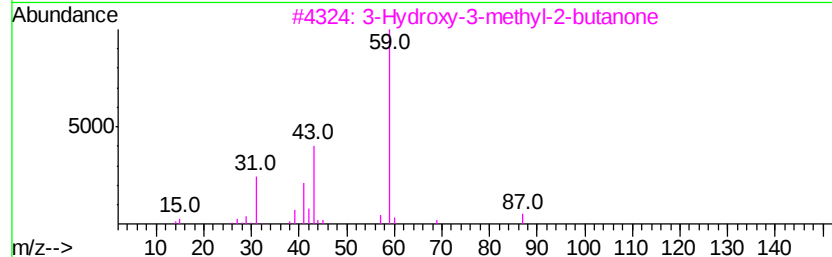
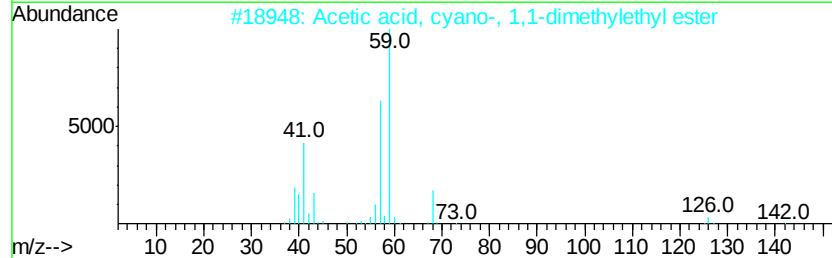
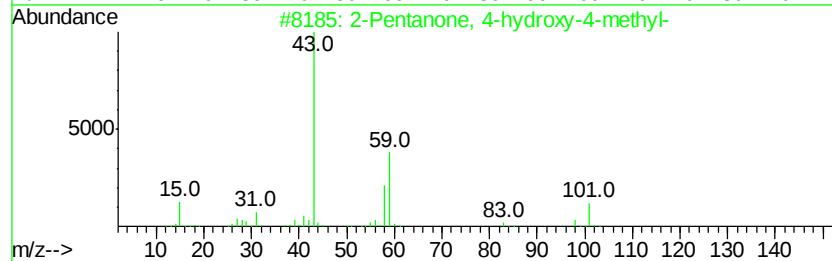
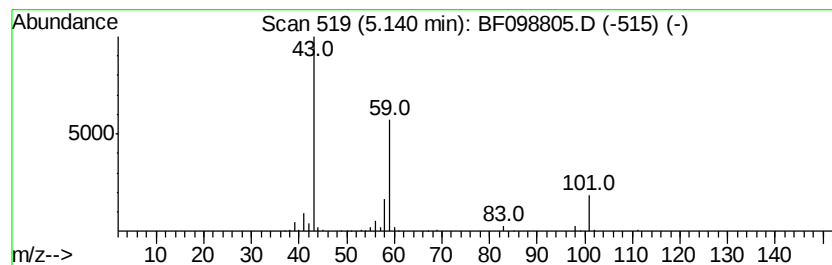
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.87 ng	618179	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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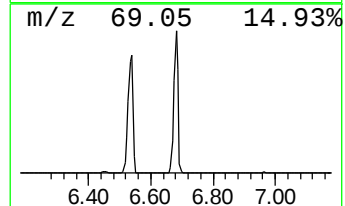
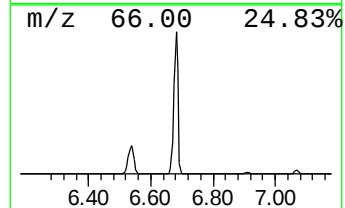
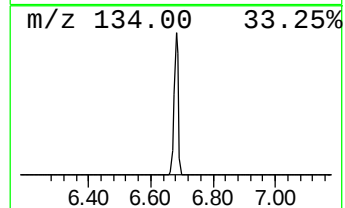
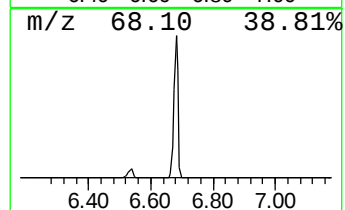
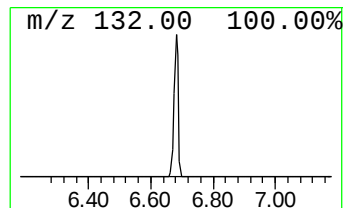
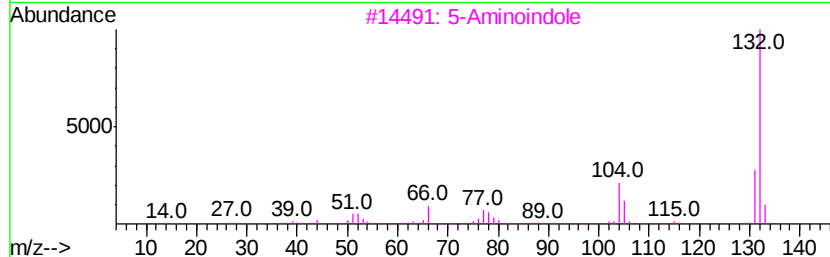
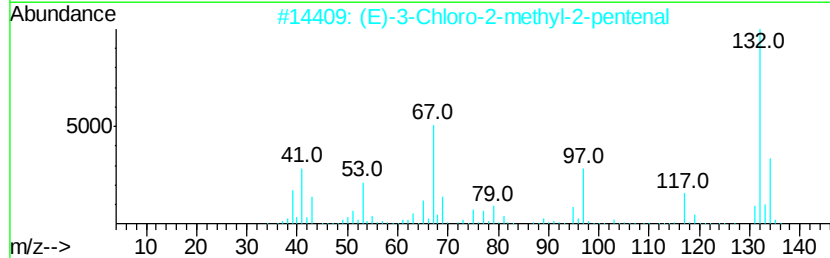
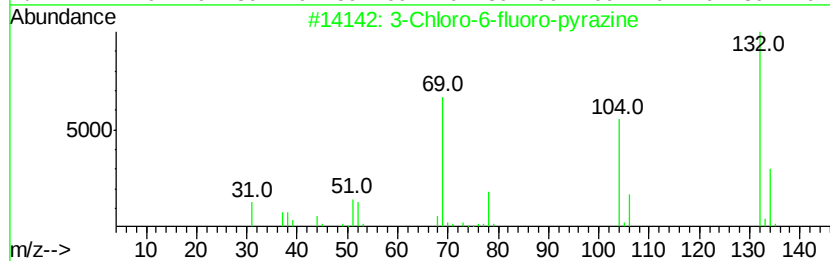
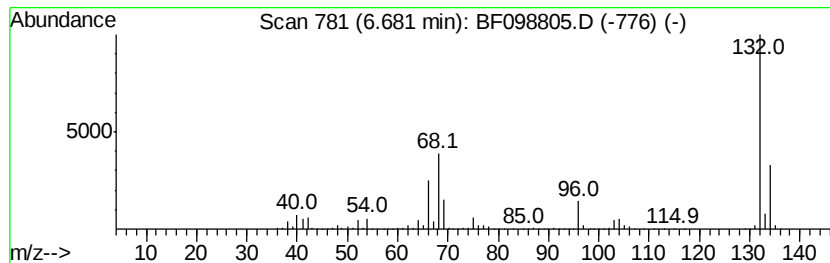
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	70.70 ng	3150810	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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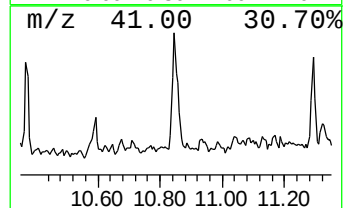
