

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
 Data File : BF096852.D
 Acq On : 18 Jul 2017 17:42
 Operator : SJ/JU
 Sample : I4245-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-01-071717-C

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-BF071317.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	2.857	145	148	162	rBV	107098	203397	7.39%	0.763%
2	4.775	470	474	485	rVB	187588	273326	9.93%	1.025%
3	5.210	543	548	551	rBV	2586557	2651453	96.33%	9.942%
4	6.251	719	725	728	rBV	2455183	2752329	100.00%	10.320%
5	6.369	740	745	748	rBV	2668877	2637852	95.84%	9.891%
6	6.598	780	784	792	rBV	819060	706518	25.67%	2.649%
7	6.681	794	798	806	rBV	76771	123384	4.48%	0.463%
8	6.751	806	810	814	rBV	1902501	1922238	69.84%	7.208%
9	7.163	874	880	883	rBV	1772727	1684664	61.21%	6.317%
10	7.286	896	901	906	rVB	55683	62283	2.26%	0.234%
11	7.798	984	988	992	rBV	74559	68977	2.51%	0.259%
12	7.880	997	1002	1005	rBV	1175006	1001862	36.40%	3.757%
13	8.957	1180	1185	1188	rBV	2669888	2468882	89.70%	9.258%
14	9.051	1199	1201	1206	rVB2	36293	29781	1.08%	0.112%
15	9.351	1248	1252	1255	rBV	886627	751472	27.30%	2.818%
16	9.486	1273	1275	1279	rBV	41588	30747	1.12%	0.115%
17	9.580	1288	1291	1294	rVB	44517	35917	1.30%	0.135%
18	9.627	1294	1299	1302	rBV	1067040	928011	33.72%	3.480%
19	9.833	1326	1334	1338	rBV3	30623	48710	1.77%	0.183%
20	10.045	1365	1370	1372	rBV4	21826	27721	1.01%	0.104%
21	10.074	1372	1375	1379	rVB	71746	58540	2.13%	0.220%
22	10.169	1389	1391	1394	rVB	35991	27704	1.01%	0.104%
23	10.298	1408	1413	1415	rBV	34162	38215	1.39%	0.143%
24	10.410	1428	1432	1436	rBV	1369900	1338307	48.62%	5.018%
25	10.545	1452	1455	1463	rVB	103152	135606	4.93%	0.508%
26	10.745	1486	1489	1492	rBV4	21700	27734	1.01%	0.104%