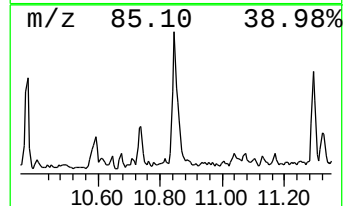
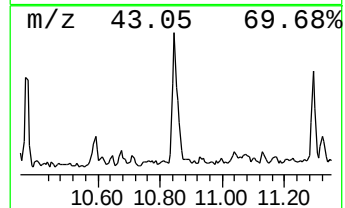
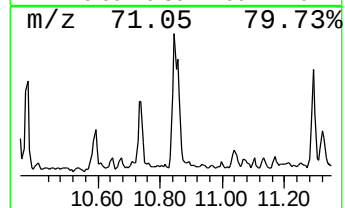
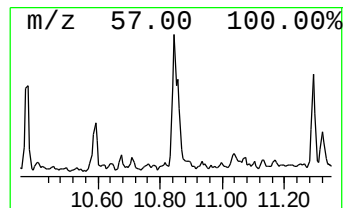
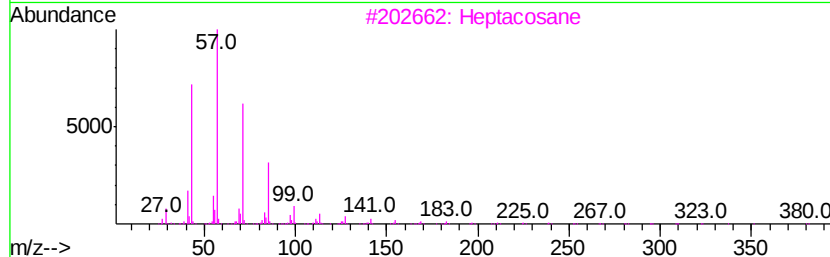
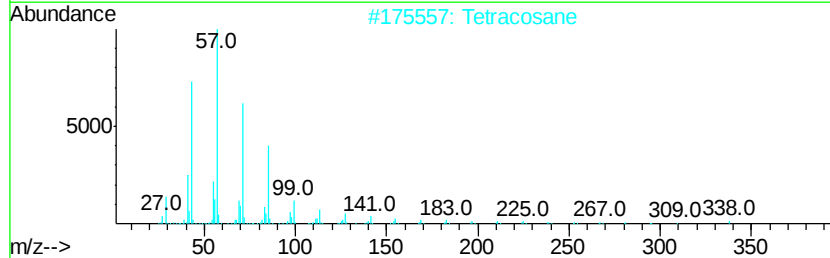
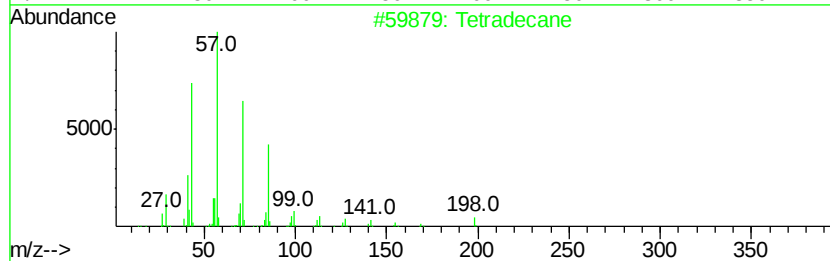
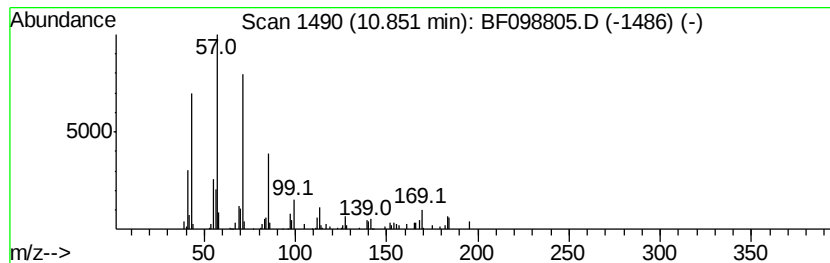
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	3.30 ng	204353	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	87
2		Tetracosane	338	C24H50	000646-31-1	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Pentadecane	212	C15H32	000629-62-9	87
5		Eicosane	282	C20H42	000112-95-8	87



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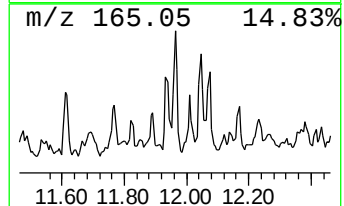
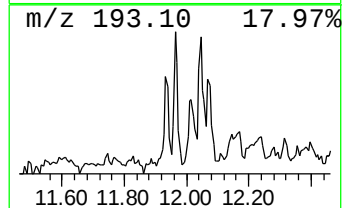
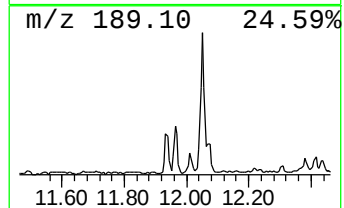