27	10.992	1528	1531	1534	rBV2	111721	92966	3.38%	0.349%
28	11.021	1534	1536	1541	rVB	68565	70750	2.57%	0.265%
29	11.098	1544	1549	1552	rBV	806788	802753	29.17%	3.010%
30	11.121	1552	1553	1558	rVB	287010	200291	7.28%	0.751%
31	11.174	1558	1562	1567	rBV	98860	96149	3.49%	0.361%
32	11.416	1601	1603	1609	rVB2	66505	66303	2.41%	0.249%
33	11.515	1617	1620	1623	rVB3	35718	30898	1.12%	0.116%
34	11.598	1632	1634	1637	rBV	42933	34888	1.27%	0.131%

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Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.627	1637	1639	1641	rBV	48627	40789	1.48%	0.153%
36	11.674	1645	1647	1650	rBV	132604	102871	3.74%	0.386%
37	11.710	1650	1653	1655	rBV	92575	81771	2.97%	0.307%
38	11.733	1655	1657	1660	rVB2	31326	31019	1.13%	0.116%
39	11.798	1665	1668	1670	rBV2	28911	31400	1.14%	0.118%
40	11.821	1670	1672	1676	rVV3	59185	62575	2.27%	0.235%
41	11.974	1695	1698	1704	rBV6	34419	69114	2.51%	0.259%
42	12.104	1717	1720	1724	rBV2	57711	59094	2.15%	0.222%
43	12.151	1725	1728	1730	rBV2	44038	45024	1.64%	0.169%
44	12.210	1736	1738	1741	rBV2	49218	45072	1.64%	0.169%
45	12.304	1751	1754	1759	rBV	298621	288443	10.48%	1.082%
46	12.351	1760	1762	1765	rBV2	38328	42098	1.53%	0.158%
47	12.527	1789	1792	1795	rVB	217907	207434	7.54%	0.778%
48	12.580	1799	1801	1803	rBV	64732	58130	2.11%	0.218%
49	12.686	1815	1819	1822	rBV	1466976	1385786	50.35%	5.196%
50	12.933	1858	1861	1864	rBV3	71169	85484	3.11%	0.321%
51	12.962	1864	1866	1873	rVV4	78458	134988	4.90%	0.506%
52	13.057	1880	1882	1886	rBV	80942	94769	3.44%	0.355%
53	13.574	1967	1970	1977	rBV3	184533	387681	14.09%	1.454%
54	13.727	1991	1996	1998	rBV2	653337	689323	25.05%	2.585%
55	14.721	2163	2165	2174	rVB	149617	244023	8.87%	0.915%