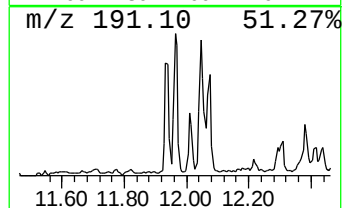
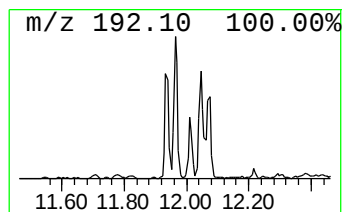
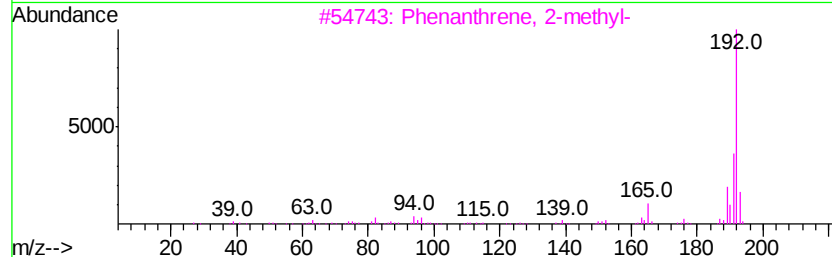
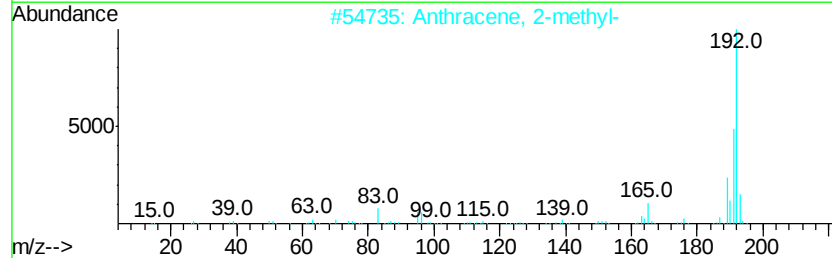
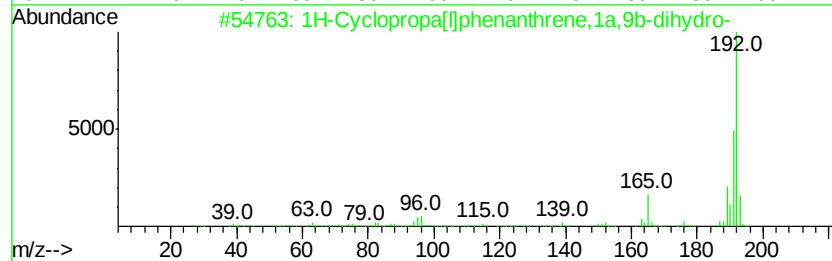
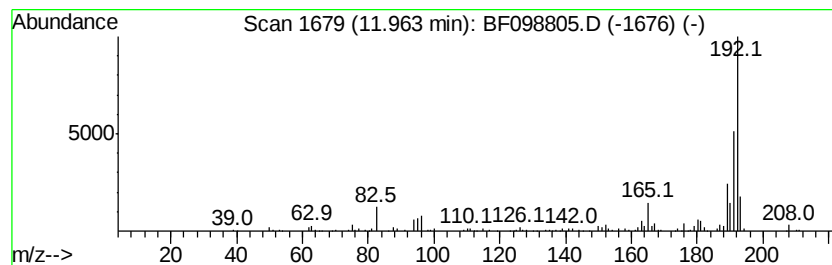
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1H-Cyclopropa[l]phenanthrene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	3.21 ng	198476	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Cyclopropa[l]phenanthrene, 1a, ...	192	C15H12	000949-41-7	98
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098805.D
Acq On : 26 Sep 2017 1:49
Operator : SJ/JU
Sample : I5362-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

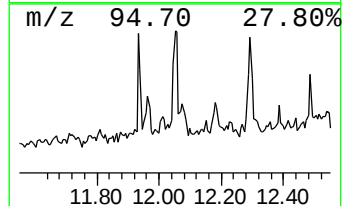
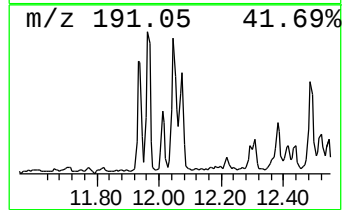
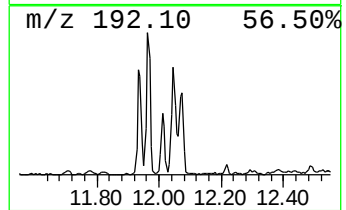
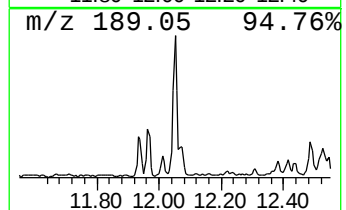