56	15.098	2226	2229	2233	rBV	373081	394242	14.32%	1.478%
57	15.721	2332	2335	2349	rVB2	181985	352858	12.82%	1.323%
58	16.098	2397	2399	2410	rVB3	169191	304105	11.05%	1.140%

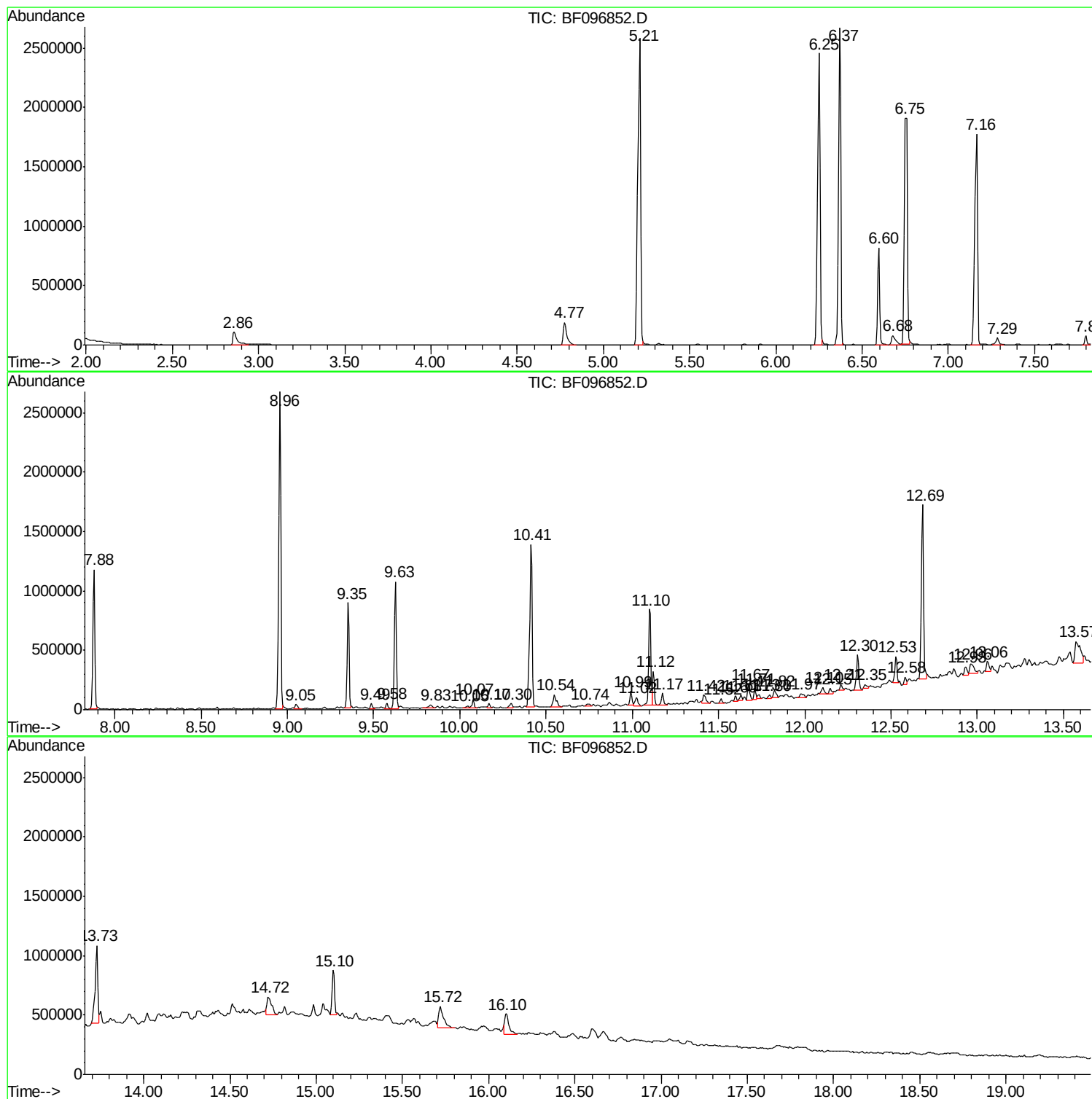
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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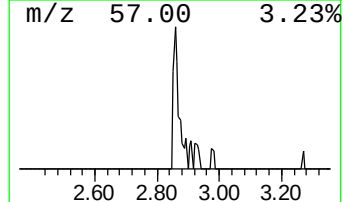
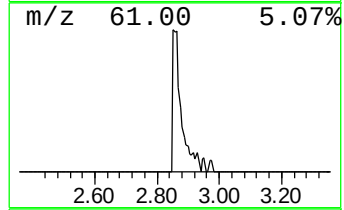
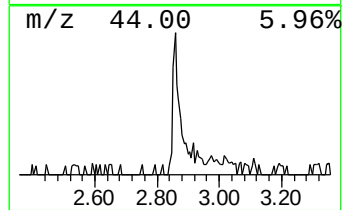
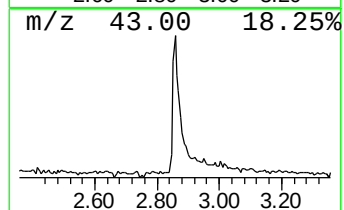
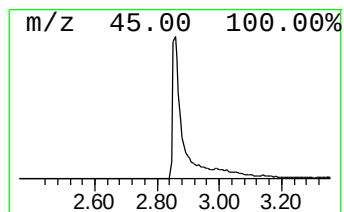
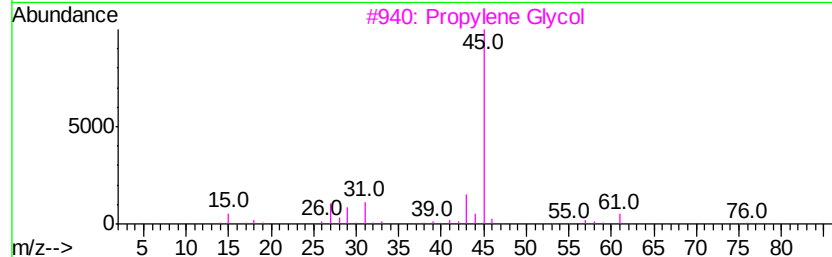
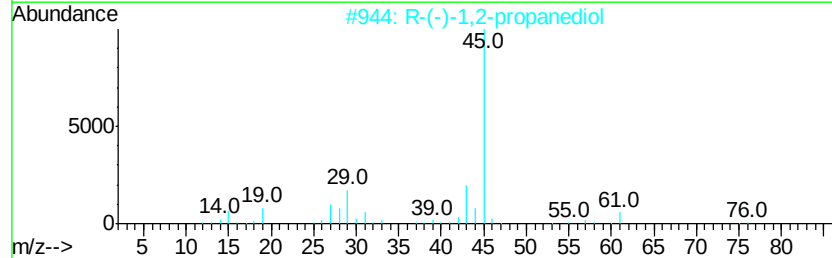
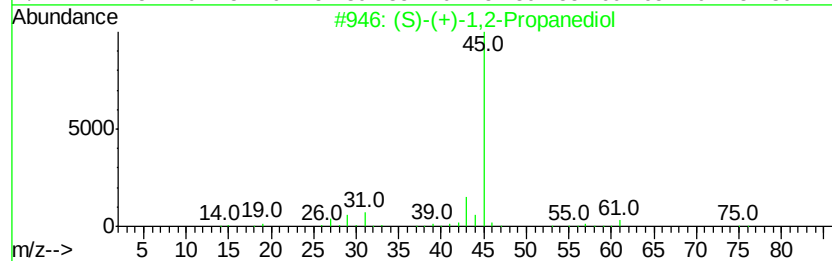
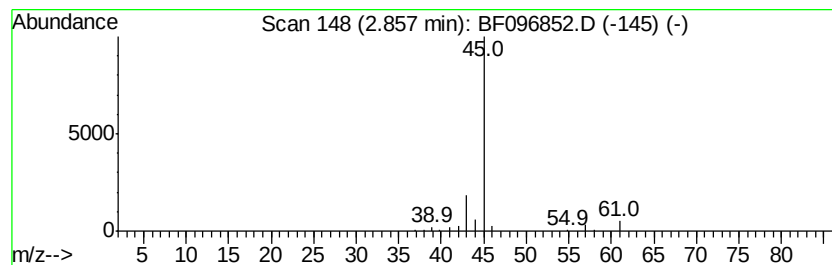
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	5.76 ng	203397	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5		Formamide	45	CH3NO	000075-12-7	7



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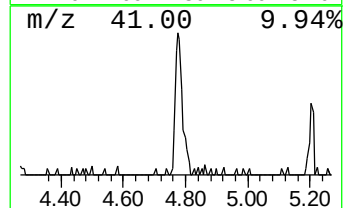
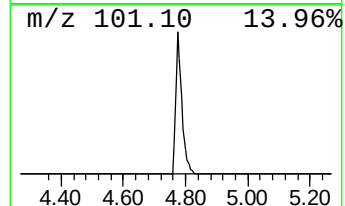
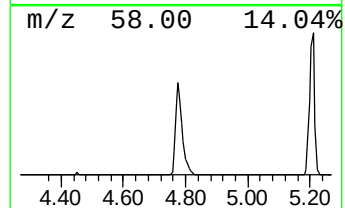
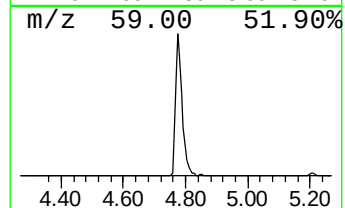
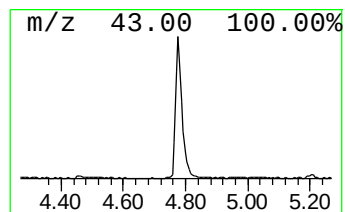
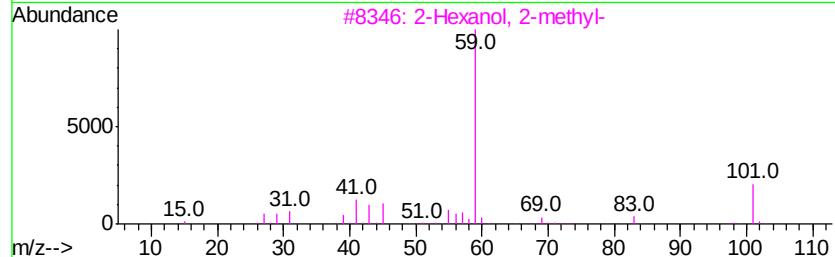
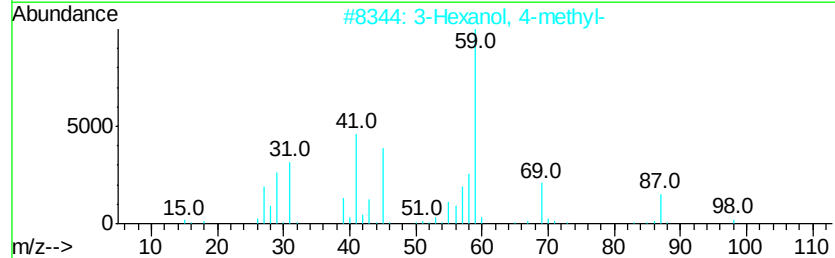
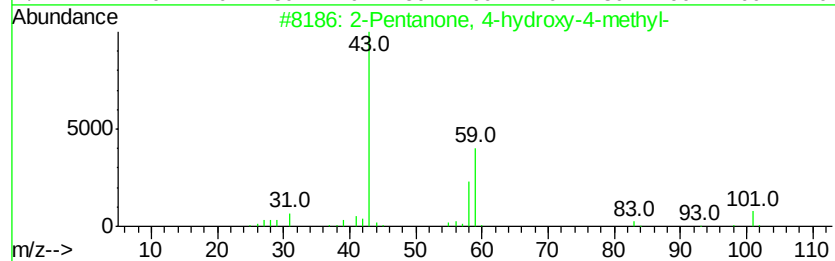
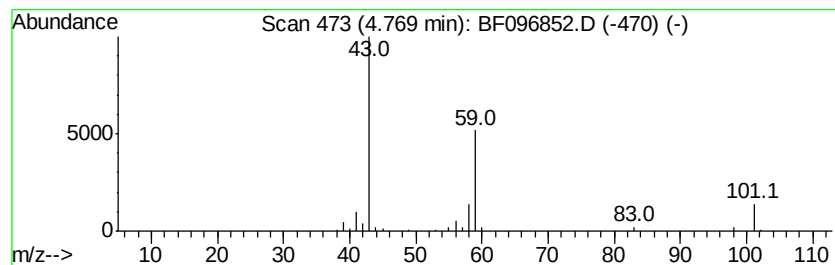
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	7.74 ng	273326	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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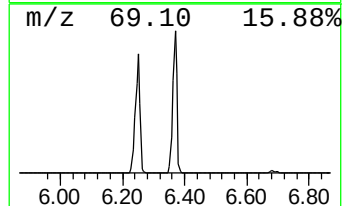
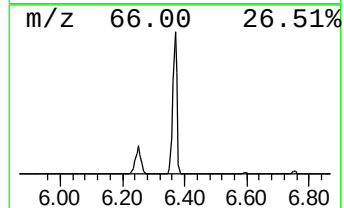
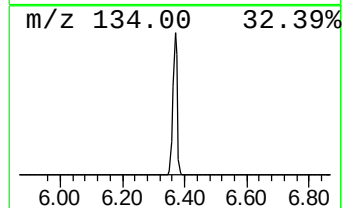
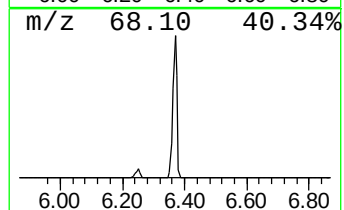
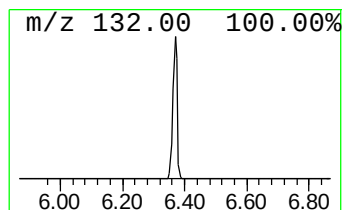
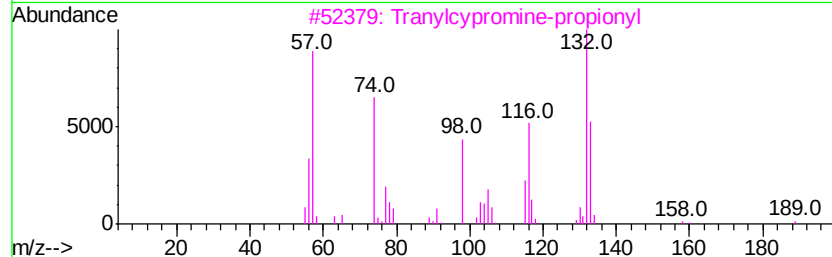