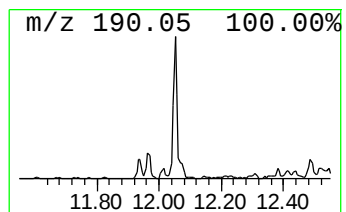
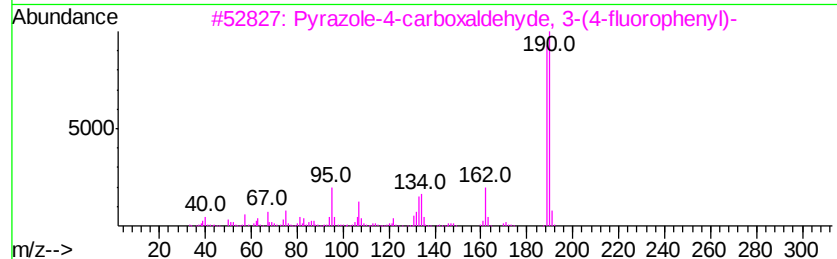
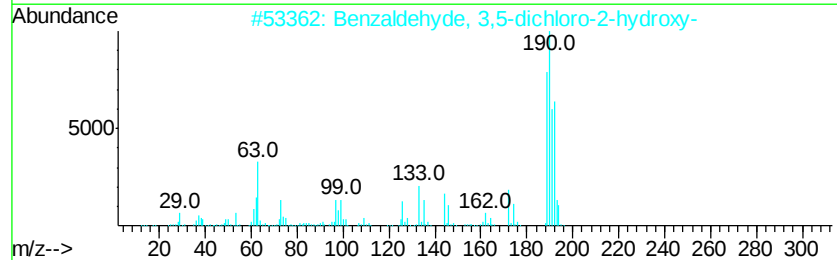
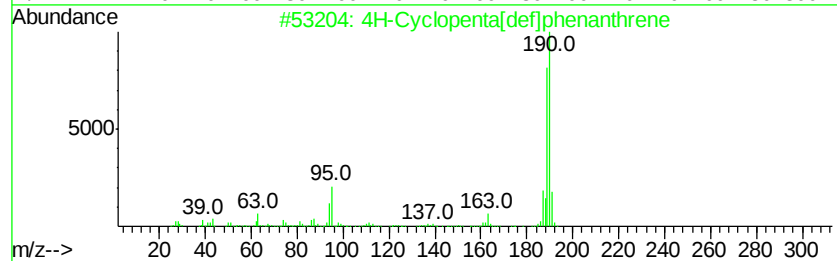
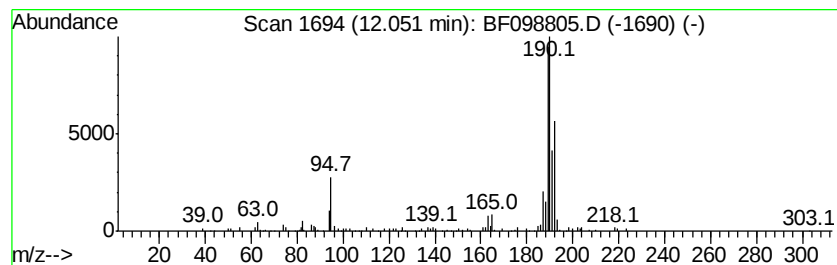
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.05	2.45 ng	151458	Phenanthrene-d10	11.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2		Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
5		Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Sample : I5362-01
Misc :
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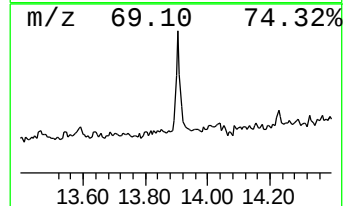
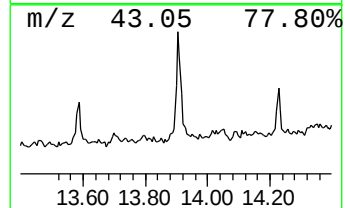
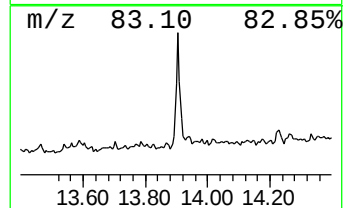
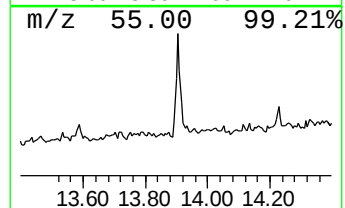
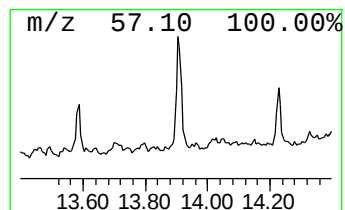
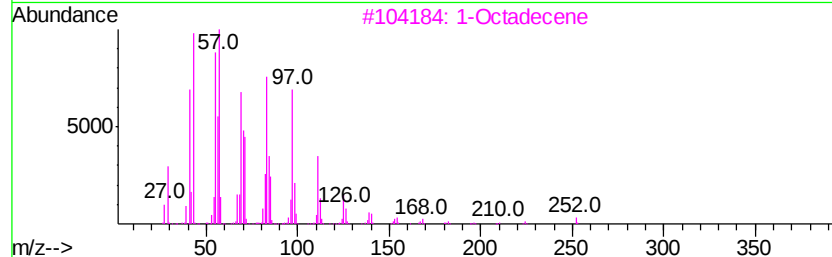
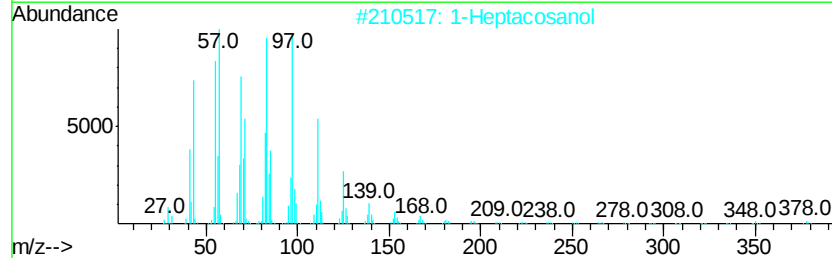
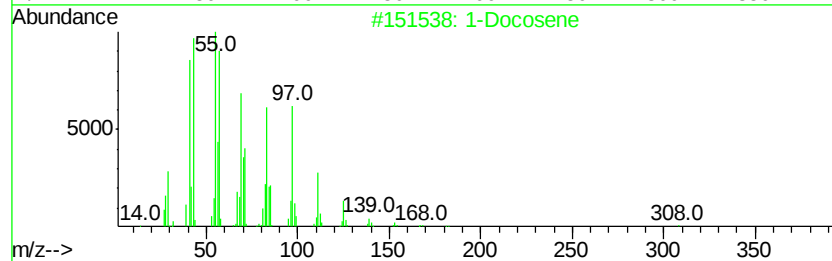
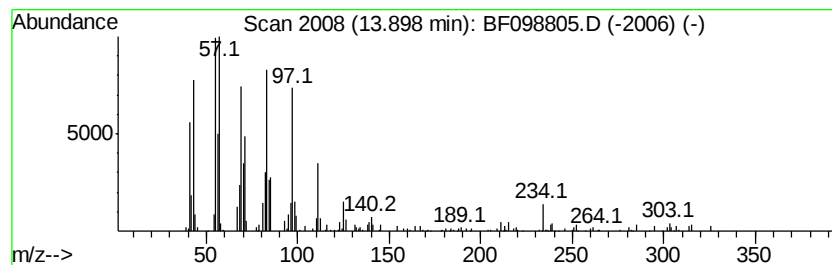
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.90	4.72 ng	264719	Chrysene-d12		14.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	90
2	1-Heptacosanol	396	C27H56O	002004-39-9	90
3	1-Octadecene	252	C18H36	000112-88-9	90
4	3-Octadecene, (E)-	252	C18H36	007206-19-1	86
5	17-Pentatriacontene	491	C35H70	006971-40-0	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098805.D
 Acq On : 26 Sep 2017 1:49
 Operator : SJ/JU
 Sample : I5362-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

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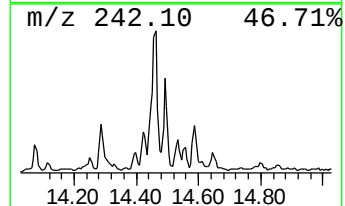
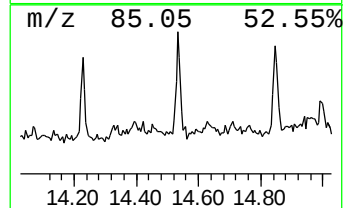
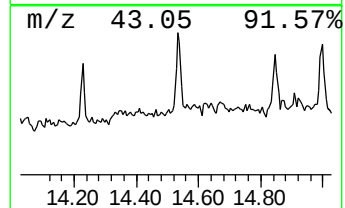
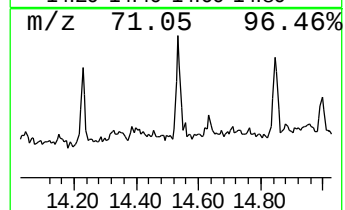
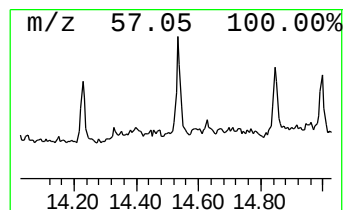
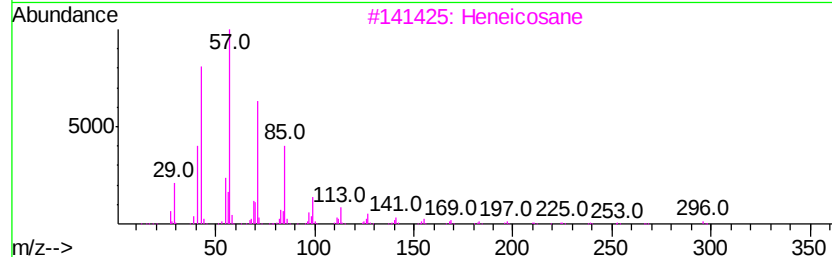
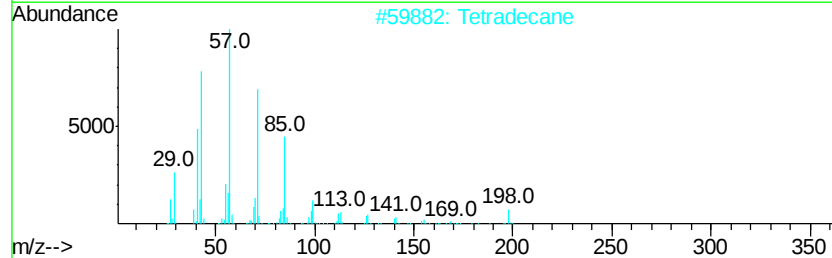