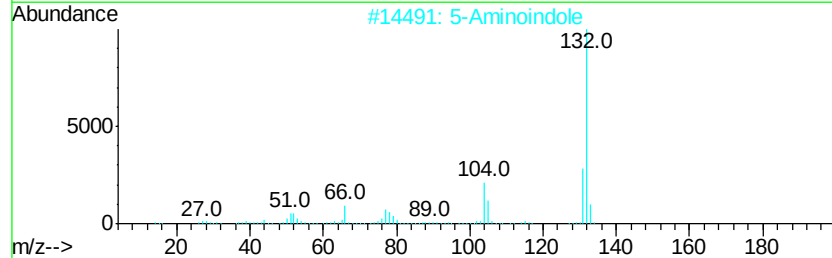
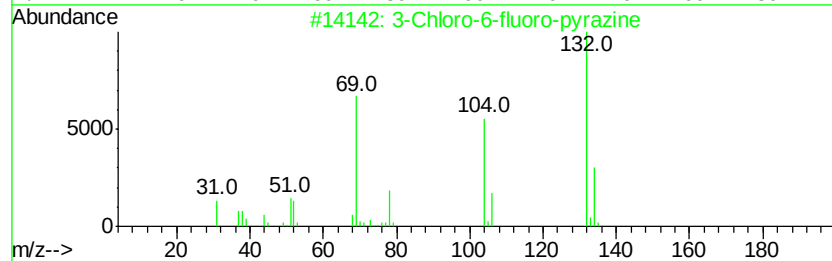
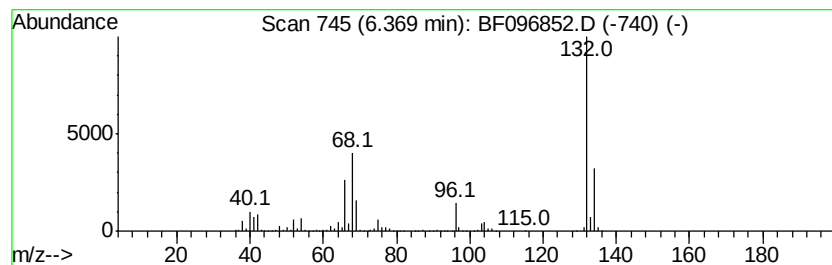
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	74.67 ng	2637850	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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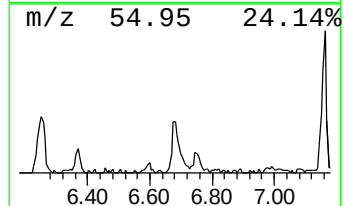
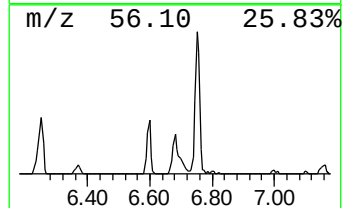
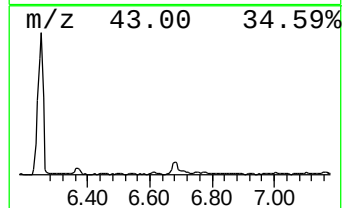
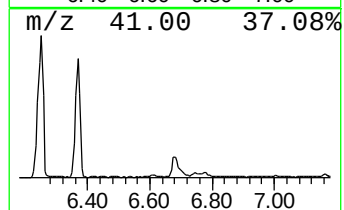
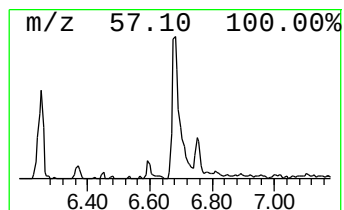
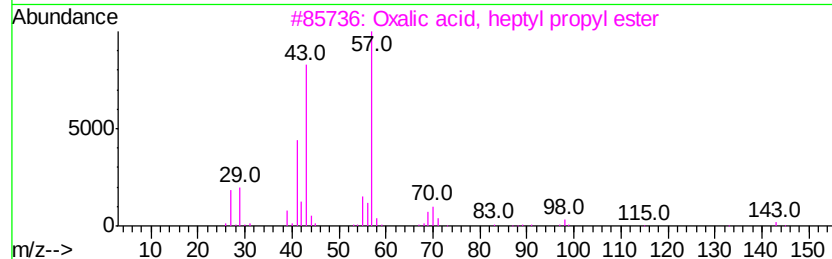
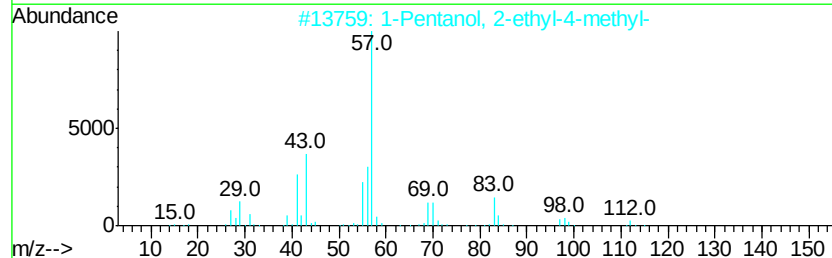
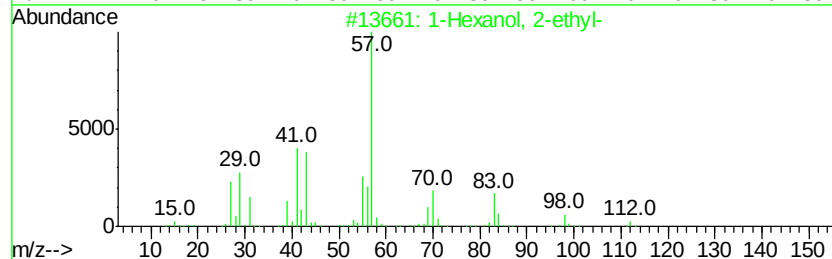
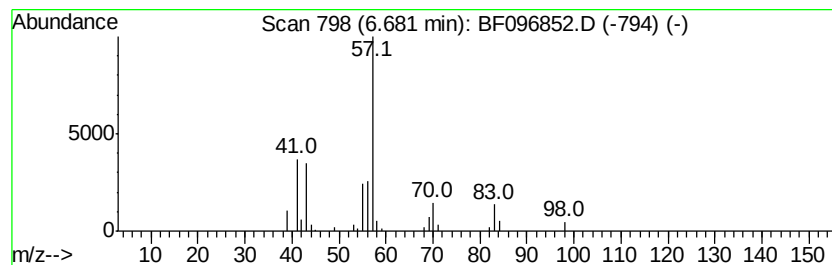
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	3.49 ng	123384	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	37
4		Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	37
5		3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	36



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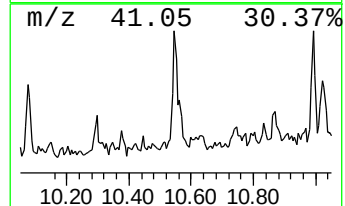
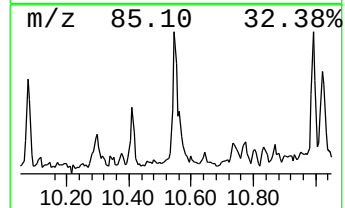
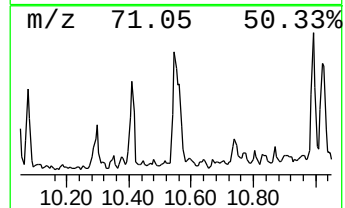
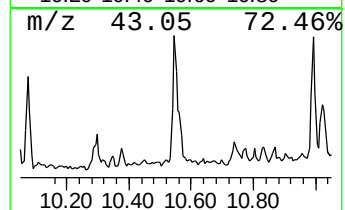
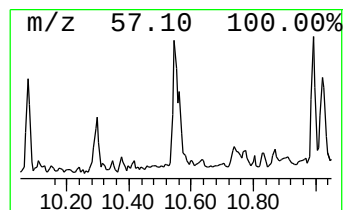
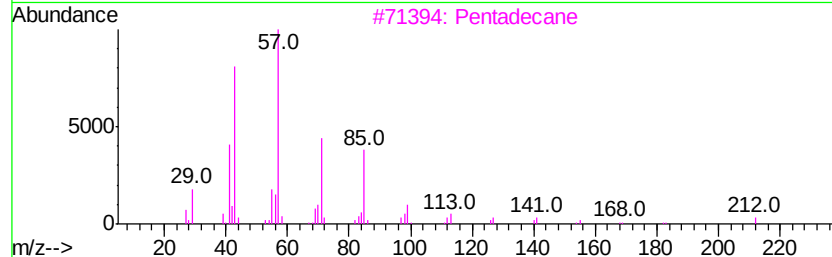
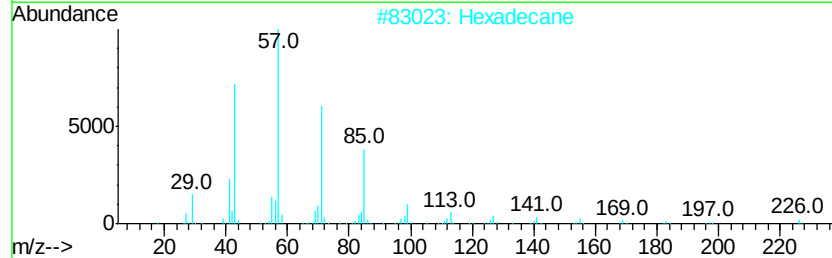
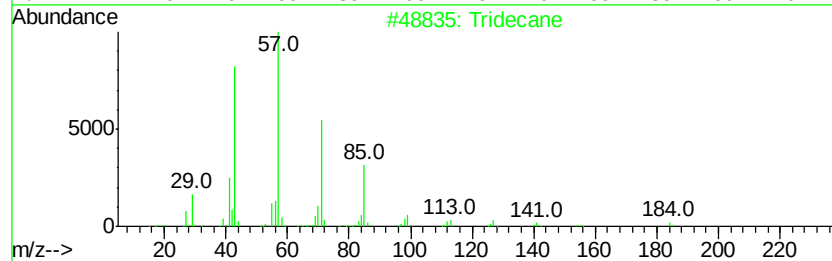
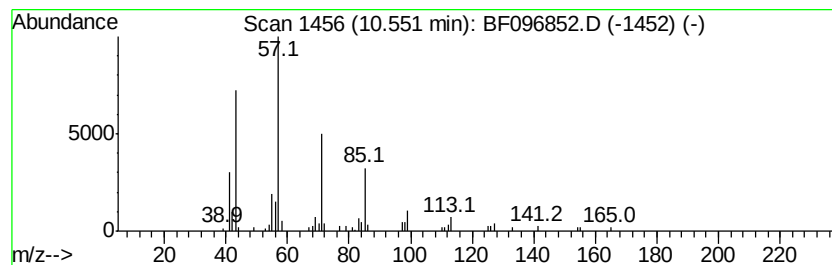
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.55	3.38 ng	135606	Phenanthrene-d10		11.10
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
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Acq On : 18 Jul 2017 17:42
Operator : SJ/JU
Sample : I4245-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

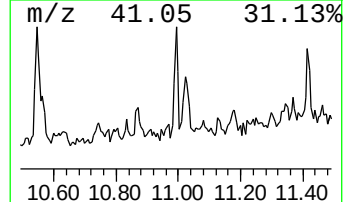