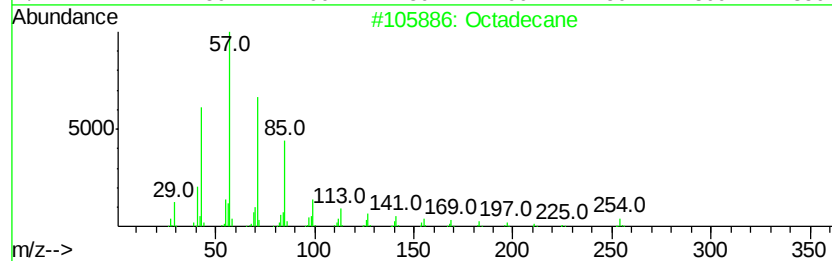
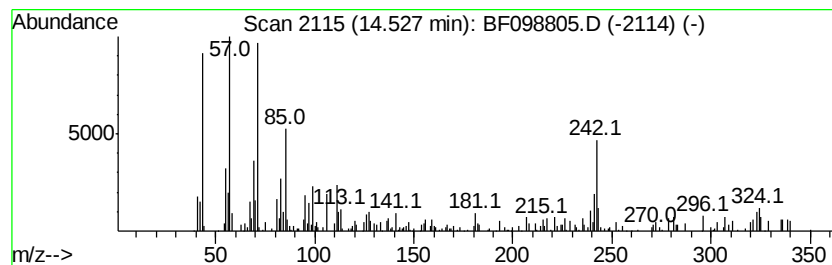
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.59 ng	145348	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	90
2		Tetradecane	198	C14H30	000629-59-4	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Hexadecane	226	C16H34	000544-76-3	70
5		Eicosane	282	C20H42	000112-95-8	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Operator : SJ/JU
Sample : I5362-01
Misc :
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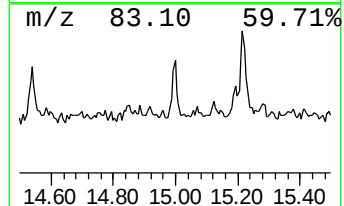
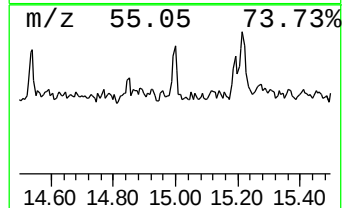
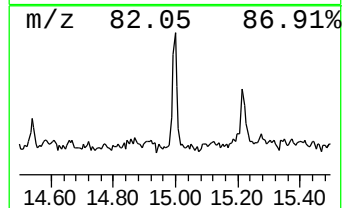
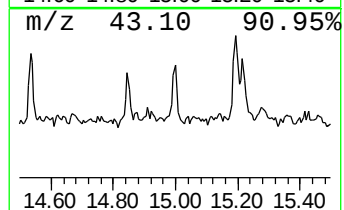
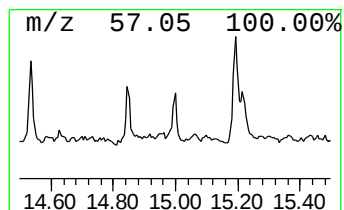
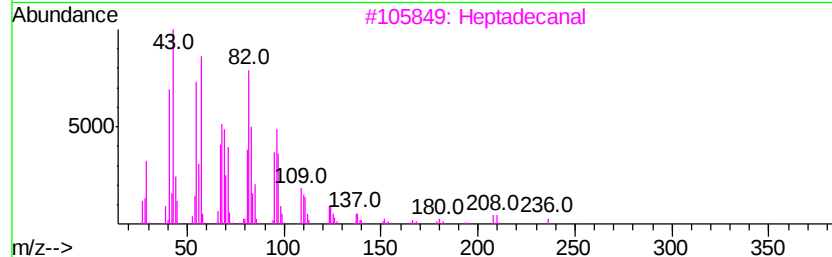
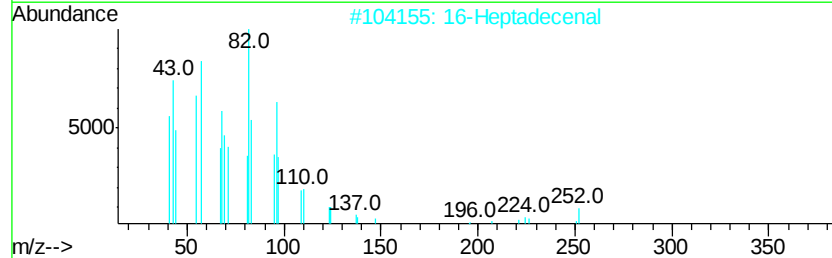
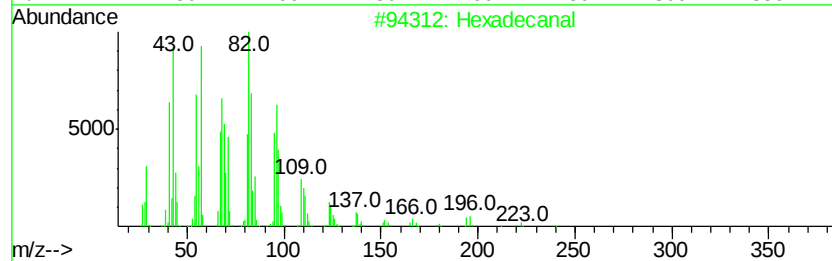