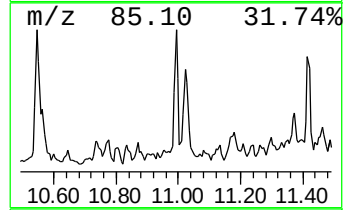
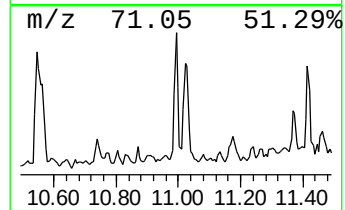
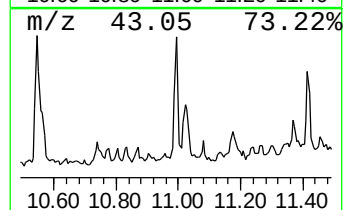
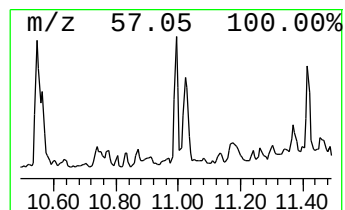
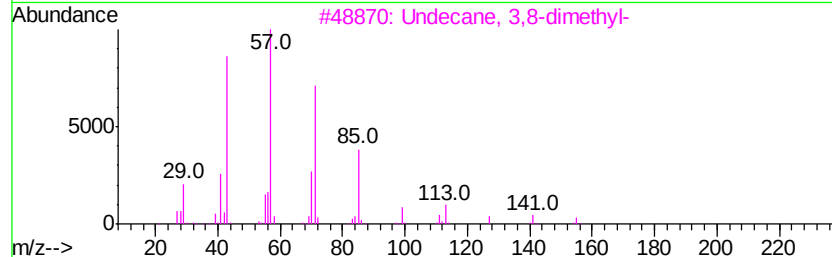
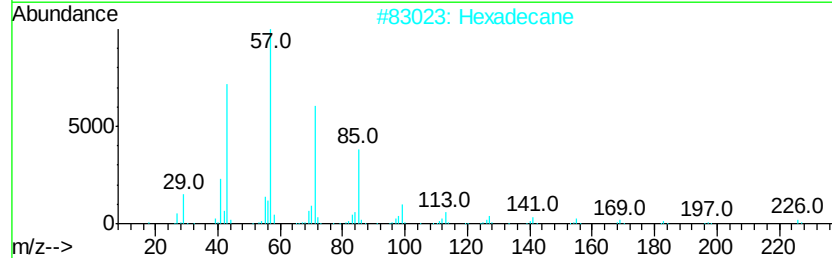
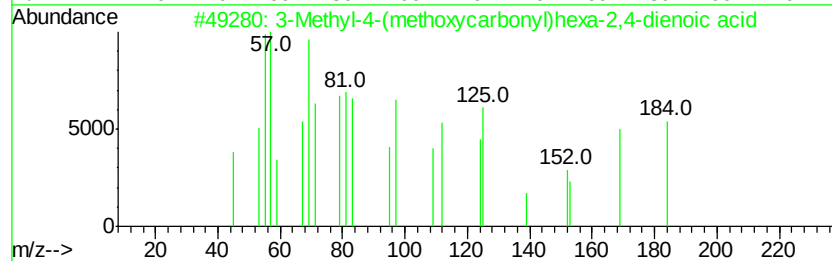
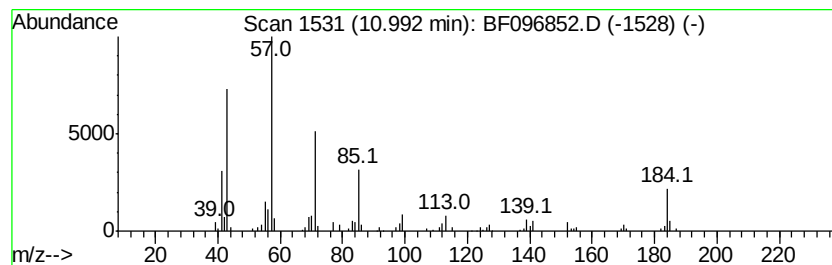
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Methyl-4-(methoxycarbonyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.99	2.32 ng	92966	Phenanthrene-d10		11.10
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	60
2	Hexadecane	226	C16H34	000544-76-3	58
3	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	53
4	Tridecane	184	C13H28	000629-50-5	53
5	Heptacosane	380	C27H56	000593-49-7	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
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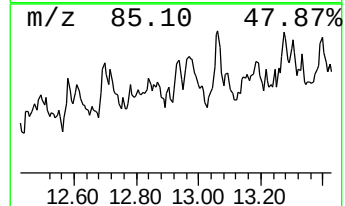
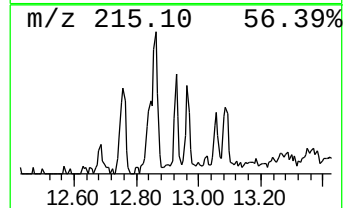
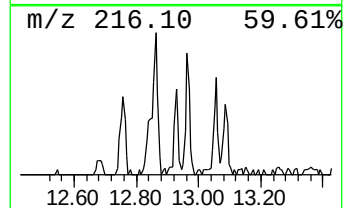
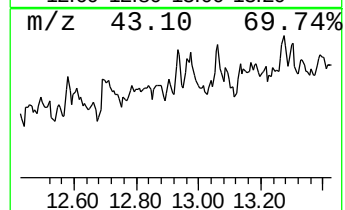
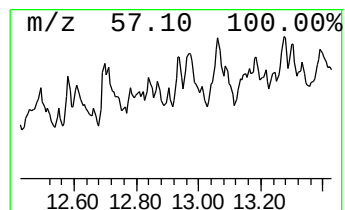
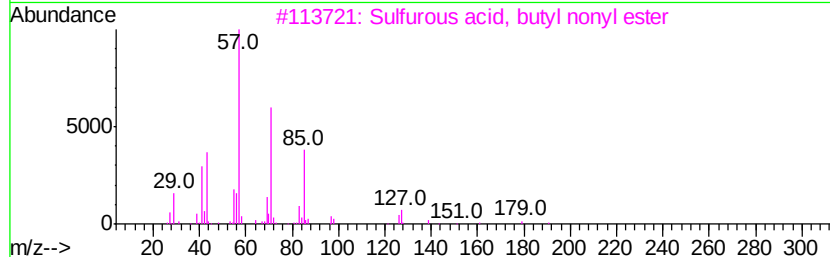
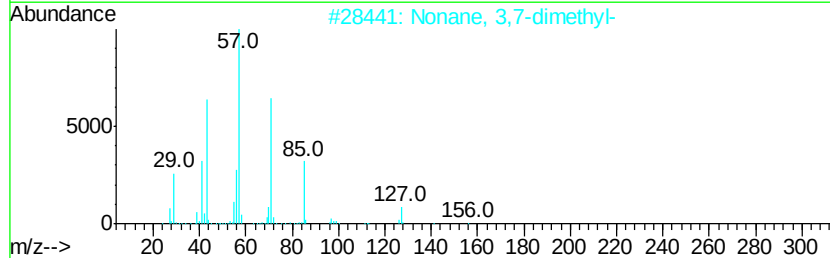
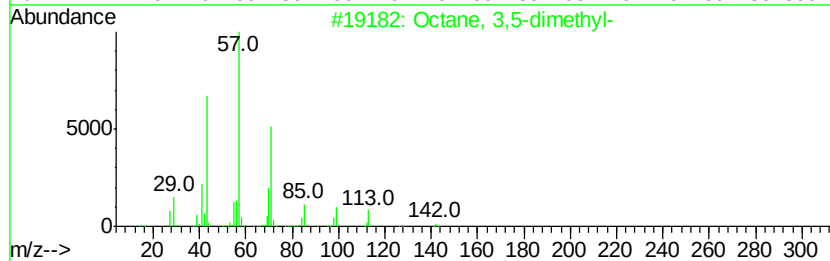
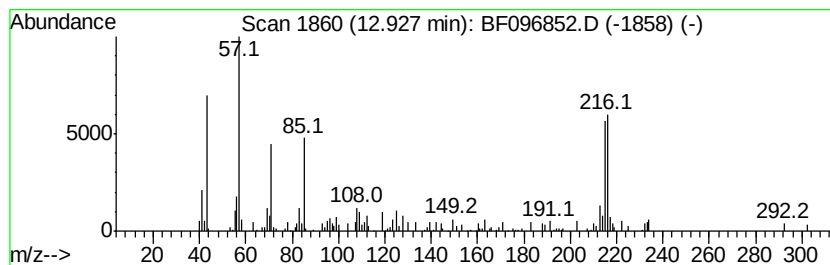
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.93 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.48 ng	85484	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
2		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	47
3		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47
4		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	38
5		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	38



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Data File : BF096852.D
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Operator : SJ/JU
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ALS Vial : 19 Sample Multiplier: 1

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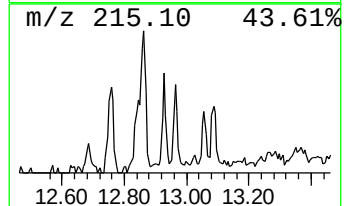
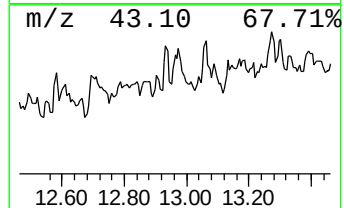
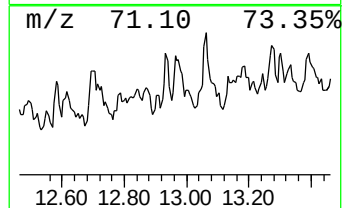
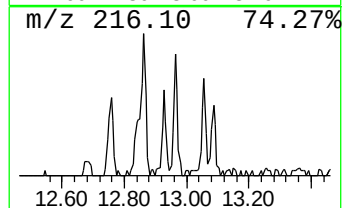
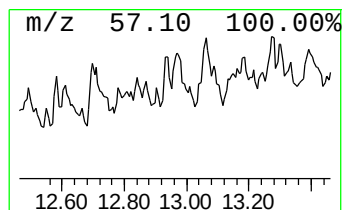
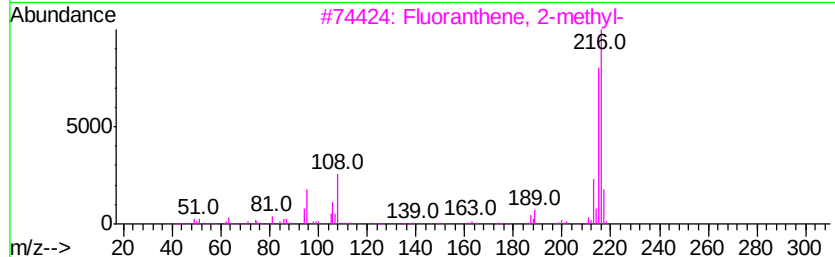
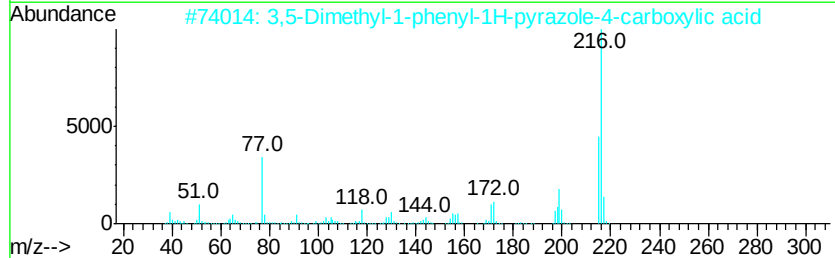
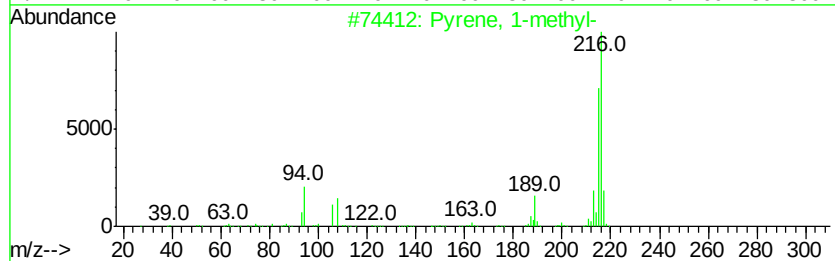
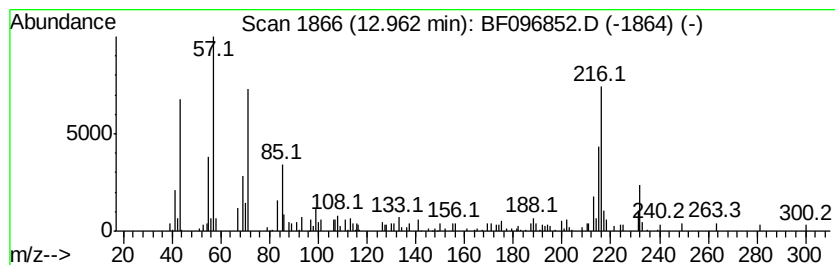
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 10 unknown12.96 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	3.92 ng	134988	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	46
2		3,5-Dimethyl-1-phenyl-1H-pyrazol...	216	C12H12N2O2	061226-19-5	41
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	41
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	38
5		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
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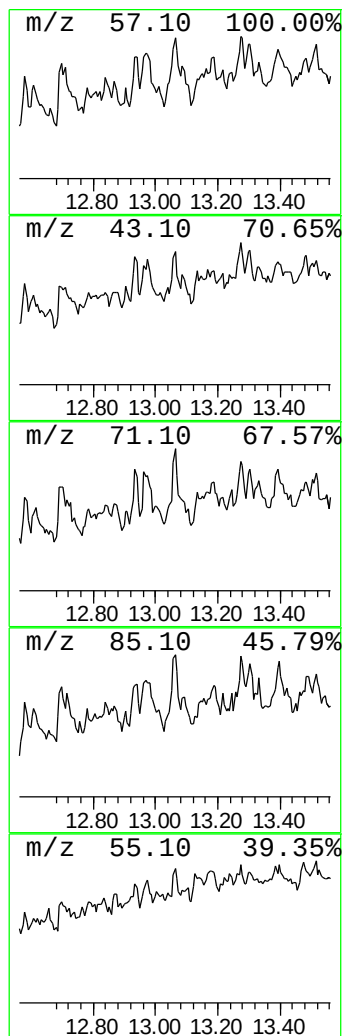
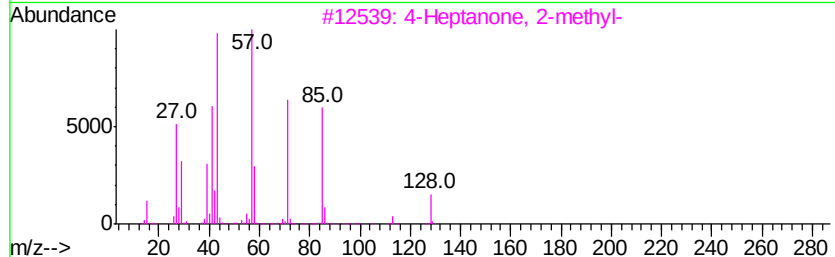
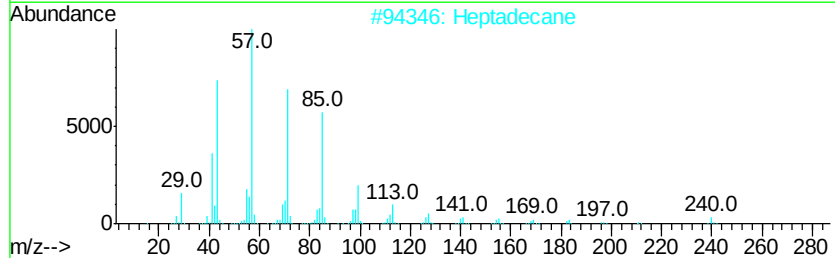
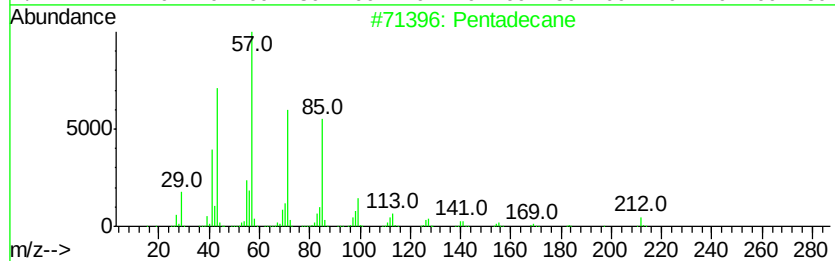
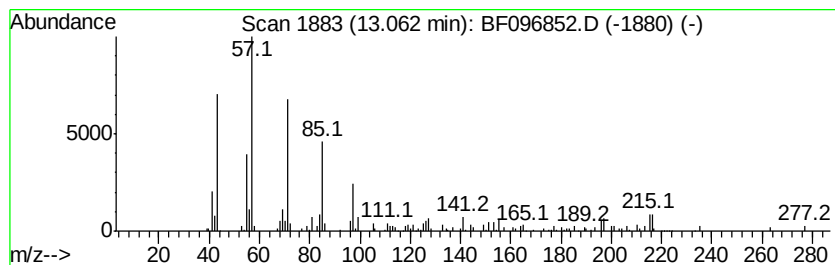
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown13.06 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	2.75 ng	94769	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	38
2		Heptadecane	240	C17H36	000629-78-7	35
3		4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	22
4		4-Methyl-5-nonanone	156	C10H20O	035900-26-6	22
5		Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	22



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Data File : BF096852.D