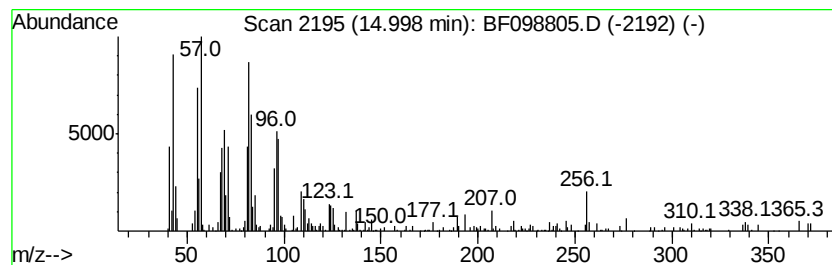
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.00	2.86 ng	136672	Perylene-d12		15.57
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	81
2	16-Heptadecenal	252	C17H32O	1000144-57-9	80
3	Heptadecanal	254	C17H34O	1000376-70-0	76
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	76
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Acq On : 26 Sep 2017 1:49
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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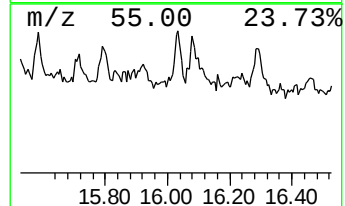
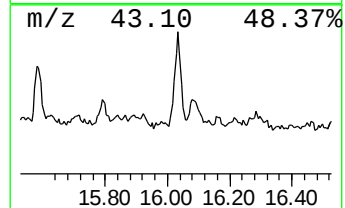
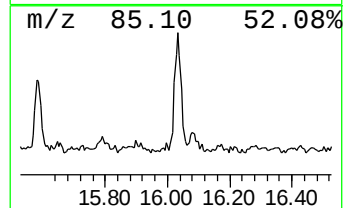
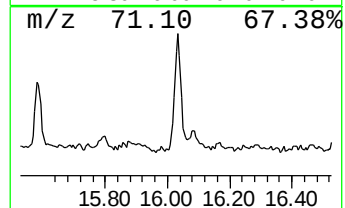
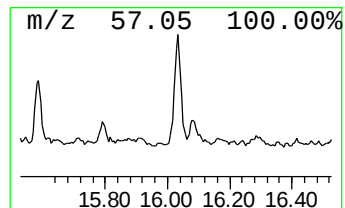
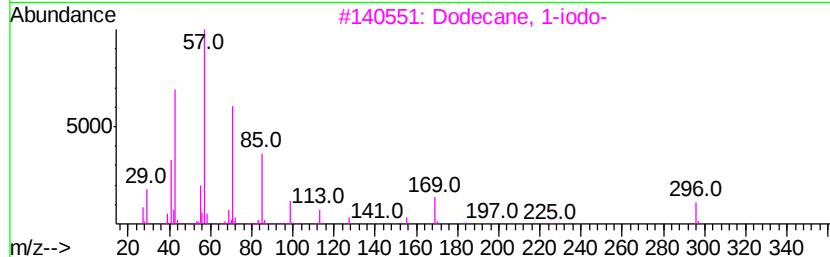
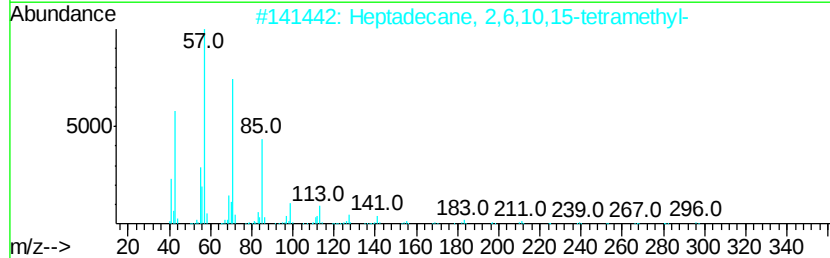
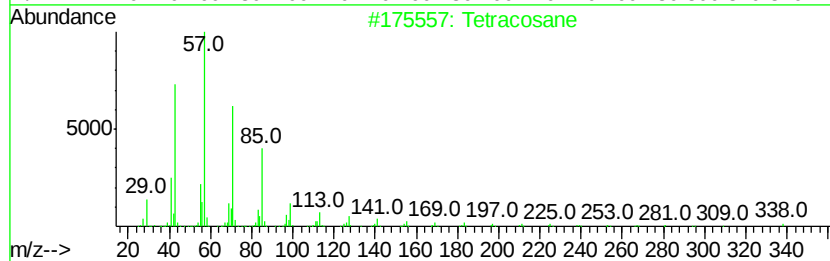
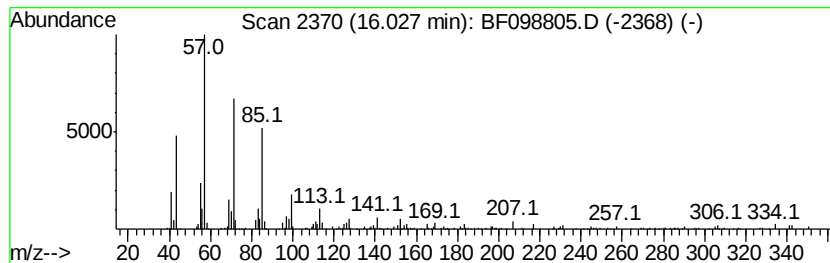
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	3.20 ng	152681	Perylene-d12	15.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	93
4			Octadecane	254	C18H38	000593-45-3	90
5			Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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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
2-Pentanone, 4-hy...	5.14	13.9	ng	618179	1	6.92	891309	20.0
unknown6.68	6.68	70.7	ng	3150810	1	6.92	891309	20.0
Tetradecane	10.85	3.3	ng	204353	4	11.44	1238100	20.0
1H-Cyclopropa[l]p...	11.96	3.2	ng	198476	4	11.44	1238100	20.0
4H-Cyclopenta[def...	12.05	2.5	ng	151458	4	11.44	1238100	20.0
1-Docosene	13.90	4.7	ng	264719	5	14.07	1122100	20.0
Octadecane	14.53	2.6	ng	145348	5	14.07	1122100	20.0
Hexadecanal	15.00	2.9	ng	136672	6	15.57	955100	20.0
Tetracosane	16.03	3.2	ng	152681	6	15.57	955100	20.0