Acq On : 18 Jul 2017 17:42
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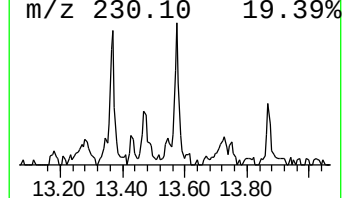
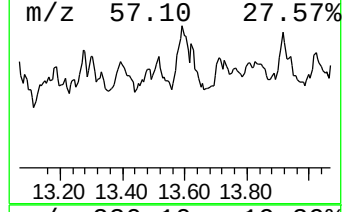
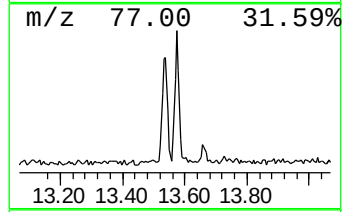
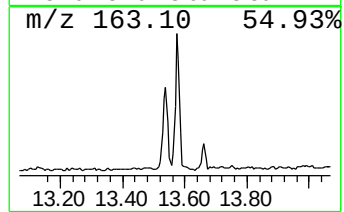
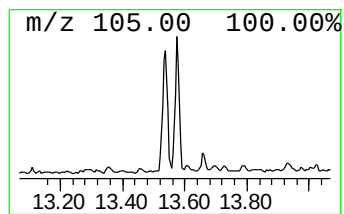
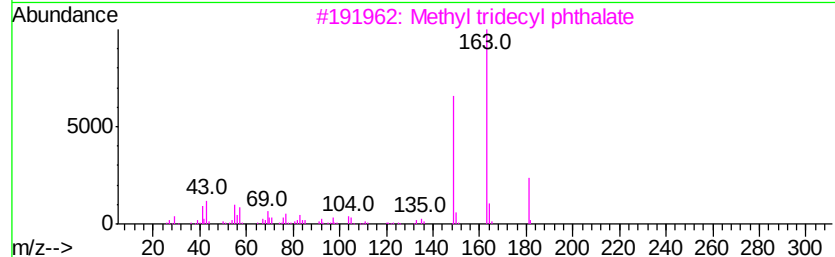
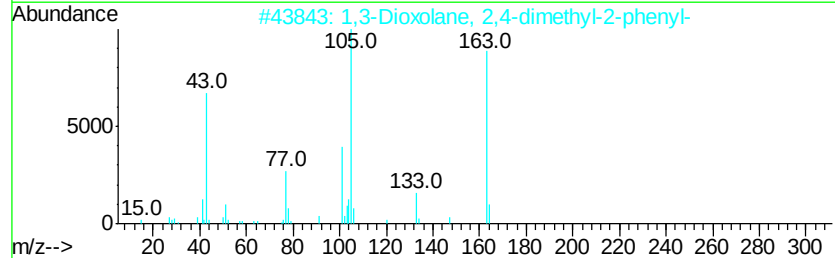
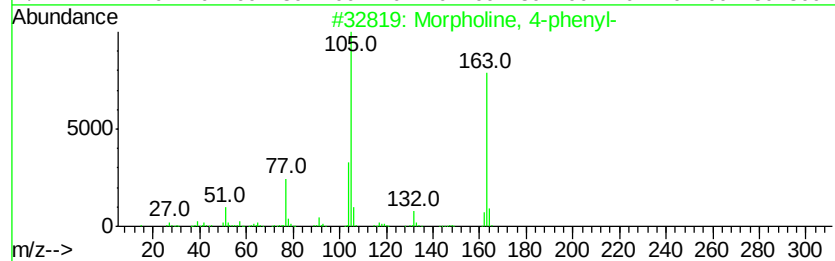
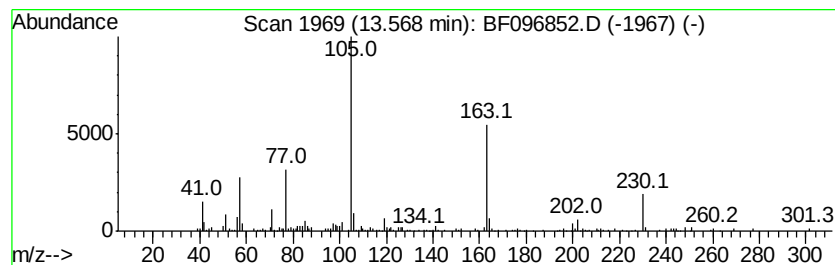
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	11.25 ng	387681	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2		1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	59
3		Methyl tridecyl phthalate	362	C22H34O4	256481-40-0	35
4		Methyl undecyl phthalate	334	C20H30O4	070794-29-5	35
5		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
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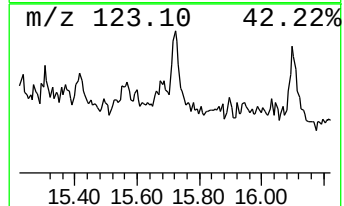
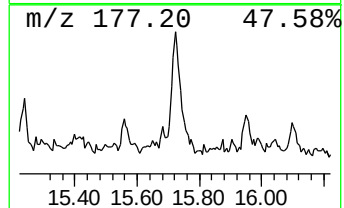
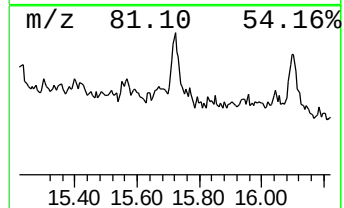
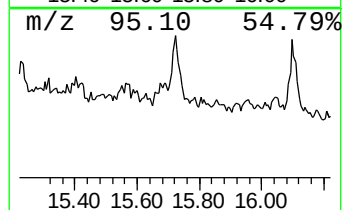
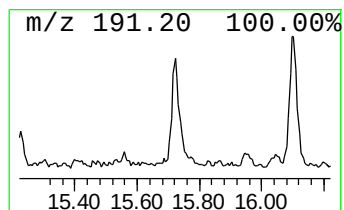
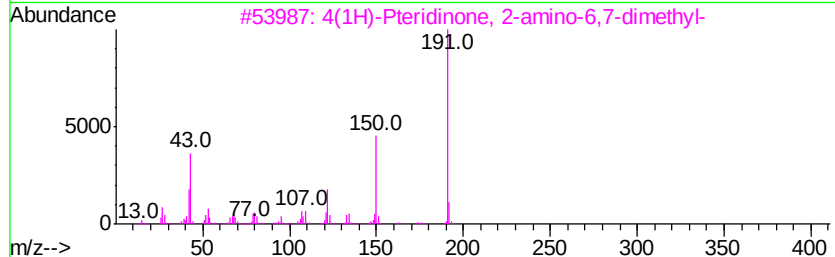
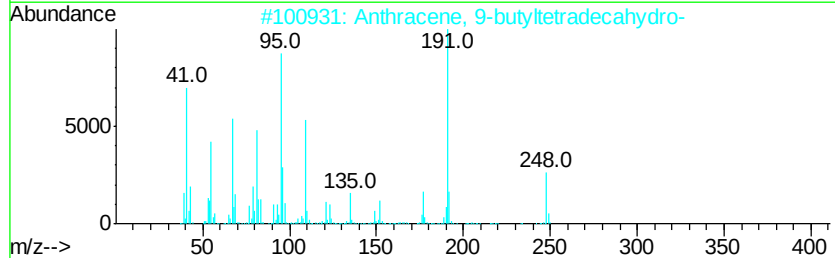
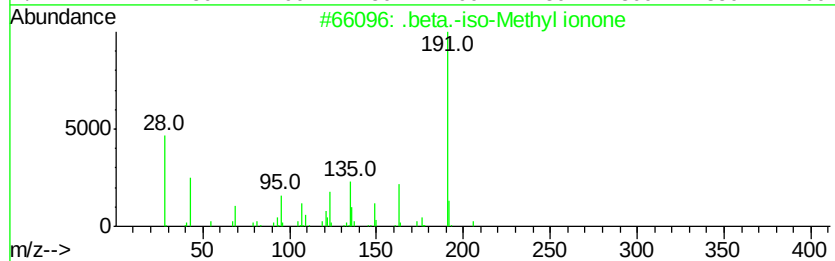
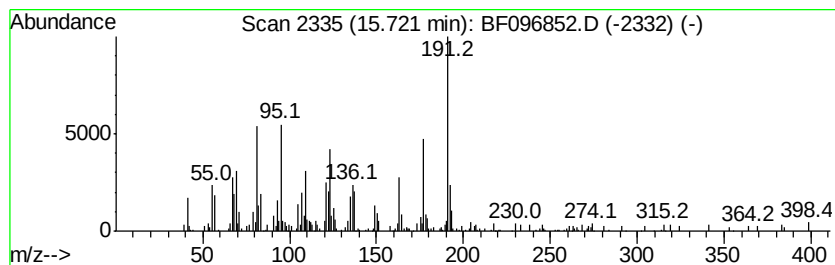
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown15.72 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	17.90 ng	352858	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	27
3		4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	27
4		Pyrrolo[3,4-d]pyrimidine-2,4(1H,3...	191	C9H9N3O2	022389-83-9	18
5		5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
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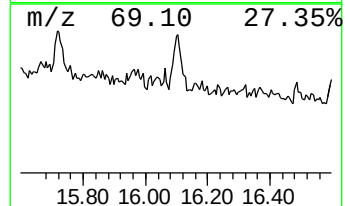
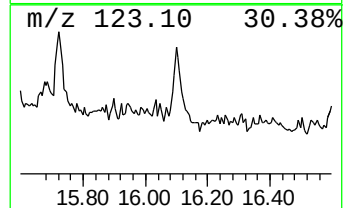
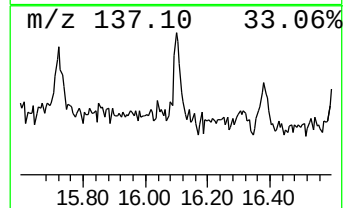
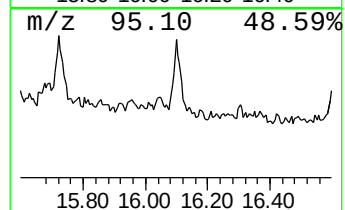
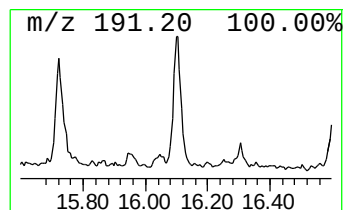
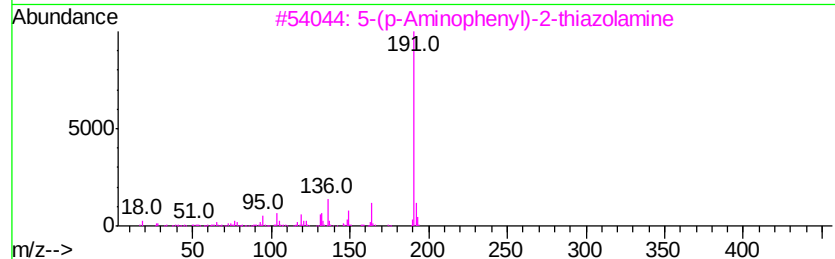
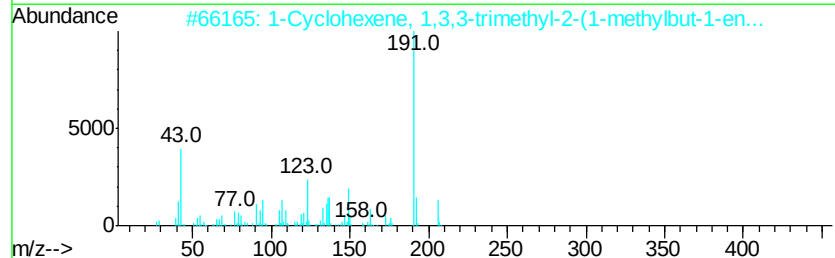
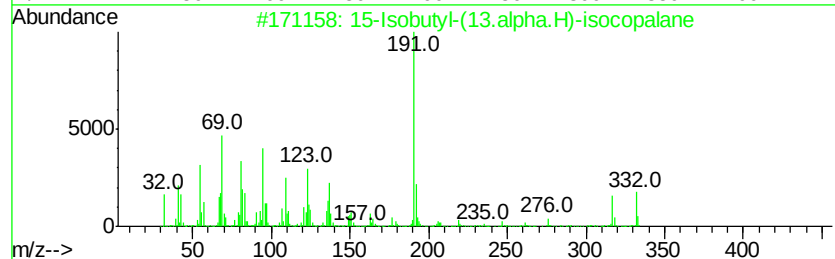
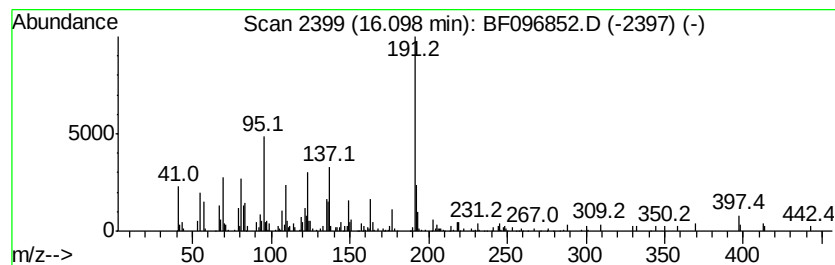
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 15-Isobutyl-(13.alpha.H)-is... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	15.43 ng	304105	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	64
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
3		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35
4		N-[2-Oxo-1,2'-bi(tricyclo[3.3.1...	355	C23H33NO2	1000305-39-6	27
5		2-Fluoro-6-trifluoromethylbenzoi...	390	C21H30F4O2	1000338-53-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
 Data File : BF096852.D
 Acq On : 18 Jul 2017 17:42
 Operator : SJ/JU
 Sample : I4245-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-01-071717-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
(S)-(+)-1,2-Propa...	2.86	5.8	ng	203397	1	6.60	706518	20.0
2-Pentanone, 4-hy...	4.77	7.7	ng	273326	1	6.60	706518	20.0
unknown6.37	6.37	74.7	ng	2637850	1	6.60	706518	20.0
1-Hexanol, 2-ethyl-	6.68	3.5	ng	123384	1	6.60	706518	20.0
Tridecane	10.55	3.4	ng	135606	4	11.10	802753	20.0
3-Methyl-4-(metho...	10.99	2.3	ng	92966	4	11.10	802753	20.0
unknown12.93	12.93	2.5	ng	85484	5	13.73	689323	20.0
unknown12.96	12.96	3.9	ng	134988	5	13.73	689323	20.0
unknown13.06	13.06	2.8	ng	94769	5	13.73	689323	20.0
Morpholine, 4-phe...	13.57	11.3	ng	387681	5	13.73	689323	20.0
unknown15.72	15.72	17.9	ng	352858	6	15.10	394242	20.0
15-Isobutyl-(13.a...	16.10	15.4	ng	304105	6	15.10	394242	20.0